



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:10 AM UTC

PDB ID : 7W73 / pdb_00007w73
EMDB ID : EMD-32338
Title : Cryo-EM map of PEDV S protein with one protomer in the D0-up conformation while the other two in the D0-down conformation
Authors : Hsu, S.T.D.; Drackowski, P.; Wang, Y.S.
Deposited on : 2021-12-03
Resolution : 6.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

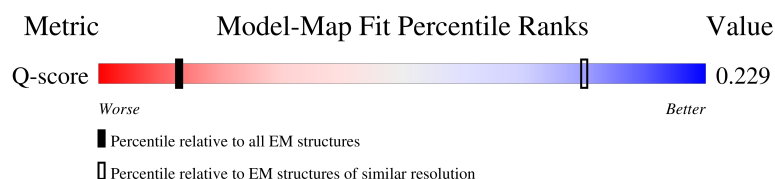
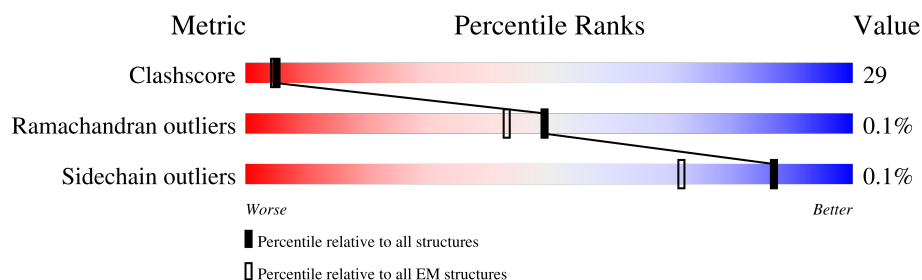
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 6.40 Å.

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



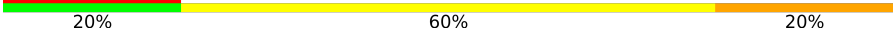
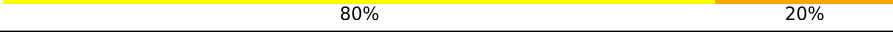
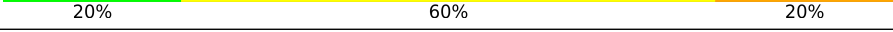
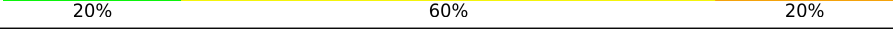
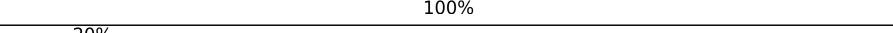
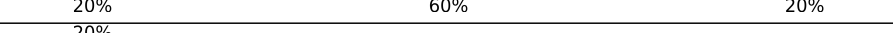
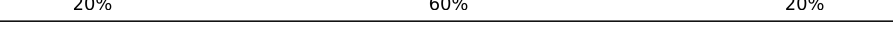
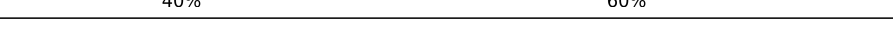
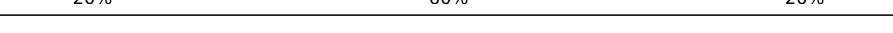
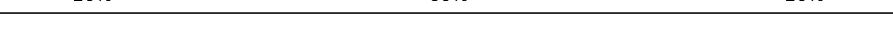
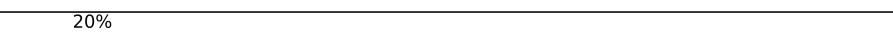
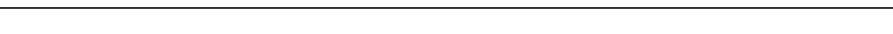
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	544 (5.90 - 6.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1386	
1	B	1386	
1	C	1386	
2	D	5	

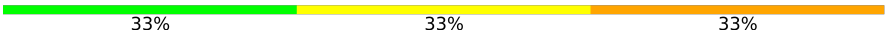
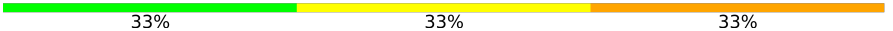
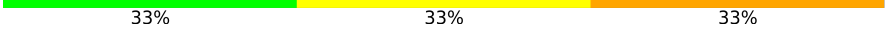
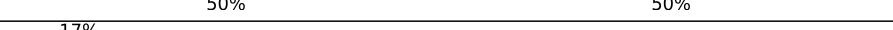
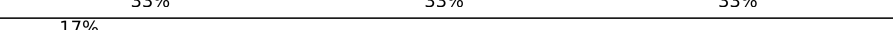
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Mol	Chain	Length	Quality of chain
2	F	5	
2	G	5	
2	H	5	
2	J	5	
2	N	5	
2	P	5	
2	R	5	
2	T	5	
2	U	5	
2	W	5	
2	X	5	
2	Y	5	
2	a	5	
2	b	5	
2	d	5	
2	g	5	
2	h	5	
2	j	5	
2	k	5	
2	m	5	
2	n	5	
2	o	5	
2	p	5	
2	u	5	
3	E	3	

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Mol	Chain	Length	Quality of chain
3	K	3	 67% 33%
3	Q	3	 33% 33% 33%
3	V	3	 33% 33% 33%
3	c	3	 33% 67%
3	f	3	 33% 33% 33%
3	l	3	 67% 33%
3	q	3	 67% 33%
3	r	3	 67% 33%
4	I	4	 25% 50% 50%
4	M	4	 50% 25% 25%
4	Z	4	 50% 50%
4	t	4	 25% 25% 75%
5	L	4	 25% 75%
6	O	6	 17% 50% 50%
6	S	6	 17% 50% 33% 17%
6	e	6	 17% 33% 33% 33%
6	i	6	 17% 67% 33%
7	s	2	 50% 50%

2 Entry composition [i](#)

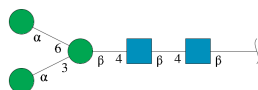
There are 8 unique types of molecules in this entry. The entry contains 30896 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1224	Total	C	N	O	S	0	0
			9400	5974	1556	1829	41		
1	B	1224	Total	C	N	O	S	0	0
			9400	5974	1556	1829	41		
1	C	1224	Total	C	N	O	S	0	0
			9400	5974	1556	1829	41		

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



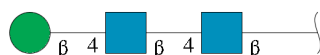
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	5	Total	C	N	O	0	0
			61	34	2	25		
2	F	5	Total	C	N	O	0	0
			61	34	2	25		
2	G	5	Total	C	N	O	0	0
			61	34	2	25		
2	H	5	Total	C	N	O	0	0
			61	34	2	25		
2	J	5	Total	C	N	O	0	0
			61	34	2	25		
2	N	5	Total	C	N	O	0	0
			61	34	2	25		
2	P	5	Total	C	N	O	0	0
			61	34	2	25		
2	R	5	Total	C	N	O	0	0
			61	34	2	25		
2	T	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	U	5	Total	C	N	O	0	0
			61	34	2	25		
2	W	5	Total	C	N	O	0	0
			61	34	2	25		
2	X	5	Total	C	N	O	0	0
			61	34	2	25		
2	Y	5	Total	C	N	O	0	0
			61	34	2	25		
2	a	5	Total	C	N	O	0	0
			61	34	2	25		
2	b	5	Total	C	N	O	0	0
			61	34	2	25		
2	d	5	Total	C	N	O	0	0
			61	34	2	25		
2	g	5	Total	C	N	O	0	0
			61	34	2	25		
2	h	5	Total	C	N	O	0	0
			61	34	2	25		
2	j	5	Total	C	N	O	0	0
			61	34	2	25		
2	k	5	Total	C	N	O	0	0
			61	34	2	25		
2	m	5	Total	C	N	O	0	0
			61	34	2	25		
2	n	5	Total	C	N	O	0	0
			61	34	2	25		
2	o	5	Total	C	N	O	0	0
			61	34	2	25		
2	p	5	Total	C	N	O	0	0
			61	34	2	25		
2	u	5	Total	C	N	O	0	0
			61	34	2	25		

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



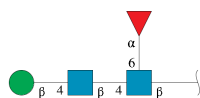
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	c	3	Total	C	N	O	0	0
			39	22	2	15		
3	f	3	Total	C	N	O	0	0
			39	22	2	15		
3	l	3	Total	C	N	O	0	0
			39	22	2	15		
3	q	3	Total	C	N	O	0	0
			39	22	2	15		
3	r	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



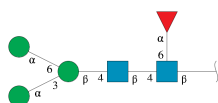
Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	4	Total	C	N	O	0	0
			49	28	2	19		
4	M	4	Total	C	N	O	0	0
			49	28	2	19		
4	Z	4	Total	C	N	O	0	0
			49	28	2	19		
4	t	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	6	Total	C	N	O	0	0
			71	40	2	29		
6	S	6	Total	C	N	O	0	0
			71	40	2	29		
6	e	6	Total	C	N	O	0	0
			71	40	2	29		
6	i	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	s	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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

3 Residue-property plots

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

• Molecule 1: Spike glycoprotein

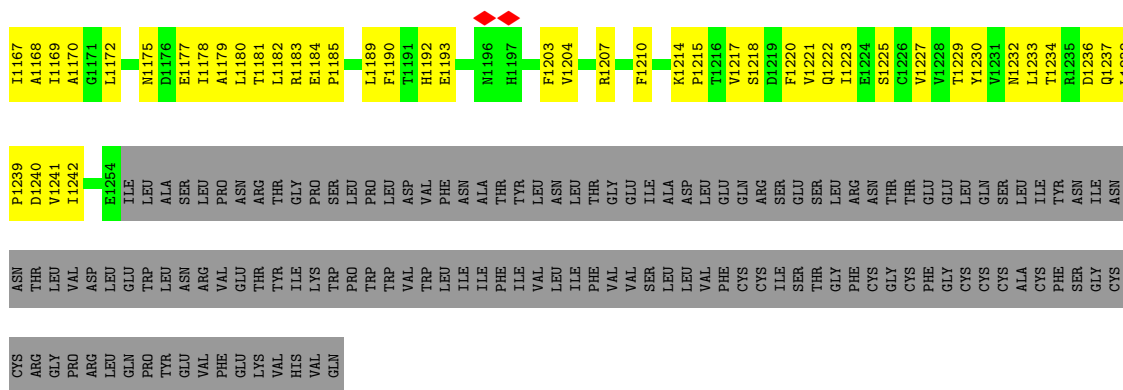


PHE GLY CYS GLN CYS SER GLU ALA CYS PHE SER GLY CYS ASN THR GLY PRO ARG LEU GLN PRO TYR LEU ASN GLU VAL PHE GLU LYS THR GLY PRO SER LEU PRO LEU ASP VAL PHE ILE ALA SER LEU PRO GLY THR GLY VAL VAL GLN	GLU	V1231	T1156	S1092	T1030	E948	Q860	P785	A693	Y606	G522	E452	K376
	GLU	M1232	V1157	A1093	V1031	H951	A862	T786	V694	G612	G523	V453	V377
	GLU	L1233	L1158	A1032	H1033	H951	A862	T787	Y695	G612	H524	Q454	
	GLN	M1095	V1159	N1095	H1034	Y953	D870	F788	S696	K614		G455	V384
	CYS	R1234	P1160	A1096	A1034	Y953	D870	S789	E704		L529	T456	Y385
	ALA	D1236	S1161	V1098	L1035	S954	G871	M790	E705		I530	K386	F387
	CYS	Q1237		F1098	T1036		Y872	S791	Q705		I530	I458	L388
	ILE			V1164	L1037	L957	L957	K1037	A706		S617	A531	
	THR			D1165	V1038	P958	T875	R792	A707		L618	Q469	
	ASN	V1241	V1166	T1101	Q1039		N876	F793	D533		S532	R460	
	ASN	D1244	I1167	L1102	E1040	L963	V877	T794	W708		F620	I461	
	ASN			T1103	V1041		L878	E795	W709		T621	L462	
	ASN			K1104	V1042		G879	Y796	D710		F622	Y463	
	THR	N1249	L1172	T1172	K1105	F966	C879	L797	D711		I536	C644	
	GLY	K1250	C1173	V1173	T1106	P967	V880	Q798	D712		K624	C644	
	PRO	T1251	V1174		L1106	A968	S881	L799	I713		G625	D466	
	ARG		N1175		E1107	A969	V882	Y800	V714		E626	P467	
	LEU	E1254			V1108				G715		L627	V468	
	LEU				A1048	P885		C808	G715		E627		
	GLN	ILE	L1180	T1180	Q1109	P973	P973	L1049	W716		D545		
TRP	LEU	L1181	L1181	A1110	F974	F974	T1050	I717		I628			
LEU		L1182		S1111	S975	S975	Q1051	T629		T629			
ASN	SER	R1183	L1182	K1112	Y976	Y976	S817	S718					
GLU	LEU	E1184	E1184	R1113	A977	A977	R818	S719					
VAL	ARG	PRO	ASN	L1114	V1054	V978	C819						
GLU	ASN	ASN	ASN	A1115	Q1055		Q892	F725		L553			
THR	ARG	ARG	ARG	Q1116	L1056		K893	W726					
VAL	THR	L1188	V1188	Q1117	Q1057		R894	F643		N556			
VAL	VAL	F1190	L1189	K1118	H058		S895	R729		V557			
HIS	VAL			V1119	L1058		R822	L646		T558			
VAL	VAL	PRO	GLY	N1119	V1059		F896			N559			
GLN	THR	SER	SER	N1120	F1060		I897						
	PRO	LEU	LEU	Q1061	Q1061		E898			K651			
	PRO			V1123			D899			Y652			
	TRP	H1197			A1062					T653			
	TRP	T1198			I1063					I654			
	LEU	A1199			S1064					Y655			
	ASP			Q1126			F902						
	VAL	S1127		S1127	S1065		N903						
	THR			Q1128	S1066		K904						
	PHE	Y1202		R1129	I1067		Q993						
	ILE	F1203		ASN			R994						
	ALA			Y1130	D1068		V906						
	THR	L1204		D1069			T907						
	PHE	S1205		F1132	D1069		N995						
	ILE				I1070		Q996						
	VAL	LEU			Y1071		Q997						
	LEU	M1209		G1135	S1072		G909						
	ASN	F1210		D1136	R1073		L998						
	LEU	E1211		GLU	L1074		S840						
	THR	P1212		H1137	R1073		A841						
	VAL	P1214		E1138	D1075		Y917						
	VAL	P1215		H1139	I1076		S1002						
	GLY	K1214		I1140	L1077		F1003						
	THR	P1216		ILE	S1078		N922						
	LEU	V1217		S1142	A1079		G923						
	ASP	V1217		L1143	D1080		R924						
	VAL	S1218		V1144	V1081		G1008						
	PHE	D1219		Q1145	D1081		N1009						
	GLN	F1220		V1145	Q1082		L929						
	CYS	ARG		A1146	A1013		N849						
	CYS	ILE			D1084		L852						
	SER	GLU		Q1149	Q932		T853						
	THR	SER		G1150	Q933		R854						
	GLY	LEU		L1151	Y934		S855						
	PHE	ARG		L1152	T1087		S936						
	ASN	C1226		F1153	T1084		S937						
	THR	V1227		L1154	S1025		V938						
	GLY	THR		H1155	R1091		L1091						

• Molecule 1: Spike glycoprotein







- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 60% 40%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 40% 60%



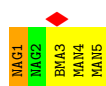
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 20% 80%

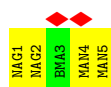


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 20% 20% 60% 20%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



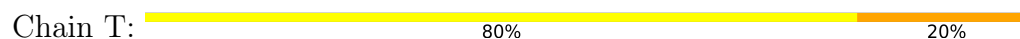
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



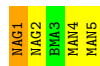
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



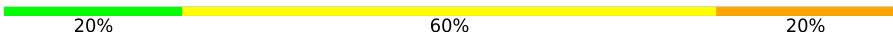
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

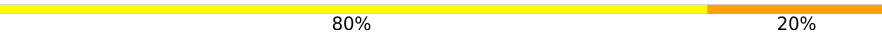


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 

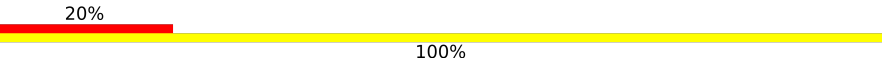


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

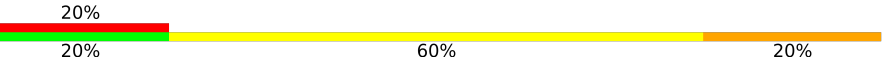


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 

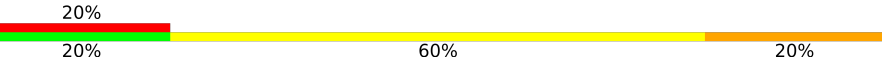


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

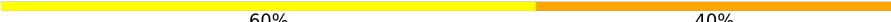


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  60% 40%

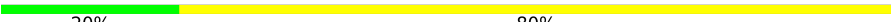


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  40% 60%

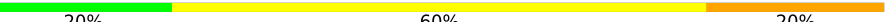


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  20% 80%

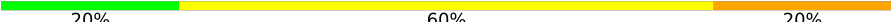


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  20% 60% 20%

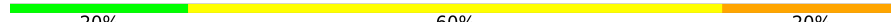


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  20% 60% 20%



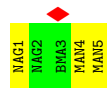
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  20% 60% 20%



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

nose



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



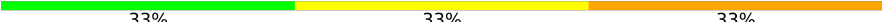
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

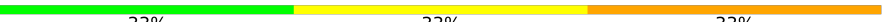


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  33% 33% 33%

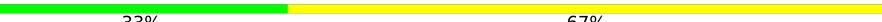


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  33% 33% 33%

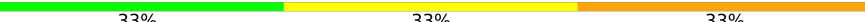


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  33% 67%

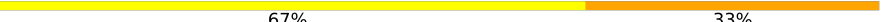


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  33% 33% 33%



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

Chain l:  67% 33%



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

Chain q:  67% 33%



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

Chain r:  67% 33%



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  25% 50% 50%



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 25% 25%



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 50%

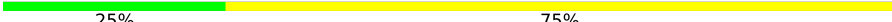


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  25% 25% 75%

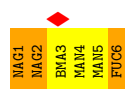


- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

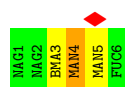
Chain L:  25% 75%



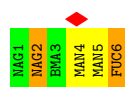
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



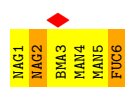
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9319	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 ($e^-/\text{\AA}^2$)	55.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.512	Depositor
Minimum map value	-0.687	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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: MAN, FUC, BMA, 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	0.26	0/9610	0.48	0/13095
1	B	0.25	0/9610	0.46	0/13095
1	C	0.26	0/9610	0.47	0/13095
All	All	0.25	0/28830	0.47	0/39285

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	9400	0	9090	606	0
1	B	9400	0	9090	595	0
1	C	9400	0	9090	569	0
2	D	61	0	52	3	0
2	F	61	0	52	3	0
2	G	61	0	52	8	0
2	H	61	0	52	1	0
2	J	61	0	52	1	0
2	N	61	0	52	2	0
2	P	61	0	52	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	61	0	52	4	0
2	T	61	0	52	2	0
2	U	61	0	52	4	0
2	W	61	0	52	2	0
2	X	61	0	52	4	0
2	Y	61	0	52	1	0
2	a	61	0	52	1	0
2	b	61	0	52	1	0
2	d	61	0	52	4	0
2	g	61	0	52	1	0
2	h	61	0	52	2	0
2	j	61	0	52	2	0
2	k	61	0	52	3	0
2	m	61	0	52	1	0
2	n	61	0	52	0	0
2	o	61	0	52	5	0
2	p	61	0	52	0	0
2	u	61	0	52	7	0
3	E	39	0	34	2	0
3	K	39	0	34	0	0
3	Q	39	0	34	2	0
3	V	39	0	34	4	0
3	c	39	0	34	1	0
3	f	39	0	34	3	0
3	l	39	0	34	1	0
3	q	39	0	34	1	0
3	r	39	0	34	1	0
4	I	49	0	43	3	0
4	M	49	0	43	1	0
4	Z	49	0	43	0	0
4	t	49	0	43	4	0
5	L	50	0	43	6	0
6	O	71	0	61	5	0
6	S	71	0	61	1	0
6	e	71	0	61	2	0
6	i	71	0	61	2	0
7	s	24	0	22	5	0
8	A	84	0	78	6	0
8	B	98	0	91	10	0
8	C	84	0	78	1	0
All	All	30896	0	29604	1756	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 29.

All (1756) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:VAL:HG12	1:B:472:LYS:HZ2	1.35	0.90
1:C:795:GLU:HB3	1:C:1153:PHE:HB2	1.51	0.90
1:A:337:LEU:HB2	1:A:345:PHE:HB2	1.55	0.87
1:A:1140:ILE:HG13	1:A:1158:LEU:HD23	1.55	0.85
1:B:1069:ASP:O	1:B:1073:ARG:NH1	2.09	0.85
1:A:687:LYS:HG3	1:A:694:VAL:HG12	1.57	0.85
1:B:933:GLN:HB3	1:B:938:VAL:HB	1.60	0.83
1:B:751:TYR:HA	1:C:842:ARG:HH22	1.42	0.83
1:C:690:THR:HG22	2:u:1:NAG:HN2	1.44	0.83
1:A:518:SER:HA	1:A:556:ASN:HB3	1.61	0.82
1:B:91:PHE:HB2	1:B:111:LYS:HB3	1.60	0.82
1:A:797:LEU:HD23	1:A:1115:ALA:HB2	1.62	0.82
1:C:488:SER:HA	1:C:703:SER:HA	1.61	0.82
1:A:1172:LEU:HB3	1:A:1180:LEU:HB3	1.60	0.82
1:A:1061:GLN:O	1:A:1085:ARG:NH1	2.13	0.81
1:B:892:GLN:NE2	1:B:893:LYS:O	2.14	0.81
1:A:280:LEU:HB3	1:A:445:ASN:HB2	1.63	0.81
1:C:916:ASP:O	1:C:919:ARG:NH1	2.14	0.80
1:C:798:GLN:HE21	1:C:1149:GLN:HG2	1.46	0.80
1:C:798:GLN:NE2	1:C:800:TYR:O	2.15	0.80
1:A:675:TYR:HA	1:A:686:PHE:HA	1.64	0.80
1:A:811:TYR:O	1:A:1090:ARG:NH2	2.15	0.80
1:C:675:TYR:HB2	1:C:683:LEU:HD11	1.64	0.80
1:C:793:ARG:HB3	1:C:1029:ASN:HB3	1.63	0.80
1:A:689:VAL:HG22	2:G:1:NAG:H81	1.62	0.79
1:B:518:SER:HA	1:B:556:ASN:HB2	1.64	0.79
1:B:678:SER:N	1:B:682:GLN:O	2.15	0.79
1:C:83:SER:HB2	1:C:163:VAL:HA	1.65	0.79
1:B:716:VAL:HB	1:B:737:HIS:HB2	1.64	0.79
2:P:1:NAG:H3	2:P:1:NAG:H83	1.65	0.79
1:A:994:ARG:NH1	1:A:995:ASN:OD1	2.15	0.79
1:A:663:ILE:HD11	1:A:695:TYR:HB3	1.64	0.79
1:A:793:ARG:NH1	1:A:1135:GLY:O	2.16	0.78
1:C:179:LYS:NZ	1:C:180:ILE:O	2.17	0.78
1:B:651:LYS:NZ	1:B:652:TYR:O	2.17	0.78
1:B:922:ASN:O	1:B:924:ARG:NH1	2.17	0.78
1:B:475:GLN:HA	1:C:831:LYS:HE2	1.65	0.78
1:B:882:VAL:HA	1:B:890:VAL:HG13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LYS:NZ	1:B:180:ILE:O	2.16	0.77
1:B:351:ASN:HB3	8:B:1407:NAG:N2	1.98	0.77
1:B:586:SER:HB3	1:B:625:GLY:HA3	1.67	0.77
1:A:798:GLN:NE2	1:A:800:TYR:O	2.16	0.77
1:A:1139:HIS:NE2	1:A:1142:SER:OG	2.17	0.77
1:B:585:PHE:CE2	1:B:622:PHE:HB2	2.20	0.77
1:C:1140:ILE:HD11	1:C:1158:LEU:HB2	1.65	0.77
1:B:565:SER:HB3	1:B:606:TYR:HB2	1.67	0.76
1:A:718:SER:OG	1:A:737:HIS:NE2	2.10	0.76
1:B:709:VAL:N	1:B:712:ASP:O	2.16	0.76
1:C:1144:VAL:O	1:C:1145:GLN:NE2	2.18	0.76
1:B:258:ASN:O	1:B:320:ARG:NH2	2.18	0.76
1:A:547:ARG:O	1:A:629:THR:N	2.19	0.76
1:A:300:ASN:HD21	4:M:4:FUC:H61	1.50	0.75
1:A:172:ARG:NH1	1:A:427:THR:OG1	2.20	0.75
1:B:112:ALA:HB3	1:B:119:ALA:HA	1.68	0.75
1:B:97:GLN:HA	1:B:190:SER:H	1.51	0.75
1:B:800:TYR:N	1:B:1149:GLN:OE1	2.20	0.75
1:C:882:VAL:HA	1:C:890:VAL:HG13	1.68	0.75
1:B:576:LEU:O	1:B:580:ASN:ND2	2.20	0.74
1:C:718:SER:HG	1:C:737:HIS:HE2	1.33	0.74
1:B:586:SER:OG	1:B:623:THR:O	2.04	0.74
1:A:868:ASN:ND2	1:A:971:ALA:O	2.20	0.74
1:C:986:ALA:O	1:C:988:GLN:NE2	2.19	0.74
1:A:130:SER:OG	1:A:141:ASP:OD2	2.06	0.74
1:B:167:THR:OG1	1:B:174:THR:OG1	2.05	0.74
1:B:113:THR:HB	8:B:1401:NAG:H81	1.69	0.74
1:B:148:CYS:SG	1:B:151:ASN:ND2	2.60	0.74
1:C:800:TYR:O	1:C:1149:GLN:NE2	2.20	0.74
1:A:274:VAL:HG22	1:A:450:LEU:HA	1.70	0.73
1:B:793:ARG:NH1	1:B:1135:GLY:O	2.21	0.73
1:C:270:HIS:ND1	1:C:453:VAL:O	2.20	0.73
1:C:667:ASN:HB2	7:s:1:NAG:H2	1.70	0.73
1:C:521:PHE:N	1:C:558:THR:O	2.21	0.73
1:A:670:PHE:HB3	1:B:456:THR:HG21	1.71	0.73
1:A:270:HIS:ND1	1:A:453:VAL:O	2.20	0.73
1:C:263:SER:OG	1:C:265:ASP:O	2.05	0.72
1:C:168:TRP:NE1	1:C:170:ASN:O	2.22	0.72
1:A:1252:ARG:NH2	1:B:1254:GLU:O	2.23	0.72
1:B:1061:GLN:O	1:B:1085:ARG:NH1	2.21	0.72
1:A:135:GLY:HA2	1:A:195:LYS:HE2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:LYS:NZ	1:C:594:LEU:O	2.18	0.71
1:B:173:VAL:HB	1:B:183:PHE:HB2	1.72	0.71
1:B:881:SER:HA	1:B:892:GLN:HA	1.72	0.71
1:B:1126:GLN:O	1:B:1128:GLN:NE2	2.23	0.71
1:B:35:PHE:O	1:B:38:LYS:NZ	2.23	0.71
1:B:677:THR:HA	1:B:683:LEU:HA	1.72	0.71
1:B:1042:VAL:O	1:B:1045:GLN:NE2	2.22	0.71
1:B:795:GLU:HB3	1:B:1153:PHE:HB2	1.72	0.71
1:C:102:PRO:O	1:C:143:THR:OG1	2.07	0.71
1:C:481:ASP:O	1:C:485:TYR:OH	2.05	0.70
1:B:146:ARG:NE	1:B:904:LYS:O	2.23	0.70
1:B:34:ARG:NH2	1:B:222:GLU:O	2.25	0.70
1:B:750:VAL:O	1:C:842:ARG:NH2	2.25	0.70
1:A:666:THR:OG1	8:A:1402:NAG:O7	2.09	0.70
1:B:798:GLN:OE1	1:B:798:GLN:N	2.25	0.70
1:B:889:ARG:NH1	1:B:890:VAL:O	2.25	0.70
1:A:262:LEU:HD22	1:A:277:GLN:HB3	1.74	0.70
1:A:674:VAL:HA	1:A:687:LYS:HB2	1.73	0.70
1:C:736:TYR:OH	1:C:760:GLY:O	2.09	0.69
1:C:893:LYS:NZ	1:C:894:ARG:O	2.24	0.69
1:A:376:LYS:HE3	1:A:383:THR:HB	1.71	0.69
1:A:712:ASP:OD1	1:A:713:ILE:N	2.25	0.69
1:C:269:VAL:HG23	1:C:456:THR:HG23	1.74	0.69
1:C:816:ASN:OD1	1:C:817:SER:N	2.25	0.69
1:C:793:ARG:NH1	1:C:1135:GLY:O	2.25	0.69
1:C:893:LYS:O	1:C:951:HIS:NE2	2.25	0.69
1:A:508:ASN:ND2	1:A:635:LEU:O	2.24	0.69
1:B:249:HIS:NE2	1:B:465:ASP:OD2	2.25	0.69
1:B:585:PHE:HE2	1:B:622:PHE:HB2	1.57	0.69
1:B:981:ARG:NE	1:B:1140:ILE:O	2.26	0.69
1:C:48:VAL:HA	1:C:214:MET:HA	1.75	0.69
1:A:488:SER:HA	1:A:703:SER:HA	1.74	0.69
1:B:1126:GLN:NE2	1:B:1139:HIS:O	2.26	0.69
1:C:718:SER:OG	1:C:737:HIS:NE2	2.20	0.69
6:O:2:NAG:HN2	6:O:6:FUC:H3	1.57	0.69
2:P:2:NAG:H61	2:P:3:BMA:H2	1.74	0.69
1:A:821:GLN:O	1:A:824:THR:OG1	2.10	0.69
1:B:33:ARG:NE	1:B:224:GLY:O	2.23	0.69
6:e:2:NAG:H2	6:e:6:FUC:H61	1.75	0.69
1:A:33:ARG:NE	1:A:224:GLY:O	2.24	0.69
1:C:127:GLN:HG3	1:C:144:ILE:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1205:SER:HB2	1:A:1211:GLU:H	1.58	0.69
1:B:856:GLU:OE1	1:B:860:GLN:NE2	2.25	0.69
1:A:889:ARG:NH1	1:A:890:VAL:O	2.26	0.68
1:A:1144:VAL:O	1:A:1145:GLN:NE2	2.26	0.68
1:A:795:GLU:HB3	1:A:1153:PHE:HB2	1.75	0.68
1:B:1036:THR:O	1:B:1039:GLN:HG3	1.93	0.68
2:d:1:NAG:O6	2:d:2:NAG:N2	2.26	0.68
1:B:481:ASP:O	1:B:485:TYR:OH	2.10	0.68
1:B:726:ASN:N	1:B:739:ASN:OD1	2.27	0.68
1:B:818:ARG:NE	1:B:1071:TYR:OH	2.21	0.68
1:B:83:SER:HB2	1:B:163:VAL:HG12	1.76	0.68
1:C:1035:LEU:HA	1:C:1038:VAL:HG12	1.74	0.68
1:A:209:GLU:OE1	1:A:209:GLU:N	2.27	0.68
1:A:225:ILE:HG21	6:O:1:NAG:H5	1.75	0.68
1:C:167:THR:OG1	1:C:174:THR:OG1	2.12	0.68
1:A:322:ASN:O	1:A:439:TRP:N	2.25	0.68
1:B:799:LEU:HG	1:B:1150:GLY:HA2	1.76	0.68
1:B:932:ALA:O	1:B:936:SER:N	2.27	0.68
1:B:1217:VAL:HA	1:B:1220:PHE:CE2	2.29	0.68
1:B:799:LEU:HD21	1:B:1151:LEU:HD23	1.76	0.68
1:A:521:PHE:N	1:A:558:THR:O	2.26	0.67
1:B:793:ARG:HB3	1:B:1029:ASN:HB3	1.74	0.67
1:C:941:LEU:HD12	1:C:942:PRO:HD2	1.75	0.67
1:C:352:SER:H	1:C:364:LEU:HD22	1.59	0.67
1:A:1222:GLN:OE1	1:B:1213:ARG:NH2	2.28	0.67
1:B:529:LEU:HD21	1:B:532:SER:HB3	1.74	0.67
1:C:895:SER:N	1:C:898:GLU:OE2	2.24	0.67
1:C:982:LEU:O	1:C:988:GLN:NE2	2.26	0.67
1:A:502:VAL:HB	1:A:654:ILE:HD12	1.77	0.67
1:B:377:VAL:HB	1:B:384:VAL:HG23	1.76	0.67
1:B:969:ALA:HA	2:R:2:NAG:H82	1.75	0.67
1:C:1066:SER:OG	1:C:1068:ASP:OD1	2.13	0.67
1:A:349:CYS:HA	1:A:373:CYS:HA	1.75	0.67
1:A:1224:GLU:OE1	1:B:1213:ARG:NH1	2.26	0.67
1:C:1138:GLU:N	1:C:1138:GLU:OE1	2.27	0.67
1:A:386:LYS:NZ	1:A:387:PHE:O	2.26	0.67
1:A:787:ASN:ND2	1:A:1162:ASP:OD2	2.27	0.67
1:B:958:ILE:HD11	1:B:1144:VAL:HG12	1.77	0.67
1:A:93:ILE:HB	1:A:109:LEU:HB3	1.75	0.67
1:A:588:PHE:HE1	1:A:620:PHE:HB3	1.60	0.67
1:B:515:ILE:HD13	1:B:536:ILE:HG13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:SER:OG	1:A:265:ASP:O	2.12	0.66
1:C:717:ILE:HD13	1:C:736:TYR:HA	1.77	0.66
1:A:497:GLN:NE2	1:A:660:GLU:OE2	2.29	0.66
1:C:812:VAL:HG12	1:C:1090:ARG:HE	1.61	0.66
1:C:1054:VAL:HG12	1:C:1058:HIS:HE1	1.58	0.66
1:C:1074:LEU:HD21	1:C:1078:SER:HB2	1.76	0.66
1:A:485:TYR:N	1:A:705:GLN:OE1	2.26	0.66
1:A:1031:VAL:HG22	1:A:1035:LEU:HD23	1.76	0.66
1:C:812:VAL:HB	1:C:1090:ARG:HH21	1.59	0.66
1:B:895:SER:N	1:B:898:GLU:OE2	2.28	0.66
1:B:1064:SER:HB3	1:B:1070:ILE:HD11	1.78	0.66
1:C:294:GLY:HA2	1:C:425:ASN:HB3	1.78	0.66
1:C:944:VAL:HG23	1:C:945:VAL:HG23	1.76	0.66
1:A:322:ASN:HB3	1:A:440:THR:H	1.61	0.66
1:A:768:GLN:NE2	1:A:769:SER:O	2.28	0.66
1:B:968:ALA:HA	2:R:1:NAG:H83	1.77	0.66
1:C:716:VAL:HB	1:C:737:HIS:HB2	1.77	0.66
1:B:60:GLY:HA2	1:B:206:TYR:HE2	1.61	0.65
1:C:679:ASP:OD1	1:C:680:SER:N	2.29	0.65
1:B:546:THR:OG1	1:B:548:GLN:O	2.14	0.65
1:B:585:PHE:O	1:B:628:ILE:N	2.28	0.65
1:B:588:PHE:HE1	1:B:620:PHE:HB3	1.60	0.65
1:C:1057:GLN:O	1:C:1057:GLN:NE2	2.29	0.65
1:A:281:VAL:HG23	1:A:442:ALA:HB1	1.77	0.65
1:A:47:VAL:HA	1:A:237:TYR:HB2	1.79	0.65
1:A:983:ASN:HB3	1:A:987:LEU:HD13	1.78	0.65
1:A:1000:ALA:HA	1:A:1003:PHE:HD2	1.61	0.65
1:A:1051:GLN:OE1	1:A:1051:GLN:N	2.30	0.65
1:A:1121:GLU:HG2	1:A:1122:CYS:N	2.12	0.65
1:B:233:ASN:OD1	2:U:1:NAG:O3	2.15	0.65
1:B:1031:VAL:HG22	1:B:1035:LEU:HD23	1.76	0.65
1:B:1048:ALA:HA	1:B:1051:GLN:HE22	1.60	0.65
1:B:1167:ILE:HD11	1:B:1194:LEU:HG	1.79	0.65
1:C:314:ARG:NH2	1:C:317:GLU:OE2	2.29	0.65
1:A:1115:ALA:HA	1:A:1118:LYS:HE2	1.78	0.65
1:B:282:ASN:OD1	1:B:445:ASN:ND2	2.29	0.65
1:C:816:ASN:O	1:C:820:LYS:NZ	2.30	0.65
1:A:267:THR:HG21	1:C:676:TYR:HA	1.79	0.65
1:B:688:ASN:N	1:B:693:ALA:O	2.27	0.65
1:A:601:ILE:HB	1:A:618:LEU:HB2	1.79	0.64
1:A:664:THR:N	1:A:696:SER:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ASP:O	1:C:470:GLN:N	2.25	0.64
1:B:1132:PHE:H	1:B:1139:HIS:CE1	2.16	0.64
1:B:778:VAL:HG21	1:C:979:GLN:HE22	1.62	0.64
1:B:792:ILE:HA	1:B:1155:HIS:O	1.97	0.64
1:C:976:TYR:O	1:C:979:GLN:NE2	2.31	0.64
1:A:564:VAL:HG22	1:A:607:PRO:HA	1.79	0.64
1:B:584:SER:O	1:B:624:LYS:NZ	2.31	0.64
1:C:304:ASP:OD1	1:C:305:GLY:N	2.31	0.64
1:C:1179:ALA:HB3	1:C:1223:ILE:HB	1.80	0.64
1:A:95:ILE:HG22	1:A:107:LEU:H	1.63	0.64
1:A:676:TYR:N	1:A:685:ALA:O	2.30	0.64
1:A:986:ALA:O	1:A:988:GLN:NE2	2.30	0.64
1:A:1192:HIS:HB3	1:A:1201:GLU:HB3	1.80	0.63
1:B:787:ASN:OD1	2:b:1:NAG:N2	2.31	0.63
1:B:1174:VAL:HG22	1:B:1235:ARG:HD3	1.80	0.63
1:A:733:GLY:HA2	1:B:916:ASP:HA	1.81	0.63
1:C:771:GLN:NE2	1:C:772:VAL:O	2.31	0.63
2:W:1:NAG:O3	2:W:2:NAG:H2	1.99	0.63
1:A:466:ASP:O	1:A:470:GLN:N	2.18	0.63
1:C:1232:ASN:OD1	3:r:1:NAG:N2	2.31	0.63
1:A:264:ASN:OD1	1:A:265:ASP:N	2.32	0.63
1:C:47:VAL:HA	1:C:237:TYR:HE1	1.64	0.63
1:A:339:THR:HA	1:A:419:LEU:HD13	1.80	0.63
1:A:979:GLN:O	1:A:983:ASN:ND2	2.21	0.63
1:C:1185:PRO:O	1:C:1207:ARG:NE	2.31	0.63
1:A:103:SER:O	1:A:127:GLN:NE2	2.31	0.63
1:B:984:TYR:OH	1:B:1128:GLN:OE1	2.16	0.63
1:C:1061:GLN:O	1:C:1085:ARG:NH1	2.31	0.63
1:B:252:GLU:N	1:B:252:GLU:OE1	2.31	0.63
1:A:1114:LEU:O	1:A:1117:GLN:HB3	1.99	0.63
1:B:1209:MET:HE3	1:B:1210:PHE:N	2.14	0.63
1:C:1178:ILE:HG23	1:C:1222:GLN:HG2	1.81	0.63
1:A:1027:GLY:O	1:A:1030:THR:OG1	2.12	0.63
1:C:343:THR:HG23	1:C:379:THR:HB	1.81	0.63
1:C:834:GLU:OE2	1:C:838:GLN:NE2	2.32	0.63
1:C:1050:THR:O	1:C:1053:THR:OG1	2.14	0.63
1:A:709:VAL:N	1:A:712:ASP:O	2.20	0.62
1:A:726:ASN:OD1	1:A:727:SER:N	2.32	0.62
1:B:354:ASN:ND2	1:B:363:PRO:O	2.32	0.62
1:A:646:LEU:HD12	1:A:663:ILE:HG23	1.80	0.62
1:C:639:THR:HG23	2:u:4:MAN:H62	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:NE1	1:A:187:ASN:OD1	2.32	0.62
1:A:895:SER:N	1:A:898:GLU:OE2	2.33	0.62
1:C:86:ARG:HH21	1:C:200:GLY:HA3	1.64	0.62
1:C:690:THR:HG22	2:u:1:NAG:N2	2.15	0.62
1:C:801:ASN:HA	1:C:1149:GLN:NE2	2.14	0.62
1:B:340:ALA:N	1:B:418:LEU:O	2.32	0.62
1:B:817:SER:O	1:B:820:LYS:HG2	2.00	0.62
1:B:1032:ALA:HA	1:B:1035:LEU:HG	1.82	0.62
1:B:97:GLN:HB3	1:B:188:ASP:O	1.98	0.62
1:B:1113:LYS:O	1:B:1116:GLN:NE2	2.33	0.62
1:B:1175:ASN:HB2	1:B:1235:ARG:HD2	1.81	0.62
1:C:930:VAL:HA	1:C:933:GLN:NE2	2.15	0.62
1:A:930:VAL:O	1:A:933:GLN:NE2	2.33	0.61
1:B:411:PHE:HD2	1:B:413:TYR:HD1	1.48	0.61
1:B:1014:PHE:HA	1:B:1031:VAL:HG21	1.82	0.61
1:C:870:ASP:OD2	1:C:975:SER:N	2.25	0.61
1:A:1228:VAL:H	5:L:2:NAG:H82	1.65	0.61
1:B:357:LEU:HD22	1:B:374:PHE:HD2	1.64	0.61
1:A:806:VAL:HG22	1:A:938:VAL:HG22	1.82	0.61
1:B:675:TYR:OH	1:C:266:SER:N	2.23	0.61
1:C:174:THR:HB	1:C:180:ILE:HD11	1.82	0.61
1:A:175:VAL:HB	1:A:181:TYR:HB2	1.81	0.61
1:A:1145:GLN:HB2	1:A:1152:LEU:HD11	1.82	0.61
1:B:1209:MET:HE3	1:B:1210:PHE:H	1.64	0.61
1:A:1057:GLN:NE2	1:C:679:ASP:O	2.33	0.61
1:A:933:GLN:O	1:A:936:SER:OG	2.12	0.61
1:B:468:VAL:HA	1:B:471:LEU:HD12	1.83	0.61
1:C:840:SER:O	1:C:843:LEU:HG	2.01	0.61
1:B:475:GLN:HA	1:C:831:LYS:CE	2.31	0.61
1:C:67:CYS:SG	1:C:68:ALA:N	2.74	0.61
1:C:502:VAL:HB	1:C:654:ILE:HD12	1.83	0.61
1:C:805:SER:N	1:C:939:MET:O	2.31	0.61
2:G:3:BMA:H5	2:G:5:MAN:H5	1.83	0.61
1:A:1112:ARG:NH1	1:A:1113:LYS:HG3	2.15	0.61
1:B:130:SER:OG	1:B:141:ASP:OD2	2.17	0.61
1:A:420:ASP:OD1	1:A:421:ALA:N	2.34	0.61
1:A:535:THR:HB	1:A:538:GLY:H	1.65	0.61
1:A:918:LYS:NZ	1:C:719:SER:HA	2.15	0.61
1:C:92:GLU:O	1:C:194:THR:OG1	2.09	0.61
1:A:92:GLU:HB3	1:A:195:LYS:HB2	1.83	0.61
1:A:781:ASN:HB3	1:A:1167:ILE:HG13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TYR:CD1	1:A:229:PRO:HD3	2.36	0.60
1:A:364:LEU:HG	1:A:372:TYR:HB2	1.83	0.60
1:A:1015:GLU:OE2	1:A:1016:SER:OG	2.17	0.60
1:C:817:SER:HA	1:C:820:LYS:HZ3	1.66	0.60
1:A:1185:PRO:O	1:A:1207:ARG:NH1	2.28	0.60
1:A:798:GLN:HA	1:A:1150:GLY:HA3	1.82	0.60
1:A:1146:ALA:HA	1:A:1151:LEU:HD13	1.82	0.60
1:C:280:LEU:O	1:C:445:ASN:N	2.34	0.60
1:C:482:ASP:OD2	1:C:710:ASP:N	2.34	0.60
1:C:677:THR:HA	1:C:683:LEU:HA	1.82	0.60
1:A:219:SER:HB3	1:A:225:ILE:HD11	1.84	0.60
1:A:792:ILE:HA	1:A:1155:HIS:O	2.00	0.60
1:B:1053:THR:O	1:B:1056:LEU:HG	2.00	0.60
1:C:1178:ILE:HA	1:C:1222:GLN:HE21	1.66	0.60
1:B:744:CYS:SG	1:B:757:CYS:N	2.74	0.60
1:C:796:TYR:CZ	1:C:1147:ALA:HB3	2.37	0.60
1:C:847:GLU:HA	1:C:850:SER:HB3	1.83	0.60
1:C:887:ARG:HH22	1:C:891:VAL:HG11	1.67	0.60
1:A:676:TYR:HB3	1:A:685:ALA:HB3	1.84	0.60
1:B:96:SER:O	1:B:190:SER:N	2.35	0.60
1:B:105:TYR:HA	1:B:127:GLN:HG2	1.84	0.60
1:B:111:LYS:HA	1:B:121:ALA:HA	1.83	0.60
1:B:321:PHE:HD2	1:B:398:ILE:HB	1.67	0.60
1:C:120:THR:HA	1:C:155:PRO:HA	1.83	0.60
1:C:150:PHE:HZ	1:C:154:ILE:HD11	1.66	0.60
1:C:400:ILE:HG13	1:C:406:VAL:HG13	1.84	0.60
1:C:404:GLY:O	1:C:416:LEU:N	2.35	0.60
1:A:676:TYR:CE1	1:B:269:VAL:HG23	2.36	0.60
1:A:748:VAL:HG21	1:A:758:LYS:HG2	1.84	0.60
1:A:887:ARG:HA	4:t:3:BMA:H4	1.84	0.60
1:A:1228:VAL:N	5:L:2:NAG:H82	2.16	0.60
1:B:57:GLU:HA	1:B:205:GLN:HG2	1.84	0.60
1:B:222:GLU:OE1	1:B:222:GLU:N	2.35	0.60
1:B:816:ASN:OD1	1:B:817:SER:N	2.34	0.60
1:C:426:PHE:O	1:C:427:THR:OG1	2.18	0.60
2:P:2:NAG:H3	2:P:2:NAG:H83	1.83	0.60
1:A:252:GLU:OE1	1:A:252:GLU:N	2.34	0.60
1:B:586:SER:HA	1:B:627:LEU:HB2	1.83	0.60
1:B:667:ASN:ND2	1:C:924:ARG:HH22	1.99	0.60
1:C:1121:GLU:HG2	1:C:1122:CYS:H	1.66	0.60
1:A:522:GLY:HA2	1:A:526:GLY:HA2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:LEU:HD11	1:C:775:ALA:H	1.67	0.59
1:C:219:SER:OG	1:C:223:ASP:O	2.18	0.59
1:B:214:MET:HG3	1:B:230:CYS:HB2	1.83	0.59
1:C:351:ASN:HB2	1:C:368:GLN:HA	1.84	0.59
1:A:284:LEU:HD11	1:A:440:THR:HB	1.83	0.59
1:C:1123:VAL:HG21	1:C:1144:VAL:HG21	1.84	0.59
1:B:322:ASN:HB3	1:B:440:THR:H	1.67	0.59
1:B:469:SER:HA	1:B:472:LYS:HE2	1.83	0.59
1:A:47:VAL:O	1:A:215:LEU:N	2.34	0.59
1:C:280:LEU:HB3	1:C:445:ASN:HB2	1.84	0.59
1:C:856:GLU:O	1:C:859:LEU:HG	2.02	0.59
1:A:753:ASN:O	1:A:765:VAL:N	2.32	0.59
1:B:361:ALA:O	1:B:362:ILE:HG22	2.03	0.59
1:C:781:ASN:HB3	2:o:1:NAG:N2	2.17	0.59
1:C:1032:ALA:HA	1:C:1035:LEU:HG	1.84	0.59
1:A:125:ILE:N	1:A:150:PHE:O	2.35	0.59
1:A:317:GLU:OE1	1:A:317:GLU:N	2.36	0.59
1:B:290:ILE:HA	1:B:429:HIS:CE1	2.38	0.59
1:B:665:LEU:HD13	1:B:695:TYR:CE1	2.37	0.59
1:C:420:ASP:OD1	1:C:421:ALA:N	2.35	0.59
1:C:820:LYS:HA	1:C:823:LEU:HG	1.85	0.59
2:T:1:NAG:O7	2:T:1:NAG:O4	2.21	0.59
1:B:1102:LEU:O	1:B:1106:THR:HG23	2.02	0.59
1:B:1143:LEU:HB2	1:B:1154:LEU:HD11	1.84	0.59
1:C:122:ARG:NH1	1:C:151:ASN:OD1	2.33	0.59
1:C:150:PHE:CZ	1:C:152:LYS:HB2	2.38	0.59
1:C:454:GLN:OE1	1:C:454:GLN:N	2.36	0.59
1:A:81:PHE:N	1:A:205:GLN:O	2.34	0.59
1:A:892:GLN:O	1:A:894:ARG:NH2	2.36	0.59
1:C:1112:ARG:HH22	1:C:1113:LYS:HG3	1.67	0.59
1:A:1227:VAL:O	5:L:1:NAG:O6	2.15	0.59
1:B:454:GLN:N	1:B:457:ALA:O	2.35	0.59
1:B:753:ASN:O	1:B:765:VAL:N	2.34	0.59
1:A:82:VAL:O	1:A:163:VAL:HA	2.03	0.58
1:B:396:ARG:NH1	1:B:409:ASN:OD1	2.36	0.58
1:C:809:ALA:O	1:C:813:CYS:N	2.28	0.58
1:A:288:PRO:HG2	1:A:436:SER:HB3	1.84	0.58
1:B:283:CYS:SG	1:B:284:LEU:N	2.76	0.58
1:B:725:PHE:HB3	1:B:738:SER:O	2.03	0.58
1:B:808:CYS:SG	1:B:809:ALA:N	2.76	0.58
1:C:1101:THR:HA	1:C:1104:LYS:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1:NAG:H5	2:T:2:NAG:C7	2.33	0.58
1:A:790:MET:HB3	1:A:1158:LEU:HD13	1.84	0.58
1:A:898:GLU:OE1	1:A:898:GLU:N	2.27	0.58
1:B:784:ILE:O	1:B:1164:VAL:N	2.33	0.58
1:C:929:LEU:O	1:C:932:ALA:N	2.35	0.58
1:B:129:PRO:HB2	1:B:140:ASN:HB2	1.84	0.58
1:B:327:SER:HA	1:B:330:LEU:HD12	1.86	0.58
2:N:2:NAG:O6	2:N:5:MAN:O2	2.13	0.58
1:A:35:PHE:HE1	1:A:162:SER:HA	1.68	0.58
1:A:840:SER:O	1:A:843:LEU:HG	2.04	0.58
1:A:1031:VAL:O	1:A:1035:LEU:N	2.26	0.58
1:C:1003:PHE:O	1:C:1007:ILE:HG12	2.04	0.58
1:A:789:SER:O	1:A:1159:VAL:N	2.37	0.58
1:B:832:THR:O	1:B:835:SER:OG	2.19	0.58
1:C:804:VAL:HA	1:C:940:VAL:HA	1.86	0.58
1:C:408:VAL:HB	1:C:413:TYR:CE2	2.39	0.58
1:A:1172:LEU:HD12	1:A:1231:VAL:O	2.04	0.58
1:B:974:PHE:O	1:B:978:VAL:HG23	2.04	0.58
1:B:1051:GLN:OE1	1:B:1051:GLN:N	2.33	0.58
1:C:338:HIS:ND1	1:C:344:ASN:OD1	2.36	0.58
1:C:790:MET:HE3	1:C:999:LEU:HD12	1.85	0.58
1:C:792:ILE:HA	1:C:1155:HIS:O	2.04	0.58
1:C:1027:GLY:O	1:C:1030:THR:OG1	2.16	0.58
1:B:482:ASP:HB3	1:B:749:LEU:HD11	1.85	0.58
1:B:678:SER:OG	1:B:682:GLN:OE1	2.22	0.58
1:A:85:ILE:HG12	1:A:113:THR:HG21	1.86	0.58
1:B:588:PHE:HZ	1:B:620:PHE:HD2	1.51	0.58
1:B:791:SER:OG	1:B:1157:VAL:O	2.19	0.58
1:C:1114:LEU:O	1:C:1118:LYS:NZ	2.32	0.58
1:A:801:ASN:OD1	1:A:802:THR:N	2.37	0.57
1:C:529:LEU:HD21	1:C:532:SER:HB3	1.86	0.57
1:C:898:GLU:HA	1:C:901:LEU:HG	1.86	0.57
1:A:48:VAL:HA	1:A:214:MET:HA	1.85	0.57
1:A:788:PHE:HA	1:A:1160:PRO:HA	1.86	0.57
1:B:298:SER:OG	1:B:299:PHE:N	2.34	0.57
1:B:853:THR:H	1:B:953:TYR:HE1	1.52	0.57
1:B:858:ALA:O	1:B:862:ALA:N	2.37	0.57
1:B:1063:ILE:HG12	1:B:1082:GLN:OE1	2.05	0.57
1:C:664:THR:N	1:C:696:SER:O	2.38	0.57
1:C:805:SER:O	1:C:939:MET:N	2.34	0.57
1:A:1053:THR:HA	1:A:1056:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:HG12	1:A:438:PHE:CD1	2.39	0.57
1:A:371:TYR:H	1:A:391:LEU:HB3	1.69	0.57
1:B:675:TYR:HB2	1:B:683:LEU:HD23	1.84	0.57
1:C:895:SER:OG	1:C:898:GLU:OE1	2.22	0.57
1:C:1138:GLU:HG2	1:C:1158:LEU:HB3	1.85	0.57
1:B:280:LEU:HB3	1:B:445:ASN:HB2	1.87	0.57
1:B:989:THR:N	1:B:1211:GLU:OE1	2.36	0.57
1:B:1189:LEU:HD11	1:B:1202:TYR:HB3	1.87	0.57
1:C:278:PRO:HA	1:C:446:PHE:HA	1.85	0.57
1:A:278:PRO:HA	1:A:445:ASN:C	2.30	0.57
1:A:480:LEU:HG	1:A:708:TYR:CE2	2.39	0.57
1:A:976:TYR:HA	1:A:979:GLN:NE2	2.19	0.57
1:B:406:VAL:O	1:B:412:GLY:HA2	2.04	0.57
1:B:1145:GLN:HB2	1:B:1152:LEU:HD11	1.87	0.57
1:C:287:ILE:O	1:C:289:LYS:NZ	2.36	0.57
1:C:489:SER:N	1:C:702:PHE:O	2.37	0.57
1:C:1183:ARG:NH2	1:C:1220:PHE:O	2.37	0.57
1:A:667:ASN:HB2	8:A:1402:NAG:H2	1.85	0.57
1:A:901:LEU:O	1:A:905:VAL:HG12	2.03	0.57
1:A:1049:LEU:HA	1:A:1052:LEU:HD23	1.87	0.57
1:C:146:ARG:NH1	1:C:903:ASN:O	2.38	0.57
1:C:1183:ARG:NH2	1:C:1218:SER:O	2.37	0.57
1:A:999:LEU:O	1:A:1002:SER:OG	2.19	0.57
1:A:1252:ARG:NH2	1:B:1251:THR:O	2.38	0.57
1:B:1074:LEU:HG	1:B:1075:ASP:O	2.05	0.57
1:B:1233:LEU:HD21	1:B:1237:GLN:HB2	1.86	0.57
1:A:97:GLN:HG3	1:A:189:TRP:HA	1.87	0.57
1:A:121:ALA:O	1:A:153:ALA:HA	2.05	0.57
1:B:588:PHE:CE1	1:B:620:PHE:HB3	2.37	0.57
2:u:2:NAG:H3	2:u:2:NAG:H83	1.87	0.57
1:A:250:ILE:HG22	1:A:463:TYR:HE1	1.70	0.56
1:A:667:ASN:HB2	8:A:1402:NAG:H83	1.86	0.56
1:B:892:GLN:O	1:B:894:ARG:NH2	2.38	0.56
4:t:2:NAG:H83	4:t:2:NAG:H3	1.87	0.56
1:A:340:ALA:N	1:A:418:LEU:O	2.33	0.56
1:B:338:HIS:O	1:B:419:LEU:HG	2.06	0.56
1:B:502:VAL:HB	1:B:654:ILE:HD12	1.87	0.56
1:B:719:SER:HA	1:C:918:LYS:NZ	2.20	0.56
1:B:1205:SER:HB2	1:B:1211:GLU:H	1.69	0.56
1:C:577:GLN:OE1	1:C:577:GLN:N	2.38	0.56
1:A:330:LEU:HD21	1:A:391:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:709:VAL:O	1:C:711:ASP:N	2.38	0.56
1:A:235:ILE:HA	1:A:238:ALA:HB3	1.87	0.56
1:A:323:ILE:O	1:A:396:ARG:HA	2.05	0.56
1:B:718:SER:OG	1:B:719:SER:N	2.38	0.56
1:C:919:ARG:O	1:C:923:GLY:N	2.33	0.56
1:B:479:ASP:OD1	1:B:480:LEU:N	2.38	0.56
1:C:91:PHE:HB2	1:C:111:LYS:HB3	1.87	0.56
1:C:356:HIS:O	1:C:359:THR:OG1	2.22	0.56
1:A:398:ILE:HD13	1:A:408:VAL:HA	1.88	0.56
1:A:799:LEU:HD13	1:A:1150:GLY:HA2	1.86	0.56
1:A:1066:SER:O	1:A:1070:ILE:HG12	2.06	0.56
1:B:75:SER:HB2	1:B:78:HIS:NE2	2.20	0.56
1:B:691:SER:OG	2:X:1:NAG:N2	2.38	0.56
1:C:983:ASN:ND2	1:C:988:GLN:OE1	2.39	0.56
1:C:1051:GLN:N	1:C:1051:GLN:OE1	2.38	0.56
1:A:947:ALA:O	1:A:951:HIS:N	2.38	0.56
1:A:1003:PHE:O	1:A:1007:ILE:HG12	2.06	0.56
1:B:168:TRP:NE1	1:B:170:ASN:O	2.39	0.56
1:B:507:PHE:HE2	1:B:509:ALA:HB2	1.71	0.56
1:C:686:PHE:CE1	1:C:695:TYR:HB2	2.40	0.56
2:u:4:MAN:HO2	2:u:5:MAN:HO4	1.51	0.56
1:B:122:ARG:HD3	1:B:153:ALA:HB2	1.88	0.56
1:B:665:LEU:HD13	1:B:695:TYR:HE1	1.69	0.56
1:B:788:PHE:HA	1:B:1160:PRO:HA	1.87	0.56
1:C:89:HIS:NE2	1:C:196:CYS:SG	2.79	0.56
1:A:404:GLY:HA3	1:A:419:LEU:HD23	1.87	0.56
1:A:767:SER:HB2	1:B:854:ILE:HG21	1.87	0.56
1:B:259:TRP:HB3	1:B:458:ILE:HD11	1.88	0.56
1:B:373:CYS:O	1:B:388:LEU:HB2	2.05	0.56
1:B:1069:ASP:N	1:B:1069:ASP:OD1	2.38	0.56
1:A:588:PHE:CD1	1:A:622:PHE:HB3	2.40	0.56
1:B:716:VAL:O	1:B:737:HIS:N	2.33	0.56
1:B:747:PRO:O	1:B:1023:GLN:NE2	2.29	0.56
1:B:1114:LEU:O	1:B:1117:GLN:HB2	2.06	0.56
1:C:726:ASN:HB2	1:C:739:ASN:HA	1.87	0.56
1:C:1120:ASN:O	1:C:1124:LYS:HB3	2.05	0.56
1:A:728:THR:HA	1:A:736:TYR:O	2.07	0.55
1:A:1178:ILE:HA	1:A:1222:GLN:HE21	1.71	0.55
1:B:54:PRO:HA	1:B:207:VAL:HG21	1.87	0.55
1:B:567:SER:OG	1:B:604:PHE:HB2	2.07	0.55
1:C:173:VAL:O	1:C:182:TYR:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:2:NAG:H3	6:e:2:NAG:H83	1.87	0.55
1:A:218:THR:HG23	6:O:1:NAG:HN2	1.71	0.55
1:B:897:ILE:H	1:B:897:ILE:HD12	1.69	0.55
1:B:833:ILE:HD13	1:B:1094:LEU:HD13	1.88	0.55
1:B:1069:ASP:O	1:B:1073:ARG:HG2	2.05	0.55
1:B:1146:ALA:HA	1:B:1151:LEU:HD13	1.88	0.55
1:C:667:ASN:HB2	7:s:1:NAG:C2	2.36	0.55
1:A:1042:VAL:HA	1:A:1045:GLN:HG3	1.88	0.55
1:A:812:VAL:HA	1:A:1090:ARG:CZ	2.37	0.55
1:B:840:SER:O	1:B:843:LEU:HG	2.06	0.55
1:C:780:GLY:N	1:C:1168:ALA:HB3	2.21	0.55
1:C:1040:GLU:O	1:C:1044:SER:OG	2.17	0.55
1:A:899:ASP:O	1:A:903:ASN:ND2	2.39	0.55
1:B:719:SER:HA	1:C:918:LYS:HZ2	1.70	0.55
1:B:1039:GLN:NE2	1:B:1040:GLU:OE2	2.40	0.55
1:C:396:ARG:HE	1:C:409:ASN:HB3	1.72	0.55
1:C:599:CYS:O	1:C:619:TYR:HA	2.06	0.55
1:A:513:VAL:HG23	1:A:551:ILE:HA	1.88	0.55
1:B:82:VAL:HG23	1:B:204:MET:HE1	1.88	0.55
1:B:879:GLY:HA3	1:B:892:GLN:HE22	1.71	0.55
1:C:796:TYR:HA	1:C:1152:LEU:HA	1.88	0.55
2:U:1:NAG:H3	2:U:1:NAG:H83	1.89	0.55
1:A:948:GLU:HB2	1:A:952:MET:HE1	1.88	0.55
1:B:485:TYR:N	1:B:705:GLN:OE1	2.38	0.55
2:D:4:MAN:O6	2:D:5:MAN:O6	2.24	0.55
1:A:667:ASN:HB2	8:A:1402:NAG:C2	2.37	0.55
1:B:671:LEU:HD23	1:B:671:LEU:H	1.72	0.55
1:B:1197:HIS:CE1	1:B:1199:ALA:HB3	2.42	0.55
1:C:367:THR:OG1	1:C:368:GLN:OE1	2.25	0.55
1:C:499:ILE:HA	1:C:651:LYS:HB3	1.89	0.55
1:A:313:GLN:OE1	1:A:313:GLN:N	2.40	0.54
1:A:1183:ARG:NH2	1:A:1220:PHE:O	2.40	0.54
1:B:487:PHE:O	1:B:704:GLU:N	2.39	0.54
1:B:1074:LEU:HD23	1:B:1074:LEU:H	1.72	0.54
1:C:503:THR:HA	1:C:655:TYR:CE1	2.42	0.54
1:C:744:CYS:SG	1:C:757:CYS:N	2.80	0.54
1:B:1074:LEU:HD21	1:B:1079:ALA:HB2	1.88	0.54
1:C:335:ILE:HB	1:C:347:PHE:HB3	1.90	0.54
1:C:652:TYR:HD1	1:C:654:ILE:HG12	1.71	0.54
1:B:966:PHE:O	2:R:1:NAG:H81	2.08	0.54
1:B:1033:HIS:HD2	1:B:1037:LYS:NZ	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1223:ILE:HG22	1:B:1225:SER:H	1.72	0.54
1:B:488:SER:O	1:B:490:ARG:NH1	2.39	0.54
1:B:872:TYR:HD2	1:B:974:PHE:HD2	1.53	0.54
1:B:1140:ILE:HG12	1:B:1157:VAL:HA	1.90	0.54
1:A:80:ILE:O	1:A:165:GLY:HA2	2.07	0.54
1:B:585:PHE:N	1:B:628:ILE:O	2.39	0.54
1:B:999:LEU:HD11	1:B:1158:LEU:HD11	1.89	0.54
1:C:793:ARG:NH2	1:C:1136:ASP:OD2	2.34	0.54
1:A:81:PHE:HB2	1:A:205:GLN:HB2	1.89	0.54
1:A:120:THR:HG22	1:A:153:ALA:HB1	1.89	0.54
1:A:131:ILE:HG22	1:A:133:THR:H	1.72	0.54
1:A:1042:VAL:O	1:A:1045:GLN:NE2	2.41	0.54
1:B:278:PRO:HA	1:B:446:PHE:HA	1.88	0.54
1:B:524:HIS:H	1:B:530:ILE:HD11	1.72	0.54
1:B:1037:LYS:HA	1:B:1040:GLU:OE1	2.08	0.54
2:P:1:NAG:H3	2:P:1:NAG:C8	2.36	0.54
1:A:51:GLY:O	1:A:211:THR:N	2.39	0.54
1:A:242:PHE:CG	1:A:251:PRO:HG3	2.43	0.54
1:A:716:VAL:O	1:A:737:HIS:N	2.27	0.54
1:B:134:LEU:HD22	1:B:193:ALA:HB2	1.89	0.54
1:C:125:ILE:HB	1:C:150:PHE:HB3	1.90	0.54
1:A:282:ASN:HB2	1:A:443:SER:HB3	1.89	0.54
1:A:736:TYR:OH	1:A:760:GLY:O	2.18	0.54
1:C:324:ASN:HB3	1:C:437:GLY:HA2	1.90	0.54
1:C:1068:ASP:HA	1:C:1071:TYR:HB3	1.90	0.54
1:A:297:PHE:N	1:A:422:VAL:O	2.41	0.54
1:A:689:VAL:H	2:G:1:NAG:H81	1.71	0.54
1:B:836:ALA:O	1:B:840:SER:OG	2.21	0.54
1:A:946:ASP:OD1	1:A:947:ALA:N	2.41	0.54
1:B:468:VAL:O	1:B:471:LEU:HB2	2.08	0.54
1:B:1113:LYS:O	1:B:1117:GLN:HG3	2.07	0.54
1:C:487:PHE:HB3	1:C:704:GLU:OE2	2.08	0.54
1:C:695:TYR:OH	2:u:1:NAG:H62	2.08	0.54
1:C:726:ASN:N	1:C:739:ASN:OD1	2.28	0.54
1:A:1175:ASN:HB2	1:A:1235:ARG:HD2	1.90	0.53
1:C:106:GLN:OE1	1:C:130:SER:OG	2.22	0.53
1:C:277:GLN:HB3	1:C:279:LEU:HD23	1.90	0.53
1:C:470:GLN:O	1:C:474:SER:OG	2.24	0.53
1:C:654:ILE:HG22	1:C:655:TYR:CD2	2.43	0.53
1:C:781:ASN:HB3	2:o:1:NAG:C7	2.37	0.53
1:A:924:ARG:NH2	7:s:2:FUC:O4	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:VAL:HG12	1:C:831:LYS:HZ3	1.73	0.53
1:C:150:PHE:CZ	1:C:154:ILE:HD11	2.42	0.53
1:C:374:PHE:HD2	1:C:385:TYR:HB3	1.73	0.53
1:C:1102:LEU:HA	1:C:1105:TYR:HB2	1.90	0.53
1:C:1145:GLN:O	1:C:1152:LEU:HG	2.09	0.53
1:A:588:PHE:CE1	1:A:620:PHE:HB3	2.43	0.53
1:B:117:THR:O	1:B:120:THR:OG1	2.27	0.53
1:B:816:ASN:OD1	1:B:818:ARG:N	2.41	0.53
1:C:262:LEU:HD13	1:C:278:PRO:HD3	1.90	0.53
1:A:547:ARG:HH21	1:A:627:LEU:HB3	1.73	0.53
1:A:568:GLN:HE22	1:A:570:SER:HB2	1.73	0.53
1:A:787:ASN:O	1:A:1161:SER:N	2.42	0.53
1:A:889:ARG:HH11	1:A:891:VAL:HG12	1.73	0.53
1:B:898:GLU:OE1	1:B:898:GLU:N	2.41	0.53
1:B:902:PHE:O	1:B:906:VAL:N	2.41	0.53
1:A:31:ASN:OD1	1:A:161:HIS:ND1	2.42	0.53
1:B:501:PHE:N	1:B:643:PHE:O	2.38	0.53
1:B:1129:ARG:HG3	1:B:1132:PHE:HB2	1.89	0.53
1:A:691:SER:HB3	2:G:1:NAG:H5	1.91	0.53
1:B:1080:ASP:HA	1:B:1083:VAL:HG12	1.91	0.53
1:C:930:VAL:HA	1:C:933:GLN:HE22	1.73	0.53
1:A:338:HIS:HB3	2:N:1:NAG:H82	1.90	0.53
1:A:820:LYS:O	1:A:824:THR:HG23	2.08	0.53
1:C:257:ASN:OD1	1:C:258:ASN:N	2.41	0.53
1:C:485:TYR:N	1:C:705:GLN:OE1	2.41	0.53
1:A:678:SER:OG	1:A:680:SER:OG	2.17	0.53
1:A:847:GLU:O	1:A:851:MET:HG2	2.09	0.53
1:B:549:PHE:HE1	1:B:628:ILE:HB	1.72	0.53
1:B:711:ASP:OD1	1:B:711:ASP:N	2.41	0.53
1:B:947:ALA:O	1:B:951:HIS:ND1	2.42	0.53
1:A:433:ASP:OD1	1:A:434:ASP:N	2.42	0.53
1:B:42:GLN:HG3	1:B:244:THR:O	2.08	0.53
1:B:67:CYS:SG	1:B:68:ALA:N	2.82	0.53
1:B:725:PHE:HB3	1:B:738:SER:C	2.34	0.53
1:B:793:ARG:NH2	1:B:1136:ASP:OD2	2.28	0.53
1:C:77:VAL:HG11	1:C:80:ILE:HB	1.90	0.53
1:C:97:GLN:NE2	1:C:101:ASP:HB2	2.23	0.53
1:C:283:CYS:SG	1:C:284:LEU:N	2.82	0.53
1:B:273:VAL:O	1:B:451:ILE:N	2.40	0.53
1:C:870:ASP:OD2	1:C:974:PHE:N	2.41	0.53
1:C:327:SER:HA	1:C:330:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:SER:HB3	1:C:625:GLY:HA3	1.91	0.52
1:A:896:PHE:CE2	1:A:900:LEU:HD11	2.44	0.52
1:C:97:GLN:HB2	1:C:99:PRO:HD2	1.92	0.52
1:C:901:LEU:HA	1:C:904:LYS:HE3	1.92	0.52
1:A:498:PRO:O	1:A:650:THR:OG1	2.23	0.52
1:A:894:ARG:HE	1:A:951:HIS:CD2	2.28	0.52
1:B:667:ASN:HD21	1:C:924:ARG:HH22	1.55	0.52
1:C:516:THR:O	1:C:534:THR:HA	2.10	0.52
1:C:901:LEU:HA	1:C:904:LYS:HG2	1.90	0.52
1:A:520:SER:HA	1:A:558:THR:HB	1.92	0.52
1:B:354:ASN:HB3	1:B:357:LEU:HB2	1.91	0.52
1:B:1082:GLN:HG2	1:B:1085:ARG:NH1	2.24	0.52
1:C:1042:VAL:O	1:C:1045:GLN:NE2	2.43	0.52
1:C:1110:ALA:HA	1:C:1113:LYS:HD2	1.91	0.52
1:C:1145:GLN:HB2	1:C:1152:LEU:HD11	1.91	0.52
1:C:1189:LEU:HA	1:C:1204:VAL:HG12	1.91	0.52
1:A:66:TYR:HB3	1:A:190:SER:O	2.10	0.52
1:A:296:PHE:HA	1:A:423:THR:HA	1.92	0.52
1:A:1168:ALA:HA	1:A:1190:PHE:HA	1.92	0.52
1:B:75:SER:HB2	1:B:78:HIS:CE1	2.45	0.52
1:B:335:ILE:O	1:B:346:SER:HA	2.09	0.52
1:B:514:ASN:N	1:B:537:ASN:OD1	2.34	0.52
1:B:1215:PRO:HB2	1:B:1220:PHE:CE1	2.44	0.52
1:C:131:ILE:HD12	1:C:136:PRO:HA	1.92	0.52
1:C:515:ILE:HG23	1:C:553:LEU:HA	1.90	0.52
1:A:216:ASN:HB3	1:A:226:SER:OG	2.10	0.52
1:A:1032:ALA:HA	1:A:1035:LEU:HG	1.90	0.52
1:A:1069:ASP:O	1:A:1073:ARG:NH1	2.42	0.52
1:B:740:ASP:OD2	1:B:761:SER:N	2.42	0.52
1:B:818:ARG:HH21	1:B:1071:TYR:HE2	1.55	0.52
1:B:1069:ASP:CG	1:B:1070:ILE:HD12	2.35	0.52
1:C:812:VAL:HB	1:C:1090:ARG:NH2	2.24	0.52
1:B:214:MET:N	1:B:228:GLN:O	2.41	0.52
1:B:895:SER:OG	1:B:898:GLU:OE1	2.25	0.52
1:C:292:GLY:HA2	1:C:426:PHE:H	1.75	0.52
5:L:1:NAG:O3	5:L:2:NAG:O5	2.27	0.52
1:A:515:ILE:HG23	1:A:553:LEU:HA	1.91	0.52
1:A:597:SER:OG	1:A:621:GLN:NE2	2.43	0.52
1:A:992:LEU:HD13	1:A:994:ARG:HE	1.74	0.52
1:C:662:ILE:O	1:C:698:THR:N	2.43	0.52
1:A:184:TYR:OH	1:A:186:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:SER:N	1:A:1159:VAL:O	2.43	0.52
1:B:108:TYR:HB3	1:B:124:ARG:HH21	1.75	0.52
1:B:250:ILE:HD12	1:B:251:PRO:HD2	1.90	0.52
1:B:250:ILE:HG21	1:B:256:PHE:HZ	1.75	0.52
1:B:549:PHE:CE1	1:B:628:ILE:HB	2.44	0.52
1:C:947:ALA:O	1:C:951:HIS:N	2.41	0.52
1:A:468:VAL:O	1:A:471:LEU:HG	2.09	0.52
1:B:751:TYR:HE1	1:C:944:VAL:HG12	1.75	0.52
1:B:1131:GLY:O	1:B:1135:GLY:HA2	2.10	0.52
1:B:1227:VAL:HG22	1:B:1230:TYR:CE2	2.45	0.52
1:C:396:ARG:NE	1:C:409:ASN:HB3	2.24	0.52
1:C:863:THR:N	1:C:866:SER:OG	2.43	0.52
1:A:125:ILE:HB	1:A:150:PHE:HB3	1.92	0.51
1:B:49:LEU:HD23	1:B:215:LEU:HD12	1.92	0.51
1:B:501:PHE:O	1:B:643:PHE:N	2.43	0.51
1:C:33:ARG:HB3	1:C:34:ARG:HH21	1.74	0.51
1:A:184:TYR:OH	3:Q:1:NAG:O3	2.25	0.51
1:A:217:VAL:HG22	1:A:224:GLY:HA2	1.92	0.51
1:A:501:PHE:HB3	1:A:643:PHE:CE1	2.45	0.51
1:A:857:GLU:HA	1:A:860:GLN:CD	2.35	0.51
1:A:867:PHE:CE2	1:A:869:GLY:HA2	2.45	0.51
1:A:894:ARG:HE	1:A:951:HIS:CG	2.29	0.51
1:A:1105:TYR:HA	1:A:1108:VAL:HG12	1.91	0.51
1:A:1213:ARG:NH2	1:A:1214:LYS:O	2.43	0.51
1:B:110:HIS:N	1:B:124:ARG:HH12	2.08	0.51
1:B:364:LEU:HG	1:B:372:TYR:HE2	1.75	0.51
1:C:270:HIS:HD1	1:C:454:GLN:HA	1.74	0.51
1:C:569:ASP:OD1	1:C:570:SER:N	2.43	0.51
1:A:336:VAL:HB	1:A:423:THR:OG1	2.09	0.51
1:A:353:SER:HB2	8:A:1401:NAG:H82	1.92	0.51
1:A:992:LEU:HB3	1:A:994:ARG:HG2	1.92	0.51
1:B:789:SER:O	1:B:1159:VAL:N	2.42	0.51
1:B:1115:ALA:HA	1:B:1118:LYS:HE2	1.93	0.51
1:A:286:ALA:HA	1:A:440:THR:HG22	1.91	0.51
1:A:469:SER:HA	1:A:472:LYS:HE2	1.92	0.51
1:A:512:PHE:CD1	1:A:550:THR:HB	2.46	0.51
1:A:658:LYS:NZ	1:B:1069:ASP:HA	2.25	0.51
1:A:1121:GLU:HG2	1:A:1122:CYS:H	1.76	0.51
1:B:556:ASN:HD21	2:W:1:NAG:H83	1.75	0.51
1:C:521:PHE:CE1	1:C:529:LEU:HD13	2.45	0.51
1:C:1077:LEU:HD12	1:C:1078:SER:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:SER:OG	1:A:600:THR:O	2.23	0.51
1:A:596:ALA:O	1:A:621:GLN:NE2	2.42	0.51
1:A:1228:VAL:HB	5:L:2:NAG:C7	2.41	0.51
1:B:209:GLU:N	1:B:209:GLU:OE1	2.44	0.51
1:B:434:ASP:HB3	2:U:2:NAG:H62	1.91	0.51
1:B:1157:VAL:HG12	1:B:1158:LEU:O	2.10	0.51
2:F:1:NAG:H83	2:F:2:NAG:H82	1.93	0.51
1:A:63:SER:HB2	1:A:74:ALA:HB3	1.93	0.51
1:B:299:PHE:CZ	1:B:402:LYS:HA	2.46	0.51
1:B:345:PHE:HE1	1:B:377:VAL:HG13	1.76	0.51
1:C:793:ARG:HD3	1:C:1029:ASN:ND2	2.26	0.51
1:C:821:GLN:NE2	1:C:822:LEU:HG	2.26	0.51
1:A:301:GLN:OE1	1:A:301:GLN:N	2.43	0.51
1:A:1116:GLN:O	1:A:1119:VAL:HG12	2.10	0.51
1:B:290:ILE:HG23	1:B:429:HIS:HE1	1.76	0.51
1:B:993:GLN:HA	1:B:996:GLN:OE1	2.11	0.51
1:C:250:ILE:HD12	1:C:251:PRO:HD2	1.91	0.51
1:A:688:ASN:HB2	1:A:693:ALA:HB3	1.92	0.51
1:C:521:PHE:HE1	1:C:529:LEU:HD13	1.76	0.51
1:A:895:SER:OG	1:A:898:GLU:OE1	2.28	0.51
1:A:918:LYS:HZ2	1:C:719:SER:HA	1.75	0.51
1:A:981:ARG:HH12	1:C:776:PRO:HG2	1.75	0.51
1:B:667:ASN:HB2	8:B:1402:NAG:H83	1.91	0.51
1:B:818:ARG:HD3	1:B:818:ARG:H	1.76	0.51
1:C:368:GLN:HG2	8:C:1406:NAG:H82	1.93	0.51
1:C:395:VAL:HA	1:C:409:ASN:HD21	1.76	0.51
1:C:687:LYS:HB2	1:C:694:VAL:HG22	1.91	0.51
1:C:1233:LEU:HD21	1:C:1241:VAL:HG11	1.93	0.51
1:B:377:VAL:N	1:B:384:VAL:O	2.36	0.51
1:C:471:LEU:HA	1:C:474:SER:HB2	1.91	0.51
1:A:680:SER:HA	1:B:1057:GLN:HG2	1.93	0.50
1:A:718:SER:HG	1:A:737:HIS:CD2	2.25	0.50
1:A:898:GLU:O	1:A:901:LEU:HG	2.11	0.50
1:A:954:SER:O	1:A:958:ILE:HG12	2.12	0.50
1:C:216:ASN:O	1:C:225:ILE:N	2.44	0.50
1:C:286:ALA:HB2	1:C:440:THR:HG22	1.92	0.50
1:C:407:TYR:CD1	1:C:412:GLY:HA2	2.46	0.50
1:A:78:HIS:ND1	1:A:168:TRP:O	2.24	0.50
1:A:276:ASN:OD1	1:A:446:PHE:HB3	2.11	0.50
1:A:333:GLY:HA2	1:A:426:PHE:HA	1.94	0.50
1:A:1119:VAL:O	1:A:1123:VAL:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:THR:HA	1:B:658:LYS:HA	1.92	0.50
1:B:745:THR:N	1:B:757:CYS:SG	2.84	0.50
1:C:108:TYR:N	1:C:128:PHE:HE2	2.09	0.50
1:C:598:ALA:HB1	1:C:619:TYR:HB3	1.93	0.50
1:C:816:ASN:OD1	1:C:818:ARG:N	2.43	0.50
1:C:879:GLY:HA2	1:C:895:SER:HA	1.92	0.50
1:A:568:GLN:HG2	1:A:602:ASP:O	2.10	0.50
1:A:748:VAL:N	1:A:756:VAL:O	2.44	0.50
1:A:796:TYR:HA	1:A:1152:LEU:HA	1.93	0.50
1:A:1035:LEU:HA	1:A:1038:VAL:HG22	1.94	0.50
1:C:711:ASP:N	1:C:711:ASP:OD1	2.45	0.50
1:A:831:LYS:HE3	1:C:475:GLN:HA	1.92	0.50
1:A:1007:ILE:HD13	1:A:1010:ILE:HD12	1.92	0.50
1:C:35:PHE:O	1:C:38:LYS:NZ	2.38	0.50
1:C:796:TYR:OH	1:C:1147:ALA:HB3	2.12	0.50
1:C:1169:ILE:HG12	1:C:1190:PHE:HA	1.94	0.50
1:B:122:ARG:HH22	1:B:151:ASN:HB3	1.77	0.50
1:B:487:PHE:HB2	1:B:704:GLU:OE2	2.11	0.50
1:B:512:PHE:HB3	3:V:2:NAG:H81	1.94	0.50
1:C:181:TYR:HB3	1:C:183:PHE:CE2	2.47	0.50
1:C:262:LEU:HD23	2:h:1:NAG:H81	1.93	0.50
1:A:270:HIS:HB2	1:A:455:GLY:H	1.77	0.50
1:A:325:ASP:OD1	1:A:327:SER:OG	2.23	0.50
1:A:337:LEU:HD23	1:A:422:VAL:HG23	1.94	0.50
1:A:501:PHE:CD2	1:A:642:SER:HA	2.46	0.50
1:A:504:LEU:HB2	1:A:626:GLU:CG	2.42	0.50
1:A:665:LEU:HB2	1:A:695:TYR:CE2	2.46	0.50
1:A:932:ALA:O	1:A:935:TYR:HB2	2.11	0.50
1:A:1184:GLU:OE1	1:A:1187:LEU:N	2.45	0.50
1:A:357:LEU:HA	1:A:360:PHE:HB2	1.93	0.50
1:B:91:PHE:HD2	1:B:111:LYS:HD2	1.76	0.50
1:C:93:ILE:HD13	1:C:109:LEU:HD22	1.93	0.50
1:C:217:VAL:HG23	1:C:224:GLY:HA2	1.94	0.50
1:A:450:LEU:O	1:A:461:ILE:HA	2.12	0.50
1:A:983:ASN:O	1:A:987:LEU:HD22	2.12	0.50
1:A:1113:LYS:O	1:A:1116:GLN:HG3	2.12	0.50
1:B:259:TRP:CD1	1:B:320:ARG:HH12	2.30	0.50
1:B:1101:THR:HA	1:B:1104:LYS:HE2	1.94	0.50
1:C:321:PHE:HB3	1:C:438:PHE:CE1	2.47	0.50
1:C:501:PHE:CE2	1:C:642:SER:HA	2.45	0.50
1:C:1011:THR:HA	1:C:1014:PHE:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1086:LEU:HD21	1:C:1090:ARG:HH12	1.77	0.50
1:A:709:VAL:O	1:A:711:ASP:N	2.45	0.50
1:B:747:PRO:HB3	1:B:755:GLY:HA3	1.94	0.50
1:B:870:ASP:OD2	1:B:974:PHE:N	2.45	0.50
1:C:487:PHE:O	1:C:704:GLU:N	2.43	0.50
1:C:569:ASP:O	1:C:601:ILE:HD12	2.12	0.50
1:C:678:SER:N	1:C:682:GLN:O	2.39	0.50
1:C:909:GLY:H	1:C:913:VAL:HG21	1.77	0.50
3:l:1:NAG:O6	3:l:1:NAG:O3	2.24	0.50
1:A:783:SER:HB3	1:A:1163:PHE:CD1	2.47	0.49
1:B:97:GLN:HA	1:B:190:SER:N	2.24	0.49
1:B:567:SER:O	1:B:604:PHE:N	2.37	0.49
1:C:1214:LYS:NZ	1:C:1241:VAL:O	2.39	0.49
1:A:117:THR:HB	8:A:1406:NAG:HN2	1.77	0.49
1:A:1110:ALA:HA	1:A:1113:LYS:HD2	1.94	0.49
1:B:1120:ASN:C	1:B:1120:ASN:HD22	2.20	0.49
1:A:274:VAL:HG13	1:A:449:ALA:O	2.12	0.49
1:A:439:TRP:CD1	1:A:440:THR:HG23	2.47	0.49
1:C:795:GLU:O	1:C:1153:PHE:N	2.36	0.49
1:A:521:PHE:HB2	1:A:559:ASN:HB3	1.94	0.49
1:A:676:TYR:CD1	1:B:267:THR:HG23	2.47	0.49
1:A:1174:VAL:HG21	1:A:1238:LEU:HD11	1.94	0.49
1:A:1241:VAL:HG23	1:A:1242:ILE:HG12	1.95	0.49
1:B:345:PHE:CE1	1:B:377:VAL:HG13	2.47	0.49
1:B:787:ASN:O	1:B:1161:SER:N	2.46	0.49
1:B:820:LYS:HA	1:B:823:LEU:HG	1.94	0.49
1:B:845:SER:O	1:B:849:ASN:ND2	2.45	0.49
1:B:992:LEU:HD13	1:B:994:ARG:NE	2.27	0.49
1:C:244:THR:H	1:C:309:GLY:HA3	1.78	0.49
1:A:285:LEU:O	1:A:440:THR:HA	2.13	0.49
1:A:297:PHE:HD2	1:A:422:VAL:HG13	1.78	0.49
1:A:718:SER:O	1:A:735:PHE:N	2.38	0.49
1:C:380:TYR:CD2	2:k:1:NAG:H83	2.47	0.49
1:C:1236:ASP:O	1:C:1239:PRO:HD2	2.12	0.49
1:A:270:HIS:HA	1:A:453:VAL:HG13	1.94	0.49
1:A:289:LYS:HB3	1:A:430:GLY:HA2	1.93	0.49
1:A:475:GLN:HA	1:B:831:LYS:HG2	1.95	0.49
1:B:87:GLY:N	1:B:198:ASN:O	2.46	0.49
1:B:256:PHE:HA	1:B:259:TRP:CE3	2.48	0.49
1:B:411:PHE:HB3	1:B:413:TYR:CE1	2.47	0.49
1:B:1232:ASN:ND2	3:f:1:NAG:O7	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:HIS:HB2	1:C:208:TYR:HA	1.95	0.49
1:C:106:GLN:HE21	1:C:128:PHE:H	1.60	0.49
1:C:565:SER:HB3	1:C:606:TYR:HB2	1.93	0.49
1:C:801:ASN:HA	1:C:1149:GLN:HE21	1.77	0.49
1:C:1121:GLU:HG2	1:C:1122:CYS:N	2.27	0.49
1:C:1217:VAL:HG23	1:C:1242:ILE:HG21	1.93	0.49
1:A:94:GLY:HA2	1:A:107:LEU:O	2.13	0.49
1:A:288:PRO:HD2	1:A:433:ASP:O	2.13	0.49
1:B:404:GLY:HA3	1:B:417:GLY:O	2.12	0.49
1:C:797:LEU:HD13	1:C:1115:ALA:HB2	1.95	0.49
2:j:2:NAG:H2	2:j:5:MAN:H5	1.95	0.49
1:A:350:SER:C	1:A:364:LEU:HD11	2.37	0.49
1:A:379:THR:HG23	1:A:382:SER:H	1.77	0.49
1:B:433:ASP:OD1	1:B:434:ASP:N	2.44	0.49
1:B:520:SER:HA	1:B:558:THR:HB	1.95	0.49
1:B:1094:LEU:HD12	1:B:1095:ASN:N	2.28	0.49
1:C:321:PHE:HB2	1:C:398:ILE:HB	1.95	0.49
1:C:374:PHE:CD2	1:C:385:TYR:HB3	2.48	0.49
1:C:427:THR:HG22	1:C:428:GLY:H	1.78	0.49
1:C:793:ARG:HD3	1:C:1029:ASN:HD22	1.78	0.49
1:A:323:ILE:HG12	1:A:438:PHE:HD1	1.77	0.49
1:B:107:LEU:HD21	1:B:109:LEU:HB3	1.93	0.49
1:B:671:LEU:O	1:C:396:ARG:NH1	2.46	0.49
1:C:256:PHE:HB3	1:C:259:TRP:HB2	1.94	0.49
1:C:319:LEU:O	1:C:399:VAL:HA	2.13	0.49
1:C:803:PRO:O	1:C:940:VAL:HG23	2.12	0.49
1:C:1116:GLN:O	1:C:1119:VAL:HG12	2.13	0.49
1:A:131:ILE:HD12	1:A:136:PRO:HA	1.94	0.49
1:A:287:ILE:O	1:A:433:ASP:HB2	2.13	0.49
1:A:547:ARG:NE	1:A:627:LEU:O	2.32	0.49
1:A:935:TYR:HE1	1:C:702:PHE:HE1	1.61	0.49
1:C:510:HIS:HA	1:C:548:GLN:O	2.13	0.49
1:A:122:ARG:NH1	1:A:123:LEU:O	2.45	0.48
1:A:266:SER:N	1:C:675:TYR:OH	2.46	0.48
1:A:1051:GLN:O	1:A:1054:VAL:HB	2.13	0.48
1:B:376:LYS:HD3	1:B:385:TYR:HE1	1.77	0.48
1:C:95:ILE:CG2	1:C:107:LEU:HB3	2.42	0.48
1:C:166:ILE:HD13	1:C:175:VAL:HG22	1.94	0.48
1:C:818:ARG:N	1:C:818:ARG:HD3	2.28	0.48
1:C:994:ARG:O	1:C:998:LEU:HG	2.13	0.48
1:A:258:ASN:ND2	1:A:322:ASN:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:N	1:A:384:VAL:O	2.46	0.48
1:B:270:HIS:ND1	1:B:454:GLN:HA	2.28	0.48
1:C:584:SER:HA	1:C:629:THR:HA	1.93	0.48
1:C:784:ILE:O	1:C:1164:VAL:N	2.28	0.48
1:A:77:VAL:HG13	1:A:206:TYR:HB2	1.95	0.48
1:C:752:SER:OG	1:C:753:ASN:N	2.43	0.48
4:I:1:NAG:H4	4:I:2:NAG:HN2	1.78	0.48
1:A:793:ARG:HH22	1:A:1137:GLY:HA3	1.78	0.48
1:B:274:VAL:HG13	1:B:449:ALA:C	2.39	0.48
1:B:790:MET:HE2	1:B:1156:THR:HB	1.95	0.48
1:B:830:CYS:O	1:B:833:ILE:HG12	2.13	0.48
1:C:509:ALA:HB3	1:C:547:ARG:HG2	1.96	0.48
1:C:819:CYS:SG	1:C:820:LYS:N	2.86	0.48
1:A:482:ASP:HA	1:A:708:TYR:CD2	2.48	0.48
1:B:47:VAL:HG22	1:B:241:VAL:HG12	1.96	0.48
1:C:111:LYS:HE2	1:C:119:ALA:HB1	1.95	0.48
1:C:663:ILE:HA	1:C:697:VAL:HA	1.96	0.48
1:C:781:ASN:HB3	2:o:1:NAG:C2	2.44	0.48
1:C:851:MET:O	1:C:953:TYR:OH	2.25	0.48
1:A:78:HIS:O	1:A:167:THR:HA	2.14	0.48
1:A:604:PHE:CE2	1:A:614:LYS:HG2	2.49	0.48
1:B:588:PHE:CZ	1:B:620:PHE:HD2	2.30	0.48
1:C:783:SER:HB3	1:C:1163:PHE:HB3	1.96	0.48
1:A:372:TYR:CZ	1:A:390:VAL:HG22	2.49	0.48
1:A:484:PHE:O	1:B:838:GLN:NE2	2.46	0.48
1:C:1112:ARG:NH2	1:C:1113:LYS:HG3	2.28	0.48
1:A:280:LEU:H	1:A:445:ASN:H	1.59	0.48
1:A:524:HIS:H	1:A:530:ILE:HD11	1.79	0.48
1:A:709:VAL:O	1:A:712:ASP:N	2.40	0.48
1:A:849:ASN:O	1:A:852:LEU:HG	2.14	0.48
1:A:944:VAL:HG13	1:A:945:VAL:HG13	1.95	0.48
1:A:1052:LEU:O	1:A:1056:LEU:HD23	2.14	0.48
1:A:1060:PHE:CE2	1:A:1089:GLY:HA3	2.49	0.48
1:A:296:PHE:HB3	1:A:423:THR:HG22	1.96	0.48
1:A:319:LEU:HD11	1:A:400:ILE:HB	1.96	0.48
1:A:515:ILE:HD13	1:A:536:ILE:HG13	1.94	0.48
1:A:688:ASN:N	1:A:693:ALA:O	2.36	0.48
1:B:471:LEU:O	1:B:474:SER:N	2.46	0.48
1:B:751:TYR:CE1	1:C:944:VAL:HG12	2.49	0.48
1:B:1053:THR:O	1:B:1057:GLN:NE2	2.47	0.48
1:B:1214:LYS:HD3	1:B:1215:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HE	1:C:200:GLY:N	2.12	0.48
1:A:335:ILE:O	1:A:346:SER:HA	2.13	0.48
1:A:726:ASN:N	1:A:739:ASN:OD1	2.37	0.48
1:A:729:ARG:O	1:A:736:TYR:N	2.44	0.48
1:A:963:LEU:HD11	1:C:775:ALA:N	2.27	0.48
1:B:817:SER:OG	1:B:818:ARG:HD3	2.14	0.48
1:C:127:GLN:HG3	1:C:144:ILE:HG23	1.96	0.48
1:C:1172:LEU:N	1:C:1230:TYR:HD1	2.11	0.48
6:i:1:NAG:O5	6:i:6:FUC:H5	2.14	0.48
1:A:127:GLN:O	1:A:144:ILE:HG12	2.13	0.47
1:A:844:GLU:O	1:A:847:GLU:HG3	2.14	0.47
1:A:989:THR:N	1:A:1211:GLU:OE1	2.46	0.47
1:A:1182:LEU:HA	1:A:1220:PHE:CD1	2.49	0.47
1:B:61:VAL:HA	1:B:208:TYR:CZ	2.49	0.47
1:B:666:THR:OG1	8:B:1402:NAG:O7	2.31	0.47
1:C:46:VAL:HG21	2:g:1:NAG:H82	1.96	0.47
1:C:324:ASN:OD1	1:C:439:TRP:NE1	2.43	0.47
1:C:375:PHE:CD1	1:C:388:LEU:HD11	2.48	0.47
1:C:433:ASP:HA	1:C:436:SER:HB2	1.96	0.47
1:C:654:ILE:O	1:C:657:PHE:N	2.44	0.47
1:A:131:ILE:HG21	1:A:138:ALA:HB3	1.96	0.47
1:B:297:PHE:O	1:B:422:VAL:N	2.43	0.47
1:B:351:ASN:C	8:B:1407:NAG:HN2	2.21	0.47
1:B:517:VAL:HA	1:B:534:THR:HG22	1.95	0.47
1:C:213:TYR:CE2	1:C:229:PRO:HG3	2.49	0.47
1:C:844:GLU:HA	1:C:847:GLU:OE2	2.14	0.47
1:C:898:GLU:HG2	1:C:899:ASP:N	2.30	0.47
1:C:928:ASP:OD1	1:C:930:VAL:HG22	2.15	0.47
1:C:974:PHE:O	1:C:978:VAL:HG23	2.15	0.47
1:A:487:PHE:N	1:A:704:GLU:O	2.37	0.47
1:A:510:HIS:CD2	1:A:634:PRO:HB3	2.49	0.47
1:A:653:THR:HA	1:A:658:LYS:HB3	1.95	0.47
1:B:667:ASN:HB2	8:B:1402:NAG:H2	1.95	0.47
1:B:1217:VAL:HG13	1:B:1244:ASP:HB2	1.97	0.47
1:C:286:ALA:HA	1:C:440:THR:HA	1.95	0.47
1:C:1085:ARG:O	1:C:1088:THR:OG1	2.27	0.47
1:A:577:GLN:OE1	1:A:577:GLN:N	2.40	0.47
1:A:750:VAL:HG23	1:A:765:VAL:HG21	1.95	0.47
1:B:1063:ILE:HB	1:B:1070:ILE:HG12	1.96	0.47
1:B:1075:ASP:OD2	1:B:1077:LEU:HB2	2.15	0.47
1:C:502:VAL:HB	1:C:654:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:ASN:HB3	1:C:632:PRO:HB3	1.97	0.47
1:C:602:ASP:HB2	1:C:614:LYS:HD2	1.96	0.47
1:C:750:VAL:HA	1:C:755:GLY:HA2	1.97	0.47
1:C:883:TYR:HB2	1:C:891:VAL:HG23	1.94	0.47
1:C:1017:VAL:HG13	1:C:1018:LYS:HG3	1.94	0.47
1:C:1069:ASP:OD1	1:C:1073:ARG:HD3	2.13	0.47
1:B:799:LEU:HB2	1:B:1149:GLN:OE1	2.14	0.47
1:C:527:ALA:HB2	1:C:609:PHE:CD2	2.50	0.47
1:A:548:GLN:HA	1:A:629:THR:O	2.14	0.47
1:B:375:PHE:CD2	1:B:386:LYS:HB3	2.50	0.47
1:B:820:LYS:O	1:B:824:THR:HG23	2.14	0.47
1:C:102:PRO:HB2	1:C:143:THR:HG21	1.97	0.47
1:C:520:SER:O	1:C:529:LEU:HD12	2.14	0.47
1:C:521:PHE:CD2	1:C:607:PRO:HB3	2.49	0.47
1:C:730:GLU:HB2	1:C:735:PHE:CE1	2.49	0.47
1:C:811:TYR:CE2	1:C:1090:ARG:HD2	2.50	0.47
1:C:1076:ILE:HG22	1:C:1080:ASP:OD2	2.14	0.47
1:C:1237:GLN:HA	1:C:1240:ASP:OD2	2.14	0.47
1:A:43:ALA:HB3	1:A:44:PRO:HD3	1.96	0.47
1:A:171:ASP:OD1	1:A:186:LYS:HA	2.15	0.47
1:A:270:HIS:HD1	1:A:454:GLN:HA	1.80	0.47
1:A:288:PRO:HD3	1:A:439:TRP:O	2.15	0.47
1:A:468:VAL:O	1:A:472:LYS:HG2	2.15	0.47
1:A:818:ARG:O	1:A:821:GLN:HG3	2.15	0.47
1:B:91:PHE:O	1:B:110:HIS:HA	2.15	0.47
1:B:321:PHE:HD1	1:B:441:ILE:HG12	1.80	0.47
1:B:344:ASN:CB	2:d:1:NAG:N2	2.77	0.47
1:B:663:ILE:HD12	1:B:696:SER:C	2.39	0.47
1:B:818:ARG:N	1:B:818:ARG:HD3	2.29	0.47
1:B:973:PRO:HD2	1:B:976:TYR:CD2	2.50	0.47
1:B:1050:THR:O	1:B:1053:THR:OG1	2.29	0.47
1:B:1183:ARG:HH22	1:B:1219:ASP:HA	1.78	0.47
1:B:1190:PHE:HZ	1:B:1212:PRO:HB3	1.80	0.47
1:C:95:ILE:HG23	1:C:189:TRP:CZ3	2.49	0.47
1:C:322:ASN:ND2	1:C:439:TRP:HB2	2.30	0.47
1:C:403:TYR:HE1	2:h:3:BMA:H5	1.77	0.47
1:C:408:VAL:HB	1:C:413:TYR:HE2	1.78	0.47
1:C:1175:ASN:O	1:C:1177:GLU:HG3	2.15	0.47
5:L:1:NAG:O3	5:L:2:NAG:O6	2.28	0.47
1:A:80:ILE:HD11	1:A:204:MET:HE2	1.97	0.47
1:A:97:GLN:HG2	1:A:99:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLN:HB2	1:A:279:LEU:HD23	1.96	0.47
1:A:792:ILE:HB	1:A:1010:ILE:HD11	1.95	0.47
1:A:1066:SER:OG	1:A:1068:ASP:OD1	2.31	0.47
1:A:1112:ARG:HA	1:A:1115:ALA:HB3	1.97	0.47
1:B:171:ASP:HA	1:B:185:PHE:O	2.14	0.47
1:B:586:SER:HB3	1:B:625:GLY:CA	2.42	0.47
1:C:175:VAL:O	1:C:180:ILE:HD12	2.15	0.47
1:C:1181:THR:OG1	1:C:1221:VAL:HG23	2.14	0.47
3:V:1:NAG:N2	3:V:2:NAG:O7	2.37	0.47
1:B:288:PRO:C	1:B:289:LYS:HD3	2.40	0.47
1:B:411:PHE:CD2	1:B:413:TYR:HD1	2.32	0.47
1:B:688:ASN:O	1:B:692:GLY:N	2.36	0.47
1:B:969:ALA:HB2	2:R:1:NAG:H3	1.96	0.47
1:B:1109:GLN:HA	1:B:1112:ARG:HG2	1.97	0.47
1:C:601:ILE:CG2	1:C:618:LEU:HB2	2.45	0.47
1:C:1203:PHE:HA	1:C:1215:PRO:HD3	1.97	0.47
2:o:2:NAG:H61	2:o:3:BMA:H2	1.97	0.47
1:A:278:PRO:C	1:A:279:LEU:HD22	2.40	0.47
1:A:321:PHE:O	1:A:397:GLU:HG2	2.14	0.47
1:A:662:ILE:O	1:A:697:VAL:HA	2.15	0.47
1:A:1114:LEU:HB3	1:A:1118:LYS:HZ2	1.78	0.47
1:B:545:ASP:OD1	1:B:546:THR:N	2.46	0.47
1:B:601:ILE:O	1:B:617:SER:HA	2.14	0.47
1:B:982:LEU:HB3	1:B:988:GLN:NE2	2.30	0.47
1:C:484:PHE:CE2	1:C:751:TYR:HB2	2.50	0.47
1:C:497:GLN:NE2	1:C:660:GLU:OE2	2.48	0.47
1:C:500:SER:N	1:C:651:LYS:O	2.38	0.47
1:C:666:THR:HB	7:s:1:NAG:H82	1.96	0.47
1:C:788:PHE:HB3	1:C:1158:LEU:HG	1.97	0.47
1:C:844:GLU:HA	1:C:847:GLU:CD	2.40	0.47
1:A:586:SER:HB3	1:A:625:GLY:HA3	1.97	0.46
1:A:1035:LEU:O	1:A:1039:GLN:HG3	2.15	0.46
1:B:328:VAL:HG11	1:B:437:GLY:H	1.81	0.46
1:B:588:PHE:HZ	1:B:620:PHE:CD2	2.31	0.46
1:B:840:SER:O	1:B:841:ALA:C	2.58	0.46
1:B:872:TYR:CE1	1:B:1000:ALA:HA	2.51	0.46
1:B:1003:PHE:O	1:B:1007:ILE:HG12	2.15	0.46
1:B:1089:GLY:O	1:B:1092:SER:OG	2.29	0.46
1:C:789:SER:O	1:C:1159:VAL:N	2.48	0.46
1:C:1138:GLU:CG	1:C:1158:LEU:HB3	2.45	0.46
1:A:547:ARG:NH2	1:A:627:LEU:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:PHE:CE1	1:A:1160:PRO:HB3	2.50	0.46
1:A:979:GLN:HA	1:A:982:LEU:HD12	1.97	0.46
1:A:1147:ALA:HB2	1:A:1152:LEU:HD23	1.97	0.46
1:A:1187:LEU:HD12	1:A:1205:SER:O	2.15	0.46
1:A:1237:GLN:HA	1:A:1240:ASP:OD2	2.15	0.46
1:B:122:ARG:HA	1:B:153:ALA:HA	1.98	0.46
1:B:274:VAL:HG23	1:B:476:VAL:HG23	1.97	0.46
1:B:332:GLU:HB3	1:B:426:PHE:HB2	1.97	0.46
1:C:262:LEU:HB3	1:C:277:GLN:NE2	2.30	0.46
1:C:729:ARG:NH1	4:t:1:NAG:O7	2.46	0.46
1:C:981:ARG:NH2	1:C:1139:HIS:O	2.46	0.46
2:F:4:MAN:O5	2:F:5:MAN:O6	2.32	0.46
1:A:46:VAL:HG21	1:A:233:ASN:HB2	1.97	0.46
1:A:719:SER:HA	1:B:918:LYS:HZ1	1.80	0.46
1:A:1189:LEU:HD23	1:A:1189:LEU:H	1.81	0.46
1:B:330:LEU:HD11	1:B:391:LEU:HD13	1.97	0.46
1:B:1068:ASP:OD1	1:B:1069:ASP:N	2.49	0.46
1:C:51:GLY:O	1:C:211:THR:N	2.45	0.46
1:C:334:SER:OG	1:C:425:ASN:O	2.26	0.46
1:A:66:TYR:C	1:A:190:SER:HB2	2.41	0.46
1:A:108:TYR:HB2	1:A:128:PHE:CZ	2.51	0.46
1:A:1087:ILE:HG13	1:A:1088:THR:N	2.30	0.46
1:A:1192:HIS:N	1:A:1201:GLU:O	2.48	0.46
1:B:38:LYS:HD3	1:B:180:ILE:HD11	1.97	0.46
1:B:84:HIS:HB2	1:B:203:ALA:HA	1.98	0.46
1:B:512:PHE:HB2	3:V:1:NAG:O7	2.16	0.46
1:B:514:ASN:HB3	3:V:1:NAG:O5	2.16	0.46
1:B:875:THR:HB	3:c:2:NAG:H81	1.96	0.46
1:C:73:THR:O	1:C:208:TYR:HB2	2.15	0.46
1:C:89:HIS:CE1	1:C:196:CYS:HG	2.33	0.46
1:C:277:GLN:O	1:C:446:PHE:HA	2.15	0.46
1:C:818:ARG:NE	1:C:1071:TYR:OH	2.48	0.46
1:C:903:ASN:OD1	1:C:904:LYS:N	2.49	0.46
1:C:954:SER:HA	1:C:957:LEU:HG	1.97	0.46
1:C:959:GLY:O	1:C:962:VAL:HG22	2.16	0.46
1:C:1190:PHE:CZ	1:C:1203:PHE:HB2	2.50	0.46
1:A:351:ASN:HA	1:A:364:LEU:HD21	1.96	0.46
1:B:547:ARG:NE	1:B:627:LEU:O	2.35	0.46
1:B:1022:SER:OG	1:B:1025:SER:OG	2.15	0.46
1:C:115:GLY:O	1:C:119:ALA:HB2	2.15	0.46
1:C:518:SER:HA	1:C:556:ASN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1121:GLU:HG3	1:C:1132:PHE:CE2	2.50	0.46
1:A:509:ALA:H	1:A:548:GLN:HE22	1.63	0.46
1:A:829:ALA:O	1:A:832:THR:OG1	2.28	0.46
1:A:1112:ARG:HH12	1:A:1113:LYS:HG3	1.77	0.46
1:B:411:PHE:HB3	1:B:413:TYR:HE1	1.79	0.46
1:B:1145:GLN:O	1:B:1152:LEU:HG	2.16	0.46
1:C:106:GLN:NE2	1:C:128:PHE:H	2.14	0.46
1:A:115:GLY:O	1:A:119:ALA:N	2.49	0.46
1:A:514:ASN:HA	1:A:552:SER:HB3	1.97	0.46
1:A:833:ILE:HG13	1:A:834:GLU:N	2.31	0.46
1:B:86:ARG:H	1:B:199:SER:HG	1.58	0.46
1:B:95:ILE:HG13	1:B:189:TRP:HB3	1.98	0.46
1:B:821:GLN:HA	1:B:824:THR:HG23	1.97	0.46
1:B:1140:ILE:HG22	1:B:1141:PHE:CD1	2.51	0.46
1:C:250:ILE:HG22	1:C:463:TYR:OH	2.16	0.46
1:C:323:ILE:HD12	1:C:396:ARG:C	2.41	0.46
1:C:653:THR:C	1:C:654:ILE:HD13	2.41	0.46
1:C:1145:GLN:C	1:C:1152:LEU:HG	2.41	0.46
1:A:136:PRO:HD3	1:A:195:LYS:NZ	2.31	0.46
1:A:278:PRO:HG3	1:A:446:PHE:CE1	2.50	0.46
1:A:287:ILE:HG13	1:A:289:LYS:NZ	2.30	0.46
1:A:514:ASN:OD1	3:E:1:NAG:H2	2.16	0.46
1:A:783:SER:HA	1:A:1164:VAL:O	2.15	0.46
1:A:1178:ILE:HG23	1:A:1222:GLN:HG2	1.98	0.46
1:B:32:PHE:HA	1:B:35:PHE:CD2	2.50	0.46
1:B:129:PRO:HB3	1:B:144:ILE:HD11	1.98	0.46
1:B:319:LEU:HD11	1:B:441:ILE:HG22	1.98	0.46
1:B:330:LEU:HB3	1:B:371:TYR:CG	2.50	0.46
1:B:789:SER:N	1:B:1159:VAL:O	2.34	0.46
1:A:186:LYS:NZ	3:Q:1:NAG:O3	2.49	0.46
1:A:287:ILE:C	1:A:433:ASP:HB2	2.41	0.46
1:A:930:VAL:HA	1:A:933:GLN:HE21	1.80	0.46
1:B:476:VAL:HG12	1:C:831:LYS:NZ	2.30	0.46
1:B:844:GLU:HA	1:B:847:GLU:HG3	1.98	0.46
1:B:1087:ILE:HA	1:B:1090:ARG:CD	2.45	0.46
1:C:915:GLU:HG2	1:C:919:ARG:HH12	1.81	0.46
1:A:374:PHE:CD1	1:A:387:PHE:HA	2.51	0.46
1:A:450:LEU:HD23	1:A:450:LEU:H	1.81	0.46
1:A:1145:GLN:O	1:A:1152:LEU:HG	2.16	0.46
1:B:258:ASN:H	1:B:259:TRP:HE3	1.64	0.46
1:B:276:ASN:HA	1:B:448:ASP:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:PHE:HA	1:B:639:THR:HA	1.98	0.46
1:B:729:ARG:HG3	1:B:736:TYR:HB3	1.98	0.46
1:B:1189:LEU:HD12	1:B:1203:PHE:O	2.15	0.46
1:C:150:PHE:CE2	1:C:152:LYS:HD3	2.51	0.46
1:C:555:TYR:HE2	1:C:603:LEU:HD21	1.80	0.46
1:C:709:VAL:O	1:C:712:ASP:N	2.31	0.46
1:C:1238:LEU:HB2	1:C:1239:PRO:HD3	1.97	0.46
1:A:79:GLY:HA2	1:A:166:ILE:O	2.15	0.45
1:A:287:ILE:O	1:A:289:LYS:HG3	2.16	0.45
1:A:744:CYS:HB2	1:A:761:SER:C	2.41	0.45
1:A:818:ARG:O	1:A:822:LEU:HG	2.15	0.45
1:A:1023:GLN:OE1	1:A:1026:ARG:HD2	2.16	0.45
1:B:349:CYS:HA	1:B:372:TYR:O	2.16	0.45
1:B:426:PHE:CE2	1:B:438:PHE:HE2	2.34	0.45
1:B:797:LEU:HD11	1:B:1151:LEU:HB2	1.98	0.45
1:B:1188:VAL:O	1:B:1204:VAL:HA	2.16	0.45
1:C:334:SER:OG	1:C:425:ASN:OD1	2.34	0.45
1:A:105:TYR:OH	1:A:146:ARG:HB3	2.15	0.45
1:A:391:LEU:HD12	1:A:392:PRO:HD2	1.99	0.45
1:A:605:GLY:HA3	1:A:615:PHE:CZ	2.51	0.45
1:A:818:ARG:HG3	1:A:1071:TYR:OH	2.16	0.45
1:A:868:ASN:HD21	1:A:972:LEU:C	2.25	0.45
1:B:833:ILE:HG13	1:B:834:GLU:N	2.31	0.45
1:B:1164:VAL:HG12	1:B:1166:VAL:HG13	1.99	0.45
1:C:1097:PHE:O	1:C:1100:GLN:HG2	2.15	0.45
1:A:897:ILE:HG13	1:A:898:GLU:N	2.32	0.45
1:B:218:THR:H	1:B:225:ILE:HG12	1.82	0.45
1:B:778:VAL:HG21	1:C:979:GLN:NE2	2.30	0.45
1:B:1066:SER:HB3	1:B:1069:ASP:OD2	2.16	0.45
1:C:262:LEU:HB3	1:C:277:GLN:HE22	1.82	0.45
1:A:861:LEU:HA	1:A:866:SER:HB2	1.98	0.45
1:A:979:GLN:HA	1:A:982:LEU:HB2	1.97	0.45
1:A:1121:GLU:O	1:A:1125:SER:OG	2.27	0.45
1:A:1173:CYS:SG	1:A:1230:TYR:HD2	2.39	0.45
1:A:1224:GLU:OE1	1:A:1224:GLU:N	2.40	0.45
1:B:819:CYS:HA	1:B:822:LEU:HD12	1.99	0.45
1:B:1088:THR:O	1:B:1091:LEU:HG	2.16	0.45
1:C:716:VAL:O	1:C:737:HIS:N	2.41	0.45
1:C:1164:VAL:HG11	1:C:1210:PHE:CE1	2.52	0.45
1:A:484:PHE:HB3	1:A:705:GLN:NE2	2.32	0.45
1:A:840:SER:O	1:A:841:ALA:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:VAL:O	1:A:1057:GLN:HB2	2.17	0.45
1:B:559:ASN:OD1	1:B:559:ASN:N	2.50	0.45
1:B:782:ILE:O	1:B:1165:ASP:HA	2.17	0.45
1:B:1119:VAL:O	1:B:1123:VAL:HB	2.16	0.45
1:C:1234:THR:N	1:C:1237:GLN:OE1	2.42	0.45
1:A:65:TRP:NE1	1:A:67:CYS:HB3	2.32	0.45
1:A:588:PHE:HD1	1:A:622:PHE:HB3	1.81	0.45
1:A:686:PHE:CZ	1:A:695:TYR:HB2	2.52	0.45
1:A:915:GLU:CG	1:A:919:ARG:HE	2.30	0.45
1:A:1189:LEU:HA	1:A:1204:VAL:HG12	1.97	0.45
1:B:97:GLN:HB2	1:B:99:PRO:HD2	1.99	0.45
1:B:829:ALA:O	1:B:833:ILE:HG23	2.16	0.45
1:B:1049:LEU:O	1:B:1053:THR:HG23	2.17	0.45
1:C:270:HIS:HB2	1:C:455:GLY:H	1.81	0.45
1:A:67:CYS:N	1:A:190:SER:HB2	2.32	0.45
1:A:91:PHE:HB3	1:A:111:LYS:HZ3	1.82	0.45
1:A:590:VAL:HG13	1:A:620:PHE:CE1	2.52	0.45
1:B:274:VAL:HA	1:B:450:LEU:HA	1.99	0.45
1:B:1097:PHE:O	1:B:1101:THR:HG23	2.17	0.45
1:C:570:SER:OG	1:C:571:ASN:N	2.50	0.45
1:B:217:VAL:HA	1:B:225:ILE:HG12	1.99	0.45
1:B:278:PRO:O	1:B:279:LEU:HD22	2.17	0.45
1:B:357:LEU:HD23	1:B:385:TYR:CD2	2.52	0.45
1:B:516:THR:O	1:B:534:THR:HA	2.17	0.45
1:B:880:VAL:O	1:B:893:LYS:N	2.45	0.45
1:B:1104:LYS:O	1:B:1107:GLU:HG3	2.17	0.45
1:C:43:ALA:O	1:C:218:THR:HA	2.17	0.45
1:C:1223:ILE:HG22	1:C:1225:SER:H	1.82	0.45
1:A:352:SER:H	1:A:364:LEU:HD13	1.81	0.45
1:A:432:ASP:O	1:A:436:SER:N	2.49	0.45
1:A:501:PHE:N	1:A:643:PHE:O	2.28	0.45
1:A:801:ASN:HB3	1:A:1105:TYR:CZ	2.52	0.45
1:B:269:VAL:O	1:B:453:VAL:HG22	2.17	0.45
1:B:280:LEU:N	1:B:444:THR:OG1	2.50	0.45
1:B:792:ILE:HG13	1:B:1156:THR:HA	1.99	0.45
1:C:818:ARG:HD3	1:C:818:ARG:H	1.81	0.45
2:G:2:NAG:O3	2:G:3:BMA:O6	2.34	0.45
2:G:3:BMA:H62	2:G:5:MAN:H2	1.36	0.45
3:f:1:NAG:O4	3:f:2:NAG:O7	2.35	0.45
1:A:278:PRO:HA	1:A:446:PHE:HA	1.99	0.45
1:A:788:PHE:CE2	1:A:1160:PRO:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ASP:HB3	1:B:469:SER:HB2	1.99	0.45
1:B:789:SER:O	1:B:1159:VAL:HG12	2.16	0.45
1:B:840:SER:O	1:B:843:LEU:N	2.49	0.45
1:C:47:VAL:HA	1:C:237:TYR:CE1	2.48	0.45
1:C:1153:PHE:O	1:C:1154:LEU:HD22	2.16	0.45
1:A:471:LEU:HD12	1:A:472:LYS:N	2.32	0.44
1:B:322:ASN:OD1	1:B:323:ILE:N	2.50	0.44
1:A:322:ASN:HB3	1:A:439:TRP:HB3	1.99	0.44
1:A:325:ASP:HB3	1:A:436:SER:O	2.17	0.44
1:A:518:SER:HB3	2:F:1:NAG:H61	1.99	0.44
1:A:798:GLN:HG2	1:A:1149:GLN:HG3	1.99	0.44
1:A:928:ASP:OD1	1:A:930:VAL:HG22	2.17	0.44
1:A:995:ASN:O	1:A:999:LEU:HG	2.17	0.44
1:A:1091:LEU:HA	1:A:1094:LEU:HG	1.99	0.44
1:B:66:TYR:O	1:B:190:SER:HB2	2.17	0.44
1:B:452:GLU:OE1	1:B:459:GLN:HG2	2.18	0.44
1:B:602:ASP:CG	1:B:614:LYS:HD2	2.43	0.44
1:C:398:ILE:HD13	1:C:408:VAL:HG13	1.99	0.44
1:C:729:ARG:HH22	4:t:1:NAG:C7	2.30	0.44
1:C:1128:GLN:HB2	1:C:1129:ARG:HH12	1.82	0.44
1:A:466:ASP:HB3	1:A:469:SER:OG	2.17	0.44
1:A:821:GLN:NE2	1:A:822:LEU:HG	2.32	0.44
1:A:1109:GLN:HA	1:A:1112:ARG:NE	2.32	0.44
1:B:565:SER:O	1:B:606:TYR:N	2.41	0.44
1:B:667:ASN:HB2	8:B:1402:NAG:C2	2.47	0.44
1:B:1183:ARG:HB2	1:B:1221:VAL:HG13	1.98	0.44
1:C:222:GLU:OE1	1:C:222:GLU:N	2.42	0.44
1:C:563:TYR:HB3	1:C:608:GLU:OE2	2.17	0.44
1:C:785:PRO:HA	1:C:1162:ASP:O	2.17	0.44
1:C:805:SER:OG	1:C:939:MET:HB3	2.16	0.44
1:C:1172:LEU:HB3	1:C:1180:LEU:HB3	1.99	0.44
1:A:317:GLU:CD	1:A:445:ASN:HD22	2.24	0.44
1:A:411:PHE:CE2	1:A:413:TYR:HA	2.52	0.44
1:A:918:LYS:HZ1	1:C:735:PHE:N	2.16	0.44
1:A:975:SER:O	1:A:978:VAL:HB	2.17	0.44
1:B:44:PRO:HD2	1:B:309:GLY:HA2	1.99	0.44
1:C:333:GLY:HA2	1:C:426:PHE:CE1	2.53	0.44
1:C:1048:ALA:C	1:C:1051:GLN:HE22	2.26	0.44
1:C:1064:SER:HB3	1:C:1070:ILE:HD11	1.99	0.44
1:A:270:HIS:ND1	1:A:454:GLN:HA	2.33	0.44
1:A:1197:HIS:CD2	1:A:1199:ALA:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:O	1:B:184:TYR:HA	2.17	0.44
1:B:236:GLY:HA2	1:B:239:ALA:HB3	1.98	0.44
1:B:454:GLN:CD	1:B:459:GLN:HE22	2.26	0.44
1:B:520:SER:O	1:B:529:LEU:HD12	2.17	0.44
1:B:753:ASN:O	1:B:764:TYR:HA	2.18	0.44
1:B:791:SER:N	1:B:1157:VAL:O	2.50	0.44
1:B:1085:ARG:O	1:B:1088:THR:OG1	2.35	0.44
1:C:1117:GLN:O	1:C:1120:ASN:N	2.50	0.44
1:A:292:GLY:HA2	1:A:426:PHE:H	1.83	0.44
1:A:317:GLU:O	1:A:402:LYS:N	2.51	0.44
1:A:435:VAL:O	1:A:435:VAL:HG12	2.18	0.44
1:A:740:ASP:OD2	1:A:761:SER:N	2.51	0.44
1:B:319:LEU:HD12	1:B:442:ALA:O	2.17	0.44
1:B:1050:THR:O	1:B:1054:VAL:HG23	2.18	0.44
1:C:199:SER:HB3	1:C:203:ALA:HB3	2.00	0.44
1:C:374:PHE:CD1	1:C:387:PHE:HA	2.52	0.44
1:C:1117:GLN:HB2	1:C:1118:LYS:NZ	2.33	0.44
1:A:375:PHE:CZ	1:A:388:LEU:HD11	2.52	0.44
1:A:504:LEU:HB2	1:A:626:GLU:HG3	2.00	0.44
1:A:830:CYS:O	1:A:834:GLU:HG3	2.18	0.44
1:A:990:ASP:OD1	1:A:991:VAL:N	2.51	0.44
1:A:1069:ASP:O	1:A:1073:ARG:HG2	2.18	0.44
1:B:34:ARG:HH21	1:B:37:SER:HB3	1.83	0.44
1:B:213:TYR:CE2	1:B:229:PRO:HG3	2.53	0.44
1:B:242:PHE:CZ	1:B:284:LEU:HD22	2.53	0.44
1:B:425:ASN:HD21	8:B:1406:NAG:H83	1.82	0.44
1:B:753:ASN:HA	1:B:765:VAL:HB	1.99	0.44
1:B:953:TYR:O	1:B:957:LEU:HG	2.17	0.44
1:B:1082:GLN:HG2	1:B:1085:ARG:HH12	1.83	0.44
1:B:1138:GLU:O	1:B:1157:VAL:HG13	2.17	0.44
1:C:134:LEU:HD11	1:C:193:ALA:HB1	1.99	0.44
1:C:284:LEU:O	1:C:307:CYS:HA	2.17	0.44
1:C:291:TYR:O	1:C:425:ASN:HA	2.17	0.44
1:C:796:TYR:CD1	1:C:797:LEU:N	2.85	0.44
1:C:915:GLU:CG	1:C:919:ARG:HH22	2.30	0.44
1:C:1192:HIS:NE2	1:C:1193:GLU:HG2	2.33	0.44
1:C:1227:VAL:HG22	1:C:1230:TYR:CE2	2.52	0.44
1:A:238:ALA:O	1:A:240:ASN:N	2.50	0.44
1:A:516:THR:HB	1:A:535:THR:OG1	2.17	0.44
1:A:1143:LEU:CD1	1:A:1154:LEU:HB2	2.48	0.44
1:B:1110:ALA:HA	1:B:1113:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:PRO:C	1:C:143:THR:HG1	2.19	0.44
1:C:105:TYR:CE1	1:C:149:LEU:HB2	2.53	0.44
1:C:403:TYR:HA	1:C:418:LEU:HD23	1.99	0.44
1:C:471:LEU:HD12	1:C:474:SER:HB2	2.00	0.44
1:C:906:VAL:HG13	1:C:910:LEU:HD12	2.00	0.44
6:O:2:NAG:N2	6:O:6:FUC:H3	2.30	0.44
1:A:508:ASN:OD1	1:A:548:GLN:NE2	2.51	0.44
1:A:852:LEU:HA	1:A:953:TYR:CZ	2.52	0.44
1:A:1109:GLN:HA	1:A:1112:ARG:CD	2.48	0.44
1:A:1120:ASN:O	1:A:1124:LYS:HG2	2.17	0.44
1:A:1217:VAL:HG11	1:A:1245:TYR:HA	2.00	0.44
1:B:98:GLU:H	1:B:190:SER:HG	1.56	0.44
1:B:256:PHE:HD1	1:B:259:TRP:CE2	2.36	0.44
1:B:796:TYR:CG	1:B:797:LEU:N	2.85	0.44
1:B:1142:SER:OG	1:B:1155:HIS:HA	2.18	0.44
1:B:1182:LEU:HD21	1:B:1184:GLU:C	2.43	0.44
1:C:319:LEU:HD12	1:C:442:ALA:O	2.18	0.44
1:C:490:ARG:HD2	1:C:492:LEU:H	1.83	0.44
1:C:510:HIS:HA	1:C:548:GLN:HG3	1.98	0.44
1:C:514:ASN:O	1:C:536:ILE:HA	2.18	0.44
1:C:605:GLY:O	1:C:612:GLY:HA2	2.17	0.44
1:C:652:TYR:N	1:C:659:GLY:O	2.50	0.44
1:C:900:LEU:HA	1:C:903:ASN:HD21	1.83	0.44
1:C:982:LEU:O	1:C:985:LEU:HG	2.18	0.44
1:C:1026:ARG:HG2	1:C:1032:ALA:CB	2.48	0.44
1:A:33:ARG:NH2	1:A:226:SER:HA	2.33	0.43
1:A:568:GLN:NE2	1:A:569:ASP:O	2.51	0.43
1:A:580:ASN:O	1:A:632:PRO:HD3	2.18	0.43
1:A:1048:ALA:C	1:A:1049:LEU:HD22	2.43	0.43
1:B:98:GLU:N	1:B:190:SER:OG	2.34	0.43
1:B:1087:ILE:O	1:B:1090:ARG:HG2	2.18	0.43
1:B:1099:ALA:O	1:B:1103:THR:OG1	2.32	0.43
1:B:1116:GLN:HA	1:B:1119:VAL:HG12	1.98	0.43
1:C:269:VAL:HG22	1:C:455:GLY:HA2	2.00	0.43
1:C:322:ASN:OD1	1:C:323:ILE:N	2.51	0.43
1:C:897:ILE:HG13	1:C:901:LEU:HD23	2.00	0.43
1:C:1144:VAL:HG22	1:C:1153:PHE:CD1	2.53	0.43
1:A:277:GLN:O	1:A:446:PHE:HA	2.17	0.43
1:A:395:VAL:HG13	1:A:409:ASN:ND2	2.33	0.43
1:A:665:LEU:HD13	1:A:695:TYR:CZ	2.52	0.43
1:A:788:PHE:HB3	1:A:1158:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:ILE:HD12	1:A:1063:ILE:H	1.82	0.43
1:B:576:LEU:HA	1:B:579:VAL:HG22	2.01	0.43
1:B:840:SER:O	1:B:844:GLU:OE1	2.37	0.43
1:C:270:HIS:CG	1:C:271:GLY:N	2.87	0.43
1:C:291:TYR:HB3	1:C:424:ILE:HG23	2.01	0.43
1:C:345:PHE:CE1	1:C:377:VAL:HG13	2.53	0.43
1:C:427:THR:HG22	1:C:428:GLY:N	2.33	0.43
1:C:508:ASN:ND2	1:C:635:LEU:O	2.52	0.43
1:C:873:ASN:HB3	3:q:1:NAG:HN2	1.82	0.43
1:C:1011:THR:HA	1:C:1014:PHE:HD2	1.84	0.43
2:a:2:NAG:H4	2:a:3:BMA:H2	1.80	0.43
1:A:362:ILE:HD12	1:C:507:PHE:CD1	2.54	0.43
1:A:375:PHE:CE1	1:A:388:LEU:HD11	2.53	0.43
1:A:512:PHE:HB2	3:E:1:NAG:C7	2.48	0.43
1:A:663:ILE:HD12	1:A:696:SER:C	2.42	0.43
1:A:768:GLN:O	1:B:854:ILE:HG12	2.19	0.43
1:A:818:ARG:O	1:A:821:GLN:NE2	2.51	0.43
1:B:338:HIS:HB2	1:B:421:ALA:O	2.18	0.43
1:B:349:CYS:HA	1:B:373:CYS:HA	2.01	0.43
1:B:434:ASP:OD1	2:U:1:NAG:H2	2.17	0.43
1:B:461:ILE:C	1:B:462:LEU:HD22	2.43	0.43
1:B:654:ILE:HG22	1:B:655:TYR:CD2	2.53	0.43
1:B:793:ARG:HH22	1:B:1136:ASP:CG	2.21	0.43
1:B:1072:SER:HB2	1:B:1073:ARG:NH1	2.33	0.43
1:C:250:ILE:HG12	1:C:256:PHE:CZ	2.53	0.43
1:C:601:ILE:O	1:C:617:SER:HA	2.18	0.43
1:C:1133:CYS:HB3	1:C:1155:HIS:CE1	2.53	0.43
1:C:1167:ILE:HG13	2:o:1:NAG:H81	2.00	0.43
1:C:1232:ASN:C	1:C:1233:LEU:HD12	2.42	0.43
1:A:105:TYR:CD2	1:A:127:GLN:HG3	2.53	0.43
1:A:339:THR:C	1:A:342:GLY:H	2.26	0.43
1:A:582:TYR:CE1	1:A:632:PRO:HD2	2.53	0.43
1:A:1127:SER:OG	1:A:1129:ARG:HG2	2.18	0.43
1:B:93:ILE:O	1:B:109:LEU:HG	2.19	0.43
1:B:467:PRO:O	1:B:471:LEU:HG	2.18	0.43
1:B:751:TYR:HB2	1:C:842:ARG:HH12	1.82	0.43
1:B:1187:LEU:HD13	1:B:1205:SER:C	2.44	0.43
1:C:107:LEU:HD12	1:C:125:ILE:HG13	1.99	0.43
1:C:270:HIS:ND1	1:C:454:GLN:HA	2.33	0.43
1:C:789:SER:O	1:C:790:MET:HE2	2.18	0.43
2:D:1:NAG:H61	2:D:2:NAG:H82	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:O	1:A:444:THR:HA	2.19	0.43
1:A:516:THR:O	1:A:534:THR:HA	2.18	0.43
1:A:1208:ARG:C	1:A:1209:MET:HE2	2.44	0.43
1:B:423:THR:HG22	1:B:425:ASN:OD1	2.18	0.43
1:B:585:PHE:CE1	1:B:624:LYS:HA	2.52	0.43
1:B:682:GLN:OE1	1:B:682:GLN:N	2.51	0.43
1:B:995:ASN:OD1	1:B:996:GLN:N	2.51	0.43
1:C:547:ARG:HH21	1:C:627:LEU:HA	1.83	0.43
1:C:783:SER:OG	1:C:1165:ASP:OD1	2.20	0.43
1:C:789:SER:OG	1:C:1159:VAL:HB	2.18	0.43
1:A:302:THR:HG23	1:A:314:ARG:O	2.17	0.43
1:A:524:HIS:ND1	1:A:528:ASN:HB2	2.34	0.43
1:A:601:ILE:O	1:A:617:SER:HA	2.19	0.43
1:B:569:ASP:OD1	1:B:570:SER:N	2.51	0.43
1:B:652:TYR:HE2	1:B:661:GLY:N	2.17	0.43
1:B:1138:GLU:OE1	1:B:1138:GLU:N	2.51	0.43
1:B:1249:ASN:ND2	8:B:1404:NAG:O7	2.50	0.43
1:C:32:PHE:CE2	1:C:54:PRO:HG2	2.53	0.43
1:C:513:VAL:HA	1:C:537:ASN:OD1	2.18	0.43
1:C:541:SER:HA	1:C:591:SER:HA	1.99	0.43
1:C:603:LEU:O	1:C:614:LYS:HA	2.18	0.43
1:C:817:SER:O	1:C:820:LYS:HG2	2.17	0.43
1:C:939:MET:HE3	1:C:940:VAL:O	2.18	0.43
1:C:1112:ARG:CZ	1:C:1112:ARG:HB3	2.47	0.43
1:A:1091:LEU:HD12	1:A:1092:SER:N	2.34	0.43
1:B:778:VAL:HG23	1:B:779:THR:HG22	2.00	0.43
1:B:834:GLU:O	1:B:837:LEU:HG	2.19	0.43
1:C:57:GLU:HB3	1:C:202:CYS:HB3	2.00	0.43
1:C:466:ASP:HB3	1:C:469:SER:OG	2.18	0.43
1:C:581:ASP:O	1:C:583:LEU:HD22	2.17	0.43
1:C:585:PHE:HE1	1:C:624:LYS:NZ	2.16	0.43
1:C:653:THR:O	1:C:654:ILE:HD13	2.17	0.43
1:C:745:THR:N	1:C:757:CYS:SG	2.92	0.43
1:C:799:LEU:HD12	1:C:1151:LEU:HD23	2.01	0.43
1:C:808:CYS:O	1:C:812:VAL:HG13	2.18	0.43
1:C:841:ALA:HA	1:C:844:GLU:OE1	2.18	0.43
1:C:1119:VAL:O	1:C:1123:VAL:HB	2.19	0.43
1:C:1183:ARG:HD2	1:C:1184:GLU:OE2	2.19	0.43
1:A:514:ASN:OD1	1:A:537:ASN:ND2	2.50	0.43
1:A:691:SER:CB	2:G:1:NAG:H5	2.49	0.43
1:A:1083:VAL:O	1:A:1086:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLY:HA2	1:B:167:THR:HA	2.00	0.43
1:B:86:ARG:N	1:B:199:SER:OG	2.30	0.43
1:B:182:TYR:HB3	1:B:184:TYR:CE1	2.54	0.43
1:B:281:VAL:HA	1:B:444:THR:HA	2.00	0.43
1:B:336:VAL:HB	1:B:423:THR:HB	2.01	0.43
1:B:339:THR:HA	1:B:419:LEU:HA	2.01	0.43
1:B:482:ASP:HA	1:B:708:TYR:HD2	1.83	0.43
1:B:677:THR:HG23	1:B:683:LEU:HD12	2.01	0.43
1:C:1131:GLY:O	1:C:1135:GLY:HA2	2.19	0.43
1:A:357:LEU:HD22	1:A:374:PHE:HD2	1.83	0.43
1:A:719:SER:HA	1:B:918:LYS:NZ	2.33	0.43
1:A:729:ARG:HB2	1:A:736:TYR:HD2	1.83	0.43
1:A:831:LYS:HE2	1:C:476:VAL:HG22	2.00	0.43
1:A:857:GLU:H	1:A:857:GLU:CD	2.23	0.43
1:B:120:THR:HG23	1:B:155:PRO:HD3	2.00	0.43
1:B:298:SER:HA	1:B:421:ALA:HA	1.99	0.43
1:B:450:LEU:HD11	1:B:478:PHE:CZ	2.54	0.43
1:B:573:PRO:HB2	1:C:1073:ARG:HH21	1.84	0.43
1:B:929:LEU:HD23	1:B:933:GLN:HE22	1.84	0.43
1:A:228:GLN:HB3	1:A:231:THR:OG1	2.19	0.43
1:A:287:ILE:HB	1:A:433:ASP:CG	2.44	0.43
1:A:594:LEU:HD11	1:B:614:LYS:HD3	2.01	0.43
1:A:708:TYR:CA	1:A:713:ILE:HD13	2.48	0.43
1:A:952:MET:HA	1:A:955:ALA:HB3	2.01	0.43
1:A:978:VAL:O	1:A:982:LEU:HG	2.18	0.43
1:B:507:PHE:CE2	1:B:509:ALA:HB2	2.51	0.43
1:B:540:SER:HB2	1:B:592:THR:OG1	2.18	0.43
1:B:1029:ASN:N	1:B:1033:HIS:ND1	2.67	0.43
1:B:1120:ASN:C	1:B:1120:ASN:ND2	2.77	0.43
1:C:122:ARG:HD2	1:C:153:ALA:HB2	2.01	0.43
1:C:270:HIS:HA	1:C:453:VAL:HG13	2.01	0.43
1:C:808:CYS:O	1:C:812:VAL:HG22	2.18	0.43
1:C:1018:LYS:HG2	1:C:1026:ARG:HH22	1.84	0.43
2:X:3:BMA:O4	2:X:5:MAN:O6	2.21	0.43
1:A:287:ILE:HB	1:A:433:ASP:HB2	2.00	0.42
1:A:290:ILE:O	1:A:293:LEU:N	2.51	0.42
1:A:469:SER:HA	1:A:472:LYS:CE	2.49	0.42
1:A:999:LEU:HB3	1:A:1003:PHE:CE2	2.54	0.42
1:B:78:HIS:O	1:B:167:THR:HA	2.19	0.42
1:B:107:LEU:HD12	1:B:125:ILE:HD11	2.00	0.42
1:B:515:ILE:HG23	1:B:553:LEU:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ASN:HB2	2:Y:1:NAG:O5	2.19	0.42
1:B:1049:LEU:H	1:B:1049:LEU:HD23	1.83	0.42
1:C:820:LYS:O	1:C:824:THR:HG23	2.19	0.42
1:C:821:GLN:HA	1:C:824:THR:HG23	2.01	0.42
1:A:50:GLY:HA3	1:A:212:TYR:HD1	1.84	0.42
1:A:102:PRO:HA	1:A:106:GLN:NE2	2.35	0.42
1:A:257:ASN:N	1:A:257:ASN:OD1	2.52	0.42
1:A:513:VAL:HG23	1:A:551:ILE:HD12	2.02	0.42
1:A:585:PHE:HD1	1:A:624:LYS:HA	1.84	0.42
1:A:918:LYS:HZ3	1:C:719:SER:HA	1.85	0.42
1:B:278:PRO:C	1:B:279:LEU:HD22	2.44	0.42
1:B:475:GLN:HA	1:C:831:LYS:NZ	2.34	0.42
1:B:885:PRO:O	1:B:888:GLY:N	2.51	0.42
1:B:948:GLU:HA	1:B:951:HIS:ND1	2.34	0.42
1:B:973:PRO:HG2	1:B:976:TYR:CZ	2.54	0.42
1:C:861:LEU:HA	1:C:866:SER:HB2	2.01	0.42
1:C:1069:ASP:O	1:C:1073:ARG:N	2.51	0.42
1:A:75:SER:O	1:A:75:SER:OG	2.36	0.42
1:A:167:THR:OG1	1:A:174:THR:OG1	2.34	0.42
1:A:284:LEU:HD13	1:A:442:ALA:HB2	2.01	0.42
1:A:503:THR:HA	1:A:655:TYR:CE1	2.54	0.42
1:B:93:ILE:HG13	1:B:194:THR:HG22	2.01	0.42
1:B:125:ILE:HB	1:B:150:PHE:HB3	2.00	0.42
1:B:929:LEU:O	1:B:932:ALA:N	2.52	0.42
1:B:963:LEU:HD13	1:B:963:LEU:HA	1.89	0.42
1:B:998:LEU:HA	1:B:1001:GLU:HG3	2.01	0.42
1:C:53:LEU:HD12	1:C:213:TYR:CD1	2.54	0.42
1:C:240:ASN:O	1:C:440:THR:HG21	2.18	0.42
1:C:521:PHE:HB2	1:C:559:ASN:HA	2.00	0.42
1:C:864:ILE:HD13	1:C:878:LEU:HD13	2.01	0.42
1:C:1039:GLN:NE2	1:C:1043:ASN:OD1	2.45	0.42
1:C:1091:LEU:O	1:C:1094:LEU:HG	2.20	0.42
1:A:228:GLN:HG2	1:A:229:PRO:HD2	2.02	0.42
1:B:344:ASN:HB2	2:d:1:NAG:HN2	1.84	0.42
1:B:357:LEU:HD13	1:B:374:PHE:CD2	2.54	0.42
1:B:747:PRO:HB2	1:B:750:VAL:HG12	2.00	0.42
1:B:790:MET:CE	1:B:1156:THR:HB	2.49	0.42
1:C:273:VAL:O	1:C:451:ILE:N	2.43	0.42
1:C:468:VAL:O	1:C:472:LYS:HG3	2.19	0.42
1:C:563:TYR:CG	1:C:564:VAL:N	2.87	0.42
1:C:588:PHE:HA	1:C:621:GLN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1:NAG:H61	2:J:2:NAG:H82	2.01	0.42
1:A:92:GLU:CB	1:A:195:LYS:HB2	2.48	0.42
1:A:264:ASN:HA	1:A:407:TYR:HE1	1.84	0.42
1:A:958:ILE:O	1:A:961:MET:HG3	2.19	0.42
1:C:708:TYR:CE1	1:C:711:ASP:HA	2.54	0.42
1:C:840:SER:O	1:C:844:GLU:CD	2.63	0.42
1:C:1234:THR:HG22	1:C:1237:GLN:CD	2.45	0.42
1:A:286:ALA:O	1:A:287:ILE:C	2.62	0.42
1:A:322:ASN:HA	1:A:397:GLU:HG2	2.00	0.42
1:A:950:LEU:HA	1:A:953:TYR:HB3	2.00	0.42
1:B:188:ASP:O	1:B:189:TRP:HD1	2.02	0.42
1:B:948:GLU:OE1	1:B:952:MET:HE3	2.20	0.42
1:C:513:VAL:O	1:C:551:ILE:HD12	2.19	0.42
1:C:843:LEU:HD12	1:C:844:GLU:HG3	2.02	0.42
1:A:337:LEU:O	1:A:344:ASN:HA	2.19	0.42
1:A:376:LYS:HA	1:A:385:TYR:HA	2.01	0.42
1:A:784:ILE:O	1:A:1164:VAL:N	2.42	0.42
1:B:111:LYS:HG3	1:B:119:ALA:O	2.20	0.42
1:B:168:TRP:CD1	1:B:173:VAL:HG22	2.55	0.42
1:B:351:ASN:HB2	1:B:371:TYR:CE1	2.55	0.42
1:B:515:ILE:O	1:B:553:LEU:HA	2.19	0.42
1:B:606:TYR:CD1	1:B:612:GLY:HA3	2.54	0.42
1:B:744:CYS:HB2	1:B:761:SER:O	2.19	0.42
1:B:982:LEU:O	1:B:986:ALA:N	2.48	0.42
1:B:1048:ALA:CA	1:B:1051:GLN:HE22	2.31	0.42
1:C:338:HIS:ND1	2:k:1:NAG:O5	2.53	0.42
1:C:399:VAL:CG1	1:C:407:TYR:HB2	2.50	0.42
1:C:686:PHE:O	1:C:694:VAL:HA	2.19	0.42
1:C:806:VAL:HG22	1:C:938:VAL:HG23	2.02	0.42
1:C:1088:THR:HA	1:C:1091:LEU:HG	2.01	0.42
1:C:1104:LYS:O	1:C:1108:VAL:HG12	2.20	0.42
1:A:124:ARG:O	1:A:128:PHE:HE2	2.02	0.42
1:A:217:VAL:HA	1:A:225:ILE:HG12	2.02	0.42
1:A:276:ASN:HA	1:A:447:VAL:O	2.19	0.42
1:A:357:LEU:HD22	1:A:374:PHE:CD2	2.55	0.42
1:A:470:GLN:O	1:A:474:SER:N	2.47	0.42
1:A:676:TYR:HD1	1:B:267:THR:HG23	1.83	0.42
1:A:1036:THR:O	1:A:1039:GLN:NE2	2.53	0.42
1:B:95:ILE:HD12	1:B:191:ARG:O	2.20	0.42
1:B:146:ARG:HD3	1:B:904:LYS:HG2	2.02	0.42
1:B:324:ASN:ND2	1:B:439:TRP:NE1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:HIS:HB2	1:B:385:TYR:HE2	1.85	0.42
1:B:735:PHE:N	1:C:918:LYS:HZ1	2.18	0.42
1:B:784:ILE:N	1:B:1164:VAL:O	2.45	0.42
1:C:708:TYR:HA	1:C:713:ILE:HD13	2.02	0.42
1:C:1109:GLN:HG2	1:C:1112:ARG:HH21	1.85	0.42
1:A:510:HIS:HE1	1:A:512:PHE:CD1	2.37	0.42
1:A:653:THR:HG23	1:A:658:LYS:HB3	2.01	0.42
1:A:653:THR:HG23	1:A:658:LYS:HD3	2.02	0.42
1:A:674:VAL:C	1:A:687:LYS:HE2	2.45	0.42
1:A:832:THR:O	1:A:835:SER:OG	2.32	0.42
1:A:1127:SER:OG	1:A:1128:GLN:N	2.53	0.42
1:B:284:LEU:HD13	1:B:442:ALA:HB2	2.01	0.42
1:B:521:PHE:HZ	1:B:613:VAL:HG21	1.85	0.42
1:B:1013:ALA:O	1:B:1031:VAL:HG11	2.19	0.42
1:B:1034:ALA:O	1:B:1038:VAL:HG22	2.20	0.42
1:B:1099:ALA:O	1:B:1102:LEU:HG	2.19	0.42
1:B:1172:LEU:HD22	1:B:1231:VAL:HB	2.01	0.42
1:C:278:PRO:C	1:C:279:LEU:HD22	2.45	0.42
1:C:687:LYS:HA	1:C:693:ALA:O	2.19	0.42
1:C:1117:GLN:O	1:C:1118:LYS:C	2.63	0.42
1:A:263:SER:HA	2:D:1:NAG:O7	2.20	0.42
1:A:512:PHE:HD1	1:A:550:THR:HB	1.83	0.42
1:A:879:GLY:HA2	1:A:895:SER:HB3	2.01	0.42
1:B:344:ASN:HB3	2:d:1:NAG:N2	2.35	0.42
1:B:485:TYR:HD1	1:C:838:GLN:HE22	1.67	0.42
1:B:497:GLN:OE1	1:B:498:PRO:HD2	2.20	0.42
1:B:511:SER:O	1:B:549:PHE:HA	2.20	0.42
1:B:598:ALA:HA	1:B:620:PHE:O	2.19	0.42
1:B:602:ASP:OD1	1:B:614:LYS:NZ	2.50	0.42
1:C:272:LYS:HG2	1:C:452:GLU:OE1	2.20	0.42
1:C:379:THR:HG23	1:C:381:ASN:H	1.85	0.42
1:C:691:SER:OG	2:u:1:NAG:H3	2.20	0.42
1:C:708:TYR:HE1	1:C:711:ASP:HA	1.85	0.42
1:C:834:GLU:O	1:C:837:LEU:HG	2.20	0.42
1:C:887:ARG:HD2	1:C:889:ARG:NH2	2.35	0.42
1:C:918:LYS:O	1:C:921:SER:OG	2.29	0.42
1:A:1237:GLN:O	1:A:1241:VAL:HG22	2.19	0.41
1:B:50:GLY:HA2	1:B:212:TYR:HA	2.01	0.41
1:B:216:ASN:O	1:B:225:ILE:N	2.53	0.41
1:B:248:GLY:O	1:B:463:TYR:OH	2.38	0.41
1:B:524:HIS:HD2	1:B:530:ILE:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:GLU:OE2	1:B:706:ALA:HB2	2.20	0.41
1:B:999:LEU:HD13	1:B:999:LEU:HA	1.94	0.41
1:B:1109:GLN:HG2	1:B:1113:LYS:HE3	2.02	0.41
1:C:48:VAL:HG22	1:C:214:MET:HB3	2.01	0.41
1:C:140:ASN:OD1	1:C:141:ASP:N	2.52	0.41
1:C:377:VAL:O	1:C:383:THR:HA	2.19	0.41
1:C:598:ALA:HA	1:C:620:PHE:O	2.19	0.41
1:C:905:VAL:HG23	1:C:906:VAL:HG23	2.00	0.41
1:C:1082:GLN:HG3	1:C:1085:ARG:CZ	2.50	0.41
1:C:1082:GLN:HG3	1:C:1085:ARG:NH1	2.35	0.41
1:C:1091:LEU:HD12	1:C:1092:SER:N	2.34	0.41
1:C:1118:LYS:HA	1:C:1118:LYS:HD3	1.88	0.41
1:A:665:LEU:HD12	1:A:694:VAL:O	2.19	0.41
1:A:790:MET:HE3	1:A:1158:LEU:HD11	2.03	0.41
1:A:796:TYR:CG	1:A:797:LEU:N	2.86	0.41
1:B:58:ASN:HA	1:B:206:TYR:CE1	2.55	0.41
1:B:126:CYS:HB2	1:B:128:PHE:CD2	2.54	0.41
1:B:482:ASP:OD2	1:B:710:ASP:N	2.53	0.41
1:B:585:PHE:HB3	1:B:628:ILE:HG13	2.02	0.41
1:B:1180:LEU:HA	1:B:1221:VAL:O	2.20	0.41
1:C:127:GLN:H	1:C:127:GLN:HG2	1.48	0.41
1:C:259:TRP:CD1	1:C:259:TRP:N	2.88	0.41
1:C:411:PHE:HD2	1:C:413:TYR:OH	2.04	0.41
1:C:569:ASP:HB3	1:C:602:ASP:OD1	2.20	0.41
1:C:957:LEU:HD12	1:C:958:ILE:HG12	2.02	0.41
1:C:1069:ASP:O	1:C:1073:ARG:HB2	2.19	0.41
1:A:644:MET:N	1:A:644:MET:SD	2.93	0.41
1:A:747:PRO:HB3	1:A:755:GLY:HA3	2.01	0.41
1:A:812:VAL:HG12	1:A:1090:ARG:NE	2.36	0.41
1:B:272:LYS:NZ	1:B:476:VAL:O	2.33	0.41
1:B:899:ASP:HA	1:B:902:PHE:CD2	2.55	0.41
1:C:600:THR:HA	1:C:618:LEU:O	2.20	0.41
1:C:828:ALA:O	1:C:831:LYS:HB2	2.20	0.41
1:A:464:CYS:HA	1:A:469:SER:HB3	2.01	0.41
1:A:474:SER:O	1:B:831:LYS:NZ	2.39	0.41
1:A:519:ALA:HA	1:A:531:ALA:O	2.20	0.41
1:A:791:SER:O	1:A:1157:VAL:HG12	2.20	0.41
1:A:982:LEU:O	1:A:985:LEU:HG	2.21	0.41
1:B:337:LEU:O	1:B:344:ASN:HA	2.20	0.41
1:B:517:VAL:O	1:B:556:ASN:HB2	2.20	0.41
1:C:93:ILE:O	1:C:108:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:GLN:NE2	1:C:683:LEU:O	2.53	0.41
1:C:1028:LEU:HA	1:C:1033:HIS:ND1	2.36	0.41
2:k:2:NAG:O3	2:k:5:MAN:O5	2.38	0.41
1:A:144:ILE:O	1:A:144:ILE:HG22	2.21	0.41
1:A:327:SER:HA	1:A:330:LEU:HD12	2.03	0.41
1:A:466:ASP:HB3	1:A:469:SER:CB	2.50	0.41
1:A:540:SER:HB2	1:A:592:THR:OG1	2.20	0.41
1:A:793:ARG:HB2	1:A:1155:HIS:HB2	2.01	0.41
1:A:972:LEU:HD21	1:C:778:VAL:HG22	2.01	0.41
1:A:1144:VAL:HG22	1:A:1153:PHE:CD1	2.55	0.41
1:B:565:SER:O	1:B:605:GLY:HA2	2.20	0.41
1:B:583:LEU:O	1:B:629:THR:HA	2.20	0.41
1:B:686:PHE:CE2	1:B:695:TYR:HB2	2.56	0.41
1:B:1188:VAL:N	1:B:1205:SER:O	2.52	0.41
1:C:654:ILE:HG22	1:C:655:TYR:HD2	1.86	0.41
2:H:1:NAG:O7	2:H:1:NAG:O4	2.38	0.41
1:A:46:VAL:HG13	1:A:236:GLY:HA3	2.01	0.41
1:A:278:PRO:O	1:A:279:LEU:HD22	2.20	0.41
1:A:399:VAL:HG12	1:A:407:TYR:HB2	2.02	0.41
1:A:513:VAL:O	1:A:552:SER:N	2.53	0.41
1:A:820:LYS:HA	1:A:823:LEU:HG	2.02	0.41
1:A:948:GLU:HA	1:A:951:HIS:HB3	2.02	0.41
1:A:1059:ASN:OD1	1:A:1062:ALA:HB3	2.21	0.41
1:B:242:PHE:HB2	1:B:251:PRO:CG	2.50	0.41
1:B:452:GLU:O	1:B:458:ILE:HA	2.20	0.41
1:B:709:VAL:HG21	1:B:714:VAL:HB	2.02	0.41
1:B:983:ASN:ND2	1:B:988:GLN:OE1	2.53	0.41
1:C:352:SER:N	1:C:364:LEU:HD22	2.31	0.41
1:C:564:VAL:HA	1:C:606:TYR:O	2.21	0.41
1:C:944:VAL:O	1:C:949:LYS:NZ	2.50	0.41
1:C:979:GLN:HA	1:C:982:LEU:HB3	2.02	0.41
6:S:3:BMA:H3	6:S:4:MAN:H2	1.80	0.41
2:X:1:NAG:O7	2:X:1:NAG:H3	2.20	0.41
1:A:33:ARG:HA	1:A:36:PHE:CD2	2.56	0.41
1:A:319:LEU:HD12	1:A:319:LEU:O	2.21	0.41
1:A:509:ALA:O	1:A:546:THR:HB	2.20	0.41
1:A:916:ASP:OD1	1:A:918:LYS:HG2	2.20	0.41
1:A:933:GLN:OE1	1:A:938:VAL:HB	2.21	0.41
1:A:959:GLY:O	1:A:962:VAL:HG22	2.20	0.41
1:A:1039:GLN:HA	1:A:1042:VAL:HG22	2.03	0.41
1:B:184:TYR:HD2	1:B:460:ARG:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:HD23	1:B:462:LEU:H	1.86	0.41
1:B:1059:ASN:ND2	1:B:1062:ALA:O	2.40	0.41
1:B:1142:SER:C	1:B:1143:LEU:HD22	2.46	0.41
1:C:466:ASP:HB3	1:C:469:SER:CB	2.50	0.41
1:C:1061:GLN:HG3	1:C:1085:ARG:NH1	2.36	0.41
1:A:35:PHE:N	1:A:35:PHE:CD1	2.88	0.41
1:A:376:LYS:HD2	1:A:384:VAL:C	2.46	0.41
1:A:510:HIS:NE2	1:A:634:PRO:HG3	2.36	0.41
1:A:1084:ASP:HA	1:A:1087:ILE:HG12	2.03	0.41
1:B:254:PHE:HB3	1:B:256:PHE:CZ	2.55	0.41
1:B:270:HIS:CE1	1:B:454:GLN:HA	2.55	0.41
1:B:1068:ASP:HA	1:B:1071:TYR:HB3	2.03	0.41
1:B:1143:LEU:HB2	1:B:1154:LEU:CD1	2.50	0.41
1:C:946:ASP:HB2	1:C:949:LYS:HG3	2.03	0.41
1:C:1097:PHE:O	1:C:1101:THR:HG23	2.21	0.41
1:C:1170:ALA:HB3	1:C:1229:THR:O	2.21	0.41
1:C:1227:VAL:HG22	1:C:1230:TYR:HE2	1.86	0.41
4:I:1:NAG:H62	4:I:2:NAG:N2	2.36	0.41
2:m:2:NAG:O6	2:m:4:MAN:O6	2.37	0.41
1:A:46:VAL:HG11	1:A:233:ASN:HB3	2.03	0.41
1:A:106:GLN:N	1:A:126:CYS:O	2.54	0.41
1:A:123:LEU:HD22	1:A:154:ILE:HD13	2.02	0.41
1:A:200:GLY:O	1:A:204:MET:HG3	2.21	0.41
1:A:218:THR:CG2	6:O:1:NAG:HN2	2.34	0.41
1:A:454:GLN:HG3	1:A:457:ALA:HB3	2.03	0.41
1:A:897:ILE:HG13	1:A:898:GLU:H	1.86	0.41
1:B:78:HIS:HB3	1:B:168:TRP:O	2.21	0.41
1:B:159:SER:HB3	1:B:162:SER:HB3	2.03	0.41
1:B:325:ASP:CG	1:B:327:SER:HG	2.29	0.41
1:B:515:ILE:CD1	1:B:536:ILE:HG13	2.48	0.41
1:B:709:VAL:O	1:B:711:ASP:N	2.54	0.41
1:B:785:PRO:HB2	1:B:788:PHE:CZ	2.56	0.41
1:B:790:MET:SD	1:B:1158:LEU:HD22	2.60	0.41
1:B:876:ASN:OD1	1:B:877:VAL:N	2.53	0.41
1:B:933:GLN:HA	1:B:936:SER:HB2	2.01	0.41
1:B:954:SER:O	1:B:958:ILE:HG12	2.20	0.41
1:B:1237:GLN:O	1:B:1241:VAL:HG22	2.20	0.41
1:C:77:VAL:HG22	1:C:206:TYR:HB2	2.03	0.41
1:C:324:ASN:ND2	2:j:1:NAG:O7	2.54	0.41
1:C:396:ARG:HG2	1:C:409:ASN:OD1	2.20	0.41
1:C:471:LEU:O	1:C:475:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:VAL:HG23	1:C:551:ILE:CD1	2.51	0.41
1:C:518:SER:O	1:C:532:SER:HA	2.20	0.41
1:C:555:TYR:CE2	1:C:603:LEU:HD21	2.55	0.41
1:C:820:LYS:HA	1:C:823:LEU:CG	2.50	0.41
1:C:1182:LEU:HD21	1:C:1184:GLU:C	2.45	0.41
1:A:334:SER:OG	1:A:425:ASN:ND2	2.53	0.41
1:A:640:ASP:OD2	2:G:2:NAG:O6	2.33	0.41
1:A:679:ASP:OD1	1:A:680:SER:N	2.53	0.41
1:A:702:PHE:HE1	1:B:935:TYR:CE1	2.39	0.41
1:A:793:ARG:O	1:A:1154:LEU:HA	2.21	0.41
1:A:924:ARG:HH21	7:s:2:FUC:H63	1.85	0.41
1:A:1039:GLN:O	1:A:1042:VAL:HG22	2.21	0.41
1:B:95:ILE:HD13	1:B:192:VAL:HB	2.02	0.41
1:B:257:ASN:OD1	1:B:257:ASN:N	2.54	0.41
1:B:852:LEU:HA	1:B:953:TYR:CZ	2.56	0.41
1:C:504:LEU:HD23	1:C:505:PRO:O	2.21	0.41
1:C:1068:ASP:OD1	1:C:1069:ASP:N	2.54	0.41
1:A:90:GLY:HA3	1:A:111:LYS:O	2.21	0.40
1:A:92:GLU:HA	1:A:109:LEU:O	2.21	0.40
1:A:354:ASN:HB3	1:A:357:LEU:HB2	2.03	0.40
1:A:790:MET:N	1:A:790:MET:SD	2.93	0.40
1:A:1129:ARG:HD3	1:A:1132:PHE:CG	2.56	0.40
1:B:150:PHE:CZ	1:B:152:LYS:HB2	2.56	0.40
1:C:47:VAL:HG22	1:C:241:VAL:HG12	2.04	0.40
1:C:48:VAL:C	1:C:49:LEU:HD22	2.46	0.40
1:C:497:GLN:OE1	1:C:498:PRO:HD2	2.21	0.40
1:C:517:VAL:CG1	1:C:555:TYR:HA	2.52	0.40
1:C:896:PHE:O	1:C:900:LEU:HG	2.21	0.40
1:C:1049:LEU:O	1:C:1052:LEU:HB2	2.22	0.40
1:A:491:ASN:ND2	1:A:700:CYS:O	2.54	0.40
1:A:676:TYR:CZ	1:B:269:VAL:HG23	2.57	0.40
1:A:689:VAL:O	1:B:393:PRO:HG2	2.20	0.40
1:B:717:ILE:HA	1:B:735:PHE:O	2.21	0.40
1:B:1009:ASN:N	8:B:1403:NAG:O7	2.54	0.40
1:C:280:LEU:N	1:C:445:ASN:O	2.53	0.40
1:C:833:ILE:HG13	1:C:834:GLU:N	2.36	0.40
1:C:881:SER:HA	1:C:892:GLN:HA	2.03	0.40
6:i:2:NAG:H5	6:i:3:BMA:H2	2.03	0.40
1:A:116:ASN:HD21	1:A:157:HIS:HA	1.85	0.40
1:A:240:ASN:OD1	1:A:241:VAL:N	2.55	0.40
1:A:289:LYS:HG2	1:A:433:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LYS:O	1:A:476:VAL:N	2.54	0.40
1:A:706:ALA:HB1	1:A:713:ILE:HD12	2.03	0.40
1:A:836:ALA:O	1:A:839:LEU:HG	2.22	0.40
1:A:1204:VAL:N	1:A:1213:ARG:O	2.49	0.40
1:B:448:ASP:O	1:B:464:CYS:HB2	2.20	0.40
1:B:748:VAL:N	1:B:756:VAL:O	2.53	0.40
1:C:405:ASP:CG	1:C:407:TYR:HE1	2.29	0.40
1:C:484:PHE:HE2	1:C:751:TYR:HB2	1.84	0.40
1:C:616:THR:OG1	1:C:617:SER:N	2.54	0.40
1:C:985:LEU:HD12	1:C:986:ALA:N	2.36	0.40
1:C:1183:ARG:HB3	1:C:1184:GLU:OE1	2.21	0.40
4:I:1:NAG:H4	4:I:2:NAG:N2	2.36	0.40
2:X:2:NAG:H4	2:X:3:BMA:H2	1.87	0.40
1:A:468:VAL:HG12	1:A:472:LYS:NZ	2.36	0.40
1:A:704:GLU:OE1	1:A:704:GLU:N	2.54	0.40
1:A:793:ARG:HB3	1:A:1029:ASN:HB3	2.04	0.40
1:A:1060:PHE:HE2	1:A:1089:GLY:HA3	1.86	0.40
1:B:259:TRP:CG	1:B:320:ARG:HH22	2.38	0.40
1:B:320:ARG:O	1:B:441:ILE:HA	2.20	0.40
1:C:337:LEU:HD12	1:C:419:LEU:HD11	2.03	0.40
1:C:717:ILE:HA	1:C:735:PHE:O	2.21	0.40
1:A:454:GLN:OE1	1:A:459:GLN:NE2	2.55	0.40
1:A:708:TYR:HA	1:A:713:ILE:HD13	2.02	0.40
1:A:963:LEU:HD11	1:C:774:ILE:HA	2.03	0.40
1:A:1091:LEU:O	1:A:1094:LEU:HG	2.20	0.40
1:A:1183:ARG:NH1	1:A:1218:SER:O	2.48	0.40
1:B:35:PHE:HE1	1:B:162:SER:HA	1.86	0.40
1:B:41:VAL:HG13	1:B:243:ALA:HB2	2.04	0.40
1:B:600:THR:HA	1:B:618:LEU:O	2.21	0.40
1:B:646:LEU:HA	1:B:663:ILE:HG23	2.03	0.40
1:B:830:CYS:O	1:B:831:LYS:C	2.64	0.40
1:B:876:ASN:HB2	1:B:896:PHE:CB	2.52	0.40
1:B:966:PHE:O	1:B:967:THR:OG1	2.34	0.40
1:C:116:ASN:HB3	1:C:157:HIS:ND1	2.37	0.40
1:C:336:VAL:C	1:C:337:LEU:HD22	2.46	0.40
1:C:1070:ILE:HD12	1:C:1070:ILE:H	1.86	0.40
3:f:1:NAG:H61	3:f:2:NAG:C1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1222/1386 (88%)	1127 (92%)	93 (8%)	2 (0%)	43	77
1	B	1222/1386 (88%)	1119 (92%)	101 (8%)	2 (0%)	43	77
1	C	1222/1386 (88%)	1124 (92%)	97 (8%)	1 (0%)	48	83
All	All	3666/4158 (88%)	3370 (92%)	291 (8%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	ALA
1	A	710	ASP
1	B	353	SER
1	C	710	ASP
1	B	710	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1049/1199 (88%)	1049 (100%)	0	100	100
1	B	1049/1199 (88%)	1048 (100%)	1 (0%)	88	89
1	C	1049/1199 (88%)	1047 (100%)	2 (0%)	87	87
All	All	3147/3597 (88%)	3144 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	351	ASN
1	C	126	CYS
1	C	127	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	233	ASN
1	A	470	GLN
1	A	568	GLN
1	A	1029	ASN
1	A	1043	ASN
1	A	1145	GLN
1	B	59	GLN
1	B	157	HIS
1	B	524	HIS
1	B	849	ASN
1	B	908	ASN
1	B	983	ASN
1	B	1126	GLN
1	C	445	ASN
1	C	470	GLN
1	C	508	ASN
1	C	524	HIS
1	C	768	GLN
1	C	798	GLN
1	C	838	GLN
1	C	979	GLN
1	C	1058	HIS
1	C	1100	GLN
1	C	1128	GLN
1	C	1155	HIS
1	C	1222	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

198 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	2,1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.51	0
2	BMA	D	3	2	11,11,12	0.86	0	15,15,17	1.04	2 (13%)
2	MAN	D	4	2	11,11,12	0.64	0	15,15,17	1.03	2 (13%)
2	MAN	D	5	2	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.94	2 (14%)	17,19,21	1.53	1 (5%)
3	NAG	E	2	3	14,14,15	0.30	0	17,19,21	0.89	1 (5%)
3	BMA	E	3	3	11,11,12	0.58	0	15,15,17	0.88	0
2	NAG	F	1	2,1	14,14,15	0.62	1 (7%)	17,19,21	1.43	1 (5%)
2	NAG	F	2	2	14,14,15	0.46	0	17,19,21	0.42	0
2	BMA	F	3	2	11,11,12	1.09	1 (9%)	15,15,17	1.05	1 (6%)
2	MAN	F	4	2	11,11,12	0.76	1 (9%)	15,15,17	1.15	2 (13%)
2	MAN	F	5	2	11,11,12	0.79	0	15,15,17	1.03	2 (13%)
2	NAG	G	1	2,1	14,14,15	0.60	1 (7%)	17,19,21	0.85	0
2	NAG	G	2	2	14,14,15	0.50	0	17,19,21	0.80	1 (5%)
2	BMA	G	3	2	11,11,12	0.72	0	15,15,17	1.46	3 (20%)
2	MAN	G	4	2	11,11,12	0.60	0	15,15,17	1.07	2 (13%)
2	MAN	G	5	2	11,11,12	1.60	2 (18%)	15,15,17	1.85	3 (20%)
2	NAG	H	1	2,1	14,14,15	0.76	1 (7%)	17,19,21	0.79	0
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.59	0
2	BMA	H	3	2	11,11,12	0.79	0	15,15,17	0.89	1 (6%)
2	MAN	H	4	2	11,11,12	0.87	1 (9%)	15,15,17	1.33	2 (13%)
2	MAN	H	5	2	11,11,12	0.78	0	15,15,17	0.95	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	I	1	4,1	14,14,15	0.57	0	17,19,21	0.69	1 (5%)
4	NAG	I	2	4	14,14,15	0.57	0	17,19,21	0.79	1 (5%)
4	BMA	I	3	4	11,11,12	0.84	0	15,15,17	0.83	0
4	FUC	I	4	4	10,10,11	0.74	0	14,14,16	0.73	0
2	NAG	J	1	2,1	14,14,15	0.24	0	17,19,21	0.54	0
2	NAG	J	2	2	14,14,15	0.20	0	17,19,21	0.55	0
2	BMA	J	3	2	11,11,12	0.71	0	15,15,17	0.91	0
2	MAN	J	4	2	11,11,12	0.71	0	15,15,17	0.87	1 (6%)
2	MAN	J	5	2	11,11,12	0.73	1 (9%)	15,15,17	1.09	2 (13%)
3	NAG	K	1	3,1	14,14,15	0.64	1 (7%)	17,19,21	0.58	0
3	NAG	K	2	3	14,14,15	0.19	0	17,19,21	0.47	0
3	BMA	K	3	3	11,11,12	0.50	0	15,15,17	0.73	0
5	NAG	L	1	5,1	14,14,15	0.51	0	17,19,21	0.77	0
5	NAG	L	2	5	14,14,15	0.46	0	17,19,21	0.50	0
5	BMA	L	3	5	11,11,12	0.48	0	15,15,17	0.67	0
5	MAN	L	4	5	11,11,12	0.58	0	15,15,17	1.01	2 (13%)
4	NAG	M	1	4,1	14,14,15	0.60	0	17,19,21	1.07	1 (5%)
4	NAG	M	2	4	14,14,15	0.46	0	17,19,21	0.41	0
4	BMA	M	3	4	11,11,12	0.47	0	15,15,17	0.79	0
4	FUC	M	4	4	10,10,11	0.69	0	14,14,16	0.93	1 (7%)
2	NAG	N	1	2,1	14,14,15	0.44	0	17,19,21	0.72	0
2	NAG	N	2	2	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
2	BMA	N	3	2	11,11,12	0.88	1 (9%)	15,15,17	1.03	2 (13%)
2	MAN	N	4	2	11,11,12	0.94	1 (9%)	15,15,17	1.03	1 (6%)
2	MAN	N	5	2	11,11,12	0.91	1 (9%)	15,15,17	1.25	1 (6%)
6	NAG	O	1	6,1	14,14,15	0.71	1 (7%)	17,19,21	0.94	1 (5%)
6	NAG	O	2	6	14,14,15	0.62	1 (7%)	17,19,21	0.94	1 (5%)
6	BMA	O	3	6	11,11,12	0.89	1 (9%)	15,15,17	1.48	3 (20%)
6	MAN	O	4	6	11,11,12	0.77	0	15,15,17	1.56	2 (13%)
6	MAN	O	5	6	11,11,12	0.86	1 (9%)	15,15,17	1.84	3 (20%)
6	FUC	O	6	6	10,10,11	0.71	0	14,14,16	0.92	1 (7%)
2	NAG	P	1	2,1	14,14,15	1.02	1 (7%)	17,19,21	2.13	4 (23%)
2	NAG	P	2	2	14,14,15	0.96	2 (14%)	17,19,21	1.47	2 (11%)
2	BMA	P	3	2	11,11,12	0.59	0	15,15,17	1.03	0
2	MAN	P	4	2	11,11,12	1.21	1 (9%)	15,15,17	2.17	5 (33%)
2	MAN	P	5	2	11,11,12	0.68	0	15,15,17	0.85	1 (6%)
3	NAG	Q	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	0.58	0
3	NAG	Q	2	3	14,14,15	0.27	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	Q	3	3	11,11,12	0.51	0	15,15,17	0.87	1 (6%)
2	NAG	R	1	2,1	14,14,15	0.97	1 (7%)	17,19,21	0.78	0
2	NAG	R	2	2	14,14,15	0.28	0	17,19,21	0.89	1 (5%)
2	BMA	R	3	2	11,11,12	0.67	0	15,15,17	0.89	1 (6%)
2	MAN	R	4	2	11,11,12	0.70	0	15,15,17	1.36	2 (13%)
2	MAN	R	5	2	11,11,12	0.60	0	15,15,17	0.91	1 (6%)
6	NAG	S	1	6,1	14,14,15	0.29	0	17,19,21	0.40	0
6	NAG	S	2	6	14,14,15	0.22	0	17,19,21	0.48	0
6	BMA	S	3	6	11,11,12	0.69	0	15,15,17	0.89	0
6	MAN	S	4	6	11,11,12	0.70	0	15,15,17	1.00	1 (6%)
6	MAN	S	5	6	11,11,12	0.75	0	15,15,17	1.05	2 (13%)
6	FUC	S	6	6	10,10,11	0.67	0	14,14,16	0.75	0
2	NAG	T	1	2,1	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
2	NAG	T	2	2	14,14,15	0.31	0	17,19,21	0.51	0
2	BMA	T	3	2	11,11,12	0.94	0	15,15,17	1.31	2 (13%)
2	MAN	T	4	2	11,11,12	0.80	0	15,15,17	1.06	2 (13%)
2	MAN	T	5	2	11,11,12	0.64	0	15,15,17	1.09	2 (13%)
2	NAG	U	1	2,1	14,14,15	0.40	0	17,19,21	1.34	2 (11%)
2	NAG	U	2	2	14,14,15	0.22	0	17,19,21	0.58	0
2	BMA	U	3	2	11,11,12	0.70	0	15,15,17	0.66	0
2	MAN	U	4	2	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
2	MAN	U	5	2	11,11,12	0.63	0	15,15,17	0.89	1 (6%)
3	NAG	V	1	3,1	14,14,15	0.40	0	17,19,21	1.36	1 (5%)
3	NAG	V	2	3	14,14,15	0.24	0	17,19,21	0.47	0
3	BMA	V	3	3	11,11,12	0.58	0	15,15,17	0.69	0
2	NAG	W	1	2,1	14,14,15	0.33	0	17,19,21	0.70	0
2	NAG	W	2	2	14,14,15	1.11	1 (7%)	17,19,21	1.14	1 (5%)
2	BMA	W	3	2	11,11,12	0.83	0	15,15,17	0.92	0
2	MAN	W	4	2	11,11,12	0.59	0	15,15,17	0.96	2 (13%)
2	MAN	W	5	2	11,11,12	0.55	0	15,15,17	0.99	2 (13%)
2	NAG	X	1	2,1	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	X	2	2	14,14,15	0.38	0	17,19,21	0.77	0
2	BMA	X	3	2	11,11,12	0.58	0	15,15,17	0.74	0
2	MAN	X	4	2	11,11,12	0.52	0	15,15,17	1.01	2 (13%)
2	MAN	X	5	2	11,11,12	0.64	0	15,15,17	1.13	2 (13%)
2	NAG	Y	1	2,1	14,14,15	0.18	0	17,19,21	0.58	0
2	NAG	Y	2	2	14,14,15	0.82	1 (7%)	17,19,21	1.43	1 (5%)
2	BMA	Y	3	2	11,11,12	0.97	0	15,15,17	0.86	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	Y	4	2	11,11,12	0.53	0	15,15,17	1.03	2 (13%)
2	MAN	Y	5	2	11,11,12	0.68	0	15,15,17	1.02	2 (13%)
4	NAG	Z	1	4,1	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
4	NAG	Z	2	4	14,14,15	0.29	0	17,19,21	0.41	0
4	BMA	Z	3	4	11,11,12	0.57	0	15,15,17	0.76	0
4	FUC	Z	4	4	10,10,11	0.71	0	14,14,16	1.43	2 (14%)
2	NAG	a	1	2,1	14,14,15	0.49	0	17,19,21	0.50	0
2	NAG	a	2	2	14,14,15	0.49	0	17,19,21	1.41	2 (11%)
2	BMA	a	3	2	11,11,12	0.94	0	15,15,17	0.97	0
2	MAN	a	4	2	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
2	MAN	a	5	2	11,11,12	0.75	1 (9%)	15,15,17	1.11	2 (13%)
2	NAG	b	1	2,1	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
2	NAG	b	2	2	14,14,15	0.35	0	17,19,21	1.49	1 (5%)
2	BMA	b	3	2	11,11,12	0.64	0	15,15,17	0.79	0
2	MAN	b	4	2	11,11,12	0.68	0	15,15,17	1.29	2 (13%)
2	MAN	b	5	2	11,11,12	0.87	0	15,15,17	1.14	2 (13%)
3	NAG	c	1	3,1	14,14,15	0.40	0	17,19,21	0.40	0
3	NAG	c	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	BMA	c	3	3	11,11,12	0.85	1 (9%)	15,15,17	0.90	0
2	NAG	d	1	2,1	14,14,15	1.07	1 (7%)	17,19,21	1.06	1 (5%)
2	NAG	d	2	2	14,14,15	0.71	1 (7%)	17,19,21	0.74	0
2	BMA	d	3	2	11,11,12	0.49	0	15,15,17	1.03	1 (6%)
2	MAN	d	4	2	11,11,12	0.61	0	15,15,17	0.90	1 (6%)
2	MAN	d	5	2	11,11,12	0.63	0	15,15,17	0.94	1 (6%)
6	NAG	e	1	6,1	14,14,15	0.33	0	17,19,21	0.52	0
6	NAG	e	2	6	14,14,15	0.61	1 (7%)	17,19,21	1.38	2 (11%)
6	BMA	e	3	6	11,11,12	0.71	0	15,15,17	0.72	0
6	MAN	e	4	6	11,11,12	0.57	0	15,15,17	0.98	2 (13%)
6	MAN	e	5	6	11,11,12	0.72	0	15,15,17	1.07	2 (13%)
6	FUC	e	6	6	10,10,11	1.61	2 (20%)	14,14,16	1.59	3 (21%)
3	NAG	f	1	3,1	14,14,15	0.77	1 (7%)	17,19,21	0.80	1 (5%)
3	NAG	f	2	3	14,14,15	0.22	0	17,19,21	0.38	0
3	BMA	f	3	3	11,11,12	0.65	0	15,15,17	0.72	0
2	NAG	g	1	2,1	14,14,15	0.18	0	17,19,21	0.56	0
2	NAG	g	2	2	14,14,15	0.19	0	17,19,21	0.52	0
2	BMA	g	3	2	11,11,12	0.70	0	15,15,17	0.75	0
2	MAN	g	4	2	11,11,12	0.50	0	15,15,17	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	g	5	2	11,11,12	0.71	1 (9%)	15,15,17	1.25	2 (13%)
2	NAG	h	1	2,1	14,14,15	0.18	0	17,19,21	0.67	0
2	NAG	h	2	2	14,14,15	0.21	0	17,19,21	0.46	0
2	BMA	h	3	2	11,11,12	0.65	0	15,15,17	0.77	0
2	MAN	h	4	2	11,11,12	0.66	0	15,15,17	0.96	1 (6%)
2	MAN	h	5	2	11,11,12	0.81	1 (9%)	15,15,17	1.22	2 (13%)
6	NAG	i	1	6,1	14,14,15	0.57	0	17,19,21	0.71	0
6	NAG	i	2	6	14,14,15	0.30	0	17,19,21	1.26	1 (5%)
6	BMA	i	3	6	11,11,12	0.64	0	15,15,17	0.63	0
6	MAN	i	4	6	11,11,12	0.92	1 (9%)	15,15,17	1.45	2 (13%)
6	MAN	i	5	6	11,11,12	0.66	0	15,15,17	1.16	2 (13%)
6	FUC	i	6	6	10,10,11	0.63	0	14,14,16	1.02	2 (14%)
2	NAG	j	1	2,1	14,14,15	0.39	0	17,19,21	0.43	0
2	NAG	j	2	2	14,14,15	0.24	0	17,19,21	0.41	0
2	BMA	j	3	2	11,11,12	0.78	0	15,15,17	0.71	0
2	MAN	j	4	2	11,11,12	0.84	0	15,15,17	1.32	2 (13%)
2	MAN	j	5	2	11,11,12	0.82	1 (9%)	15,15,17	1.25	2 (13%)
2	NAG	k	1	2,1	14,14,15	0.27	0	17,19,21	0.47	0
2	NAG	k	2	2	14,14,15	0.35	0	17,19,21	0.54	0
2	BMA	k	3	2	11,11,12	0.58	0	15,15,17	0.73	0
2	MAN	k	4	2	11,11,12	0.59	0	15,15,17	0.98	2 (13%)
2	MAN	k	5	2	11,11,12	0.68	0	15,15,17	1.24	2 (13%)
3	NAG	l	1	3,1	14,14,15	0.88	1 (7%)	17,19,21	1.89	1 (5%)
3	NAG	l	2	3	14,14,15	0.65	0	17,19,21	1.12	1 (5%)
3	BMA	l	3	3	11,11,12	0.91	1 (9%)	15,15,17	1.03	1 (6%)
2	NAG	m	1	2,1	14,14,15	0.52	0	17,19,21	1.35	1 (5%)
2	NAG	m	2	2	14,14,15	0.27	0	17,19,21	0.59	0
2	BMA	m	3	2	11,11,12	0.57	0	15,15,17	0.64	0
2	MAN	m	4	2	11,11,12	0.62	0	15,15,17	1.10	2 (13%)
2	MAN	m	5	2	11,11,12	0.73	0	15,15,17	0.92	1 (6%)
2	NAG	n	1	2,1	14,14,15	0.64	1 (7%)	17,19,21	0.69	0
2	NAG	n	2	2	14,14,15	0.16	0	17,19,21	0.49	0
2	BMA	n	3	2	11,11,12	1.10	0	15,15,17	0.79	0
2	MAN	n	4	2	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
2	MAN	n	5	2	11,11,12	0.59	0	15,15,17	0.96	2 (13%)
2	NAG	o	1	2,1	14,14,15	0.70	1 (7%)	17,19,21	0.53	0
2	NAG	o	2	2	14,14,15	0.34	0	17,19,21	0.73	0
2	BMA	o	3	2	11,11,12	1.12	2 (18%)	15,15,17	1.05	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	o	4	2	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
2	MAN	o	5	2	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
2	NAG	p	1	2,1	14,14,15	0.58	0	17,19,21	1.01	1 (5%)
2	NAG	p	2	2	14,14,15	0.57	0	17,19,21	0.99	1 (5%)
2	BMA	p	3	2	11,11,12	0.73	0	15,15,17	1.10	0
2	MAN	p	4	2	11,11,12	0.64	0	15,15,17	1.15	2 (13%)
2	MAN	p	5	2	11,11,12	0.68	0	15,15,17	1.11	2 (13%)
3	NAG	q	1	3,1	14,14,15	0.29	0	17,19,21	0.44	0
3	NAG	q	2	3	14,14,15	0.20	0	17,19,21	0.45	0
3	BMA	q	3	3	11,11,12	0.72	0	15,15,17	0.67	0
3	NAG	r	1	3,1	14,14,15	0.25	0	17,19,21	0.54	0
3	NAG	r	2	3	14,14,15	0.28	0	17,19,21	0.55	0
3	BMA	r	3	3	11,11,12	0.61	0	15,15,17	0.65	0
7	NAG	s	1	7,1	14,14,15	0.48	0	17,19,21	0.57	0
7	FUC	s	2	7	10,10,11	0.90	0	14,14,16	0.95	1 (7%)
4	NAG	t	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.56	0
4	NAG	t	2	4	14,14,15	0.64	0	17,19,21	1.35	2 (11%)
4	BMA	t	3	4	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
4	FUC	t	4	4	10,10,11	0.88	1 (10%)	14,14,16	1.04	1 (7%)
2	NAG	u	1	2,1	14,14,15	0.87	2 (14%)	17,19,21	0.60	0
2	NAG	u	2	2	14,14,15	0.46	0	17,19,21	1.44	3 (17%)
2	BMA	u	3	2	11,11,12	1.19	2 (18%)	15,15,17	0.99	0
2	MAN	u	4	2	11,11,12	0.71	0	15,15,17	0.85	1 (6%)
2	MAN	u	5	2	11,11,12	0.93	0	15,15,17	1.35	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	1/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1
2	MAN	N	4	2	-	0/2/19/22	1/1/1/1
2	MAN	N	5	2	-	0/2/19/22	1/1/1/1
6	NAG	O	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	1/2/19/22	0/1/1/1
6	MAN	O	4	6	-	2/2/19/22	1/1/1/1
6	MAN	O	5	6	-	1/2/19/22	0/1/1/1
6	FUC	O	6	6	-	-	0/1/1/1
2	NAG	P	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	P	2	2	-	6/6/23/26	0/1/1/1
2	BMA	P	3	2	-	2/2/19/22	0/1/1/1
2	MAN	P	4	2	-	0/2/19/22	0/1/1/1
2	MAN	P	5	2	-	0/2/19/22	1/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
2	NAG	R	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	BMA	R	3	2	-	2/2/19/22	0/1/1/1
2	MAN	R	4	2	-	0/2/19/22	0/1/1/1
2	MAN	R	5	2	-	0/2/19/22	0/1/1/1
6	NAG	S	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1
6	MAN	S	4	6	-	0/2/19/22	0/1/1/1
6	MAN	S	5	6	-	0/2/19/22	1/1/1/1
6	FUC	S	6	6	-	-	0/1/1/1
2	NAG	T	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	BMA	T	3	2	-	0/2/19/22	0/1/1/1
2	MAN	T	4	2	-	2/2/19/22	1/1/1/1
2	MAN	T	5	2	-	0/2/19/22	0/1/1/1
2	NAG	U	1	2,1	-	6/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	BMA	U	3	2	-	2/2/19/22	0/1/1/1
2	MAN	U	4	2	-	0/2/19/22	0/1/1/1
2	MAN	U	5	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	V	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
2	NAG	W	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	BMA	W	3	2	-	2/2/19/22	0/1/1/1
2	MAN	W	4	2	-	0/2/19/22	0/1/1/1
2	MAN	W	5	2	-	0/2/19/22	0/1/1/1
2	NAG	X	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	X	2	2	-	4/6/23/26	0/1/1/1
2	BMA	X	3	2	-	2/2/19/22	0/1/1/1
2	MAN	X	4	2	-	0/2/19/22	0/1/1/1
2	MAN	X	5	2	-	0/2/19/22	1/1/1/1
2	NAG	Y	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
2	BMA	Y	3	2	-	0/2/19/22	0/1/1/1
2	MAN	Y	4	2	-	0/2/19/22	0/1/1/1
2	MAN	Y	5	2	-	0/2/19/22	0/1/1/1
4	NAG	Z	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	4/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1
4	FUC	Z	4	4	-	-	0/1/1/1
2	NAG	a	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	BMA	a	3	2	-	2/2/19/22	0/1/1/1
2	MAN	a	4	2	-	0/2/19/22	0/1/1/1
2	MAN	a	5	2	-	0/2/19/22	0/1/1/1
2	NAG	b	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	b	2	2	-	2/6/23/26	0/1/1/1
2	BMA	b	3	2	-	0/2/19/22	0/1/1/1
2	MAN	b	4	2	-	1/2/19/22	1/1/1/1
2	MAN	b	5	2	-	0/2/19/22	0/1/1/1
3	NAG	c	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	BMA	c	3	3	-	2/2/19/22	0/1/1/1
2	NAG	d	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	d	2	2	-	3/6/23/26	0/1/1/1
2	BMA	d	3	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	d	4	2	-	0/2/19/22	0/1/1/1
2	MAN	d	5	2	-	2/2/19/22	0/1/1/1
6	NAG	e	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	6/6/23/26	0/1/1/1
6	BMA	e	3	6	-	1/2/19/22	0/1/1/1
6	MAN	e	4	6	-	0/2/19/22	0/1/1/1
6	MAN	e	5	6	-	0/2/19/22	0/1/1/1
6	FUC	e	6	6	-	-	0/1/1/1
3	NAG	f	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	0/6/23/26	0/1/1/1
3	BMA	f	3	3	-	0/2/19/22	0/1/1/1
2	NAG	g	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	g	2	2	-	0/6/23/26	0/1/1/1
2	BMA	g	3	2	-	0/2/19/22	0/1/1/1
2	MAN	g	4	2	-	0/2/19/22	0/1/1/1
2	MAN	g	5	2	-	0/2/19/22	0/1/1/1
2	NAG	h	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	h	2	2	-	2/6/23/26	0/1/1/1
2	BMA	h	3	2	-	1/2/19/22	0/1/1/1
2	MAN	h	4	2	-	1/2/19/22	0/1/1/1
2	MAN	h	5	2	-	0/2/19/22	0/1/1/1
6	NAG	i	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	i	2	6	-	2/6/23/26	0/1/1/1
6	BMA	i	3	6	-	0/2/19/22	0/1/1/1
6	MAN	i	4	6	-	1/2/19/22	1/1/1/1
6	MAN	i	5	6	-	1/2/19/22	1/1/1/1
6	FUC	i	6	6	-	-	0/1/1/1
2	NAG	j	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	j	2	2	-	2/6/23/26	0/1/1/1
2	BMA	j	3	2	-	2/2/19/22	0/1/1/1
2	MAN	j	4	2	-	1/2/19/22	1/1/1/1
2	MAN	j	5	2	-	0/2/19/22	1/1/1/1
2	NAG	k	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	k	2	2	-	2/6/23/26	0/1/1/1
2	BMA	k	3	2	-	2/2/19/22	0/1/1/1
2	MAN	k	4	2	-	1/2/19/22	0/1/1/1
2	MAN	k	5	2	-	0/2/19/22	1/1/1/1
3	NAG	l	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	l	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	l	3	3	-	0/2/19/22	0/1/1/1
2	NAG	m	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	m	2	2	-	2/6/23/26	0/1/1/1
2	BMA	m	3	2	-	2/2/19/22	0/1/1/1
2	MAN	m	4	2	-	0/2/19/22	0/1/1/1
2	MAN	m	5	2	-	0/2/19/22	0/1/1/1
2	NAG	n	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	n	2	2	-	4/6/23/26	0/1/1/1
2	BMA	n	3	2	-	2/2/19/22	0/1/1/1
2	MAN	n	4	2	-	2/2/19/22	0/1/1/1
2	MAN	n	5	2	-	0/2/19/22	0/1/1/1
2	NAG	o	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	o	2	2	-	2/6/23/26	0/1/1/1
2	BMA	o	3	2	-	1/2/19/22	0/1/1/1
2	MAN	o	4	2	-	0/2/19/22	0/1/1/1
2	MAN	o	5	2	-	0/2/19/22	0/1/1/1
2	NAG	p	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	p	2	2	-	0/6/23/26	0/1/1/1
2	BMA	p	3	2	-	2/2/19/22	0/1/1/1
2	MAN	p	4	2	-	0/2/19/22	0/1/1/1
2	MAN	p	5	2	-	2/2/19/22	1/1/1/1
3	NAG	q	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	q	2	3	-	0/6/23/26	0/1/1/1
3	BMA	q	3	3	-	0/2/19/22	0/1/1/1
3	NAG	r	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	r	2	3	-	0/6/23/26	0/1/1/1
3	BMA	r	3	3	-	0/2/19/22	0/1/1/1
7	NAG	s	1	7,1	-	2/6/23/26	0/1/1/1
7	FUC	s	2	7	-	-	0/1/1/1
4	NAG	t	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	t	2	4	-	6/6/23/26	0/1/1/1
4	BMA	t	3	4	-	2/2/19/22	0/1/1/1
4	FUC	t	4	4	-	-	0/1/1/1
2	NAG	u	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	u	2	2	-	6/6/23/26	0/1/1/1
2	BMA	u	3	2	-	2/2/19/22	0/1/1/1
2	MAN	u	4	2	-	0/2/19/22	0/1/1/1
2	MAN	u	5	2	-	1/2/19/22	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	5	MAN	C1-C2	4.41	1.62	1.52
2	d	1	NAG	O5-C1	-3.81	1.37	1.43
6	e	6	FUC	C1-C2	3.69	1.61	1.52
2	P	1	NAG	O5-C1	-3.60	1.37	1.43
2	R	1	NAG	O5-C1	-3.45	1.37	1.43
2	W	2	NAG	O5-C1	-3.38	1.38	1.43
2	P	4	MAN	C1-C2	3.17	1.59	1.52
3	l	1	NAG	O5-C1	3.09	1.48	1.43
6	e	6	FUC	O5-C1	2.85	1.48	1.43
3	f	1	NAG	O5-C1	-2.84	1.38	1.43
2	Y	2	NAG	O5-C1	2.76	1.48	1.43
2	H	1	NAG	O5-C1	-2.72	1.39	1.43
3	E	1	NAG	O5-C1	2.69	1.48	1.43
4	t	1	NAG	O5-C1	-2.57	1.39	1.43
2	o	1	NAG	C1-C2	2.53	1.55	1.52
2	P	2	NAG	O5-C1	-2.53	1.39	1.43
3	c	3	BMA	C1-C2	2.45	1.58	1.52
3	Q	1	NAG	O5-C1	-2.43	1.39	1.43
4	t	4	FUC	C1-C2	2.43	1.58	1.52
2	T	1	NAG	O5-C1	-2.39	1.39	1.43
2	N	2	NAG	O5-C1	-2.39	1.39	1.43
2	o	3	BMA	C4-C3	2.37	1.58	1.52
2	d	2	NAG	O5-C1	-2.32	1.39	1.43
2	u	3	BMA	C4-C3	2.31	1.58	1.52
3	K	1	NAG	O5-C1	-2.31	1.39	1.43
2	h	5	MAN	C1-C2	2.30	1.57	1.52
2	a	5	MAN	C1-C2	2.29	1.57	1.52
2	J	5	MAN	C1-C2	2.22	1.57	1.52
2	n	1	NAG	O5-C1	-2.22	1.40	1.43
2	u	1	NAG	O5-C1	-2.21	1.40	1.43
2	P	2	NAG	C1-C2	2.19	1.55	1.52
6	O	1	NAG	O5-C1	-2.19	1.40	1.43
6	O	2	NAG	O5-C1	-2.19	1.40	1.43
3	E	1	NAG	C1-C2	2.18	1.55	1.52
2	g	5	MAN	C1-C2	2.18	1.57	1.52
6	i	4	MAN	C1-C2	2.16	1.57	1.52
2	o	3	BMA	C4-C5	2.16	1.57	1.53
2	F	1	NAG	O5-C1	2.16	1.47	1.43
2	F	3	BMA	O3-C3	2.14	1.48	1.43
2	j	5	MAN	C1-C2	2.11	1.57	1.52
3	l	3	BMA	C4-C5	2.11	1.57	1.53
2	u	3	BMA	O3-C3	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O5-C1	-2.09	1.40	1.43
6	O	5	MAN	O5-C5	2.07	1.47	1.43
2	N	3	BMA	C1-C2	2.07	1.57	1.52
6	e	2	NAG	C1-C2	2.07	1.55	1.52
2	G	5	MAN	O5-C1	2.06	1.47	1.43
2	u	1	NAG	C1-C2	-2.05	1.49	1.52
6	O	3	BMA	O3-C3	2.04	1.48	1.43
2	N	4	MAN	C1-C2	2.03	1.57	1.52
2	F	4	MAN	C1-C2	2.03	1.57	1.52
2	H	4	MAN	O5-C5	2.02	1.47	1.43
2	N	5	MAN	C1-C2	2.02	1.57	1.52

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	l	1	NAG	C1-O5-C5	7.47	122.20	112.19
2	P	4	MAN	C1-O5-C5	6.35	120.69	112.19
6	O	5	MAN	C1-O5-C5	5.87	120.05	112.19
3	E	1	NAG	C1-O5-C5	5.74	119.88	112.19
2	b	2	NAG	C1-O5-C5	5.69	119.81	112.19
2	F	1	NAG	C1-O5-C5	5.52	119.58	112.19
2	Y	2	NAG	C1-O5-C5	5.49	119.54	112.19
3	V	1	NAG	C1-O5-C5	5.17	119.11	112.19
2	m	1	NAG	C1-O5-C5	5.07	118.99	112.19
2	a	2	NAG	C1-O5-C5	5.05	118.95	112.19
2	P	1	NAG	C2-N2-C7	5.02	129.63	122.90
6	O	4	MAN	C1-O5-C5	4.98	118.86	112.19
6	i	2	NAG	C1-O5-C5	4.71	118.50	112.19
2	P	2	NAG	C2-N2-C7	4.63	129.11	122.90
6	i	4	MAN	C1-O5-C5	4.54	118.26	112.19
2	U	1	NAG	C2-N2-C7	4.50	128.94	122.90
2	u	2	NAG	C2-N2-C7	4.48	128.91	122.90
6	e	2	NAG	C2-N2-C7	4.47	128.88	122.90
2	G	5	MAN	C1-O5-C5	4.37	118.04	112.19
4	t	2	NAG	C2-N2-C7	4.29	128.65	122.90
2	P	1	NAG	C1-O5-C5	4.17	117.78	112.19
2	j	4	MAN	C1-O5-C5	4.16	117.76	112.19
2	P	1	NAG	C3-C4-C5	4.13	117.72	110.23
2	R	4	MAN	C1-O5-C5	4.01	117.57	112.19
2	H	4	MAN	C1-O5-C5	3.99	117.54	112.19
2	b	4	MAN	C1-O5-C5	3.96	117.50	112.19
2	N	5	MAN	C1-O5-C5	3.87	117.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	MAN	C1-C2-C3	3.83	115.22	109.64
2	k	5	MAN	C1-O5-C5	3.82	117.31	112.19
6	e	6	FUC	C1-O5-C5	3.79	121.92	112.97
2	j	5	MAN	C1-O5-C5	3.67	117.10	112.19
4	M	1	NAG	C1-O5-C5	3.55	116.95	112.19
2	T	3	BMA	C1-C2-C3	3.50	114.73	109.64
6	i	5	MAN	C1-O5-C5	3.47	116.83	112.19
3	l	2	NAG	C1-O5-C5	3.43	116.78	112.19
2	g	5	MAN	C1-O5-C5	3.43	116.78	112.19
2	h	5	MAN	C1-O5-C5	3.37	116.70	112.19
4	Z	4	FUC	C1-O5-C5	3.36	120.89	112.97
6	O	3	BMA	C1-O5-C5	3.33	116.65	112.19
2	X	5	MAN	C1-O5-C5	3.32	116.64	112.19
2	G	3	BMA	C1-O5-C5	3.30	116.61	112.19
2	W	2	NAG	C4-C3-C2	3.21	115.73	111.02
2	p	5	MAN	C1-O5-C5	3.18	116.44	112.19
2	g	4	MAN	C1-O5-C5	3.15	116.41	112.19
2	P	4	MAN	C1-C2-C3	3.11	114.17	109.64
2	p	4	MAN	C1-O5-C5	3.11	116.35	112.19
6	e	6	FUC	C1-C2-C3	2.99	113.99	109.64
6	O	3	BMA	O3-C3-C2	2.97	116.12	110.05
4	Z	4	FUC	O5-C5-C4	2.96	114.88	109.55
6	S	5	MAN	C1-O5-C5	2.95	116.14	112.19
2	m	4	MAN	C1-O5-C5	2.95	116.13	112.19
2	p	1	NAG	C1-O5-C5	2.94	116.12	112.19
2	N	4	MAN	C1-O5-C5	2.92	116.10	112.19
2	u	5	MAN	C1-O5-C5	2.90	116.08	112.19
6	e	5	MAN	C1-O5-C5	2.90	116.07	112.19
2	F	5	MAN	C1-O5-C5	2.89	116.06	112.19
2	G	3	BMA	C3-C4-C5	-2.88	105.01	110.23
2	T	5	MAN	C1-O5-C5	2.87	116.03	112.19
4	t	4	FUC	O2-C2-C1	2.77	115.56	109.22
2	X	4	MAN	C1-O5-C5	2.77	115.89	112.19
3	E	2	NAG	C1-O5-C5	2.75	115.88	112.19
2	u	2	NAG	C1-O5-C5	2.75	115.88	112.19
2	F	4	MAN	C1-O5-C5	2.74	115.86	112.19
2	p	2	NAG	C3-C4-C5	2.74	115.19	110.23
2	J	5	MAN	C1-O5-C5	2.73	115.84	112.19
2	a	5	MAN	C1-O5-C5	2.72	115.83	112.19
2	U	4	MAN	C1-O5-C5	2.70	115.81	112.19
2	P	4	MAN	O5-C1-C2	2.69	117.21	110.79
2	T	4	MAN	C1-O5-C5	2.69	115.79	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C1-O5-C5	2.66	115.75	112.19
2	Y	5	MAN	C1-O5-C5	2.65	115.73	112.19
2	D	4	MAN	C1-O5-C5	2.62	115.70	112.19
2	b	5	MAN	C1-O5-C5	2.58	115.65	112.19
2	d	3	BMA	C1-O5-C5	2.57	115.63	112.19
2	Y	4	MAN	C1-O5-C5	2.55	115.61	112.19
6	O	1	NAG	C3-C4-C5	2.54	114.83	110.23
2	P	1	NAG	C1-C2-N2	2.53	114.42	110.43
2	n	4	MAN	O2-C2-C3	-2.49	104.99	110.15
2	u	5	MAN	O2-C2-C3	-2.49	105.00	110.15
2	p	4	MAN	O2-C2-C3	-2.47	105.04	110.15
2	b	1	NAG	C1-O5-C5	2.47	115.50	112.19
2	d	1	NAG	C3-C4-C5	2.47	114.70	110.23
2	W	4	MAN	C1-O5-C5	2.47	115.49	112.19
2	D	4	MAN	O2-C2-C3	-2.46	105.06	110.15
2	R	4	MAN	O2-C2-C3	-2.45	105.08	110.15
2	D	5	MAN	O2-C2-C3	-2.45	105.08	110.15
2	k	4	MAN	C1-O5-C5	2.44	115.46	112.19
6	S	4	MAN	O2-C2-C3	-2.44	105.09	110.15
2	H	5	MAN	C1-O5-C5	2.43	115.44	112.19
2	T	4	MAN	O2-C2-C3	-2.42	105.14	110.15
2	a	5	MAN	O2-C2-C3	-2.41	105.15	110.15
2	W	5	MAN	C1-O5-C5	2.41	115.41	112.19
5	L	4	MAN	C1-O5-C5	2.40	115.40	112.19
2	F	3	BMA	C3-C4-C5	2.39	114.57	110.23
6	O	3	BMA	C1-C2-C3	-2.39	106.16	109.64
6	O	4	MAN	O2-C2-C3	-2.39	105.20	110.15
6	e	4	MAN	C1-O5-C5	2.39	115.39	112.19
4	Z	1	NAG	C1-O5-C5	2.39	115.39	112.19
2	J	5	MAN	O2-C2-C3	-2.38	105.21	110.15
6	e	4	MAN	O2-C2-C3	-2.37	105.23	110.15
2	U	4	MAN	O2-C2-C3	-2.37	105.23	110.15
2	F	4	MAN	O2-C2-C3	-2.37	105.24	110.15
2	g	4	MAN	O2-C2-C3	-2.37	105.25	110.15
5	L	4	MAN	O2-C2-C3	-2.37	105.25	110.15
6	O	2	NAG	C3-C4-C5	2.36	114.50	110.23
3	f	1	NAG	C1-O5-C5	2.35	115.34	112.19
6	i	6	FUC	C1-O5-C5	2.35	118.50	112.97
2	h	5	MAN	O2-C2-C3	-2.35	105.29	110.15
2	G	4	MAN	C1-O5-C5	2.34	115.32	112.19
2	R	2	NAG	O4-C4-C5	-2.34	103.57	109.32
2	T	5	MAN	O2-C2-C3	-2.34	105.31	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	4	MAN	O2-C2-C3	-2.33	105.32	110.15
2	a	4	MAN	O2-C2-C3	-2.33	105.32	110.15
2	d	5	MAN	C1-O5-C5	2.32	115.30	112.19
2	h	4	MAN	O2-C2-C3	-2.32	105.35	110.15
6	i	5	MAN	O2-C2-C3	-2.31	105.38	110.15
2	P	2	NAG	C1-C2-N2	2.30	114.06	110.43
2	o	4	MAN	O2-C2-C3	-2.30	105.39	110.15
6	O	5	MAN	O2-C2-C3	-2.30	105.39	110.15
2	o	5	MAN	C1-O5-C5	2.29	115.26	112.19
2	Y	4	MAN	O2-C2-C3	-2.29	105.41	110.15
2	R	5	MAN	O2-C2-C3	-2.29	105.41	110.15
2	H	4	MAN	O2-C2-C3	-2.28	105.43	110.15
2	W	5	MAN	O2-C2-C3	-2.28	105.43	110.15
2	b	5	MAN	O2-C2-C3	-2.28	105.43	110.15
2	D	3	BMA	O2-C2-C3	-2.27	105.45	110.15
2	m	4	MAN	O2-C2-C3	-2.26	105.47	110.15
2	o	3	BMA	C2-C3-C4	2.26	114.83	110.86
2	D	5	MAN	C1-O5-C5	2.25	115.21	112.19
6	e	5	MAN	O2-C2-C3	-2.25	105.49	110.15
2	N	3	BMA	C1-C2-C3	-2.25	106.37	109.64
2	X	5	MAN	O2-C2-C3	-2.24	105.51	110.15
2	g	5	MAN	O2-C2-C3	-2.24	105.51	110.15
2	b	4	MAN	O2-C2-C3	-2.23	105.52	110.15
2	H	5	MAN	O2-C2-C3	-2.23	105.53	110.15
2	X	4	MAN	O2-C2-C3	-2.23	105.53	110.15
2	p	5	MAN	O2-C2-C3	-2.23	105.54	110.15
2	o	5	MAN	O2-C2-C3	-2.22	105.54	110.15
2	d	4	MAN	O2-C2-C3	-2.22	105.55	110.15
6	i	4	MAN	O2-C2-C3	-2.22	105.55	110.15
6	S	5	MAN	O2-C2-C3	-2.21	105.57	110.15
2	n	5	MAN	C1-O5-C5	2.21	115.15	112.19
2	J	4	MAN	O2-C2-C3	-2.21	105.58	110.15
6	i	6	FUC	O5-C5-C4	2.20	113.52	109.55
2	n	5	MAN	O2-C2-C3	-2.20	105.59	110.15
2	R	3	BMA	C1-O5-C5	2.19	115.12	112.19
2	U	1	NAG	C1-C2-N2	2.19	113.88	110.43
2	o	3	BMA	C3-C4-C5	2.18	114.18	110.23
2	G	5	MAN	O2-C2-C3	-2.18	105.64	110.15
2	P	4	MAN	C3-C4-C5	-2.18	106.29	110.23
2	u	4	MAN	O2-C2-C3	-2.18	105.64	110.15
2	U	5	MAN	O2-C2-C3	-2.17	105.65	110.15
2	F	5	MAN	O2-C2-C3	-2.17	105.65	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	l	3	BMA	C3-C4-C5	2.15	114.13	110.23
3	Q	3	BMA	C1-O5-C5	2.14	115.06	112.19
2	j	5	MAN	O2-C2-C3	-2.14	105.71	110.15
2	k	5	MAN	O2-C2-C3	-2.14	105.72	110.15
2	Y	3	BMA	C1-O5-C5	2.14	115.05	112.19
2	H	3	BMA	C1-O5-C5	2.14	115.05	112.19
4	t	3	BMA	O2-C2-C3	-2.14	105.73	110.15
2	Y	5	MAN	O2-C2-C3	-2.13	105.74	110.15
2	W	4	MAN	O2-C2-C3	-2.13	105.75	110.15
2	G	2	NAG	C3-C4-C5	2.13	114.08	110.23
2	k	4	MAN	O2-C2-C3	-2.12	105.76	110.15
6	O	5	MAN	C3-C4-C5	2.11	114.06	110.23
2	n	4	MAN	C1-O5-C5	2.11	115.01	112.19
2	m	5	MAN	O2-C2-C3	-2.10	105.79	110.15
4	I	1	NAG	C1-O5-C5	2.10	115.00	112.19
2	T	3	BMA	O2-C2-C3	-2.08	105.83	110.15
2	j	4	MAN	O2-C2-C3	-2.08	105.83	110.15
4	t	2	NAG	C1-C2-N2	2.08	113.71	110.43
6	e	6	FUC	O5-C5-C4	2.08	113.29	109.55
6	O	6	FUC	O5-C5-C4	2.07	113.29	109.55
4	M	4	FUC	C1-O5-C5	2.07	117.85	112.97
2	a	2	NAG	C3-C4-C5	2.07	113.98	110.23
2	a	4	MAN	C1-O5-C5	2.06	114.95	112.19
2	u	5	MAN	C1-C2-C3	2.06	112.64	109.64
2	u	2	NAG	C1-C2-N2	2.04	113.65	110.43
2	G	3	BMA	O3-C3-C2	2.03	114.19	110.05
2	G	4	MAN	O2-C2-C3	-2.02	105.97	110.15
7	s	2	FUC	O5-C5-C4	2.02	113.18	109.55
6	e	2	NAG	C1-C2-N2	2.01	113.61	110.43
4	t	3	BMA	C1-O5-C5	2.01	114.88	112.19
2	N	3	BMA	O3-C3-C2	2.01	114.15	110.05
2	D	3	BMA	C1-C2-C3	2.01	112.57	109.64
2	P	5	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (263) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	2	NAG	C4-C5-C6-O6
2	k	3	BMA	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
2	o	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	X	3	BMA	O5-C5-C6-O6
2	d	5	MAN	O5-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6
2	W	3	BMA	C4-C5-C6-O6
4	t	2	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6
7	s	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	P	3	BMA	O5-C5-C6-O6
2	U	3	BMA	O5-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	d	3	BMA	O5-C5-C6-O6
2	n	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
6	i	2	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	h	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
7	s	1	NAG	C4-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	p	3	BMA	O5-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	P	3	BMA	C4-C5-C6-O6
2	X	3	BMA	C4-C5-C6-O6
2	n	3	BMA	C4-C5-C6-O6
2	o	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	r	1	NAG	C4-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
6	i	1	NAG	O5-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6
6	S	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	R	2	NAG	O5-C5-C6-O6
2	m	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
2	d	5	MAN	C4-C5-C6-O6
2	k	3	BMA	C4-C5-C6-O6
2	p	3	BMA	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
2	j	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	H	3	BMA	C4-C5-C6-O6
2	j	3	BMA	C4-C5-C6-O6
2	p	5	MAN	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	T	4	MAN	O5-C5-C6-O6
2	W	3	BMA	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
4	t	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	j	3	BMA	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
2	d	3	BMA	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
6	i	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	U	3	BMA	C4-C5-C6-O6
2	n	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
2	p	5	MAN	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
3	r	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	S	2	NAG	O5-C5-C6-O6
2	R	3	BMA	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
2	P	2	NAG	C8-C7-N2-C2
2	P	2	NAG	O7-C7-N2-C2
2	U	1	NAG	C8-C7-N2-C2
2	U	1	NAG	O7-C7-N2-C2
2	W	1	NAG	C8-C7-N2-C2
2	W	1	NAG	O7-C7-N2-C2
2	Y	1	NAG	C8-C7-N2-C2
2	Y	1	NAG	O7-C7-N2-C2
2	Y	2	NAG	C8-C7-N2-C2
2	Y	2	NAG	O7-C7-N2-C2
2	a	1	NAG	C8-C7-N2-C2
2	a	1	NAG	O7-C7-N2-C2
2	b	2	NAG	C8-C7-N2-C2
2	b	2	NAG	O7-C7-N2-C2
2	d	1	NAG	C8-C7-N2-C2
2	d	1	NAG	O7-C7-N2-C2
2	d	2	NAG	C8-C7-N2-C2
2	d	2	NAG	O7-C7-N2-C2
2	n	2	NAG	C8-C7-N2-C2
2	n	2	NAG	O7-C7-N2-C2
2	p	1	NAG	C8-C7-N2-C2
2	p	1	NAG	O7-C7-N2-C2
2	u	1	NAG	C8-C7-N2-C2
2	u	1	NAG	O7-C7-N2-C2
2	u	2	NAG	C8-C7-N2-C2
2	u	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	l	1	NAG	C8-C7-N2-C2
3	l	1	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	Z	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	t	2	NAG	C8-C7-N2-C2
4	t	2	NAG	O7-C7-N2-C2
6	e	2	NAG	C8-C7-N2-C2
6	e	2	NAG	O7-C7-N2-C2
5	L	2	NAG	O5-C5-C6-O6
2	h	2	NAG	O5-C5-C6-O6
2	n	2	NAG	O5-C5-C6-O6
2	u	3	BMA	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	R	3	BMA	C4-C5-C6-O6
2	a	1	NAG	C4-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
2	n	3	BMA	O5-C5-C6-O6
2	a	3	BMA	C4-C5-C6-O6
2	n	2	NAG	C4-C5-C6-O6
2	u	3	BMA	C4-C5-C6-O6
2	u	2	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	T	4	MAN	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
3	f	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	a	3	BMA	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	f	1	NAG	C4-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
2	m	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	F	3	BMA	O5-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
2	j	2	NAG	O5-C5-C6-O6
6	i	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	j	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
6	O	4	MAN	C4-C5-C6-O6
4	t	3	BMA	C4-C5-C6-O6
6	e	2	NAG	C4-C5-C6-O6
4	t	1	NAG	O5-C5-C6-O6
6	O	4	MAN	O5-C5-C6-O6
6	i	4	MAN	O5-C5-C6-O6
2	k	4	MAN	O5-C5-C6-O6
4	t	3	BMA	O5-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
2	n	4	MAN	O5-C5-C6-O6
2	u	5	MAN	O5-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
3	c	3	BMA	C4-C5-C6-O6
6	i	5	MAN	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
6	O	3	BMA	O5-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	g	1	NAG	C4-C5-C6-O6
2	h	3	BMA	O5-C5-C6-O6
2	o	3	BMA	O5-C5-C6-O6
2	j	4	MAN	O5-C5-C6-O6
2	X	1	NAG	C3-C2-N2-C7
2	b	1	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	n	4	MAN	C4-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	c	3	BMA	O5-C5-C6-O6
2	F	4	MAN	O5-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	T	1	NAG	C1-C2-N2-C7
2	U	1	NAG	C1-C2-N2-C7
2	X	2	NAG	C1-C2-N2-C7
2	h	1	NAG	C1-C2-N2-C7
2	D	1	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
6	O	5	MAN	O5-C5-C6-O6
2	F	4	MAN	C4-C5-C6-O6
2	u	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C3-C2-N2-C7
2	P	1	NAG	C3-C2-N2-C7
2	T	1	NAG	C3-C2-N2-C7
2	U	1	NAG	C3-C2-N2-C7
2	X	2	NAG	C3-C2-N2-C7
2	b	1	NAG	C3-C2-N2-C7
2	n	1	NAG	C3-C2-N2-C7
4	M	1	NAG	C3-C2-N2-C7
5	L	2	NAG	C3-C2-N2-C7
2	g	1	NAG	O5-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
2	m	3	BMA	C4-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	b	4	MAN	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	m	3	BMA	O5-C5-C6-O6
2	H	1	NAG	C1-C2-N2-C7
2	P	2	NAG	C1-C2-N2-C7
2	b	1	NAG	C1-C2-N2-C7
2	n	1	NAG	C1-C2-N2-C7
2	u	2	NAG	C1-C2-N2-C7
4	M	1	NAG	C1-C2-N2-C7
4	t	2	NAG	C1-C2-N2-C7
6	e	2	NAG	C1-C2-N2-C7
2	P	2	NAG	C3-C2-N2-C7
2	R	1	NAG	C3-C2-N2-C7
2	h	1	NAG	C3-C2-N2-C7
2	u	2	NAG	C3-C2-N2-C7
4	t	2	NAG	C3-C2-N2-C7
5	L	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	e	2	NAG	C3-C2-N2-C7
6	e	3	BMA	C4-C5-C6-O6
2	h	4	MAN	C4-C5-C6-O6
2	j	2	NAG	C4-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
3	q	1	NAG	C4-C5-C6-O6

All (18) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	j	5	MAN	C1-C2-C3-C4-C5-O5
6	i	4	MAN	C1-C2-C3-C4-C5-O5
2	P	5	MAN	C1-C2-C3-C4-C5-O5
6	O	4	MAN	C1-C2-C3-C4-C5-O5
2	H	5	MAN	C1-C2-C3-C4-C5-O5
2	T	4	MAN	C1-C2-C3-C4-C5-O5
2	F	5	MAN	C1-C2-C3-C4-C5-O5
2	H	4	MAN	C1-C2-C3-C4-C5-O5
6	S	5	MAN	C1-C2-C3-C4-C5-O5
2	N	5	MAN	C1-C2-C3-C4-C5-O5
6	i	5	MAN	C1-C2-C3-C4-C5-O5
2	p	5	MAN	C1-C2-C3-C4-C5-O5
2	X	5	MAN	C1-C2-C3-C4-C5-O5
2	j	4	MAN	C1-C2-C3-C4-C5-O5
2	D	4	MAN	C1-C2-C3-C4-C5-O5
2	k	5	MAN	C1-C2-C3-C4-C5-O5
2	b	4	MAN	C1-C2-C3-C4-C5-O5
2	N	4	MAN	C1-C2-C3-C4-C5-O5

88 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	2	NAG	2	0
4	M	4	FUC	1	0
2	u	4	MAN	2	0
6	i	1	NAG	1	0
4	I	2	NAG	3	0
2	k	2	NAG	1	0
2	P	2	NAG	2	0
2	a	2	NAG	1	0
2	F	2	NAG	1	0

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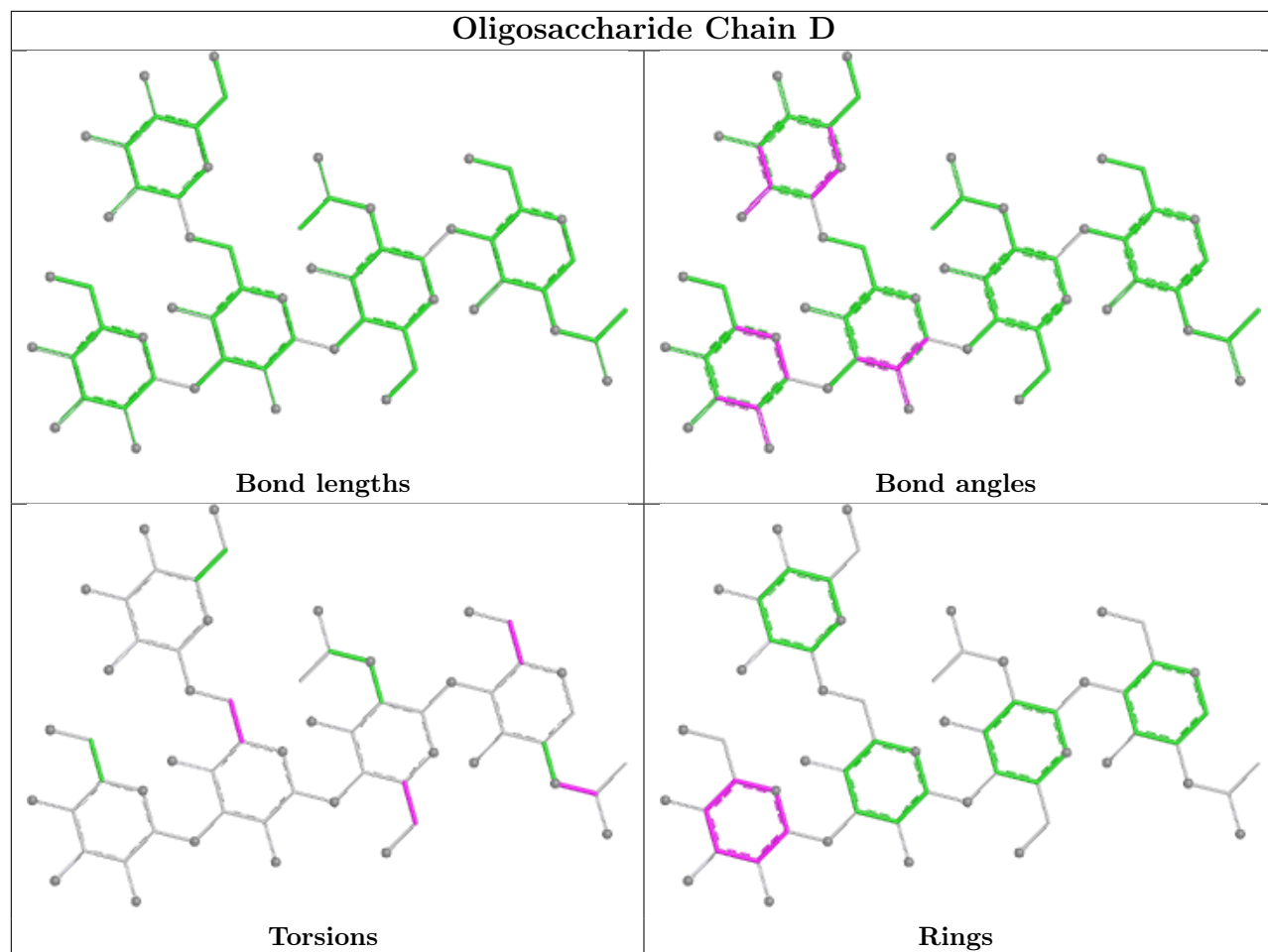
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	NAG	1	0
2	d	1	NAG	4	0
2	k	5	MAN	1	0
2	G	3	BMA	3	0
3	f	1	NAG	3	0
2	H	1	NAG	1	0
2	J	1	NAG	1	0
2	U	1	NAG	3	0
5	L	1	NAG	3	0
3	f	2	NAG	2	0
2	N	1	NAG	1	0
6	S	3	BMA	1	0
2	u	5	MAN	1	0
2	N	5	MAN	1	0
2	W	2	NAG	1	0
2	u	2	NAG	1	0
3	V	1	NAG	3	0
2	N	2	NAG	1	0
2	j	2	NAG	1	0
2	X	1	NAG	2	0
2	g	1	NAG	1	0
2	m	2	NAG	1	0
2	T	1	NAG	2	0
2	o	1	NAG	4	0
2	X	5	MAN	1	0
2	m	4	MAN	1	0
2	R	2	NAG	1	0
2	D	1	NAG	2	0
3	l	1	NAG	1	0
2	h	1	NAG	1	0
7	s	1	NAG	3	0
4	t	3	BMA	1	0
6	i	3	BMA	1	0
2	j	1	NAG	1	0
6	O	1	NAG	3	0
4	t	2	NAG	1	0
2	D	4	MAN	1	0
2	U	2	NAG	1	0
3	Q	1	NAG	2	0
2	G	2	NAG	2	0
2	R	1	NAG	3	0
2	j	5	MAN	1	0

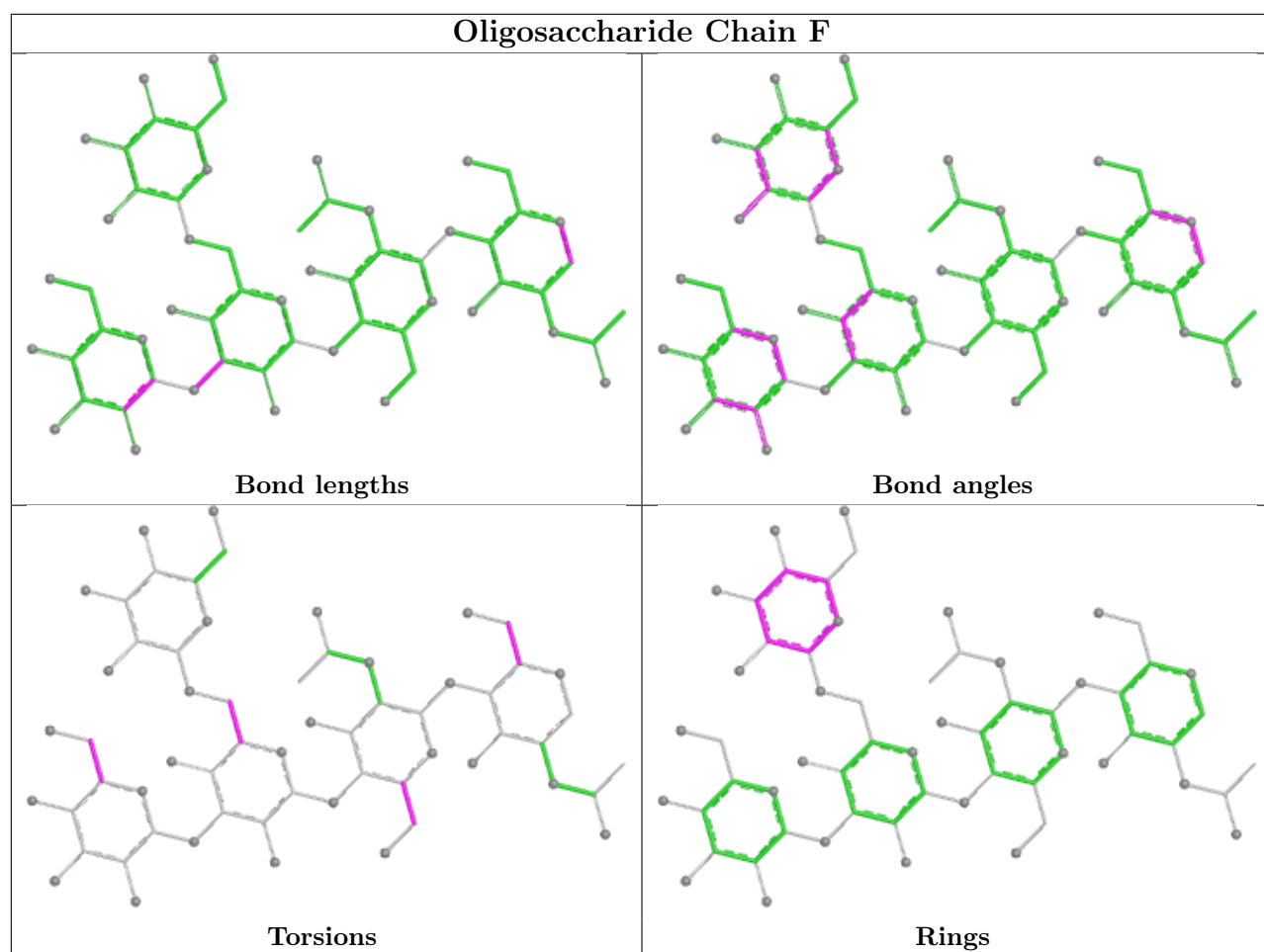
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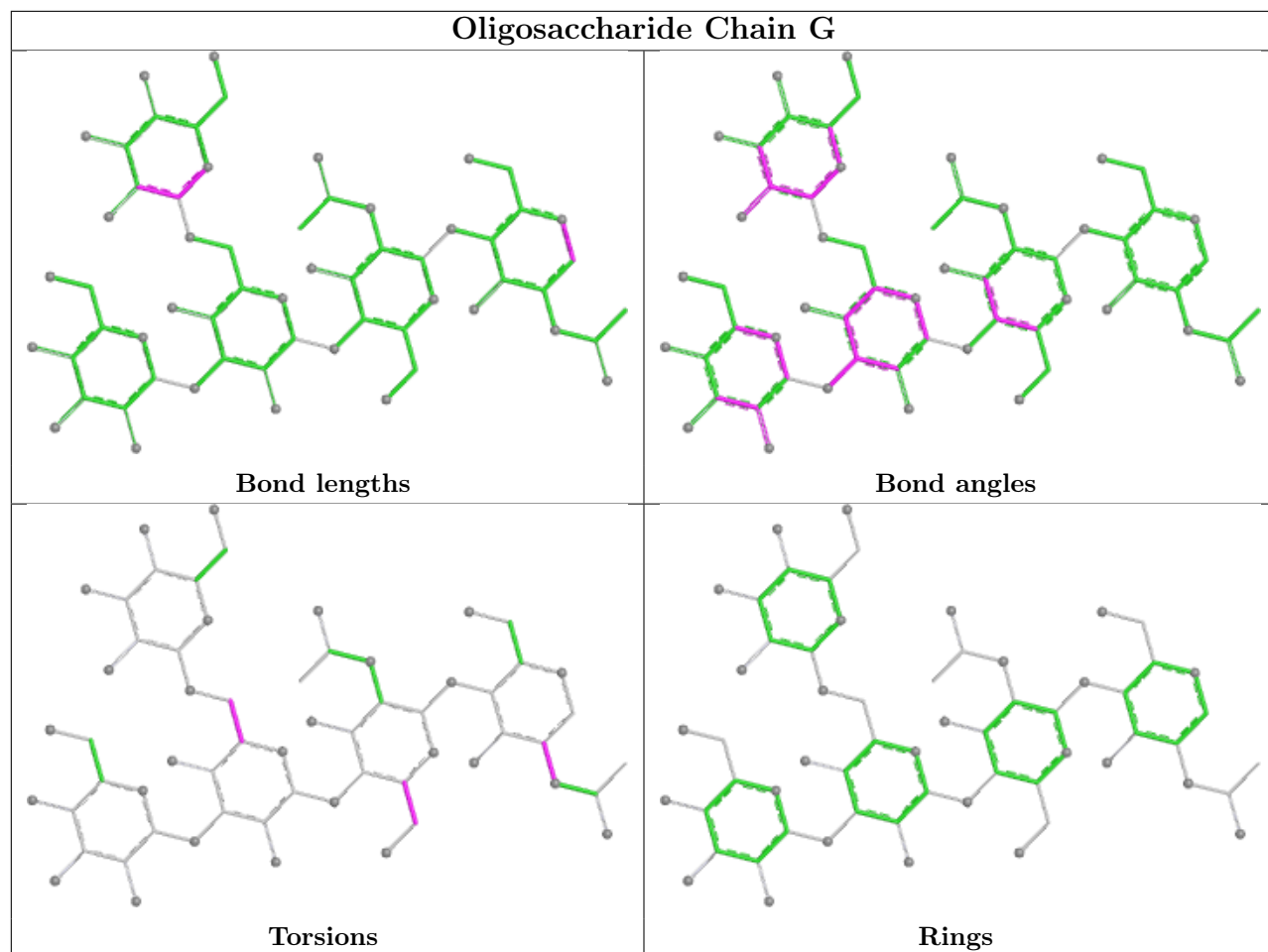
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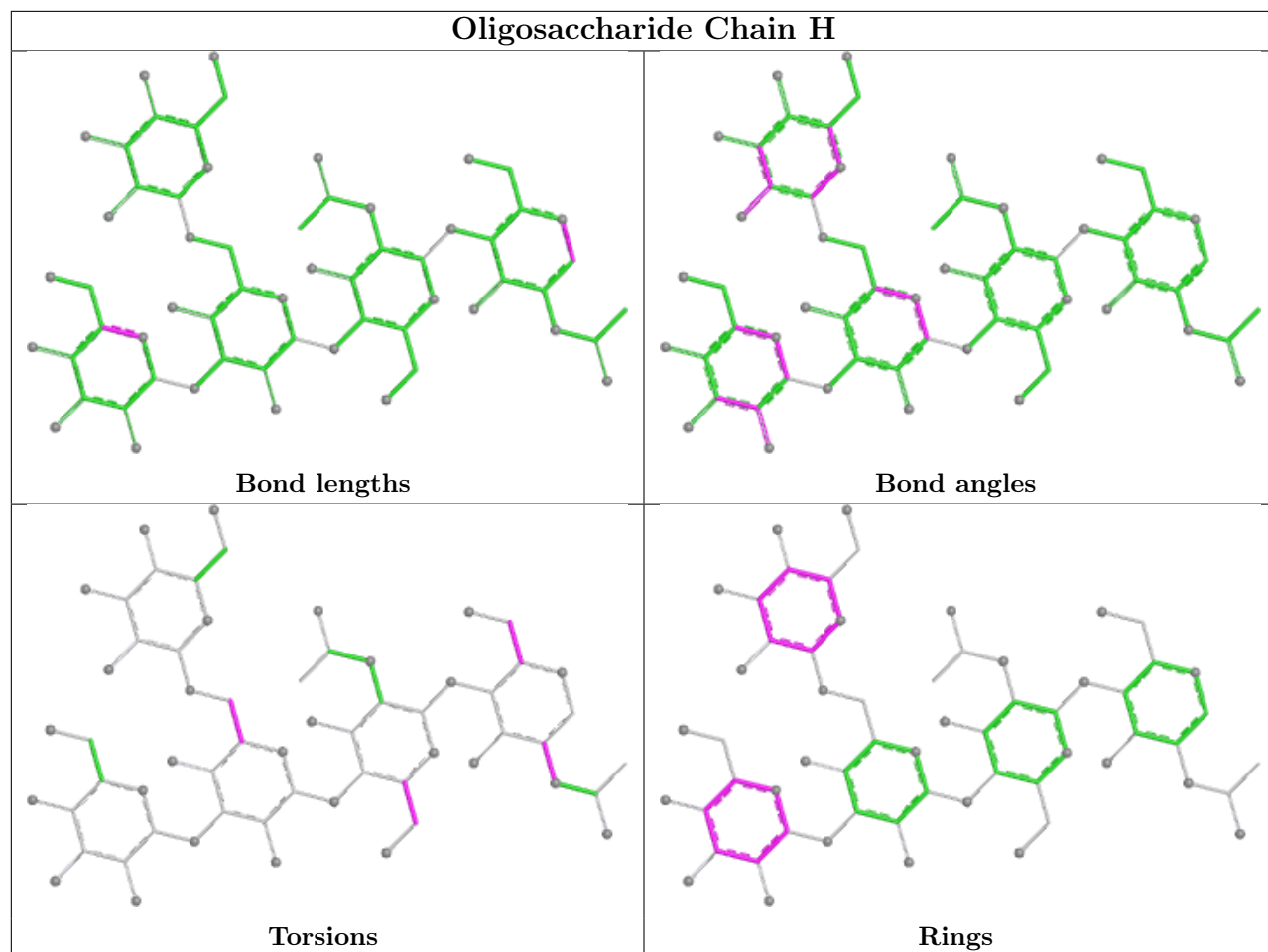
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	2	NAG	2	0
2	b	1	NAG	1	0
2	Y	1	NAG	1	0
6	S	4	MAN	1	0
4	I	1	NAG	3	0
2	h	3	BMA	1	0
2	o	3	BMA	1	0
2	X	2	NAG	1	0
5	L	2	NAG	5	0
2	F	5	MAN	1	0
2	u	1	NAG	4	0
2	F	4	MAN	1	0
2	T	2	NAG	1	0
4	t	1	NAG	2	0
2	G	1	NAG	4	0
2	P	1	NAG	2	0
2	F	1	NAG	2	0
3	c	2	NAG	1	0
7	s	2	FUC	2	0
6	i	6	FUC	1	0
2	a	3	BMA	1	0
3	E	1	NAG	2	0
6	i	2	NAG	1	0
6	O	6	FUC	2	0
3	r	1	NAG	1	0
2	W	1	NAG	2	0
2	o	2	NAG	1	0
2	k	1	NAG	2	0
3	q	1	NAG	1	0
2	D	5	MAN	1	0
2	P	3	BMA	1	0
6	e	6	FUC	1	0
2	X	3	BMA	2	0
2	D	2	NAG	1	0
2	G	5	MAN	2	0
6	e	2	NAG	2	0
2	d	2	NAG	1	0

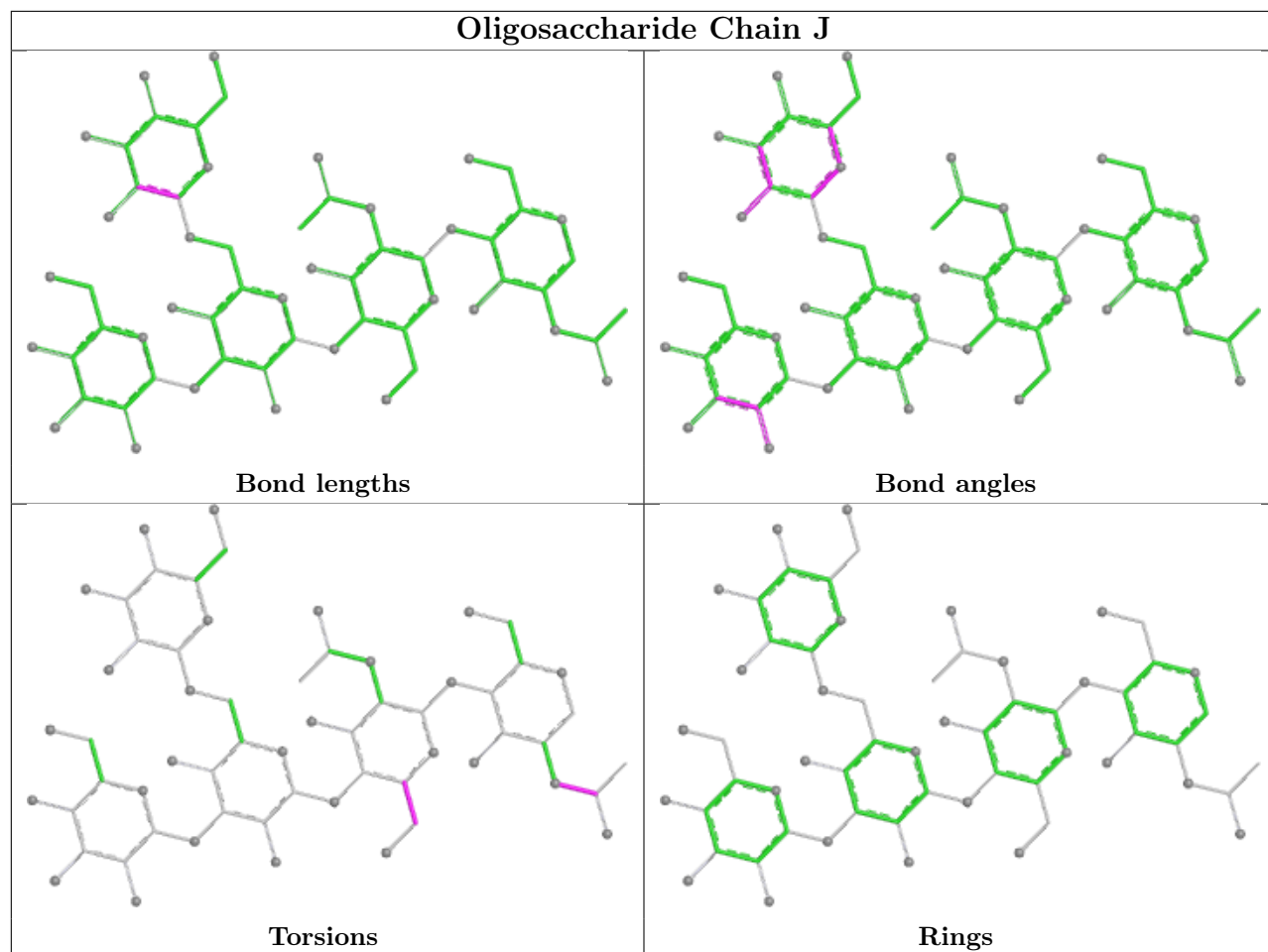
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

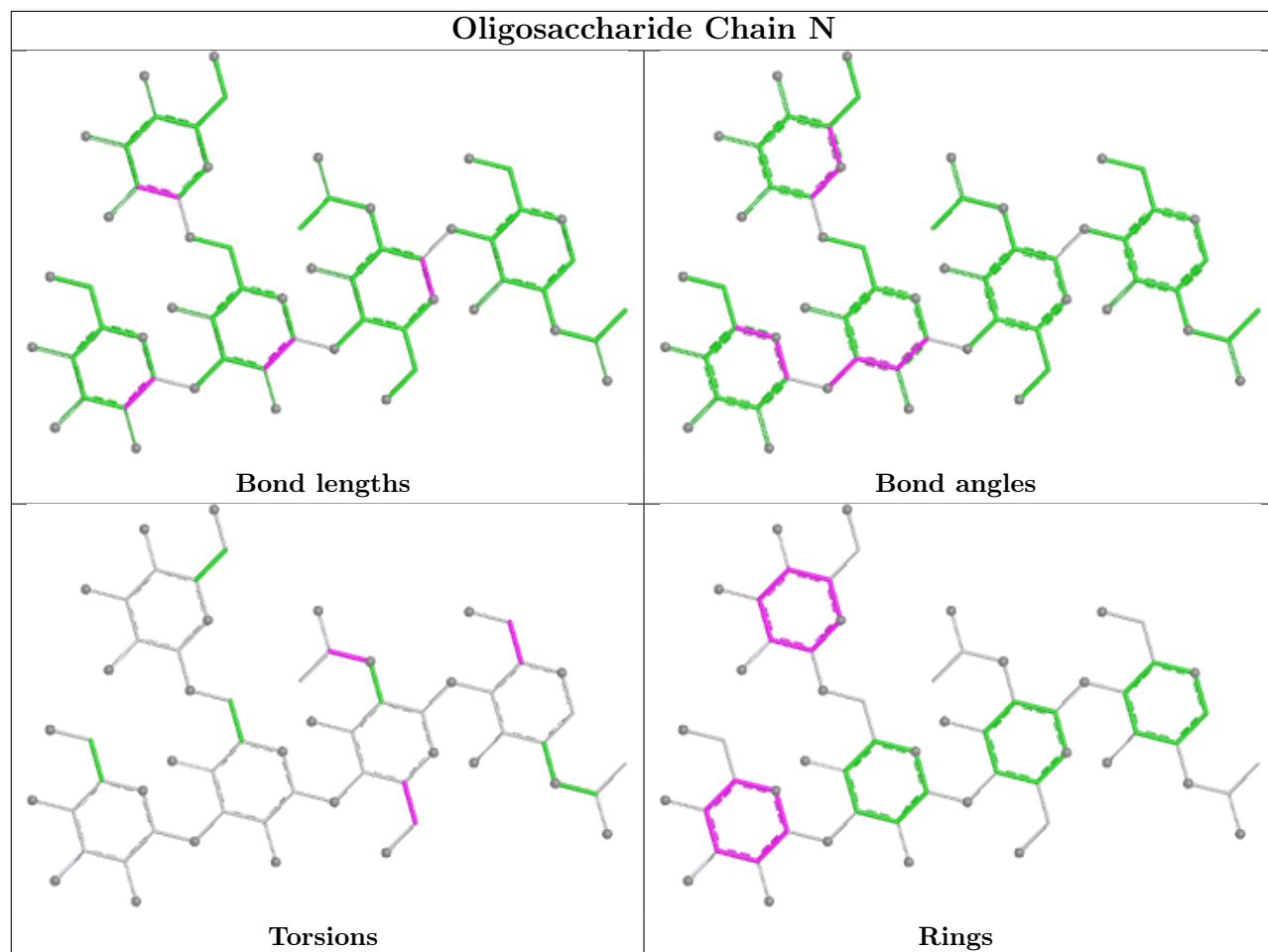


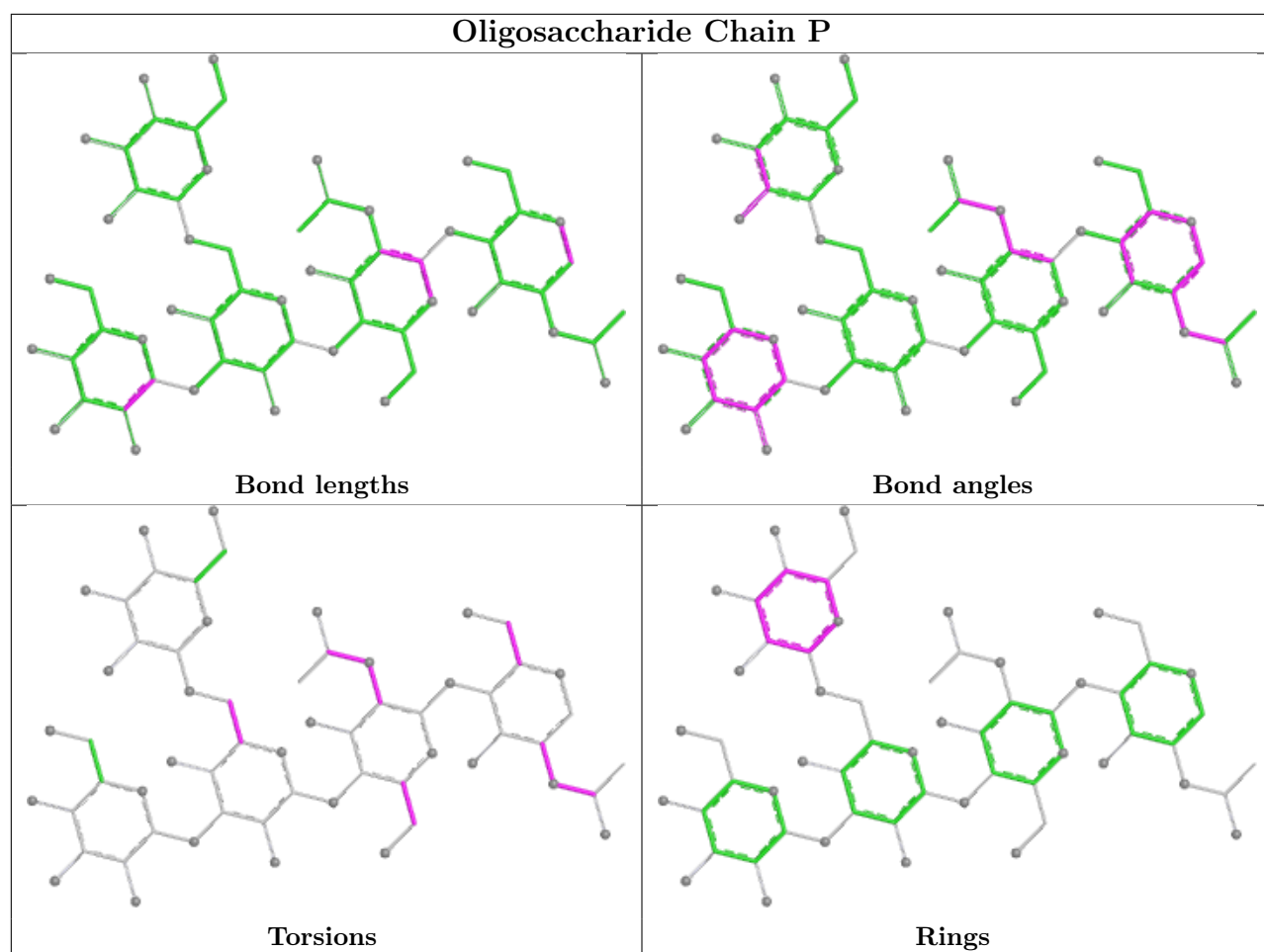


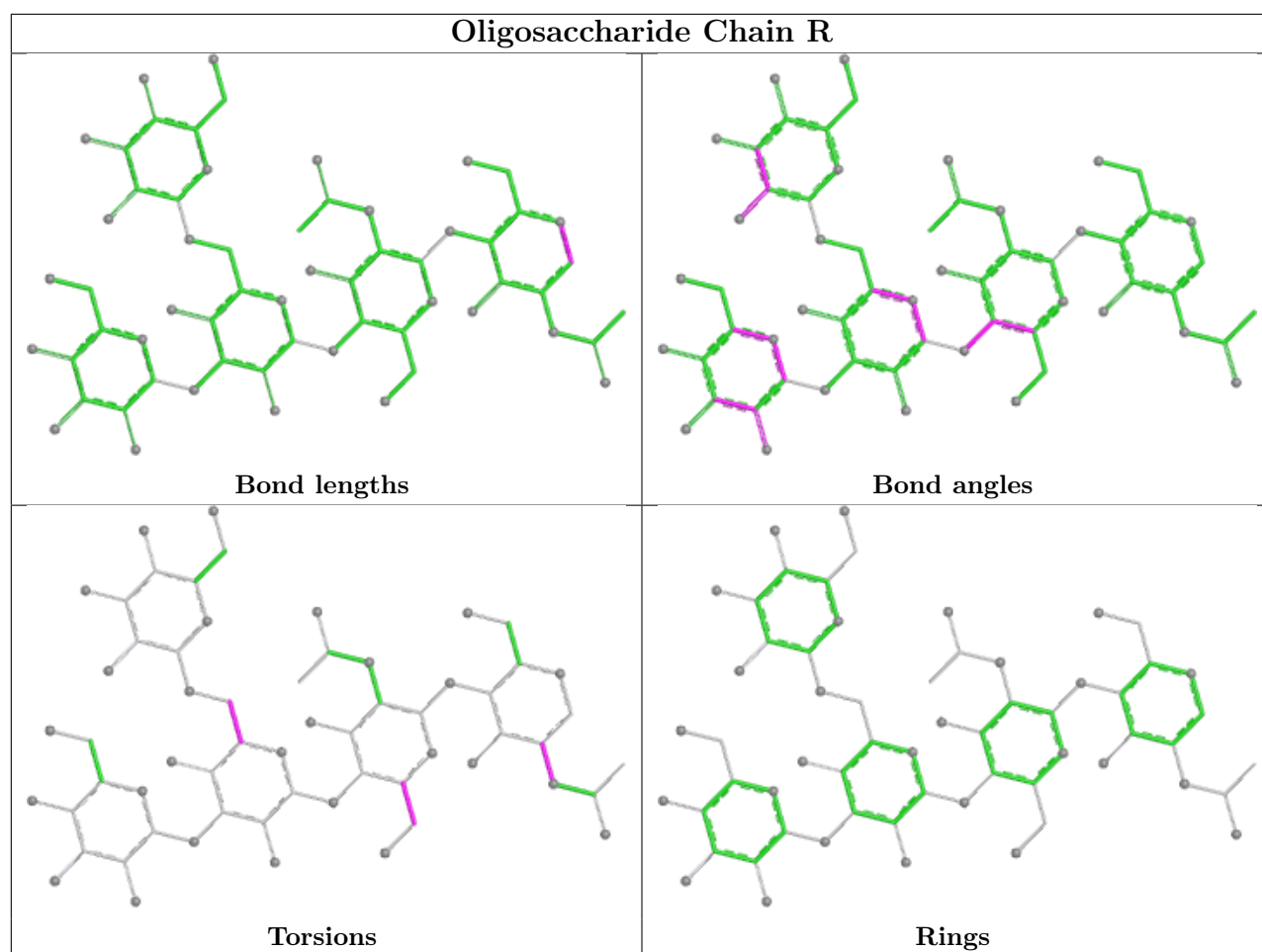


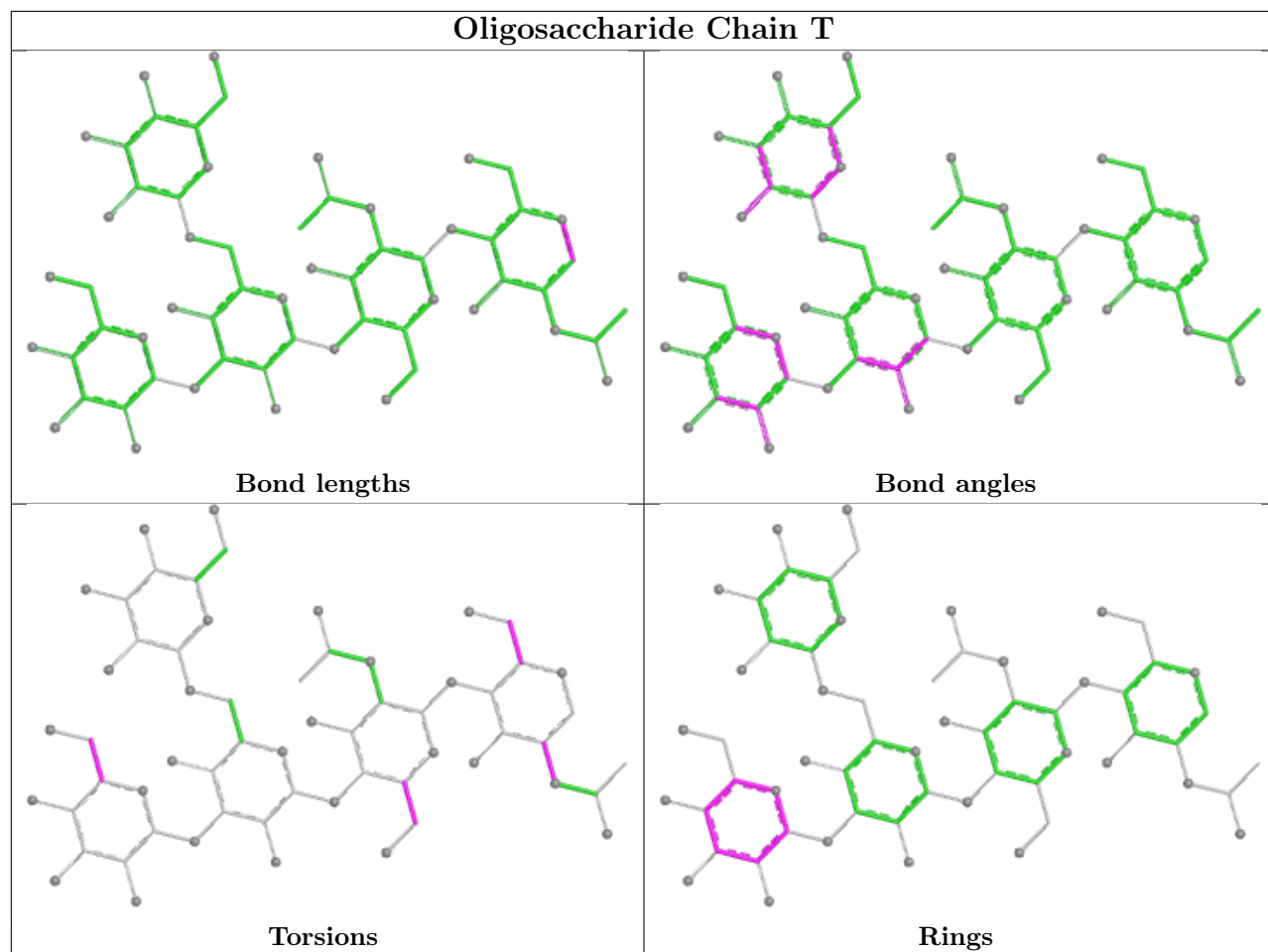


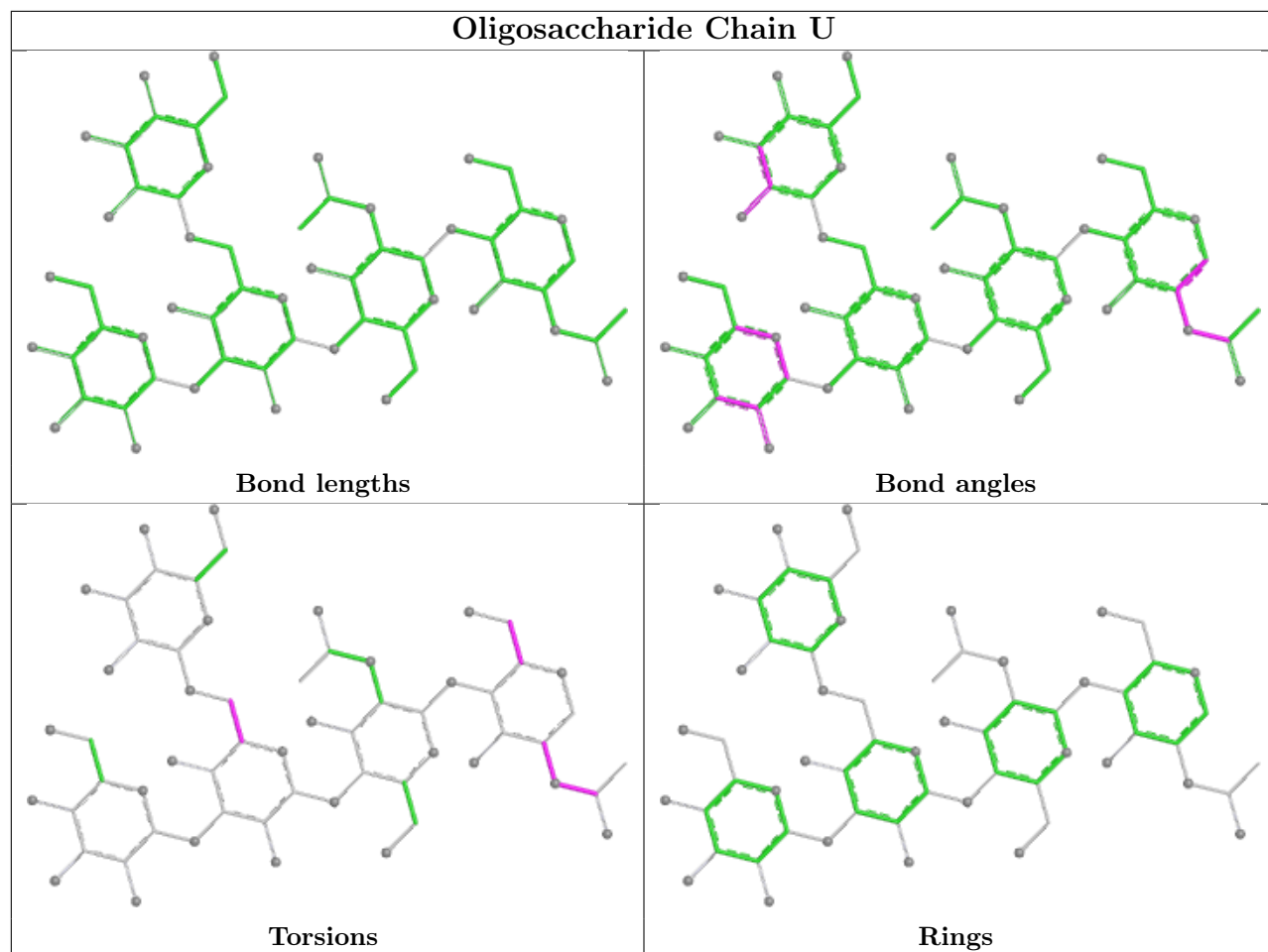


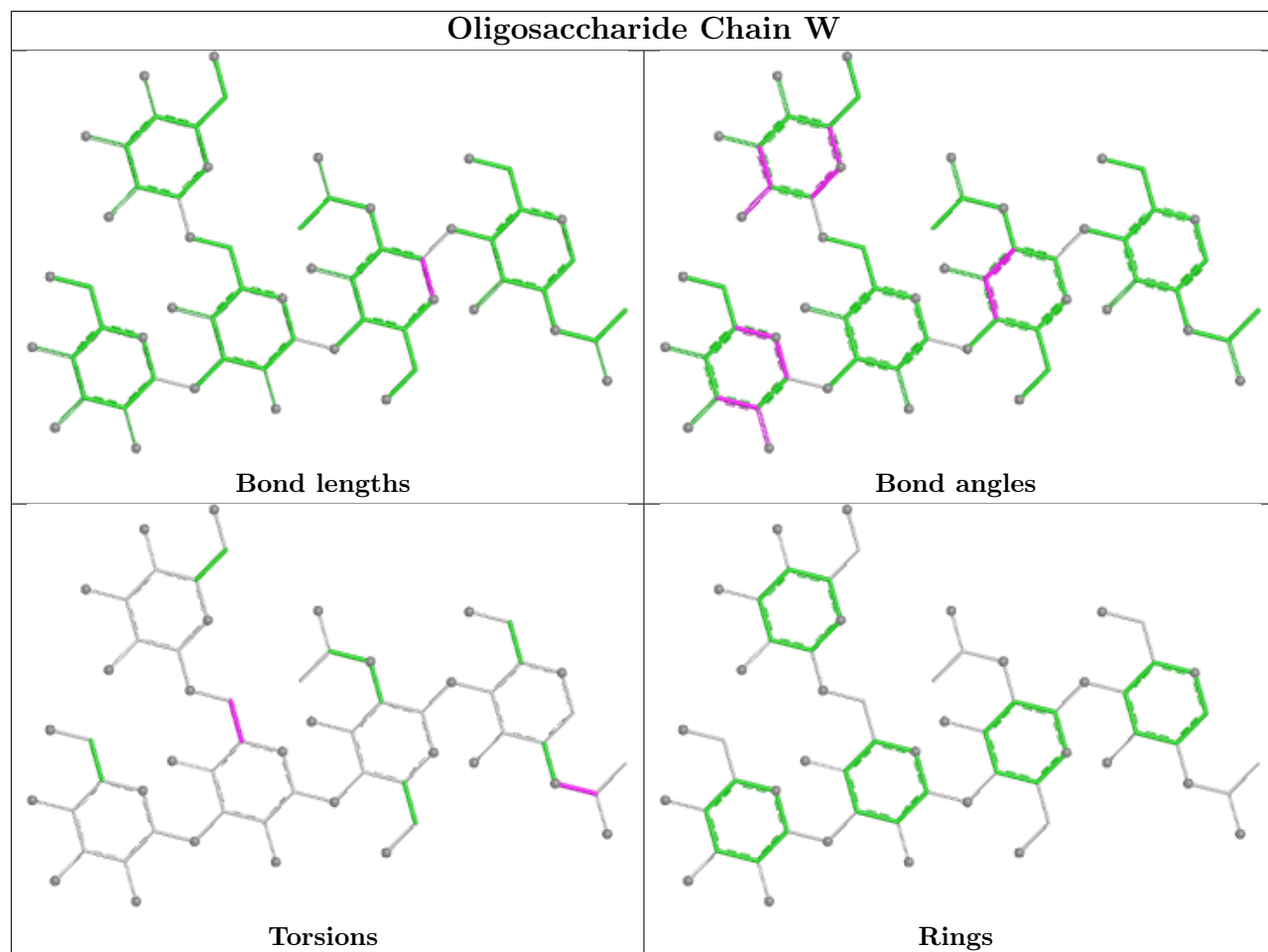


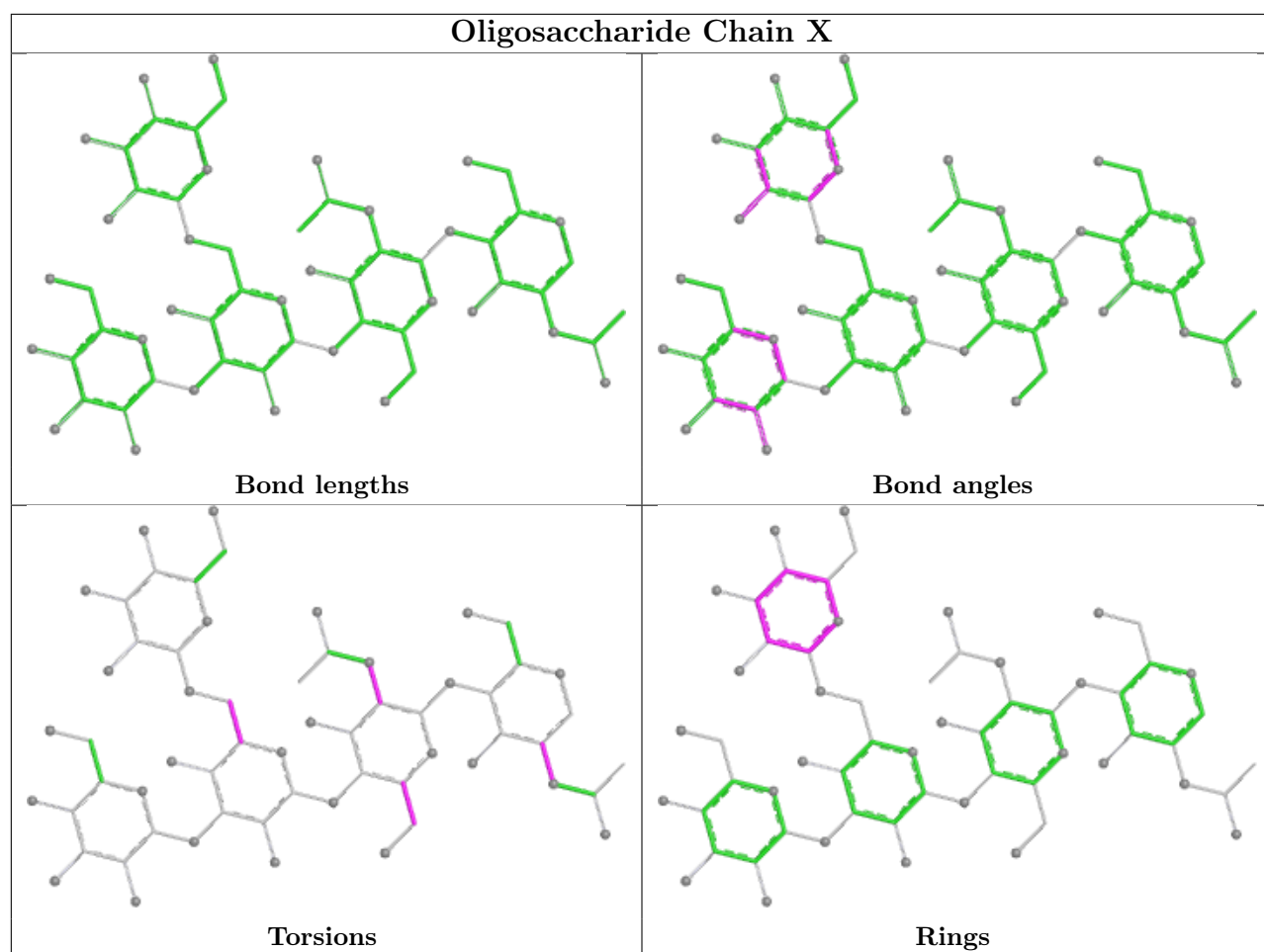


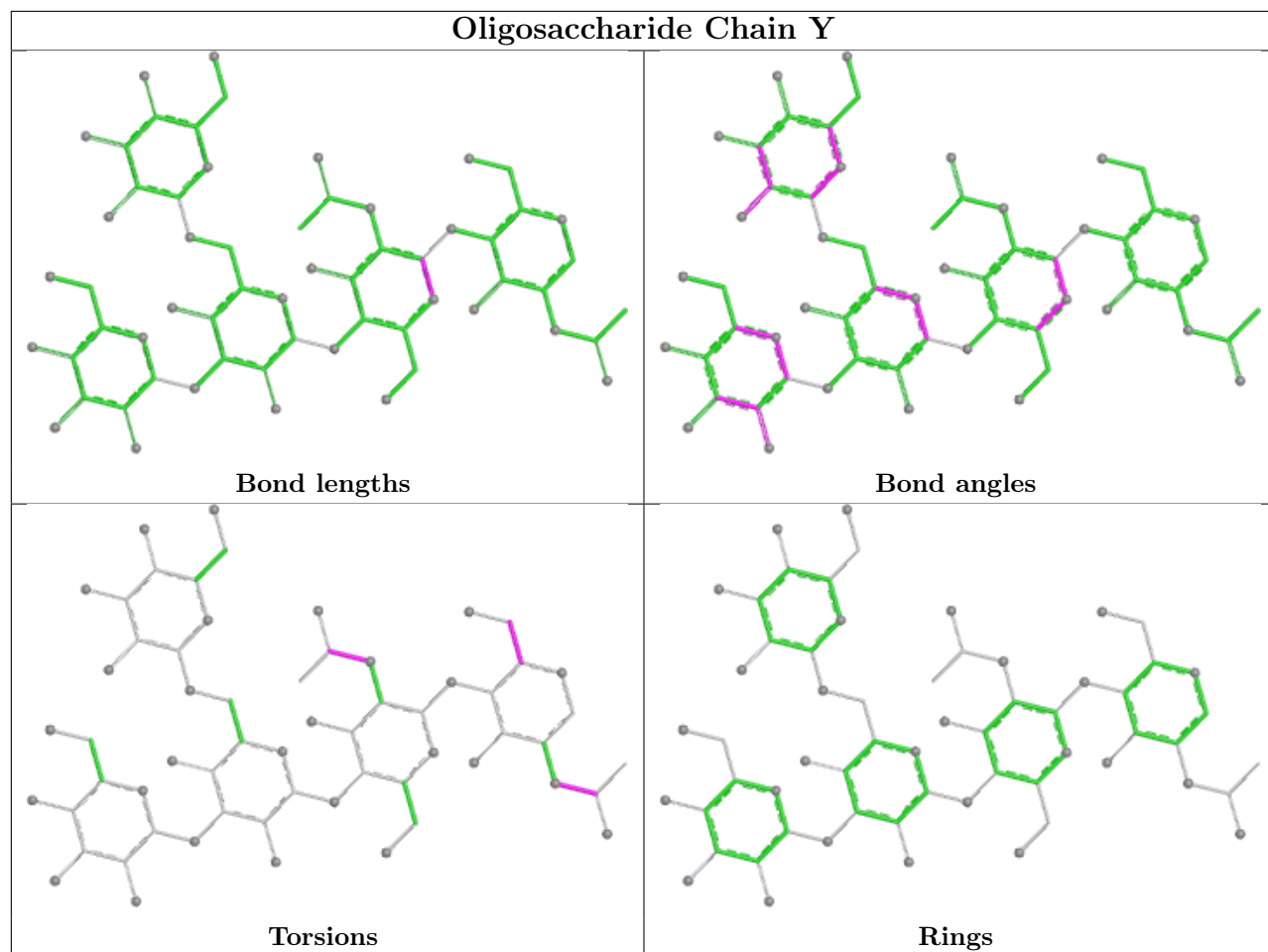


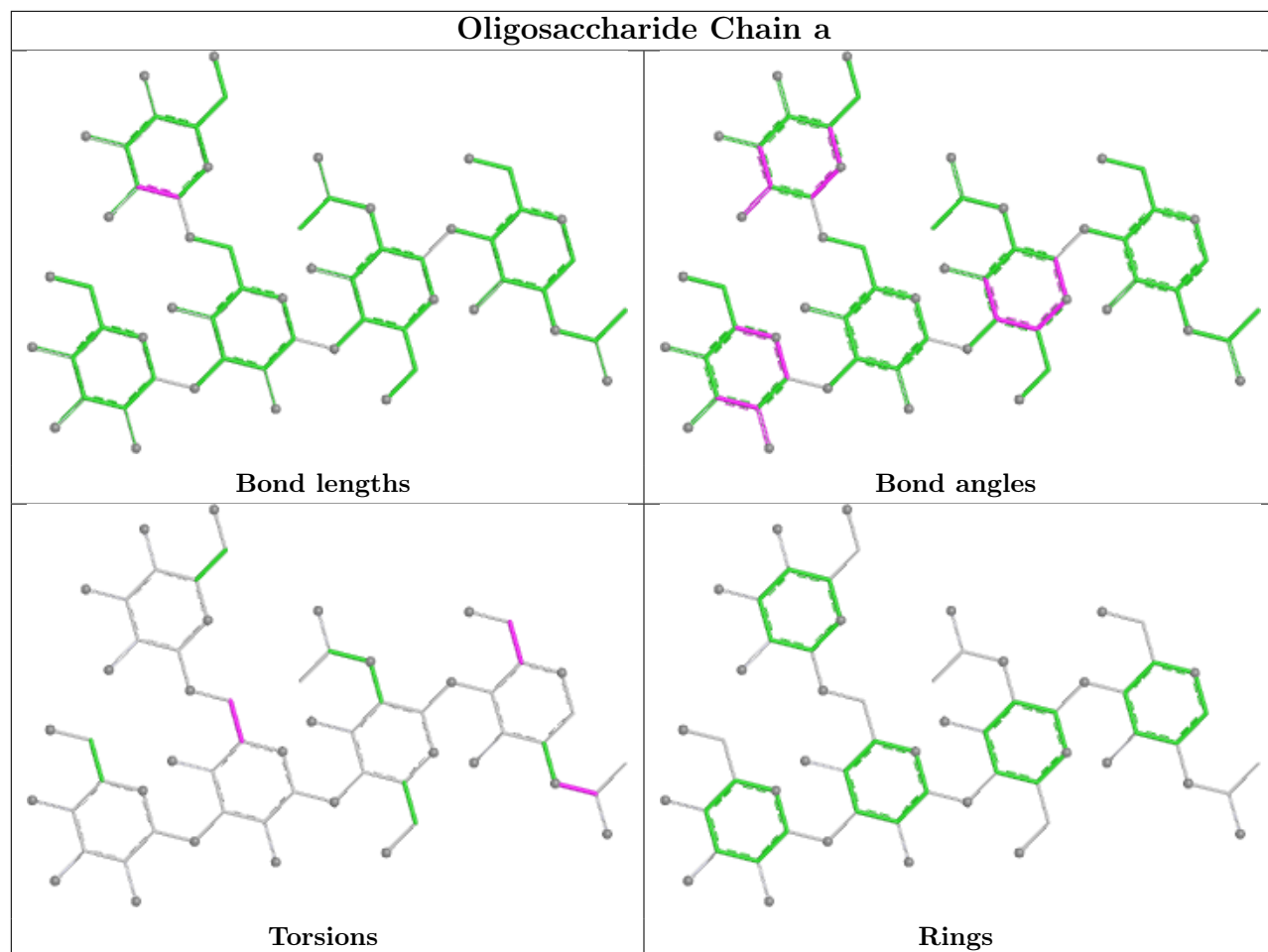


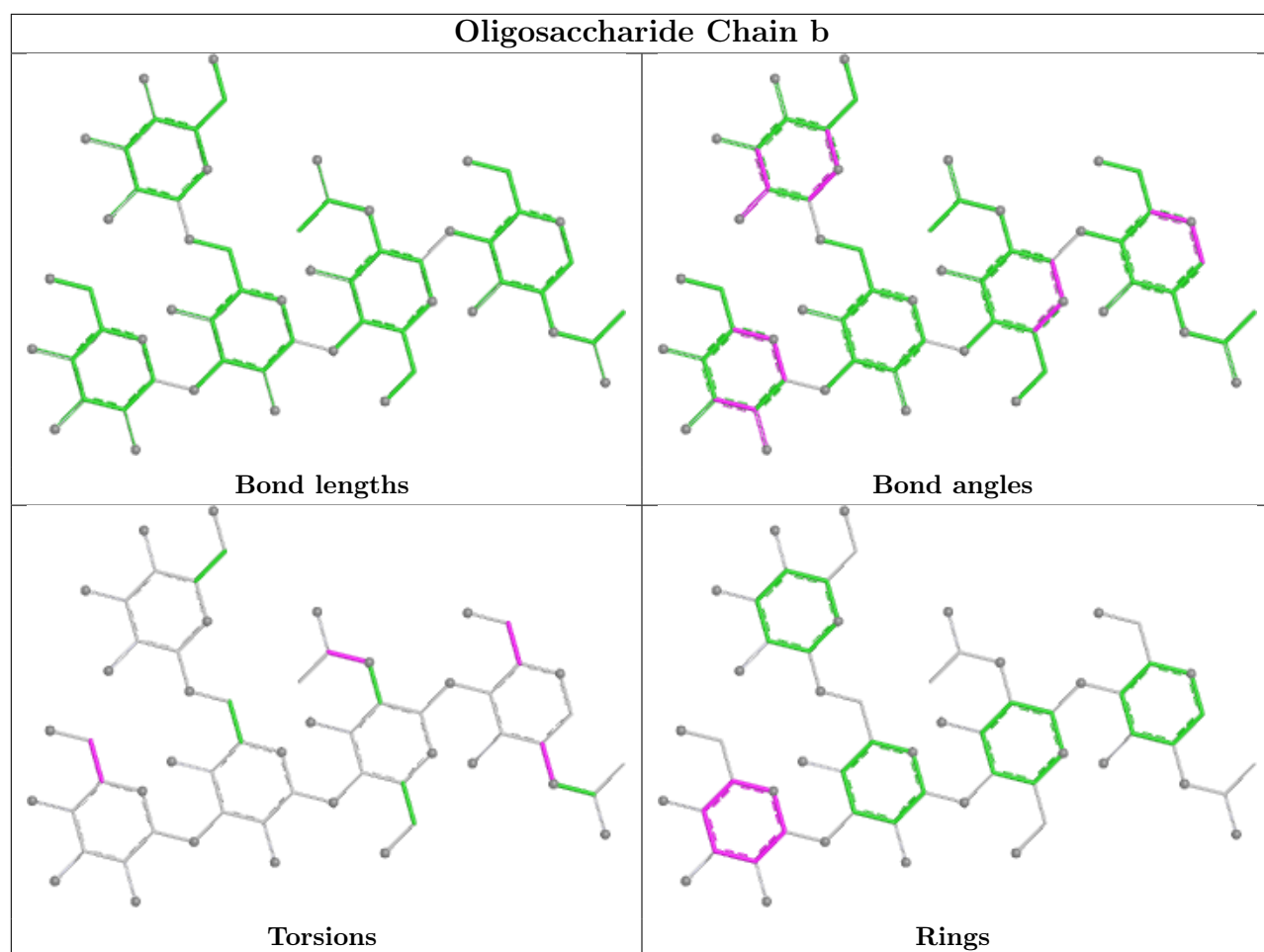


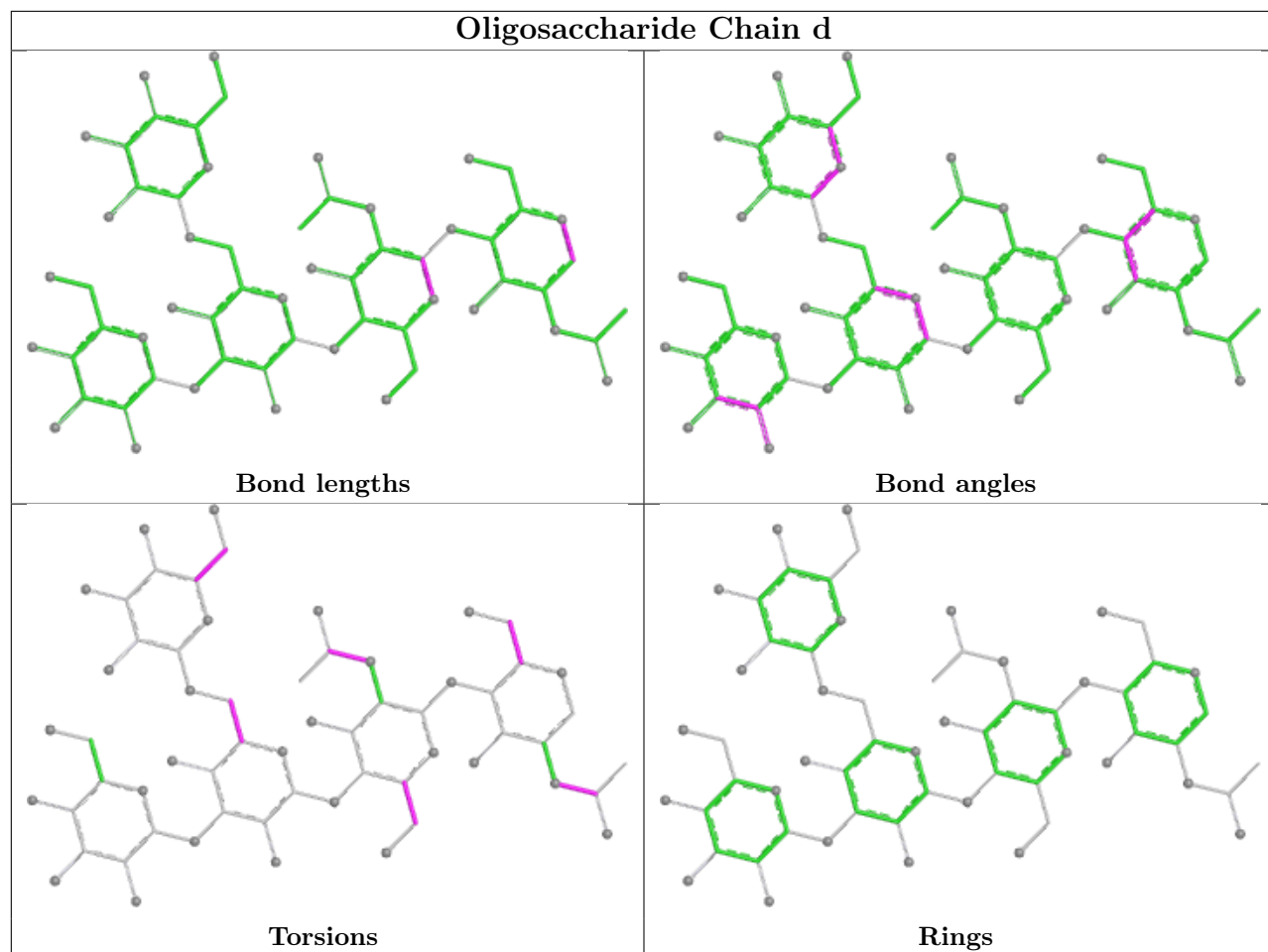


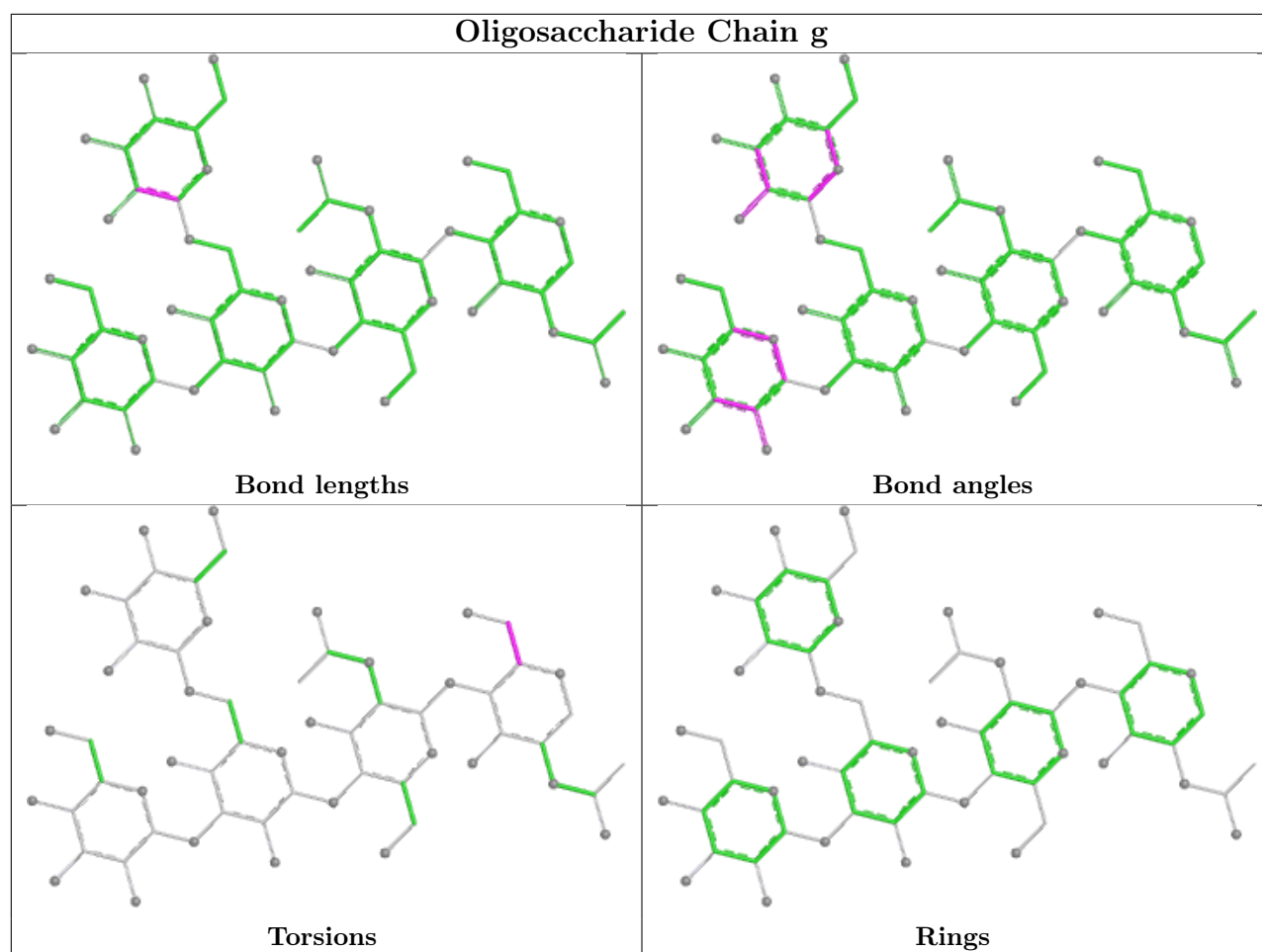


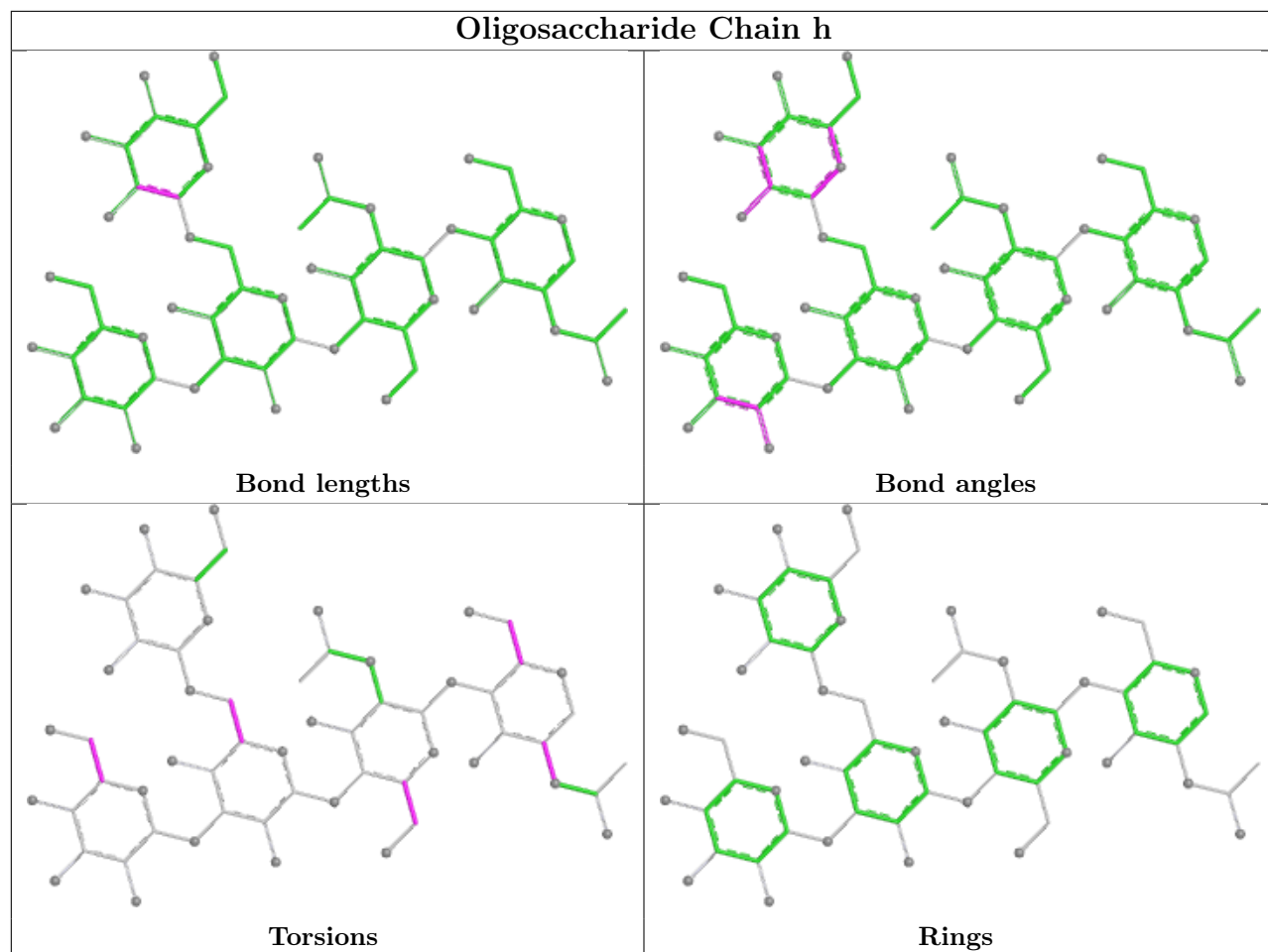


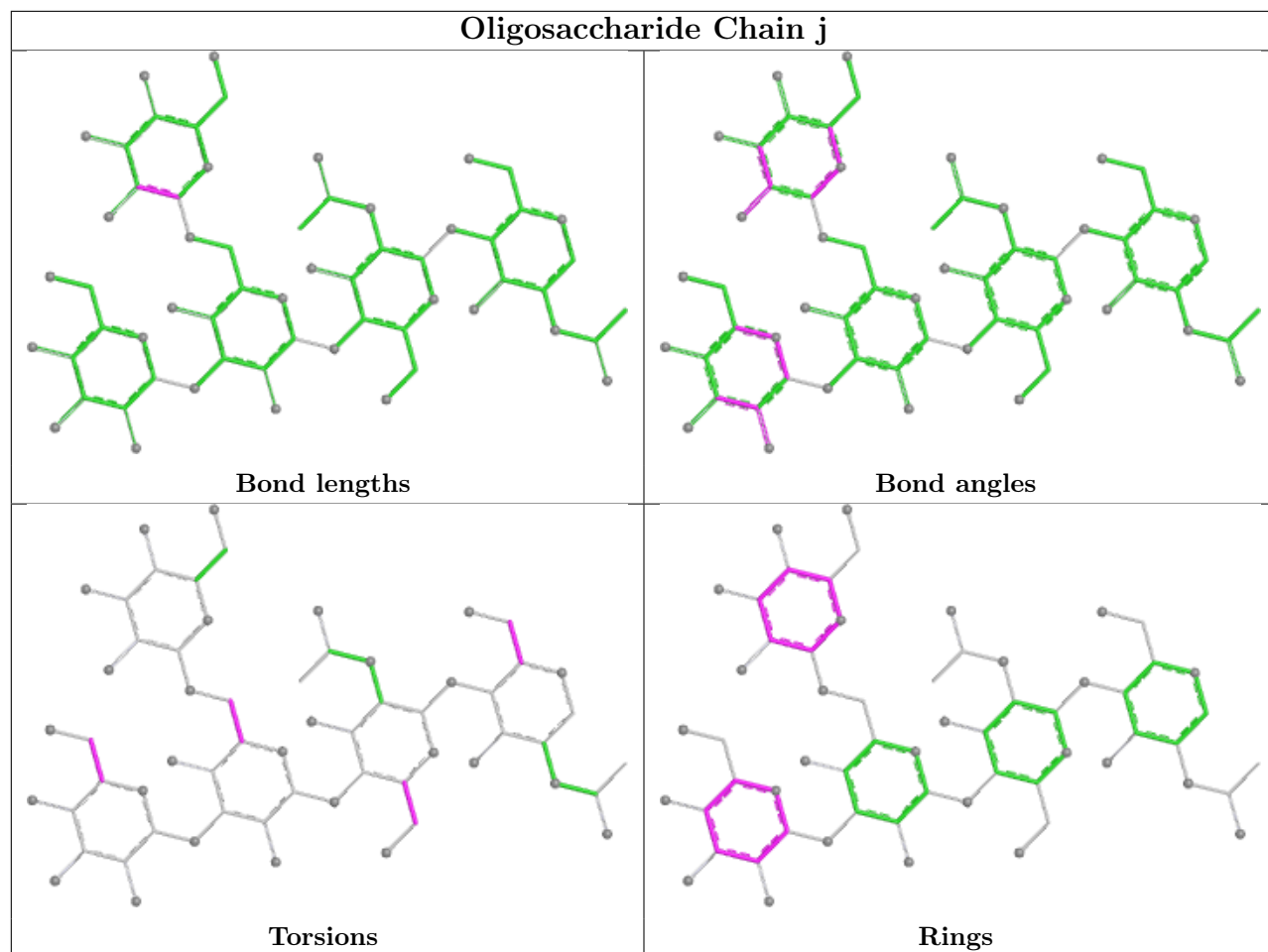


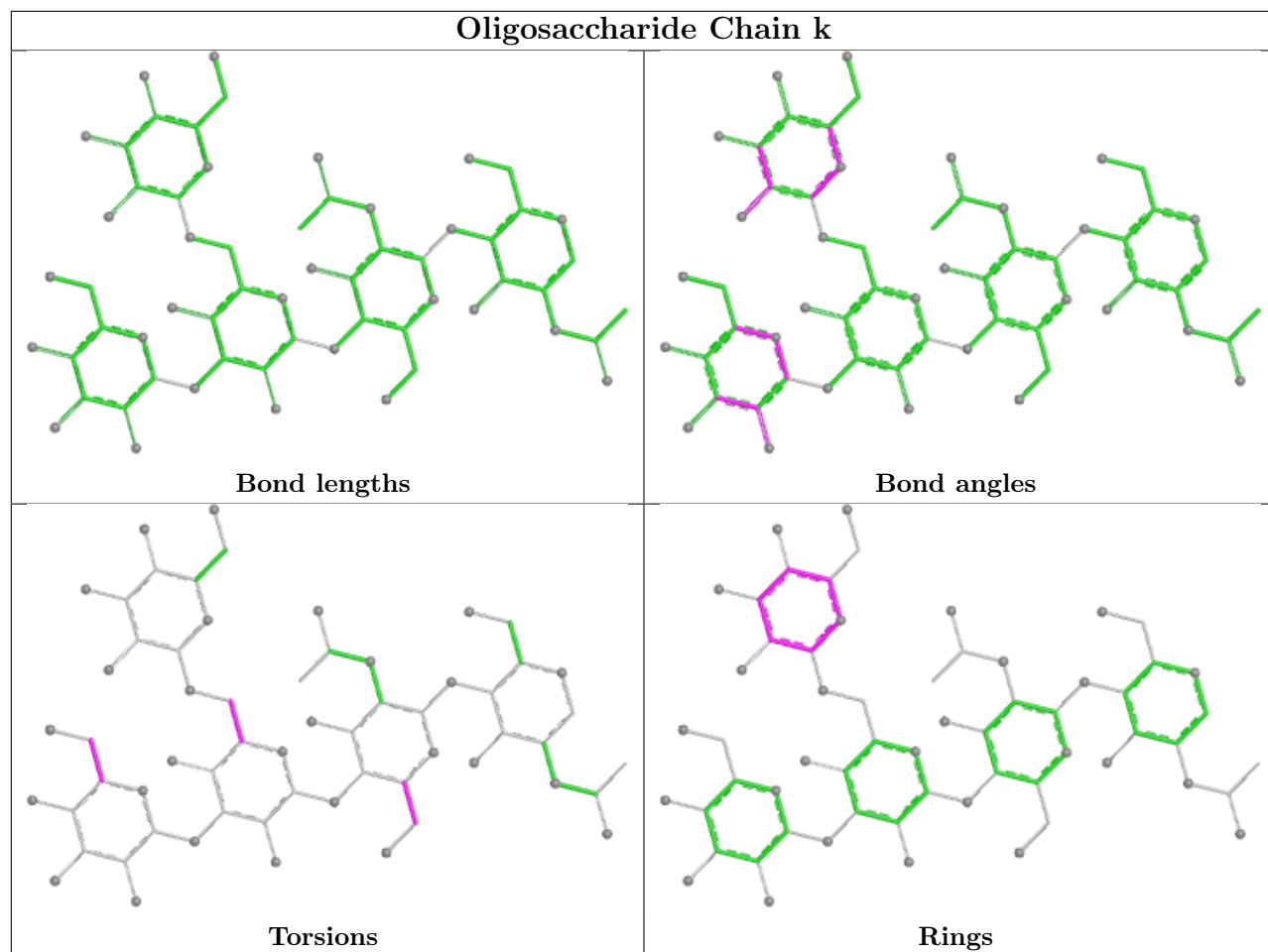


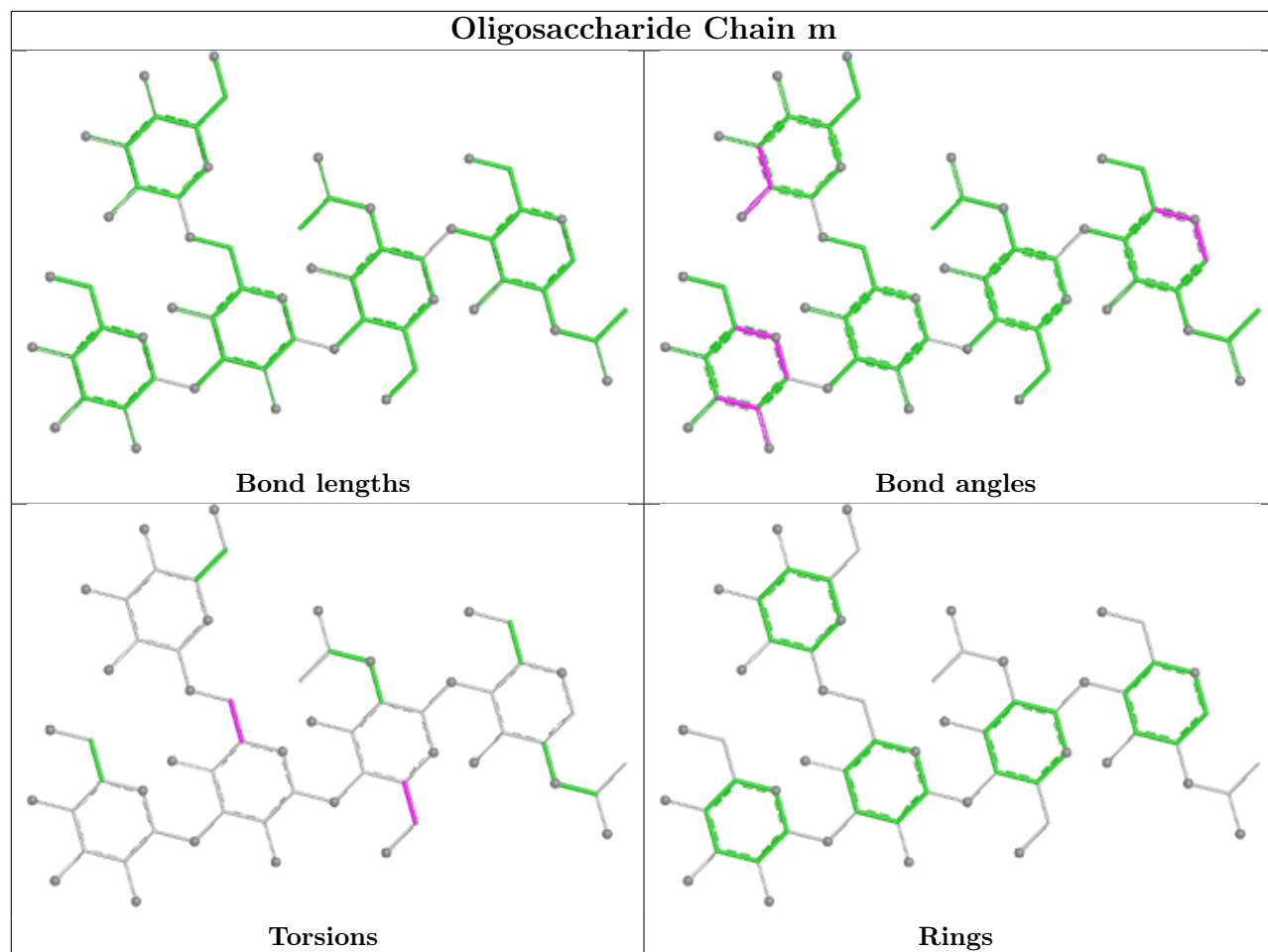


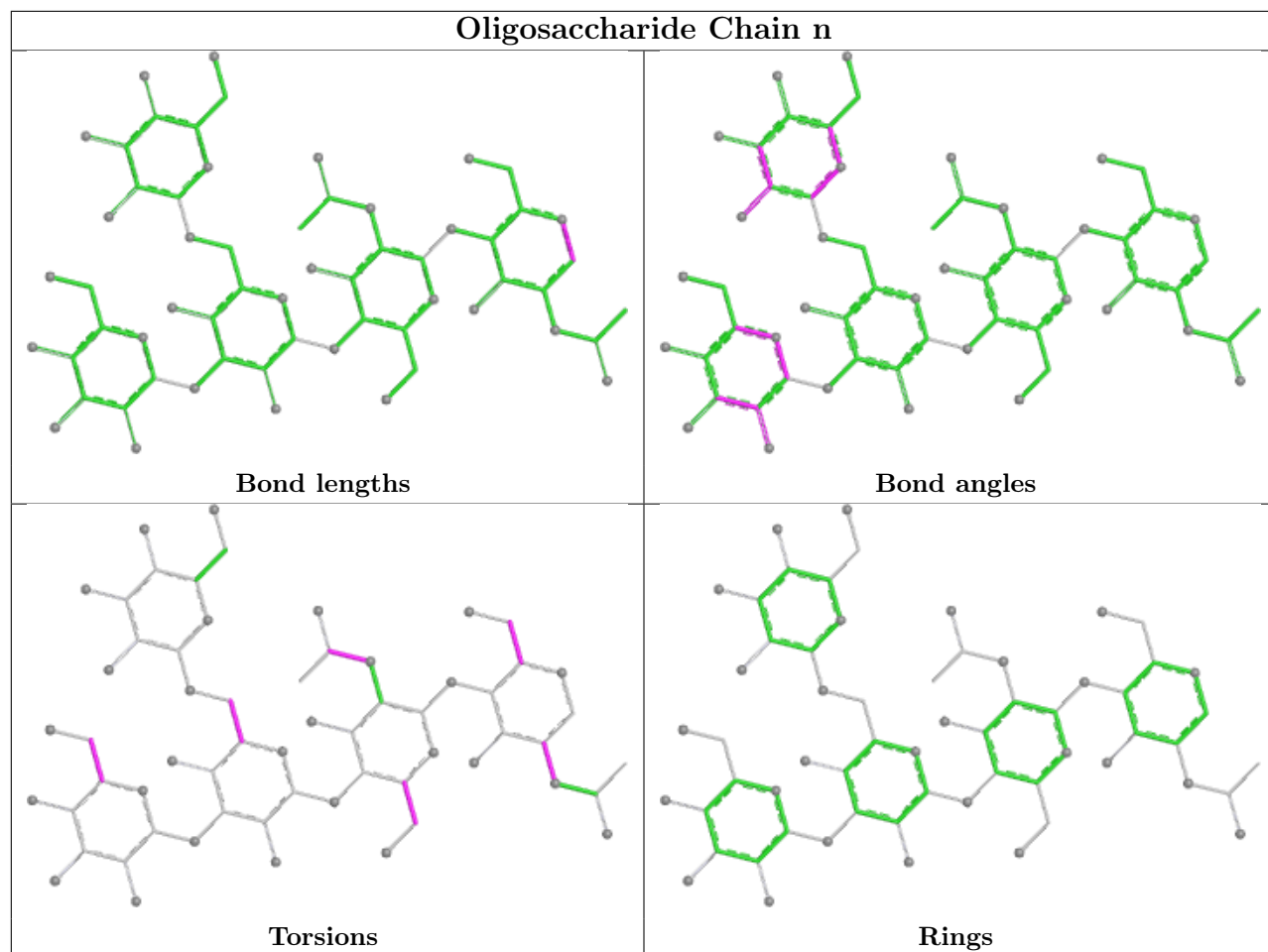


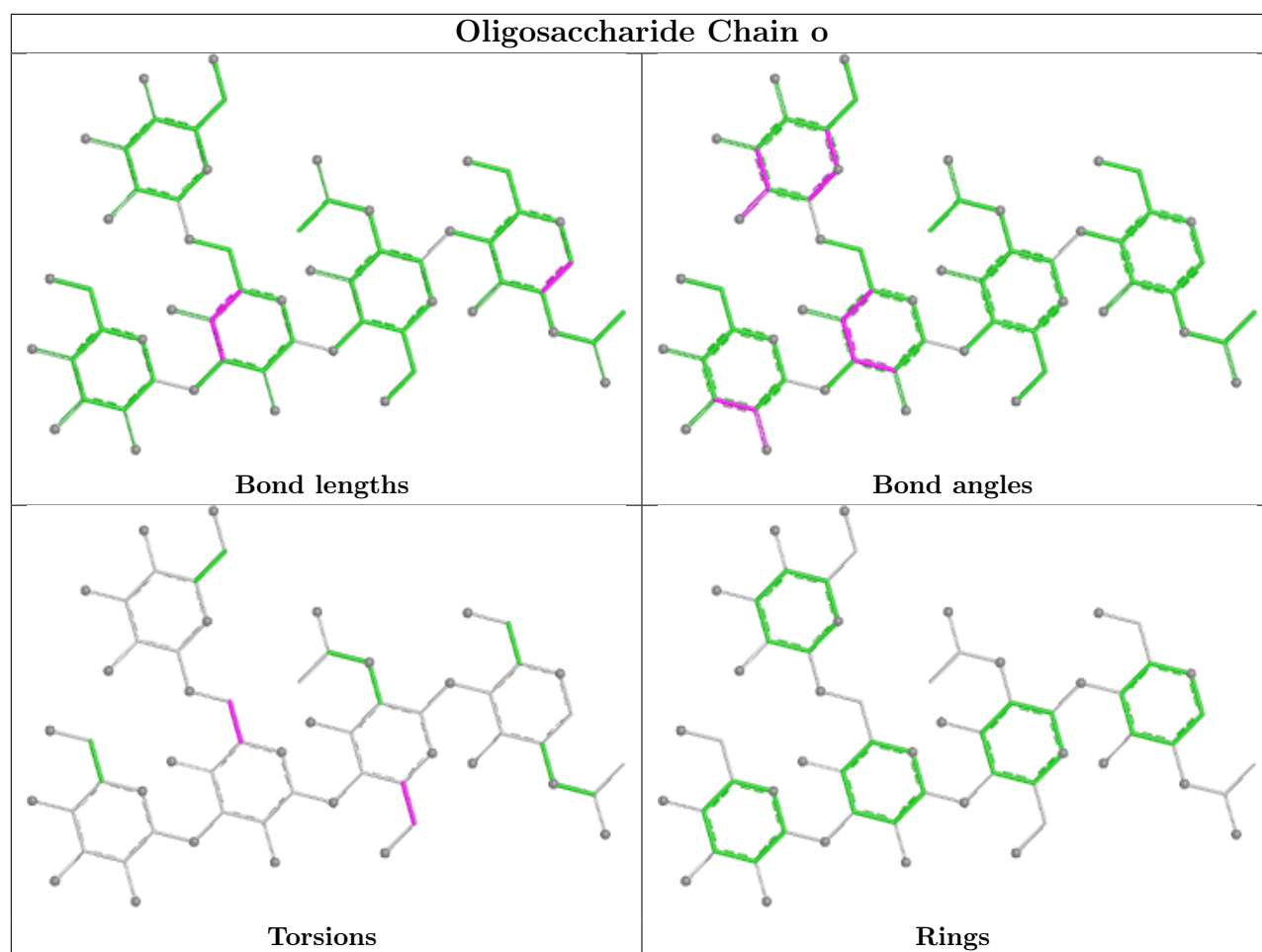


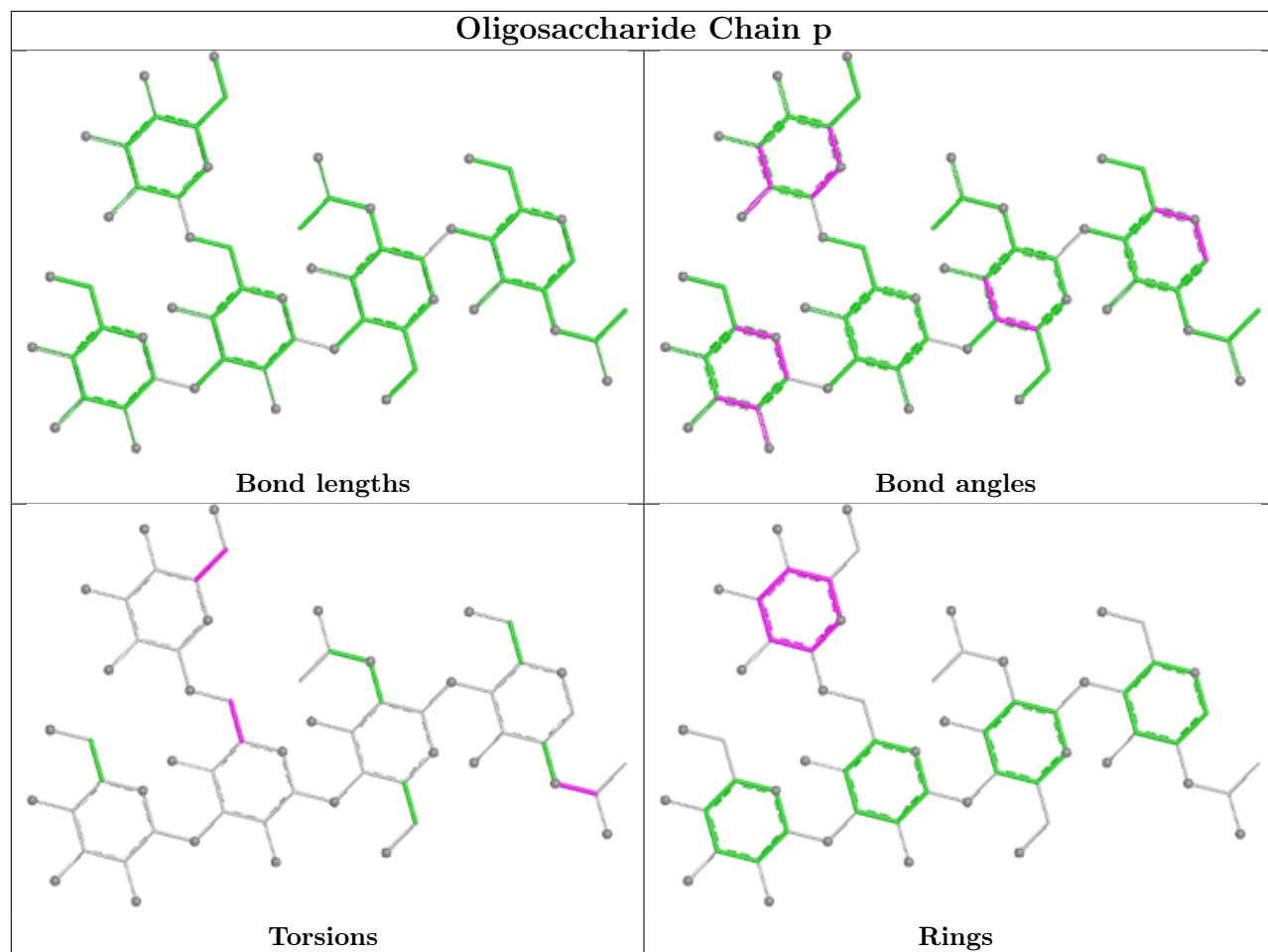


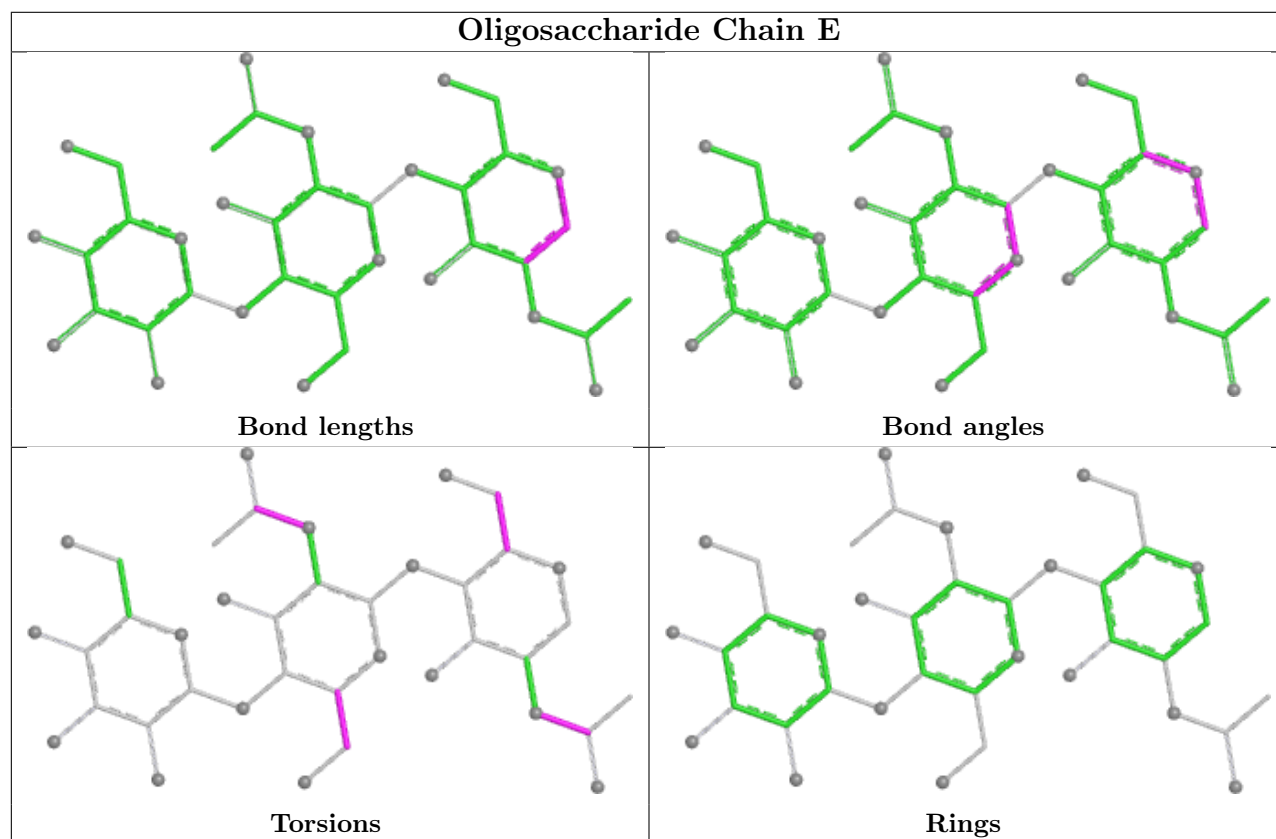
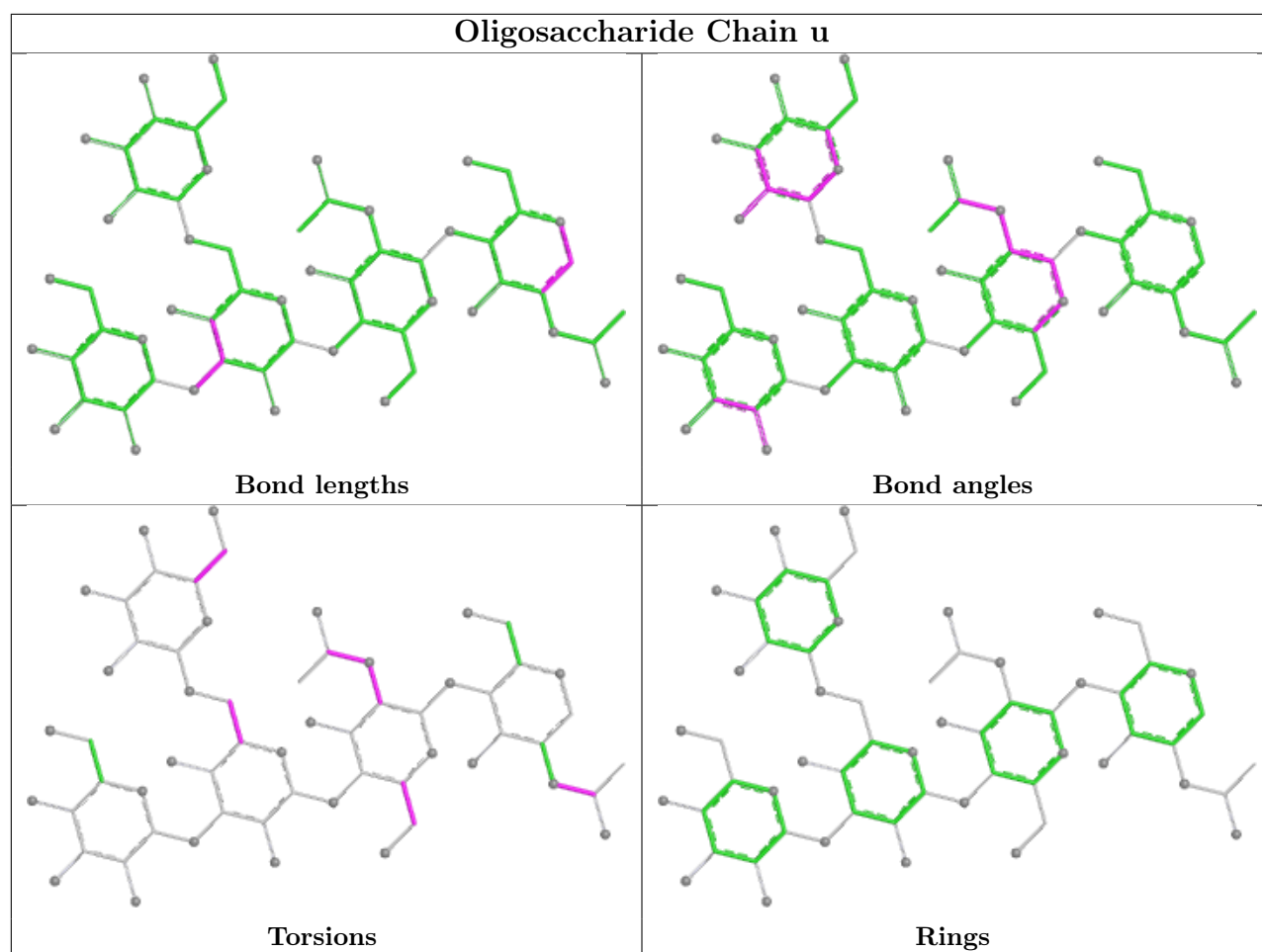


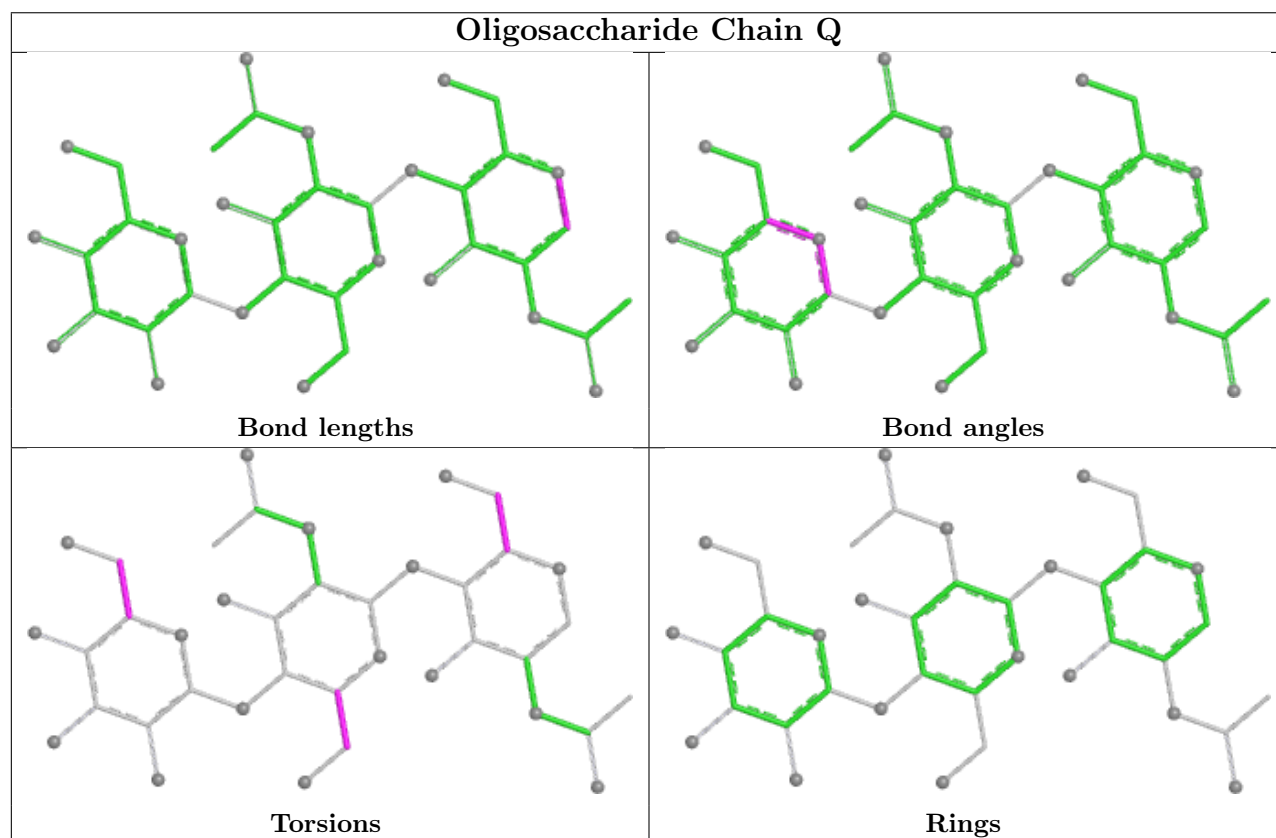
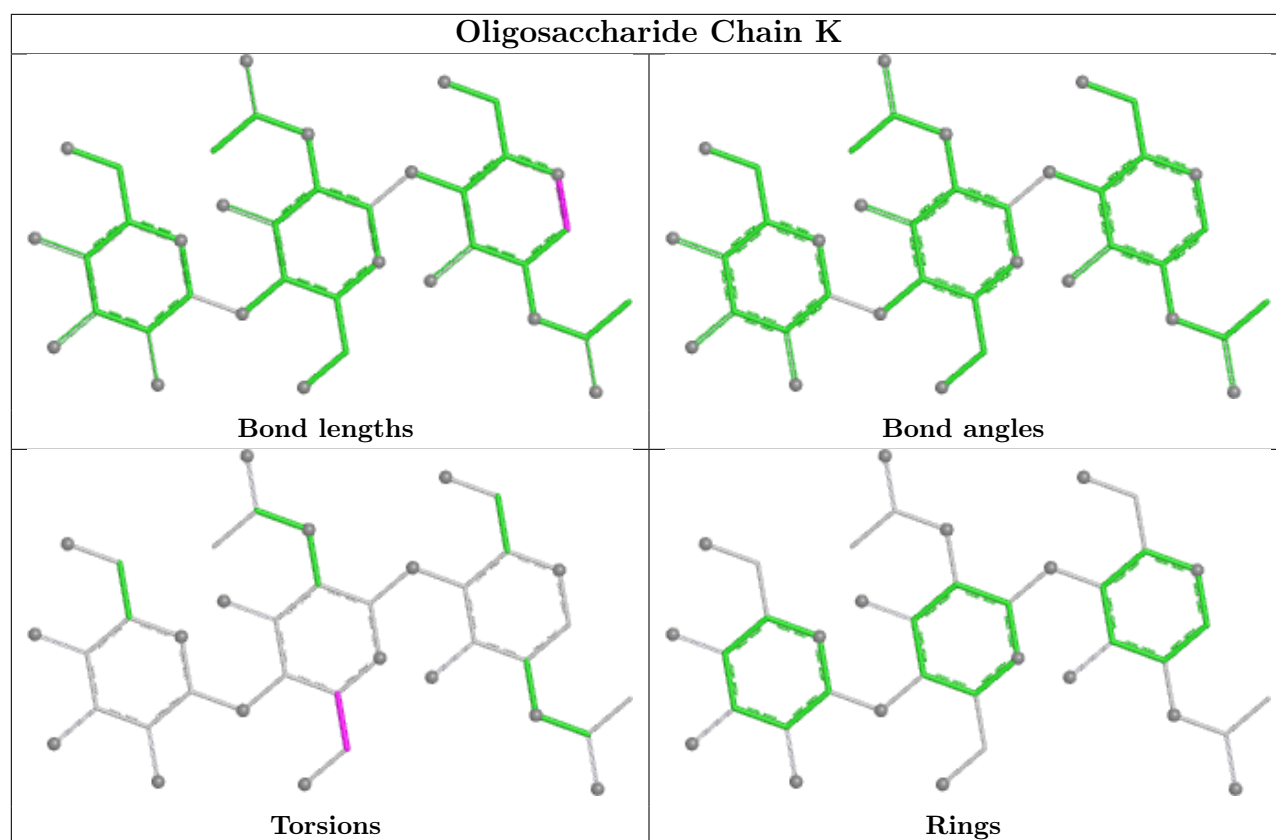


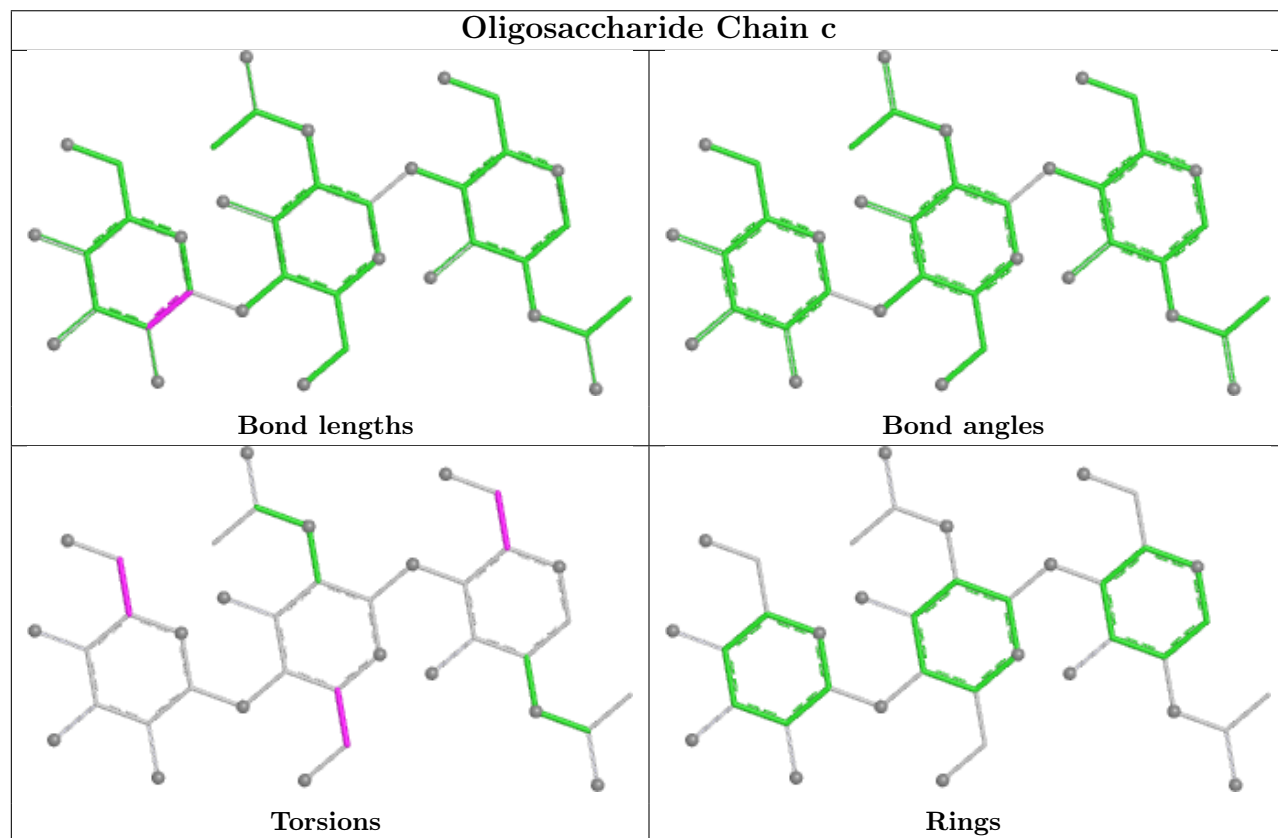
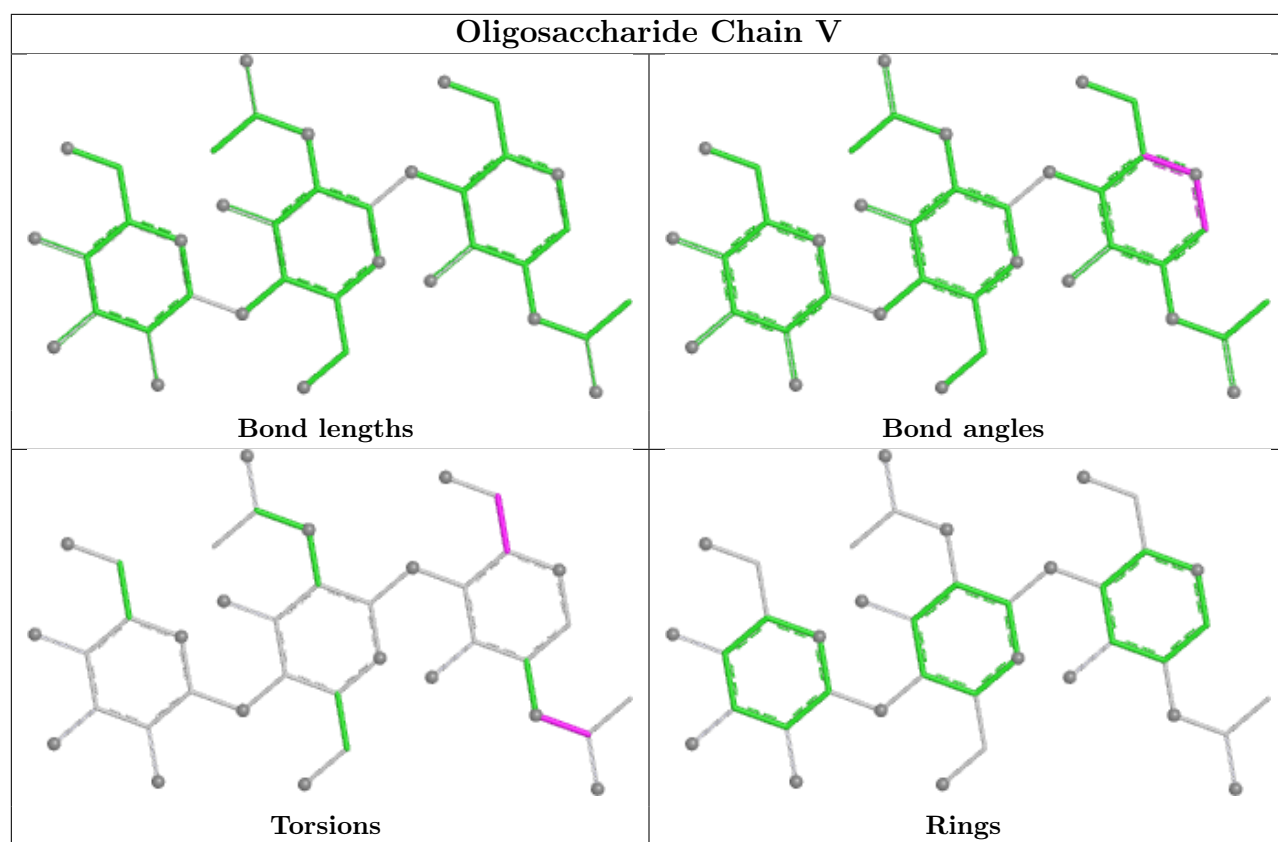


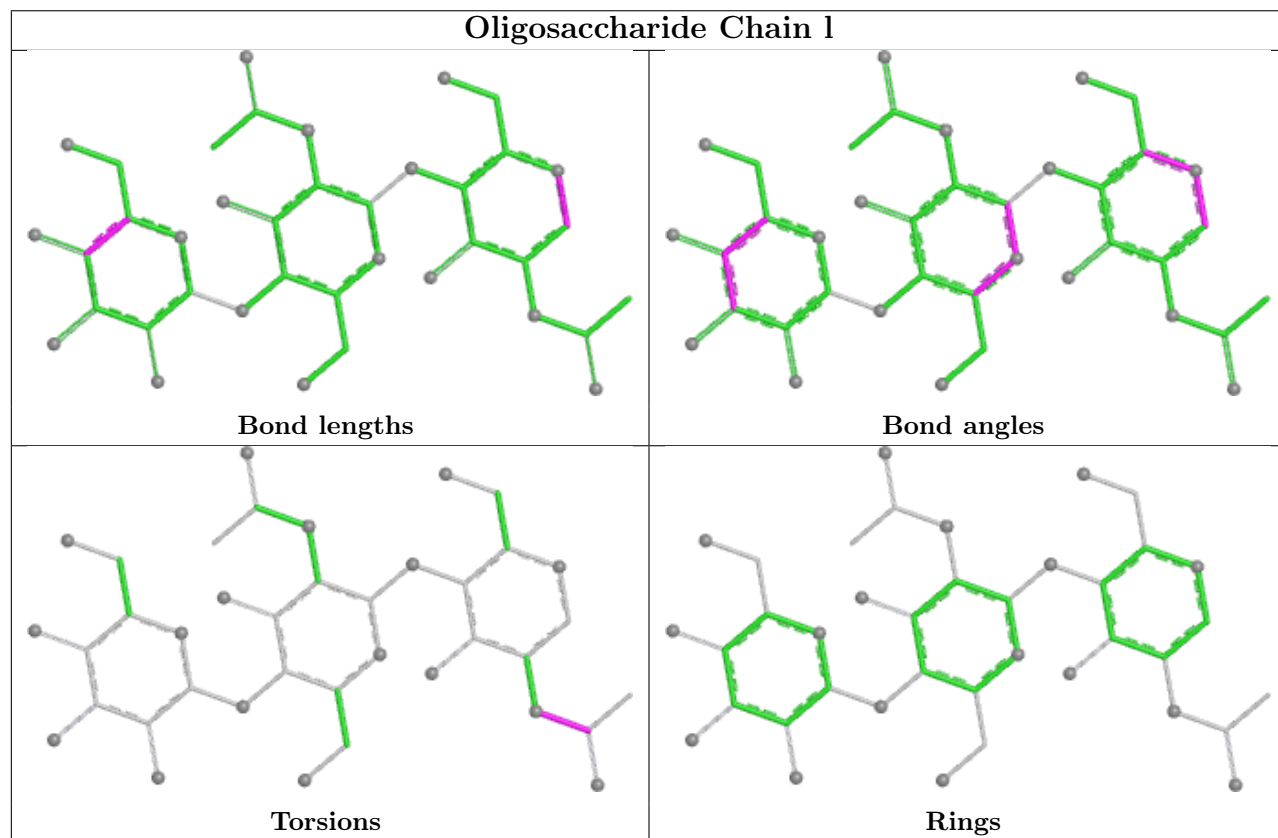
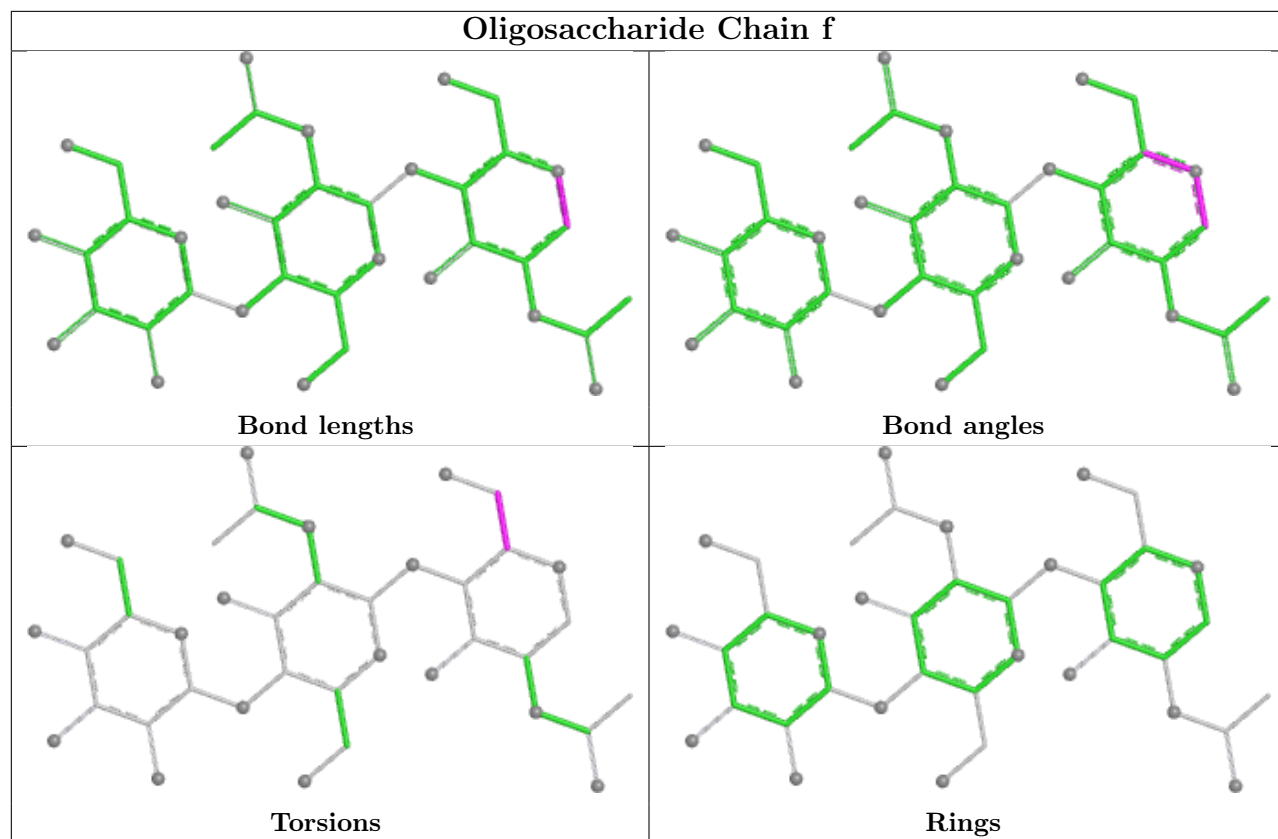


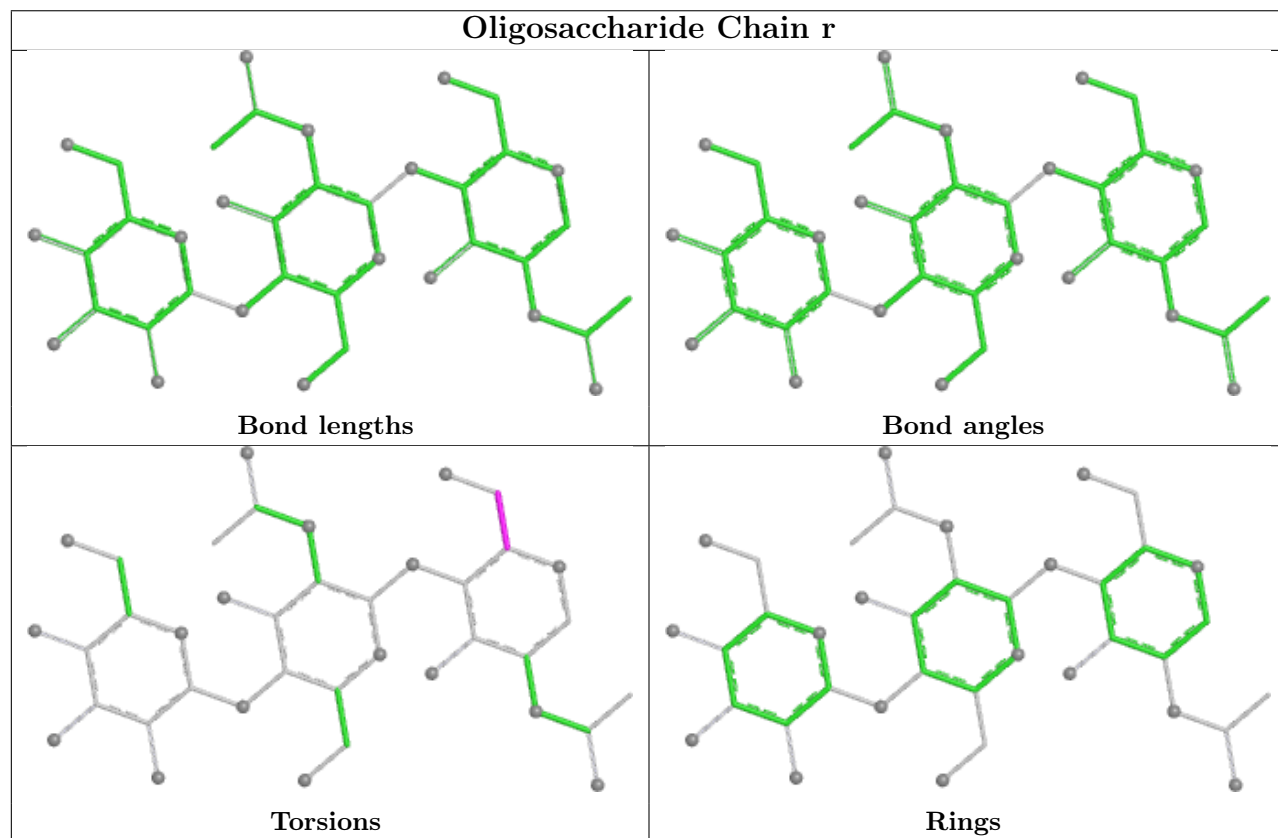
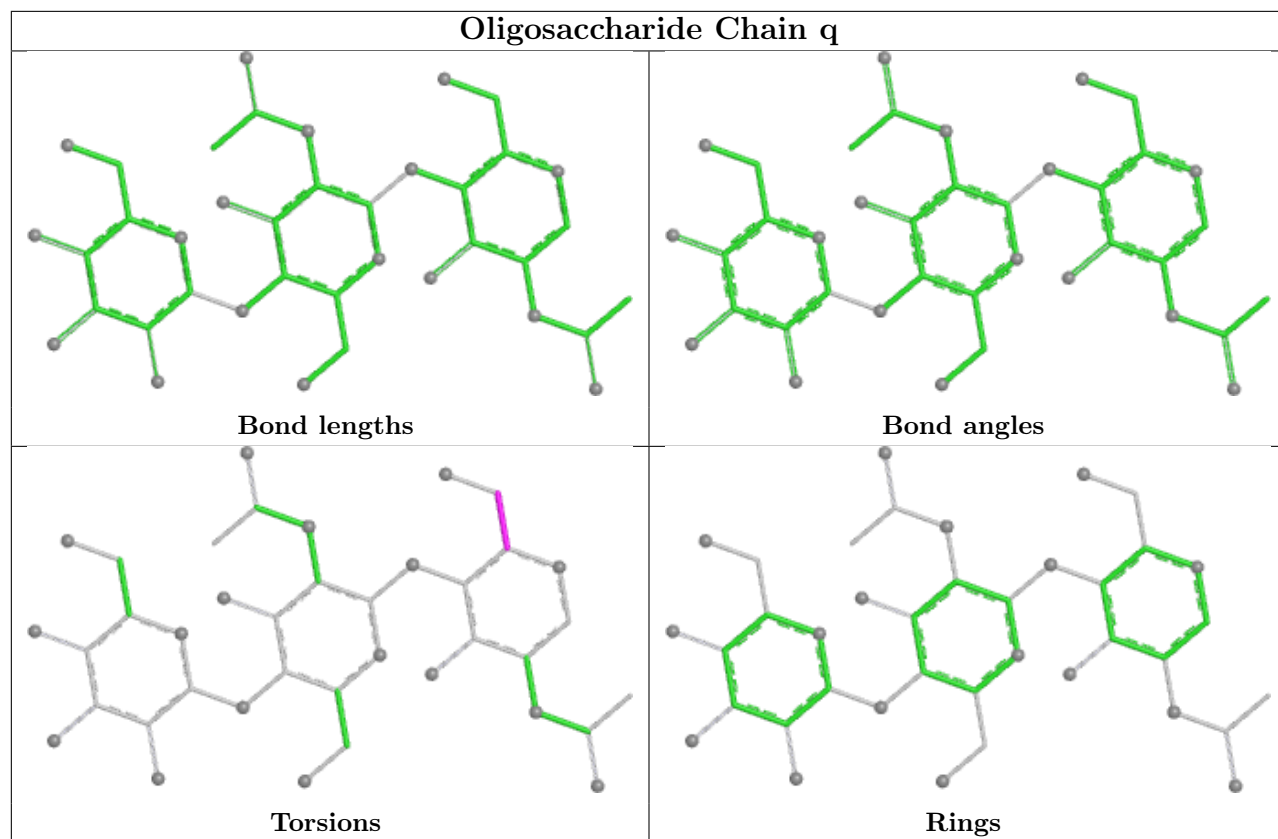


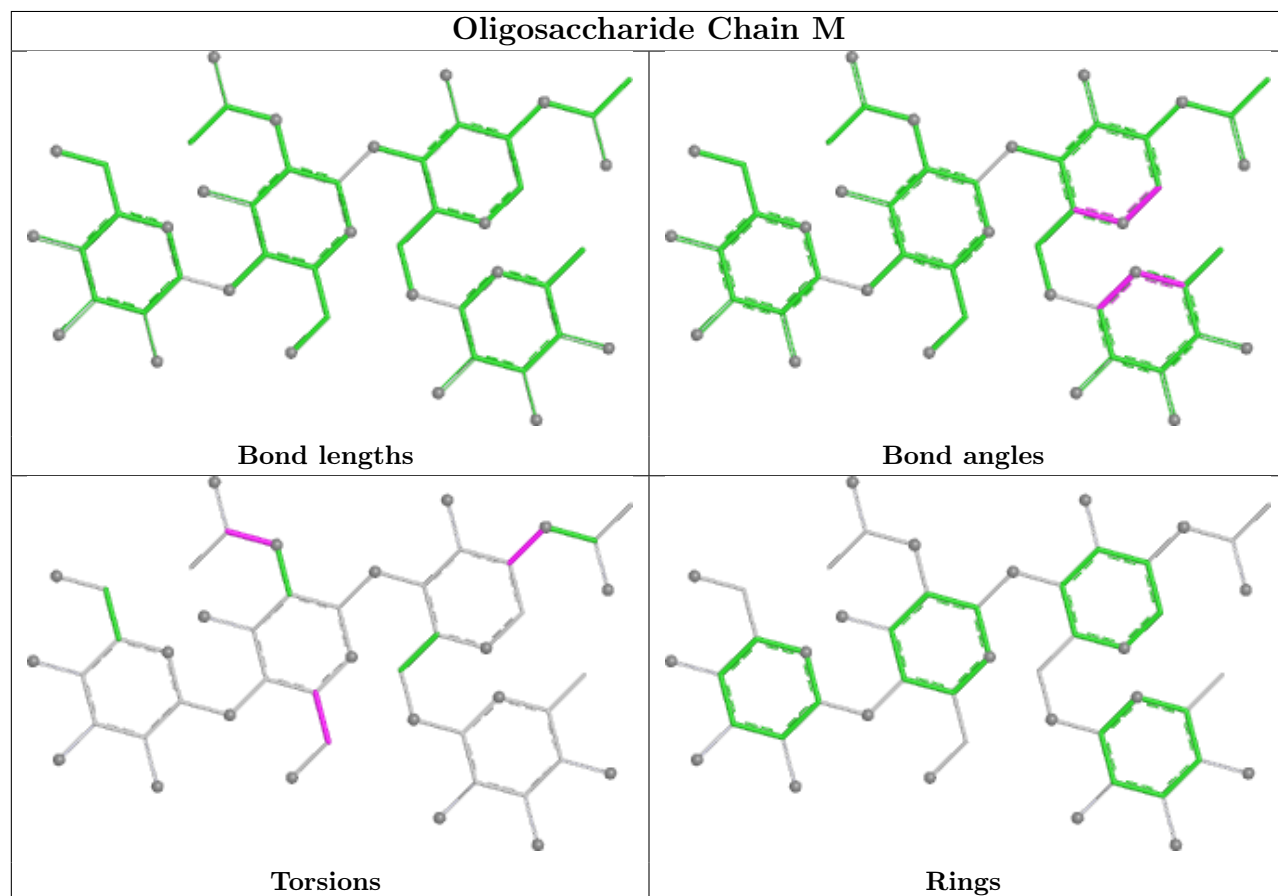
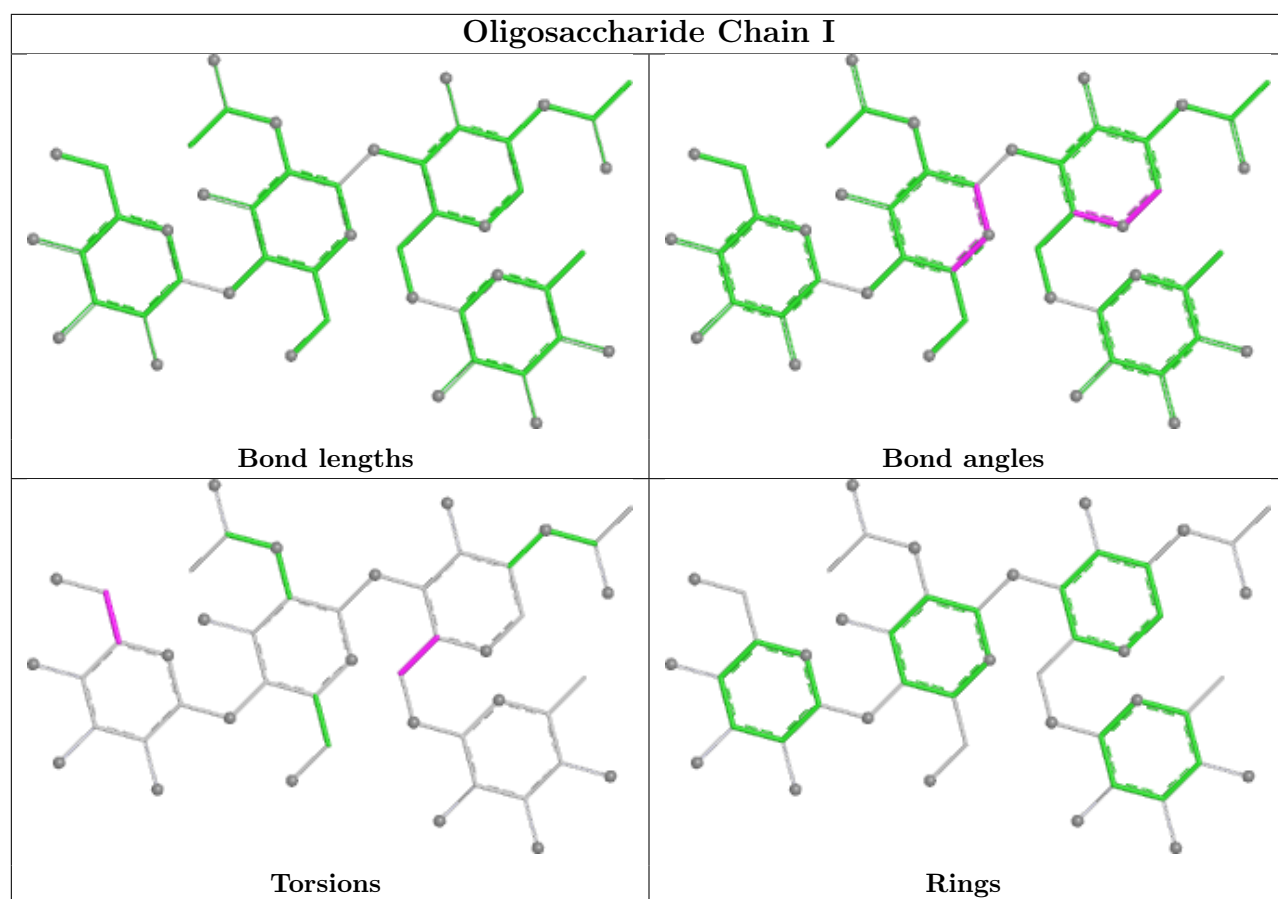


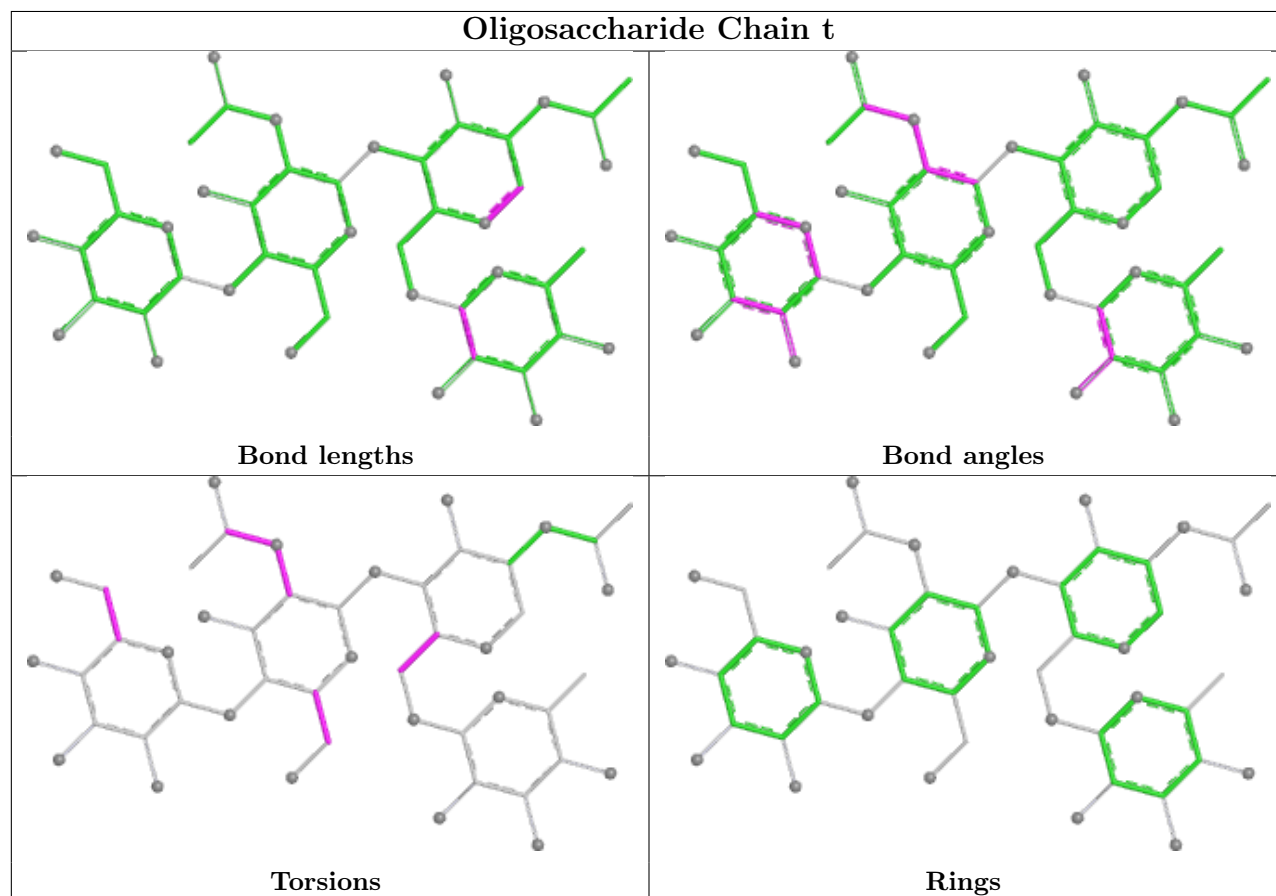
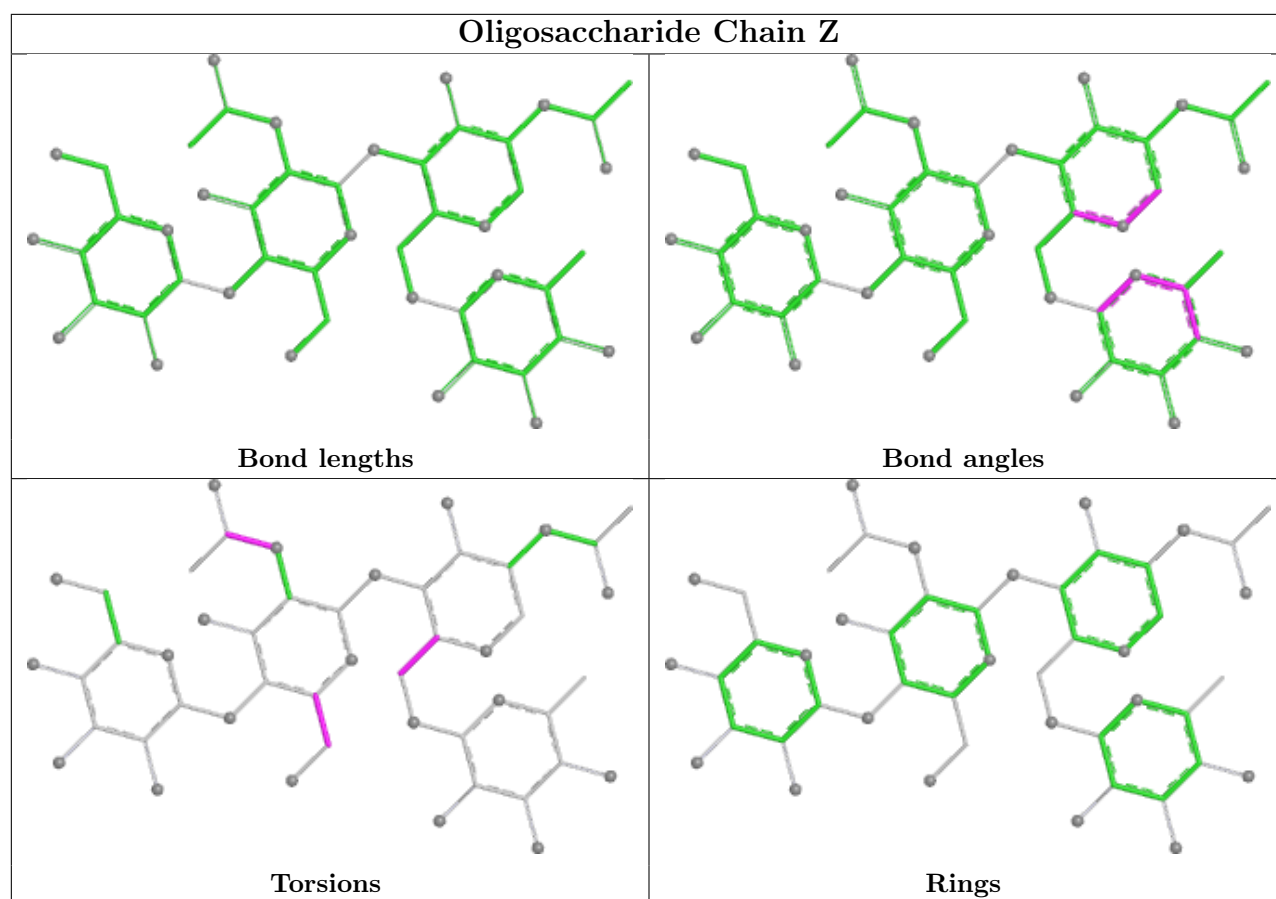


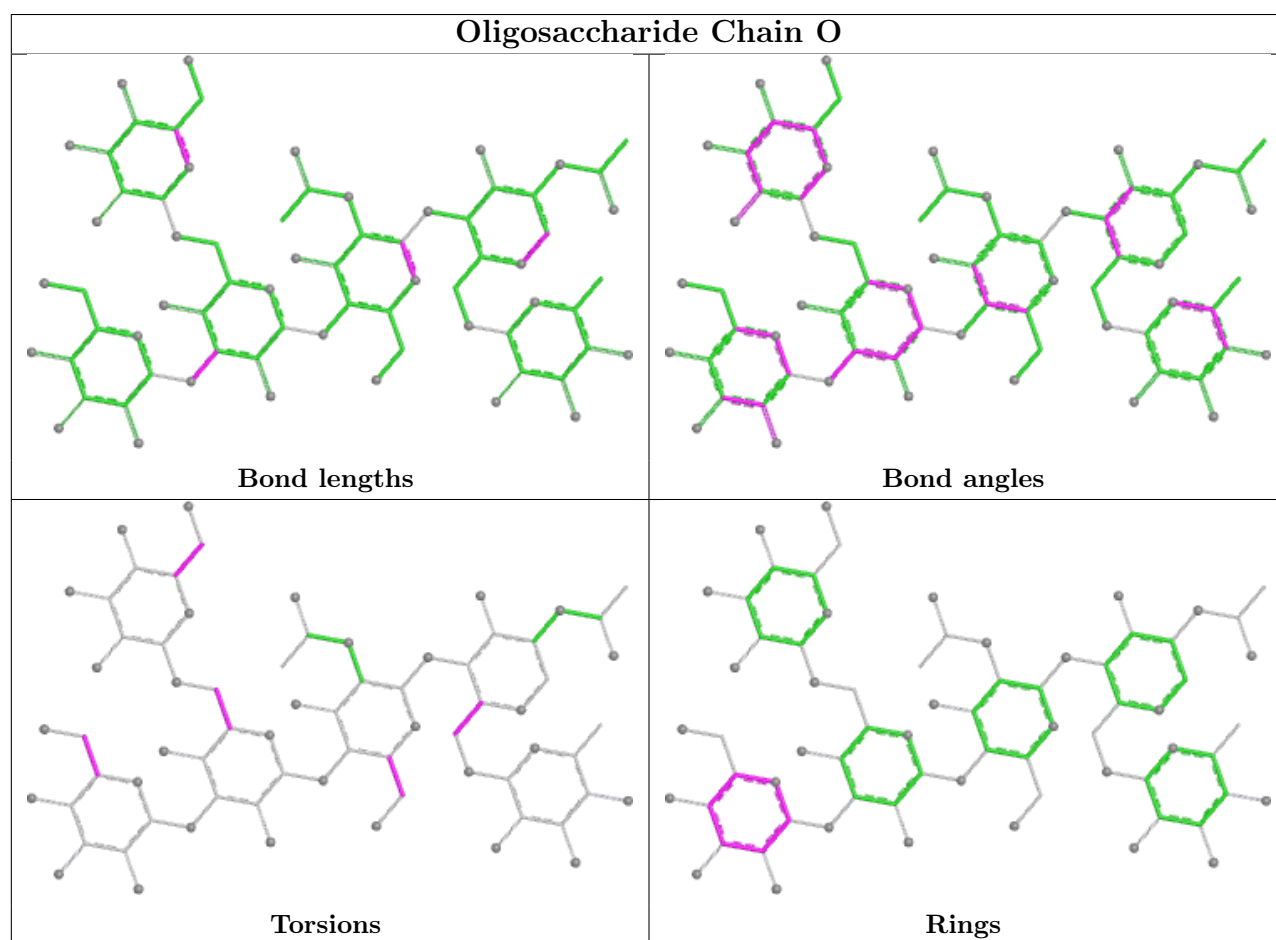
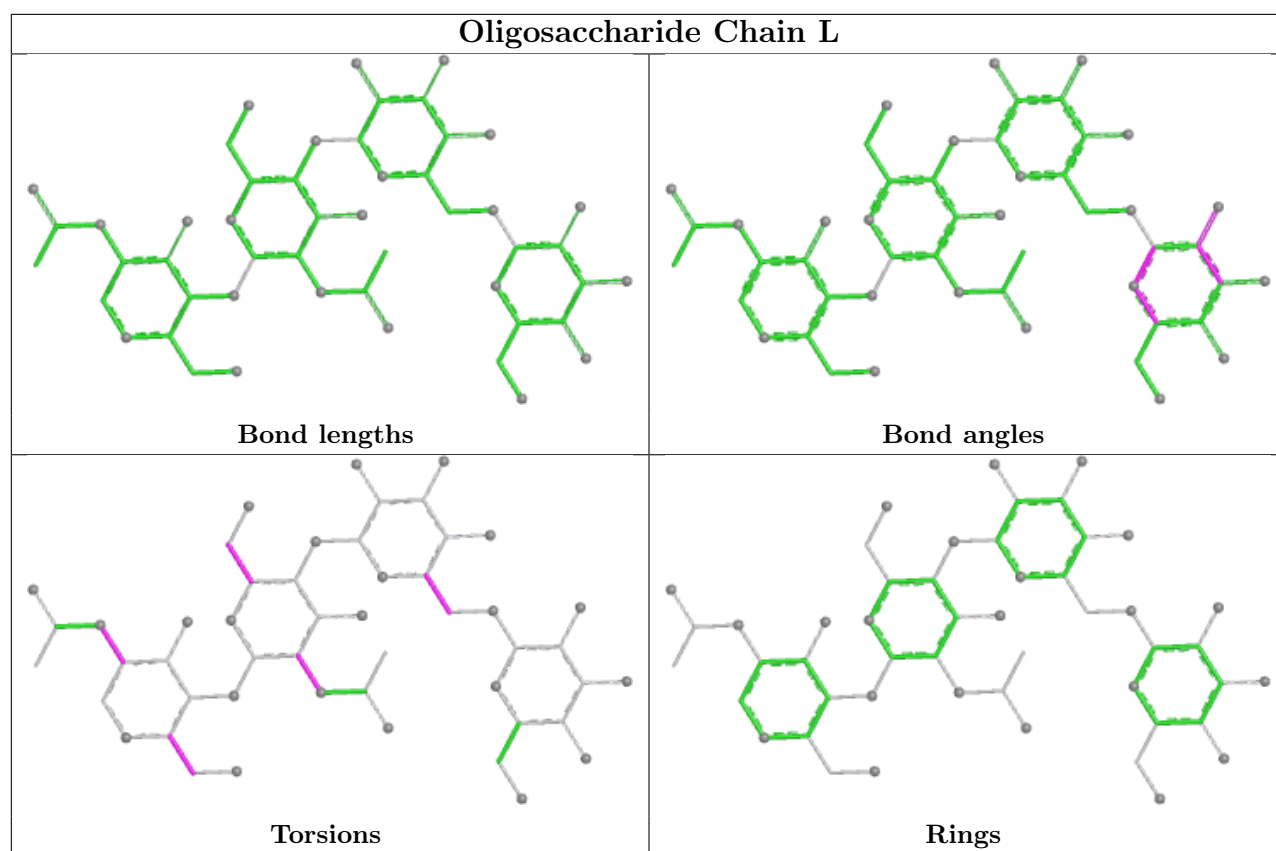


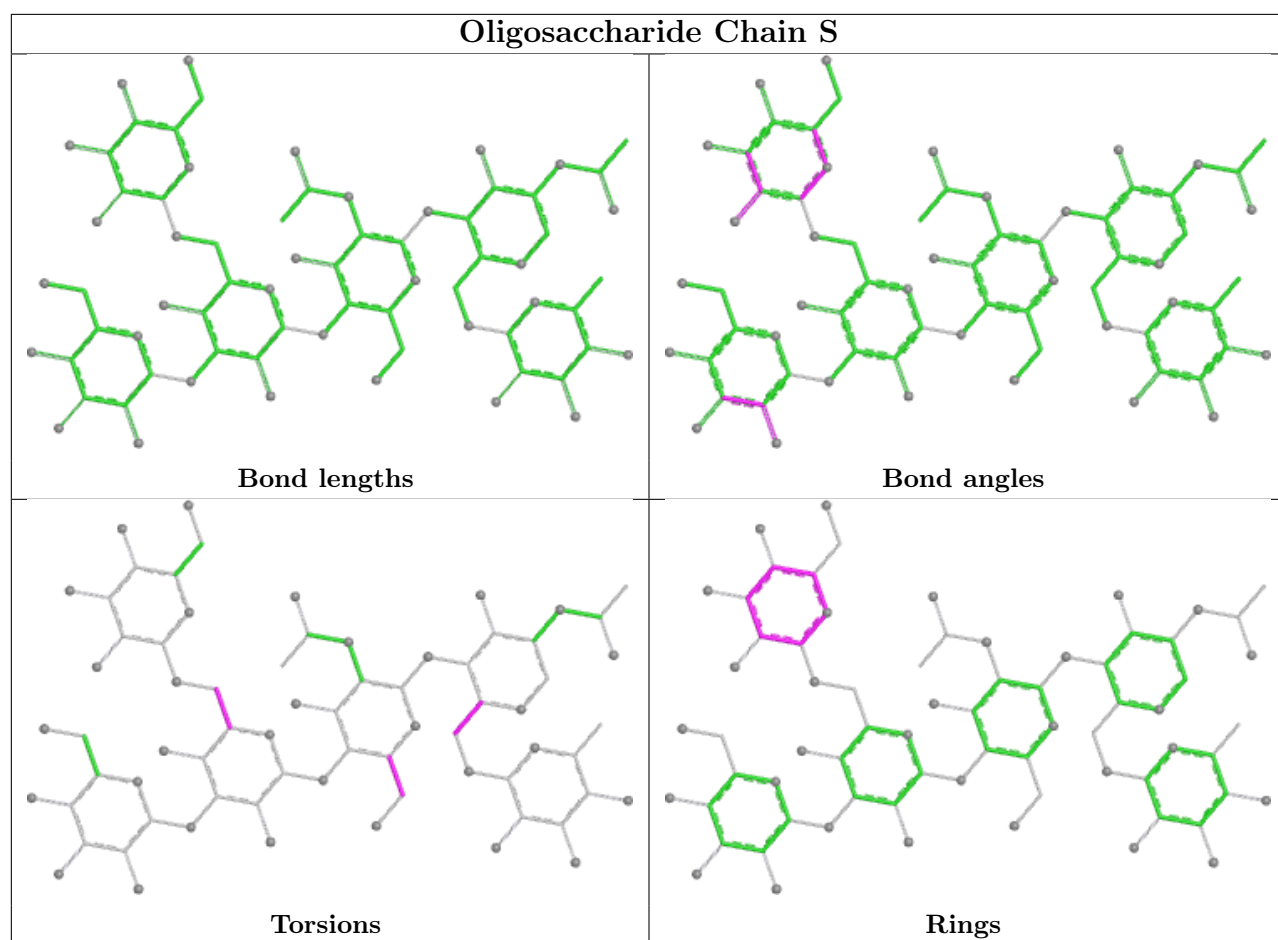


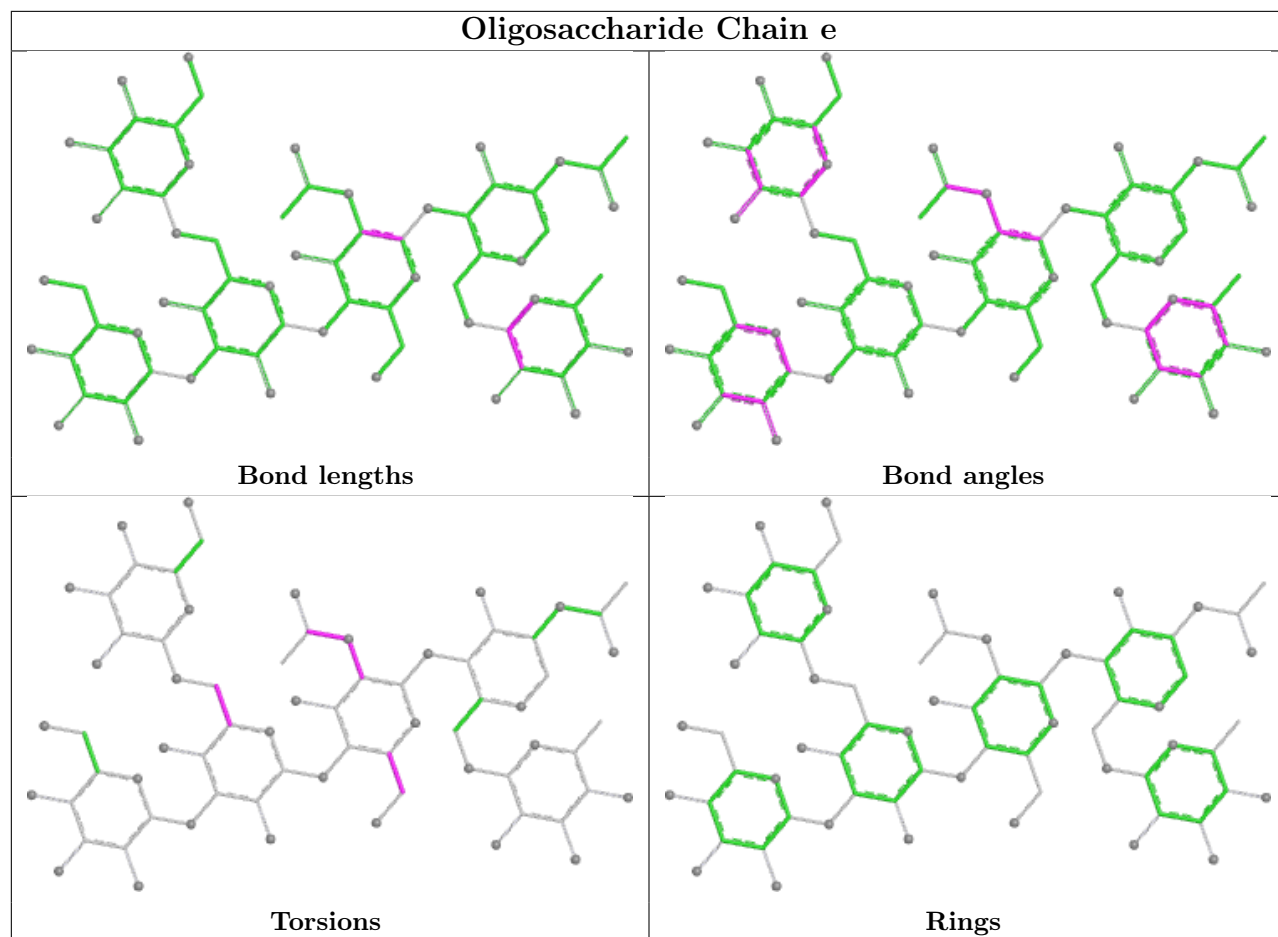


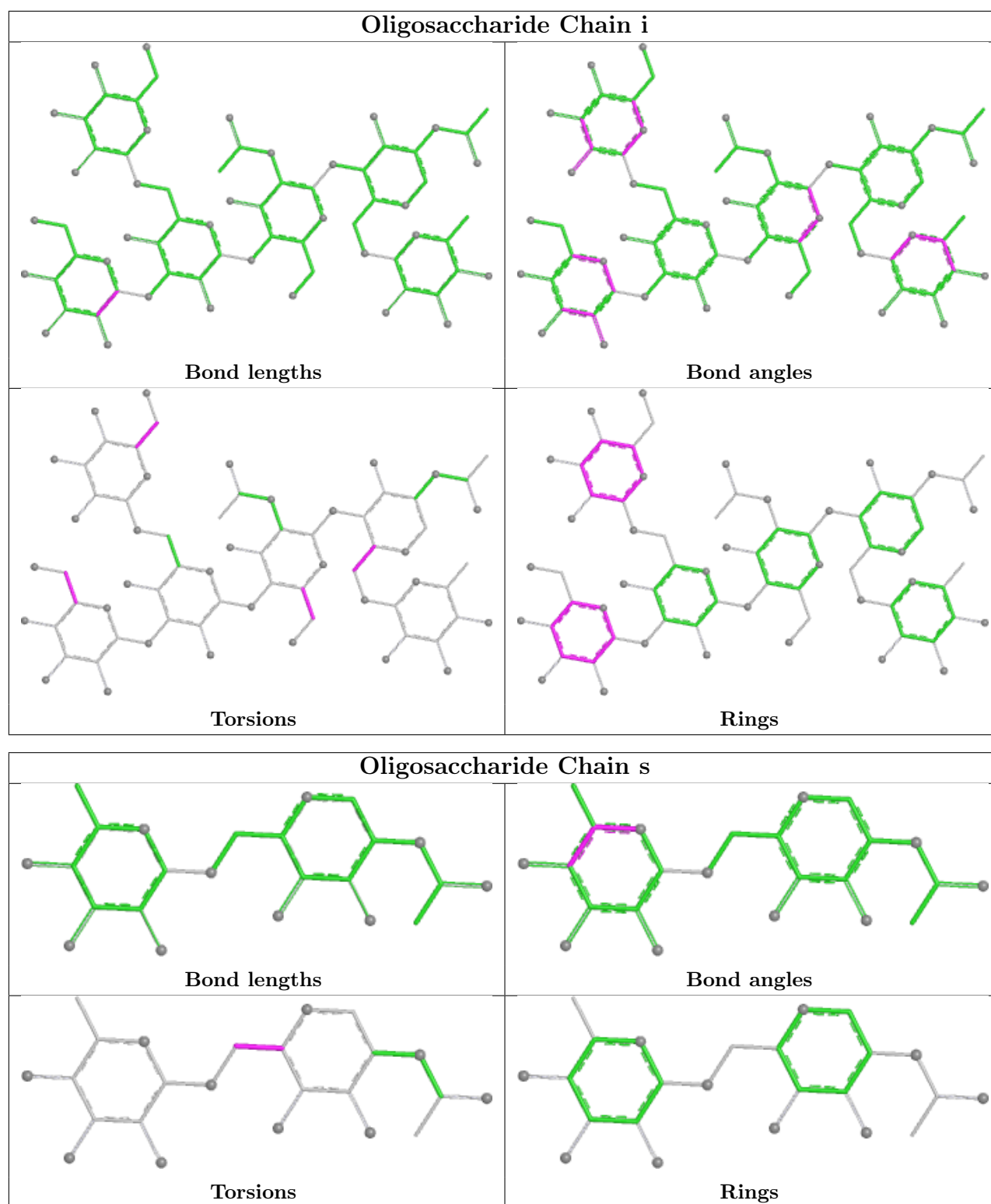












5.6 Ligand geometry [i](#)

19 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$
8	NAG	B	1404	1	14,14,15	0.27	0	17,19,21	0.46	0
8	NAG	A	1402	1	14,14,15	0.50	0	17,19,21	0.47	0
8	NAG	B	1407	1	14,14,15	0.82	1 (7%)	17,19,21	0.62	0
8	NAG	A	1406	1	14,14,15	0.27	0	17,19,21	0.47	0
8	NAG	A	1404	1	14,14,15	0.21	0	17,19,21	0.41	0
8	NAG	B	1406	1	14,14,15	0.19	0	17,19,21	0.42	0
8	NAG	C	1406	1	14,14,15	1.16	1 (7%)	17,19,21	0.59	0
8	NAG	B	1401	1	14,14,15	0.26	0	17,19,21	0.48	0
8	NAG	C	1403	1	14,14,15	0.27	0	17,19,21	0.55	0
8	NAG	A	1403	1	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	C	1405	1	14,14,15	0.42	0	17,19,21	0.48	0
8	NAG	A	1405	1	14,14,15	0.24	0	17,19,21	0.36	0
8	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.40	0
8	NAG	C	1404	1	14,14,15	0.20	0	17,19,21	0.44	0
8	NAG	B	1403	1	14,14,15	0.26	0	17,19,21	0.46	0
8	NAG	C	1402	1	14,14,15	0.29	0	17,19,21	0.34	0
8	NAG	C	1401	1	14,14,15	0.26	0	17,19,21	0.55	0
8	NAG	B	1405	1	14,14,15	0.26	0	17,19,21	0.52	0
8	NAG	A	1401	1	14,14,15	0.28	0	17,19,21	0.54	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
8	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1402	1	-	4/6/23/26	0/1/1/1
8	NAG	B	1407	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1406	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1404	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
8	NAG	C	1406	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1401	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1402	1	-	3/6/23/26	0/1/1/1
8	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1405	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1401	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1406	NAG	C1-C2	3.91	1.57	1.52
8	B	1407	NAG	C1-C2	2.99	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1403	NAG	O5-C5-C6-O6
8	C	1401	NAG	O5-C5-C6-O6
8	A	1401	NAG	C4-C5-C6-O6
8	A	1401	NAG	O5-C5-C6-O6
8	B	1404	NAG	O5-C5-C6-O6
8	B	1405	NAG	O5-C5-C6-O6
8	B	1407	NAG	C4-C5-C6-O6
8	A	1403	NAG	C4-C5-C6-O6
8	C	1401	NAG	C4-C5-C6-O6
8	C	1405	NAG	O5-C5-C6-O6
8	A	1402	NAG	C4-C5-C6-O6
8	C	1404	NAG	O5-C5-C6-O6
8	A	1405	NAG	O5-C5-C6-O6
8	B	1405	NAG	C4-C5-C6-O6
8	B	1401	NAG	O5-C5-C6-O6
8	B	1404	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	1404	NAG	C4-C5-C6-O6
8	A	1402	NAG	C8-C7-N2-C2
8	A	1402	NAG	O7-C7-N2-C2
8	A	1406	NAG	C8-C7-N2-C2
8	A	1406	NAG	O7-C7-N2-C2
8	B	1402	NAG	C8-C7-N2-C2
8	B	1402	NAG	O7-C7-N2-C2
8	B	1405	NAG	C8-C7-N2-C2
8	B	1405	NAG	O7-C7-N2-C2
8	B	1406	NAG	C8-C7-N2-C2
8	B	1406	NAG	O7-C7-N2-C2
8	B	1407	NAG	O5-C5-C6-O6
8	A	1402	NAG	O5-C5-C6-O6
8	B	1401	NAG	C4-C5-C6-O6
8	A	1405	NAG	C4-C5-C6-O6
8	C	1405	NAG	C4-C5-C6-O6
8	A	1406	NAG	O5-C5-C6-O6
8	B	1402	NAG	O5-C5-C6-O6
8	B	1406	NAG	O5-C5-C6-O6
8	B	1407	NAG	C3-C2-N2-C7
8	C	1406	NAG	C3-C2-N2-C7
8	A	1406	NAG	C4-C5-C6-O6
8	B	1407	NAG	C1-C2-N2-C7
8	A	1404	NAG	O5-C5-C6-O6

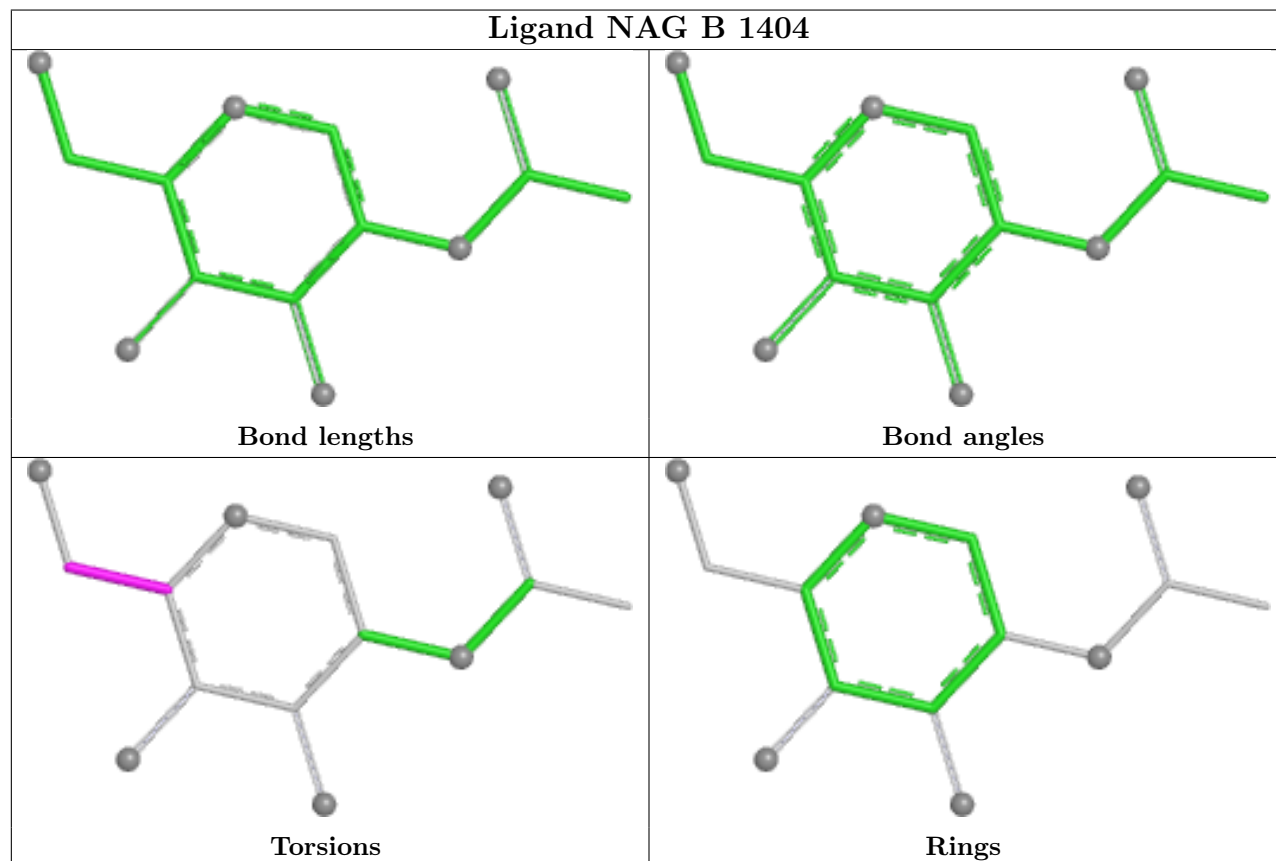
There are no ring outliers.

10 monomers are involved in 17 short contacts:

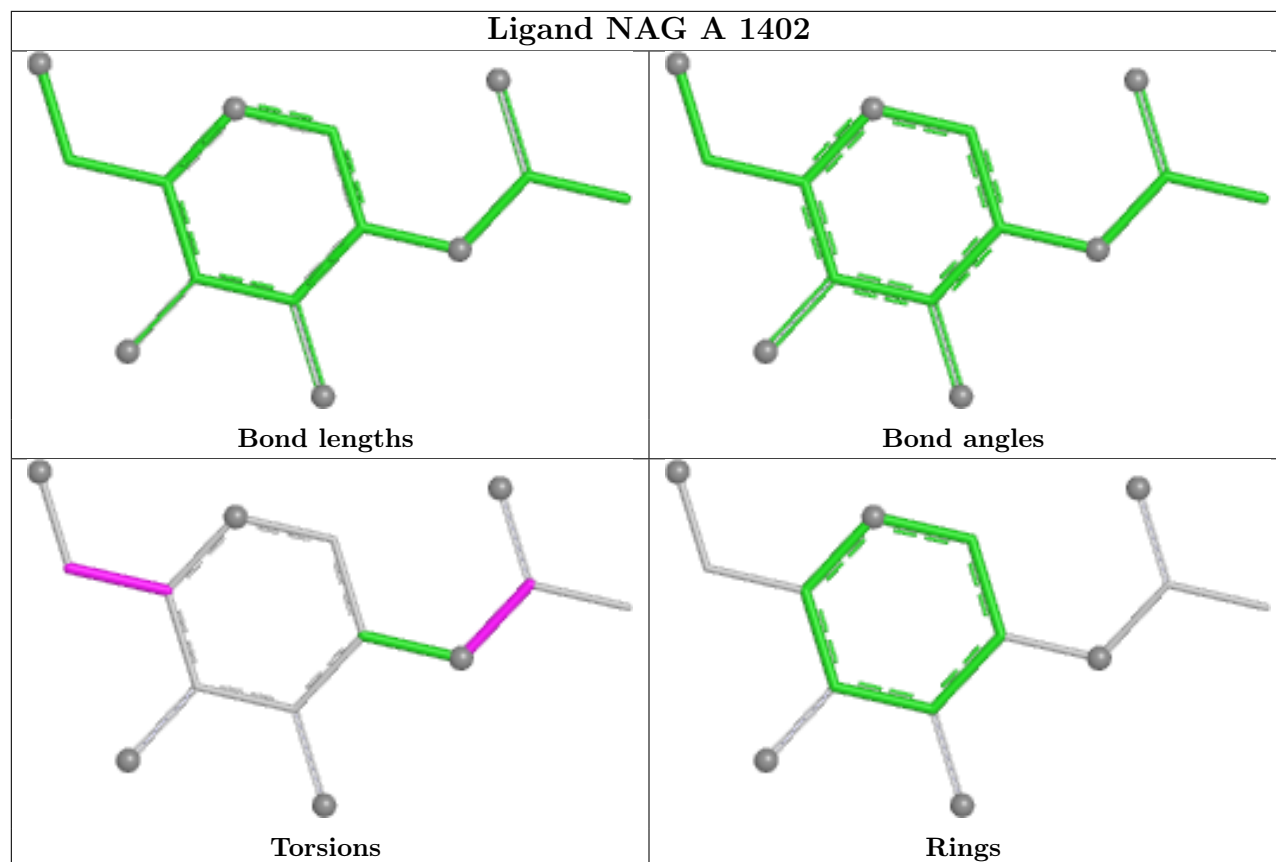
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1404	NAG	1	0
8	A	1402	NAG	4	0
8	B	1407	NAG	2	0
8	A	1406	NAG	1	0
8	B	1406	NAG	1	0
8	C	1406	NAG	1	0
8	B	1401	NAG	1	0
8	B	1402	NAG	4	0
8	B	1403	NAG	1	0
8	A	1401	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

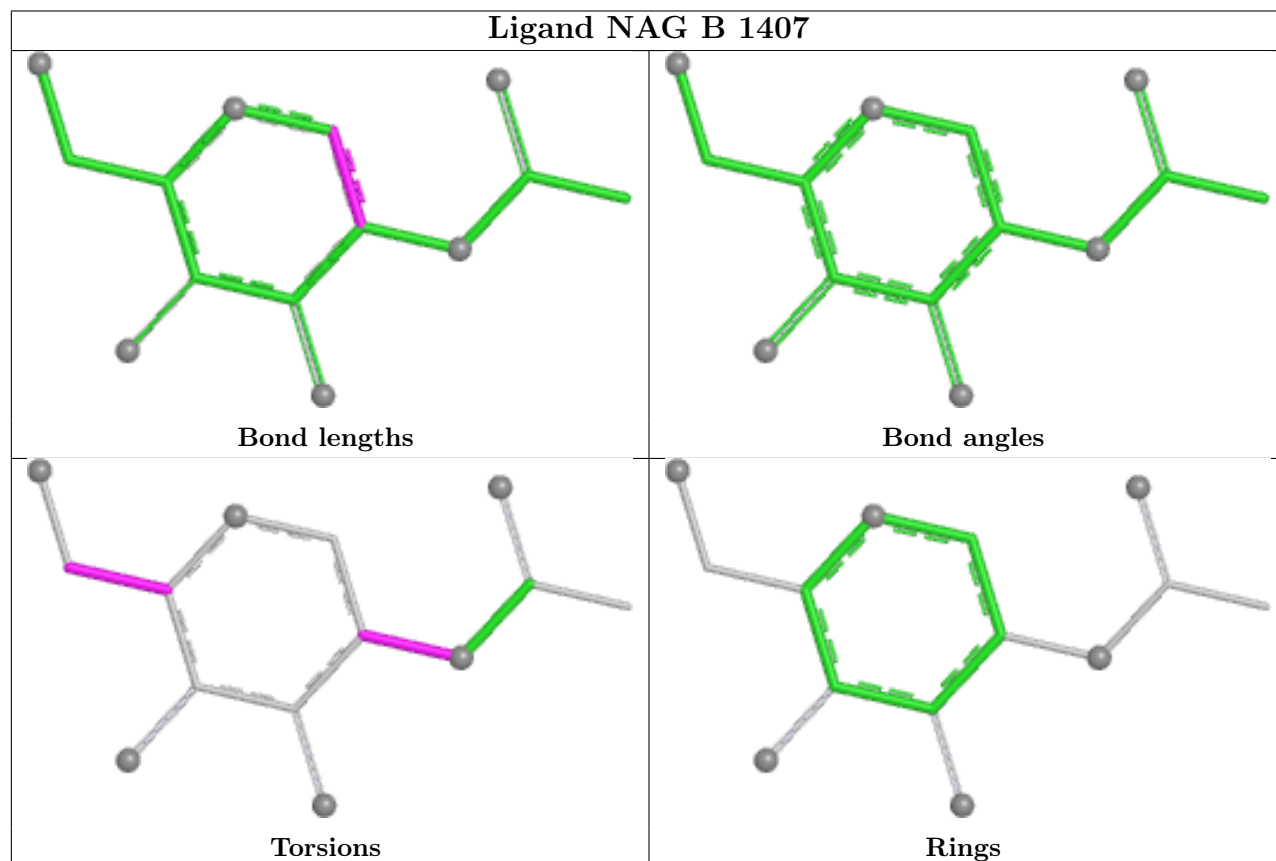
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



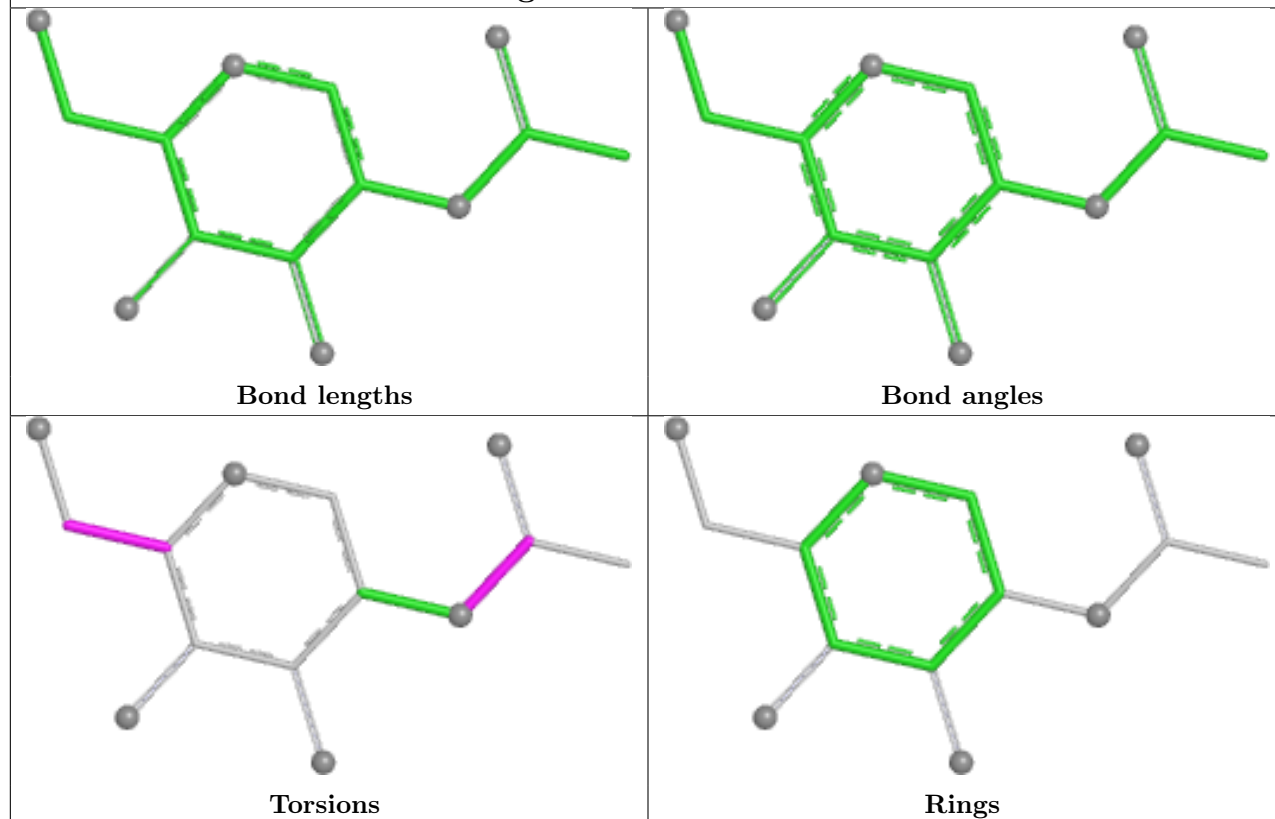
Ligand NAG A 1402



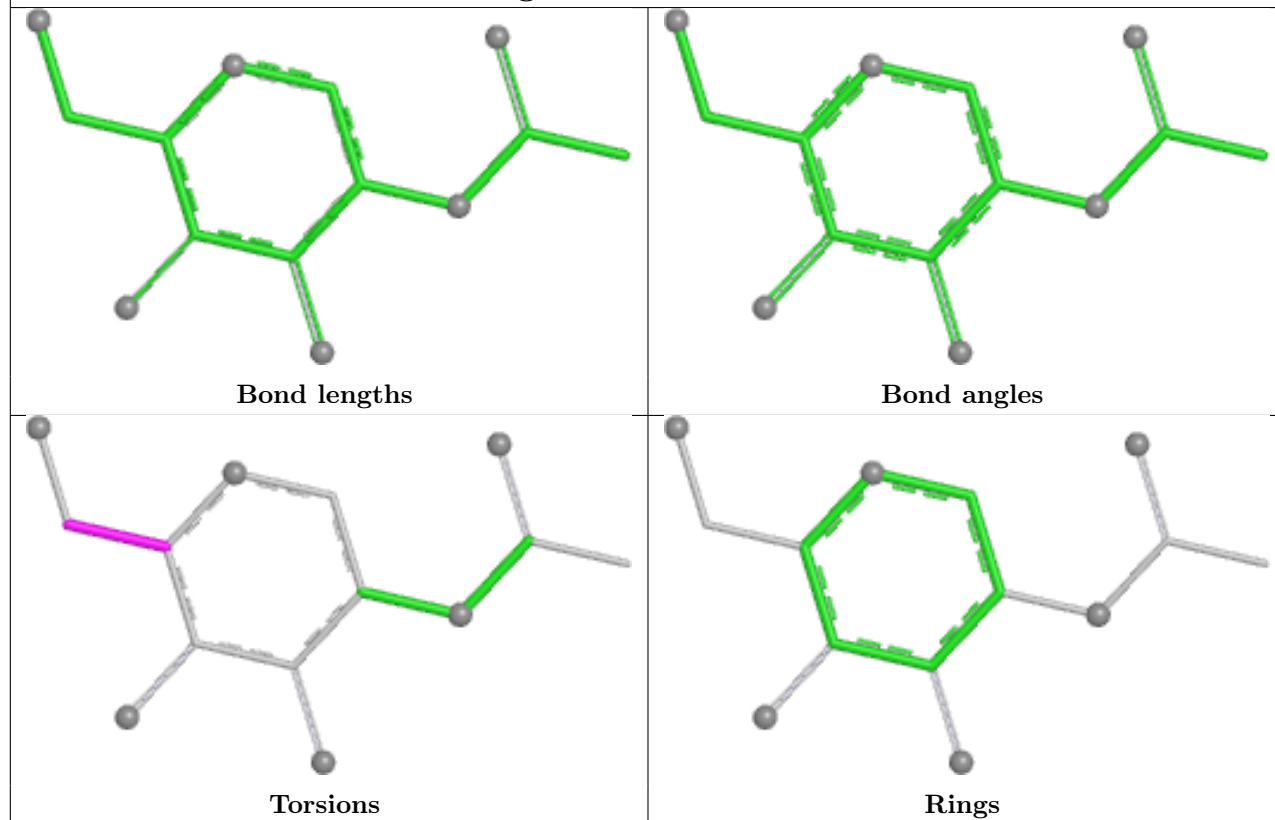
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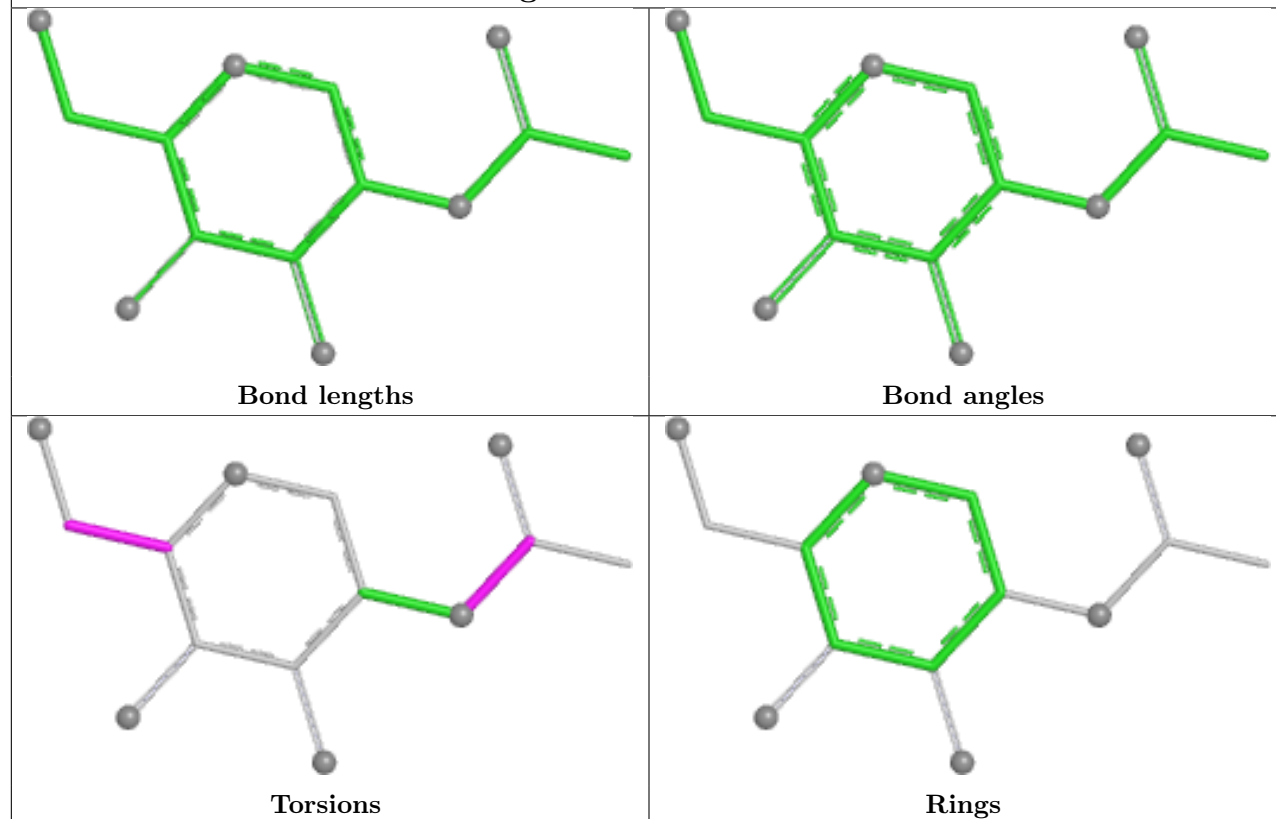
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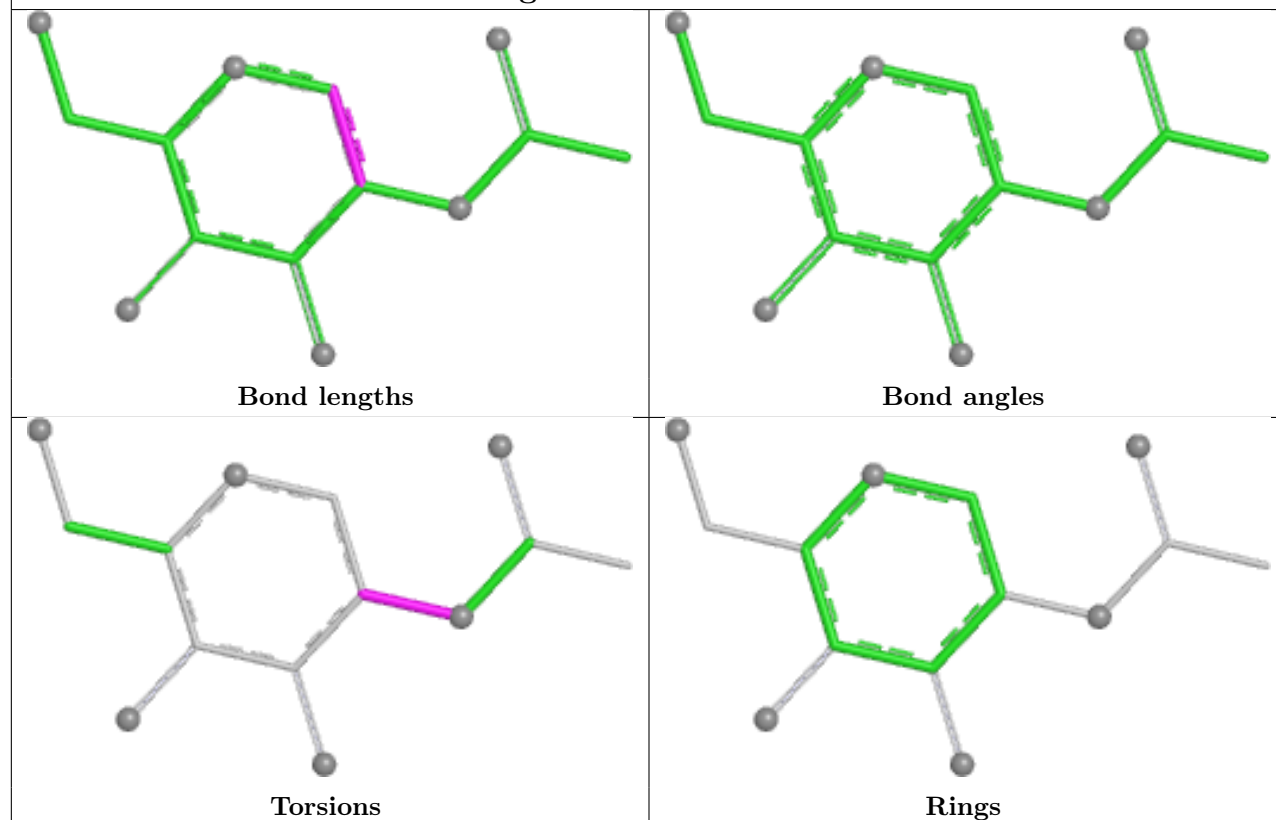
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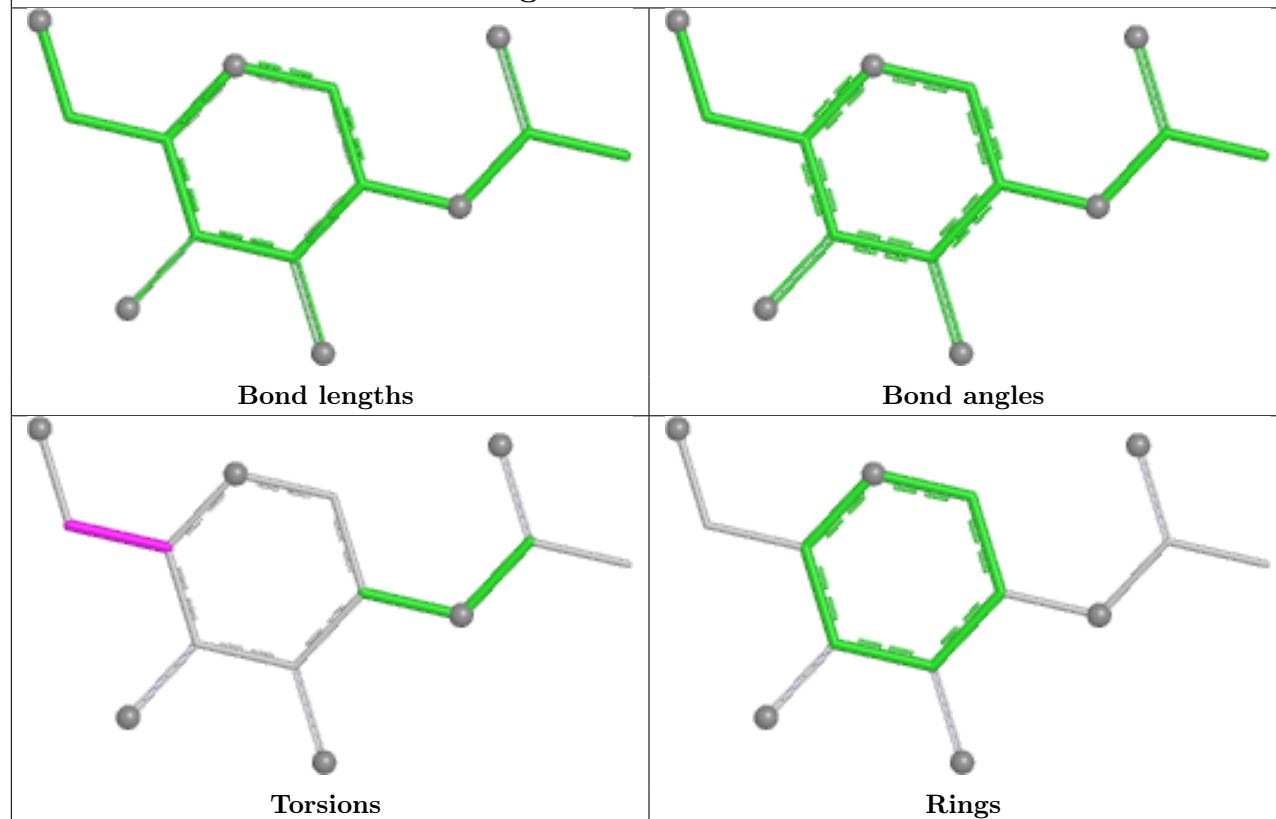
Ligand NAG B 1406



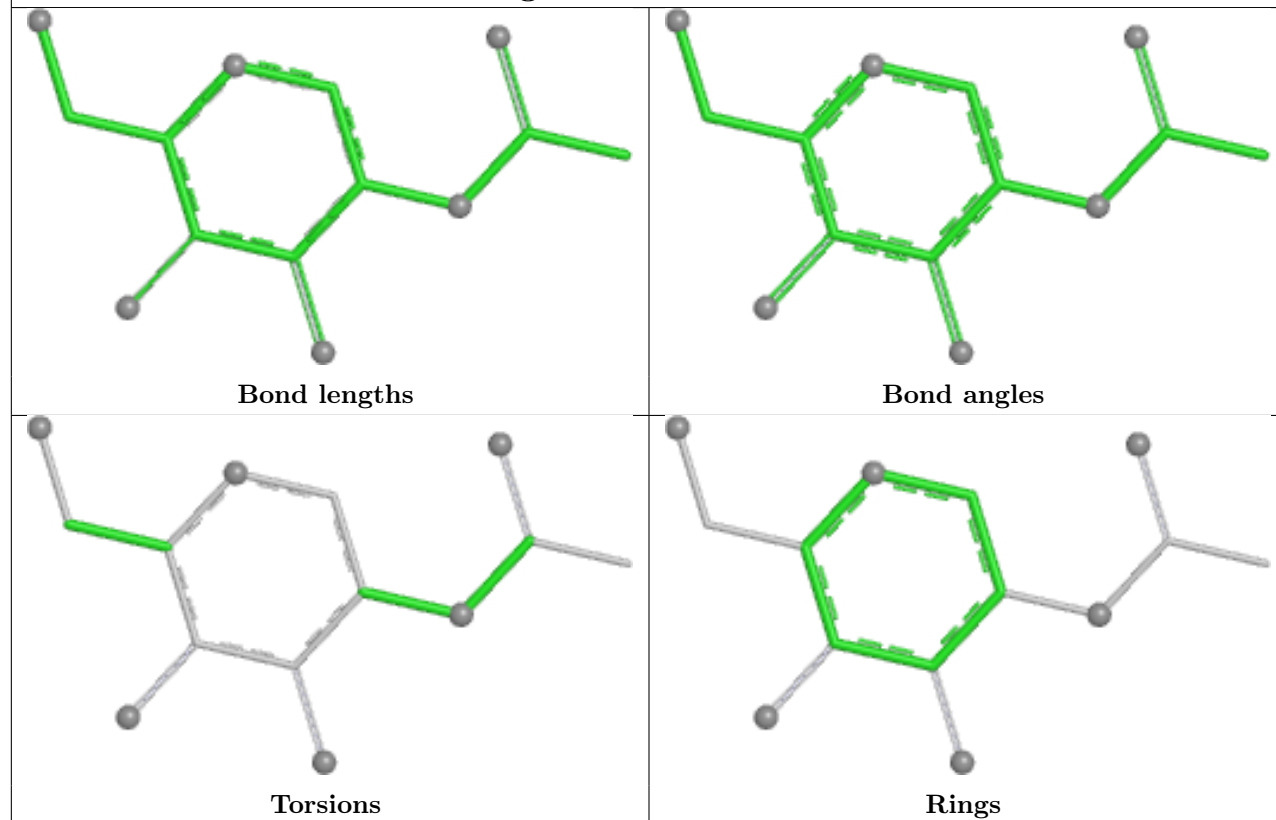
Ligand NAG C 1406



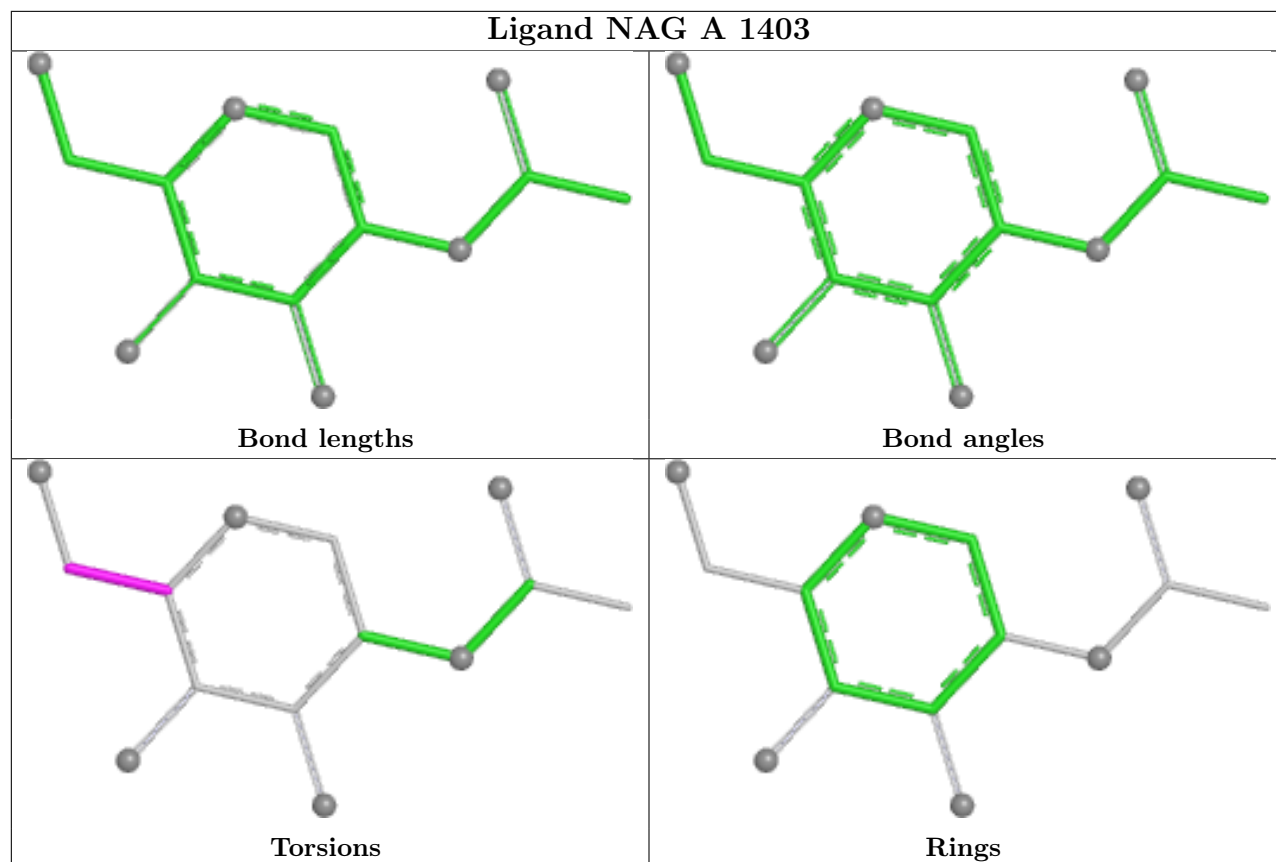
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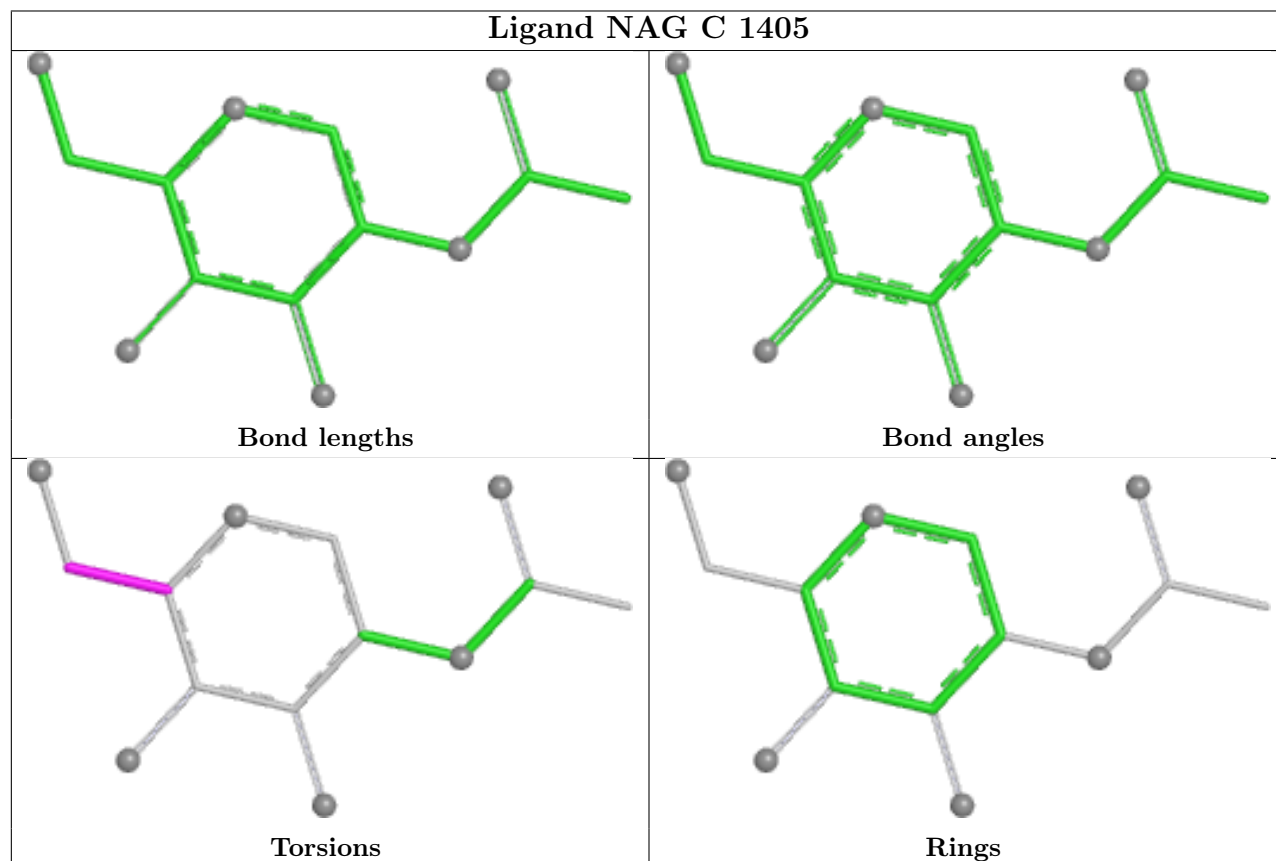
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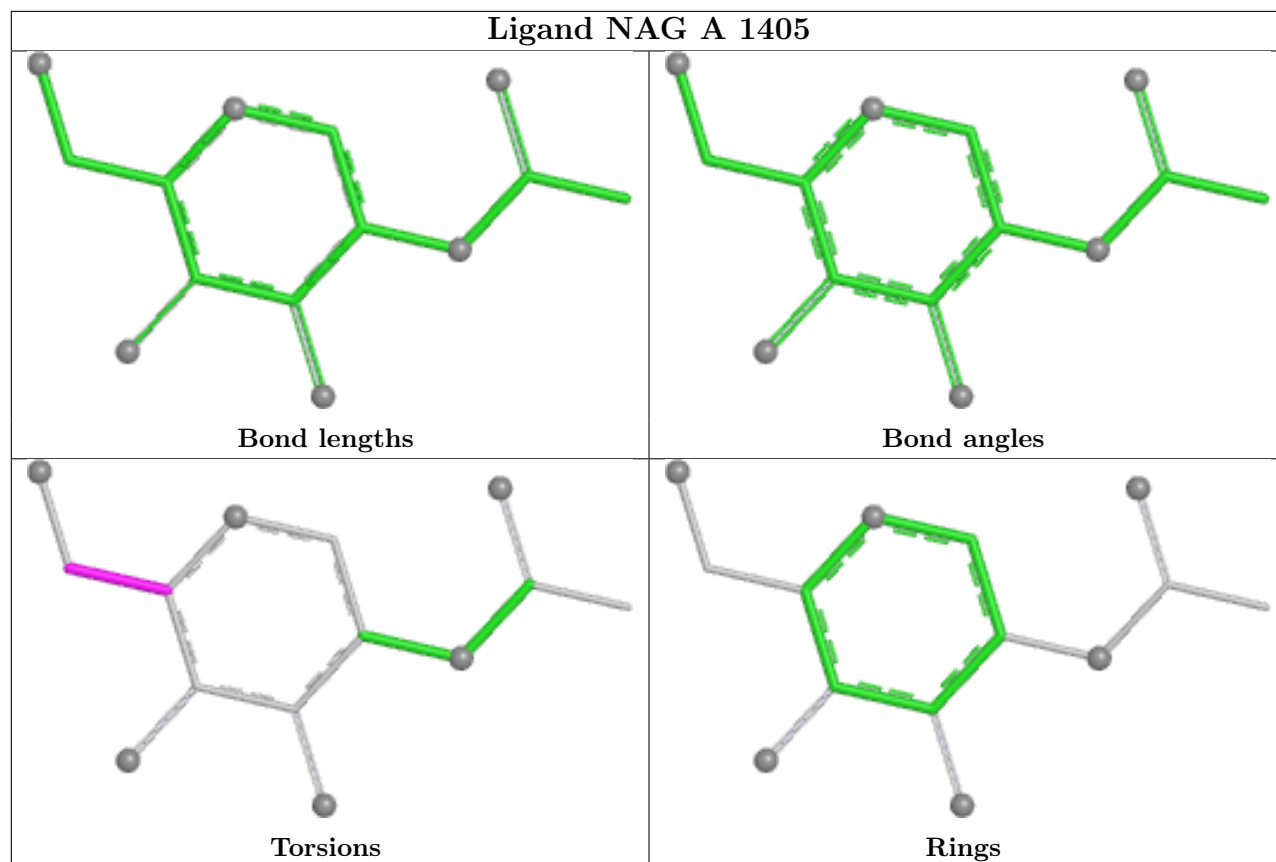
Ligand NAG A 1403



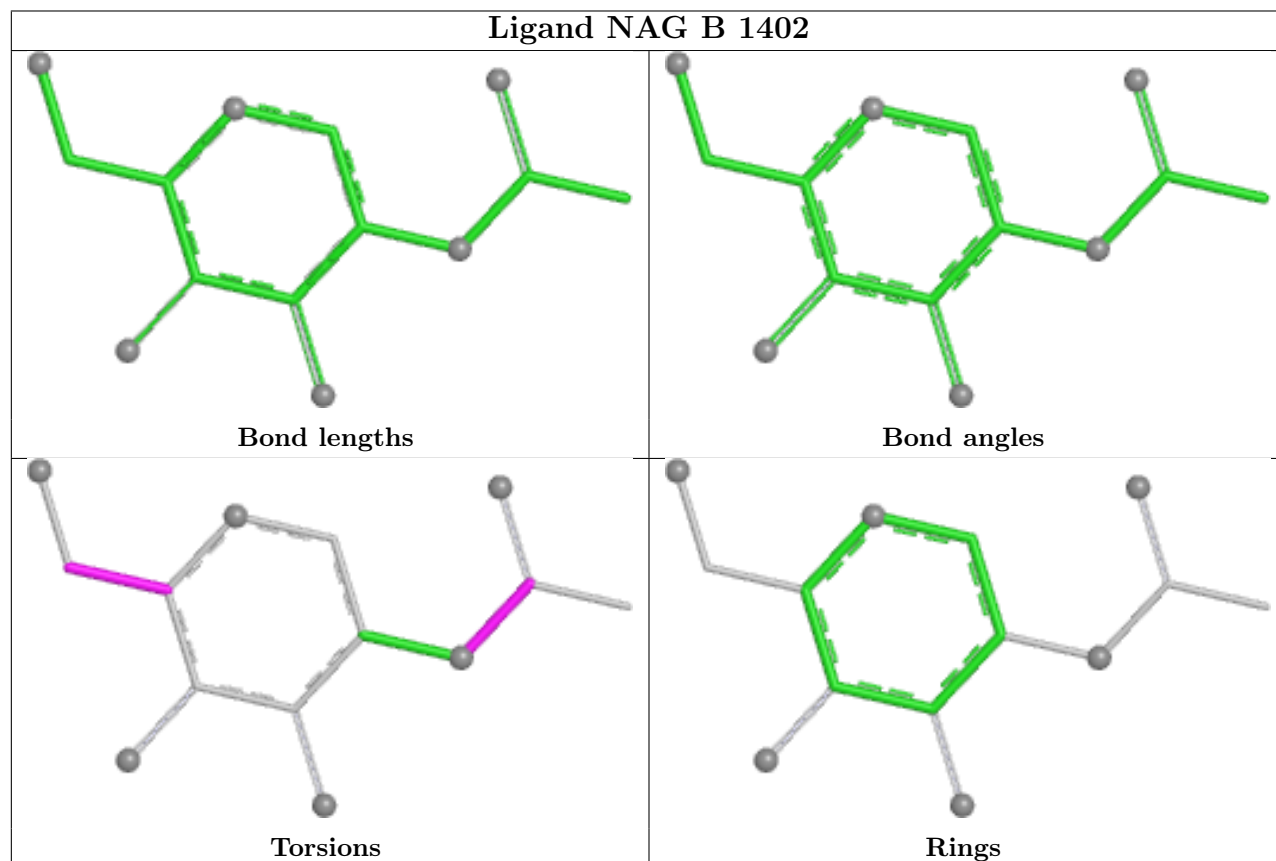
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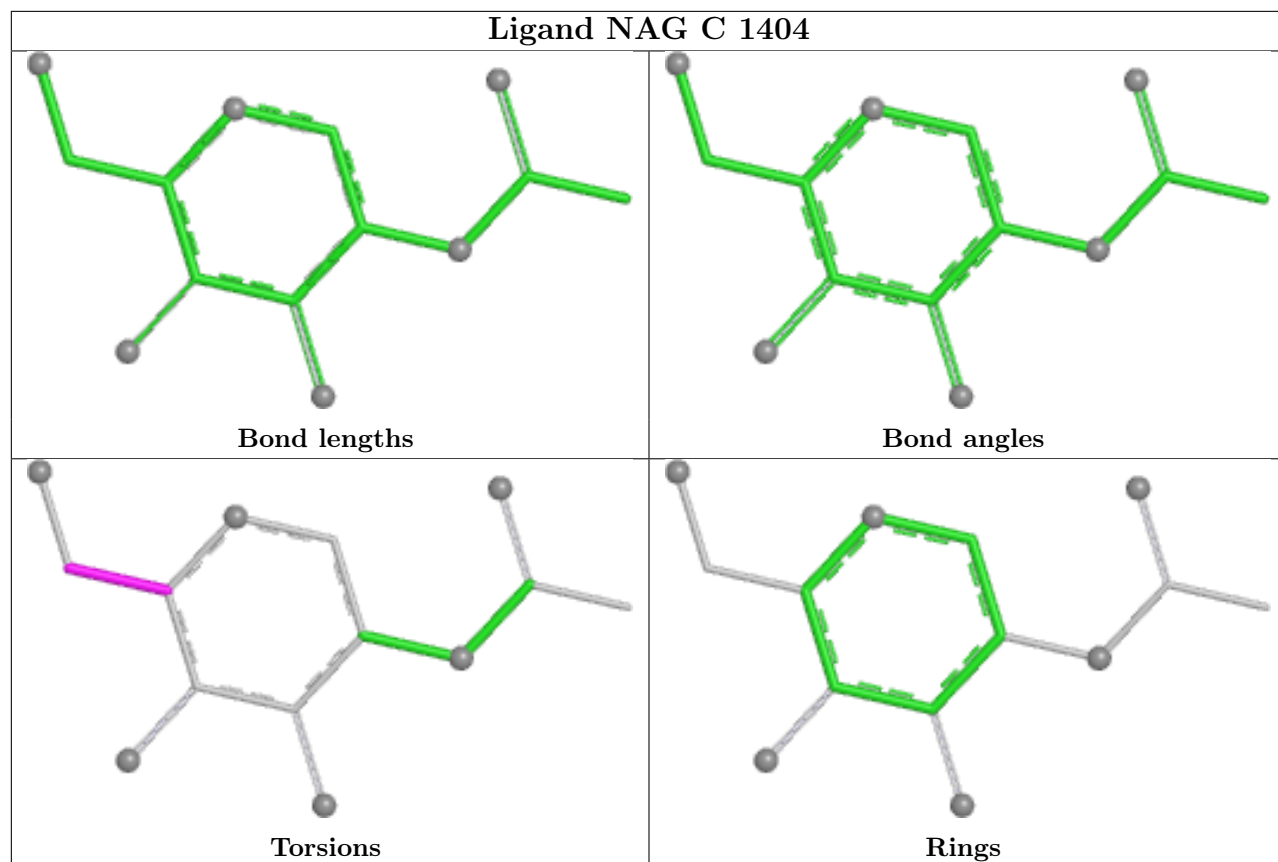
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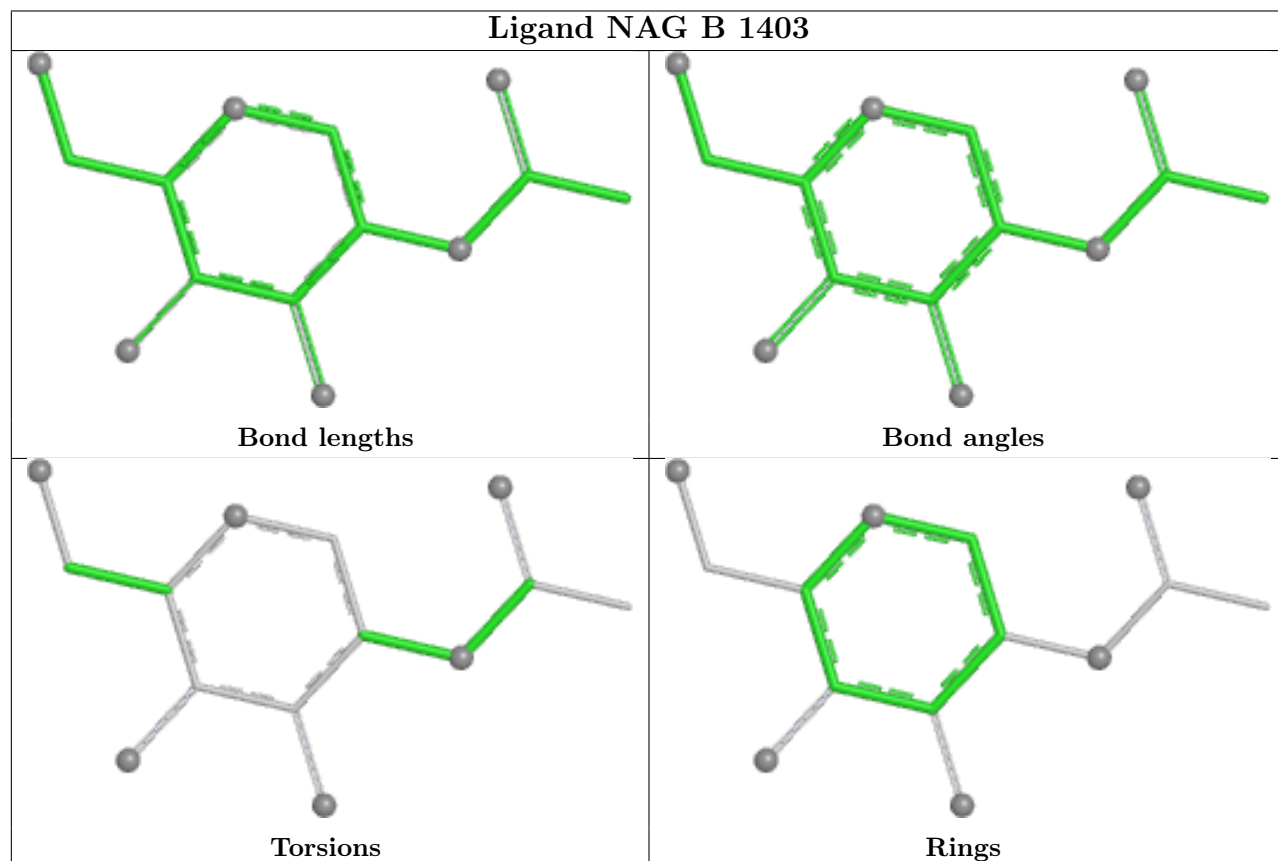
Ligand NAG B 1402



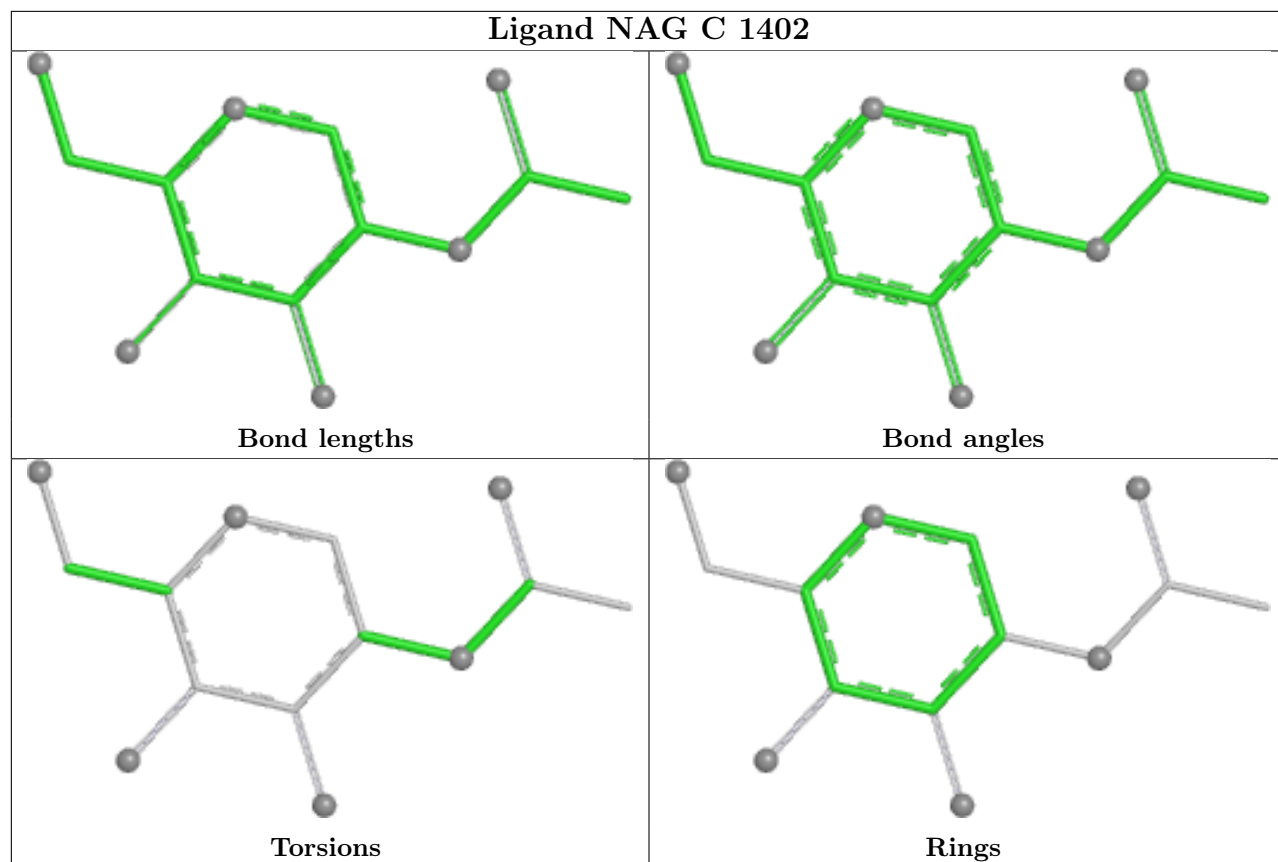
Ligand NAG C 1404



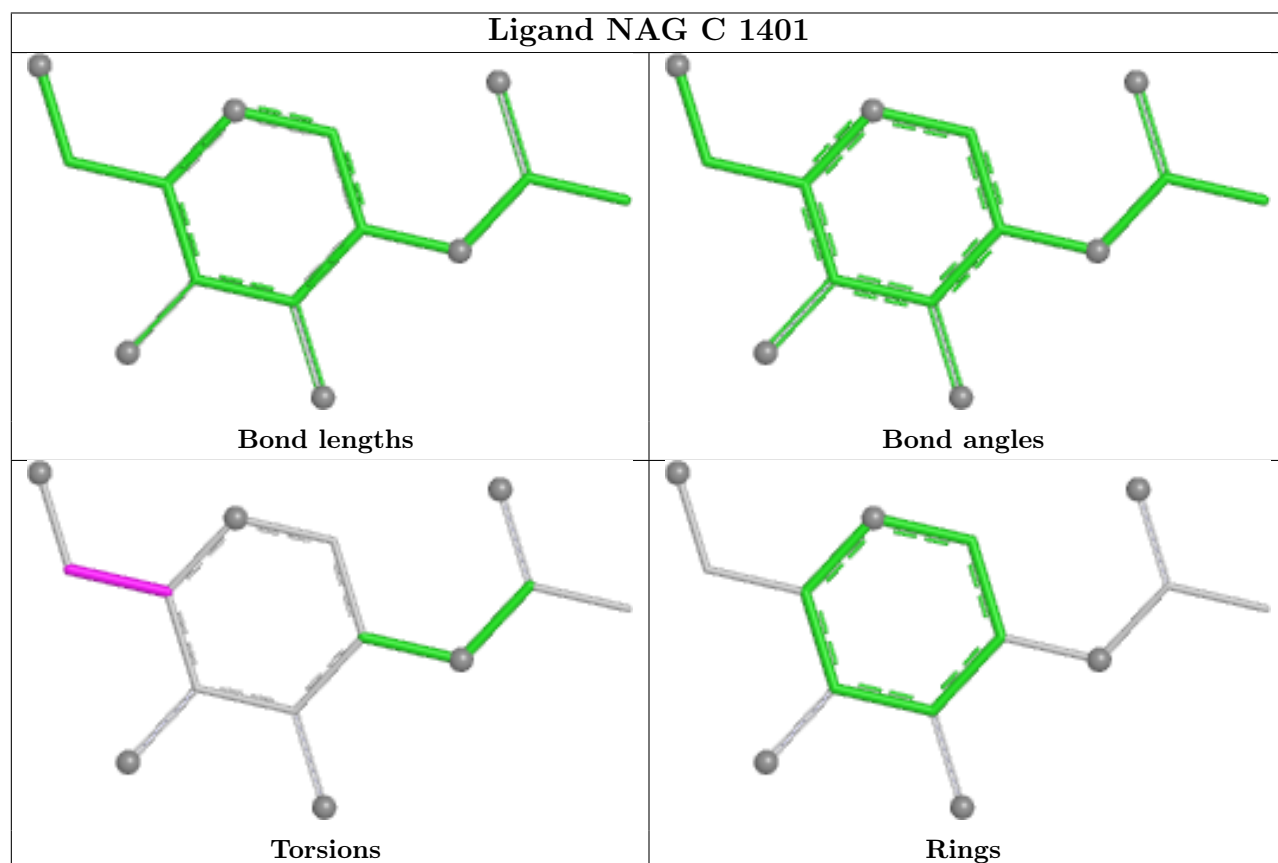
Ligand NAG B 1403



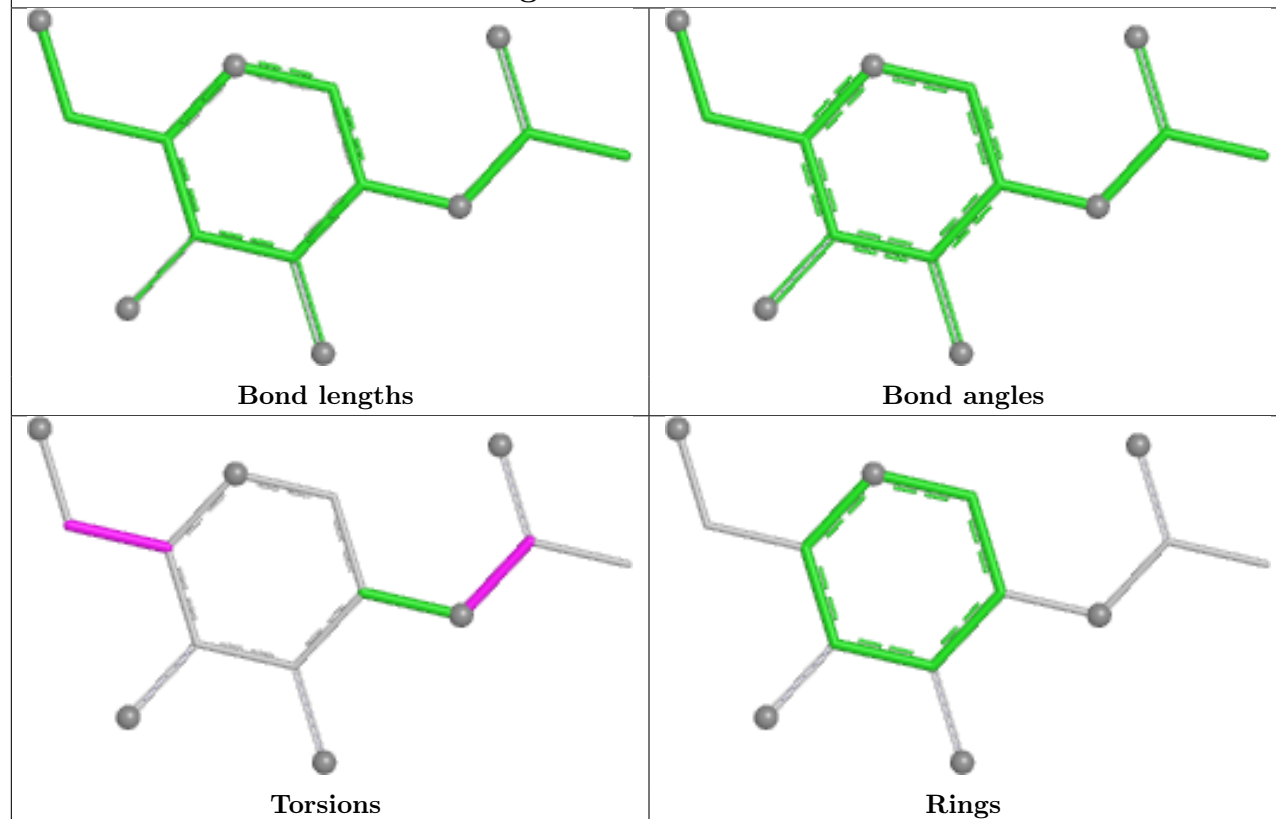
Ligand NAG C 1402



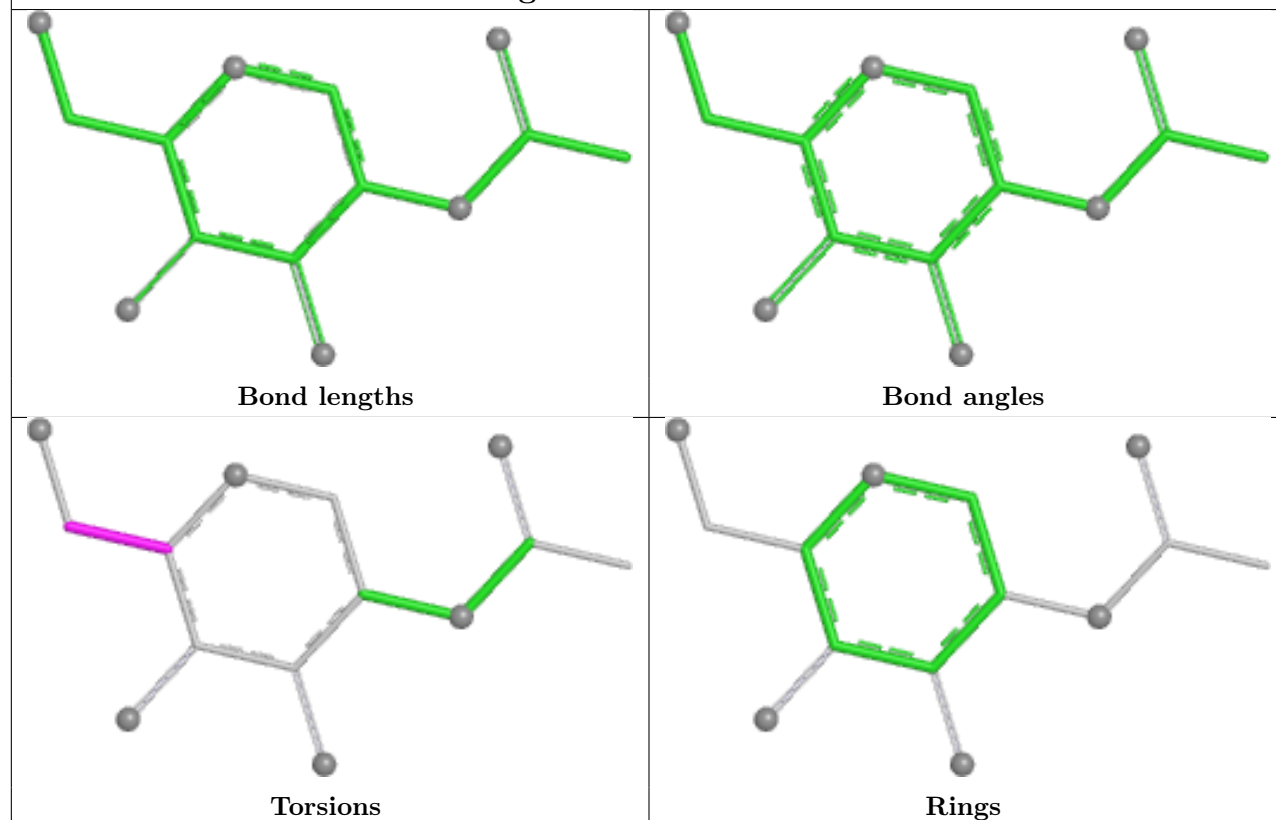
Ligand NAG C 1401



Ligand NAG B 1405



Ligand NAG A 1401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

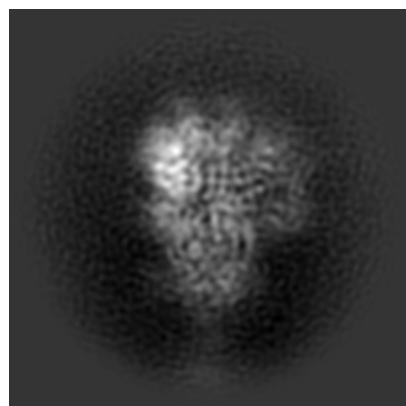
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32338. These allow visual inspection of the internal detail of the map and identification of artifacts.

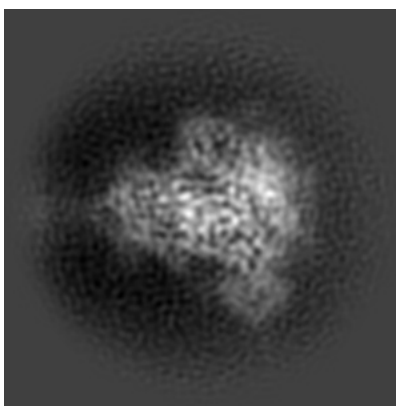
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

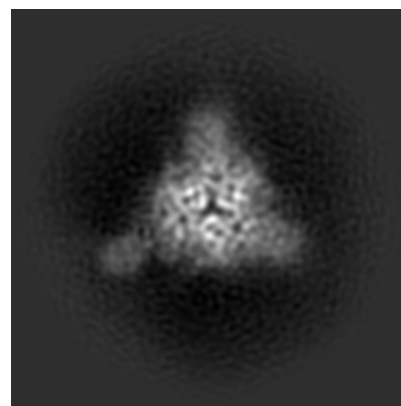
6.1.1 Primary map



X

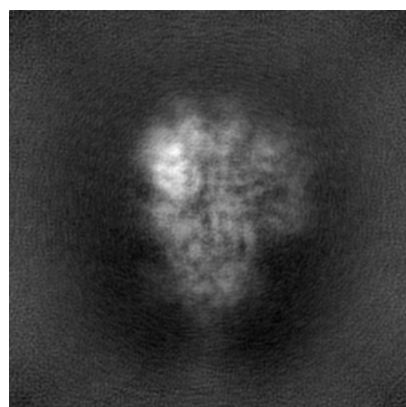


Y

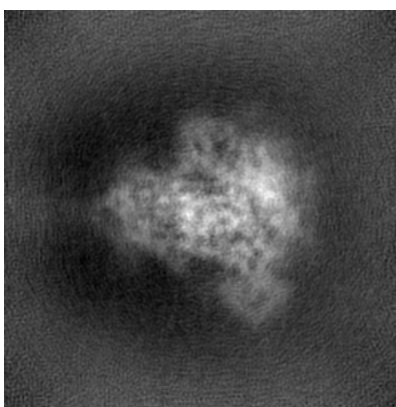


Z

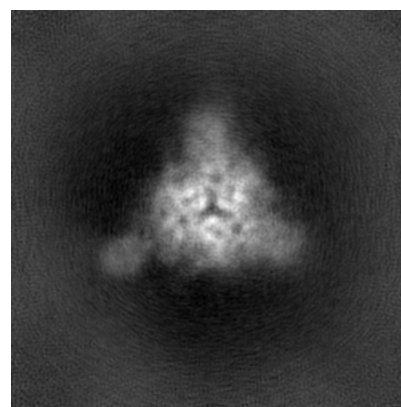
6.1.2 Raw map



X



Y

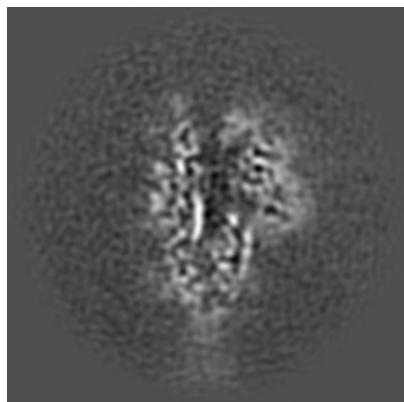


Z

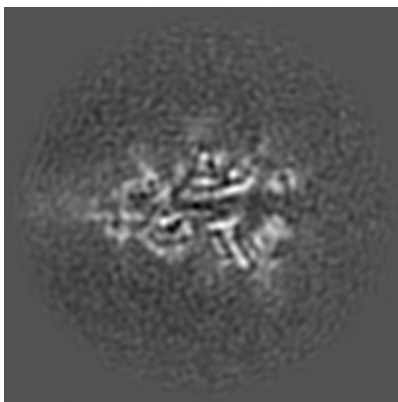
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

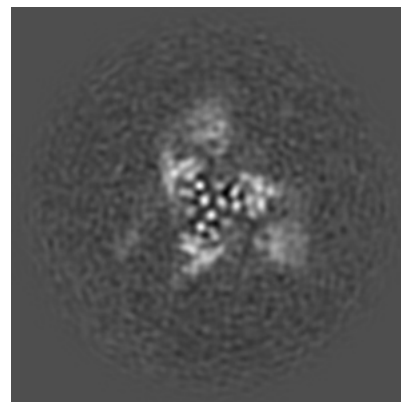
6.2.1 Primary map



X Index: 110

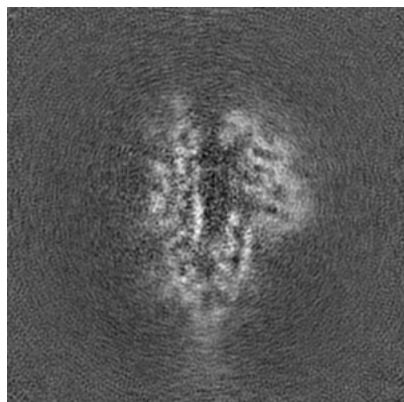


Y Index: 110

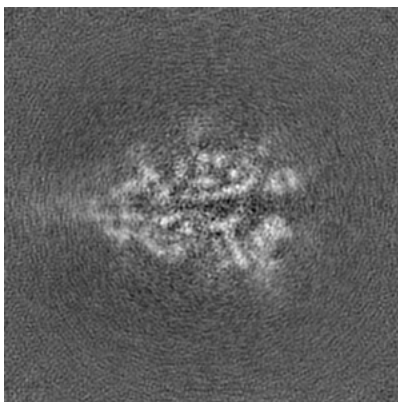


Z Index: 110

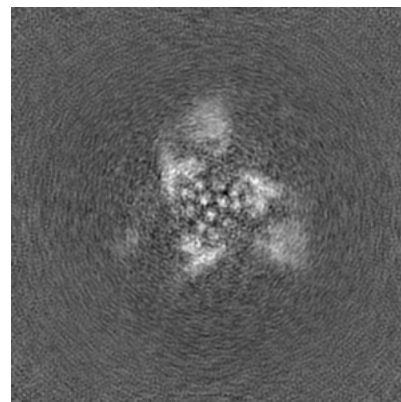
6.2.2 Raw map



X Index: 110



Y Index: 110

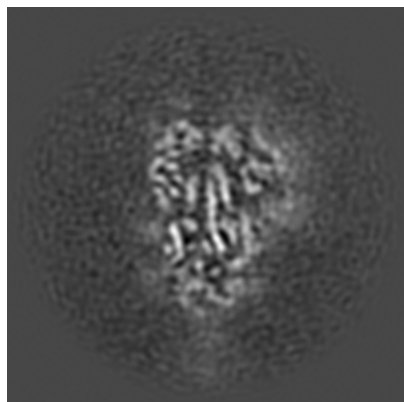


Z Index: 110

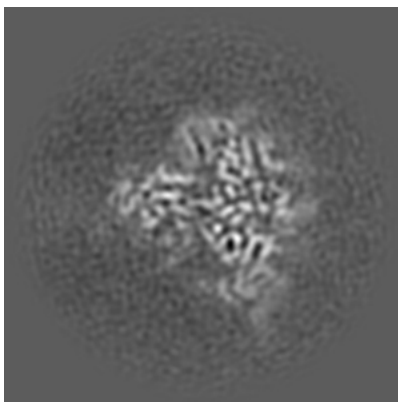
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

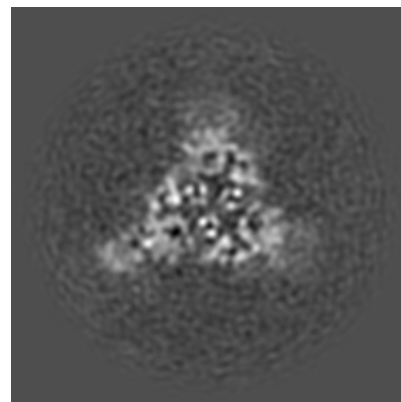
6.3.1 Primary map



X Index: 116

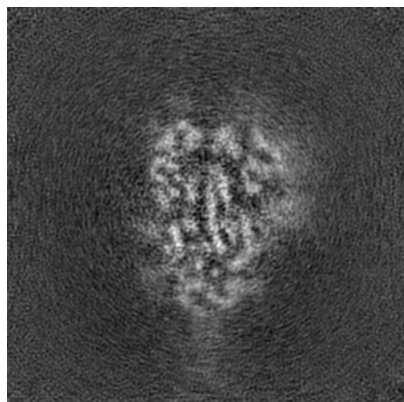


Y Index: 94

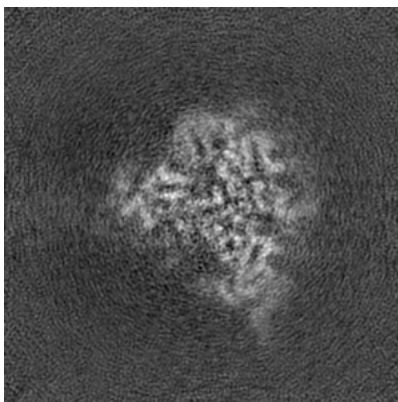


Z Index: 132

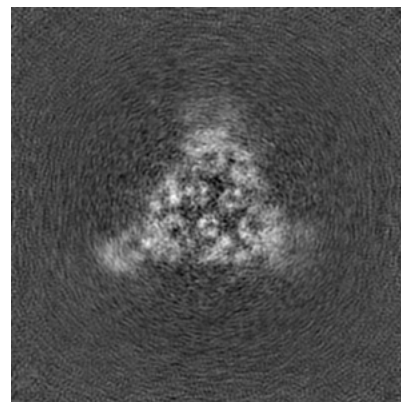
6.3.2 Raw map



X Index: 116



Y Index: 93

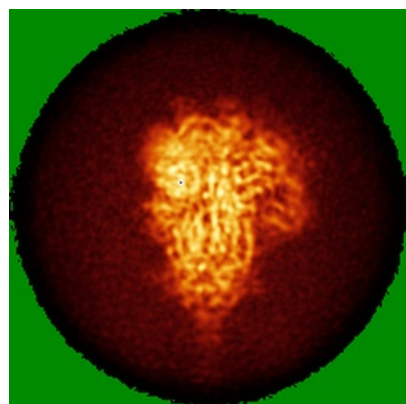


Z Index: 132

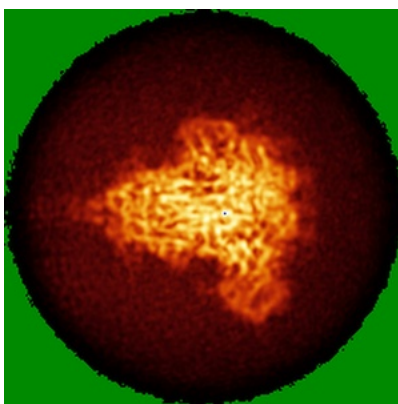
The images above show the largest variance slices of the map in three orthogonal directions.

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

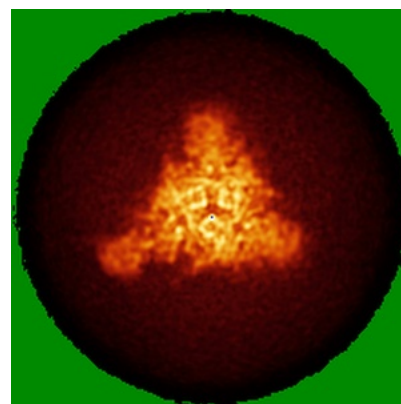
6.4.1 Primary map



X

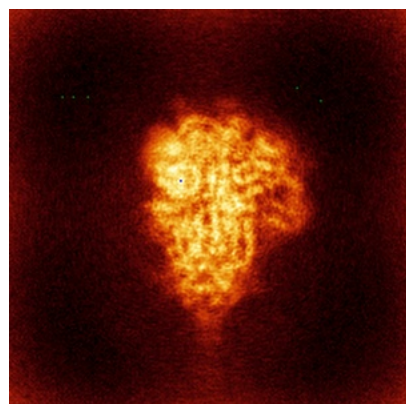


Y

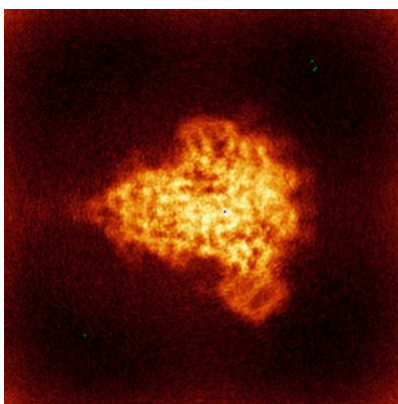


Z

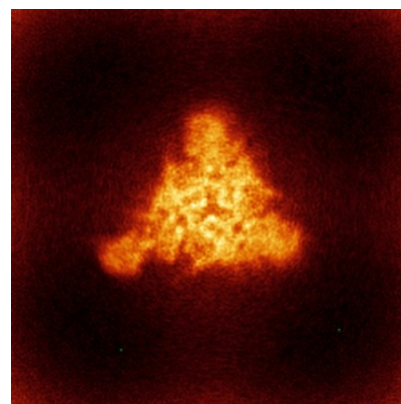
6.4.2 Raw map



X



Y



Z

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

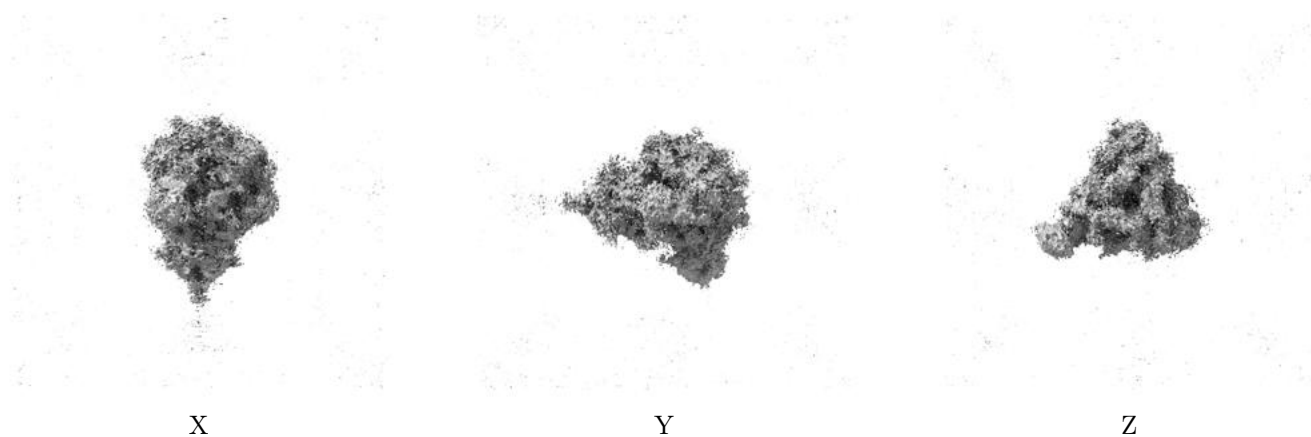
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

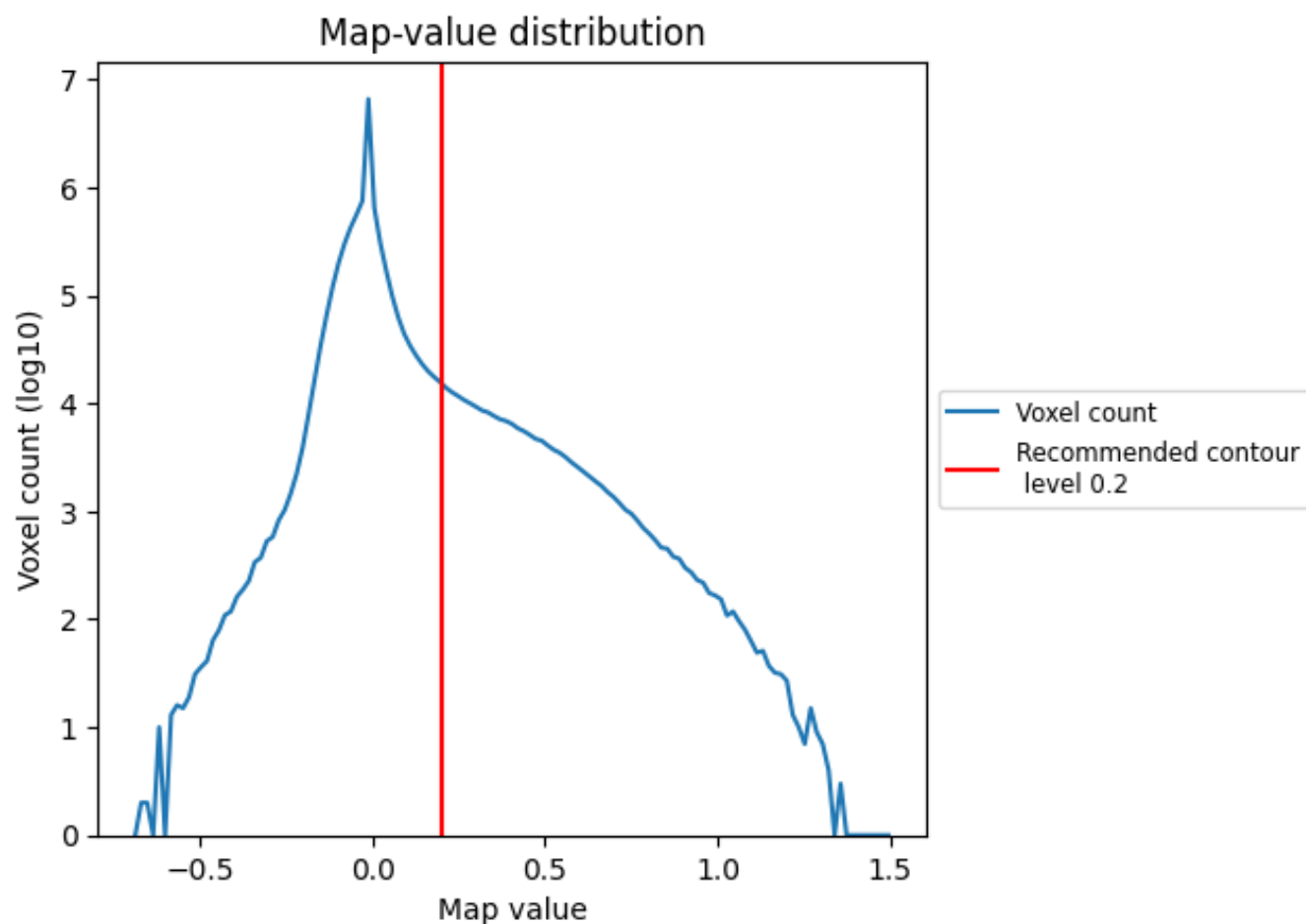
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

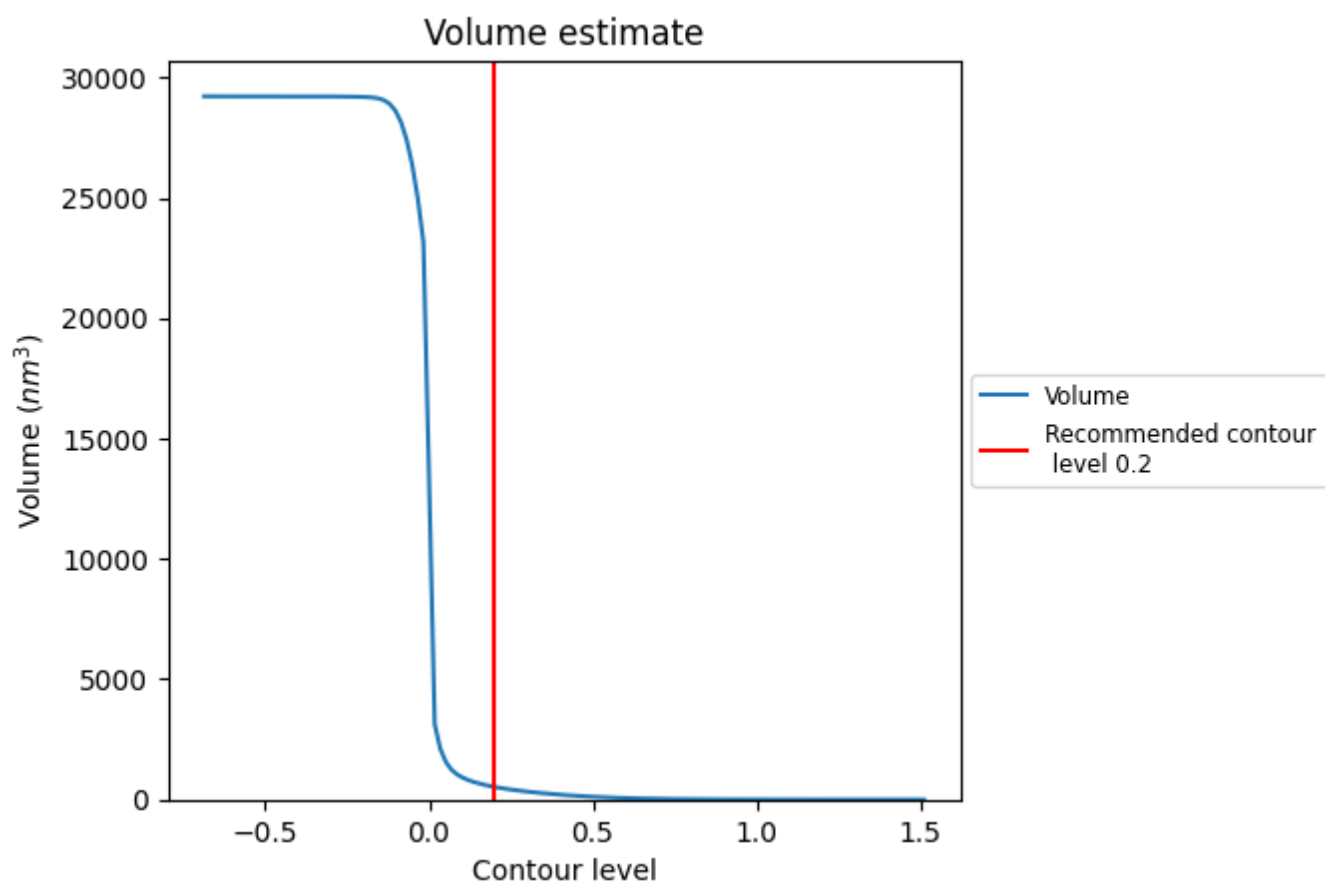
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

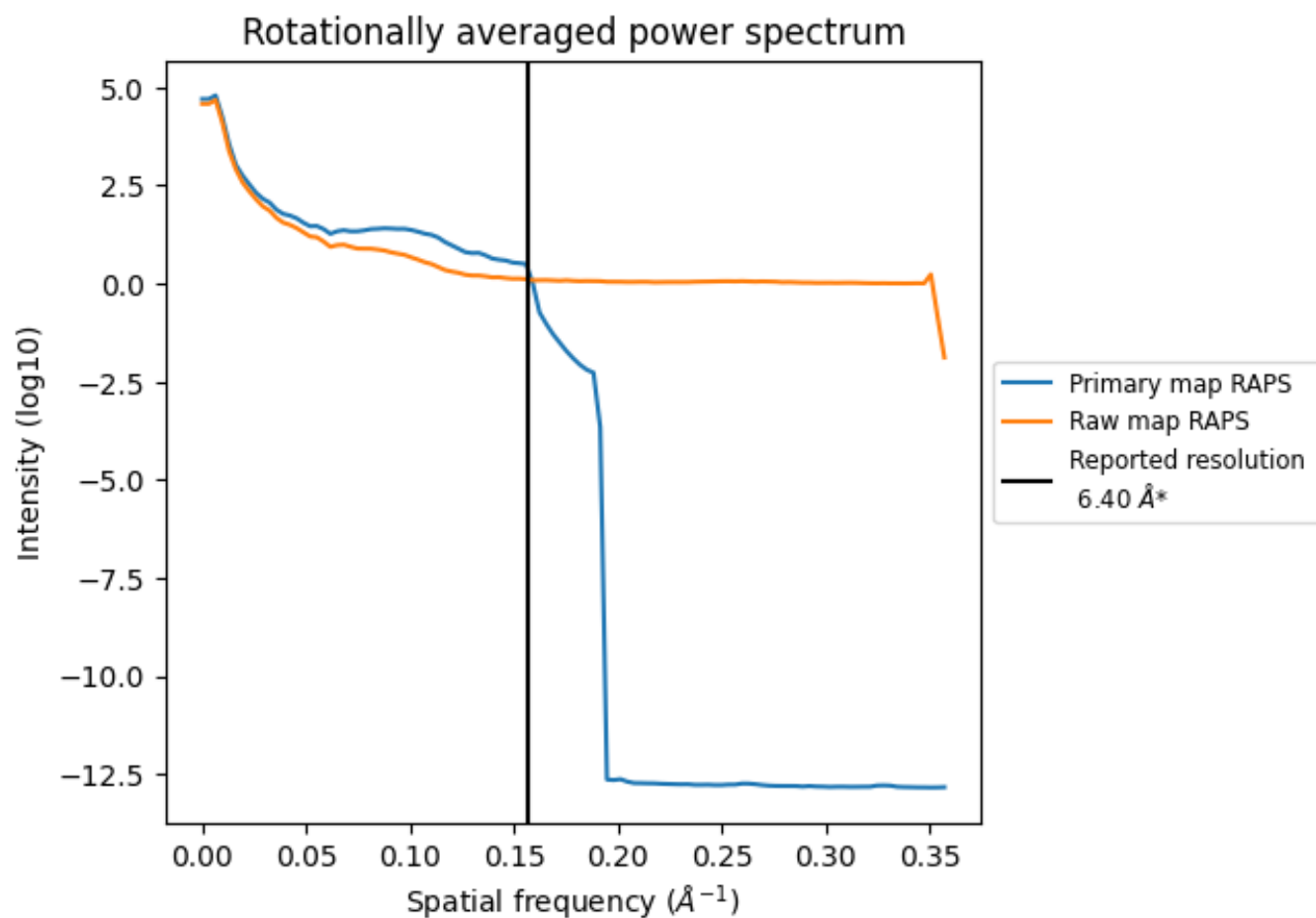
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 524 nm³; this corresponds to an approximate mass of 473 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

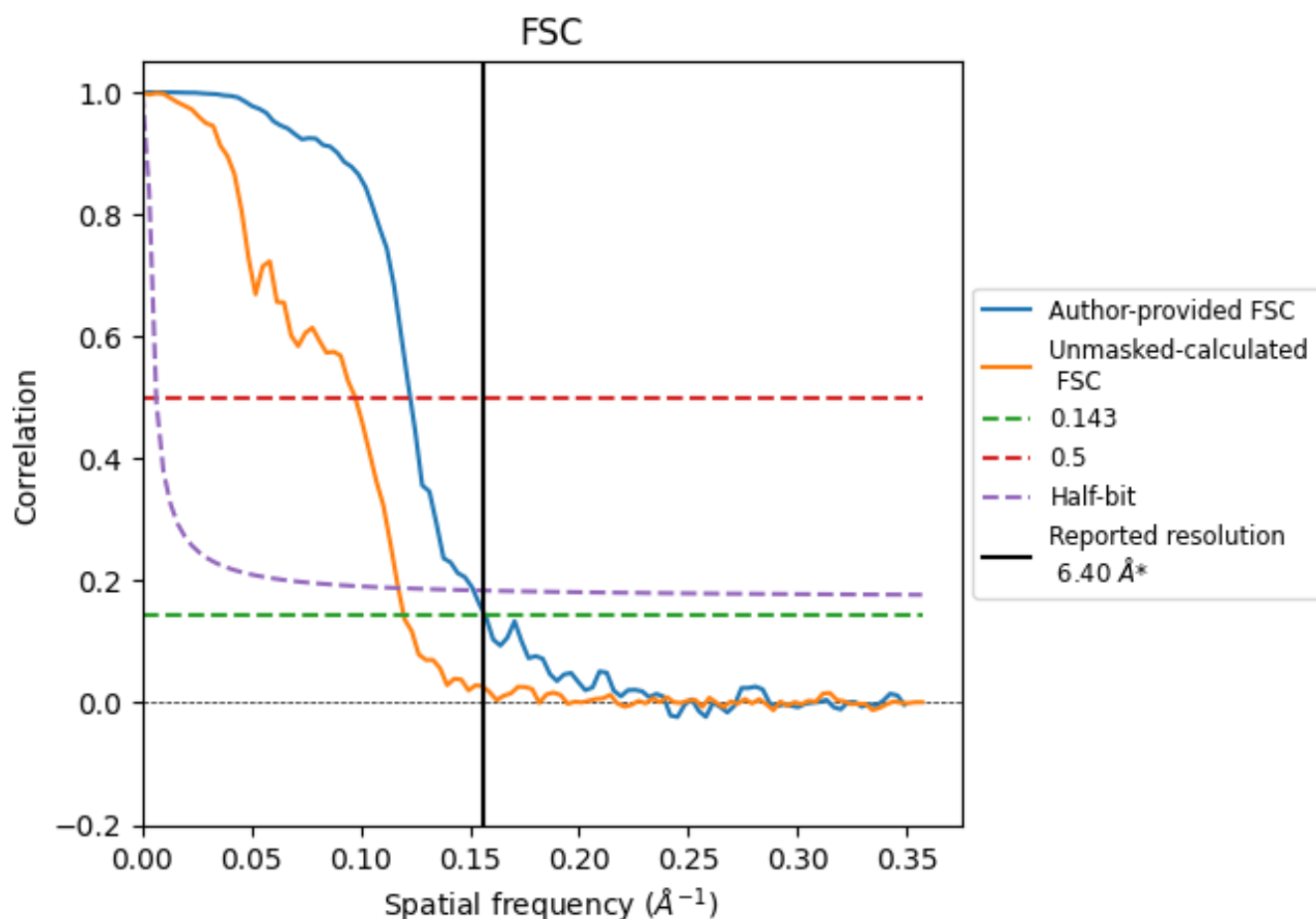


*Reported resolution corresponds to spatial frequency of 0.156 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.156 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

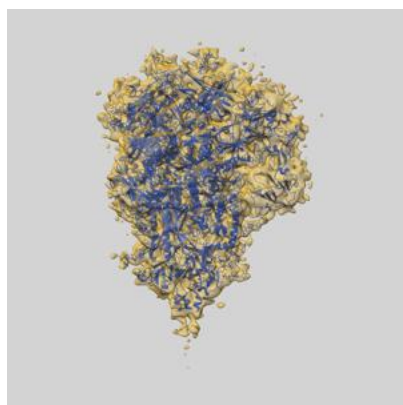
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.40	-	-
Author-provided FSC curve	6.37	8.15	6.60
Unmasked-calculated*	8.35	10.26	8.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.35 differs from the reported value 6.4 by more than 10 %

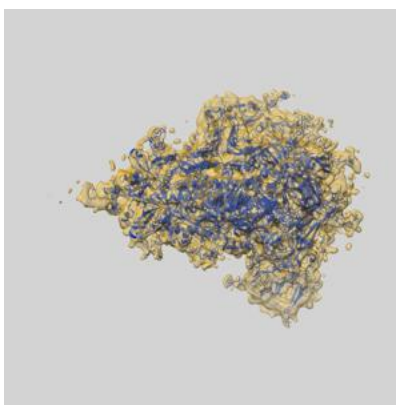
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32338 and PDB model 7W73. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

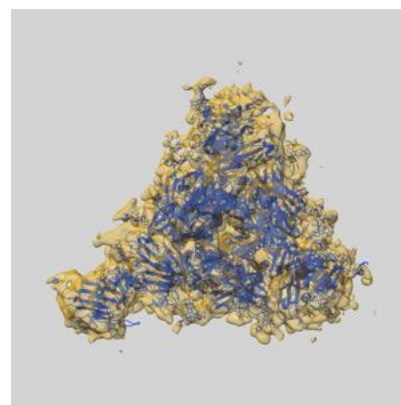
9.1 Map-model overlay [i](#)



X



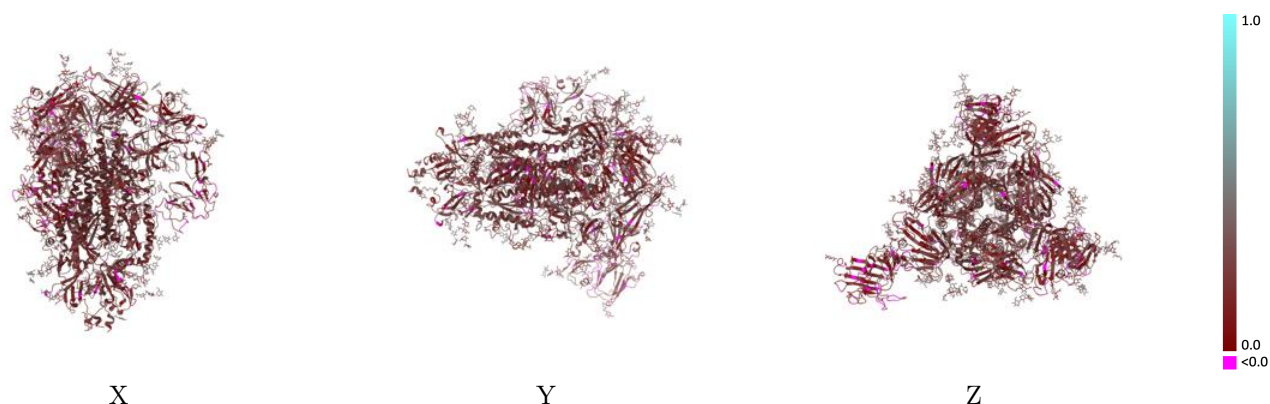
Y



Z

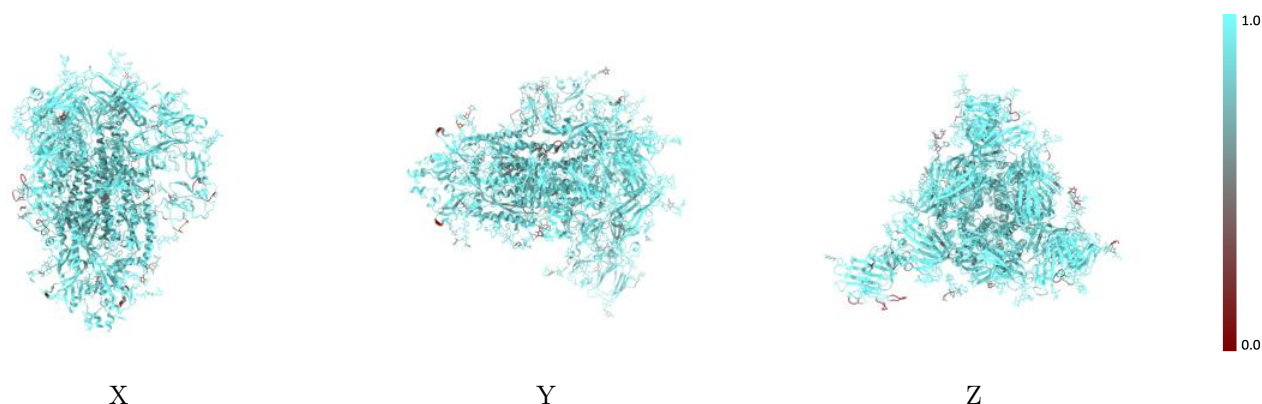
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



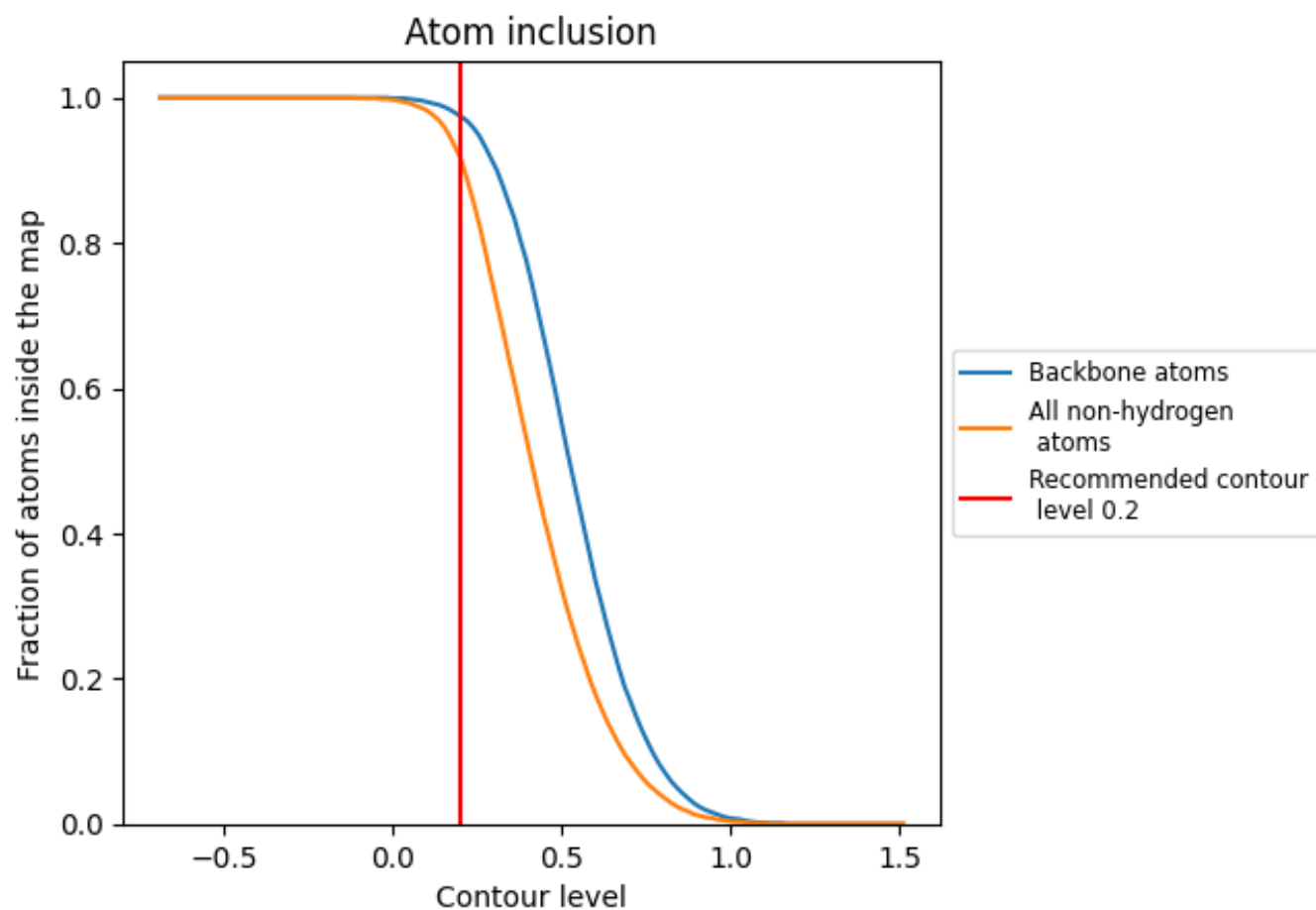
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9180	 0.2290
A	 0.9250	 0.2190
B	 0.9180	 0.2210
C	 0.9240	 0.2230
D	 0.9840	 0.3790
E	 0.9490	 0.3570
F	 0.9840	 0.2650
G	 0.9670	 0.3020
H	 0.7050	 0.3130
I	 0.6330	 0.2430
J	 0.6390	 0.2700
K	 0.9490	 0.4320
L	 0.9400	 0.3350
M	 0.8570	 0.3100
N	 0.9840	 0.2810
O	 0.8450	 0.2370
P	 0.9020	 0.2930
Q	 1.0000	 0.2760
R	 0.9020	 0.3530
S	 0.7180	 0.3240
T	 0.9840	 0.4080
U	 0.9840	 0.3230
V	 0.9230	 0.2930
W	 1.0000	 0.3490
X	 0.9510	 0.3330
Y	 0.7050	 0.2440
Z	 0.8980	 0.3360
a	 0.8200	 0.3270
b	 0.7210	 0.2970
c	 1.0000	 0.3650
d	 0.9670	 0.2600
e	 0.7320	 0.3460
f	 0.9490	 0.3120
g	 0.8530	 0.3540
h	 0.9840	 0.4160



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Chain	Atom inclusion	Q-score
i	 0.7040	 0.3660
j	 0.9840	 0.2680
k	 0.9020	 0.3110
l	 0.9230	 0.3220
m	 0.9020	 0.3260
n	 0.6890	 0.2970
o	 0.8200	 0.3050
p	 0.7380	 0.3410
q	 0.9490	 0.3860
r	 0.8720	 0.3840
s	 0.9580	 0.2960
t	 0.7550	 0.2920
u	 0.8690	 0.2270