



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:27 AM UTC

PDB ID : 7Y6T / pdb_00007y6t
EMDB ID : EMD-33647
Title : Cryo-EM map of IPEC-J2 cell-derived PEDV PT52 S protein one D0-down and two D0-up
Authors : Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on : 2022-06-21
Resolution : 4.20 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

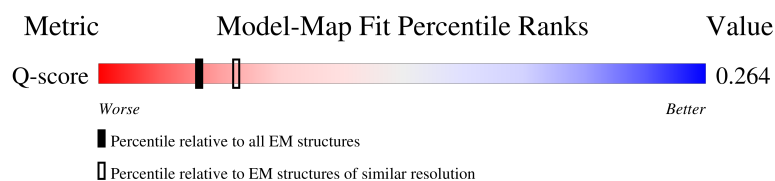
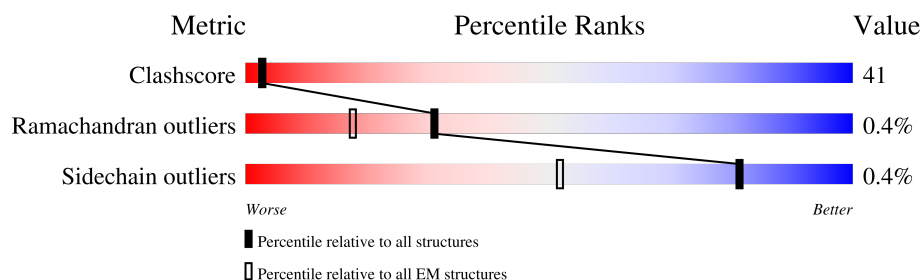
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



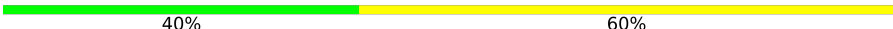
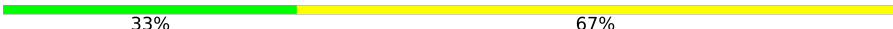
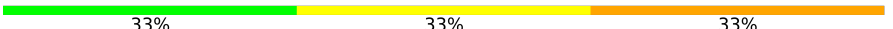
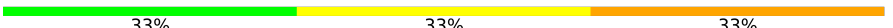
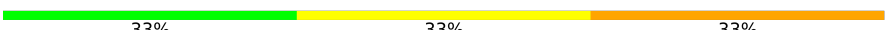
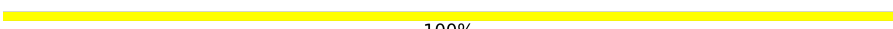
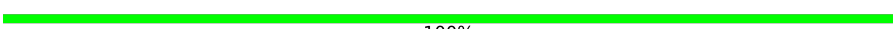
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	1402	
1	B	1402	
1	C	1402	
2	D	5	

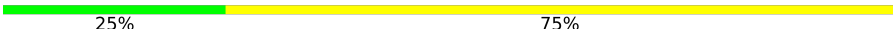
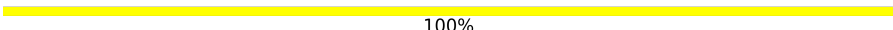
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Mol	Chain	Length	Quality of chain
2	O	5	 20% 80%
2	b	5	 40% 60%
3	E	3	 33% 67%
3	F	3	 33% 33% 33%
3	G	3	 33% 67%
3	K	3	 33% 67%
3	Q	3	 67% 33%
3	T	3	 33% 33% 33%
3	V	3	 33% 67%
3	X	3	 33% 67%
3	d	3	 67% 33%
3	g	3	 33% 67%
3	h	3	 33% 33% 33%
3	j	3	 33% 67%
4	H	2	 100%
4	I	2	 50% 50%
4	J	2	 50% 50%
4	L	2	 50% 50%
4	R	2	 50% 50%
4	U	2	 100%
4	W	2	 100%
4	Y	2	 100%
4	e	2	 50% 50%
4	i	2	 50% 50%
5	M	3	 33% 67%

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Mol	Chain	Length	Quality of chain
5	Z	3	 67%33%
6	N	4	 50%50%
6	a	4	 25%75%
6	k	4	 50%25%25%
7	P	2	 100%
7	S	2	 50%50%
7	c	2	 50%50%
7	f	2	 50%50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27988 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	1124	Total	C	N	O	S	0	0
			8648	5493	1442	1676	37		
1	C	1098	Total	C	N	O	S	0	0
			8440	5359	1407	1637	37		
1	B	1224	Total	C	N	O	S	0	0
			9398	5972	1556	1829	41		

There are 231 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1076	PRO	ILE	engineered mutation	UNP A0A1Y0DD46
A	1077	PRO	LEU	engineered mutation	UNP A0A1Y0DD46
A	1328	GLU	-	expression tag	UNP A0A1Y0DD46
A	1329	PHE	-	expression tag	UNP A0A1Y0DD46
A	1330	GLY	-	expression tag	UNP A0A1Y0DD46
A	1331	SER	-	expression tag	UNP A0A1Y0DD46
A	1332	GLY	-	expression tag	UNP A0A1Y0DD46
A	1333	GLY	-	expression tag	UNP A0A1Y0DD46
A	1334	TYR	-	expression tag	UNP A0A1Y0DD46
A	1335	ILE	-	expression tag	UNP A0A1Y0DD46
A	1336	PRO	-	expression tag	UNP A0A1Y0DD46
A	1337	GLU	-	expression tag	UNP A0A1Y0DD46
A	1338	ALA	-	expression tag	UNP A0A1Y0DD46
A	1339	PRO	-	expression tag	UNP A0A1Y0DD46
A	1340	ARG	-	expression tag	UNP A0A1Y0DD46
A	1341	ASP	-	expression tag	UNP A0A1Y0DD46
A	1342	GLY	-	expression tag	UNP A0A1Y0DD46
A	1343	GLN	-	expression tag	UNP A0A1Y0DD46
A	1344	ALA	-	expression tag	UNP A0A1Y0DD46
A	1345	TYR	-	expression tag	UNP A0A1Y0DD46
A	1346	VAL	-	expression tag	UNP A0A1Y0DD46
A	1347	ARG	-	expression tag	UNP A0A1Y0DD46
A	1348	LYS	-	expression tag	UNP A0A1Y0DD46
A	1349	ASP	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1350	GLY	-	expression tag	UNP A0A1Y0DD46
A	1351	GLU	-	expression tag	UNP A0A1Y0DD46
A	1352	TRP	-	expression tag	UNP A0A1Y0DD46
A	1353	VAL	-	expression tag	UNP A0A1Y0DD46
A	1354	LEU	-	expression tag	UNP A0A1Y0DD46
A	1355	LEU	-	expression tag	UNP A0A1Y0DD46
A	1356	SER	-	expression tag	UNP A0A1Y0DD46
A	1357	THR	-	expression tag	UNP A0A1Y0DD46
A	1358	PHE	-	expression tag	UNP A0A1Y0DD46
A	1359	LEU	-	expression tag	UNP A0A1Y0DD46
A	1360	LYS	-	expression tag	UNP A0A1Y0DD46
A	1361	GLY	-	expression tag	UNP A0A1Y0DD46
A	1362	GLN	-	expression tag	UNP A0A1Y0DD46
A	1363	ASP	-	expression tag	UNP A0A1Y0DD46
A	1364	ASN	-	expression tag	UNP A0A1Y0DD46
A	1365	SER	-	expression tag	UNP A0A1Y0DD46
A	1366	ALA	-	expression tag	UNP A0A1Y0DD46
A	1367	ASP	-	expression tag	UNP A0A1Y0DD46
A	1368	ILE	-	expression tag	UNP A0A1Y0DD46
A	1369	GLN	-	expression tag	UNP A0A1Y0DD46
A	1370	HIS	-	expression tag	UNP A0A1Y0DD46
A	1371	SER	-	expression tag	UNP A0A1Y0DD46
A	1372	GLY	-	expression tag	UNP A0A1Y0DD46
A	1373	ARG	-	expression tag	UNP A0A1Y0DD46
A	1374	PRO	-	expression tag	UNP A0A1Y0DD46
A	1375	LEU	-	expression tag	UNP A0A1Y0DD46
A	1376	GLU	-	expression tag	UNP A0A1Y0DD46
A	1377	SER	-	expression tag	UNP A0A1Y0DD46
A	1378	ARG	-	expression tag	UNP A0A1Y0DD46
A	1379	GLY	-	expression tag	UNP A0A1Y0DD46
A	1380	PRO	-	expression tag	UNP A0A1Y0DD46
A	1381	PHE	-	expression tag	UNP A0A1Y0DD46
A	1382	GLU	-	expression tag	UNP A0A1Y0DD46
A	1383	GLN	-	expression tag	UNP A0A1Y0DD46
A	1384	LYS	-	expression tag	UNP A0A1Y0DD46
A	1385	LEU	-	expression tag	UNP A0A1Y0DD46
A	1386	ILE	-	expression tag	UNP A0A1Y0DD46
A	1387	SER	-	expression tag	UNP A0A1Y0DD46
A	1388	GLU	-	expression tag	UNP A0A1Y0DD46
A	1389	GLU	-	expression tag	UNP A0A1Y0DD46
A	1390	ASP	-	expression tag	UNP A0A1Y0DD46
A	1391	LEU	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1392	ASN	-	expression tag	UNP A0A1Y0DD46
A	1393	MET	-	expression tag	UNP A0A1Y0DD46
A	1394	HIS	-	expression tag	UNP A0A1Y0DD46
A	1395	THR	-	expression tag	UNP A0A1Y0DD46
A	1396	GLY	-	expression tag	UNP A0A1Y0DD46
A	1397	HIS	-	expression tag	UNP A0A1Y0DD46
A	1398	HIS	-	expression tag	UNP A0A1Y0DD46
A	1399	HIS	-	expression tag	UNP A0A1Y0DD46
A	1400	HIS	-	expression tag	UNP A0A1Y0DD46
A	1401	HIS	-	expression tag	UNP A0A1Y0DD46
A	1402	HIS	-	expression tag	UNP A0A1Y0DD46
C	1076	PRO	ILE	conflict	UNP A0A1Y0DD46
C	1077	PRO	LEU	conflict	UNP A0A1Y0DD46
C	1328	GLU	-	expression tag	UNP A0A1Y0DD46
C	1329	PHE	-	expression tag	UNP A0A1Y0DD46
C	1330	GLY	-	expression tag	UNP A0A1Y0DD46
C	1331	SER	-	expression tag	UNP A0A1Y0DD46
C	1332	GLY	-	expression tag	UNP A0A1Y0DD46
C	1333	GLY	-	expression tag	UNP A0A1Y0DD46
C	1334	TYR	-	expression tag	UNP A0A1Y0DD46
C	1335	ILE	-	expression tag	UNP A0A1Y0DD46
C	1336	PRO	-	expression tag	UNP A0A1Y0DD46
C	1337	GLU	-	expression tag	UNP A0A1Y0DD46
C	1338	ALA	-	expression tag	UNP A0A1Y0DD46
C	1339	PRO	-	expression tag	UNP A0A1Y0DD46
C	1340	ARG	-	expression tag	UNP A0A1Y0DD46
C	1341	ASP	-	expression tag	UNP A0A1Y0DD46
C	1342	GLY	-	expression tag	UNP A0A1Y0DD46
C	1343	GLN	-	expression tag	UNP A0A1Y0DD46
C	1344	ALA	-	expression tag	UNP A0A1Y0DD46
C	1345	TYR	-	expression tag	UNP A0A1Y0DD46
C	1346	VAL	-	expression tag	UNP A0A1Y0DD46
C	1347	ARG	-	expression tag	UNP A0A1Y0DD46
C	1348	LYS	-	expression tag	UNP A0A1Y0DD46
C	1349	ASP	-	expression tag	UNP A0A1Y0DD46
C	1350	GLY	-	expression tag	UNP A0A1Y0DD46
C	1351	GLU	-	expression tag	UNP A0A1Y0DD46
C	1352	TRP	-	expression tag	UNP A0A1Y0DD46
C	1353	VAL	-	expression tag	UNP A0A1Y0DD46
C	1354	LEU	-	expression tag	UNP A0A1Y0DD46
C	1355	LEU	-	expression tag	UNP A0A1Y0DD46
C	1356	SER	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
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C	1358	PHE	-	expression tag	UNP A0A1Y0DD46
C	1359	LEU	-	expression tag	UNP A0A1Y0DD46
C	1360	LYS	-	expression tag	UNP A0A1Y0DD46
C	1361	GLY	-	expression tag	UNP A0A1Y0DD46
C	1362	GLN	-	expression tag	UNP A0A1Y0DD46
C	1363	ASP	-	expression tag	UNP A0A1Y0DD46
C	1364	ASN	-	expression tag	UNP A0A1Y0DD46
C	1365	SER	-	expression tag	UNP A0A1Y0DD46
C	1366	ALA	-	expression tag	UNP A0A1Y0DD46
C	1367	ASP	-	expression tag	UNP A0A1Y0DD46
C	1368	ILE	-	expression tag	UNP A0A1Y0DD46
C	1369	GLN	-	expression tag	UNP A0A1Y0DD46
C	1370	HIS	-	expression tag	UNP A0A1Y0DD46
C	1371	SER	-	expression tag	UNP A0A1Y0DD46
C	1372	GLY	-	expression tag	UNP A0A1Y0DD46
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C	1389	GLU	-	expression tag	UNP A0A1Y0DD46
C	1390	ASP	-	expression tag	UNP A0A1Y0DD46
C	1391	LEU	-	expression tag	UNP A0A1Y0DD46
C	1392	ASN	-	expression tag	UNP A0A1Y0DD46
C	1393	MET	-	expression tag	UNP A0A1Y0DD46
C	1394	HIS	-	expression tag	UNP A0A1Y0DD46
C	1395	THR	-	expression tag	UNP A0A1Y0DD46
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C	1397	HIS	-	expression tag	UNP A0A1Y0DD46
C	1398	HIS	-	expression tag	UNP A0A1Y0DD46

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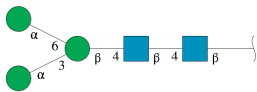
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C	1401	HIS	-	expression tag	UNP A0A1Y0DD46
C	1402	HIS	-	expression tag	UNP A0A1Y0DD46
B	1076	PRO	ILE	conflict	UNP A0A1Y0DD46
B	1077	PRO	LEU	conflict	UNP A0A1Y0DD46
B	1328	GLU	-	expression tag	UNP A0A1Y0DD46
B	1329	PHE	-	expression tag	UNP A0A1Y0DD46
B	1330	GLY	-	expression tag	UNP A0A1Y0DD46
B	1331	SER	-	expression tag	UNP A0A1Y0DD46
B	1332	GLY	-	expression tag	UNP A0A1Y0DD46
B	1333	GLY	-	expression tag	UNP A0A1Y0DD46
B	1334	TYR	-	expression tag	UNP A0A1Y0DD46
B	1335	ILE	-	expression tag	UNP A0A1Y0DD46
B	1336	PRO	-	expression tag	UNP A0A1Y0DD46
B	1337	GLU	-	expression tag	UNP A0A1Y0DD46
B	1338	ALA	-	expression tag	UNP A0A1Y0DD46
B	1339	PRO	-	expression tag	UNP A0A1Y0DD46
B	1340	ARG	-	expression tag	UNP A0A1Y0DD46
B	1341	ASP	-	expression tag	UNP A0A1Y0DD46
B	1342	GLY	-	expression tag	UNP A0A1Y0DD46
B	1343	GLN	-	expression tag	UNP A0A1Y0DD46
B	1344	ALA	-	expression tag	UNP A0A1Y0DD46
B	1345	TYR	-	expression tag	UNP A0A1Y0DD46
B	1346	VAL	-	expression tag	UNP A0A1Y0DD46
B	1347	ARG	-	expression tag	UNP A0A1Y0DD46
B	1348	LYS	-	expression tag	UNP A0A1Y0DD46
B	1349	ASP	-	expression tag	UNP A0A1Y0DD46
B	1350	GLY	-	expression tag	UNP A0A1Y0DD46
B	1351	GLU	-	expression tag	UNP A0A1Y0DD46
B	1352	TRP	-	expression tag	UNP A0A1Y0DD46
B	1353	VAL	-	expression tag	UNP A0A1Y0DD46
B	1354	LEU	-	expression tag	UNP A0A1Y0DD46
B	1355	LEU	-	expression tag	UNP A0A1Y0DD46
B	1356	SER	-	expression tag	UNP A0A1Y0DD46
B	1357	THR	-	expression tag	UNP A0A1Y0DD46
B	1358	PHE	-	expression tag	UNP A0A1Y0DD46
B	1359	LEU	-	expression tag	UNP A0A1Y0DD46
B	1360	LYS	-	expression tag	UNP A0A1Y0DD46
B	1361	GLY	-	expression tag	UNP A0A1Y0DD46
B	1362	GLN	-	expression tag	UNP A0A1Y0DD46
B	1363	ASP	-	expression tag	UNP A0A1Y0DD46

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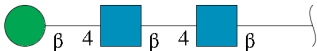
Chain	Residue	Modelled	Actual	Comment	Reference
B	1364	ASN	-	expression tag	UNP A0A1Y0DD46
B	1365	SER	-	expression tag	UNP A0A1Y0DD46
B	1366	ALA	-	expression tag	UNP A0A1Y0DD46
B	1367	ASP	-	expression tag	UNP A0A1Y0DD46
B	1368	ILE	-	expression tag	UNP A0A1Y0DD46
B	1369	GLN	-	expression tag	UNP A0A1Y0DD46
B	1370	HIS	-	expression tag	UNP A0A1Y0DD46
B	1371	SER	-	expression tag	UNP A0A1Y0DD46
B	1372	GLY	-	expression tag	UNP A0A1Y0DD46
B	1373	ARG	-	expression tag	UNP A0A1Y0DD46
B	1374	PRO	-	expression tag	UNP A0A1Y0DD46
B	1375	LEU	-	expression tag	UNP A0A1Y0DD46
B	1376	GLU	-	expression tag	UNP A0A1Y0DD46
B	1377	SER	-	expression tag	UNP A0A1Y0DD46
B	1378	ARG	-	expression tag	UNP A0A1Y0DD46
B	1379	GLY	-	expression tag	UNP A0A1Y0DD46
B	1380	PRO	-	expression tag	UNP A0A1Y0DD46
B	1381	PHE	-	expression tag	UNP A0A1Y0DD46
B	1382	GLU	-	expression tag	UNP A0A1Y0DD46
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B	1385	LEU	-	expression tag	UNP A0A1Y0DD46
B	1386	ILE	-	expression tag	UNP A0A1Y0DD46
B	1387	SER	-	expression tag	UNP A0A1Y0DD46
B	1388	GLU	-	expression tag	UNP A0A1Y0DD46
B	1389	GLU	-	expression tag	UNP A0A1Y0DD46
B	1390	ASP	-	expression tag	UNP A0A1Y0DD46
B	1391	LEU	-	expression tag	UNP A0A1Y0DD46
B	1392	ASN	-	expression tag	UNP A0A1Y0DD46
B	1393	MET	-	expression tag	UNP A0A1Y0DD46
B	1394	HIS	-	expression tag	UNP A0A1Y0DD46
B	1395	THR	-	expression tag	UNP A0A1Y0DD46
B	1396	GLY	-	expression tag	UNP A0A1Y0DD46
B	1397	HIS	-	expression tag	UNP A0A1Y0DD46
B	1398	HIS	-	expression tag	UNP A0A1Y0DD46
B	1399	HIS	-	expression tag	UNP A0A1Y0DD46
B	1400	HIS	-	expression tag	UNP A0A1Y0DD46
B	1401	HIS	-	expression tag	UNP A0A1Y0DD46
B	1402	HIS	-	expression tag	UNP A0A1Y0DD46

- 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	O	5	Total	C	N	O	0	0
			61	34	2	25		
2	b	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.



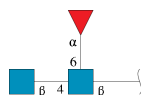
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		
3	T	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	d	3	Total	C	N	O	0	0
			39	22	2	15		
3	g	3	Total	C	N	O	0	0
			39	22	2	15		
3	h	3	Total	C	N	O	0	0
			39	22	2	15		
3	j	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		

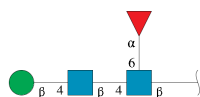
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	3	Total	C	N	O	0	0
			38	22	2	14		
5	Z	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 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.

ranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	4	Total	C	N	O	0	0
			49	28	2	19		
6	a	4	Total	C	N	O	0	0
			49	28	2	19		
6	k	4	Total	C	N	O	0	0
			49	28	2	19		

- 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	P	2	Total	C	N	O	0	0
			24	14	1	9		
7	S	2	Total	C	N	O	0	0
			24	14	1	9		
7	c	2	Total	C	N	O	0	0
			24	14	1	9		
7	f	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).

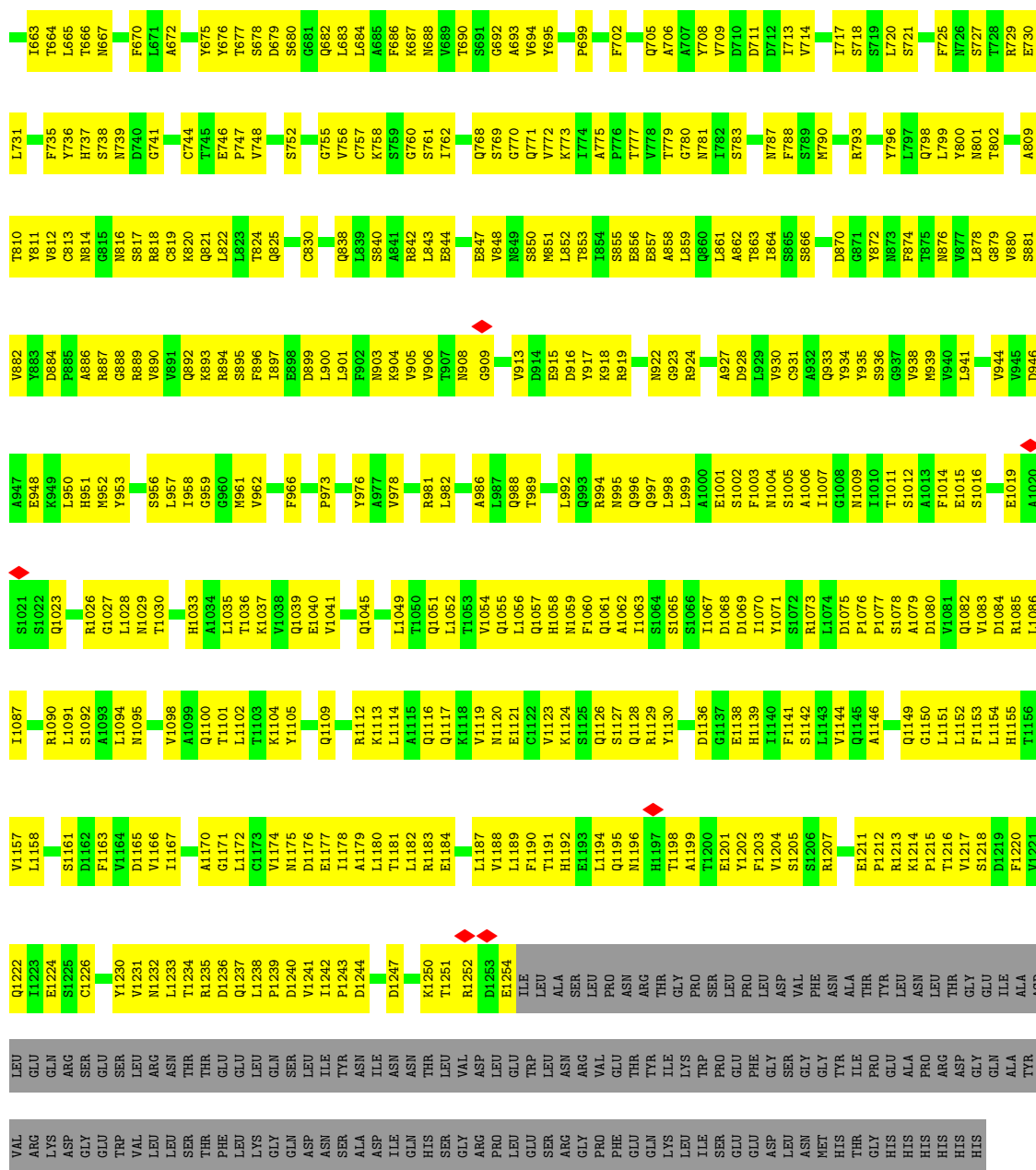


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8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

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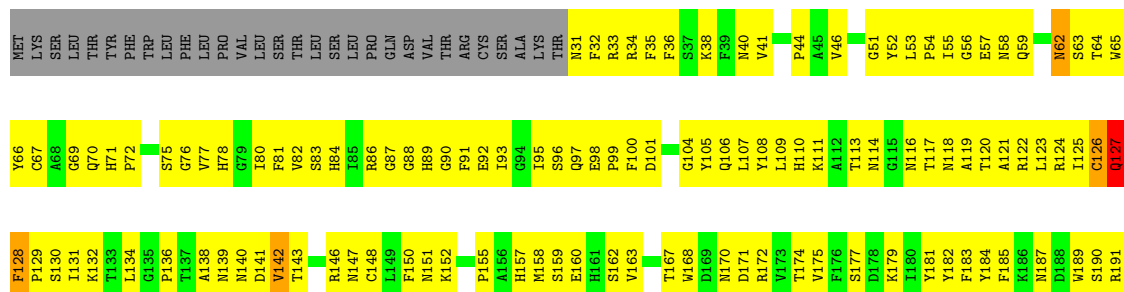
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Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	

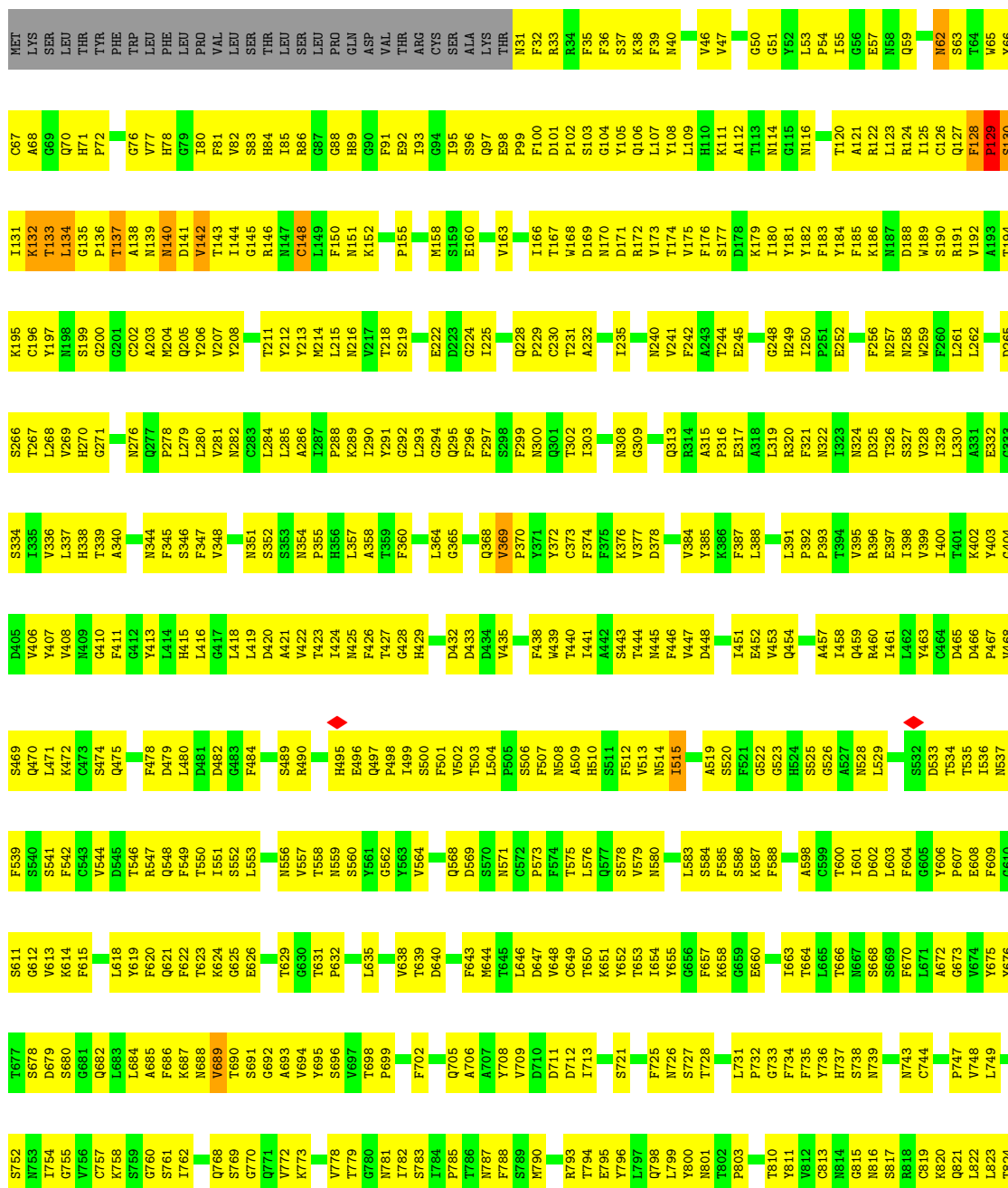
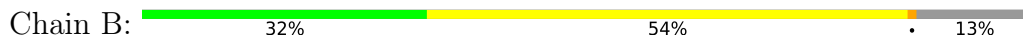


● Molecule 1: Spike glycoprotein

Chain C: 30% 48% 22%



C1173	V1105	A1032	G888	E746	S668	THR	SER	V476	F411	V336	L261	V192
V1174	T1106	H1033	Q892	F747	S669	ILE	SER	A477	H415	L337	L262	A193
N1176	Q1109	A1034	Q893	L748	F670	LEU	PHE	D479	L416	H338	D265	K194
D1176	L1035	L1035	K893	V749	L671	LEU	CYS	L480	G417	T339	S266	K195
E1177	T1036	R894	R894	Y750	A672	PHE	VAL	D481	L418	A340	D265	C196
I1178	K1037	S895	T824	S751	G673	GLY	ASP	D482	L419	L341	V269	Y197
A1179	V1038	F896	Q825	S752	V674	THR	THR	G483	D420	G342	H270	H198
Q1039	Q1039	I897	Q826	N753	Y675	PRO	ARG	G484	A421	G271	H271	S199
E1040	L972	E898	T827	I754	T677	GLU	GLU	F484	V422	T343	G272	C202
Q1116	P973	D899	A828	G755	T677	PHE	PHE	Y485	V422	N344	K272	A203
Q1117	V1042	L900	G756	S678	S678	GLY	THR	T423	G223	F345	V273	M204
E1184	Y976	L901	K831	C757	D679	SER	ILE	S489	I424	N274	S274	Q205
P1185	V1119	F902	T832	K758	S680	GLY	SER	R490	N425	S275	Q205	M204
N1120	R981	N903	I833			VAL	LEU		F426	S352	N276	Q205
E1121	E834	E904	E834	S761	L683	LYS	SER	L493	T427	S353	Q277	Y207
C1122	V1054	V905	S835	I762	L684	PHE	THR	S494	G428	N354	P278	Y208
V1123	L985	N906	S835	Q768	A685	THR	ASN	H495	H429	P355	L279	E209
K1124	A986	T907	Q838	S769	F686	SER	VAL	E496		H356	L280	P210
F1190	A986	N908	L839	G770	K687	LEU	THR	Q497	D432	L357	V281	T211
T1191	L987	C909	S840		N688	THR	ASN	P498	D433		N282	Y212
S1126	Q988	L910	L843	T777	V689	PHE	SER	I499	D434	F360		Y213
Q1126	T989	V913	E844	T778	T690	GLN	GLY	S500	V435	P363	L285	M214
Y1130	D990	V913	E844	V778	G692	THR	TYR	F501	F438	L364	L215	N216
G1131	V991	V913	S845	T779	G692	THR	TYR	V502	F438		N216	N217
D1136	N985	D916	V846	G780	A693	LYS	VAL		V439	V369	K269	N218
G1137	R986	Y917	E847	N781	V694	GLY	SER		T440		L290	
E1138	Q997	K918	V848	I782	Y695	GLU	ASN		I441		Y291	
H1139	R998	R919	V848	S783	S696	LEU	SER		F374	F374	G292	G221
D1069	L999	C920	M851	I784	S696	ILE	GLN	N508	F375	F375	L293	D223
F1141	A1000	S921	L852	P785	P699	THR	ASP	A509	K376	K376	G294	E222
S1142	E1001	N922	T853	T786		GLY	SER	HIS	N445	V377	Q295	G224
L1143	S1002	G923		N787	F702	THR	ASN	SER	F446	D378	F296	T225
R1073	F1003	R924	E856	F788		PRO	CYS	PHE	V447	T379	S226	S226
D1074	P1003	A927	E857	S789	Q705	LYS	PRO	VAL	D448	Y380	Y227	Y227
P1075	N1004	D928	Q860	M790	A706	THR	PHE	ASN	A449	N381	F299	N300
P1077	S1005	L928	L861	I792	I708	LEU	THR	ILE	L450	S382	N300	T231
S1078	I1007	V930	A862	R793	V709	GLN	VAL	VAL	I451	V384	Q301	T231
A1079	N1009	C931	S863		D710	SER	SER	SER	V452	V385	T302	A232
D1080	T1010	Q933	I864	Y796	D711	VAL	ALA	ALA	K396	F387	N308	I235
V1083	T1011	S865	S865	L797	D712	ASN	ASN	PHE	G455	G309	A238	A238
D1084	S1012	S866	S866	Q798	I713	ASP	ASP	GLY	T456	A389	A239	A239
R1085	Y934			L799	I713	TYR	TYR	GLY	A457	V390	N240	N240
L1086	M939	D870	D870	Y800	S721	LEU	LEU	HIS	R460	L391	R313	R313
I1087	V940	G871	G871	N801	S722	SER	SER	GLY	L461	P392	R314	R314
S1016	L941	Y872	Y872	S805	F725	PHE	PHE	GLY	L462		A315	A315
V1017	V944	N873	N873	D807	N726	LYS	LYS	ALA	Y463	R396	P316	P316
K1018	V945	F874	F874	V806	T728	PHE	PHE	ASN	C464	E397	E317	T244
E1019	D946	N876	N876	C808	T728	CYS	CYS	LEU	D465	I398	R320	N247
A1020	A847	V877	V877	A809	R729	VAL	VAL	ILE	D466		F321	G248
Q1023	E948	L878	L878	T810	T735	ALA	ALA	ALA	P467	T401	F321	G248
T1024	K949	G879	G879	Y811	I654	THR	THR	SER	V468	K402	I323	H249
S1025	V950	V880	V880	V812	Y736	SER	SER	ASP	S469	N324	E252	E252
R1026	H951	S881	S881	C813	H737	LEU	THR	THR	Q470	G404	D325	F256
G1027	M952	V882	V882	N814	S738	LEU	LEU	THR	L471		T326	F256
L1028	Y953	Y883	Y883	C815	N739	ALA	ALA	ILE	K472	Y407	S327	N257
N1029	S954	D884	D884	N816	N739	SER	SER	ASN	C473	V408	V328	N258
T1030	A955	P885	P885	S817	C744	ALA	ALA	GLY	S474	N409	I329	W259
V1031	S956			R818	T745		CYS	PHE	Q475	G410	L330	F260





- 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



- 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

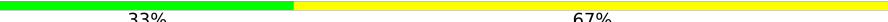


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  33% 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 X:  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 d:  67% 33%

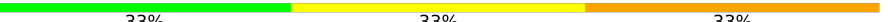


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  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 h:  33% 33% 33%

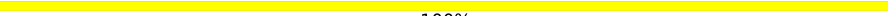


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  33% 67%



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

Chain H:  100%

NAG1
NAG2

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

Chain I:  50% 50%

NAG1
NAG2

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

Chain J:  50% 50%

NAG1
NAG2

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

Chain L:  50% 50%

NAG1
NAG2

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

Chain R:  50% 50%

NAG1
NAG2

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

Chain U:  100%

NAG1
NAG2

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

Chain W:  100%

NAG1
NAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain e:  50% 50%

MAG1
MAG2

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

Chain i:  50% 50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 67%

MAG1
MAG2
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  67% 33%

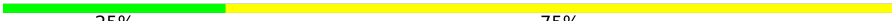
MAG1
MAG2
FUC3

- Molecule 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

Chain N:  50% 50%

MAG1
MAG2
BMA3
FUC4

- Molecule 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

Chain a:  25% 75%



- Molecule 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



- Molecule 7: 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



- 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, Not provided	
Number of particles used	51124	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	0.810	Depositor
Minimum map value	-0.175	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	385.83997, 385.83997, 385.83997	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/8838	0.52	0/12039
1	B	0.38	0/9610	0.51	0/13097
1	C	0.39	0/8626	0.53	1/11756 (0.0%)
All	All	0.38	0/27074	0.52	1/36892 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	GLN	N-CA-C	-5.42	99.26	110.80

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	8648	0	8399	769	0
1	B	9398	0	9085	802	0
1	C	8440	0	8178	730	0
2	D	61	0	52	4	0
2	O	61	0	52	1	0
2	b	61	0	52	2	0
3	E	39	0	34	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	39	0	34	3	0
3	G	39	0	34	3	0
3	K	39	0	34	2	0
3	Q	39	0	34	1	0
3	T	39	0	34	3	0
3	V	39	0	34	6	0
3	X	39	0	34	1	0
3	d	39	0	34	2	0
3	g	39	0	34	3	0
3	h	39	0	34	3	0
3	j	39	0	34	2	0
4	H	28	0	25	0	0
4	I	28	0	25	2	0
4	J	28	0	25	4	0
4	L	28	0	25	2	0
4	R	28	0	25	1	0
4	U	28	0	25	4	0
4	W	28	0	25	0	0
4	Y	28	0	25	3	0
4	e	28	0	25	1	0
4	i	28	0	25	1	0
5	M	38	0	34	4	0
5	Z	38	0	34	2	0
6	N	49	0	43	3	0
6	a	49	0	43	6	0
6	k	49	0	43	5	0
7	P	24	0	22	3	0
7	S	24	0	22	6	0
7	c	24	0	22	1	0
7	f	24	0	22	1	0
8	A	84	0	78	5	0
8	B	98	0	91	4	0
8	C	70	0	65	2	0
All	All	27988	0	26995	2243	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 41.

All (2243) 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:A:482:ASP:HA	1:A:708:TYR:O	1.52	1.06
1:C:218:THR:HG21	6:N:1:NAG:H62	1.40	1.00
1:A:510:HIS:HB2	1:A:634:PRO:HB3	1.45	0.97
1:B:482:ASP:HA	1:B:708:TYR:O	1.66	0.96
1:C:96:SER:O	1:C:191:ARG:HB3	1.63	0.96
1:A:258:ASN:HB3	1:A:396:ARG:HB3	1.48	0.95
1:A:1054:VAL:HA	1:A:1057:GLN:HE22	1.30	0.94
1:C:126:CYS:HB2	1:C:128:PHE:HB3	1.50	0.94
1:B:96:SER:O	1:B:191:ARG:HB3	1.69	0.93
1:A:405:ASP:HA	1:A:415:HIS:HA	1.52	0.91
1:A:66:TYR:HE2	1:A:206:TYR:H	1.18	0.91
1:B:1116:GLN:NE2	1:B:1120:ASN:OD1	2.04	0.91
1:C:497:GLN:HB3	1:C:650:THR:HA	1.54	0.90
1:C:1177:GLU:HG3	1:C:1178:ILE:HD12	1.53	0.90
1:A:1068:ASP:H	1:B:658:LYS:HZ3	1.20	0.89
1:A:404:GLY:HA2	1:A:419:LEU:HG	1.55	0.88
1:B:466:ASP:O	1:B:470:GLN:N	2.07	0.88
1:A:240:ASN:HD22	1:A:439:TRP:HB3	1.38	0.87
1:A:59:GLN:NE2	1:A:213:TYR:OH	2.08	0.86
1:C:452:GLU:HB3	1:C:460:ARG:HG2	1.54	0.86
1:C:466:ASP:O	1:C:470:GLN:N	2.07	0.86
1:B:131:ILE:HG23	1:B:138:ALA:HB3	1.58	0.86
1:A:117:THR:HA	1:A:157:HIS:HB3	1.58	0.85
1:A:1068:ASP:HB2	1:B:658:LYS:HD3	1.59	0.85
1:A:508:ASN:HD22	1:A:636:GLU:HA	1.39	0.84
1:B:727:SER:HB3	1:B:738:SER:O	1.77	0.84
1:A:324:ASN:HB2	1:A:439:TRP:CG	2.13	0.83
1:B:497:GLN:NE2	1:B:649:CYS:SG	2.51	0.83
1:C:507:PHE:HA	1:C:637:GLY:HA2	1.61	0.83
1:A:59:GLN:O	1:A:62:ASN:ND2	2.11	0.83
1:C:1195:GLN:HB3	1:C:1201:GLU:HB2	1.59	0.83
1:A:320:ARG:NH1	1:A:397:GLU:OE1	2.10	0.83
1:C:71:HIS:ND1	1:C:194:THR:O	2.11	0.83
1:C:126:CYS:HB3	1:C:148:CYS:HA	1.61	0.83
1:C:651:LYS:NZ	1:C:653:THR:OG1	2.11	0.83
1:B:881:SER:HA	1:B:892:GLN:HA	1.60	0.82
1:A:466:ASP:O	1:A:470:GLN:N	2.11	0.82
1:C:131:ILE:HG12	1:C:138:ALA:HB3	1.58	0.82
1:B:132:LYS:HD3	1:B:191:ARG:HE	1.44	0.82
1:C:328:VAL:HG13	1:C:427:THR:H	1.45	0.82
1:C:482:ASP:HA	1:C:708:TYR:O	1.80	0.82
1:B:515:ILE:HA	1:B:535:THR:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:GLN:OE1	1:A:1055:GLN:NE2	2.13	0.81
1:B:783:SER:HB3	1:B:1163:PHE:HB3	1.63	0.81
1:B:338:HIS:ND1	1:B:344:ASN:OD1	2.13	0.80
1:C:33:ARG:HB3	1:C:222:GLU:HB3	1.64	0.80
1:C:232:ALA:HA	1:C:235:ILE:HD13	1.62	0.80
1:B:1195:GLN:HB3	1:B:1201:GLU:HB3	1.62	0.80
1:A:727:SER:HB3	1:A:738:SER:O	1.82	0.80
1:C:317:GLU:OE2	1:C:446:PHE:N	2.14	0.80
1:A:790:MET:HE3	1:A:1003:PHE:HB2	1.61	0.80
1:B:529:LEU:HD11	1:B:613:VAL:HG11	1.62	0.80
1:A:280:LEU:HB3	1:A:445:ASN:HB2	1.64	0.80
1:A:1069:ASP:H	1:B:658:LYS:HE2	1.48	0.79
1:A:96:SER:O	1:A:191:ARG:HB3	1.82	0.79
1:C:744:CYS:SG	1:C:757:CYS:N	2.56	0.79
1:A:773:LYS:HE2	1:C:1124:LYS:HE2	1.62	0.79
1:A:916:ASP:HB2	1:A:918:LYS:HE3	1.63	0.79
1:B:514:ASN:OD1	1:B:537:ASN:ND2	2.16	0.79
1:B:1189:LEU:HD11	1:B:1202:TYR:HB3	1.62	0.79
1:A:1216:THR:HG22	1:A:1218:SER:H	1.48	0.79
1:A:322:ASN:HB3	1:A:440:THR:HG22	1.62	0.79
1:B:497:GLN:HE22	1:B:660:GLU:HG3	1.46	0.79
1:C:289:LYS:HB2	1:C:435:VAL:H	1.48	0.79
1:B:803:PRO:HB2	1:B:941:LEU:HB2	1.63	0.79
1:B:915:GLU:OE1	1:B:919:ARG:NH2	2.15	0.79
1:B:1054:VAL:O	1:B:1057:GLN:NE2	2.14	0.79
1:A:256:PHE:HB3	1:A:259:TRP:HB2	1.64	0.79
1:A:752:SER:HB3	1:C:941:LEU:HD21	1.64	0.78
1:A:137:THR:O	1:A:140:ASN:ND2	2.17	0.78
1:A:747:PRO:O	1:A:1026:ARG:NH2	2.15	0.78
1:A:1082:GLN:HG3	1:A:1085:ARG:HH22	1.48	0.78
1:B:338:HIS:HB2	1:B:421:ALA:HB3	1.66	0.78
1:B:508:ASN:OD1	1:B:548:GLN:NE2	2.15	0.78
1:C:1131:GLY:HA2	1:C:1136:ASP:HA	1.65	0.78
1:B:33:ARG:HB3	1:B:222:GLU:HB3	1.64	0.78
1:C:881:SER:HA	1:C:892:GLN:HA	1.65	0.77
1:B:78:HIS:ND1	1:B:208:TYR:O	2.16	0.77
1:C:783:SER:HB3	1:C:1163:PHE:HB3	1.65	0.77
1:C:282:ASN:ND2	1:C:445:ASN:OD1	2.16	0.77
1:B:334:SER:HA	1:B:425:ASN:HB3	1.66	0.77
1:B:799:LEU:HD23	1:B:1150:GLY:HA2	1.66	0.77
1:A:374:PHE:HB3	1:A:385:TYR:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:VAL:HG13	1:A:708:TYR:HE1	1.49	0.77
1:B:92:GLU:HB2	1:B:195:LYS:HB3	1.67	0.77
1:B:177:SER:HB2	1:B:181:TYR:HE2	1.50	0.76
1:C:65:TRP:HB3	1:C:202:CYS:HA	1.68	0.76
1:C:78:HIS:ND1	1:C:208:TYR:O	2.18	0.76
1:A:1189:LEU:HD11	1:A:1202:TYR:HB3	1.66	0.75
1:A:115:GLY:H	1:A:119:ALA:HB2	1.51	0.75
1:B:874:PHE:HB3	1:B:878:LEU:HD13	1.67	0.75
1:A:801:ASN:HB2	1:A:1105:TYR:HE1	1.52	0.75
1:B:587:LYS:HE3	1:B:623:THR:HG23	1.68	0.75
1:B:1177:GLU:HG3	1:B:1178:ILE:HD12	1.67	0.75
1:B:1051:GLN:O	1:B:1055:GLN:NE2	2.15	0.74
1:C:337:LEU:O	1:C:344:ASN:HA	1.86	0.74
1:B:853:THR:H	1:B:953:TYR:HE1	1.33	0.74
1:C:798:GLN:NE2	1:C:800:TYR:O	2.20	0.74
1:B:666:THR:HG23	1:B:694:VAL:HG23	1.69	0.74
1:B:547:ARG:O	1:B:629:THR:N	2.20	0.74
1:B:128:PHE:HB2	1:B:144:ILE:HA	1.69	0.74
1:B:958:ILE:HA	1:B:961:MET:HE2	1.70	0.74
1:B:969:ALA:HB1	3:X:1:NAG:H5	1.68	0.74
1:A:97:GLN:HG2	1:A:99:PRO:HD2	1.69	0.74
1:C:812:VAL:O	1:C:1090:ARG:NH1	2.21	0.73
1:B:129:PRO:HB3	1:B:140:ASN:CG	2.12	0.73
1:C:242:PHE:O	1:C:308:ASN:ND2	2.20	0.73
1:B:337:LEU:O	1:B:344:ASN:HA	1.89	0.73
1:B:498:PRO:O	1:B:650:THR:OG1	2.05	0.73
1:B:787:ASN:HB3	1:B:1161:SER:HB2	1.70	0.73
1:A:248:GLY:O	1:A:281:VAL:N	2.16	0.73
1:A:1252:ARG:NH1	1:C:1250:LYS:O	2.21	0.73
1:B:364:LEU:HB2	7:f:1:NAG:H61	1.69	0.73
1:A:508:ASN:ND2	1:C:354:ASN:OD1	2.18	0.73
1:B:35:PHE:HA	1:B:38:LYS:HE2	1.71	0.73
1:B:370:PRO:HG3	1:B:393:PRO:HG3	1.71	0.73
1:C:69:GLY:HA2	1:C:196:CYS:H	1.51	0.73
1:B:322:ASN:ND2	1:B:397:GLU:OE2	2.21	0.73
1:A:498:PRO:O	1:A:650:THR:OG1	2.06	0.73
1:A:1078:SER:O	1:A:1082:GLN:NE2	2.22	0.73
1:B:1234:THR:OG1	1:B:1236:ASP:OD1	2.07	0.73
1:B:282:ASN:HD21	1:B:445:ASN:HD21	1.37	0.72
1:A:282:ASN:ND2	1:A:445:ASN:OD1	2.20	0.72
1:B:670:PHE:O	1:B:687:LYS:NZ	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:VAL:HG22	1:A:713:ILE:HG12	1.71	0.72
1:C:1051:GLN:NE2	1:C:1055:GLN:OE1	2.21	0.72
1:A:265:ASP:OD1	1:A:266:SER:N	2.23	0.72
1:C:1091:LEU:O	1:C:1095:ASN:ND2	2.23	0.72
1:B:231:THR:HG22	1:B:232:ALA:H	1.55	0.72
1:A:508:ASN:ND2	1:A:636:GLU:HA	2.04	0.72
1:C:729:ARG:HD3	1:C:762:ILE:HG22	1.71	0.72
1:A:1086:LEU:HD11	1:A:1090:ARG:HE	1.54	0.71
1:B:108:TYR:CD1	1:B:131:ILE:HG21	2.25	0.71
1:B:278:PRO:HA	1:B:446:PHE:HA	1.72	0.71
1:B:788:PHE:HA	1:B:1159:VAL:O	1.89	0.71
1:B:744:CYS:SG	1:B:757:CYS:N	2.64	0.71
1:A:452:GLU:HG2	1:A:459:GLN:HB2	1.69	0.71
1:C:768:GLN:NE2	1:C:769:SER:O	2.23	0.71
1:C:86:ARG:O	1:C:89:HIS:ND1	2.23	0.71
1:C:688:ASN:HB3	1:C:693:ALA:H	1.54	0.71
1:B:65:TRP:HA	1:B:204:MET:O	1.91	0.71
1:B:726:ASN:OD1	1:B:739:ASN:ND2	2.24	0.71
1:A:105:TYR:HD1	1:A:127:GLN:HG3	1.56	0.71
1:A:683:LEU:HD21	1:A:686:PHE:HB3	1.72	0.71
1:C:1189:LEU:HD11	1:C:1202:TYR:HB3	1.72	0.71
1:B:647:ASP:N	1:B:663:ILE:O	2.17	0.71
1:A:83:SER:OG	1:A:202:CYS:O	2.09	0.71
1:A:821:GLN:O	1:A:824:THR:OG1	2.08	0.71
1:C:67:CYS:SG	1:C:199:SER:N	2.60	0.71
1:B:747:PRO:HB3	1:B:755:GLY:HA3	1.72	0.71
1:C:240:ASN:HD21	1:C:438:PHE:H	1.39	0.71
1:C:793:ARG:NH1	1:C:1136:ASP:O	2.23	0.71
1:B:177:SER:HB2	1:B:181:TYR:CE2	2.25	0.71
1:A:510:HIS:CE1	1:C:356:HIS:HB3	2.26	0.70
1:B:901:LEU:O	1:B:905:VAL:HB	1.91	0.70
1:A:55:ILE:O	1:A:59:GLN:NE2	2.23	0.70
1:A:838:GLN:OE1	1:B:484:PHE:N	2.20	0.70
1:B:1059:ASN:ND2	1:B:1062:ALA:O	2.24	0.70
1:A:879:GLY:O	1:A:892:GLN:NE2	2.20	0.70
1:A:182:TYR:HB3	1:A:252:GLU:HG2	1.74	0.70
1:B:586:SER:N	1:B:623:THR:O	2.24	0.70
1:A:510:HIS:HE1	1:C:356:HIS:HB3	1.56	0.70
1:A:1041:VAL:O	1:A:1045:GLN:NE2	2.24	0.70
1:C:876:ASN:O	1:C:895:SER:OG	2.10	0.70
1:B:934:TYR:CD1	1:B:939:MET:HE1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:ALA:HA	1:A:1085:ARG:HH21	1.56	0.70
1:B:252:GLU:N	1:B:252:GLU:OE1	2.25	0.70
1:B:320:ARG:NH1	1:B:397:GLU:OE1	2.24	0.70
1:A:236:GLY:H	3:E:1:NAG:H61	1.56	0.70
1:A:679:ASP:O	1:C:1057:GLN:NE2	2.25	0.70
1:B:614:LYS:NZ	1:B:615:PHE:O	2.21	0.70
1:A:930:VAL:O	1:A:933:GLN:NE2	2.24	0.70
1:B:256:PHE:HB3	1:B:259:TRP:HB2	1.72	0.70
1:B:523:GLY:HA3	1:B:528:ASN:HB2	1.73	0.70
1:B:70:GLN:HG3	1:B:72:PRO:HD3	1.72	0.69
1:B:230:CYS:SG	1:B:231:THR:N	2.58	0.69
1:B:908:ASN:HB3	1:B:913:VAL:HG21	1.74	0.69
1:A:39:PHE:HA	1:A:180:ILE:HD11	1.74	0.69
1:A:904:LYS:NZ	1:A:1014:PHE:O	2.24	0.69
1:B:482:ASP:HB3	1:B:709:VAL:HG12	1.73	0.69
1:A:66:TYR:HB3	1:A:72:PRO:HG3	1.73	0.69
1:B:38:LYS:NZ	1:B:163:VAL:O	2.26	0.69
1:A:399:VAL:HG13	1:A:407:TYR:HB3	1.74	0.69
1:A:684:LEU:HD12	1:C:927:ALA:HB3	1.73	0.69
1:A:918:LYS:NZ	1:B:731:LEU:O	2.25	0.69
1:C:138:ALA:O	1:C:140:ASN:ND2	2.25	0.69
1:C:1138:GLU:HB2	1:C:1158:LEU:HB2	1.75	0.69
1:B:472:LYS:NZ	1:B:478:PHE:O	2.22	0.69
1:B:826:TYR:OH	1:B:1084:ASP:OD1	2.11	0.69
1:A:768:GLN:NE2	1:A:769:SER:O	2.26	0.69
1:B:151:ASN:H	1:B:152:LYS:HZ3	1.41	0.69
1:B:365:GLY:O	1:B:368:GLN:NE2	2.23	0.69
1:B:1033:HIS:O	1:B:1036:THR:OG1	2.10	0.69
1:C:172:ARG:NH1	1:C:182:TYR:OH	2.26	0.68
1:B:76:GLY:H	1:B:190:SER:HB2	1.57	0.68
1:B:84:HIS:HE2	1:B:160:GLU:HB3	1.58	0.68
1:B:261:LEU:HB3	1:B:458:ILE:HD11	1.75	0.68
1:A:411:PHE:HE1	1:B:673:GLY:HA2	1.58	0.68
1:A:1172:LEU:HD13	1:A:1231:VAL:HB	1.76	0.68
1:C:670:PHE:O	1:C:687:LYS:NZ	2.27	0.68
1:C:708:TYR:CZ	1:C:711:ASP:HA	2.29	0.68
1:B:302:THR:HG21	1:B:313:GLN:HA	1.75	0.68
6:a:1:NAG:H4	6:a:4:FUC:H5	1.76	0.68
1:B:133:THR:HG23	1:B:139:ASN:ND2	2.09	0.68
1:B:504:LEU:O	1:B:547:ARG:NH2	2.26	0.68
1:B:985:LEU:HB3	1:B:1208:ARG:HH22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:688:ASN:HB2	1:C:695:TYR:HE1	1.58	0.68
1:B:1172:LEU:HB3	1:B:1180:LEU:O	1.94	0.68
1:A:127:GLN:N	1:A:147:ASN:O	2.26	0.68
1:C:123:LEU:HD21	1:C:125:ILE:HG13	1.76	0.68
1:C:678:SER:HB3	1:C:684:LEU:HD21	1.75	0.68
1:A:41:VAL:HA	1:A:243:ALA:HB1	1.76	0.68
1:B:68:ALA:O	1:B:196:CYS:HB2	1.94	0.68
1:A:892:GLN:HB3	1:A:952:MET:HE1	1.76	0.68
1:C:1175:ASN:N	1:C:1233:LEU:O	2.26	0.67
1:A:38:LYS:NZ	1:A:163:VAL:O	2.24	0.67
1:C:289:LYS:HA	1:C:439:TRP:HD1	1.59	0.67
1:C:90:GLY:N	1:C:114:ASN:OD1	2.27	0.67
1:A:1116:GLN:NE2	1:A:1120:ASN:OD1	2.27	0.67
1:C:821:GLN:O	1:C:824:THR:OG1	2.10	0.67
1:B:134:LEU:HB2	1:B:195:LYS:HB2	1.77	0.67
1:A:729:ARG:NH1	1:A:762:ILE:O	2.27	0.67
1:C:1193:GLU:OE2	1:C:1195:GLN:NE2	2.27	0.67
1:C:1234:THR:OG1	1:C:1236:ASP:OD1	2.12	0.67
1:B:299:PHE:HD1	1:B:317:GLU:HA	1.59	0.67
1:C:403:TYR:H	1:C:418:LEU:HD23	1.60	0.67
1:B:88:GLY:O	1:B:114:ASN:ND2	2.28	0.67
1:B:903:ASN:HA	1:B:909:GLY:HA2	1.77	0.67
1:C:706:ALA:HB1	1:C:713:ILE:HD12	1.76	0.67
1:B:134:LEU:HD13	1:B:195:LYS:HD2	1.75	0.67
1:B:536:ILE:N	1:B:539:PHE:O	2.22	0.67
4:Y:1:NAG:H83	4:Y:1:NAG:H3	1.76	0.67
1:B:876:ASN:HA	1:B:896:PHE:HB3	1.75	0.67
1:B:1085:ARG:O	1:B:1088:THR:OG1	2.12	0.67
1:A:282:ASN:HB2	1:A:443:SER:HB2	1.75	0.67
1:C:92:GLU:OE1	1:C:110:HIS:ND1	2.27	0.67
1:C:108:TYR:HE2	1:C:110:HIS:HB2	1.59	0.67
1:C:124:ARG:HG2	1:C:151:ASN:HA	1.77	0.67
1:C:779:THR:HB	1:C:1170:ALA:HB2	1.77	0.66
1:C:265:ASP:OD1	1:C:266:SER:N	2.27	0.66
1:B:72:PRO:O	1:B:206:TYR:OH	2.09	0.66
1:B:876:ASN:O	1:B:895:SER:OG	2.13	0.66
1:A:381:ASN:HB3	8:A:1506:NAG:HN2	1.60	0.66
1:C:338:HIS:HB2	1:C:421:ALA:HB3	1.77	0.66
1:C:754:ILE:HD12	1:C:762:ILE:HD11	1.77	0.66
1:B:678:SER:N	1:B:682:GLN:O	2.27	0.66
1:A:757:CYS:HB2	1:A:761:SER:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:770:GLY:H	1:B:853:THR:HB	1.61	0.66
1:C:986:ALA:O	1:C:988:GLN:NE2	2.28	0.66
1:C:1116:GLN:NE2	1:C:1120:ASN:OD1	2.28	0.66
1:B:89:HIS:O	1:B:111:LYS:NZ	2.28	0.66
1:B:122:ARG:NH1	1:B:123:LEU:O	2.29	0.66
1:A:414:LEU:HG	1:A:416:LEU:HB2	1.77	0.66
3:V:1:NAG:H61	3:V:2:NAG:N2	2.11	0.66
3:V:1:NAG:H83	3:V:1:NAG:H3	1.76	0.66
1:A:680:SER:HB2	1:A:682:GLN:HE22	1.59	0.66
1:B:332:GLU:OE2	1:B:346:SER:OG	2.14	0.66
1:A:1234:THR:OG1	1:A:1236:ASP:OD1	2.13	0.66
1:B:799:LEU:O	1:B:1112:ARG:NH1	2.28	0.66
1:C:215:LEU:HD23	1:C:227:TYR:HB3	1.78	0.66
1:C:833:ILE:HG21	1:C:1094:LEU:HD21	1.78	0.66
1:B:242:PHE:O	1:B:308:ASN:ND2	2.27	0.66
1:B:513:VAL:O	1:B:552:SER:N	2.28	0.66
1:A:881:SER:HA	1:A:892:GLN:HA	1.76	0.66
1:C:172:ARG:NH2	1:C:425:ASN:OD1	2.23	0.66
1:A:324:ASN:HB2	1:A:439:TRP:CD1	2.30	0.65
1:C:403:TYR:H	1:C:418:LEU:HA	1.60	0.65
1:B:265:ASP:OD1	1:B:266:SER:N	2.30	0.65
1:B:624:LYS:NZ	1:B:626:GLU:OE2	2.29	0.65
1:A:688:ASN:HB3	1:A:693:ALA:HB3	1.77	0.65
1:B:86:ARG:HB2	1:B:199:SER:HA	1.78	0.65
1:A:95:ILE:HG22	1:A:189:TRP:HB3	1.78	0.65
1:A:746:GLU:OE2	1:A:758:LYS:NZ	2.30	0.65
1:A:77:VAL:HG22	1:A:208:TYR:HE1	1.62	0.65
1:C:231:THR:HG22	1:C:232:ALA:H	1.61	0.65
1:A:747:PRO:HB3	1:A:755:GLY:HA3	1.79	0.65
1:C:122:ARG:NH1	1:C:123:LEU:O	2.29	0.65
1:C:1059:ASN:ND2	1:C:1062:ALA:O	2.29	0.65
1:B:59:GLN:O	1:B:62:ASN:ND2	2.28	0.65
1:B:523:GLY:N	1:B:560:SER:OG	2.30	0.65
1:B:817:SER:O	1:B:821:GLN:NE2	2.21	0.65
1:A:323:ILE:HD11	1:A:328:VAL:HG11	1.77	0.65
1:A:903:ASN:OD1	1:A:904:LYS:N	2.30	0.65
1:B:1239:PRO:HG3	1:B:1245:TYR:CD2	2.32	0.65
1:A:184:TYR:CZ	1:A:454:GLN:HG2	2.32	0.65
1:C:919:ARG:HH22	1:C:930:VAL:HB	1.62	0.65
1:C:1166:VAL:HG12	1:C:1192:HIS:HB2	1.79	0.65
1:B:398:ILE:HD12	1:B:408:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:796:TYR:HD2	1:C:1037:LYS:HE3	1.59	0.65
1:B:40:ASN:ND2	1:B:432:ASP:O	2.28	0.65
1:B:467:PRO:HA	1:B:470:GLN:HB2	1.78	0.65
1:A:1068:ASP:N	1:B:658:LYS:HZ3	1.91	0.64
1:A:1175:ASN:N	1:A:1233:LEU:O	2.23	0.64
5:Z:1:NAG:H4	5:Z:3:FUC:H5	1.79	0.64
1:A:729:ARG:NH2	1:A:741:GLY:O	2.30	0.64
1:A:781:ASN:HB3	4:I:1:NAG:N2	2.13	0.64
1:A:853:THR:H	1:A:953:TYR:HE1	1.45	0.64
1:A:897:ILE:HA	1:A:900:LEU:HD12	1.80	0.64
1:B:340:ALA:N	1:B:418:LEU:O	2.19	0.64
1:B:280:LEU:HB3	1:B:445:ASN:HB2	1.79	0.64
1:B:1009:ASN:O	1:B:1012:SER:OG	2.14	0.64
1:A:250:ILE:HD12	1:A:251:PRO:HD2	1.77	0.64
1:C:92:GLU:HB2	1:C:195:LYS:HB3	1.79	0.64
1:B:876:ASN:HB3	1:B:897:ILE:HG13	1.78	0.64
1:B:988:GLN:NE2	1:B:1211:GLU:OE2	2.31	0.64
1:A:1174:VAL:HG21	1:A:1238:LEU:HD11	1.78	0.64
1:B:515:ILE:HG12	1:B:536:ILE:HA	1.79	0.64
5:Z:1:NAG:O6	5:Z:2:NAG:N2	2.29	0.64
1:A:35:PHE:HA	1:A:38:LYS:HE2	1.80	0.64
1:A:355:PRO:HG3	1:A:360:PHE:CE2	2.33	0.64
1:A:848:VAL:HA	1:A:851:MET:SD	2.38	0.64
1:C:124:ARG:HA	1:C:150:PHE:O	1.97	0.64
1:B:404:GLY:HA2	1:B:419:LEU:HD23	1.79	0.64
1:A:586:SER:N	1:A:623:THR:O	2.27	0.64
1:C:901:LEU:O	1:C:905:VAL:HB	1.97	0.64
1:C:1194:LEU:O	1:C:1198:THR:OG1	2.08	0.64
1:B:92:GLU:HB3	1:B:108:TYR:OH	1.97	0.64
1:B:137:THR:O	1:B:140:ASN:ND2	2.28	0.64
1:A:889:ARG:NH1	1:A:890:VAL:O	2.31	0.64
1:B:895:SER:N	1:B:898:GLU:OE1	2.24	0.64
1:A:86:ARG:HG3	1:A:89:HIS:ND1	2.13	0.63
1:C:240:ASN:ND2	1:C:438:PHE:O	2.31	0.63
1:A:128:PHE:HE2	1:A:131:ILE:HD11	1.63	0.63
1:C:67:CYS:HA	1:C:203:ALA:HB3	1.80	0.63
1:C:828:ALA:O	1:C:832:THR:N	2.21	0.63
1:A:1177:GLU:OE1	1:A:1235:ARG:NH2	2.29	0.63
1:B:95:ILE:HG12	1:B:192:VAL:HG23	1.80	0.63
1:A:1009:ASN:O	1:A:1012:SER:OG	2.15	0.63
1:C:262:LEU:HB3	1:C:407:TYR:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:HIS:NE2	1:B:160:GLU:HB3	2.13	0.63
1:A:783:SER:HB3	1:A:1163:PHE:HB3	1.79	0.63
1:A:816:ASN:OD1	1:A:819:CYS:N	2.29	0.63
1:B:78:HIS:N	1:B:207:VAL:O	2.28	0.63
1:B:568:GLN:HA	1:B:603:LEU:HD13	1.79	0.63
1:C:793:ARG:HB3	1:C:1029:ASN:OD1	1.99	0.63
1:C:872:TYR:HB3	1:C:874:PHE:CE1	2.33	0.63
1:B:706:ALA:HB1	1:B:713:ILE:HD12	1.80	0.63
1:A:263:SER:O	1:A:407:TYR:OH	2.16	0.63
1:C:105:TYR:CE1	1:C:127:GLN:HB2	2.34	0.63
1:C:134:LEU:HD13	1:C:195:LYS:HB2	1.79	0.63
1:C:179:LYS:HB2	1:C:181:TYR:CZ	2.34	0.63
1:A:918:LYS:NZ	1:B:734:PHE:O	2.31	0.63
1:B:120:THR:HA	1:B:155:PRO:HA	1.79	0.63
1:B:218:THR:CG2	6:a:1:NAG:H62	2.29	0.63
1:A:374:PHE:HE1	1:A:387:PHE:HD1	1.47	0.62
1:C:83:SER:OG	1:C:202:CYS:O	2.14	0.62
1:C:1033:HIS:O	1:C:1036:THR:OG1	2.15	0.62
1:C:1144:VAL:HA	1:C:1152:LEU:O	1.98	0.62
1:B:1012:SER:HA	1:B:1015:GLU:CD	2.24	0.62
1:C:1239:PRO:HG3	1:C:1245:TYR:HD2	1.64	0.62
1:B:328:VAL:HG13	1:B:427:THR:H	1.64	0.62
1:B:688:ASN:O	1:B:690:THR:N	2.29	0.62
1:A:322:ASN:ND2	1:A:397:GLU:OE2	2.18	0.62
1:C:748:VAL:N	1:C:756:VAL:O	2.32	0.62
1:B:584:SER:HB3	1:B:624:LYS:HE2	1.81	0.62
1:A:1016:SER:HB3	1:A:1019:GLU:HB3	1.81	0.62
1:A:1051:GLN:O	1:A:1055:GLN:HG2	1.99	0.62
1:B:212:TYR:CD1	1:B:235:ILE:HD11	2.34	0.62
1:B:403:TYR:HA	1:B:418:LEU:HD23	1.81	0.62
1:A:953:TYR:O	1:A:957:LEU:HG	1.98	0.62
1:C:1239:PRO:HG3	1:C:1245:TYR:CD2	2.34	0.62
1:B:289:LYS:O	1:B:429:HIS:ND1	2.33	0.62
1:A:66:TYR:HH	1:A:208:TYR:HH	1.40	0.62
1:A:337:LEU:O	1:A:338:HIS:ND1	2.33	0.62
1:A:1056:LEU:HB2	1:A:1090:ARG:CZ	2.30	0.62
1:C:494:SER:OG	1:C:496:GLU:OE1	2.18	0.62
1:B:84:HIS:CE1	1:B:86:ARG:HD2	2.35	0.62
1:B:472:LYS:HA	1:B:480:LEU:HD11	1.80	0.62
1:A:274:VAL:HG22	1:A:450:LEU:HB2	1.81	0.62
1:C:77:VAL:HG22	1:C:208:TYR:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ASP:HA	1:C:470:GLN:HE21	1.62	0.62
1:A:376:LYS:HA	1:A:385:TYR:HA	1.81	0.62
1:A:394:THR:O	1:A:396:ARG:NH1	2.32	0.62
1:A:876:ASN:OD1	3:K:1:NAG:O6	2.17	0.62
1:C:981:ARG:NE	1:C:1141:PHE:HB3	2.14	0.62
1:B:182:TYR:HE2	1:B:292:GLY:H	1.48	0.62
1:A:744:CYS:SG	1:A:757:CYS:N	2.73	0.62
1:C:468:VAL:HG22	1:C:713:ILE:HG12	1.80	0.62
1:B:680:SER:O	1:B:682:GLN:NE2	2.33	0.62
1:C:89:HIS:HB3	1:C:197:TYR:HB2	1.82	0.61
1:C:752:SER:OG	1:C:753:ASN:N	2.31	0.61
1:B:795:GLU:O	1:B:1152:LEU:HD12	2.01	0.61
1:B:1239:PRO:HG3	1:B:1245:TYR:HD2	1.63	0.61
1:B:123:LEU:HD22	1:B:150:PHE:CD1	2.34	0.61
1:A:134:LEU:HD11	1:A:195:LYS:HD2	1.82	0.61
1:A:283:CYS:HA	1:A:307:CYS:HB3	1.81	0.61
1:C:120:THR:HA	1:C:155:PRO:HA	1.82	0.61
1:B:902:PHE:O	1:B:906:VAL:N	2.33	0.61
1:B:1192:HIS:HB3	1:B:1203:PHE:CD1	2.35	0.61
1:A:801:ASN:HB2	1:A:1105:TYR:CE1	2.35	0.61
1:C:91:PHE:H	1:C:111:LYS:HG3	1.64	0.61
1:C:505:PRO:HG2	1:C:639:THR:HA	1.82	0.61
1:C:1183:ARG:NH1	1:B:1219:ASP:OD1	2.33	0.61
4:J:1:NAG:H3	4:J:2:NAG:C7	2.30	0.61
1:A:549:PHE:O	1:A:631:THR:N	2.32	0.61
1:C:256:PHE:HB3	1:C:259:TRP:HB2	1.82	0.61
1:C:299:PHE:HA	1:C:316:PRO:HG2	1.82	0.61
1:A:129:PRO:HB3	1:A:140:ASN:OD1	2.01	0.61
1:A:260:PHE:H	1:A:320:ARG:HH12	1.47	0.61
1:A:428:GLY:HA2	1:A:432:ASP:HB3	1.81	0.61
1:A:796:TYR:O	1:A:1037:LYS:NZ	2.34	0.61
1:C:471:LEU:O	1:C:474:SER:OG	2.19	0.61
1:B:32:PHE:CD1	1:B:163:VAL:HG21	2.35	0.61
1:B:1028:LEU:HG	1:B:1033:HIS:CE1	2.35	0.61
1:C:282:ASN:N	1:C:443:SER:O	2.27	0.61
1:C:818:ARG:NH1	1:C:818:ARG:O	2.34	0.61
1:B:107:LEU:HB2	1:B:125:ILE:HD13	1.82	0.61
1:B:218:THR:N	1:B:224:GLY:O	2.29	0.61
1:B:297:PHE:HB2	1:B:422:VAL:HB	1.83	0.61
1:B:428:GLY:O	1:B:429:HIS:ND1	2.34	0.61
1:A:489:SER:HB2	1:A:702:PHE:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:HIS:ND1	1:C:344:ASN:OD1	2.30	0.61
1:B:240:ASN:HD21	1:B:438:PHE:H	1.46	0.61
1:B:489:SER:OG	1:B:702:PHE:O	2.16	0.61
1:B:501:PHE:HD1	1:B:653:THR:HB	1.64	0.61
1:A:992:LEU:HD12	1:A:994:ARG:HH21	1.65	0.61
1:C:126:CYS:CB	1:C:148:CYS:HA	2.30	0.61
1:A:892:GLN:HG2	1:A:951:HIS:HE1	1.65	0.60
1:C:425:ASN:HB2	3:T:1:NAG:C7	2.31	0.60
1:B:324:ASN:O	1:B:396:ARG:NE	2.33	0.60
1:B:959:GLY:HA2	1:B:962:VAL:HG22	1.83	0.60
1:A:242:PHE:CE2	1:A:244:THR:HG22	2.36	0.60
1:A:838:GLN:HG2	1:A:842:ARG:HE	1.65	0.60
1:B:244:THR:N	1:B:309:GLY:HA3	2.15	0.60
1:A:406:VAL:HB	1:A:414:LEU:HB3	1.82	0.60
1:C:97:GLN:HG3	1:C:189:TRP:CD1	2.36	0.60
1:C:55:ILE:HG23	1:C:207:VAL:HG22	1.83	0.60
1:C:747:PRO:HB3	1:C:755:GLY:HA3	1.84	0.60
1:C:1012:SER:HB2	1:C:1020:ALA:HB1	1.83	0.60
1:B:1205:SER:HB2	1:B:1211:GLU:H	1.66	0.60
1:C:726:ASN:N	1:C:739:ASN:OD1	2.33	0.60
1:B:503:THR:HB	1:B:626:GLU:HB3	1.84	0.60
1:A:337:LEU:HB3	1:A:345:PHE:HB2	1.83	0.60
1:B:280:LEU:O	1:B:445:ASN:N	2.34	0.60
1:B:402:LYS:HA	1:B:419:LEU:HB2	1.82	0.60
1:B:1190:PHE:CE2	1:B:1203:PHE:HB2	2.37	0.60
1:A:195:LYS:HE2	1:A:197:TYR:HE1	1.67	0.60
1:A:982:LEU:HB3	1:A:988:GLN:NE2	2.17	0.60
1:A:1234:THR:N	1:A:1237:GLN:OE1	2.34	0.60
1:C:1205:SER:HB2	1:C:1211:GLU:H	1.66	0.60
1:B:465:ASP:OD1	1:B:466:ASP:N	2.34	0.60
1:B:1213:ARG:NH2	1:B:1219:ASP:OD2	2.34	0.60
1:A:370:PRO:HB3	1:A:391:LEU:O	2.02	0.60
1:B:322:ASN:HA	1:B:397:GLU:HG2	1.83	0.60
1:B:654:ILE:O	1:B:657:PHE:HB2	2.01	0.60
1:B:984:TYR:HD2	1:B:985:LEU:HD12	1.66	0.60
1:A:1242:ILE:HG22	1:A:1244:ASP:H	1.67	0.60
1:C:95:ILE:HD12	1:C:107:LEU:HD23	1.84	0.60
1:B:92:GLU:HA	1:B:109:LEU:O	2.00	0.60
1:B:129:PRO:HD2	1:B:144:ILE:HG13	1.84	0.60
1:A:961:MET:HE1	1:A:1124:LYS:HA	1.83	0.59
1:A:1144:VAL:HG22	1:A:1151:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:HIS:CG	1:C:199:SER:HB3	2.37	0.59
1:C:777:THR:HB	1:B:972:LEU:HD21	1.83	0.59
1:C:919:ARG:NH1	1:C:931:CYS:SG	2.74	0.59
1:B:922:ASN:HD21	1:B:924:ARG:CZ	2.15	0.59
1:C:72:PRO:HD2	1:C:194:THR:OG1	2.02	0.59
1:C:172:ARG:N	1:C:187:ASN:HD21	2.00	0.59
1:C:252:GLU:OE1	1:C:252:GLU:N	2.36	0.59
1:C:811:TYR:OH	1:C:1052:LEU:O	2.20	0.59
1:B:1109:GLN:HG2	1:B:1113:LYS:NZ	2.17	0.59
4:U:1:NAG:H5	4:U:2:NAG:C7	2.32	0.59
6:k:1:NAG:H4	6:k:4:FUC:H5	1.84	0.59
1:A:1062:ALA:HA	1:A:1085:ARG:NH2	2.17	0.59
1:A:1063:ILE:HD11	1:B:573:PRO:HB3	1.83	0.59
1:A:1069:ASP:N	1:B:658:LYS:HE2	2.17	0.59
1:B:743:ASN:OD1	8:B:1505:NAG:N2	2.35	0.59
1:A:278:PRO:HB2	1:A:444:THR:HB	1.83	0.59
1:A:317:GLU:O	1:A:402:LYS:N	2.34	0.59
1:A:923:GLY:HA3	1:B:698:THR:HG21	1.84	0.59
1:C:407:TYR:HA	1:C:411:PHE:O	2.03	0.59
1:C:689:VAL:HG23	1:C:690:THR:H	1.65	0.59
1:A:316:PRO:HB3	1:A:443:SER:HB3	1.83	0.59
1:A:647:ASP:N	1:A:663:ILE:O	2.28	0.59
1:C:171:ASP:O	1:C:185:PHE:N	2.33	0.59
1:C:1055:GLN:HA	1:C:1058:HIS:ND1	2.17	0.59
1:B:131:ILE:HA	1:B:140:ASN:HD22	1.68	0.59
1:B:257:ASN:OD1	1:B:258:ASN:N	2.36	0.59
1:B:994:ARG:NH1	1:B:995:ASN:HB2	2.18	0.59
4:Y:2:NAG:H83	4:Y:2:NAG:H3	1.83	0.59
1:A:374:PHE:CE1	1:A:387:PHE:HD1	2.20	0.59
1:C:34:ARG:HH21	1:C:163:VAL:N	2.01	0.59
1:C:34:ARG:HH21	1:C:163:VAL:H	1.51	0.59
1:C:108:TYR:CE2	1:C:110:HIS:HB2	2.37	0.59
1:B:793:ARG:HB3	1:B:1029:ASN:OD1	2.03	0.59
1:C:82:VAL:O	1:C:163:VAL:HA	2.03	0.59
1:B:86:ARG:NH2	1:B:160:GLU:OE2	2.36	0.59
1:A:171:ASP:HA	1:A:187:ASN:OD1	2.03	0.59
1:A:328:VAL:HB	1:A:437:GLY:H	1.68	0.59
1:A:665:LEU:HD13	1:A:693:ALA:HB1	1.84	0.59
1:A:672:ALA:O	1:A:676:TYR:OH	2.21	0.59
1:C:672:ALA:O	1:C:676:TYR:OH	2.21	0.59
1:C:1067:ILE:HD11	1:C:1090:ARG:HH12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ASN:HB2	1:B:358:ALA:HB3	1.84	0.59
1:A:240:ASN:ND2	1:A:439:TRP:HB3	2.14	0.59
1:A:505:PRO:HD2	1:A:640:ASP:H	1.67	0.59
1:C:34:ARG:HD2	1:C:38:LYS:HE3	1.84	0.59
1:C:840:SER:O	1:C:1105:TYR:OH	2.17	0.59
1:A:371:TYR:O	1:A:391:LEU:HB2	2.03	0.58
1:C:241:VAL:HG11	1:C:286:ALA:HB2	1.85	0.58
1:C:989:THR:OG1	1:C:1211:GLU:OE1	2.19	0.58
1:B:408:VAL:HB	1:B:413:TYR:CE2	2.38	0.58
1:A:799:LEU:HD23	1:A:1150:GLY:HA2	1.85	0.58
1:C:856:GLU:CD	1:C:856:GLU:H	2.10	0.58
1:B:447:VAL:HG11	1:B:463:TYR:CE2	2.37	0.58
1:B:798:GLN:NE2	1:B:801:ASN:OD1	2.36	0.58
1:A:53:LEU:HB2	1:A:211:THR:HG23	1.83	0.58
1:A:933:GLN:O	1:A:936:SER:OG	2.16	0.58
1:C:317:GLU:O	1:C:401:THR:OG1	2.14	0.58
1:B:127:GLN:O	1:B:146:ARG:HB2	2.03	0.58
1:A:457:ALA:O	1:A:459:GLN:NE2	2.28	0.58
1:B:86:ARG:O	1:B:89:HIS:ND1	2.37	0.58
1:B:544:VAL:HG11	1:B:549:PHE:CD1	2.38	0.58
1:A:770:GLY:N	1:C:853:THR:HB	2.19	0.58
1:C:728:THR:OG1	1:C:737:HIS:ND1	2.30	0.58
1:C:1098:VAL:O	1:C:1101:THR:OG1	2.20	0.58
1:B:82:VAL:HG23	1:B:204:MET:SD	2.44	0.58
1:B:326:THR:HG22	1:B:395:VAL:HB	1.84	0.58
1:A:377:VAL:O	1:A:383:THR:HA	2.03	0.58
1:C:84:HIS:HA	1:C:160:GLU:O	2.03	0.58
1:C:508:ASN:OD1	1:C:638:VAL:N	2.36	0.58
1:B:954:SER:HA	1:B:957:LEU:HD12	1.84	0.58
1:B:1010:ILE:HG22	1:B:1014:PHE:CE2	2.39	0.58
1:A:1011:THR:HA	1:A:1014:PHE:HD2	1.69	0.58
1:A:1166:VAL:HA	1:A:1192:HIS:CD2	2.37	0.58
1:B:468:VAL:HG22	1:B:713:ILE:HG12	1.86	0.58
1:A:272:LYS:HB3	1:A:450:LEU:HD11	1.85	0.58
1:A:334:SER:O	1:A:424:ILE:HG23	2.04	0.58
1:A:490:ARG:NH2	1:A:491:ASN:OD1	2.36	0.58
1:A:872:TYR:HB3	1:A:874:PHE:HE1	1.68	0.58
1:A:1188:VAL:O	1:A:1204:VAL:HA	2.03	0.58
1:C:108:TYR:HB2	1:C:131:ILE:HD12	1.86	0.58
1:B:1036:THR:HA	1:B:1039:GLN:OE1	2.04	0.58
1:A:86:ARG:HG3	1:A:89:HIS:HD1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:O	1:A:122:ARG:NH1	2.35	0.58
1:A:283:CYS:H	1:A:311:ALA:HB1	1.69	0.58
1:C:377:VAL:HG12	1:C:379:THR:HG22	1.84	0.58
1:C:796:TYR:HE1	1:C:1150:GLY:HA3	1.68	0.58
1:B:1183:ARG:HB2	1:B:1221:VAL:HG13	1.85	0.58
1:A:218:THR:N	1:A:224:GLY:O	2.36	0.58
1:C:87:GLY:H	1:C:160:GLU:HG2	1.68	0.58
1:C:89:HIS:HD2	1:C:197:TYR:HB3	1.69	0.58
1:C:1174:VAL:HA	1:C:1233:LEU:HB3	1.86	0.58
1:B:1204:VAL:HG23	1:B:1213:ARG:HB3	1.85	0.58
4:I:1:NAG:H83	4:I:1:NAG:H3	1.86	0.58
3:K:2:NAG:H3	3:K:2:NAG:H83	1.85	0.58
1:A:337:LEU:HD21	1:A:419:LEU:HD22	1.85	0.57
1:C:272:LYS:HB3	1:C:450:LEU:HD11	1.86	0.57
1:C:404:GLY:O	1:C:416:LEU:N	2.35	0.57
1:A:289:LYS:HE3	3:E:2:NAG:H5	1.86	0.57
1:C:289:LYS:HA	1:C:439:TRP:CD1	2.39	0.57
1:B:847:GLU:OE2	1:B:1112:ARG:NH2	2.37	0.57
3:j:2:NAG:H3	3:j:2:NAG:H83	1.86	0.57
1:A:472:LYS:HA	1:A:480:LEU:HD11	1.86	0.57
1:C:76:GLY:H	1:C:190:SER:HB2	1.69	0.57
1:C:1085:ARG:O	1:C:1088:THR:OG1	2.19	0.57
1:B:63:SER:O	1:B:205:GLN:NE2	2.37	0.57
1:C:953:TYR:O	1:C:957:LEU:HG	2.04	0.57
1:B:89:HIS:HB3	1:B:197:TYR:HB3	1.87	0.57
1:B:798:GLN:NE2	1:B:800:TYR:O	2.26	0.57
5:M:2:NAG:H3	5:M:2:NAG:H83	1.86	0.57
1:A:48:VAL:H	1:A:241:VAL:HG21	1.69	0.57
1:A:87:GLY:O	1:A:116:ASN:ND2	2.30	0.57
1:A:1059:ASN:ND2	1:A:1062:ALA:O	2.36	0.57
1:C:56:GLY:O	1:C:65:TRP:NE1	2.36	0.57
1:C:72:PRO:HD2	1:C:194:THR:HG1	1.69	0.57
1:C:688:ASN:HB2	1:C:695:TYR:CE1	2.39	0.57
1:C:696:SER:OG	1:B:923:GLY:O	2.18	0.57
1:C:1066:SER:O	1:C:1070:ILE:HG12	2.05	0.57
1:B:793:ARG:HB3	1:B:1029:ASN:HD21	1.70	0.57
1:A:1033:HIS:O	1:A:1036:THR:OG1	2.22	0.57
1:A:1165:ASP:O	1:A:1192:HIS:NE2	2.38	0.57
1:C:97:GLN:HE21	1:C:189:TRP:HE1	1.53	0.57
1:C:97:GLN:HE22	1:C:106:GLN:HE22	1.51	0.57
1:A:708:TYR:CE2	1:A:711:ASP:HA	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:HIS:HD1	1:C:344:ASN:CG	2.13	0.57
1:C:744:CYS:HB2	1:C:761:SER:C	2.30	0.57
1:C:843:LEU:O	1:C:846:VAL:HG12	2.05	0.57
1:C:845:SER:HA	1:C:944:VAL:HG11	1.87	0.57
1:A:98:GLU:HA	1:A:191:ARG:HB2	1.87	0.57
1:A:362:ILE:HG13	1:A:364:LEU:H	1.69	0.57
1:A:381:ASN:HB3	8:A:1506:NAG:N2	2.19	0.57
1:A:706:ALA:HB1	1:A:713:ILE:HD12	1.86	0.57
1:C:428:GLY:O	1:C:429:HIS:ND1	2.37	0.57
1:B:218:THR:HG22	6:a:1:NAG:H62	1.86	0.57
1:B:281:VAL:HA	1:B:444:THR:HG22	1.87	0.57
1:B:404:GLY:HA3	1:B:416:LEU:C	2.30	0.57
1:A:67:CYS:O	1:A:198:ASN:ND2	2.38	0.57
1:A:285:LEU:HD12	1:A:441:ILE:HD11	1.87	0.57
1:C:1216:THR:HB	1:C:1219:ASP:HB2	1.87	0.57
1:B:175:VAL:O	1:B:180:ILE:HA	2.04	0.57
1:B:985:LEU:HB3	1:B:1208:ARG:NH2	2.19	0.57
1:A:181:TYR:HB3	1:A:183:PHE:HE2	1.68	0.57
1:A:652:TYR:HB2	1:A:654:ILE:HD11	1.87	0.57
1:A:1052:LEU:HD11	1:A:1094:LEU:HD23	1.87	0.57
1:C:84:HIS:NE2	1:C:160:GLU:HB3	2.20	0.57
1:C:295:GLN:NE2	1:C:296:PHE:O	2.28	0.57
1:C:857:GLU:HA	1:C:860:GLN:CD	2.30	0.57
3:T:1:NAG:H61	3:T:2:NAG:HN2	1.70	0.57
1:A:1054:VAL:CA	1:A:1057:GLN:HE22	2.11	0.56
1:C:32:PHE:CD2	1:C:163:VAL:HG21	2.40	0.56
1:C:798:GLN:NE2	1:C:801:ASN:OD1	2.37	0.56
1:C:1017:VAL:O	1:C:1018:LYS:HG3	2.05	0.56
1:A:55:ILE:HG12	1:A:205:GLN:HG3	1.87	0.56
1:A:336:VAL:HB	1:A:423:THR:OG1	2.05	0.56
1:A:386:LYS:NZ	1:A:387:PHE:O	2.37	0.56
1:A:508:ASN:O	1:A:547:ARG:HB3	2.05	0.56
1:C:793:ARG:HD3	1:C:1029:ASN:HD21	1.70	0.56
1:C:874:PHE:HB3	1:C:878:LEU:HD13	1.87	0.56
1:B:374:PHE:CE1	1:B:387:PHE:HD1	2.23	0.56
1:C:407:TYR:OH	2:O:1:NAG:N2	2.36	0.56
1:C:796:TYR:CE1	1:C:1150:GLY:HA3	2.40	0.56
1:C:1055:GLN:HA	1:C:1058:HIS:CE1	2.39	0.56
1:A:462:LEU:HD21	1:A:472:LYS:HD3	1.87	0.56
1:A:727:SER:HB2	3:F:1:NAG:H81	1.87	0.56
1:C:292:GLY:HA3	1:C:426:PHE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:808:CYS:HB3	1:C:834:GLU:OE2	2.05	0.56
1:A:34:ARG:NH2	1:A:178:ASP:OD1	2.38	0.56
1:A:289:LYS:HD3	1:A:434:ASP:O	2.05	0.56
1:A:731:LEU:O	1:C:918:LYS:NZ	2.32	0.56
1:C:636:GLU:OE2	1:B:357:LEU:N	2.31	0.56
1:B:125:ILE:HG22	1:B:150:PHE:HB3	1.87	0.56
1:C:355:PRO:HG2	1:C:385:TYR:CG	2.40	0.56
1:C:1214:LYS:HE3	1:C:1215:PRO:HD2	1.88	0.56
1:B:66:TYR:HB3	1:B:70:GLN:CD	2.31	0.56
1:B:122:ARG:HG2	1:B:124:ARG:NH2	2.21	0.56
1:B:289:LYS:HA	1:B:439:TRP:CD1	2.40	0.56
1:B:526:GLY:HA3	1:B:609:PHE:HB2	1.88	0.56
1:B:856:GLU:H	1:B:856:GLU:CD	2.13	0.56
1:A:86:ARG:HH21	1:A:197:TYR:HB3	1.71	0.56
1:A:168:TRP:HB2	1:A:187:ASN:ND2	2.21	0.56
1:A:345:PHE:HB3	1:A:375:PHE:CZ	2.39	0.56
1:A:813:CYS:HB2	1:A:820:LYS:NZ	2.21	0.56
1:A:1222:GLN:HE21	1:C:1214:LYS:HB2	1.71	0.56
1:C:150:PHE:CZ	1:C:152:LYS:HB2	2.40	0.56
1:C:666:THR:HG23	1:C:694:VAL:HG23	1.86	0.56
1:C:883:TYR:HE1	1:C:888:GLY:HA2	1.70	0.56
1:C:1187:LEU:HD21	1:C:1204:VAL:HB	1.87	0.56
1:B:241:VAL:HG12	1:B:440:THR:HB	1.88	0.56
1:B:675:TYR:HA	1:B:686:PHE:HA	1.88	0.56
1:A:1166:VAL:HG12	1:A:1192:HIS:CG	2.41	0.56
1:C:83:SER:HA	1:C:163:VAL:HG22	1.88	0.56
1:C:182:TYR:HH	1:C:292:GLY:HA3	1.71	0.56
1:C:863:THR:HG23	1:C:866:SER:H	1.70	0.56
1:B:1031:VAL:HG12	1:B:1035:LEU:HD23	1.87	0.56
1:A:115:GLY:N	1:A:119:ALA:HB2	2.20	0.56
1:A:263:SER:OG	1:A:266:SER:O	2.23	0.56
1:A:498:PRO:HG2	1:A:648:VAL:HG11	1.88	0.56
1:A:1232:ASN:OD1	4:L:1:NAG:N2	2.39	0.56
1:C:502:VAL:HA	1:C:642:SER:HB3	1.88	0.56
1:C:816:ASN:ND2	1:C:1068:ASP:OD1	2.38	0.56
1:B:420:ASP:OD1	1:B:421:ALA:N	2.39	0.56
1:B:768:GLN:NE2	1:B:769:SER:O	2.35	0.56
1:B:795:GLU:OE2	1:B:1155:HIS:NE2	2.24	0.56
1:B:1129:ARG:HG2	1:B:1132:PHE:HB2	1.88	0.56
1:A:36:PHE:HA	1:A:39:PHE:CE2	2.41	0.56
1:A:90:GLY:HA2	1:A:111:LYS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:CYS:O	1:C:128:PHE:N	2.39	0.56
1:C:502:VAL:O	1:C:655:TYR:N	2.23	0.56
1:B:651:LYS:NZ	1:B:660:GLU:HB2	2.21	0.56
1:B:688:ASN:N	1:B:693:ALA:O	2.28	0.56
1:C:853:THR:H	1:C:953:TYR:HE1	1.52	0.55
1:A:179:LYS:HB2	1:A:181:TYR:CZ	2.41	0.55
1:C:256:PHE:HA	1:C:259:TRP:CD1	2.40	0.55
1:C:325:ASP:OD2	1:C:327:SER:OG	2.17	0.55
1:C:856:GLU:OE1	1:C:856:GLU:N	2.36	0.55
1:B:219:SER:HB3	1:B:224:GLY:HA3	1.86	0.55
1:A:240:ASN:OD1	1:A:241:VAL:N	2.40	0.55
1:A:344:ASN:C	1:A:378:ASP:HB2	2.31	0.55
1:A:499:ILE:HB	1:A:651:LYS:HZ2	1.71	0.55
1:A:548:GLN:HG2	1:A:635:LEU:HG	1.87	0.55
1:A:1180:LEU:HG	1:A:1220:PHE:HB3	1.87	0.55
1:C:736:TYR:CE2	1:C:762:ILE:HB	2.41	0.55
1:C:818:ARG:NH1	1:C:821:GLN:HB2	2.20	0.55
1:B:71:HIS:ND1	1:B:195:LYS:HA	2.22	0.55
1:B:86:ARG:HB3	1:B:89:HIS:ND1	2.21	0.55
1:B:240:ASN:ND2	1:B:438:PHE:O	2.39	0.55
1:B:548:GLN:OE1	1:B:635:LEU:N	2.38	0.55
1:A:77:VAL:HG22	1:A:208:TYR:CE1	2.42	0.55
1:B:92:GLU:HG2	1:B:111:LYS:H	1.70	0.55
1:B:811:TYR:CE1	1:B:1056:LEU:HD21	2.41	0.55
1:B:1233:LEU:HD22	1:B:1237:GLN:HB3	1.88	0.55
1:A:777:THR:O	1:A:1207:ARG:NH2	2.39	0.55
1:C:212:TYR:CD1	1:C:235:ILE:HD11	2.41	0.55
1:C:665:LEU:HD12	1:C:694:VAL:O	2.07	0.55
1:B:35:PHE:HB2	1:B:163:VAL:HB	1.88	0.55
1:A:282:ASN:HB2	1:A:443:SER:CB	2.36	0.55
1:A:1067:ILE:HA	1:A:1070:ILE:HD12	1.88	0.55
1:A:1194:LEU:O	1:A:1198:THR:OG1	2.20	0.55
1:C:218:THR:CG2	6:N:1:NAG:H62	2.28	0.55
1:A:502:VAL:HB	1:A:654:ILE:HG23	1.89	0.55
1:C:345:PHE:HB3	1:C:375:PHE:CD1	2.42	0.55
1:C:403:TYR:N	1:C:418:LEU:HD23	2.22	0.55
1:B:509:ALA:C	1:B:546:THR:HB	2.31	0.55
1:B:757:CYS:HB2	1:B:761:SER:HB2	1.88	0.55
1:A:788:PHE:HB3	1:A:1158:LEU:HB3	1.89	0.55
1:C:451:ILE:HG12	1:C:461:ILE:HG13	1.88	0.55
1:C:946:ASP:HB3	1:C:949:LYS:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:TRP:NE1	1:B:189:TRP:O	2.40	0.55
1:A:233:ASN:OD1	3:E:2:NAG:O6	2.11	0.55
1:A:720:LEU:HD23	1:C:921:SER:HB2	1.88	0.55
1:C:691:SER:HB3	3:V:1:NAG:H62	1.89	0.55
1:C:1185:PRO:O	1:C:1207:ARG:NH1	2.34	0.55
1:C:1225:SER:OG	1:B:990:ASP:OD1	2.21	0.55
1:B:571:ASN:HB2	1:B:600:THR:HB	1.88	0.55
1:A:103:SER:O	1:A:127:GLN:NE2	2.40	0.55
1:A:356:HIS:CE1	1:A:384:VAL:HA	2.42	0.55
1:A:495:HIS:CG	1:A:496:GLU:H	2.25	0.55
1:A:793:ARG:HB3	1:A:1029:ASN:OD1	2.07	0.55
1:A:982:LEU:O	1:A:986:ALA:N	2.32	0.55
1:C:40:ASN:HB3	1:C:432:ASP:O	2.07	0.55
1:C:351:ASN:HB3	7:S:1:NAG:C7	2.36	0.55
1:C:498:PRO:O	1:C:650:THR:OG1	2.25	0.55
1:B:289:LYS:HA	1:B:439:TRP:HD1	1.72	0.55
1:B:790:MET:SD	1:B:1002:SER:OG	2.60	0.55
1:A:260:PHE:HE1	1:B:672:ALA:HA	1.72	0.54
1:A:328:VAL:HG23	1:A:426:PHE:CD1	2.42	0.54
1:B:513:VAL:N	1:B:550:THR:O	2.40	0.54
1:B:606:TYR:CD1	1:B:612:GLY:HA2	2.42	0.54
1:A:236:GLY:O	1:A:240:ASN:N	2.41	0.54
1:C:316:PRO:HB3	1:C:443:SER:OG	2.07	0.54
1:C:748:VAL:HG21	1:C:758:LYS:HB3	1.89	0.54
1:C:817:SER:O	1:C:821:GLN:NE2	2.24	0.54
1:C:916:ASP:OD2	1:C:918:LYS:HB2	2.06	0.54
1:C:989:THR:HG23	1:C:1211:GLU:HB3	1.89	0.54
1:B:67:CYS:SG	1:B:199:SER:N	2.61	0.54
1:B:71:HIS:HE1	1:B:195:LYS:HG3	1.72	0.54
1:B:652:TYR:O	1:B:658:LYS:HA	2.06	0.54
4:U:1:NAG:H3	4:U:1:NAG:H83	1.90	0.54
1:A:177:SER:O	1:A:181:TYR:OH	2.24	0.54
1:A:237:TYR:CD1	1:A:288:PRO:HB3	2.42	0.54
1:A:1027:GLY:O	1:A:1030:THR:OG1	2.15	0.54
1:A:1100:GLN:O	1:A:1104:LYS:HG2	2.06	0.54
1:C:215:LEU:HB3	1:C:217:VAL:HG23	1.90	0.54
1:C:280:LEU:O	1:C:445:ASN:N	2.40	0.54
1:B:793:ARG:HB3	1:B:1029:ASN:ND2	2.22	0.54
1:A:481:ASP:O	1:A:485:TYR:OH	2.23	0.54
1:A:822:LEU:HA	1:A:825:GLN:OE1	2.08	0.54
1:A:915:GLU:HB2	1:A:919:ARG:HH21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LEU:HB3	1:C:407:TYR:HD2	1.73	0.54
1:C:1011:THR:HA	1:C:1014:PHE:CD2	2.43	0.54
1:B:296:PHE:CZ	1:B:421:ALA:HB1	2.41	0.54
1:B:339:THR:HA	1:B:419:LEU:HA	1.89	0.54
1:B:1164:VAL:HG12	1:B:1166:VAL:HG13	1.89	0.54
1:A:80:ILE:HG12	1:A:168:TRP:CZ3	2.42	0.54
1:A:748:VAL:N	1:A:756:VAL:O	2.41	0.54
1:C:818:ARG:NH1	1:C:822:LEU:HG	2.22	0.54
1:B:578:SER:O	1:B:583:LEU:HD23	2.07	0.54
1:B:946:ASP:OD1	1:B:947:ALA:N	2.41	0.54
1:A:239:ALA:HB1	1:A:257:ASN:HB3	1.89	0.54
1:A:583:LEU:HB3	1:A:585:PHE:HE2	1.72	0.54
1:A:664:THR:HG21	1:C:924:ARG:HA	1.89	0.54
1:C:302:THR:HG21	1:C:313:GLN:HA	1.88	0.54
1:C:844:GLU:HA	1:C:847:GLU:OE2	2.07	0.54
1:C:981:ARG:HE	1:C:1141:PHE:HB3	1.73	0.54
1:B:172:ARG:NH2	1:B:426:PHE:O	2.41	0.54
1:B:502:VAL:O	1:B:655:TYR:N	2.22	0.54
1:B:607:PRO:HG2	1:B:611:SER:H	1.73	0.54
1:B:800:TYR:CZ	1:B:1149:GLN:HG2	2.43	0.54
1:A:126:CYS:HB3	1:A:148:CYS:HA	1.89	0.54
1:A:128:PHE:HE1	1:A:144:ILE:HG23	1.73	0.54
1:A:1188:VAL:HG13	1:A:1207:ARG:HG2	1.89	0.54
1:C:177:SER:HB2	1:C:181:TYR:HE2	1.71	0.54
1:C:281:VAL:HA	1:C:444:THR:HG22	1.89	0.54
1:C:800:TYR:CZ	1:C:1149:GLN:HG2	2.43	0.54
1:C:1216:THR:HA	1:C:1244:ASP:OD2	2.08	0.54
1:B:1185:PRO:O	1:B:1207:ARG:NH1	2.34	0.54
1:A:217:VAL:HA	1:A:225:ILE:HA	1.89	0.54
1:A:752:SER:HA	1:C:944:VAL:HG22	1.89	0.54
1:A:1120:ASN:HA	1:A:1124:LYS:HE2	1.90	0.54
1:C:92:GLU:HG2	1:C:110:HIS:HA	1.90	0.54
1:C:1016:SER:OG	1:C:1019:GLU:OE2	2.25	0.54
1:B:139:ASN:H	1:B:139:ASN:HD22	1.55	0.54
1:B:173:VAL:HB	1:B:183:PHE:HB2	1.89	0.54
1:B:262:LEU:HD11	1:B:399:VAL:HG11	1.89	0.54
1:A:324:ASN:HA	3:E:1:NAG:C7	2.37	0.54
1:A:1091:LEU:HA	1:A:1094:LEU:HD12	1.90	0.54
1:C:917:TYR:CE1	1:C:934:TYR:HB2	2.43	0.54
1:B:98:GLU:HA	1:B:191:ARG:HB2	1.90	0.54
1:B:126:CYS:O	1:B:128:PHE:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:TYR:O	1:B:957:LEU:HG	2.08	0.54
1:A:38:LYS:HZ1	1:A:176:PHE:HB3	1.73	0.54
1:A:66:TYR:OH	1:A:208:TYR:OH	2.15	0.54
1:A:362:ILE:HD12	1:A:363:PRO:HD2	1.90	0.54
1:A:727:SER:OG	1:A:741:GLY:N	2.41	0.54
1:A:872:TYR:HB3	1:A:874:PHE:CE1	2.42	0.54
1:A:917:TYR:CE1	1:A:934:TYR:HB2	2.43	0.54
1:C:51:GLY:O	1:C:53:LEU:HG	2.08	0.54
1:C:128:PHE:CD2	1:C:129:PRO:HD2	2.43	0.54
1:C:344:ASN:HB2	1:C:378:ASP:HB3	1.89	0.54
1:C:500:SER:HB3	1:C:652:TYR:HA	1.90	0.54
1:C:1188:VAL:O	1:C:1204:VAL:HA	2.07	0.54
1:B:498:PRO:HG2	1:B:648:VAL:HG11	1.89	0.54
1:A:168:TRP:HB2	1:A:187:ASN:HD22	1.74	0.53
1:A:233:ASN:HA	3:E:2:NAG:H61	1.89	0.53
1:A:302:THR:HA	1:A:316:PRO:HD3	1.90	0.53
1:A:426:PHE:CZ	1:A:436:SER:HA	2.43	0.53
1:A:944:VAL:HG22	1:B:752:SER:HA	1.90	0.53
1:A:1058:HIS:HB2	1:A:1060:PHE:CZ	2.42	0.53
1:C:468:VAL:HG13	1:C:708:TYR:HE1	1.72	0.53
1:B:39:PHE:HZ	1:B:176:PHE:HE1	1.57	0.53
1:B:84:HIS:CD2	1:B:160:GLU:HB3	2.42	0.53
1:A:237:TYR:HA	1:A:240:ASN:OD1	2.07	0.53
1:C:71:HIS:CE1	1:C:134:LEU:HD22	2.43	0.53
1:C:688:ASN:N	1:C:693:ALA:O	2.41	0.53
1:C:844:GLU:HB2	1:C:1105:TYR:CE2	2.43	0.53
1:C:894:ARG:HA	1:C:951:HIS:CE1	2.42	0.53
1:A:639:THR:HG22	1:A:640:ASP:H	1.74	0.53
1:C:736:TYR:CZ	1:C:738:SER:HB3	2.43	0.53
1:B:107:LEU:O	1:B:131:ILE:HD13	2.09	0.53
1:B:132:LYS:H	1:B:139:ASN:HD21	1.55	0.53
1:B:466:ASP:HB3	1:B:469:SER:H	1.74	0.53
1:B:736:TYR:OH	1:B:760:GLY:O	2.23	0.53
1:A:166:ILE:HG13	1:A:175:VAL:HG13	1.89	0.53
1:A:338:HIS:HD1	1:A:344:ASN:HA	1.74	0.53
1:A:375:PHE:N	1:A:386:LYS:O	2.38	0.53
1:A:670:PHE:O	1:A:676:TYR:OH	2.22	0.53
1:A:680:SER:OG	1:A:682:GLN:OE1	2.22	0.53
1:A:1116:GLN:HE21	1:A:1120:ASN:HD21	1.56	0.53
1:C:92:GLU:HB3	1:C:108:TYR:OH	2.09	0.53
1:C:862:ALA:HB1	1:C:955:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:880:VAL:O	1:C:893:LYS:N	2.41	0.53
1:C:1031:VAL:HG12	1:C:1035:LEU:HD23	1.91	0.53
1:B:66:TYR:CG	1:B:72:PRO:HG3	2.43	0.53
1:A:291:TYR:CE1	1:A:293:LEU:HD12	2.43	0.53
1:A:917:TYR:HE1	1:A:933:GLN:HE22	1.56	0.53
1:A:1129:ARG:NE	1:C:1121:GLU:OE2	2.41	0.53
1:C:247:ASN:OD1	1:C:249:HIS:N	2.35	0.53
1:C:278:PRO:HA	1:C:446:PHE:HA	1.91	0.53
1:C:908:ASN:HB3	1:C:913:VAL:HG21	1.90	0.53
1:B:46:VAL:HG23	1:B:216:ASN:HA	1.90	0.53
1:B:282:ASN:HD21	1:B:445:ASN:ND2	2.05	0.53
1:B:1082:GLN:NE2	1:B:1085:ARG:HH22	2.07	0.53
1:C:300:ASN:OD1	7:P:2:FUC:H3	2.08	0.53
1:C:490:ARG:NH1	1:C:490:ARG:HA	2.23	0.53
1:B:484:PHE:O	1:B:705:GLN:NE2	2.41	0.53
1:B:490:ARG:HA	1:B:490:ARG:CZ	2.38	0.53
1:C:324:ASN:O	1:C:396:ARG:NE	2.38	0.53
1:C:481:ASP:O	1:C:485:TYR:OH	2.26	0.53
1:C:812:VAL:HA	1:C:1090:ARG:HD2	1.90	0.53
1:B:316:PRO:HB3	1:B:443:SER:OG	2.08	0.53
1:B:844:GLU:HA	1:B:847:GLU:OE2	2.09	0.53
1:A:1082:GLN:HA	1:A:1085:ARG:NH1	2.24	0.53
1:C:184:TYR:HD2	3:T:2:NAG:H82	1.73	0.53
1:B:65:TRP:HB3	1:B:202:CYS:HA	1.89	0.53
1:B:289:LYS:HB2	1:B:435:VAL:H	1.74	0.53
1:B:569:ASP:HB2	1:B:604:PHE:CZ	2.44	0.53
3:F:1:NAG:H83	3:F:1:NAG:H3	1.91	0.53
1:C:323:ILE:HD13	1:C:329:ILE:HD11	1.91	0.53
1:B:100:PHE:HZ	1:B:140:ASN:HA	1.74	0.53
1:B:559:ASN:ND2	1:B:608:GLU:H	2.06	0.53
1:B:1133:CYS:HB3	1:B:1155:HIS:ND1	2.24	0.53
1:A:1184:GLU:OE1	1:A:1184:GLU:N	2.39	0.53
1:C:280:LEU:HB3	1:C:445:ASN:HB2	1.89	0.53
1:C:990:ASP:O	1:C:995:ASN:ND2	2.42	0.53
1:B:285:LEU:HD12	1:B:441:ILE:HD11	1.91	0.53
1:B:668:SER:HB2	1:B:694:VAL:HG21	1.90	0.53
1:A:1084:ASP:HA	1:A:1087:ILE:HD12	1.91	0.52
1:C:77:VAL:O	1:C:190:SER:HA	2.09	0.52
1:C:129:PRO:HD3	1:C:143:THR:O	2.10	0.52
1:C:364:LEU:HD13	7:S:1:NAG:H61	1.91	0.52
1:C:1190:PHE:CE2	1:C:1203:PHE:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:ASP:O	1:B:903:ASN:ND2	2.42	0.52
1:B:904:LYS:NZ	1:B:1014:PHE:O	2.42	0.52
1:B:993:GLN:NE2	1:B:997:GLN:HB2	2.24	0.52
1:B:1109:GLN:HG2	1:B:1113:LYS:HZ2	1.73	0.52
3:j:1:NAG:H3	3:j:1:NAG:H83	1.90	0.52
1:A:81:PHE:O	1:A:204:MET:HA	2.10	0.52
1:A:129:PRO:HB3	1:A:140:ASN:CG	2.34	0.52
1:A:182:TYR:HB3	1:A:252:GLU:CG	2.38	0.52
1:A:583:LEU:HB3	1:A:585:PHE:CE2	2.45	0.52
1:A:1068:ASP:HA	1:A:1071:TYR:HD2	1.73	0.52
1:C:374:PHE:CD1	1:C:387:PHE:HA	2.44	0.52
1:C:466:ASP:OD2	1:C:468:VAL:HB	2.08	0.52
1:C:1139:HIS:HA	1:C:1157:VAL:HA	1.91	0.52
1:B:916:ASP:OD2	1:B:918:LYS:HB2	2.08	0.52
1:A:33:ARG:HG2	1:A:225:ILE:HD11	1.90	0.52
1:A:105:TYR:CD1	1:A:127:GLN:HG3	2.42	0.52
1:A:374:PHE:CD1	1:A:387:PHE:HA	2.44	0.52
1:A:908:ASN:HB3	1:A:913:VAL:HG21	1.92	0.52
1:B:106:GLN:HG3	1:B:130:SER:HA	1.91	0.52
1:B:501:PHE:HB3	1:B:643:PHE:CZ	2.43	0.52
1:B:894:ARG:NH2	1:B:910:LEU:HD22	2.24	0.52
1:A:109:LEU:HG	1:A:123:LEU:HG	1.90	0.52
1:C:281:VAL:HA	1:C:444:THR:HA	1.92	0.52
1:C:344:ASN:ND2	4:R:1:NAG:O7	2.42	0.52
1:C:894:ARG:HH12	1:C:910:LEU:HD22	1.75	0.52
1:C:1139:HIS:HD2	1:C:1155:HIS:HB3	1.73	0.52
1:B:93:ILE:HD12	1:B:194:THR:HG22	1.90	0.52
1:A:81:PHE:CD1	1:A:165:GLY:HA3	2.43	0.52
1:A:801:ASN:HD22	1:A:1105:TYR:HD1	1.58	0.52
1:C:80:ILE:HG23	1:C:168:TRP:HH2	1.75	0.52
1:C:212:TYR:CG	1:C:235:ILE:HD11	2.44	0.52
1:C:354:ASN:HD22	1:C:357:LEU:HD21	1.73	0.52
1:C:686:PHE:CE1	1:C:695:TYR:HB2	2.43	0.52
1:B:854:ILE:HG23	1:B:956:SER:HB2	1.91	0.52
1:A:215:LEU:HD23	1:A:225:ILE:HB	1.92	0.52
1:A:917:TYR:CE2	1:A:939:MET:HG2	2.43	0.52
1:A:1181:THR:HG22	1:A:1182:LEU:HD23	1.90	0.52
1:C:76:GLY:N	1:C:190:SER:HB2	2.25	0.52
1:C:296:PHE:CZ	1:C:421:ALA:HB1	2.44	0.52
1:B:293:LEU:H	1:B:426:PHE:HB2	1.74	0.52
1:B:856:GLU:OE1	1:B:856:GLU:N	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:1:NAG:H61	3:V:2:NAG:HN2	1.74	0.52
1:A:777:THR:H	1:A:1207:ARG:NH1	2.07	0.52
1:A:853:THR:HA	1:B:768:GLN:O	2.09	0.52
1:A:981:ARG:NE	1:A:1141:PHE:HB3	2.25	0.52
1:A:1117:GLN:O	1:A:1121:GLU:HG3	2.10	0.52
1:A:1217:VAL:HG13	1:A:1242:ILE:HG21	1.91	0.52
1:B:55:ILE:HD11	1:B:205:GLN:HE22	1.72	0.52
1:B:108:TYR:HD1	1:B:131:ILE:HG21	1.73	0.52
1:B:282:ASN:N	1:B:443:SER:O	2.41	0.52
1:B:433:ASP:O	3:d:1:NAG:O6	2.22	0.52
1:B:675:TYR:HB3	1:B:686:PHE:HB2	1.92	0.52
1:A:42:GLN:CD	1:A:44:PRO:HD2	2.34	0.52
1:A:343:THR:HG23	1:A:379:THR:HB	1.92	0.52
1:C:484:PHE:HD2	1:C:705:GLN:HB3	1.74	0.52
1:C:946:ASP:OD1	1:C:948:GLU:N	2.37	0.52
1:B:126:CYS:HB2	1:B:128:PHE:HB3	1.92	0.52
1:B:181:TYR:HB3	1:B:183:PHE:CZ	2.44	0.52
1:B:1057:GLN:N	1:B:1057:GLN:OE1	2.37	0.52
1:C:98:GLU:HA	1:C:191:ARG:HB2	1.92	0.52
1:C:991:VAL:HA	1:C:995:ASN:HD22	1.74	0.52
1:A:45:ALA:HA	1:A:308:ASN:CG	2.35	0.52
1:A:278:PRO:HA	1:A:446:PHE:HA	1.92	0.52
1:A:670:PHE:HB3	1:C:456:THR:HG21	1.91	0.52
1:A:850:SER:HB2	1:B:1028:LEU:HD13	1.91	0.52
1:C:107:LEU:HD13	1:C:125:ILE:HG12	1.92	0.52
1:C:843:LEU:HB3	1:C:1105:TYR:OH	2.09	0.52
1:B:57:GLU:HB2	1:B:202:CYS:CB	2.40	0.52
1:A:258:ASN:O	1:A:397:GLU:HG3	2.10	0.51
1:C:194:THR:HG21	1:C:204:MET:HE2	1.92	0.51
1:C:699:PRO:HD2	1:C:702:PHE:HE1	1.75	0.51
1:B:199:SER:HB2	1:B:203:ALA:HB2	1.92	0.51
1:B:319:LEU:HD23	1:B:400:ILE:O	2.09	0.51
1:A:317:GLU:OE1	1:A:445:ASN:HA	2.09	0.51
1:C:175:VAL:HB	1:C:181:TYR:HB2	1.91	0.51
1:C:1142:SER:HA	1:C:1154:LEU:O	2.10	0.51
1:B:299:PHE:CD1	1:B:317:GLU:HA	2.43	0.51
1:B:1122:CYS:O	1:B:1142:SER:OG	2.28	0.51
1:A:86:ARG:HE	1:A:197:TYR:HB3	1.75	0.51
1:A:372:TYR:HD2	1:A:374:PHE:HE1	1.58	0.51
1:C:269:VAL:O	1:C:456:THR:N	2.31	0.51
1:C:1080:ASP:HA	1:C:1083:VAL:HG22	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1094:LEU:O	1:C:1098:VAL:HG23	2.10	0.51
1:B:329:ILE:HG22	1:B:347:PHE:CE2	2.46	0.51
1:B:542:PHE:HE2	1:B:544:VAL:HG22	1.75	0.51
1:B:672:ALA:O	1:B:676:TYR:OH	2.20	0.51
1:A:507:PHE:CD1	1:C:387:PHE:HB2	2.45	0.51
1:A:636:GLU:HB3	1:C:354:ASN:CG	2.36	0.51
1:A:858:ALA:O	1:A:862:ALA:N	2.43	0.51
1:C:77:VAL:HG12	1:C:168:TRP:CZ2	2.45	0.51
1:C:244:THR:N	1:C:309:GLY:HA3	2.25	0.51
1:C:277:GLN:HB2	1:C:279:LEU:HD23	1.91	0.51
1:C:1036:THR:HA	1:C:1039:GLN:OE1	2.10	0.51
1:B:603:LEU:O	1:B:615:PHE:N	2.31	0.51
1:B:721:SER:O	1:B:728:THR:HG21	2.10	0.51
1:B:985:LEU:HD11	1:B:1126:GLN:HG3	1.92	0.51
1:A:469:SER:HA	1:A:472:LYS:HD2	1.90	0.51
1:C:260:PHE:HD2	1:C:409:ASN:HA	1.75	0.51
1:C:652:TYR:HB2	1:C:654:ILE:HD11	1.93	0.51
1:B:105:TYR:CE1	1:B:127:GLN:HB2	2.46	0.51
1:B:453:VAL:HG23	1:B:457:ALA:C	2.36	0.51
1:B:1017:VAL:O	1:B:1019:GLU:HG2	2.11	0.51
1:B:1171:GLY:O	1:B:1231:VAL:N	2.42	0.51
1:B:1228:VAL:HG23	6:k:1:NAG:O4	2.09	0.51
1:B:127:GLN:OE1	1:B:146:ARG:NE	2.40	0.51
1:B:1194:LEU:O	1:B:1198:THR:OG1	2.19	0.51
1:A:210:PRO:HB2	1:A:212:TYR:HE1	1.74	0.51
1:A:465:ASP:N	1:A:465:ASP:OD1	2.43	0.51
1:A:800:TYR:CE1	1:A:1149:GLN:HA	2.45	0.51
1:A:886:ALA:O	1:A:887:ARG:HG2	2.11	0.51
1:A:1191:THR:OG1	1:A:1196:ASN:O	2.23	0.51
1:C:172:ARG:HH21	1:C:294:GLY:N	2.09	0.51
1:C:1142:SER:HB3	1:C:1155:HIS:HA	1.93	0.51
1:B:547:ARG:NH1	1:B:626:GLU:O	2.44	0.51
1:B:918:LYS:O	1:B:921:SER:OG	2.29	0.51
1:A:748:VAL:C	1:A:1026:ARG:HH22	2.18	0.51
1:A:887:ARG:CZ	1:A:889:ARG:HB3	2.41	0.51
1:C:97:GLN:HE22	1:C:106:GLN:NE2	2.08	0.51
1:C:880:VAL:HG23	1:C:893:LYS:HB2	1.93	0.51
1:A:347:PHE:CD1	1:A:388:LEU:HD13	2.46	0.51
1:A:367:THR:C	1:A:369:VAL:H	2.19	0.51
1:A:1204:VAL:HG13	1:A:1215:PRO:HG3	1.92	0.51
1:C:688:ASN:HB3	1:C:693:ALA:N	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1217:VAL:HG13	1:C:1244:ASP:HB2	1.93	0.51
1:B:102:PRO:HB2	1:B:146:ARG:CZ	2.40	0.51
1:B:894:ARG:HG3	1:B:898:GLU:HB2	1.92	0.51
1:B:1214:LYS:HZ2	1:B:1215:PRO:HD2	1.75	0.51
1:A:509:ALA:HB3	1:A:547:ARG:H	1.76	0.51
1:A:1237:GLN:HA	1:A:1240:ASP:OD2	2.11	0.51
1:C:64:THR:HG1	1:C:205:GLN:HB2	1.75	0.51
1:C:687:LYS:HG3	1:C:694:VAL:HG12	1.93	0.51
1:C:688:ASN:O	1:C:689:VAL:C	2.53	0.51
1:C:881:SER:HB2	1:C:892:GLN:OE1	2.11	0.51
1:B:171:ASP:O	1:B:185:PHE:N	2.29	0.51
1:B:344:ASN:ND2	4:e:1:NAG:O7	2.44	0.51
1:B:391:LEU:HD12	1:B:392:PRO:HD2	1.92	0.51
1:B:512:PHE:O	1:B:537:ASN:ND2	2.44	0.51
1:B:679:ASP:OD1	1:B:680:SER:N	2.43	0.51
1:A:1121:GLU:OE1	1:A:1129:ARG:NH1	2.45	0.50
1:A:1224:GLU:OE1	1:A:1224:GLU:N	2.37	0.50
1:B:282:ASN:ND2	1:B:443:SER:OG	2.38	0.50
1:A:127:GLN:HB2	1:A:147:ASN:HB3	1.94	0.50
1:A:320:ARG:HG2	1:A:321:PHE:N	2.26	0.50
1:A:928:ASP:OD1	1:A:931:CYS:N	2.31	0.50
1:C:57:GLU:HA	1:C:65:TRP:CD1	2.46	0.50
1:C:214:MET:HB2	1:C:230:CYS:SG	2.51	0.50
1:C:828:ALA:HB1	1:C:831:LYS:HB2	1.93	0.50
1:C:870:ASP:OD1	1:C:870:ASP:N	2.42	0.50
1:B:535:THR:HB	1:B:539:PHE:N	2.26	0.50
1:B:687:LYS:HA	1:B:694:VAL:HA	1.93	0.50
1:B:734:PHE:HE2	1:B:736:TYR:HB2	1.75	0.50
1:A:636:GLU:OE1	1:C:352:SER:OG	2.30	0.50
1:A:747:PRO:HB3	1:A:755:GLY:CA	2.42	0.50
1:A:840:SER:HB3	1:A:1105:TYR:HD2	1.74	0.50
1:A:994:ARG:HD2	1:A:995:ASN:N	2.26	0.50
1:C:70:GLN:HG3	1:C:72:PRO:HD3	1.93	0.50
1:B:89:HIS:HB3	1:B:197:TYR:CB	2.42	0.50
1:B:245:GLU:CD	1:B:249:HIS:HB2	2.36	0.50
1:B:495:HIS:O	1:B:496:GLU:HG2	2.11	0.50
1:B:744:CYS:HB2	1:B:761:SER:C	2.37	0.50
1:B:1119:VAL:HA	1:B:1123:VAL:HB	1.93	0.50
1:A:36:PHE:HA	1:A:39:PHE:HE2	1.76	0.50
1:A:244:THR:H	1:A:309:GLY:HA3	1.75	0.50
1:A:1098:VAL:O	1:A:1101:THR:OG1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:PHE:CE2	1:C:377:VAL:HG22	2.47	0.50
1:C:843:LEU:HB3	1:C:1105:TYR:HH	1.77	0.50
1:C:958:ILE:O	1:C:961:MET:HB3	2.11	0.50
1:B:55:ILE:HD11	1:B:205:GLN:NE2	2.27	0.50
1:B:122:ARG:NH2	1:B:151:ASN:O	2.45	0.50
1:B:317:GLU:OE1	1:B:445:ASN:ND2	2.34	0.50
1:B:559:ASN:HB3	1:B:562:GLY:O	2.11	0.50
1:A:108:TYR:HB3	1:A:124:ARG:CZ	2.42	0.50
1:A:637:GLY:N	1:C:353:SER:HB2	2.25	0.50
1:A:771:GLN:HB3	1:A:1136:ASP:OD2	2.11	0.50
1:C:380:TYR:CG	1:C:380:TYR:O	2.65	0.50
1:B:281:VAL:HA	1:B:444:THR:HA	1.92	0.50
1:B:673:GLY:HA3	1:B:676:TYR:HE1	1.77	0.50
1:B:796:TYR:CE1	1:B:1150:GLY:HA3	2.46	0.50
1:B:821:GLN:O	1:B:824:THR:OG1	2.29	0.50
1:A:108:TYR:O	1:A:124:ARG:HD3	2.11	0.50
1:A:549:PHE:HE1	1:A:628:ILE:HB	1.76	0.50
1:A:1058:HIS:HB2	1:A:1060:PHE:CE1	2.47	0.50
1:C:77:VAL:HG12	1:C:168:TRP:HZ2	1.77	0.50
1:C:355:PRO:HD3	1:C:374:PHE:HE2	1.77	0.50
1:C:721:SER:HA	1:C:735:PHE:CE2	2.46	0.50
1:C:1180:LEU:HG	1:C:1220:PHE:HB3	1.92	0.50
1:C:1201:GLU:OE1	1:C:1214:LYS:NZ	2.44	0.50
1:B:506:SER:HB3	1:B:547:ARG:HD2	1.93	0.50
1:B:654:ILE:HG22	1:B:655:TYR:CD2	2.46	0.50
1:B:958:ILE:O	1:B:961:MET:HG2	2.11	0.50
1:A:897:ILE:HD12	1:A:897:ILE:H	1.77	0.50
1:C:280:LEU:HD23	1:C:314:ARG:NH1	2.27	0.50
1:C:302:THR:HA	1:C:316:PRO:HD3	1.94	0.50
1:C:489:SER:HB2	1:C:702:PHE:H	1.76	0.50
1:C:894:ARG:HA	1:C:951:HIS:CD2	2.47	0.50
1:B:232:ALA:HA	1:B:235:ILE:HD13	1.93	0.50
1:B:368:GLN:O	1:B:369:VAL:HG12	2.12	0.50
1:B:1003:PHE:O	1:B:1007:ILE:HG12	2.12	0.50
1:A:989:THR:HG23	1:A:1211:GLU:HB3	1.93	0.50
1:A:1171:GLY:HA3	1:A:1230:TYR:CZ	2.47	0.50
1:C:1191:THR:HB	1:C:1196:ASN:HA	1.92	0.50
1:B:103:SER:HA	1:B:146:ARG:HH21	1.77	0.50
1:B:344:ASN:HB2	1:B:378:ASP:HB3	1.94	0.50
1:B:712:ASP:OD1	1:B:713:ILE:N	2.44	0.50
1:B:863:THR:HG23	1:B:866:SER:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLY:HA3	3:E:1:NAG:O5	2.12	0.50
1:C:270:HIS:HB2	1:C:454:GLN:HA	1.92	0.50
1:C:391:LEU:HD12	1:C:392:PRO:HD2	1.92	0.50
1:C:1100:GLN:C	1:C:1104:LYS:HZ3	2.19	0.50
1:B:72:PRO:HD2	1:B:194:THR:OG1	2.11	0.50
1:B:276:ASN:HA	1:B:448:ASP:HA	1.93	0.50
1:B:514:ASN:H	1:B:537:ASN:CG	2.20	0.50
1:A:237:TYR:HA	1:A:240:ASN:CG	2.37	0.49
1:A:347:PHE:CE1	1:A:373:CYS:HB3	2.46	0.49
1:A:351:ASN:H	1:A:362:ILE:HD13	1.76	0.49
1:A:899:ASP:O	1:A:903:ASN:ND2	2.45	0.49
1:A:916:ASP:HA	1:B:733:GLY:HA2	1.94	0.49
1:A:1005:SER:HA	8:A:1505:NAG:H81	1.94	0.49
1:A:1055:GLN:HA	1:A:1058:HIS:CE1	2.47	0.49
1:A:1146:ALA:HA	1:A:1151:LEU:HD13	1.93	0.49
1:C:62:ASN:O	1:C:64:THR:HG23	2.12	0.49
1:C:105:TYR:CD1	1:C:127:GLN:HB2	2.47	0.49
1:C:109:LEU:HD13	1:C:123:LEU:HD12	1.94	0.49
1:C:883:TYR:CZ	1:C:885:PRO:HA	2.47	0.49
1:B:141:ASP:O	1:B:142:VAL:C	2.55	0.49
1:C:475:GLN:HG3	1:B:831:LYS:HE2	1.93	0.49
1:C:922:ASN:HD21	1:C:924:ARG:CZ	2.24	0.49
1:B:452:GLU:OE2	1:B:459:GLN:NE2	2.44	0.49
2:D:1:NAG:H3	2:D:1:NAG:H83	1.94	0.49
4:U:1:NAG:H83	4:U:2:NAG:HN2	1.76	0.49
1:A:175:VAL:HB	1:A:181:TYR:HB2	1.93	0.49
1:A:214:MET:HB3	1:A:230:CYS:HB3	1.93	0.49
1:A:858:ALA:HB1	1:A:959:GLY:HA3	1.95	0.49
1:A:1190:PHE:CE2	1:A:1203:PHE:HB2	2.47	0.49
1:A:1236:ASP:O	1:A:1239:PRO:HD2	2.13	0.49
1:C:64:THR:HB	1:C:66:TYR:CZ	2.46	0.49
1:C:77:VAL:HG22	1:C:208:TYR:CE1	2.45	0.49
1:C:501:PHE:CD2	1:C:642:SER:HA	2.48	0.49
1:C:676:TYR:HB3	1:B:269:VAL:HB	1.94	0.49
1:C:1120:ASN:O	1:C:1124:LYS:HB2	2.12	0.49
1:B:525:SER:C	1:B:609:PHE:HD2	2.21	0.49
1:B:793:ARG:NH1	1:B:1136:ASP:O	2.45	0.49
1:A:1138:GLU:OE1	1:A:1138:GLU:N	2.44	0.49
1:C:100:PHE:CZ	1:C:130:SER:HB3	2.46	0.49
1:C:101:ASP:O	1:C:106:GLN:NE2	2.46	0.49
1:C:783:SER:HB2	1:B:966:PHE:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:THR:HG23	1:B:139:ASN:CG	2.37	0.49
1:B:872:TYR:HB3	1:B:874:PHE:HE1	1.78	0.49
1:A:55:ILE:O	1:A:62:ASN:ND2	2.45	0.49
1:A:185:PHE:HE2	1:A:189:TRP:HH2	1.60	0.49
1:A:676:TYR:HE1	1:A:687:LYS:HG3	1.78	0.49
1:A:946:ASP:OD2	1:A:948:GLU:HB3	2.12	0.49
1:C:91:PHE:CE2	1:C:93:ILE:HD11	2.48	0.49
1:C:129:PRO:HB3	1:C:140:ASN:CG	2.37	0.49
1:C:209:GLU:OE1	1:C:209:GLU:N	2.45	0.49
1:C:248:GLY:O	1:C:281:VAL:HG12	2.12	0.49
1:C:341:LEU:C	1:C:343:THR:H	2.18	0.49
1:C:770:GLY:N	1:B:853:THR:HB	2.25	0.49
1:B:240:ASN:HD21	1:B:438:PHE:N	2.09	0.49
1:B:519:ALA:O	1:B:557:VAL:HA	2.12	0.49
1:B:983:ASN:OD1	1:B:988:GLN:N	2.41	0.49
1:B:1073:ARG:HB3	1:B:1074:LEU:HD12	1.95	0.49
1:A:644:MET:N	1:A:644:MET:SD	2.85	0.49
1:A:679:ASP:OD1	1:A:680:SER:N	2.45	0.49
1:C:96:SER:HB2	1:C:191:ARG:HD3	1.94	0.49
1:C:476:VAL:H	1:B:831:LYS:HZ1	1.60	0.49
1:C:781:ASN:HB3	1:C:1167:ILE:HG12	1.95	0.49
1:B:128:PHE:CZ	1:B:131:ILE:HD11	2.47	0.49
1:B:292:GLY:CA	1:B:428:GLY:H	2.26	0.49
1:B:295:GLN:NE2	1:B:296:PHE:O	2.44	0.49
1:A:391:LEU:HD12	1:A:392:PRO:HD2	1.95	0.49
1:A:509:ALA:HB1	1:A:546:THR:HA	1.94	0.49
1:A:798:GLN:NE2	1:A:800:TYR:O	2.36	0.49
1:C:35:PHE:HB2	1:C:163:VAL:HB	1.94	0.49
1:C:847:GLU:O	1:C:851:MET:HE3	2.11	0.49
1:C:903:ASN:HA	1:C:909:GLY:HA2	1.94	0.49
1:B:36:PHE:HB2	1:B:225:ILE:HD13	1.93	0.49
1:B:39:PHE:HZ	1:B:176:PHE:CE1	2.31	0.49
1:B:497:GLN:HE21	1:B:649:CYS:C	2.20	0.49
1:A:124:ARG:HB3	1:A:151:ASN:OD1	2.13	0.49
1:C:793:ARG:HD3	1:C:1029:ASN:ND2	2.27	0.49
1:B:833:ILE:HG23	1:B:1098:VAL:HG21	1.95	0.49
1:B:989:THR:HG21	1:B:1213:ARG:HB2	1.94	0.49
1:B:1017:VAL:O	1:B:1018:LYS:HG3	2.13	0.49
1:B:1138:GLU:C	1:B:1157:VAL:HG23	2.38	0.49
1:B:1175:ASN:N	1:B:1233:LEU:O	2.28	0.49
1:A:36:PHE:CG	1:A:215:LEU:HD21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLY:H	1:A:176:PHE:HB2	1.77	0.49
1:A:400:ILE:HA	1:A:405:ASP:O	2.12	0.49
1:A:676:TYR:H	1:A:683:LEU:HD11	1.77	0.49
1:A:876:ASN:HB3	1:A:896:PHE:HD2	1.76	0.49
1:C:317:GLU:HG2	1:C:445:ASN:HA	1.94	0.49
1:C:1192:HIS:O	1:C:1193:GLU:HG2	2.13	0.49
1:B:778:VAL:HG23	1:B:779:THR:HG22	1.93	0.49
1:B:1036:THR:O	1:B:1040:GLU:OE1	2.31	0.49
1:C:447:VAL:HG11	1:C:463:TYR:HE2	1.78	0.49
1:C:688:ASN:O	1:C:690:THR:N	2.46	0.49
1:C:843:LEU:O	1:C:846:VAL:N	2.46	0.49
1:C:1138:GLU:CD	1:C:1208:ARG:HE	2.19	0.49
1:B:324:ASN:OD1	3:d:1:NAG:H2	2.12	0.49
1:B:930:VAL:O	1:B:933:GLN:HG2	2.13	0.49
1:B:1184:GLU:H	1:B:1184:GLU:CD	2.21	0.49
1:A:509:ALA:O	1:A:547:ARG:N	2.46	0.48
1:C:65:TRP:CH2	1:C:83:SER:HB3	2.47	0.48
1:C:501:PHE:HB3	1:C:643:PHE:CE1	2.48	0.48
1:C:835:SER:O	1:C:838:GLN:HG3	2.13	0.48
1:C:1011:THR:O	1:C:1014:PHE:HB2	2.13	0.48
1:C:1233:LEU:HD21	1:C:1238:LEU:HA	1.94	0.48
1:B:396:ARG:HD3	1:B:396:ARG:HA	1.47	0.48
1:B:607:PRO:CG	1:B:611:SER:H	2.26	0.48
1:B:894:ARG:HA	1:B:951:HIS:CE1	2.48	0.48
1:A:38:LYS:NZ	1:A:176:PHE:HB3	2.28	0.48
1:A:128:PHE:CD1	1:A:129:PRO:HD2	2.48	0.48
1:A:798:GLN:NE2	1:A:801:ASN:OD1	2.32	0.48
1:A:887:ARG:NE	1:A:889:ARG:HB3	2.27	0.48
1:A:1080:ASP:O	1:A:1083:VAL:HG12	2.14	0.48
1:C:40:ASN:OD1	1:C:41:VAL:N	2.45	0.48
1:C:257:ASN:OD1	1:C:258:ASN:N	2.42	0.48
1:C:786:THR:HG21	1:C:1164:VAL:HG23	1.95	0.48
1:C:894:ARG:HG3	1:C:898:GLU:HB2	1.95	0.48
1:B:80:ILE:HG23	1:B:168:TRP:HH2	1.79	0.48
1:B:195:LYS:HD3	1:B:197:TYR:HE1	1.79	0.48
1:A:456:THR:HG21	1:B:670:PHE:HB3	1.94	0.48
1:A:748:VAL:HG22	1:A:756:VAL:O	2.12	0.48
1:A:1090:ARG:O	1:A:1094:LEU:HG	2.12	0.48
1:C:75:SER:HB3	1:C:98:GLU:HG3	1.94	0.48
1:C:91:PHE:N	1:C:111:LYS:HG3	2.28	0.48
1:C:168:TRP:CD1	1:C:189:TRP:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ILE:H	1:B:537:ASN:H	1.59	0.48
1:B:949:LYS:HA	1:B:952:MET:HE3	1.94	0.48
1:A:57:GLU:HB2	1:A:202:CYS:SG	2.53	0.48
1:A:318:ALA:HB2	1:A:401:THR:HG23	1.94	0.48
1:A:499:ILE:HB	1:A:651:LYS:NZ	2.28	0.48
1:A:505:PRO:HG2	1:A:639:THR:HA	1.94	0.48
1:A:959:GLY:HA2	1:A:962:VAL:HG22	1.95	0.48
1:B:1011:THR:HA	1:B:1014:PHE:HD2	1.77	0.48
1:A:665:LEU:HD12	1:A:694:VAL:O	2.13	0.48
1:A:817:SER:HA	1:A:820:LYS:HB2	1.95	0.48
1:A:1109:GLN:O	1:A:1113:LYS:HD3	2.14	0.48
1:C:285:LEU:HB2	1:C:441:ILE:HG12	1.95	0.48
1:C:722:SER:HA	1:C:737:HIS:CE1	2.48	0.48
1:B:31:ASN:ND2	1:B:33:ARG:HH11	2.12	0.48
1:B:91:PHE:HB3	1:B:111:LYS:HE3	1.95	0.48
1:B:184:TYR:H	3:g:2:NAG:H81	1.77	0.48
1:B:880:VAL:O	1:B:893:LYS:N	2.46	0.48
1:B:1214:LYS:NZ	1:B:1215:PRO:HD2	2.28	0.48
1:A:38:LYS:NZ	1:A:176:PHE:O	2.37	0.48
1:A:379:THR:HG22	1:A:382:SER:HB3	1.96	0.48
1:A:500:SER:O	1:A:652:TYR:HA	2.14	0.48
1:C:158:MET:HG2	1:C:159:SER:O	2.13	0.48
1:C:847:GLU:C	1:C:851:MET:HE3	2.38	0.48
1:C:949:LYS:HA	1:C:952:MET:HG2	1.96	0.48
1:B:169:ASP:O	1:B:172:ARG:HB2	2.14	0.48
1:B:993:GLN:HE22	1:B:997:GLN:HB2	1.76	0.48
1:B:1055:GLN:HA	1:B:1058:HIS:ND1	2.29	0.48
1:A:247:ASN:O	1:A:280:LEU:HD11	2.14	0.48
1:A:780:GLY:C	1:A:1167:ILE:HD12	2.39	0.48
1:C:852:LEU:HD12	1:C:945:VAL:HG11	1.95	0.48
1:C:899:ASP:O	1:C:903:ASN:ND2	2.47	0.48
1:C:1202:TYR:CD2	1:C:1241:VAL:HG13	2.49	0.48
1:B:131:ILE:HD12	1:B:131:ILE:H	1.77	0.48
1:B:520:SER:HA	1:B:558:THR:O	2.13	0.48
1:A:129:PRO:HD3	1:A:143:THR:O	2.13	0.48
1:A:214:MET:HE1	5:M:3:FUC:H62	1.94	0.48
1:A:236:GLY:H	3:E:1:NAG:C6	2.23	0.48
1:A:736:TYR:OH	1:A:760:GLY:O	2.23	0.48
1:A:821:GLN:O	1:A:825:GLN:NE2	2.46	0.48
1:C:104:GLY:O	1:C:106:GLN:NE2	2.46	0.48
1:C:300:ASN:HB3	1:C:301:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:THR:HA	1:C:419:LEU:HD13	1.95	0.48
1:C:800:TYR:CE1	1:C:1149:GLN:HA	2.49	0.48
1:C:897:ILE:O	1:C:901:LEU:HG	2.14	0.48
1:B:55:ILE:HG22	1:B:211:THR:HG21	1.95	0.48
1:B:76:GLY:N	1:B:190:SER:HB2	2.25	0.48
1:B:171:ASP:CG	1:B:186:LYS:HA	2.39	0.48
1:B:519:ALA:HB3	1:B:557:VAL:HG22	1.96	0.48
1:B:586:SER:HB3	1:B:625:GLY:HA3	1.96	0.48
1:B:788:PHE:CE1	1:B:1160:PRO:HB3	2.49	0.48
1:A:56:GLY:HA3	1:A:59:GLN:HE22	1.79	0.48
1:C:490:ARG:HA	1:C:490:ARG:CZ	2.44	0.48
1:C:712:ASP:OD1	1:C:713:ILE:N	2.47	0.48
1:C:747:PRO:HB3	1:C:755:GLY:CA	2.44	0.48
1:C:946:ASP:OD1	1:C:947:ALA:N	2.47	0.48
1:C:1073:ARG:HA	1:C:1073:ARG:CZ	2.44	0.48
1:B:213:TYR:CG	1:B:229:PRO:HA	2.49	0.48
1:B:214:MET:HE3	1:B:228:GLN:HG2	1.94	0.48
1:B:499:ILE:HG22	1:B:643:PHE:HE1	1.78	0.48
1:B:754:ILE:HD12	1:B:762:ILE:HD11	1.96	0.48
1:B:857:GLU:O	1:B:861:LEU:HG	2.14	0.48
1:B:1236:ASP:C	1:B:1239:PRO:HD2	2.39	0.48
1:A:94:GLY:O	1:A:192:VAL:HA	2.14	0.48
1:A:108:TYR:CD2	1:A:131:ILE:HD12	2.48	0.48
1:A:127:GLN:O	1:A:146:ARG:HB3	2.13	0.48
1:A:195:LYS:HE2	1:A:197:TYR:CE1	2.48	0.48
1:A:919:ARG:HH12	1:A:928:ASP:CG	2.22	0.48
1:A:1045:GLN:O	1:A:1049:LEU:HG	2.14	0.48
1:A:1183:ARG:NH2	1:A:1184:GLU:OE2	2.47	0.48
1:C:84:HIS:CD2	1:C:160:GLU:HB3	2.49	0.48
1:B:66:TYR:CD1	1:B:72:PRO:HG3	2.49	0.48
1:B:513:VAL:HB	1:B:551:ILE:HA	1.96	0.48
1:B:793:ARG:HB3	1:B:1029:ASN:CG	2.38	0.48
1:B:822:LEU:HA	1:B:825:GLN:CD	2.38	0.48
1:B:1023:GLN:O	1:B:1026:ARG:HB2	2.14	0.48
1:B:1174:VAL:CG1	1:B:1178:ILE:HB	2.44	0.48
1:B:1191:THR:HB	1:B:1196:ASN:HA	1.95	0.48
1:A:718:SER:HB3	1:A:737:HIS:CE1	2.49	0.47
1:A:811:TYR:HE2	1:A:1090:ARG:HB3	1.79	0.47
1:C:34:ARG:NH2	1:C:163:VAL:O	2.47	0.47
1:C:46:VAL:HG23	1:C:216:ASN:HA	1.95	0.47
1:C:116:ASN:O	1:C:157:HIS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:HH22	1:C:151:ASN:HB2	1.79	0.47
1:C:129:PRO:HA	1:C:141:ASP:O	2.14	0.47
1:C:820:LYS:O	1:C:824:THR:HG23	2.14	0.47
1:C:826:TYR:OH	1:C:1084:ASP:OD1	2.25	0.47
1:C:1003:PHE:O	1:C:1007:ILE:HG12	2.13	0.47
1:C:1109:GLN:O	1:C:1112:ARG:HG2	2.14	0.47
1:C:1193:GLU:HG3	1:C:1195:GLN:H	1.79	0.47
1:B:99:PRO:HB2	1:B:101:ASP:OD1	2.14	0.47
1:B:167:THR:HB	1:B:174:THR:OG1	2.14	0.47
1:B:327:SER:HA	1:B:330:LEU:HB2	1.95	0.47
1:B:355:PRO:HG3	1:B:360:PHE:CE2	2.49	0.47
1:A:282:ASN:O	1:A:443:SER:HB2	2.14	0.47
1:A:376:LYS:HA	1:A:384:VAL:O	2.14	0.47
1:A:549:PHE:CE1	1:A:628:ILE:HB	2.48	0.47
1:A:935:TYR:CE1	1:B:699:PRO:HD2	2.49	0.47
1:C:129:PRO:HB3	1:C:140:ASN:ND2	2.29	0.47
1:C:130:SER:N	1:C:140:ASN:HB2	2.29	0.47
1:C:351:ASN:HB3	7:S:1:NAG:N2	2.29	0.47
1:C:844:GLU:N	1:C:1105:TYR:OH	2.47	0.47
1:C:927:ALA:HB1	1:C:931:CYS:CB	2.44	0.47
1:B:218:THR:HG21	6:a:1:NAG:H62	1.95	0.47
1:B:887:ARG:C	1:B:889:ARG:H	2.21	0.47
1:B:1037:LYS:HA	1:B:1040:GLU:OE2	2.14	0.47
1:A:100:PHE:CZ	1:A:130:SER:HB3	2.49	0.47
1:A:105:TYR:CE2	1:A:149:LEU:HB2	2.49	0.47
1:A:373:CYS:O	1:A:388:LEU:N	2.47	0.47
1:A:447:VAL:HG11	1:A:463:TYR:HE2	1.79	0.47
1:A:818:ARG:HH12	1:A:822:LEU:HD21	1.80	0.47
1:A:917:TYR:HE1	1:A:934:TYR:HB2	1.77	0.47
1:A:1027:GLY:C	1:A:1033:HIS:HB2	2.39	0.47
1:C:790:MET:HE2	1:C:999:LEU:C	2.39	0.47
1:B:170:ASN:O	1:B:172:ARG:HD3	2.14	0.47
1:B:482:ASP:CG	1:B:709:VAL:HA	2.40	0.47
1:B:504:LEU:HG	1:B:626:GLU:HB2	1.96	0.47
1:B:1183:ARG:NH1	1:B:1218:SER:O	2.43	0.47
1:A:934:TYR:HA	1:A:938:VAL:O	2.13	0.47
1:C:355:PRO:HG3	1:C:360:PHE:CE2	2.49	0.47
1:C:1236:ASP:O	1:C:1239:PRO:HD2	2.14	0.47
1:B:184:TYR:CD2	3:g:1:NAG:H5	2.49	0.47
1:B:279:LEU:O	1:B:463:TYR:OH	2.31	0.47
1:B:1138:GLU:OE1	1:B:1208:ARG:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:HG13	1:A:433:ASP:HB2	1.96	0.47
1:A:490:ARG:NH1	1:A:490:ARG:HA	2.30	0.47
1:A:507:PHE:O	1:A:547:ARG:NH1	2.33	0.47
1:A:748:VAL:HG11	1:A:758:LYS:HB3	1.96	0.47
1:A:864:ILE:HD12	1:A:864:ILE:H	1.80	0.47
1:A:1057:GLN:O	1:A:1065:SER:OG	2.20	0.47
1:C:182:TYR:HE2	1:C:292:GLY:H	1.60	0.47
1:C:472:LYS:HA	1:C:480:LEU:HD11	1.97	0.47
1:C:973:PRO:HD2	1:C:976:TYR:CD2	2.50	0.47
1:B:150:PHE:HA	1:B:152:LYS:NZ	2.29	0.47
1:B:407:TYR:HD2	1:B:410:GLY:C	2.22	0.47
1:B:880:VAL:C	1:B:892:GLN:HG3	2.39	0.47
1:B:1119:VAL:HG22	1:B:1124:LYS:HG3	1.95	0.47
1:A:302:THR:HG21	1:A:313:GLN:HA	1.96	0.47
1:A:586:SER:HB3	1:A:625:GLY:HA3	1.95	0.47
1:A:864:ILE:HD13	1:A:880:VAL:HG12	1.96	0.47
1:A:992:LEU:HD12	1:A:994:ARG:HE	1.80	0.47
1:C:88:GLY:O	1:C:114:ASN:HA	2.15	0.47
1:C:107:LEU:HD12	1:C:108:TYR:N	2.30	0.47
1:C:168:TRP:NE1	1:C:189:TRP:O	2.47	0.47
1:C:639:THR:HG22	1:C:640:ASP:H	1.80	0.47
1:C:750:VAL:HG21	1:B:846:VAL:HB	1.97	0.47
1:B:400:ILE:HG12	1:B:406:VAL:HG23	1.97	0.47
1:B:452:GLU:HB3	1:B:460:ARG:HG3	1.97	0.47
1:B:651:LYS:HE2	1:B:651:LYS:HA	1.96	0.47
1:B:1184:GLU:OE1	1:B:1184:GLU:N	2.47	0.47
1:B:1232:ASN:ND2	6:k:1:NAG:H62	2.29	0.47
1:A:372:TYR:CE1	1:B:639:THR:HG23	2.50	0.47
1:A:501:PHE:HB3	1:A:643:PHE:CZ	2.50	0.47
1:A:856:GLU:OE1	1:A:856:GLU:N	2.47	0.47
1:A:870:ASP:OD1	1:A:870:ASP:N	2.43	0.47
1:C:185:PHE:O	1:C:187:ASN:ND2	2.48	0.47
1:C:317:GLU:HB2	1:C:402:LYS:HE2	1.96	0.47
1:C:791:SER:OG	1:C:792:ILE:N	2.47	0.47
1:C:897:ILE:HB	1:C:1145:GLN:OE1	2.14	0.47
1:C:1204:VAL:HG23	1:C:1213:ARG:HB3	1.96	0.47
1:B:332:GLU:HG2	1:B:348:VAL:HA	1.96	0.47
1:B:507:PHE:CD2	1:B:509:ALA:HB2	2.50	0.47
1:B:569:ASP:HB3	1:B:602:ASP:HB2	1.97	0.47
1:A:89:HIS:HA	1:A:114:ASN:OD1	2.14	0.47
1:A:212:TYR:O	1:A:229:PRO:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ARG:HD3	1:A:445:ASN:OD1	2.15	0.47
1:A:510:HIS:HA	1:A:548:GLN:HB2	1.96	0.47
1:A:1128:GLN:OE1	1:A:1128:GLN:N	2.32	0.47
1:A:1195:GLN:HB3	1:A:1201:GLU:HB2	1.97	0.47
1:A:1251:THR:HB	1:B:1252:ARG:CZ	2.45	0.47
1:C:464:CYS:O	1:C:470:GLN:NE2	2.47	0.47
1:C:909:GLY:O	1:C:910:LEU:HD23	2.15	0.47
1:C:1144:VAL:HG11	1:C:1151:LEU:HD13	1.97	0.47
1:C:1236:ASP:OD1	1:C:1236:ASP:N	2.46	0.47
1:B:55:ILE:HD12	1:B:62:ASN:HA	1.96	0.47
1:B:126:CYS:CB	1:B:148:CYS:HA	2.43	0.47
1:B:205:GLN:HG2	1:B:206:TYR:N	2.29	0.47
1:B:781:ASN:HA	1:B:1167:ILE:HA	1.95	0.47
1:B:825:GLN:O	1:B:827:THR:HG23	2.14	0.47
1:A:269:VAL:O	1:A:455:GLY:N	2.48	0.47
1:A:548:GLN:HB3	1:A:634:PRO:HA	1.97	0.47
1:A:739:ASN:HB3	3:F:1:NAG:H5	1.97	0.47
1:A:874:PHE:HB3	1:A:878:LEU:HD13	1.97	0.47
1:A:1247:ASP:HB3	1:A:1250:LYS:HG2	1.97	0.47
1:C:122:ARG:NH2	1:C:151:ASN:O	2.47	0.47
1:C:786:THR:HB	1:C:1210:PHE:HB3	1.96	0.47
1:C:1187:LEU:HD12	1:C:1205:SER:O	2.14	0.47
1:B:100:PHE:CE2	1:B:130:SER:HB3	2.50	0.47
1:B:211:THR:OG1	1:B:212:TYR:N	2.47	0.47
1:B:407:TYR:HA	1:B:411:PHE:O	2.15	0.47
1:B:510:HIS:HA	1:B:548:GLN:O	2.15	0.47
1:B:735:PHE:HB3	1:B:737:HIS:CE1	2.50	0.47
1:B:1144:VAL:HG11	1:B:1151:LEU:HD13	1.96	0.47
1:A:48:VAL:HG12	1:A:238:ALA:HB2	1.96	0.47
1:A:134:LEU:HD21	1:A:195:LYS:HD2	1.98	0.47
1:A:175:VAL:HB	1:A:181:TYR:HD2	1.79	0.47
1:A:978:VAL:O	1:A:982:LEU:HD23	2.15	0.47
1:A:1076:PRO:N	1:A:1077:PRO:HD2	2.30	0.47
1:A:1119:VAL:HG22	1:A:1124:LYS:NZ	2.30	0.47
1:B:85:ILE:HG13	1:B:158:MET:CG	2.44	0.47
1:B:293:LEU:N	1:B:426:PHE:HB2	2.30	0.47
1:A:245:GLU:HB2	1:A:247:ASN:OD1	2.15	0.46
1:A:328:VAL:HG23	1:A:426:PHE:CG	2.50	0.46
1:A:372:TYR:HE1	1:B:639:THR:HG23	1.80	0.46
1:A:735:PHE:CE1	1:C:918:LYS:HG2	2.50	0.46
1:C:109:LEU:HD11	1:C:121:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:SER:N	1:C:694:VAL:HG21	2.30	0.46
1:B:129:PRO:HB3	1:B:140:ASN:OD1	2.15	0.46
1:B:373:CYS:SG	1:B:391:LEU:HB2	2.55	0.46
1:B:898:GLU:OE2	1:B:1145:GLN:NE2	2.48	0.46
1:A:80:ILE:HG23	1:A:168:TRP:HH2	1.80	0.46
1:A:316:PRO:CB	1:A:443:SER:HB3	2.46	0.46
1:A:509:ALA:CB	1:A:547:ARG:H	2.27	0.46
1:A:800:TYR:HA	1:A:1112:ARG:HH21	1.80	0.46
1:A:802:THR:HG22	1:A:1045:GLN:HG2	1.98	0.46
1:A:927:ALA:HB3	1:B:684:LEU:HD13	1.98	0.46
1:A:1068:ASP:HB2	1:B:658:LYS:CD	2.39	0.46
1:C:768:GLN:O	1:B:853:THR:HA	2.15	0.46
1:C:919:ARG:NH2	1:C:930:VAL:HB	2.26	0.46
1:C:1074:LEU:HB2	1:C:1079:ALA:HB2	1.98	0.46
1:B:408:VAL:HB	1:B:413:TYR:CD2	2.50	0.46
1:B:844:GLU:O	1:B:847:GLU:HG2	2.15	0.46
1:B:864:ILE:HA	1:B:878:LEU:HD23	1.96	0.46
6:k:1:NAG:H4	6:k:4:FUC:C5	2.45	0.46
1:A:174:THR:HA	1:A:181:TYR:O	2.16	0.46
1:A:261:LEU:HD11	1:A:267:THR:HG23	1.98	0.46
1:A:309:GLY:O	1:A:311:ALA:N	2.49	0.46
1:A:1129:ARG:HB2	1:C:1121:GLU:CD	2.40	0.46
1:C:57:GLU:HG3	1:C:58:ASN:OD1	2.15	0.46
1:C:64:THR:OG1	1:C:205:GLN:HB2	2.14	0.46
1:C:327:SER:HA	1:C:330:LEU:HD23	1.97	0.46
1:C:902:PHE:HB3	1:C:909:GLY:O	2.15	0.46
1:C:1018:LYS:H	1:C:1023:GLN:CD	2.20	0.46
1:B:175:VAL:HB	1:B:181:TYR:HB2	1.97	0.46
1:B:646:LEU:HG	1:B:663:ILE:HG22	1.98	0.46
1:A:80:ILE:HG12	1:A:168:TRP:HZ3	1.80	0.46
1:A:211:THR:HG1	1:A:213:TYR:HE1	1.63	0.46
1:A:260:PHE:O	1:A:320:ARG:NH2	2.49	0.46
1:A:294:GLY:HA3	8:A:1502:NAG:HN2	1.80	0.46
1:A:489:SER:CB	1:A:702:PHE:H	2.27	0.46
1:A:1069:ASP:OD1	1:B:658:LYS:HG2	2.15	0.46
1:A:1175:ASN:O	1:A:1177:GLU:HG3	2.15	0.46
1:C:51:GLY:O	1:C:53:LEU:N	2.45	0.46
1:C:336:VAL:HB	1:C:423:THR:OG1	2.14	0.46
1:C:484:PHE:HB3	1:C:705:GLN:HE21	1.80	0.46
1:C:1001:GLU:HA	1:C:1004:ASN:ND2	2.30	0.46
1:B:292:GLY:HA2	1:B:428:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ASN:HB3	1:B:632:PRO:HA	1.98	0.46
1:A:182:TYR:HB2	1:A:253:GLY:HA2	1.97	0.46
1:A:666:THR:HB	1:C:924:ARG:O	2.16	0.46
1:A:857:GLU:H	1:A:857:GLU:CD	2.23	0.46
1:C:363:PRO:HG2	7:S:1:NAG:H5	1.96	0.46
1:C:376:LYS:HA	1:C:384:VAL:O	2.15	0.46
1:C:387:PHE:CZ	1:C:389:ALA:HA	2.51	0.46
1:C:404:GLY:O	1:C:415:HIS:HA	2.16	0.46
1:C:1106:THR:O	1:C:1109:GLN:HB3	2.15	0.46
1:C:1114:LEU:HA	1:C:1117:GLN:OE1	2.15	0.46
1:B:158:MET:N	1:B:158:MET:SD	2.88	0.46
1:B:373:CYS:O	1:B:388:LEU:HB3	2.15	0.46
1:B:794:THR:O	1:B:1029:ASN:HA	2.15	0.46
1:A:1138:GLU:CD	1:A:1138:GLU:H	2.24	0.46
1:C:107:LEU:HD13	1:C:125:ILE:CG1	2.45	0.46
1:C:322:ASN:HB2	1:C:440:THR:HG22	1.98	0.46
1:C:374:PHE:CE1	1:C:387:PHE:HD1	2.34	0.46
1:C:382:SER:O	1:C:384:VAL:HG13	2.16	0.46
1:C:404:GLY:HA2	1:C:419:LEU:HD23	1.98	0.46
1:C:783:SER:CB	1:B:966:PHE:H	2.29	0.46
1:C:833:ILE:HD13	1:C:1094:LEU:HD22	1.96	0.46
1:C:997:GLN:O	1:C:1001:GLU:HG3	2.15	0.46
1:B:97:GLN:H	1:B:97:GLN:CD	2.24	0.46
1:B:425:ASN:HD22	3:g:1:NAG:C7	2.28	0.46
1:B:902:PHE:HD1	1:B:906:VAL:HG21	1.81	0.46
1:B:1142:SER:HB3	1:B:1155:HIS:HA	1.97	0.46
1:A:123:LEU:HD22	1:A:150:PHE:CE2	2.51	0.46
1:A:355:PRO:HG2	1:A:385:TYR:CG	2.51	0.46
1:A:376:LYS:HB2	1:A:385:TYR:CE2	2.50	0.46
1:A:876:ASN:O	1:A:895:SER:OG	2.30	0.46
1:A:901:LEU:O	1:A:905:VAL:HB	2.15	0.46
1:A:922:ASN:HD21	1:A:924:ARG:CZ	2.28	0.46
1:A:1139:HIS:HD2	1:A:1155:HIS:HB3	1.79	0.46
1:A:1250:LYS:O	1:A:1254:GLU:N	2.49	0.46
1:C:1084:ASP:HA	1:C:1087:ILE:HB	1.97	0.46
1:C:1188:VAL:HG22	1:C:1205:SER:O	2.15	0.46
1:B:80:ILE:HD13	1:B:95:ILE:HD11	1.97	0.46
1:B:231:THR:HG22	1:B:232:ALA:N	2.27	0.46
1:B:300:ASN:HB3	7:c:1:NAG:H2	1.98	0.46
1:B:584:SER:OG	1:B:625:GLY:O	2.12	0.46
1:B:652:TYR:CD1	1:B:654:ILE:HG12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:CB	1:A:72:PRO:HG3	2.45	0.46
1:A:111:LYS:HA	1:A:122:ARG:NH2	2.31	0.46
1:A:502:VAL:HG11	1:A:686:PHE:CE2	2.51	0.46
1:A:714:VAL:O	1:A:738:SER:HB2	2.16	0.46
1:A:1153:PHE:C	1:A:1154:LEU:HD22	2.40	0.46
1:C:181:TYR:HB3	1:C:183:PHE:CZ	2.51	0.46
1:C:879:GLY:HA2	1:C:895:SER:HA	1.98	0.46
1:B:502:VAL:HG11	1:B:686:PHE:CE2	2.50	0.46
1:B:790:MET:HE1	1:B:999:LEU:HB3	1.97	0.46
1:B:1066:SER:O	1:B:1070:ILE:HG12	2.16	0.46
1:B:1236:ASP:O	1:B:1239:PRO:HD2	2.16	0.46
7:P:1:NAG:H4	7:P:2:FUC:O2	2.16	0.46
1:A:52:TYR:CE2	1:A:78:HIS:HB2	2.50	0.46
1:A:367:THR:OG1	1:A:368:GLN:N	2.47	0.46
1:A:690:THR:HB	3:G:1:NAG:C1	2.46	0.46
1:A:924:ARG:HG2	1:B:664:THR:HG21	1.96	0.46
1:C:374:PHE:HE1	1:C:387:PHE:HD1	1.64	0.46
1:C:467:PRO:HA	1:C:470:GLN:HB2	1.97	0.46
1:C:898:GLU:HA	1:C:901:LEU:HD12	1.98	0.46
1:C:904:LYS:HE3	1:C:1015:GLU:C	2.41	0.46
1:B:351:ASN:OD1	1:B:352:SER:N	2.49	0.46
1:B:575:THR:H	1:B:578:SER:HG	1.64	0.46
1:A:82:VAL:HB	1:A:91:PHE:CZ	2.51	0.46
1:A:209:GLU:OE1	1:A:209:GLU:N	2.49	0.46
1:A:213:TYR:HA	1:A:229:PRO:HA	1.97	0.46
1:A:372:TYR:HD2	1:A:374:PHE:CE1	2.34	0.46
1:A:1195:GLN:HG3	1:A:1199:ALA:HB3	1.97	0.46
1:C:321:PHE:HD2	1:C:441:ILE:HG22	1.81	0.46
1:C:460:ARG:HH22	1:C:478:PHE:HB2	1.81	0.46
1:C:468:VAL:HG13	1:C:708:TYR:CE1	2.51	0.46
1:C:673:GLY:O	1:C:676:TYR:OH	2.33	0.46
1:B:86:ARG:HB3	1:B:89:HIS:HD1	1.81	0.46
1:B:92:GLU:HB3	1:B:108:TYR:HH	1.78	0.46
1:B:195:LYS:HD3	1:B:197:TYR:CE1	2.51	0.46
1:B:510:HIS:HB2	1:B:548:GLN:HB2	1.97	0.46
1:B:725:PHE:HB3	1:B:738:SER:O	2.16	0.46
1:B:863:THR:O	1:B:866:SER:OG	2.27	0.46
1:B:984:TYR:CD2	1:B:985:LEU:HD12	2.50	0.46
1:B:1034:ALA:HA	1:B:1037:LYS:HZ1	1.81	0.46
2:D:3:BMA:H4	2:D:5:MAN:O5	2.16	0.46
1:A:216:ASN:HB2	5:M:3:FUC:O3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASN:HA	3:E:1:NAG:N2	2.32	0.45
1:A:872:TYR:HD1	1:A:1003:PHE:CD2	2.34	0.45
1:A:1091:LEU:HD12	1:A:1092:SER:N	2.31	0.45
1:C:89:HIS:HA	1:C:114:ASN:CG	2.41	0.45
1:C:276:ASN:OD1	1:C:446:PHE:HB3	2.16	0.45
1:C:289:LYS:N	1:C:435:VAL:HG12	2.31	0.45
1:C:363:PRO:HB2	7:S:1:NAG:O6	2.16	0.45
1:B:480:LEU:HB2	1:B:708:TYR:CE2	2.51	0.45
1:A:175:VAL:HB	1:A:181:TYR:CD2	2.51	0.45
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.82	0.45
1:A:1001:GLU:HA	1:A:1004:ASN:HD22	1.81	0.45
1:A:1144:VAL:HA	1:A:1152:LEU:O	2.16	0.45
1:C:676:TYR:O	1:C:683:LEU:HD12	2.15	0.45
1:C:722:SER:HA	1:C:737:HIS:ND1	2.30	0.45
1:B:55:ILE:O	1:B:62:ASN:ND2	2.50	0.45
1:B:245:GLU:OE1	1:B:249:HIS:HB2	2.16	0.45
1:B:1011:THR:HA	1:B:1014:PHE:CD2	2.51	0.45
1:B:1084:ASP:HA	1:B:1087:ILE:HD12	1.98	0.45
1:A:122:ARG:O	1:A:124:ARG:NH1	2.47	0.45
1:A:233:ASN:CG	1:A:288:PRO:HB2	2.41	0.45
1:A:372:TYR:OH	1:B:639:THR:HA	2.17	0.45
1:A:916:ASP:O	1:A:919:ARG:HG3	2.16	0.45
1:C:725:PHE:HB3	1:C:738:SER:C	2.41	0.45
1:C:1023:GLN:O	1:C:1026:ARG:HB2	2.15	0.45
1:B:321:PHE:O	1:B:397:GLU:HA	2.15	0.45
1:B:411:PHE:HD1	1:B:413:TYR:CD2	2.35	0.45
1:B:946:ASP:O	1:B:950:LEU:HG	2.16	0.45
1:A:337:LEU:HD11	1:A:419:LEU:HB3	1.97	0.45
1:A:508:ASN:OD1	1:A:509:ALA:N	2.49	0.45
1:C:93:ILE:O	1:C:108:TYR:HA	2.17	0.45
1:C:290:ILE:HG12	1:C:435:VAL:HG11	1.97	0.45
1:C:843:LEU:O	1:C:844:GLU:C	2.57	0.45
1:B:85:ILE:O	1:B:160:GLU:HA	2.15	0.45
1:B:218:THR:HG21	6:a:4:FUC:O5	2.17	0.45
1:B:268:LEU:HD21	1:B:271:GLY:HA3	1.98	0.45
1:B:536:ILE:HG21	1:B:542:PHE:HB3	1.98	0.45
1:B:556:ASN:HB2	8:B:1503:NAG:O7	2.17	0.45
1:B:795:GLU:OE2	1:B:1118:LYS:NZ	2.45	0.45
1:B:810:THR:HG22	1:B:815:GLY:HA2	1.99	0.45
1:B:1033:HIS:CE1	1:B:1037:LYS:HZ2	2.35	0.45
1:A:35:PHE:HB2	1:A:163:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:LEU:O	1:A:648:VAL:HG23	2.16	0.45
1:A:678:SER:HB3	1:A:684:LEU:HD23	1.98	0.45
1:C:31:ASN:O	1:C:227:TYR:OH	2.13	0.45
1:C:36:PHE:CD1	1:C:215:LEU:HD21	2.50	0.45
1:C:320:ARG:NH1	1:C:397:GLU:OE1	2.49	0.45
1:C:883:TYR:CE1	1:C:888:GLY:HA2	2.51	0.45
1:C:981:ARG:O	1:C:984:TYR:HB3	2.16	0.45
1:C:1120:ASN:HA	1:C:1124:LYS:HG3	1.98	0.45
1:C:1174:VAL:HG21	1:C:1238:LEU:HD12	1.98	0.45
1:C:1180:LEU:HD12	1:C:1222:GLN:HA	1.98	0.45
1:C:1239:PRO:HA	1:C:1242:ILE:O	2.17	0.45
1:B:116:ASN:HB3	8:B:1501:NAG:H81	1.99	0.45
1:B:548:GLN:HB3	1:B:631:THR:HG21	1.97	0.45
1:B:687:LYS:HG2	1:B:689:VAL:H	1.81	0.45
1:B:822:LEU:HA	1:B:825:GLN:NE2	2.32	0.45
1:B:1006:ALA:O	1:B:1010:ILE:HG12	2.16	0.45
1:B:1110:ALA:HA	1:B:1113:LYS:NZ	2.32	0.45
1:A:351:ASN:H	1:A:362:ILE:CD1	2.29	0.45
1:A:482:ASP:CG	1:A:709:VAL:HA	2.41	0.45
1:A:800:TYR:O	1:A:1149:GLN:HB3	2.16	0.45
1:A:1011:THR:O	1:A:1014:PHE:HB2	2.16	0.45
1:C:404:GLY:HA3	1:C:416:LEU:C	2.42	0.45
1:C:818:ARG:HH12	1:C:822:LEU:HG	1.81	0.45
1:B:262:LEU:HG	1:B:407:TYR:CD2	2.52	0.45
1:B:800:TYR:CE1	1:B:1149:GLN:HA	2.52	0.45
1:B:1174:VAL:HG12	1:B:1178:ILE:HB	1.98	0.45
1:B:1192:HIS:C	1:B:1196:ASN:HB3	2.42	0.45
1:A:37:SER:HB2	1:A:221:GLY:HA2	1.98	0.45
1:A:286:ALA:HA	1:A:440:THR:HA	1.98	0.45
1:A:291:TYR:HB3	1:A:426:PHE:CE2	2.51	0.45
1:A:818:ARG:HA	1:A:821:GLN:OE1	2.17	0.45
1:C:52:TYR:CE2	1:C:78:HIS:HB2	2.52	0.45
1:C:453:VAL:HG23	1:C:457:ALA:C	2.42	0.45
1:C:1100:GLN:HG3	1:C:1101:THR:N	2.31	0.45
1:B:51:GLY:O	1:B:53:LEU:N	2.49	0.45
1:B:258:ASN:HB2	1:B:322:ASN:ND2	2.31	0.45
1:B:411:PHE:HB3	1:B:413:TYR:CE2	2.52	0.45
1:B:579:VAL:O	1:B:583:LEU:HB2	2.17	0.45
1:B:587:LYS:NZ	1:B:621:GLN:HG2	2.31	0.45
1:B:870:ASP:OD1	1:B:870:ASP:N	2.43	0.45
1:B:949:LYS:HA	1:B:952:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:SER:OG	1:A:702:PHE:O	2.28	0.45
1:A:677:THR:HA	1:A:683:LEU:HA	1.98	0.45
1:C:208:TYR:HB2	1:C:209:GLU:OE1	2.17	0.45
1:C:699:PRO:HD2	1:C:702:PHE:CE1	2.51	0.45
1:C:883:TYR:OH	1:C:885:PRO:HA	2.17	0.45
1:C:1153:PHE:C	1:C:1154:LEU:HD22	2.42	0.45
1:B:235:ILE:HG13	1:B:438:PHE:CE2	2.52	0.45
1:B:490:ARG:HA	1:B:490:ARG:NH1	2.32	0.45
1:B:781:ASN:HD22	4:i:1:NAG:H4	1.81	0.45
1:B:1153:PHE:C	1:B:1154:LEU:HD22	2.41	0.45
1:B:1232:ASN:HD21	6:k:1:NAG:H62	1.82	0.45
1:A:88:GLY:O	1:A:114:ASN:HA	2.17	0.45
1:A:861:LEU:O	1:A:866:SER:OG	2.35	0.45
1:A:1061:GLN:HG3	1:C:1085:ARG:NH2	2.32	0.45
1:A:1174:VAL:HA	1:A:1233:LEU:HB3	1.99	0.45
1:C:34:ARG:NH2	1:C:162:SER:OG	2.50	0.45
1:C:292:GLY:CA	1:C:428:GLY:H	2.29	0.45
1:C:476:VAL:H	1:B:831:LYS:NZ	2.14	0.45
1:C:810:THR:HA	1:C:814:ASN:H	1.82	0.45
1:C:817:SER:HA	1:C:820:LYS:HE2	1.98	0.45
1:C:961:MET:HE1	1:C:981:ARG:CZ	2.46	0.45
1:C:981:ARG:HB2	1:C:1140:ILE:HD11	1.99	0.45
1:B:106:GLN:O	1:B:125:ILE:HD12	2.17	0.45
1:B:135:GLY:O	1:B:136:PRO:C	2.60	0.45
1:B:248:GLY:O	1:B:281:VAL:HG12	2.17	0.45
1:B:256:PHE:HA	1:B:259:TRP:CD1	2.52	0.45
1:B:290:ILE:HG12	1:B:435:VAL:HG11	1.99	0.45
1:B:299:PHE:O	1:B:315:ALA:HB1	2.17	0.45
1:B:497:GLN:HE22	1:B:660:GLU:CG	2.23	0.45
1:C:55:ILE:HD12	1:C:62:ASN:HA	1.99	0.45
1:C:300:ASN:O	7:P:2:FUC:H5	2.17	0.45
1:C:919:ARG:NH2	1:C:928:ASP:OD2	2.49	0.45
1:B:54:PRO:HG3	1:B:81:PHE:CD1	2.52	0.45
1:B:214:MET:O	1:B:215:LEU:HD23	2.17	0.45
1:B:509:ALA:HB3	1:B:547:ARG:H	1.80	0.45
1:B:559:ASN:HB2	1:B:564:VAL:HG22	1.99	0.45
1:B:678:SER:HB3	1:B:684:LEU:HD21	1.99	0.45
1:B:691:SER:HB3	3:h:1:NAG:O5	2.16	0.45
1:B:785:PRO:HB2	1:B:788:PHE:CZ	2.52	0.45
1:A:847:GLU:O	1:A:850:SER:HB3	2.18	0.44
1:A:880:VAL:O	1:A:892:GLN:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LYS:O	1:C:429:HIS:ND1	2.37	0.44
1:C:344:ASN:HB2	1:C:378:ASP:CB	2.46	0.44
1:C:807:ASP:O	1:C:811:TYR:N	2.34	0.44
1:C:1119:VAL:HG23	1:C:1123:VAL:HB	1.98	0.44
1:B:85:ILE:HG13	1:B:158:MET:HG2	1.99	0.44
1:B:133:THR:N	1:B:139:ASN:HD21	2.15	0.44
1:A:337:LEU:HD12	1:A:421:ALA:O	2.17	0.44
1:A:787:ASN:O	1:A:1161:SER:N	2.46	0.44
1:C:123:LEU:HD22	1:C:150:PHE:CD1	2.53	0.44
1:C:972:LEU:HD23	1:C:976:TYR:CD2	2.52	0.44
1:C:1192:HIS:CG	1:C:1193:GLU:H	2.35	0.44
1:B:37:SER:HB3	1:B:222:GLU:HG2	1.99	0.44
1:B:817:SER:HA	1:B:820:LYS:HG3	1.99	0.44
1:B:1084:ASP:O	1:B:1088:THR:HG23	2.18	0.44
3:V:1:NAG:H61	3:V:2:NAG:C7	2.47	0.44
1:A:54:PRO:HG3	1:A:81:PHE:CD1	2.52	0.44
1:A:124:ARG:HB2	1:A:126:CYS:SG	2.57	0.44
1:A:254:PHE:CZ	1:A:256:PHE:HA	2.52	0.44
1:A:324:ASN:HB2	1:A:439:TRP:CD2	2.52	0.44
1:A:775:ALA:HB2	1:C:960:GLY:O	2.17	0.44
1:A:894:ARG:HA	1:A:951:HIS:CE1	2.51	0.44
1:A:1036:THR:O	1:A:1039:GLN:HB2	2.18	0.44
1:C:57:GLU:HG3	1:C:58:ASN:CG	2.43	0.44
1:C:793:ARG:HB3	1:C:1029:ASN:CG	2.42	0.44
1:C:876:ASN:HA	1:C:896:PHE:HB3	1.99	0.44
1:A:847:GLU:HA	1:B:1028:LEU:CD1	2.48	0.44
1:A:1119:VAL:O	1:A:1123:VAL:HB	2.17	0.44
1:C:118:ASN:OD1	1:C:119:ALA:N	2.50	0.44
1:C:274:VAL:HG22	1:C:450:LEU:HB2	1.98	0.44
1:C:991:VAL:HG13	1:C:991:VAL:O	2.18	0.44
1:B:68:ALA:O	1:B:70:GLN:N	2.48	0.44
1:B:327:SER:HA	1:B:330:LEU:HD12	1.98	0.44
1:B:1010:ILE:HG22	1:B:1014:PHE:CZ	2.52	0.44
1:A:688:ASN:O	1:A:692:GLY:N	2.51	0.44
1:A:699:PRO:HD2	1:A:702:PHE:HE1	1.82	0.44
1:A:1003:PHE:CE2	1:A:1007:ILE:HD13	2.53	0.44
1:C:688:ASN:O	1:C:688:ASN:ND2	2.51	0.44
1:C:872:TYR:HB3	1:C:874:PHE:CZ	2.53	0.44
1:B:856:GLU:O	1:B:860:GLN:HG3	2.18	0.44
1:B:991:VAL:HG23	1:B:995:ASN:HD22	1.83	0.44
3:Q:3:BMA:O6	3:Q:3:BMA:O4	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PHE:CE1	1:A:152:LYS:HB2	2.53	0.44
1:A:678:SER:OG	1:A:682:GLN:OE1	2.30	0.44
1:A:779:THR:HB	1:A:1170:ALA:HB2	2.00	0.44
1:A:999:LEU:O	1:A:1002:SER:OG	2.25	0.44
1:C:89:HIS:CD2	1:C:197:TYR:HB3	2.50	0.44
1:C:244:THR:O	1:C:310:ALA:N	2.49	0.44
1:C:258:ASN:HB2	1:C:397:GLU:HG3	1.98	0.44
1:C:336:VAL:HA	1:C:345:PHE:O	2.17	0.44
1:C:343:THR:HG23	1:C:379:THR:HB	1.99	0.44
1:C:939:MET:N	1:C:939:MET:SD	2.90	0.44
1:C:1009:ASN:HA	1:C:1012:SER:HB3	1.99	0.44
1:B:145:GLY:O	1:B:146:ARG:C	2.60	0.44
1:B:500:SER:O	1:B:652:TYR:HA	2.17	0.44
1:B:917:TYR:HA	1:B:920:CYS:CB	2.47	0.44
1:B:1039:GLN:O	1:B:1042:VAL:HG22	2.18	0.44
1:A:33:ARG:HB3	1:A:222:GLU:HB3	1.99	0.44
1:A:336:VAL:HB	1:A:423:THR:HG1	1.82	0.44
1:A:810:THR:O	1:A:814:ASN:N	2.48	0.44
1:A:853:THR:N	1:A:953:TYR:HE1	2.14	0.44
1:A:864:ILE:HG13	1:A:878:LEU:HB2	2.00	0.44
1:A:989:THR:O	1:B:1223:ILE:HG23	2.18	0.44
1:A:1136:ASP:O	1:A:1157:VAL:HG21	2.18	0.44
1:C:158:MET:N	1:C:158:MET:SD	2.91	0.44
1:C:159:SER:HB3	1:C:162:SER:HB2	1.99	0.44
1:C:396:ARG:HD3	1:C:396:ARG:HA	1.62	0.44
1:B:638:VAL:C	1:B:640:ASP:H	2.26	0.44
1:A:131:ILE:HD13	1:A:135:GLY:O	2.17	0.44
1:A:184:TYR:CB	1:A:459:GLN:HB3	2.47	0.44
1:A:233:ASN:HB3	1:A:439:TRP:CZ3	2.52	0.44
1:A:262:LEU:HD22	1:A:407:TYR:CE2	2.52	0.44
1:A:1116:GLN:HE21	1:A:1120:ASN:ND2	2.15	0.44
1:C:216:ASN:O	1:C:218:THR:HG23	2.17	0.44
1:C:226:SER:OG	6:N:4:FUC:H62	2.17	0.44
1:C:744:CYS:HB2	1:C:761:SER:O	2.18	0.44
1:C:788:PHE:CZ	1:C:1160:PRO:HB3	2.53	0.44
1:C:1172:LEU:HD13	1:C:1231:VAL:HB	2.00	0.44
1:B:97:GLN:HG3	1:B:188:ASP:O	2.17	0.44
1:B:495:HIS:CD2	1:B:495:HIS:H	2.36	0.44
1:B:568:GLN:HE22	1:B:576:LEU:H	1.66	0.44
1:B:685:ALA:HA	1:B:695:TYR:O	2.18	0.44
1:B:991:VAL:HG23	1:B:995:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:HE1	1:A:195:LYS:HG3	1.83	0.44
1:A:347:PHE:HE1	1:A:373:CYS:HB3	1.82	0.44
1:A:350:SER:HB2	1:A:362:ILE:HD13	2.00	0.44
1:A:882:VAL:HG22	1:A:893:LYS:NZ	2.32	0.44
1:A:882:VAL:C	1:A:890:VAL:HG23	2.43	0.44
1:A:1073:ARG:HB3	1:B:573:PRO:O	2.18	0.44
1:A:1250:LYS:NZ	1:A:1254:GLU:OE2	2.32	0.44
1:C:313:GLN:OE1	1:C:313:GLN:N	2.51	0.44
1:C:403:TYR:N	1:C:418:LEU:HA	2.30	0.44
1:C:505:PRO:HD2	1:C:640:ASP:H	1.83	0.44
1:C:689:VAL:O	1:C:690:THR:C	2.60	0.44
1:B:134:LEU:HD12	1:B:135:GLY:N	2.33	0.44
1:B:484:PHE:HE1	1:B:749:LEU:HG	1.83	0.44
1:B:833:ILE:HG23	1:B:1098:VAL:CG2	2.48	0.44
1:B:835:SER:O	1:B:838:GLN:HG3	2.17	0.44
1:B:851:MET:HE2	1:B:851:MET:HA	1.99	0.44
1:A:291:TYR:CE2	1:A:293:LEU:HB2	2.53	0.43
1:A:317:GLU:OE2	1:A:446:PHE:N	2.43	0.43
1:A:500:SER:HB3	1:A:652:TYR:HB3	1.99	0.43
1:A:636:GLU:HB3	1:C:354:ASN:CB	2.48	0.43
1:A:787:ASN:HB2	4:J:1:NAG:O7	2.18	0.43
1:A:811:TYR:CE2	1:A:1090:ARG:HB3	2.54	0.43
1:A:852:LEU:HD23	1:A:852:LEU:HA	1.78	0.43
1:A:1023:GLN:HB3	1:A:1026:ARG:HB2	1.99	0.43
1:A:1195:GLN:CB	1:A:1201:GLU:HB2	2.48	0.43
1:C:123:LEU:CD2	1:C:125:ILE:HG13	2.46	0.43
1:C:132:LYS:HD2	1:C:139:ASN:CG	2.43	0.43
1:C:259:TRP:HA	1:C:397:GLU:OE2	2.18	0.43
1:C:272:LYS:HA	1:C:451:ILE:O	2.18	0.43
1:C:508:ASN:HD21	1:C:638:VAL:HB	1.83	0.43
1:C:1051:GLN:O	1:C:1054:VAL:HG12	2.17	0.43
1:B:415:HIS:ND1	2:b:1:NAG:O6	2.37	0.43
1:B:748:VAL:HG21	1:B:758:LYS:HB3	2.00	0.43
1:B:871:GLY:O	1:B:1000:ALA:HB1	2.18	0.43
1:B:938:VAL:C	1:B:939:MET:HE2	2.43	0.43
1:B:1082:GLN:CD	1:B:1085:ARG:HH22	2.26	0.43
1:A:52:TYR:OH	1:A:208:TYR:O	2.33	0.43
1:C:150:PHE:CE1	1:C:152:LYS:HB2	2.53	0.43
1:C:280:LEU:HD12	1:C:280:LEU:HA	1.69	0.43
1:C:507:PHE:HB2	1:B:387:PHE:CB	2.48	0.43
1:C:678:SER:OG	1:C:680:SER:OG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:PHE:CE2	1:C:900:LEU:HD11	2.53	0.43
1:C:927:ALA:HB1	1:C:931:CYS:HB2	1.99	0.43
1:B:96:SER:OG	1:B:106:GLN:HB3	2.18	0.43
1:B:881:SER:HB2	1:B:892:GLN:OE1	2.18	0.43
1:B:955:ALA:HA	1:B:958:ILE:HD12	2.01	0.43
1:A:236:GLY:N	3:E:1:NAG:H61	2.30	0.43
1:A:847:GLU:OE1	1:A:851:MET:HE1	2.19	0.43
1:A:1012:SER:O	1:A:1015:GLU:N	2.51	0.43
1:C:480:LEU:O	1:C:708:TYR:HE2	2.02	0.43
1:C:788:PHE:CE1	1:C:1160:PRO:HB3	2.53	0.43
1:C:946:ASP:HB3	1:C:949:LYS:HB3	2.00	0.43
1:B:93:ILE:O	1:B:108:TYR:HA	2.18	0.43
1:B:372:TYR:HB3	1:B:374:PHE:CE1	2.53	0.43
1:B:471:LEU:O	1:B:474:SER:OG	2.16	0.43
1:B:598:ALA:HB3	1:B:619:TYR:HB3	2.00	0.43
1:A:42:GLN:NE2	1:A:44:PRO:HD2	2.34	0.43
1:A:367:THR:HA	1:A:371:TYR:CZ	2.53	0.43
1:A:398:ILE:HD12	1:A:408:VAL:HG22	1.99	0.43
1:A:705:GLN:HB2	1:A:717:ILE:HB	1.99	0.43
1:A:844:GLU:HA	1:A:847:GLU:HG3	2.00	0.43
1:C:167:THR:HB	1:C:174:THR:OG1	2.18	0.43
1:C:320:ARG:HG2	1:C:321:PHE:N	2.34	0.43
1:C:345:PHE:HD2	1:C:375:PHE:HB3	1.84	0.43
1:B:569:ASP:HB3	1:B:602:ASP:H	1.83	0.43
1:B:725:PHE:HD1	1:B:739:ASN:ND2	2.17	0.43
1:B:782:ILE:O	1:B:1165:ASP:HA	2.18	0.43
6:a:1:NAG:O6	6:a:2:NAG:N2	2.52	0.43
1:A:299:PHE:CG	1:A:402:LYS:HD3	2.53	0.43
1:A:1139:HIS:NE2	1:A:1142:SER:HB3	2.33	0.43
1:A:1190:PHE:HZ	1:A:1212:PRO:HB3	1.82	0.43
1:C:142:VAL:HG13	1:C:146:ARG:CZ	2.48	0.43
1:C:728:THR:HA	1:C:736:TYR:O	2.18	0.43
1:C:822:LEU:HD11	1:C:1080:ASP:OD1	2.18	0.43
1:B:128:PHE:O	1:B:129:PRO:C	2.61	0.43
1:B:731:LEU:HA	1:B:731:LEU:HD13	1.88	0.43
1:B:1037:LYS:HA	1:B:1040:GLU:CD	2.43	0.43
1:B:1201:GLU:HG3	1:B:1203:PHE:CZ	2.53	0.43
1:A:86:ARG:HH21	1:A:197:TYR:HD2	1.66	0.43
1:C:44:PRO:HA	1:C:218:THR:HA	1.99	0.43
1:C:54:PRO:HG3	1:C:81:PHE:CD1	2.54	0.43
1:C:984:TYR:CE1	1:C:1126:GLN:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1130:TYR:HE1	1:C:1137:GLY:H	1.67	0.43
1:C:1139:HIS:NE2	1:C:1141:PHE:O	2.51	0.43
1:B:77:VAL:O	1:B:168:TRP:NE1	2.52	0.43
1:B:179:LYS:HE3	1:B:181:TYR:CE1	2.54	0.43
1:B:336:VAL:HA	1:B:345:PHE:O	2.18	0.43
1:B:588:PHE:CD1	1:B:622:PHE:HB3	2.53	0.43
1:B:938:VAL:O	1:B:939:MET:HE2	2.18	0.43
1:B:1136:ASP:O	1:B:1157:VAL:HG21	2.18	0.43
1:B:1204:VAL:O	1:B:1213:ARG:N	2.51	0.43
1:A:547:ARG:HD2	1:A:638:VAL:HG11	2.01	0.43
1:A:1080:ASP:HA	1:A:1083:VAL:HG12	2.00	0.43
1:A:1182:LEU:HD12	1:A:1187:LEU:HB2	2.00	0.43
1:C:177:SER:HB2	1:C:181:TYR:CE2	2.52	0.43
1:C:460:ARG:HG3	1:C:478:PHE:CZ	2.53	0.43
1:C:843:LEU:HA	1:C:846:VAL:HG12	2.00	0.43
1:C:894:ARG:HA	1:C:951:HIS:CG	2.53	0.43
1:B:794:THR:N	1:B:1029:ASN:OD1	2.52	0.43
1:A:367:THR:HA	1:A:371:TYR:CE2	2.54	0.43
1:A:655:TYR:HB3	1:A:675:TYR:OH	2.19	0.43
1:A:730:GLU:HG2	1:A:735:PHE:CD2	2.54	0.43
1:C:465:ASP:OD1	1:C:465:ASP:N	2.50	0.43
1:C:502:VAL:N	1:C:653:THR:O	2.33	0.43
1:C:667:ASN:HB3	8:C:1503:NAG:N2	2.33	0.43
1:C:857:GLU:O	1:C:861:LEU:HG	2.19	0.43
1:C:1027:GLY:O	1:C:1033:HIS:HB2	2.18	0.43
1:B:50:GLY:HA3	1:B:438:PHE:HE1	1.84	0.43
1:B:179:LYS:HE3	1:B:181:TYR:HE1	1.84	0.43
1:B:182:TYR:CZ	1:B:427:THR:HA	2.53	0.43
1:B:471:LEU:HD11	1:B:475:GLN:HE22	1.83	0.43
1:A:35:PHE:CD1	1:A:163:VAL:HB	2.54	0.43
1:A:790:MET:HE2	1:A:999:LEU:O	2.18	0.43
1:A:896:PHE:O	1:A:900:LEU:HG	2.19	0.43
1:A:1176:ASP:OD2	4:L:1:NAG:H62	2.19	0.43
1:C:297:PHE:CE2	1:C:441:ILE:HD12	2.54	0.43
1:C:651:LYS:HG2	1:C:659:GLY:O	2.19	0.43
1:C:799:LEU:HD13	1:C:1150:GLY:HA2	2.00	0.43
1:B:111:LYS:HD3	1:B:121:ALA:HB2	2.00	0.43
1:B:244:THR:H	1:B:309:GLY:HA3	1.82	0.43
1:B:289:LYS:N	1:B:435:VAL:HG12	2.33	0.43
1:B:644:MET:HG3	1:B:646:LEU:HD12	2.00	0.43
1:B:788:PHE:HB3	1:B:1158:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:LEU:O	1:B:1208:ARG:NH1	2.51	0.43
1:A:291:TYR:HB3	1:A:426:PHE:CD2	2.54	0.43
1:A:1109:GLN:O	1:A:1112:ARG:HG2	2.18	0.43
1:C:31:ASN:O	1:C:33:ARG:HD2	2.19	0.43
1:C:240:ASN:HD21	1:C:438:PHE:N	2.10	0.43
1:B:126:CYS:C	1:B:128:PHE:N	2.77	0.43
1:B:374:PHE:HA	1:B:388:LEU:H	1.84	0.43
1:B:512:PHE:CG	8:B:1502:NAG:H5	2.54	0.43
1:B:598:ALA:HB1	1:B:620:PHE:N	2.33	0.43
1:B:1028:LEU:O	1:B:1030:THR:HG23	2.19	0.43
1:A:78:HIS:HA	1:A:168:TRP:CE2	2.53	0.42
1:B:65:TRP:HD1	1:B:203:ALA:C	2.26	0.42
1:B:142:VAL:HG13	1:B:146:ARG:HD3	2.00	0.42
1:B:688:ASN:O	1:B:689:VAL:HG12	2.18	0.42
1:B:813:CYS:HA	1:B:819:CYS:SG	2.59	0.42
1:B:1100:GLN:HG3	1:B:1101:THR:N	2.34	0.42
1:A:267:THR:HG21	1:A:456:THR:OG1	2.19	0.42
1:A:331:ALA:HB3	1:A:426:PHE:CD1	2.54	0.42
1:A:402:LYS:HD2	1:A:419:LEU:O	2.19	0.42
1:A:896:PHE:CZ	1:A:900:LEU:HD21	2.54	0.42
1:A:958:ILE:O	1:A:961:MET:HB2	2.18	0.42
1:C:676:TYR:HA	1:B:267:THR:O	2.18	0.42
1:C:746:GLU:HB3	1:C:1024:THR:HG23	2.01	0.42
1:C:1147:ALA:HB3	1:C:1150:GLY:C	2.44	0.42
1:B:104:GLY:O	1:B:127:GLN:HG3	2.19	0.42
1:B:270:HIS:HB2	1:B:454:GLN:HA	2.01	0.42
1:B:372:TYR:HB3	1:B:374:PHE:CZ	2.54	0.42
1:A:82:VAL:O	1:A:163:VAL:HA	2.19	0.42
1:A:120:THR:HG23	1:A:155:PRO:HA	2.02	0.42
1:A:123:LEU:HD22	1:A:150:PHE:HE2	1.82	0.42
1:A:344:ASN:HB2	1:A:378:ASP:HB2	2.01	0.42
1:A:939:MET:HE1	1:A:941:LEU:HG	2.00	0.42
1:A:1174:VAL:CG1	1:A:1178:ILE:HB	2.50	0.42
1:C:100:PHE:HE2	1:C:141:ASP:CG	2.27	0.42
1:C:702:PHE:HB3	1:B:934:TYR:OH	2.19	0.42
1:C:1039:GLN:O	1:C:1042:VAL:HG22	2.18	0.42
1:B:618:LEU:HB3	1:B:620:PHE:CZ	2.54	0.42
1:B:1013:ALA:HA	1:B:1021:SER:OG	2.20	0.42
1:B:1169:ILE:HG23	1:B:1231:VAL:HG23	2.02	0.42
1:A:787:ASN:HB2	4:J:1:NAG:H2	2.01	0.42
1:A:1202:TYR:CE2	1:A:1241:VAL:HG22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:TYR:CZ	1:C:210:PRO:HD3	2.54	0.42
1:C:447:VAL:HG11	1:C:463:TYR:CE2	2.55	0.42
1:C:1109:GLN:HA	1:C:1112:ARG:CZ	2.49	0.42
1:C:1119:VAL:HA	1:C:1123:VAL:HB	2.01	0.42
1:C:1139:HIS:CD2	1:C:1155:HIS:HB3	2.53	0.42
1:B:325:ASP:OD1	1:B:325:ASP:N	2.39	0.42
1:B:1140:ILE:HG23	1:B:1141:PHE:CD1	2.55	0.42
1:A:184:TYR:CD2	1:A:459:GLN:HG3	2.54	0.42
1:A:214:MET:HE1	5:M:3:FUC:O4	2.19	0.42
1:A:450:LEU:HG	1:A:478:PHE:CZ	2.55	0.42
1:A:690:THR:HB	3:G:1:NAG:N2	2.35	0.42
1:A:813:CYS:HB2	1:A:820:LYS:HZ3	1.83	0.42
1:A:1068:ASP:HA	1:A:1071:TYR:CD2	2.55	0.42
1:A:1127:SER:OG	1:A:1129:ARG:HG2	2.19	0.42
1:A:1251:THR:HB	1:B:1252:ARG:NH2	2.34	0.42
1:C:86:ARG:HB3	1:C:89:HIS:CG	2.54	0.42
1:C:159:SER:O	1:C:162:SER:HB3	2.18	0.42
1:C:644:MET:HE1	1:C:646:LEU:HG	2.01	0.42
1:C:665:LEU:HD13	1:C:695:TYR:CE2	2.54	0.42
1:B:288:PRO:HG2	1:B:291:TYR:CD2	2.54	0.42
1:B:992:LEU:HB2	1:B:994:ARG:CZ	2.50	0.42
1:B:1036:THR:O	1:B:1039:GLN:N	2.53	0.42
1:A:158:MET:HB2	1:A:162:SER:OG	2.19	0.42
1:A:401:THR:HB	1:A:405:ASP:HB3	2.01	0.42
1:A:463:TYR:O	1:A:469:SER:HB3	2.20	0.42
1:A:501:PHE:HB3	1:A:643:PHE:CE1	2.53	0.42
1:A:721:SER:C	1:A:737:HIS:HE2	2.28	0.42
1:C:217:VAL:HA	1:C:224:GLY:O	2.20	0.42
1:C:260:PHE:CD2	1:C:409:ASN:HA	2.52	0.42
1:C:289:LYS:HB2	1:C:434:ASP:HB3	2.02	0.42
1:C:864:ILE:H	1:C:864:ILE:HD12	1.84	0.42
1:C:1006:ALA:O	1:C:1010:ILE:HG13	2.19	0.42
1:B:97:GLN:HB3	1:B:99:PRO:HD2	2.02	0.42
1:B:97:GLN:HE22	1:B:106:GLN:HE22	1.67	0.42
1:B:282:ASN:HB2	1:B:443:SER:OG	2.20	0.42
1:B:294:GLY:HA2	1:B:424:ILE:O	2.19	0.42
1:B:646:LEU:HA	1:B:663:ILE:HB	2.02	0.42
1:B:773:LYS:HD2	1:B:1130:TYR:CZ	2.54	0.42
1:B:813:CYS:SG	1:B:820:LYS:HG2	2.59	0.42
3:V:2:NAG:H4	3:V:3:BMA:H2	1.72	0.42
1:A:84:HIS:CG	1:A:199:SER:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:OD1	1:A:241:VAL:HG13	2.18	0.42
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.87	0.42
1:A:287:ILE:O	1:A:439:TRP:HA	2.19	0.42
1:A:946:ASP:O	1:A:950:LEU:HG	2.20	0.42
1:A:957:LEU:O	1:A:961:MET:HG2	2.19	0.42
1:C:52:TYR:O	1:C:81:PHE:HZ	2.02	0.42
1:C:65:TRP:CD1	1:C:202:CYS:HG	2.37	0.42
1:C:97:GLN:HG3	1:C:189:TRP:HD1	1.82	0.42
1:C:108:TYR:OH	1:C:134:LEU:HD12	2.19	0.42
1:C:108:TYR:CD2	1:C:136:PRO:HA	2.55	0.42
1:C:170:ASN:O	1:C:172:ARG:HG3	2.20	0.42
1:C:292:GLY:HA2	1:C:428:GLY:H	1.83	0.42
1:C:495:HIS:C	1:C:496:GLU:HG2	2.44	0.42
1:C:833:ILE:HD11	1:C:1095:ASN:OD1	2.19	0.42
1:A:34:ARG:N	1:A:222:GLU:OE1	2.52	0.42
1:A:95:ILE:HA	1:A:191:ARG:O	2.20	0.42
1:A:688:ASN:HB2	1:A:695:TYR:CE2	2.55	0.42
1:A:1006:ALA:HA	1:A:1009:ASN:OD1	2.20	0.42
1:A:1130:TYR:OH	1:A:1136:ASP:HB2	2.19	0.42
1:C:66:TYR:CD2	1:C:72:PRO:HG3	2.55	0.42
1:C:111:LYS:C	1:C:113:THR:H	2.26	0.42
1:C:493:LEU:HD13	1:C:493:LEU:HA	1.94	0.42
1:C:736:TYR:CE2	1:C:738:SER:HB3	2.55	0.42
1:B:297:PHE:CD2	1:B:303:ILE:HG12	2.54	0.42
1:B:374:PHE:CD1	1:B:387:PHE:HA	2.55	0.42
1:B:451:ILE:HG12	1:B:461:ILE:HG13	2.01	0.42
1:B:472:LYS:NZ	1:B:479:ASP:HA	2.35	0.42
1:B:673:GLY:HA3	1:B:676:TYR:CE1	2.53	0.42
1:A:72:PRO:O	1:A:206:TYR:OH	2.38	0.42
1:A:230:CYS:SG	1:A:231:THR:N	2.93	0.42
1:A:843:LEU:O	1:A:847:GLU:HG3	2.19	0.42
1:A:916:ASP:HB3	1:B:732:PRO:O	2.19	0.42
1:C:126:CYS:C	1:C:128:PHE:N	2.77	0.42
1:C:460:ARG:HG3	1:C:478:PHE:CE2	2.55	0.42
1:C:482:ASP:CG	1:C:710:ASP:H	2.27	0.42
1:B:286:ALA:HB1	1:B:438:PHE:HB2	2.02	0.42
1:B:1017:VAL:C	1:B:1019:GLU:H	2.27	0.42
1:A:78:HIS:HA	1:A:168:TRP:NE1	2.35	0.42
1:A:155:PRO:HG2	1:A:157:HIS:HE1	1.85	0.42
1:A:284:LEU:HD23	1:A:308:ASN:HB3	2.02	0.42
1:A:796:TYR:CE1	1:A:1150:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:GLU:HB3	1:A:919:ARG:HE	1.85	0.42
1:A:923:GLY:O	1:B:696:SER:OG	2.36	0.42
1:A:1139:HIS:CD2	1:A:1155:HIS:HB3	2.54	0.42
1:C:82:VAL:HA	1:C:203:ALA:O	2.20	0.42
1:C:238:ALA:HB3	1:C:241:VAL:HG22	2.01	0.42
1:C:249:HIS:HA	1:C:463:TYR:CZ	2.55	0.42
1:C:474:SER:OG	1:C:475:GLN:OE1	2.35	0.42
1:C:690:THR:O	1:B:370:PRO:HG2	2.20	0.42
1:C:788:PHE:HA	1:C:1159:VAL:O	2.20	0.42
1:B:166:ILE:HG13	1:B:175:VAL:HG22	2.01	0.42
1:B:235:ILE:H	1:B:235:ILE:HD12	1.84	0.42
1:B:546:THR:OG1	1:B:548:GLN:O	2.22	0.42
1:B:790:MET:HE3	1:B:790:MET:HB3	1.92	0.42
1:B:989:THR:OG1	1:B:1211:GLU:OE1	2.36	0.42
1:B:1016:SER:HB3	1:B:1019:GLU:O	2.20	0.42
1:A:128:PHE:CG	1:A:129:PRO:HD2	2.55	0.41
1:A:356:HIS:NE2	1:A:385:TYR:HD1	2.18	0.41
1:A:666:THR:OG1	1:A:667:ASN:N	2.53	0.41
1:A:699:PRO:HD2	1:A:702:PHE:CE1	2.55	0.41
1:A:880:VAL:C	1:A:892:GLN:HG3	2.45	0.41
1:A:1028:LEU:HD12	1:A:1029:ASN:H	1.85	0.41
1:C:132:LYS:O	1:C:193:ALA:HB2	2.19	0.41
1:B:47:VAL:HG23	1:B:215:LEU:HB2	2.02	0.41
1:B:127:GLN:OE1	1:B:146:ARG:HB3	2.20	0.41
1:B:177:SER:C	1:B:179:LYS:H	2.27	0.41
1:B:242:PHE:CE1	1:B:250:ILE:HG23	2.55	0.41
1:B:536:ILE:HD13	1:B:541:SER:HA	2.02	0.41
1:A:49:LEU:HB3	1:A:53:LEU:HD11	2.02	0.41
1:A:853:THR:HB	1:B:770:GLY:CA	2.49	0.41
1:C:134:LEU:CD1	1:C:195:LYS:HD2	2.50	0.41
1:C:894:ARG:NH1	1:C:910:LEU:HD22	2.35	0.41
1:C:906:VAL:HB	1:C:909:GLY:C	2.45	0.41
1:C:917:TYR:HE1	1:C:934:TYR:HB2	1.84	0.41
1:C:1059:ASN:O	1:C:1061:GLN:N	2.53	0.41
1:C:1153:PHE:N	1:C:1153:PHE:CD1	2.87	0.41
1:B:72:PRO:HD2	1:B:194:THR:HG1	1.85	0.41
1:B:522:GLY:HA3	1:B:559:ASN:OD1	2.19	0.41
1:B:601:ILE:HB	1:B:620:PHE:CE1	2.55	0.41
1:B:644:MET:CE	3:h:1:NAG:HN2	2.32	0.41
1:B:1151:LEU:HD23	1:B:1151:LEU:HA	1.78	0.41
1:A:32:PHE:HD1	1:A:163:VAL:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:HD22	8:A:1501:NAG:C7	2.33	0.41
1:A:349:CYS:HA	1:A:372:TYR:O	2.20	0.41
1:A:884:ASP:H	1:A:890:VAL:HA	1.84	0.41
1:A:1051:GLN:O	1:A:1054:VAL:HG12	2.20	0.41
1:A:1061:GLN:O	1:A:1085:ARG:NH2	2.53	0.41
1:C:128:PHE:CD1	1:C:128:PHE:C	2.98	0.41
1:B:108:TYR:CE1	1:B:131:ILE:HG21	2.54	0.41
3:G:2:NAG:H4	3:G:3:BMA:H2	1.58	0.41
1:A:267:THR:HB	1:B:676:TYR:HD1	1.85	0.41
1:A:855:SER:N	1:A:956:SER:OG	2.52	0.41
1:A:859:LEU:HA	1:A:862:ALA:HB3	2.01	0.41
1:A:997:GLN:OE1	1:A:998:LEU:HD22	2.20	0.41
1:A:1070:ILE:HG22	1:A:1079:ALA:HA	2.01	0.41
1:A:1102:LEU:HA	1:A:1102:LEU:HD13	1.86	0.41
1:C:31:ASN:ND2	1:C:33:ARG:HH11	2.17	0.41
1:C:77:VAL:HA	1:C:208:TYR:CD1	2.54	0.41
1:C:126:CYS:HB3	1:C:147:ASN:O	2.20	0.41
1:C:426:PHE:HD2	1:C:439:TRP:CH2	2.38	0.41
1:C:805:SER:OG	1:C:939:MET:HB2	2.20	0.41
1:C:816:ASN:O	1:C:820:LYS:HG3	2.20	0.41
1:C:879:GLY:HA3	1:C:951:HIS:CE1	2.56	0.41
1:C:1012:SER:HA	1:C:1015:GLU:OE1	2.20	0.41
1:C:1169:ILE:HG12	1:C:1190:PHE:HA	2.02	0.41
1:C:1183:ARG:HH22	1:B:1183:ARG:NH1	2.19	0.41
1:B:83:SER:OG	1:B:202:CYS:O	2.38	0.41
1:B:336:VAL:O	1:B:423:THR:OG1	2.33	0.41
1:B:415:HIS:CE1	2:b:1:NAG:HO6	2.32	0.41
1:B:606:TYR:CE1	1:B:612:GLY:HA2	2.55	0.41
1:B:629:THR:O	1:B:631:THR:HG23	2.21	0.41
1:B:721:SER:HA	1:B:735:PHE:CD2	2.55	0.41
1:B:831:LYS:HA	1:B:834:GLU:OE2	2.21	0.41
1:B:894:ARG:CZ	1:B:910:LEU:HD22	2.50	0.41
1:B:1172:LEU:HD12	1:B:1173:CYS:H	1.85	0.41
4:U:1:NAG:H3	4:U:2:NAG:N2	2.35	0.41
1:A:85:ILE:HG21	1:A:111:LYS:HZ3	1.86	0.41
1:A:257:ASN:ND2	1:A:322:ASN:HD21	2.19	0.41
1:A:404:GLY:HA2	1:A:419:LEU:CG	2.38	0.41
1:A:684:LEU:HD13	1:A:684:LEU:HA	1.88	0.41
1:A:772:VAL:HG11	1:C:966:PHE:CE1	2.56	0.41
1:A:916:ASP:OD1	1:A:916:ASP:N	2.52	0.41
1:C:793:ARG:HH12	1:C:1136:ASP:C	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1182:LEU:HD23	1:C:1182:LEU:HA	1.92	0.41
1:B:340:ALA:HA	1:B:420:ASP:OD2	2.21	0.41
1:B:820:LYS:HA	1:B:823:LEU:HB3	2.02	0.41
1:A:260:PHE:CE1	1:B:672:ALA:HA	2.54	0.41
1:A:280:LEU:O	1:A:444:THR:HA	2.20	0.41
1:A:366:ALA:C	1:A:367:THR:HG1	2.26	0.41
1:A:725:PHE:HB3	1:A:738:SER:O	2.20	0.41
1:A:748:VAL:HG13	1:A:757:CYS:HA	2.01	0.41
1:A:906:VAL:HG12	1:A:909:GLY:N	2.35	0.41
1:A:924:ARG:HA	1:B:664:THR:HG21	2.02	0.41
1:A:992:LEU:O	1:A:996:GLN:NE2	2.53	0.41
1:A:1075:ASP:OD1	1:A:1075:ASP:N	2.51	0.41
1:A:1114:LEU:HA	1:A:1117:GLN:OE1	2.20	0.41
1:A:1126:GLN:CD	1:A:1126:GLN:H	2.29	0.41
1:A:1150:GLY:C	1:A:1151:LEU:HD22	2.45	0.41
1:A:1204:VAL:O	1:A:1213:ARG:HD3	2.20	0.41
1:A:1233:LEU:HD21	1:A:1241:VAL:HG21	2.03	0.41
1:C:379:THR:HG23	1:C:381:ASN:OD1	2.20	0.41
1:C:838:GLN:NE2	1:C:839:LEU:HG	2.36	0.41
1:C:1092:SER:HA	1:C:1095:ASN:HD22	1.86	0.41
1:C:1136:ASP:N	1:C:1136:ASP:OD1	2.52	0.41
1:B:232:ALA:HA	1:B:235:ILE:CD1	2.51	0.41
1:B:376:LYS:HB2	1:B:385:TYR:CZ	2.55	0.41
1:B:708:TYR:CZ	1:B:711:ASP:HA	2.55	0.41
1:B:785:PRO:HB2	1:B:788:PHE:CE1	2.55	0.41
1:B:813:CYS:HB3	1:B:819:CYS:HB3	2.02	0.41
1:B:1080:ASP:HA	1:B:1083:VAL:HG22	2.02	0.41
1:A:276:ASN:OD1	1:A:446:PHE:HB3	2.20	0.41
1:A:405:ASP:OD1	2:D:1:NAG:H81	2.20	0.41
1:A:495:HIS:CG	1:A:496:GLU:N	2.88	0.41
1:A:787:ASN:HB2	4:J:1:NAG:C7	2.51	0.41
1:A:948:GLU:O	1:A:952:MET:HG2	2.19	0.41
1:A:1179:ALA:HB2	1:A:1226:CYS:SG	2.61	0.41
1:A:1205:SER:HB2	1:A:1211:GLU:H	1.85	0.41
1:C:65:TRP:CB	1:C:202:CYS:HA	2.43	0.41
1:C:500:SER:O	1:C:653:THR:N	2.51	0.41
1:C:1154:LEU:HD13	1:C:1154:LEU:HA	1.88	0.41
1:B:77:VAL:HG13	1:B:207:VAL:H	1.86	0.41
1:B:497:GLN:HB3	1:B:650:THR:HA	2.03	0.41
1:B:857:GLU:H	1:B:857:GLU:CD	2.27	0.41
1:B:904:LYS:HZ2	1:B:1014:PHE:C	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:1:NAG:O6	3:h:2:NAG:N2	2.54	0.41
1:A:83:SER:N	1:A:203:ALA:O	2.28	0.41
1:A:126:CYS:O	1:A:128:PHE:N	2.54	0.41
1:A:260:PHE:HE2	1:A:396:ARG:HB2	1.84	0.41
1:A:352:SER:HB3	1:A:360:PHE:CD1	2.55	0.41
1:A:453:VAL:HG23	1:A:457:ALA:C	2.46	0.41
1:A:973:PRO:HD2	1:A:976:TYR:CD2	2.55	0.41
1:C:82:VAL:O	1:C:82:VAL:HG13	2.21	0.41
1:C:508:ASN:OD1	1:C:508:ASN:N	2.50	0.41
1:C:930:VAL:HA	1:C:933:GLN:OE1	2.20	0.41
1:C:999:LEU:HD23	1:C:999:LEU:HA	1.88	0.41
1:C:1084:ASP:HA	1:C:1087:ILE:HD12	2.03	0.41
1:C:1192:HIS:C	1:C:1196:ASN:HB3	2.45	0.41
1:B:66:TYR:CD2	1:B:72:PRO:HG3	2.55	0.41
1:B:68:ALA:C	1:B:70:GLN:H	2.27	0.41
1:B:882:VAL:C	1:B:890:VAL:HG23	2.46	0.41
1:B:919:ARG:C	1:B:919:ARG:HD2	2.46	0.41
1:B:934:TYR:CE1	1:B:939:MET:HE1	2.55	0.41
1:B:1139:HIS:NE2	1:B:1141:PHE:O	2.54	0.41
1:A:84:HIS:NE2	1:A:160:GLU:OE1	2.53	0.41
1:A:185:PHE:HE2	1:A:189:TRP:CH2	2.37	0.41
1:A:225:ILE:HD12	1:A:227:TYR:HB3	2.03	0.41
1:A:502:VAL:C	1:A:503:THR:HG1	2.29	0.41
1:A:637:GLY:H	1:C:353:SER:HB2	1.86	0.41
1:A:687:LYS:HG2	1:A:694:VAL:HG12	2.03	0.41
1:A:790:MET:HB3	1:A:1158:LEU:HD23	2.01	0.41
1:A:863:THR:HG23	1:A:866:SER:H	1.85	0.41
1:A:930:VAL:C	1:A:933:GLN:HE21	2.29	0.41
1:A:966:PHE:HE1	1:B:772:VAL:HG11	1.86	0.41
1:C:99:PRO:HB2	1:C:101:ASP:OD1	2.20	0.41
1:C:326:THR:O	1:C:329:ILE:N	2.47	0.41
1:C:785:PRO:HB2	1:C:1160:PRO:HB3	2.03	0.41
1:C:816:ASN:HB3	1:C:819:CYS:HB3	2.03	0.41
1:C:1010:ILE:HG22	1:C:1014:PHE:CZ	2.55	0.41
1:C:1036:THR:O	1:C:1040:GLU:OE1	2.39	0.41
1:C:1076:PRO:N	1:C:1077:PRO:HD2	2.36	0.41
1:C:1152:LEU:HD13	1:C:1152:LEU:HA	1.88	0.41
1:C:1164:VAL:HG12	1:C:1166:VAL:HG13	2.02	0.41
1:B:50:GLY:HA3	1:B:438:PHE:CE1	2.56	0.41
1:B:259:TRP:CD1	1:B:259:TRP:N	2.88	0.41
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:GLN:NE2	1:B:660:GLU:HG3	2.25	0.41
1:B:510:HIS:CB	1:B:548:GLN:HB2	2.51	0.41
1:B:559:ASN:HB3	1:B:562:GLY:C	2.46	0.41
1:B:585:PHE:HB3	1:B:587:LYS:O	2.21	0.41
1:B:861:LEU:HD11	1:B:963:LEU:HD13	2.02	0.41
1:B:896:PHE:O	1:B:900:LEU:HG	2.21	0.41
1:B:1216:THR:HA	1:B:1244:ASP:HB2	2.03	0.41
1:A:233:ASN:O	1:A:237:TYR:HB3	2.20	0.41
1:A:272:LYS:HA	1:A:451:ILE:O	2.21	0.41
1:A:403:TYR:CZ	2:D:2:NAG:H2	2.56	0.41
1:A:809:ALA:N	1:A:830:CYS:SG	2.94	0.41
1:A:886:ALA:C	1:A:888:GLY:H	2.28	0.41
1:A:1036:THR:O	1:A:1040:GLU:OE1	2.39	0.41
1:A:1051:GLN:HA	1:A:1054:VAL:HG12	2.01	0.41
1:C:59:GLN:H	1:C:59:GLN:CD	2.25	0.41
1:C:260:PHE:CE2	1:C:397:GLU:HB2	2.56	0.41
1:C:1183:ARG:HH22	1:B:1219:ASP:HA	1.86	0.41
1:B:71:HIS:CE1	1:B:195:LYS:HA	2.55	0.41
1:B:86:ARG:HB3	1:B:89:HIS:CE1	2.56	0.41
1:B:259:TRP:HA	1:B:320:ARG:NH1	2.36	0.41
1:B:352:SER:HB3	1:B:360:PHE:CE1	2.56	0.41
1:B:515:ILE:O	1:B:553:LEU:HD12	2.21	0.41
1:B:533:ASP:OD1	1:B:534:THR:N	2.52	0.41
1:B:688:ASN:C	1:B:690:THR:N	2.79	0.41
1:B:790:MET:SD	1:B:790:MET:N	2.86	0.41
1:B:894:ARG:HA	1:B:951:HIS:ND1	2.36	0.41
1:B:946:ASP:O	1:B:949:LYS:HB3	2.21	0.41
1:B:1082:GLN:OE1	1:B:1085:ARG:NH1	2.54	0.41
1:A:242:PHE:CE2	1:A:284:LEU:HD22	2.56	0.40
1:A:452:GLU:HB2	1:A:478:PHE:CE1	2.55	0.40
1:A:812:VAL:HG13	1:A:813:CYS:SG	2.62	0.40
1:A:944:VAL:HG13	1:B:752:SER:O	2.21	0.40
1:A:1082:GLN:HG3	1:A:1085:ARG:NH2	2.24	0.40
1:C:291:TYR:O	1:C:439:TRP:NE1	2.53	0.40
1:C:847:GLU:HG2	1:C:848:VAL:N	2.37	0.40
1:C:997:GLN:NE2	1:C:1001:GLU:HG2	2.36	0.40
1:C:1188:VAL:HG23	1:C:1190:PHE:CE1	2.56	0.40
1:C:1204:VAL:HG22	1:C:1213:ARG:O	2.19	0.40
1:B:122:ARG:HH22	1:B:151:ASN:HB2	1.86	0.40
1:B:200:GLY:C	1:B:202:CYS:H	2.28	0.40
1:B:510:HIS:HE1	1:B:512:PHE:CG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:VAL:C	1:B:692:GLY:H	2.29	0.40
4:Y:1:NAG:H3	4:Y:1:NAG:C8	2.49	0.40
1:A:55:ILE:HB	1:A:62:ASN:OD1	2.22	0.40
1:A:86:ARG:NH2	1:A:197:TYR:HB3	2.36	0.40
1:A:416:LEU:HA	1:A:416:LEU:HD12	1.88	0.40
1:A:721:SER:HA	1:A:735:PHE:CG	2.56	0.40
1:A:1035:LEU:O	1:A:1039:GLN:HG3	2.22	0.40
1:A:1214:LYS:NZ	1:A:1243:PRO:HD3	2.36	0.40
1:A:1251:THR:HA	1:A:1254:GLU:OE1	2.20	0.40
1:C:92:GLU:HA	1:C:109:LEU:O	2.21	0.40
1:C:299:PHE:O	1:C:315:ALA:HB1	2.21	0.40
1:C:1192:HIS:CD2	1:C:1193:GLU:H	2.40	0.40
1:B:983:ASN:HA	1:B:986:ALA:O	2.21	0.40
1:B:1051:GLN:O	1:B:1054:VAL:HG12	2.20	0.40
1:B:1118:LYS:HB2	1:B:1118:LYS:HE3	1.91	0.40
1:B:1179:ALA:HB3	1:B:1223:ILE:O	2.21	0.40
1:A:287:ILE:HD12	1:A:290:ILE:O	2.21	0.40
1:A:451:ILE:HG13	1:A:461:ILE:CD1	2.50	0.40
1:A:678:SER:HB3	1:A:684:LEU:CD2	2.52	0.40
1:A:893:LYS:HE2	1:A:893:LYS:HB2	1.77	0.40
1:A:1045:GLN:H	1:A:1045:GLN:CD	2.29	0.40
1:A:1092:SER:HA	1:A:1095:ASN:OD1	2.21	0.40
1:C:364:LEU:HB2	7:S:1:NAG:O5	2.21	0.40
1:C:1147:ALA:HB2	1:C:1152:LEU:HD23	2.03	0.40
1:B:40:ASN:HD22	1:B:432:ASP:C	2.28	0.40
1:B:97:GLN:HE22	1:B:106:GLN:NE2	2.19	0.40
1:B:317:GLU:CD	1:B:445:ASN:HA	2.47	0.40
1:B:332:GLU:HG2	1:B:347:PHE:O	2.21	0.40
1:A:102:PRO:HB2	1:A:146:ARG:HH11	1.86	0.40
1:A:134:LEU:HA	1:A:134:LEU:HD12	1.81	0.40
1:A:376:LYS:HB2	1:A:385:TYR:CD2	2.57	0.40
1:C:55:ILE:HD11	1:C:64:THR:OG1	2.22	0.40
1:C:80:ILE:HG21	1:C:192:VAL:HG21	2.03	0.40
1:C:117:THR:HB	8:C:1501:NAG:H82	2.03	0.40
1:C:321:PHE:HD1	1:C:398:ILE:HG23	1.85	0.40
1:C:449:ALA:HA	1:C:464:CYS:SG	2.62	0.40
1:C:507:PHE:CE2	1:C:509:ALA:HB2	2.56	0.40
1:C:675:TYR:CE1	1:B:266:SER:HA	2.57	0.40
1:C:785:PRO:HB2	1:C:788:PHE:CZ	2.57	0.40
1:B:57:GLU:HB2	1:B:202:CYS:HB3	2.02	0.40
1:B:92:GLU:OE2	1:B:112:ALA:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:VAL:HB	1:B:183:PHE:HD2	1.87	0.40
1:B:242:PHE:CE1	1:B:284:LEU:HD22	2.56	0.40
1:B:280:LEU:HA	1:B:280:LEU:HD12	1.81	0.40
1:B:377:VAL:N	1:B:384:VAL:O	2.29	0.40
1:B:658:LYS:HD2	1:B:658:LYS:C	2.47	0.40
1:B:726:ASN:OD1	1:B:739:ASN:HA	2.20	0.40
1:B:793:ARG:HD3	1:B:1029:ASN:HD21	1.87	0.40
1:B:1027:GLY:O	1:B:1030:THR:OG1	2.34	0.40
1:B:1173:CYS:O	1:B:1232:ASN:HA	2.21	0.40
1:A:73:THR:HG23	1:A:192:VAL:O	2.20	0.40
1:A:172:ARG:NH2	1:A:182:TYR:OH	2.53	0.40
1:A:242:PHE:CE2	1:A:281:VAL:HG11	2.57	0.40
1:A:259:TRP:HA	1:A:320:ARG:NH1	2.36	0.40
1:A:456:THR:OG1	1:B:672:ALA:HB3	2.22	0.40
1:A:634:PRO:HB2	1:C:354:ASN:ND2	2.37	0.40
1:C:221:GLY:C	1:C:223:ASP:H	2.29	0.40
1:C:321:PHE:CD1	1:C:398:ILE:HG23	2.57	0.40
1:C:500:SER:O	1:C:652:TYR:HA	2.22	0.40
1:C:790:MET:HE3	1:C:1003:PHE:CB	2.51	0.40
1:C:1091:LEU:HD12	1:C:1091:LEU:HA	1.87	0.40
1:B:105:TYR:CE2	1:B:126:CYS:HA	2.56	0.40
1:B:259:TRP:CE3	1:B:320:ARG:CZ	3.05	0.40
1:B:472:LYS:HG2	1:B:480:LEU:HG	2.02	0.40
1:B:551:ILE:HG12	1:B:576:LEU:HD12	2.04	0.40
1:B:816:ASN:ND2	1:B:1071:TYR:HE2	2.18	0.40
1:B:833:ILE:O	1:B:837:LEU:HG	2.21	0.40
1:B:898:GLU:HG2	1:B:1145:GLN:HB3	2.04	0.40
1:B:1139:HIS:HD2	1:B:1155:HIS:HB3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1116/1402 (80%)	1005 (90%)	109 (10%)	2 (0%)	43	77
1	B	1222/1402 (87%)	1112 (91%)	103 (8%)	7 (1%)	21	58
1	C	1094/1402 (78%)	985 (90%)	103 (9%)	6 (0%)	24	62
All	All	3432/4206 (82%)	3102 (90%)	315 (9%)	15 (0%)	31	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	369	VAL
1	C	689	VAL
1	A	142	VAL
1	C	142	VAL
1	B	129	PRO
1	B	140	ASN
1	B	142	VAL
1	B	369	VAL
1	A	640	ASP
1	B	689	VAL
1	C	62	ASN
1	C	127	GLN
1	B	515	ILE
1	C	63	SER
1	B	62	ASN

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	962/1209 (80%)	962 (100%)	0	100	100
1	B	1049/1209 (87%)	1040 (99%)	9 (1%)	70	75
1	C	938/1209 (78%)	935 (100%)	3 (0%)	86	84
All	All	2949/3627 (81%)	2937 (100%)	12 (0%)	81	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	126	CYS
1	C	128	PHE
1	C	689	VAL
1	B	128	PHE
1	B	129	PRO
1	B	130	SER
1	B	132	LYS
1	B	133	THR
1	B	134	LEU
1	B	137	THR
1	B	143	THR
1	B	148	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	198	ASN
1	A	301	GLN
1	A	308	ASN
1	A	429	HIS
1	A	510	HIS
1	A	951	HIS
1	A	979	GLN
1	A	1057	GLN
1	A	1082	GLN
1	A	1116	GLN
1	C	84	HIS
1	C	97	GLN
1	C	187	ASN
1	C	240	ASN
1	C	459	GLN
1	C	470	GLN
1	C	491	ASN
1	C	705	GLN
1	C	995	ASN
1	C	1004	ASN
1	C	1095	ASN
1	C	1116	GLN
1	C	1120	ASN
1	C	1149	GLN
1	B	114	ASN
1	B	139	ASN

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Mol	Chain	Res	Type
1	B	240	ASN
1	B	258	ASN
1	B	445	ASN
1	B	470	GLN
1	B	497	GLN
1	B	566	ASN
1	B	577	GLN
1	B	922	ASN
1	B	979	GLN
1	B	988	GLN
1	B	993	GLN
1	B	1116	GLN
1	B	1120	ASN

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 ⓘ

97 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	0.44	0	17,19,21	1.38	2 (11%)
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	0.46	0
2	BMA	D	3	2	11,11,12	0.84	0	15,15,17	1.24	2 (13%)
2	MAN	D	4	2	11,11,12	0.77	0	15,15,17	0.95	1 (6%)
2	MAN	D	5	2	11,11,12	0.57	0	15,15,17	0.99	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	3,1	14,14,15	0.39	0	17,19,21	0.73	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.59	0
3	BMA	E	3	3	11,11,12	0.57	0	15,15,17	0.80	0
3	NAG	F	1	3,1	14,14,15	0.53	0	17,19,21	1.43	2 (11%)
3	NAG	F	2	3	14,14,15	0.14	0	17,19,21	0.45	0
3	BMA	F	3	3	11,11,12	0.87	0	15,15,17	1.42	1 (6%)
3	NAG	G	1	3	14,14,15	0.82	1 (7%)	17,19,21	0.68	0
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	0.51	0
3	BMA	G	3	3	11,11,12	0.65	0	15,15,17	0.82	1 (6%)
4	NAG	H	1	1,4	14,14,15	1.43	2 (14%)	17,19,21	1.18	1 (5%)
4	NAG	H	2	4	14,14,15	0.61	0	17,19,21	0.90	1 (5%)
4	NAG	I	1	1,4	14,14,15	1.02	1 (7%)	17,19,21	1.65	3 (17%)
4	NAG	I	2	4	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	J	1	1,4	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	J	2	4	14,14,15	0.50	0	17,19,21	0.73	1 (5%)
3	NAG	K	1	3,1	14,14,15	0.77	1 (7%)	17,19,21	0.60	0
3	NAG	K	2	3	14,14,15	0.40	0	17,19,21	1.43	2 (11%)
3	BMA	K	3	3	11,11,12	0.66	0	15,15,17	0.90	1 (6%)
4	NAG	L	1	1,4	14,14,15	0.27	0	17,19,21	0.55	0
4	NAG	L	2	4	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	M	1	5,1	14,14,15	1.36	1 (7%)	17,19,21	1.03	1 (5%)
5	NAG	M	2	5	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
5	FUC	M	3	5	10,10,11	0.94	0	14,14,16	1.23	2 (14%)
6	NAG	N	1	6,1	14,14,15	0.30	0	17,19,21	0.91	1 (5%)
6	NAG	N	2	6	14,14,15	0.23	0	17,19,21	0.47	0
6	BMA	N	3	6	11,11,12	0.51	0	15,15,17	0.75	0
6	FUC	N	4	6	10,10,11	0.45	0	14,14,16	0.82	1 (7%)
2	NAG	O	1	2,1	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	O	2	2	14,14,15	0.15	0	17,19,21	0.47	0
2	BMA	O	3	2	11,11,12	0.63	0	15,15,17	0.73	1 (6%)
2	MAN	O	4	2	11,11,12	0.71	1 (9%)	15,15,17	0.91	1 (6%)
2	MAN	O	5	2	11,11,12	0.62	0	15,15,17	0.96	1 (6%)
7	NAG	P	1	1,7	14,14,15	0.19	0	17,19,21	0.48	0
7	FUC	P	2	7	10,10,11	0.75	0	14,14,16	0.80	0
3	NAG	Q	1	3,1	14,14,15	0.50	0	17,19,21	0.40	0
3	NAG	Q	2	3	14,14,15	0.17	0	17,19,21	0.56	0
3	BMA	Q	3	3	11,11,12	0.61	0	15,15,17	0.80	0
4	NAG	R	1	1,4	14,14,15	0.36	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	R	2	4	14,14,15	0.26	0	17,19,21	0.42	0
7	NAG	S	1	1,7	14,14,15	0.65	1 (7%)	17,19,21	0.84	1 (5%)
7	FUC	S	2	7	10,10,11	0.56	0	14,14,16	0.76	0
3	NAG	T	1	3,1	14,14,15	1.44	1 (7%)	17,19,21	0.97	1 (5%)
3	NAG	T	2	3	14,14,15	0.28	0	17,19,21	0.50	0
3	BMA	T	3	3	11,11,12	0.50	0	15,15,17	0.85	0
4	NAG	U	1	1,4	14,14,15	0.28	0	17,19,21	1.40	1 (5%)
4	NAG	U	2	4	14,14,15	0.64	1 (7%)	17,19,21	0.97	1 (5%)
3	NAG	V	1	3,1	14,14,15	1.37	1 (7%)	17,19,21	1.50	2 (11%)
3	NAG	V	2	3	14,14,15	0.28	0	17,19,21	0.79	1 (5%)
3	BMA	V	3	3	11,11,12	0.69	0	15,15,17	0.68	0
4	NAG	W	1	1,4	14,14,15	0.58	0	17,19,21	0.75	0
4	NAG	W	2	4	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	X	1	3,1	14,14,15	0.39	0	17,19,21	0.81	0
3	NAG	X	2	3	14,14,15	0.33	0	17,19,21	0.40	0
3	BMA	X	3	3	11,11,12	0.83	0	15,15,17	0.93	1 (6%)
4	NAG	Y	1	1,4	14,14,15	0.72	1 (7%)	17,19,21	1.36	2 (11%)
4	NAG	Y	2	4	14,14,15	0.48	0	17,19,21	1.26	1 (5%)
5	NAG	Z	1	5,1	14,14,15	0.32	0	17,19,21	0.85	1 (5%)
5	NAG	Z	2	5	14,14,15	0.30	0	17,19,21	0.38	0
5	FUC	Z	3	5	10,10,11	0.49	0	14,14,16	0.87	0
6	NAG	a	1	6,1	14,14,15	0.63	0	17,19,21	0.67	0
6	NAG	a	2	6	14,14,15	0.23	0	17,19,21	0.49	0
6	BMA	a	3	6	11,11,12	0.50	0	15,15,17	0.68	0
6	FUC	a	4	6	10,10,11	0.51	0	14,14,16	0.70	0
2	NAG	b	1	2,1	14,14,15	0.18	0	17,19,21	0.38	0
2	NAG	b	2	2	14,14,15	0.21	0	17,19,21	0.48	0
2	BMA	b	3	2	11,11,12	0.64	0	15,15,17	0.92	0
2	MAN	b	4	2	11,11,12	0.82	1 (9%)	15,15,17	0.95	1 (6%)
2	MAN	b	5	2	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
7	NAG	c	1	1,7	14,14,15	0.30	0	17,19,21	0.34	0
7	FUC	c	2	7	10,10,11	0.64	0	14,14,16	0.90	0
3	NAG	d	1	3,1	14,14,15	0.42	0	17,19,21	0.41	0
3	NAG	d	2	3	14,14,15	0.18	0	17,19,21	0.50	0
3	BMA	d	3	3	11,11,12	0.56	0	15,15,17	0.91	0
4	NAG	e	1	1,4	14,14,15	0.40	0	17,19,21	0.58	0
4	NAG	e	2	4	14,14,15	0.20	0	17,19,21	0.45	0
7	NAG	f	1	1,7	14,14,15	0.16	0	17,19,21	0.52	0
7	FUC	f	2	7	10,10,11	0.76	0	14,14,16	0.69	0
3	NAG	g	1	3,1	14,14,15	0.30	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	g	2	3	14,14,15	0.19	0	17,19,21	0.38	0
3	BMA	g	3	3	11,11,12	0.50	0	15,15,17	0.80	0
3	NAG	h	1	3,1	14,14,15	0.77	1 (7%)	17,19,21	0.62	0
3	NAG	h	2	3	14,14,15	0.27	0	17,19,21	0.52	0
3	BMA	h	3	3	11,11,12	0.54	0	15,15,17	0.75	0
4	NAG	i	1	1,4	14,14,15	0.66	0	17,19,21	1.26	1 (5%)
4	NAG	i	2	4	14,14,15	0.22	0	17,19,21	0.38	0
3	NAG	j	1	3,1	14,14,15	0.56	0	17,19,21	1.29	1 (5%)
3	NAG	j	2	3	14,14,15	0.33	0	17,19,21	1.32	2 (11%)
3	BMA	j	3	3	11,11,12	1.31	2 (18%)	15,15,17	0.92	1 (6%)
6	NAG	k	1	6,1	14,14,15	0.68	1 (7%)	17,19,21	1.12	1 (5%)
6	NAG	k	2	6	14,14,15	0.30	0	17,19,21	0.50	0
6	BMA	k	3	6	11,11,12	0.58	0	15,15,17	0.64	0
6	FUC	k	4	6	10,10,11	0.59	0	14,14,16	0.84	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
2	NAG	D	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
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
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	6/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	6/6/23/26	0/1/1/1
5	FUC	M	3	5	-	-	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	FUC	N	4	6	-	-	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	0/2/19/22	0/1/1/1
2	MAN	O	5	2	-	2/2/19/22	0/1/1/1
7	NAG	P	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	P	2	7	-	-	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
7	NAG	S	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	S	2	7	-	-	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	BMA	T	3	3	-	2/2/19/22	0/1/1/1
4	NAG	U	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	U	2	4	-	4/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
4	NAG	W	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	BMA	X	3	3	-	2/2/19/22	0/1/1/1
4	NAG	Y	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	5/6/23/26	0/1/1/1
5	NAG	Z	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	4/6/23/26	0/1/1/1
5	FUC	Z	3	5	-	-	0/1/1/1
6	NAG	a	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	BMA	a	3	6	-	0/2/19/22	0/1/1/1
6	FUC	a	4	6	-	-	0/1/1/1
2	NAG	b	1	2,1	-	2/6/23/26	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	-	0/2/19/22	0/1/1/1
2	MAN	b	5	2	-	0/2/19/22	0/1/1/1
7	NAG	c	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	c	2	7	-	-	0/1/1/1
3	NAG	d	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	BMA	d	3	3	-	0/2/19/22	0/1/1/1
4	NAG	e	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
7	NAG	f	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	f	2	7	-	-	0/1/1/1
3	NAG	g	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	BMA	g	3	3	-	0/2/19/22	0/1/1/1
3	NAG	h	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	h	2	3	-	4/6/23/26	0/1/1/1
3	BMA	h	3	3	-	0/2/19/22	0/1/1/1
4	NAG	i	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	i	2	4	-	2/6/23/26	0/1/1/1

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1	NAG	O5-C1	-5.06	1.35	1.43
3	V	1	NAG	O5-C1	-5.01	1.35	1.43
5	M	1	NAG	O5-C1	-4.90	1.35	1.43
4	H	1	NAG	O5-C1	-4.73	1.35	1.43
4	I	1	NAG	C1-C2	3.55	1.57	1.52
3	j	3	BMA	C1-C2	3.24	1.59	1.52
3	G	1	NAG	O5-C1	-2.86	1.38	1.43
3	h	1	NAG	O5-C1	-2.83	1.38	1.43
3	K	1	NAG	O5-C1	-2.75	1.39	1.43
3	j	3	BMA	O5-C1	2.48	1.47	1.43
2	b	4	MAN	O5-C1	-2.41	1.39	1.43
6	k	1	NAG	O5-C1	2.20	1.47	1.43
4	Y	1	NAG	O5-C1	-2.15	1.40	1.43
2	O	4	MAN	O5-C1	-2.14	1.40	1.43
4	U	2	NAG	C1-C2	2.12	1.55	1.52
4	H	1	NAG	C1-C2	-2.11	1.49	1.52
7	S	1	NAG	C1-C2	2.06	1.55	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C2-N2-C7	4.70	129.20	122.90
4	U	1	NAG	C2-N2-C7	4.67	129.16	122.90
4	i	1	NAG	C1-O5-C5	4.58	118.32	112.19
3	j	2	NAG	C2-N2-C7	4.52	128.96	122.90
3	V	1	NAG	C2-N2-C7	4.49	128.92	122.90
3	j	1	NAG	C2-N2-C7	4.46	128.88	122.90
3	F	3	BMA	C1-O5-C5	4.44	118.13	112.19
3	K	2	NAG	C2-N2-C7	4.43	128.83	122.90
5	M	2	NAG	C2-N2-C7	4.42	128.83	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	2	NAG	C2-N2-C7	4.42	128.82	122.90
4	I	1	NAG	C2-N2-C7	4.35	128.73	122.90
4	Y	1	NAG	C2-N2-C7	4.35	128.73	122.90
4	I	1	NAG	C1-O5-C5	4.23	117.85	112.19
2	D	1	NAG	C2-N2-C7	4.19	128.51	122.90
6	k	1	NAG	C1-O5-C5	4.05	117.61	112.19
4	H	1	NAG	C3-C4-C5	3.90	117.30	110.23
4	H	2	NAG	C1-O5-C5	3.49	116.87	112.19
4	U	2	NAG	C1-O5-C5	3.46	116.83	112.19
2	D	3	BMA	C3-C4-C5	2.87	115.43	110.23
7	S	1	NAG	C1-O5-C5	2.82	115.97	112.19
5	M	3	FUC	O5-C5-C4	2.78	114.56	109.55
2	D	1	NAG	C1-C2-N2	2.74	114.75	110.43
3	T	1	NAG	C3-C4-C5	2.70	115.12	110.23
2	b	5	MAN	O2-C2-C3	-2.55	104.88	110.15
6	N	1	NAG	C1-O5-C5	2.51	115.56	112.19
2	b	4	MAN	O2-C2-C3	-2.41	105.16	110.15
5	M	3	FUC	C3-C4-C5	2.41	113.47	109.81
5	M	1	NAG	C1-O5-C5	2.39	115.39	112.19
3	V	1	NAG	C1-C2-N2	2.39	114.20	110.43
2	D	4	MAN	O2-C2-C3	-2.38	105.21	110.15
3	F	1	NAG	C1-C2-N2	2.35	114.14	110.43
3	j	3	BMA	O2-C2-C3	-2.34	105.30	110.15
3	G	3	BMA	O2-C2-C3	-2.34	105.31	110.15
5	Z	1	NAG	C1-O5-C5	2.31	115.29	112.19
4	J	2	NAG	C1-O5-C5	2.31	115.28	112.19
2	b	5	MAN	C1-O5-C5	2.30	115.27	112.19
2	O	4	MAN	O2-C2-C3	-2.29	105.40	110.15
3	V	2	NAG	C1-O5-C5	2.29	115.26	112.19
3	K	2	NAG	C1-O5-C5	2.27	115.23	112.19
2	D	5	MAN	C1-O5-C5	2.26	115.21	112.19
2	D	3	BMA	O2-C2-C3	-2.23	105.54	110.15
2	D	5	MAN	O2-C2-C3	-2.21	105.57	110.15
2	O	5	MAN	O2-C2-C3	-2.19	105.62	110.15
5	M	2	NAG	C1-C2-N2	2.17	113.85	110.43
3	K	3	BMA	C1-O5-C5	2.15	115.06	112.19
4	Y	1	NAG	C1-C2-N2	2.10	113.74	110.43
4	I	1	NAG	C1-C2-N2	2.09	113.72	110.43
3	j	2	NAG	C1-C2-N2	2.07	113.70	110.43
5	M	2	NAG	C1-O5-C5	2.04	114.93	112.19
6	N	4	FUC	C1-O5-C5	2.04	117.79	112.97
2	O	3	BMA	O2-C2-C3	-2.04	105.94	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	3	BMA	C2-C3-C4	2.00	114.38	110.86

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
2	O	5	MAN	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	b	1	NAG	O5-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
6	k	1	NAG	C4-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	M	2	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
2	O	5	MAN	C4-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
7	c	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
7	f	1	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
6	k	1	NAG	O5-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
6	a	1	NAG	C4-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	V	2	NAG	C8-C7-N2-C2
3	V	2	NAG	O7-C7-N2-C2
3	d	2	NAG	C8-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2
3	h	2	NAG	C8-C7-N2-C2
3	h	2	NAG	O7-C7-N2-C2
3	j	1	NAG	C8-C7-N2-C2
3	j	1	NAG	O7-C7-N2-C2
3	j	2	NAG	C8-C7-N2-C2
3	j	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	g	1	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	h	1	NAG	C3-C2-N2-C7
5	M	1	NAG	C3-C2-N2-C7
3	X	3	BMA	C4-C5-C6-O6
3	X	3	BMA	O5-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
3	T	3	BMA	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7
3	j	1	NAG	C1-C2-N2-C7
4	U	1	NAG	C1-C2-N2-C7
4	W	1	NAG	C1-C2-N2-C7
6	N	1	NAG	C1-C2-N2-C7
6	k	1	NAG	C1-C2-N2-C7
7	P	1	NAG	O5-C5-C6-O6
3	T	3	BMA	O5-C5-C6-O6
2	D	5	MAN	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C3-C2-N2-C7
3	V	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	X	1	NAG	C3-C2-N2-C7
3	j	1	NAG	C3-C2-N2-C7
4	J	2	NAG	C3-C2-N2-C7
4	L	1	NAG	C3-C2-N2-C7
4	U	2	NAG	C3-C2-N2-C7
4	W	1	NAG	C3-C2-N2-C7
4	Y	1	NAG	C3-C2-N2-C7
4	i	1	NAG	C3-C2-N2-C7
5	Z	1	NAG	C3-C2-N2-C7
6	a	1	NAG	C3-C2-N2-C7
6	k	1	NAG	C3-C2-N2-C7
3	Q	3	BMA	C4-C5-C6-O6
3	g	1	NAG	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	K	2	NAG	C1-C2-N2-C7
3	V	1	NAG	C1-C2-N2-C7
3	X	1	NAG	C1-C2-N2-C7
3	g	2	NAG	C1-C2-N2-C7
3	j	2	NAG	C1-C2-N2-C7
4	I	1	NAG	C1-C2-N2-C7
4	L	1	NAG	C1-C2-N2-C7
4	R	1	NAG	C1-C2-N2-C7
4	U	2	NAG	C1-C2-N2-C7
4	Y	1	NAG	C1-C2-N2-C7
4	Y	2	NAG	C1-C2-N2-C7
5	M	2	NAG	C1-C2-N2-C7
5	Z	1	NAG	C1-C2-N2-C7
6	a	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7
3	K	2	NAG	C3-C2-N2-C7
3	j	2	NAG	C3-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7
4	U	1	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
5	M	2	NAG	C3-C2-N2-C7
6	N	1	NAG	C3-C2-N2-C7
5	M	1	NAG	C4-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6

There are no ring outliers.

56 monomers are involved in 94 short contacts:

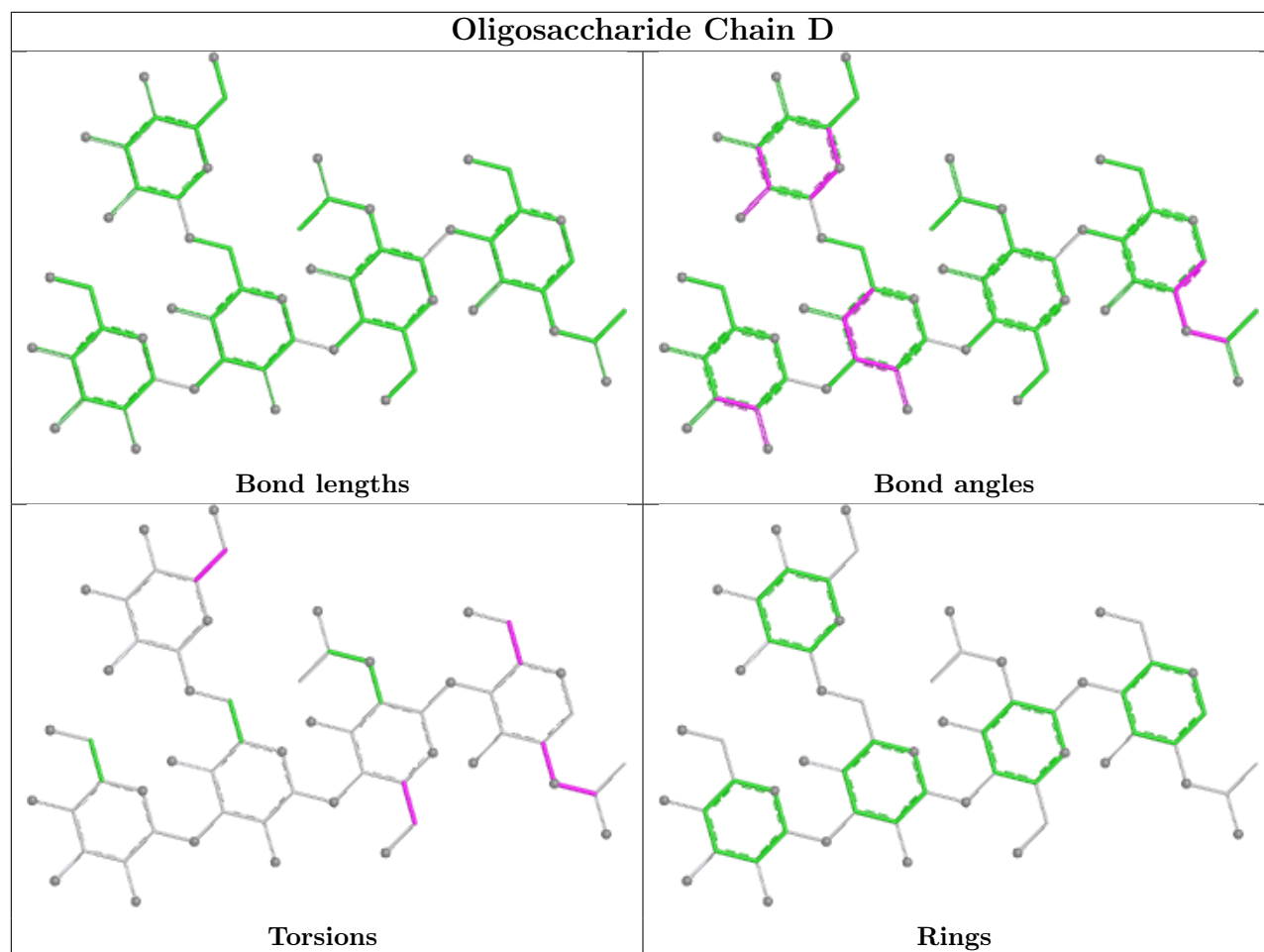
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
6	N	1	NAG	2	0
3	j	2	NAG	1	0
3	E	2	NAG	3	0
7	P	1	NAG	1	0
3	T	1	NAG	2	0
5	Z	2	NAG	1	0
3	h	2	NAG	1	0
3	h	1	NAG	3	0
3	G	2	NAG	1	0
6	k	1	NAG	5	0
3	F	1	NAG	3	0
4	R	1	NAG	1	0
4	e	1	NAG	1	0
7	f	1	NAG	1	0
3	K	1	NAG	1	0
3	V	1	NAG	5	0
7	S	1	NAG	6	0
3	G	1	NAG	2	0
4	J	2	NAG	1	0
2	D	2	NAG	1	0
6	k	4	FUC	2	0
6	N	4	FUC	1	0
3	Q	3	BMA	1	0
7	P	2	FUC	3	0
4	Y	2	NAG	1	0
6	a	2	NAG	1	0
3	g	2	NAG	1	0
4	Y	1	NAG	2	0
5	Z	3	FUC	1	0
4	U	2	NAG	3	0
7	c	1	NAG	1	0
4	i	1	NAG	1	0
4	U	1	NAG	4	0
4	I	1	NAG	2	0
3	G	3	BMA	1	0
3	T	2	NAG	2	0
2	b	1	NAG	2	0
3	K	2	NAG	1	0
3	V	2	NAG	4	0

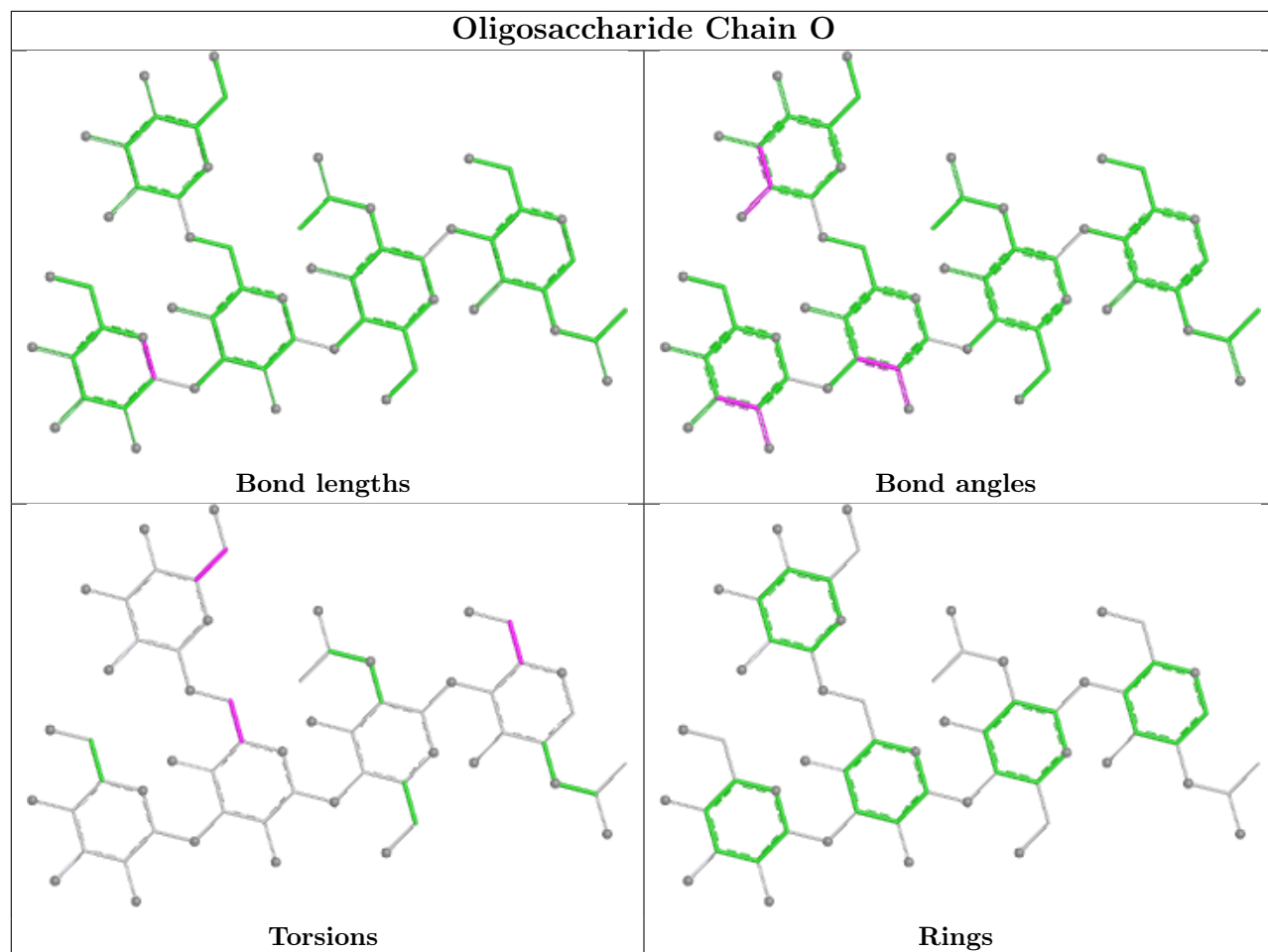
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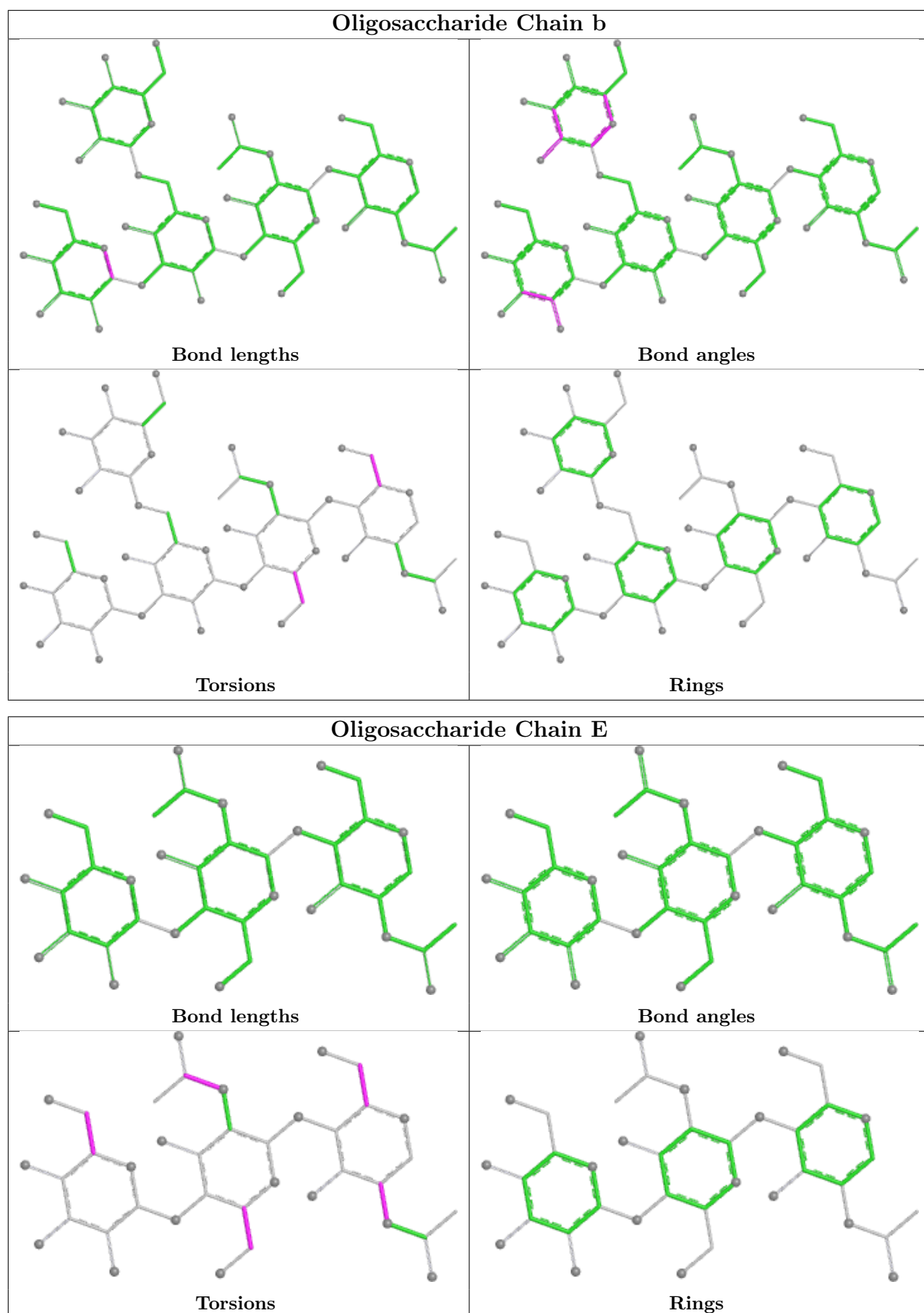
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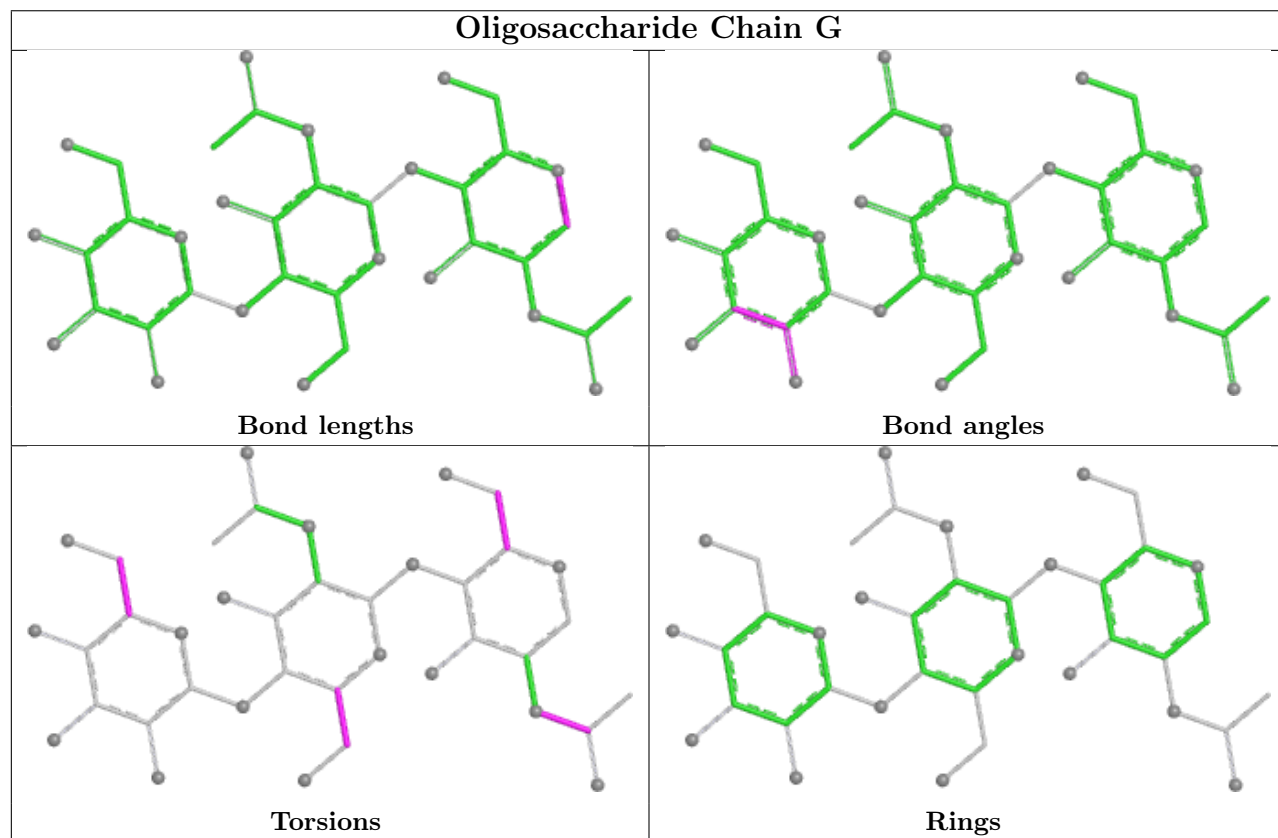
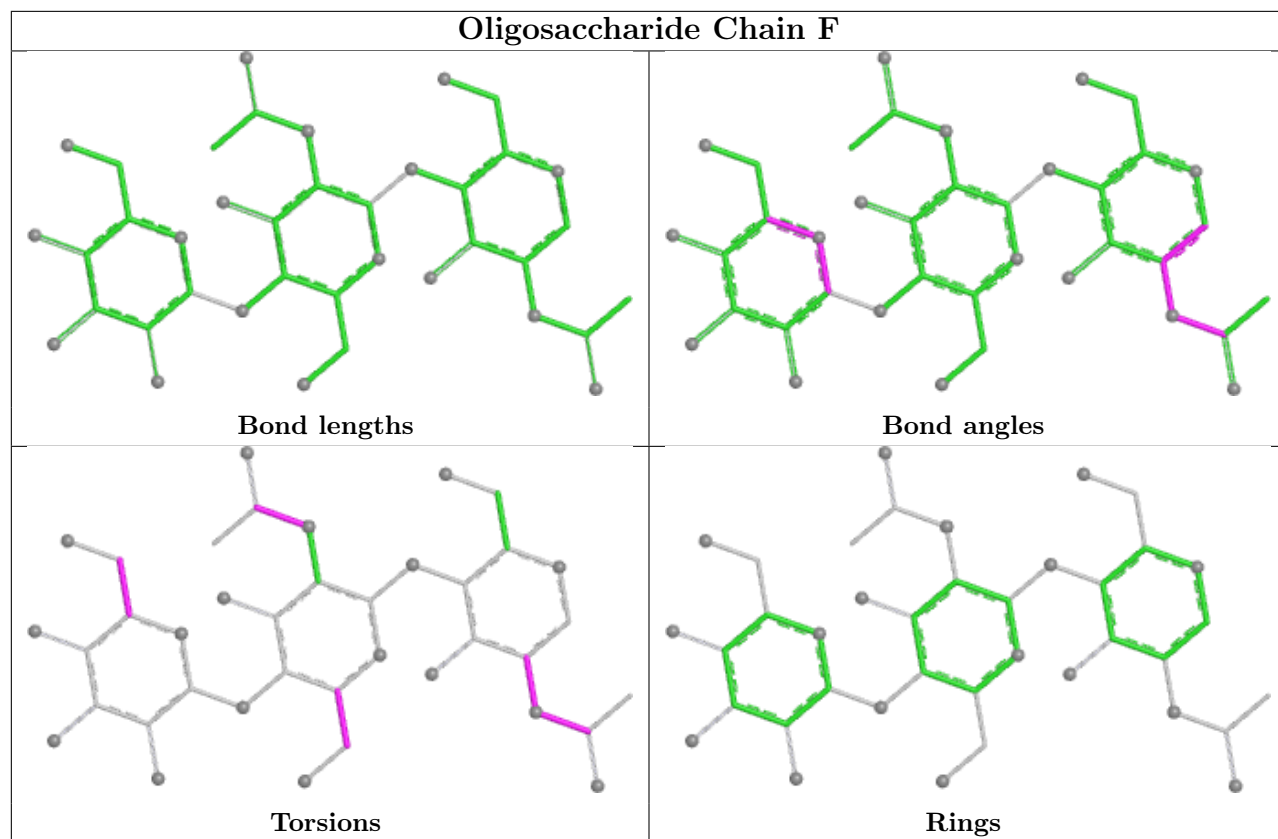
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	a	1	NAG	5	0
3	d	1	NAG	2	0
5	M	2	NAG	1	0
6	a	4	FUC	2	0
2	D	3	BMA	1	0
3	j	1	NAG	1	0
3	g	1	NAG	2	0
5	M	3	FUC	3	0
3	X	1	NAG	1	0
4	J	1	NAG	4	0
5	Z	1	NAG	2	0
2	D	5	MAN	1	0
2	O	1	NAG	1	0
4	L	1	NAG	2	0
3	E	1	NAG	6	0
3	V	3	BMA	1	0

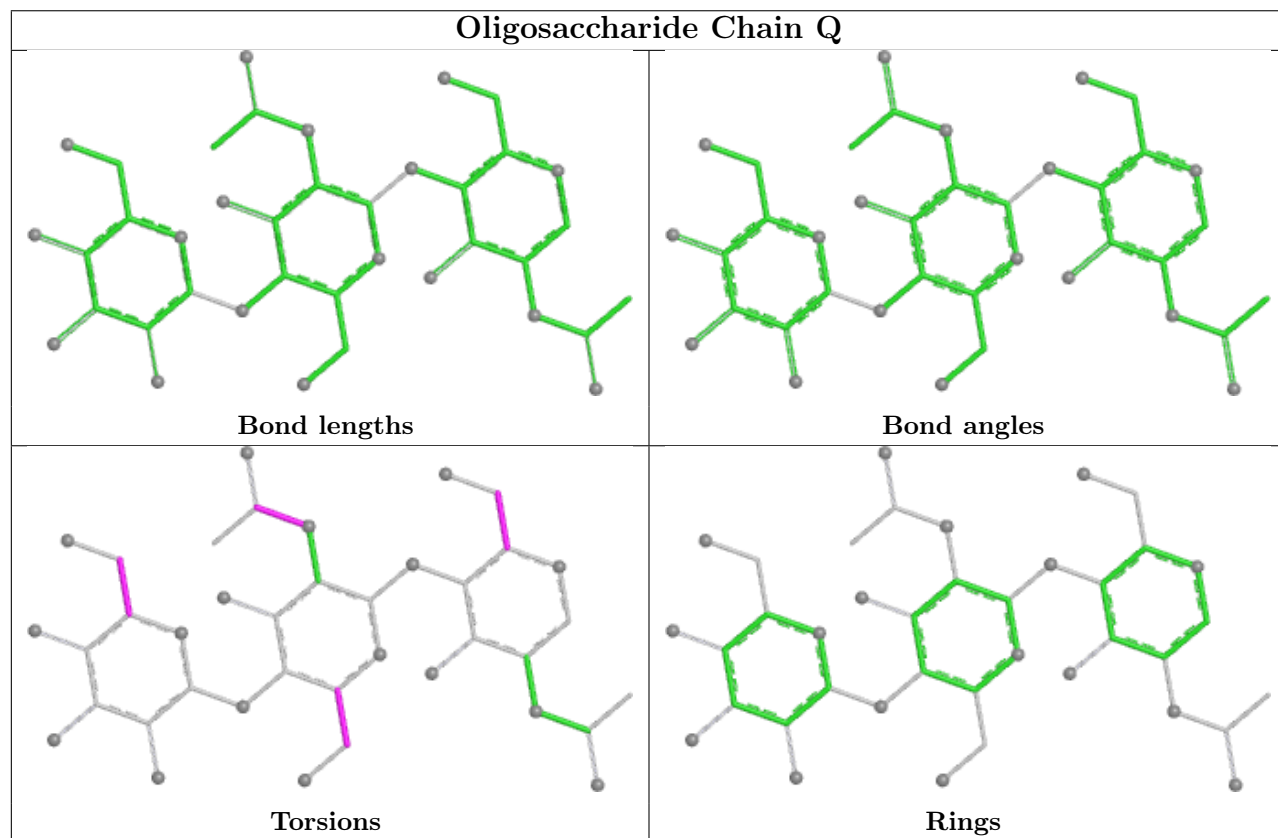
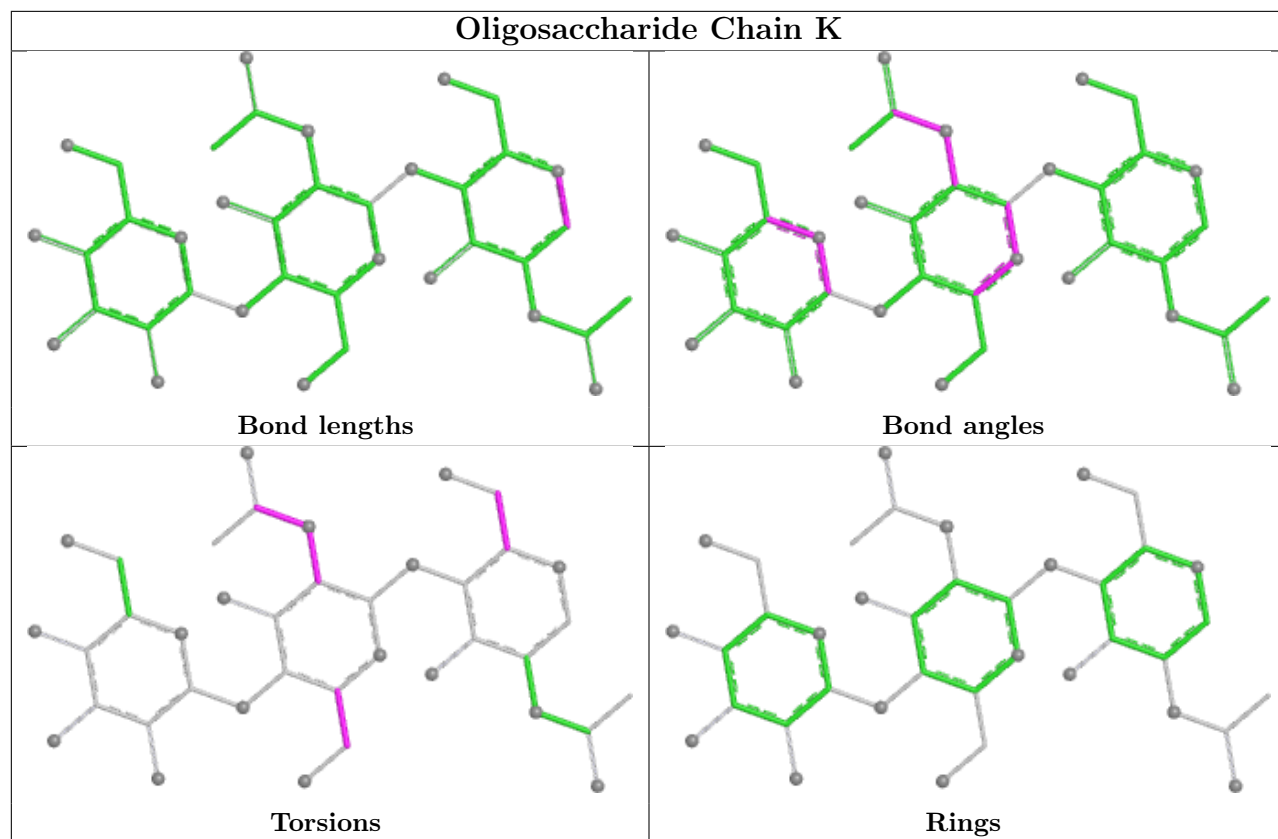
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

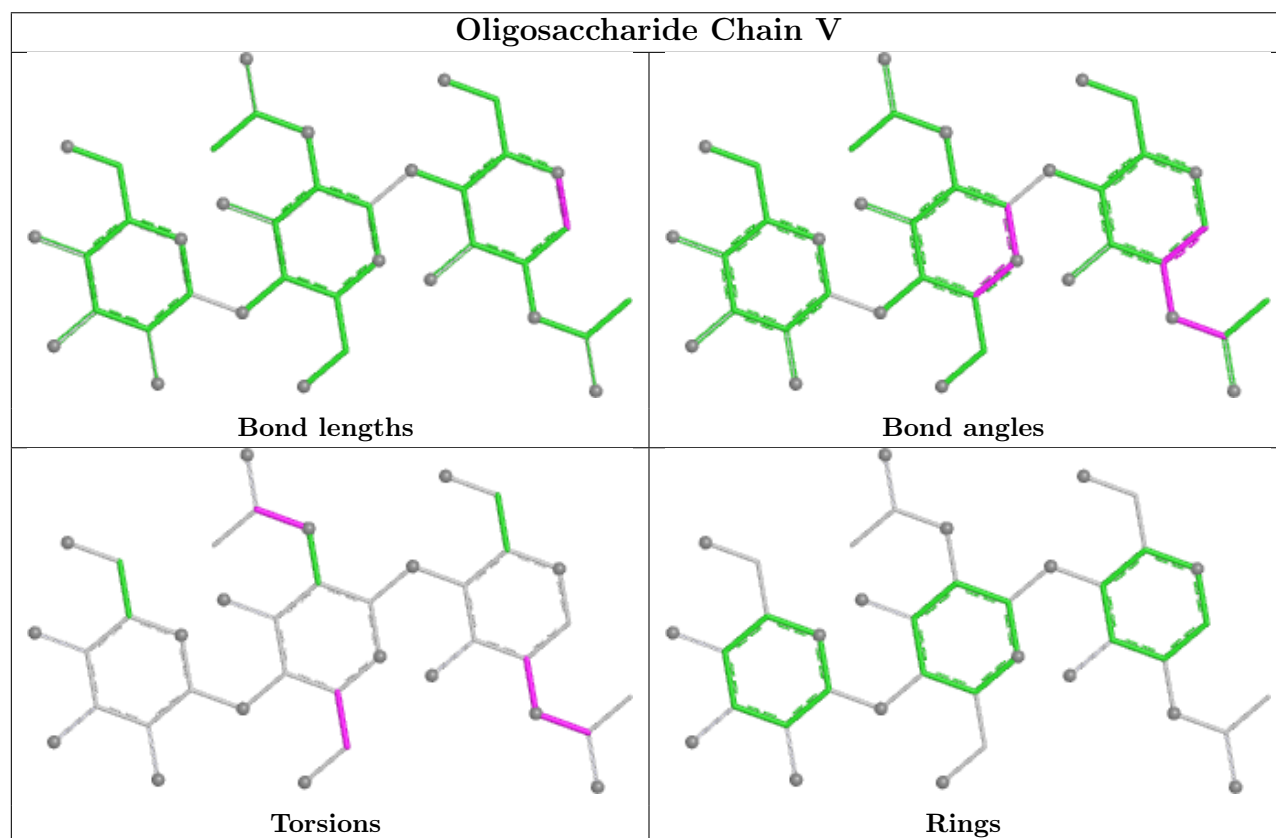
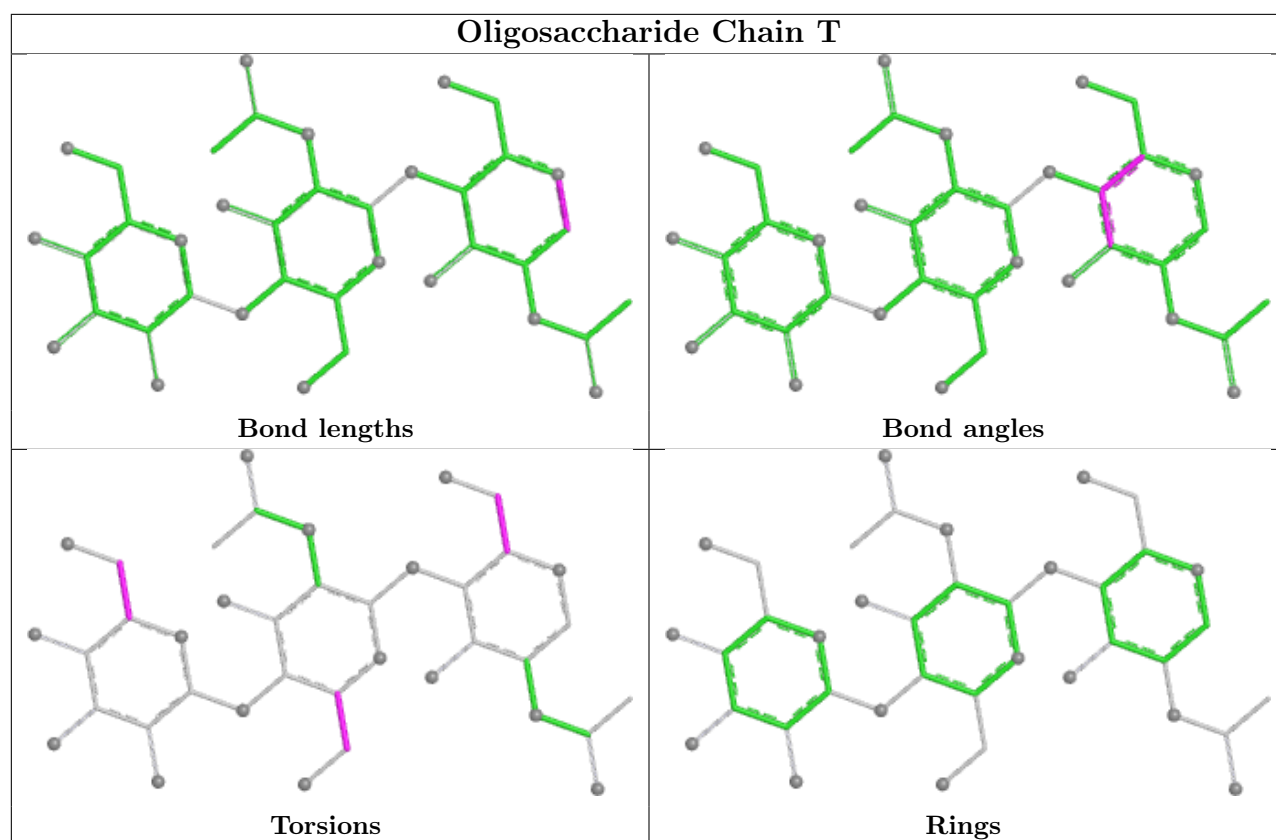


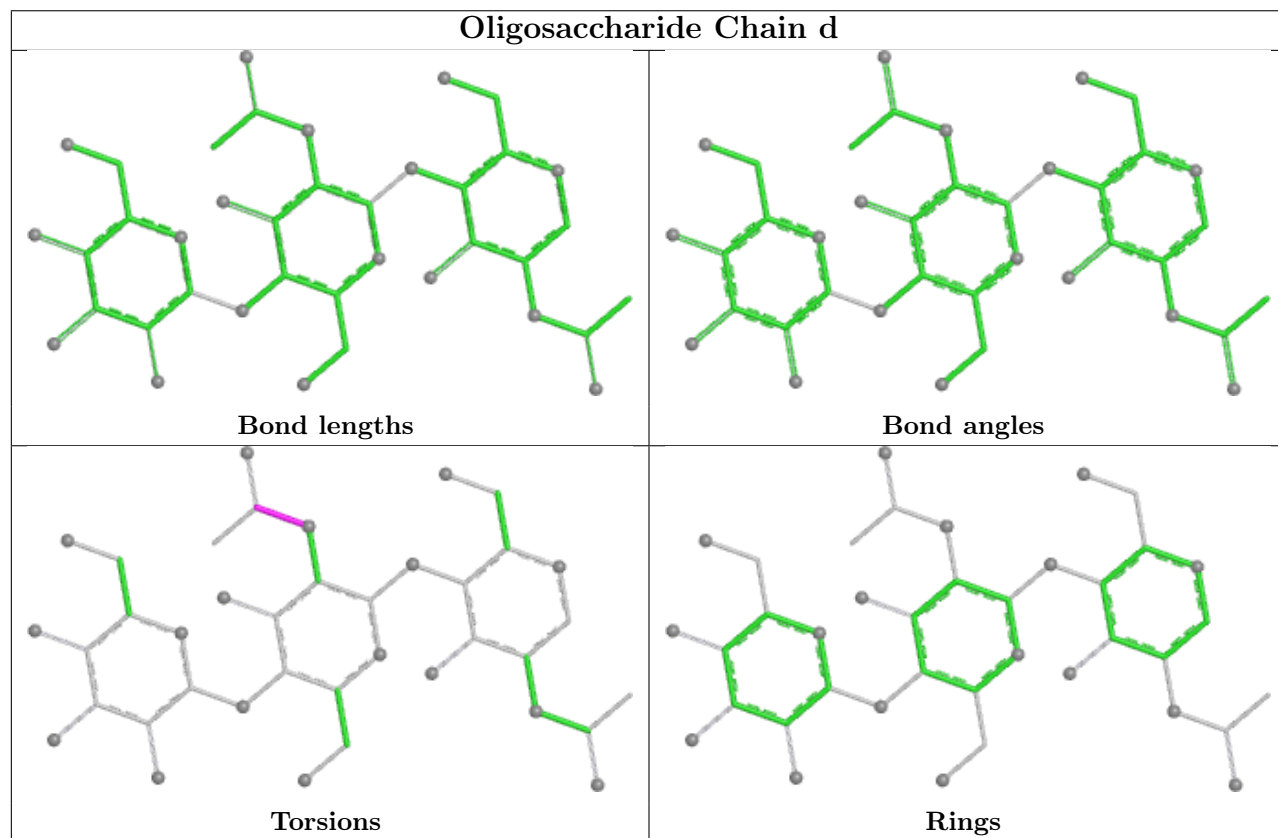
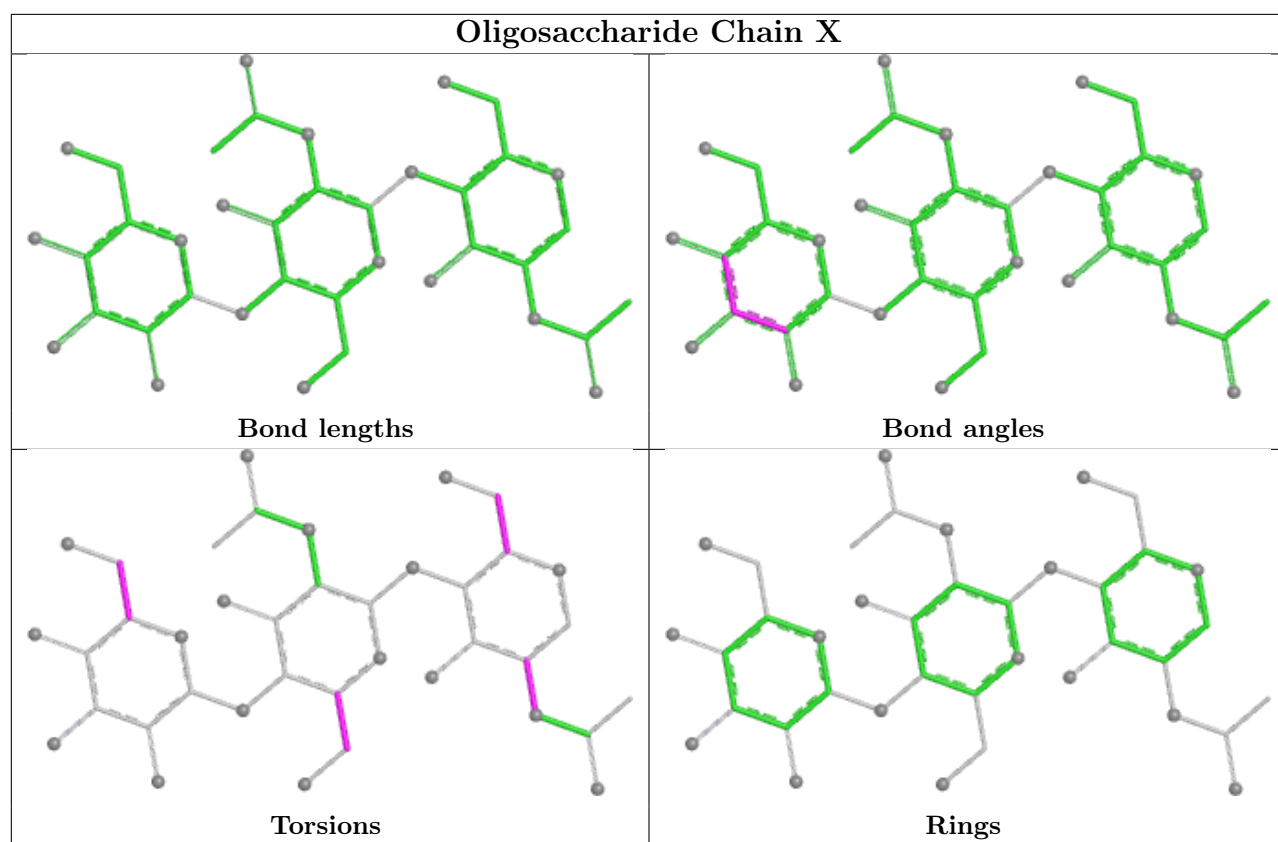


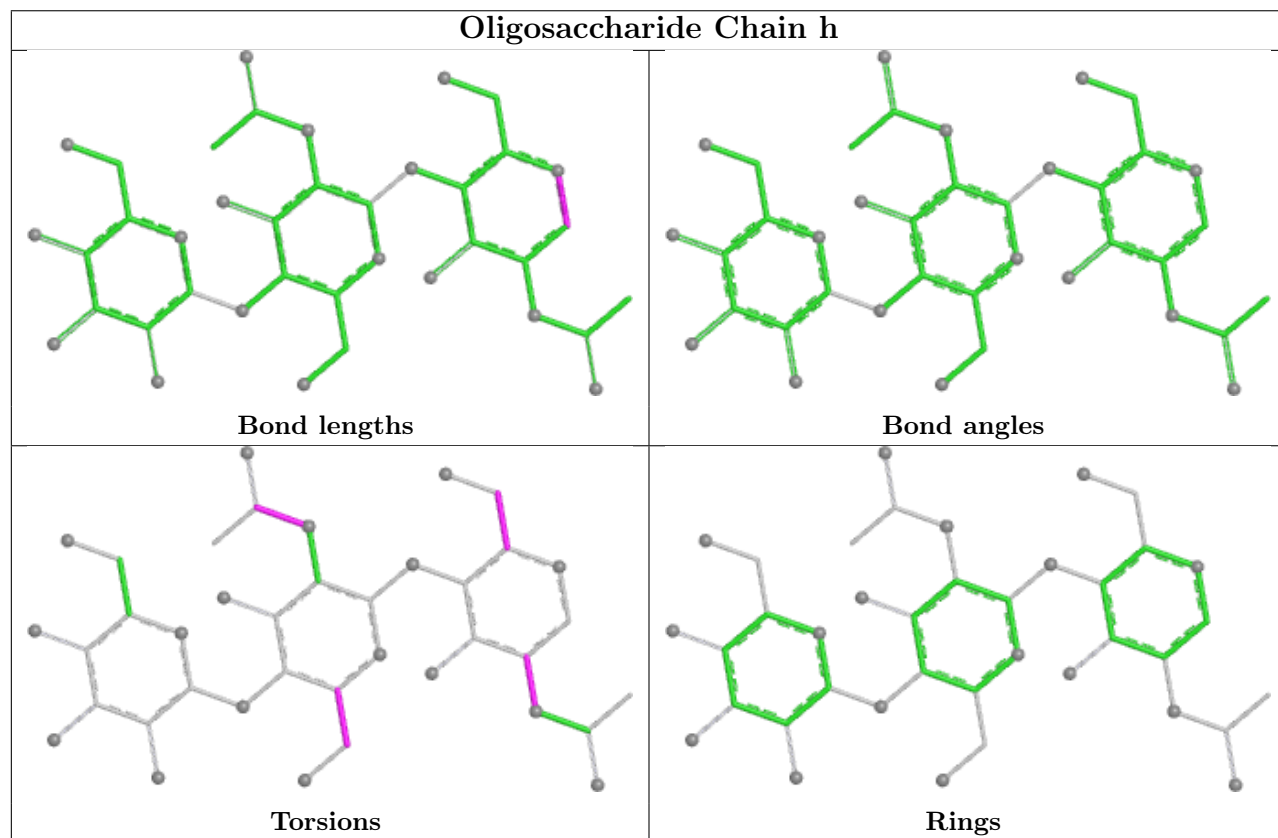
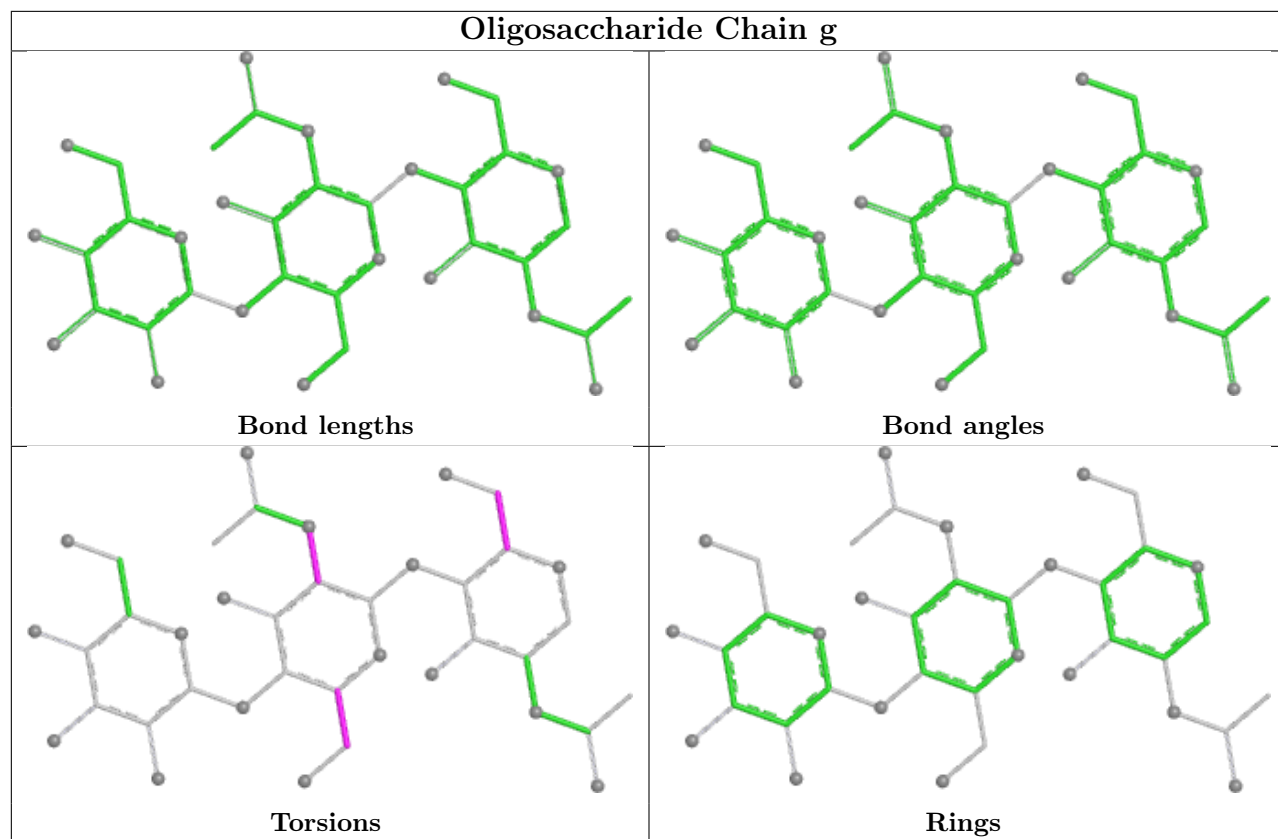


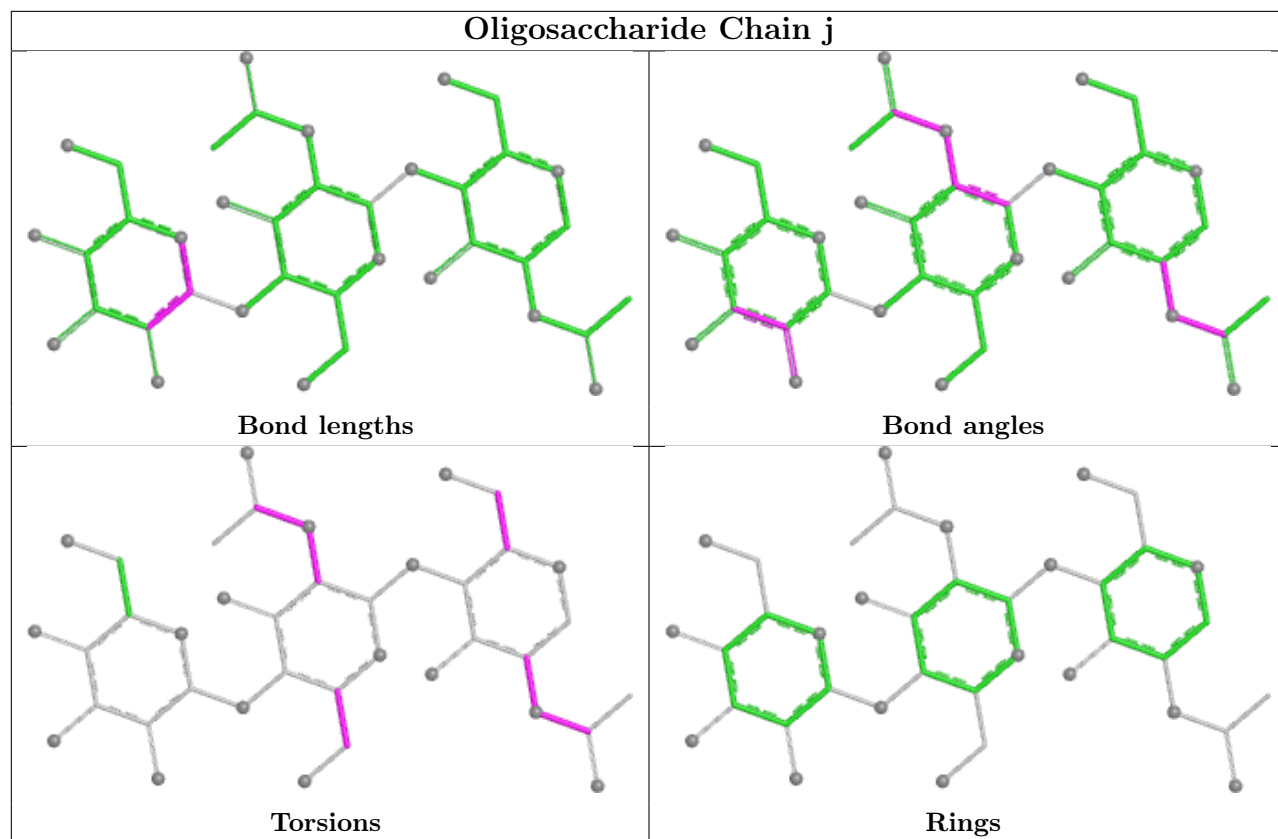


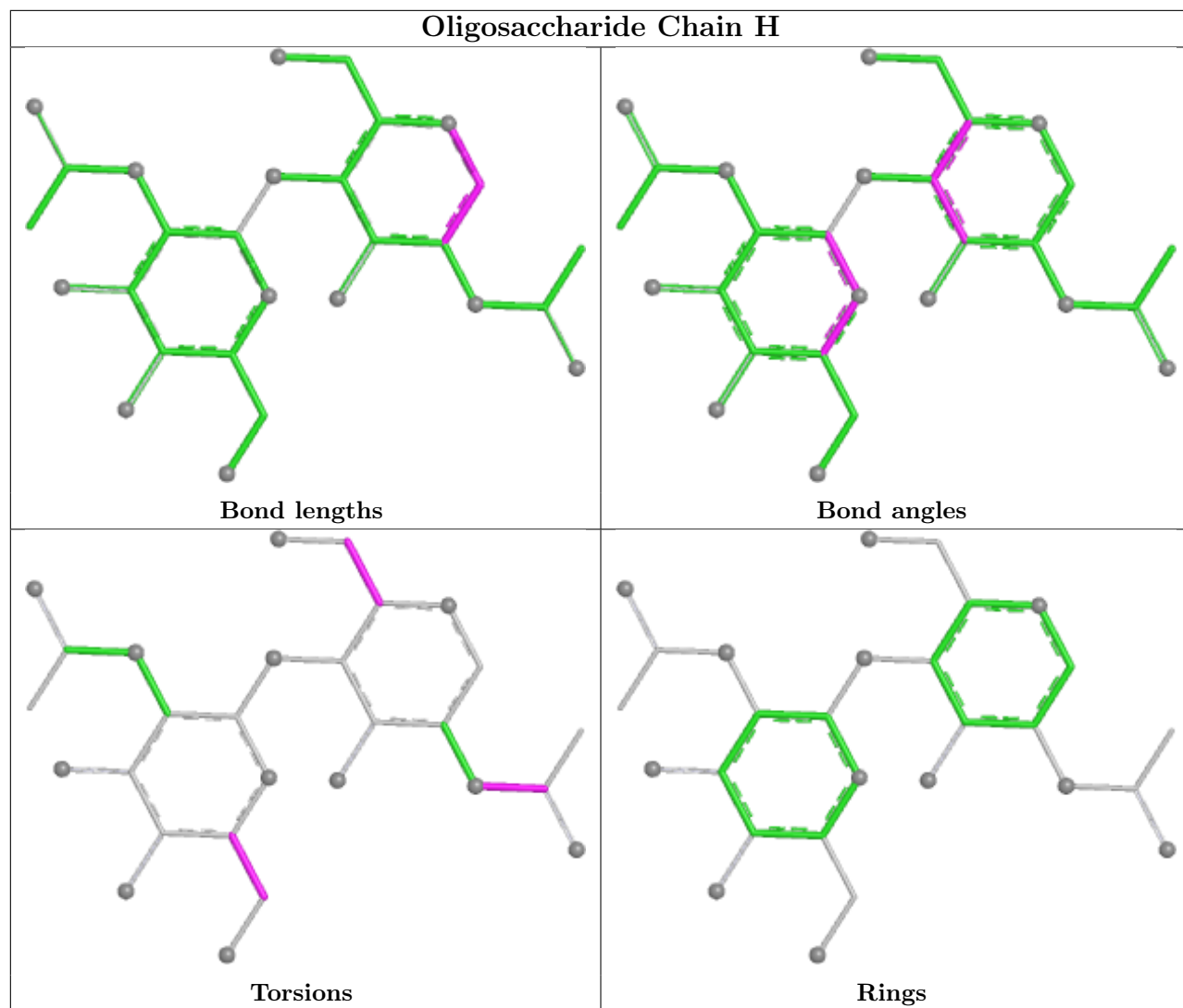


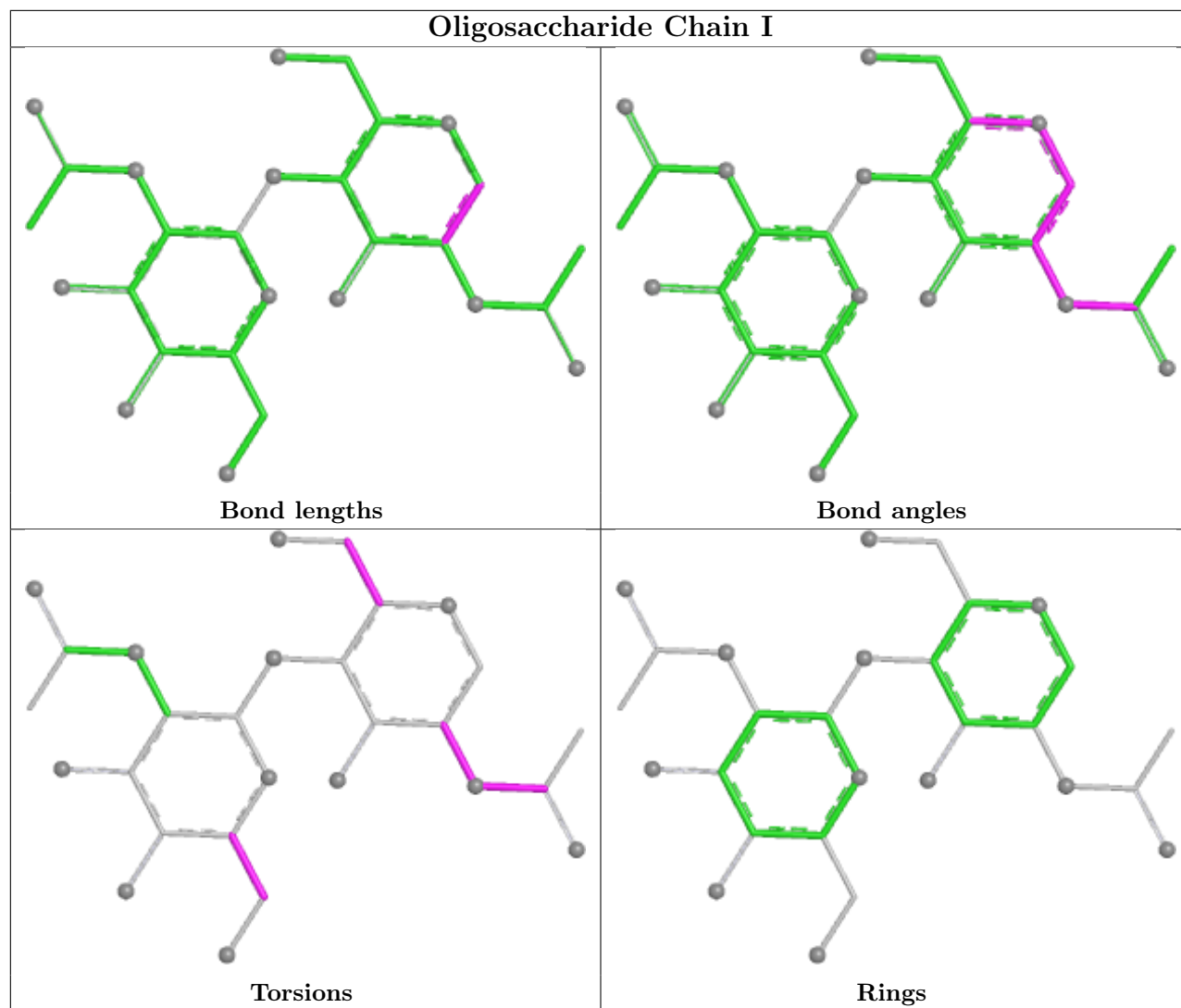


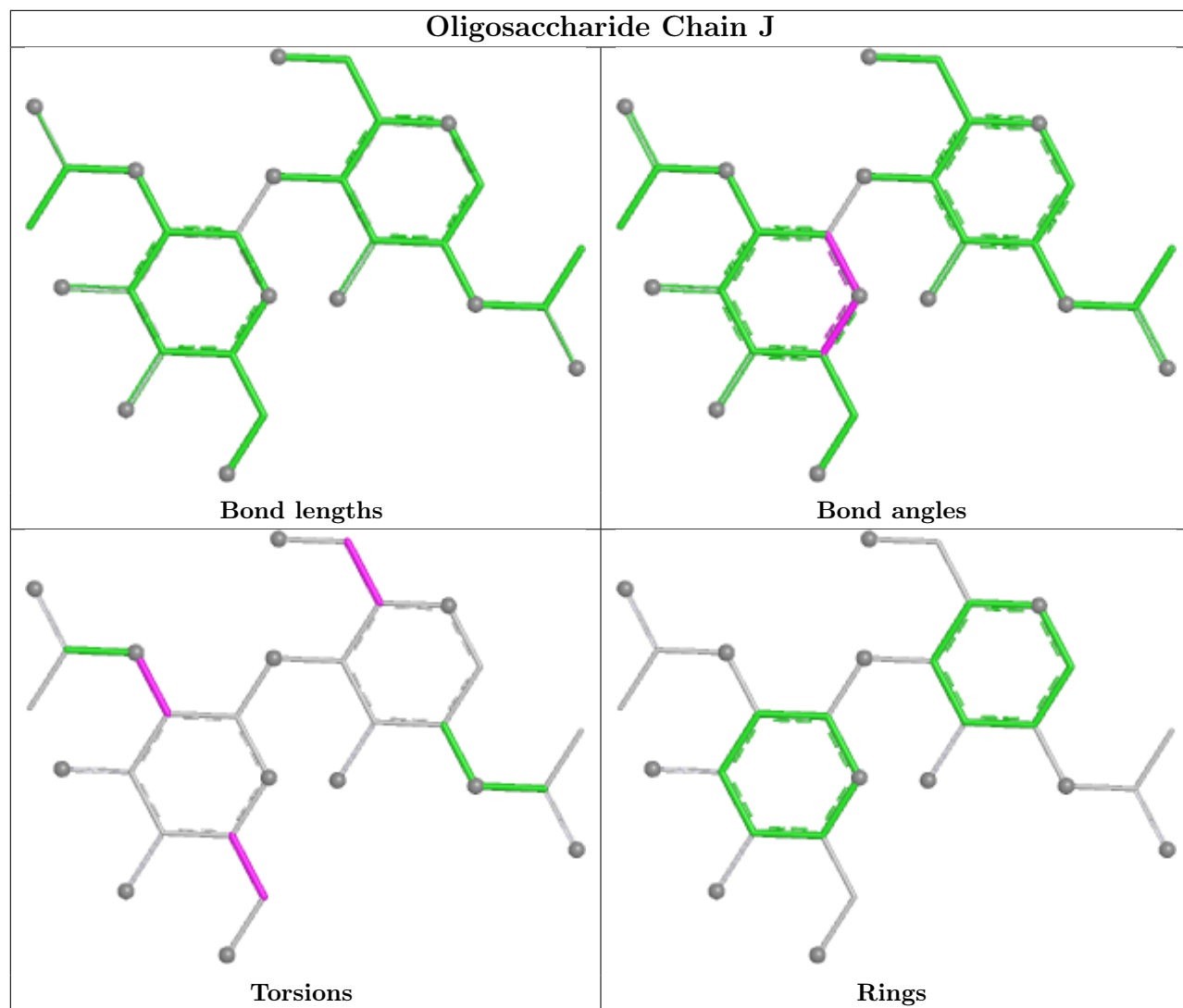


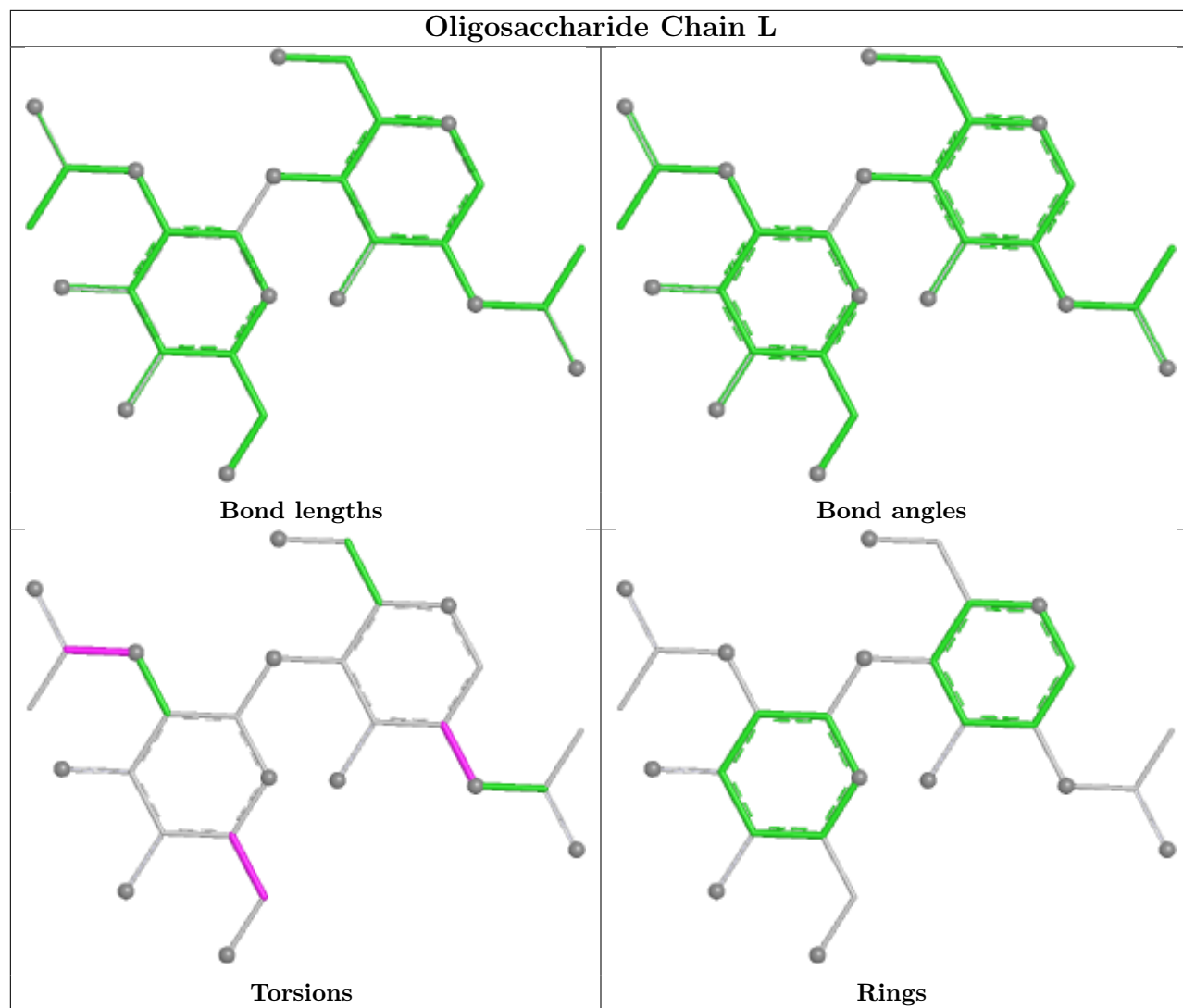


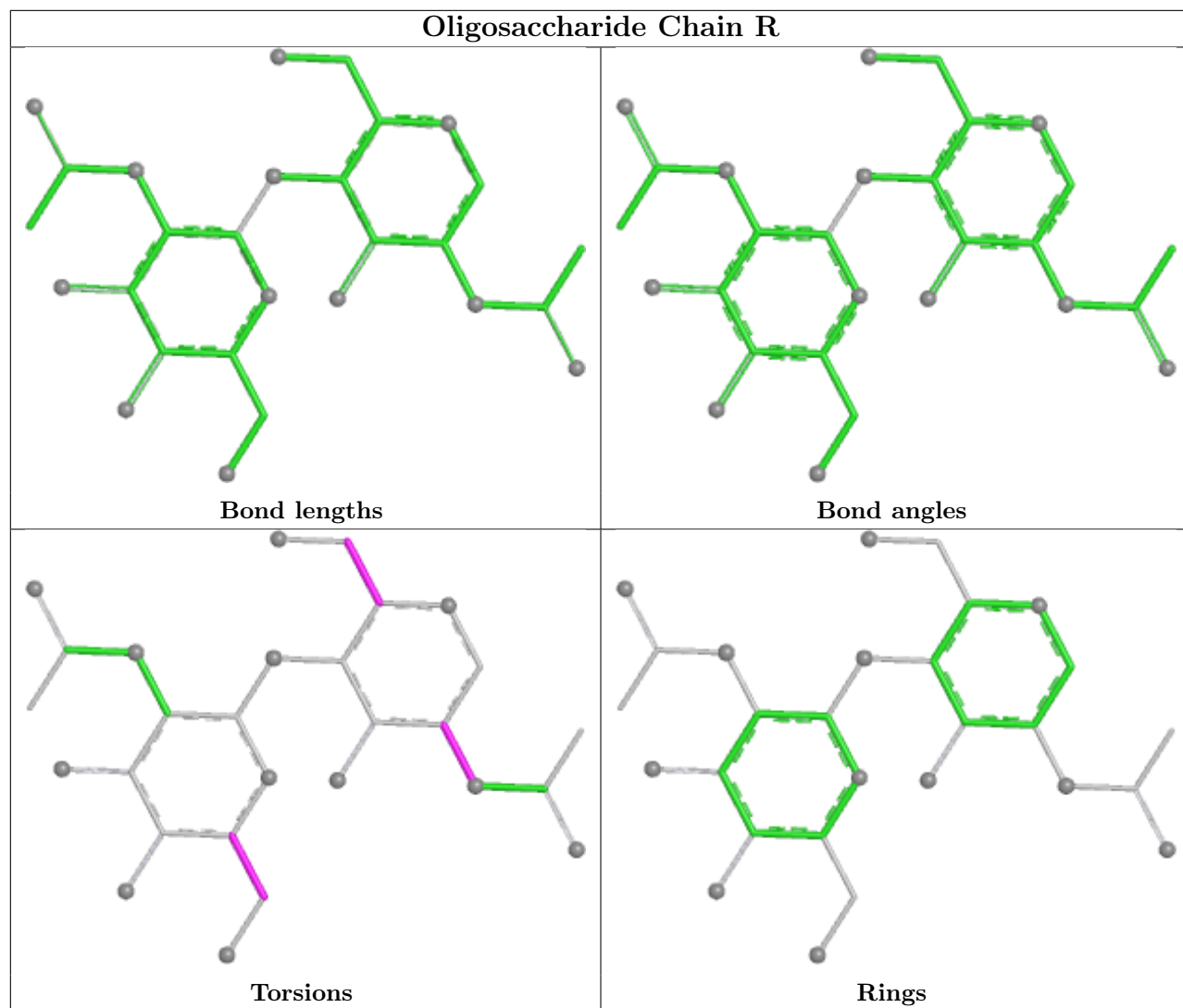


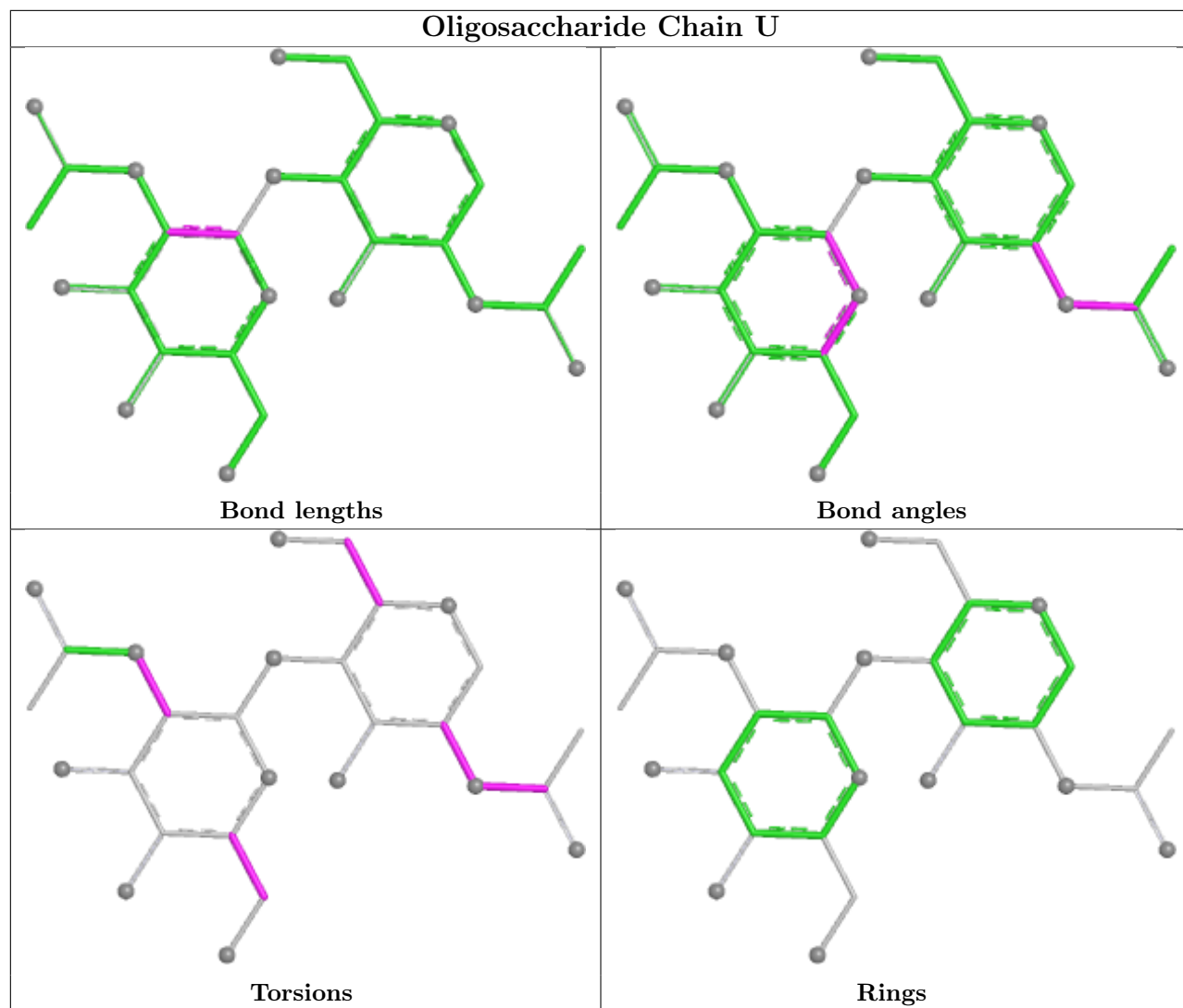


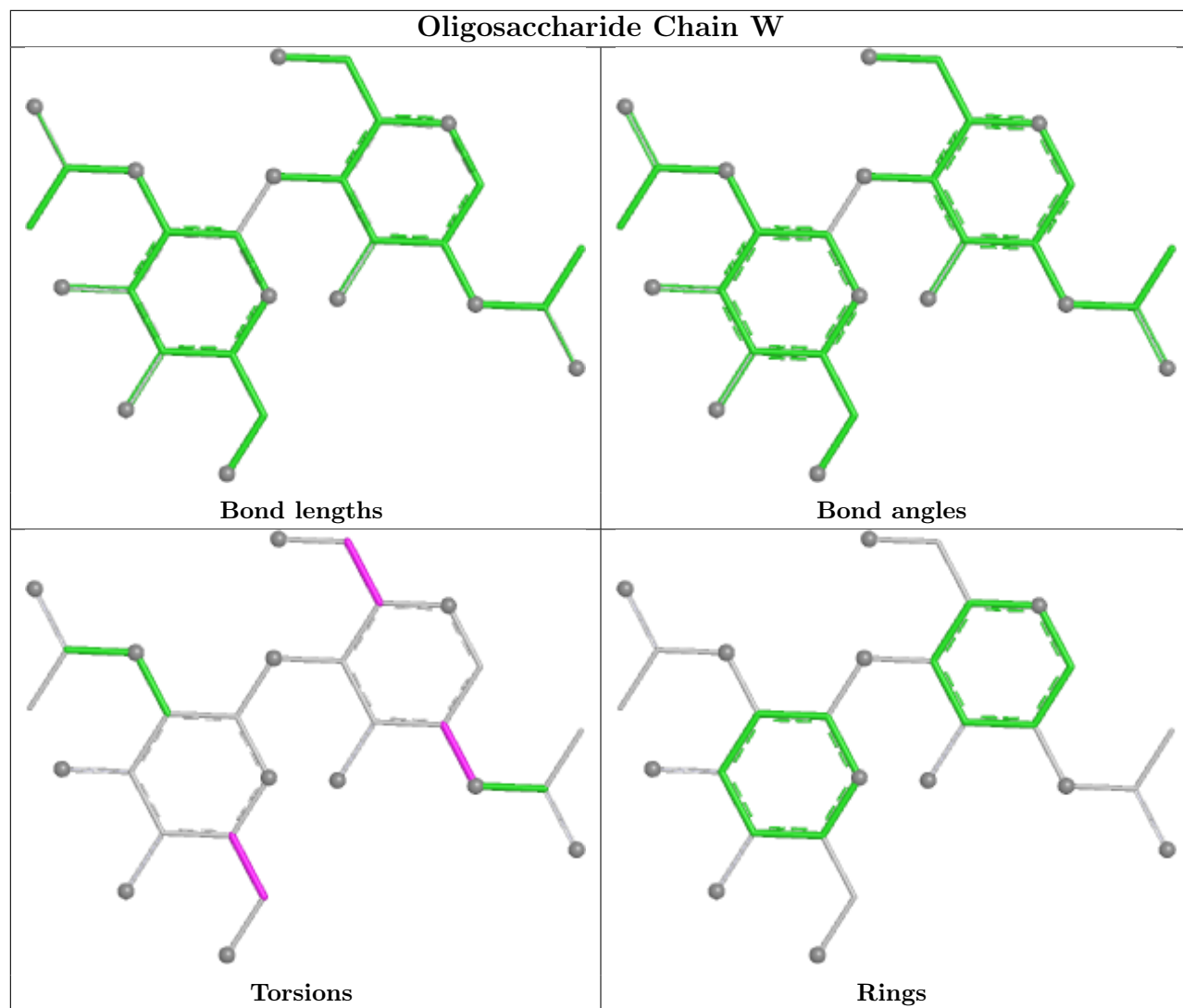


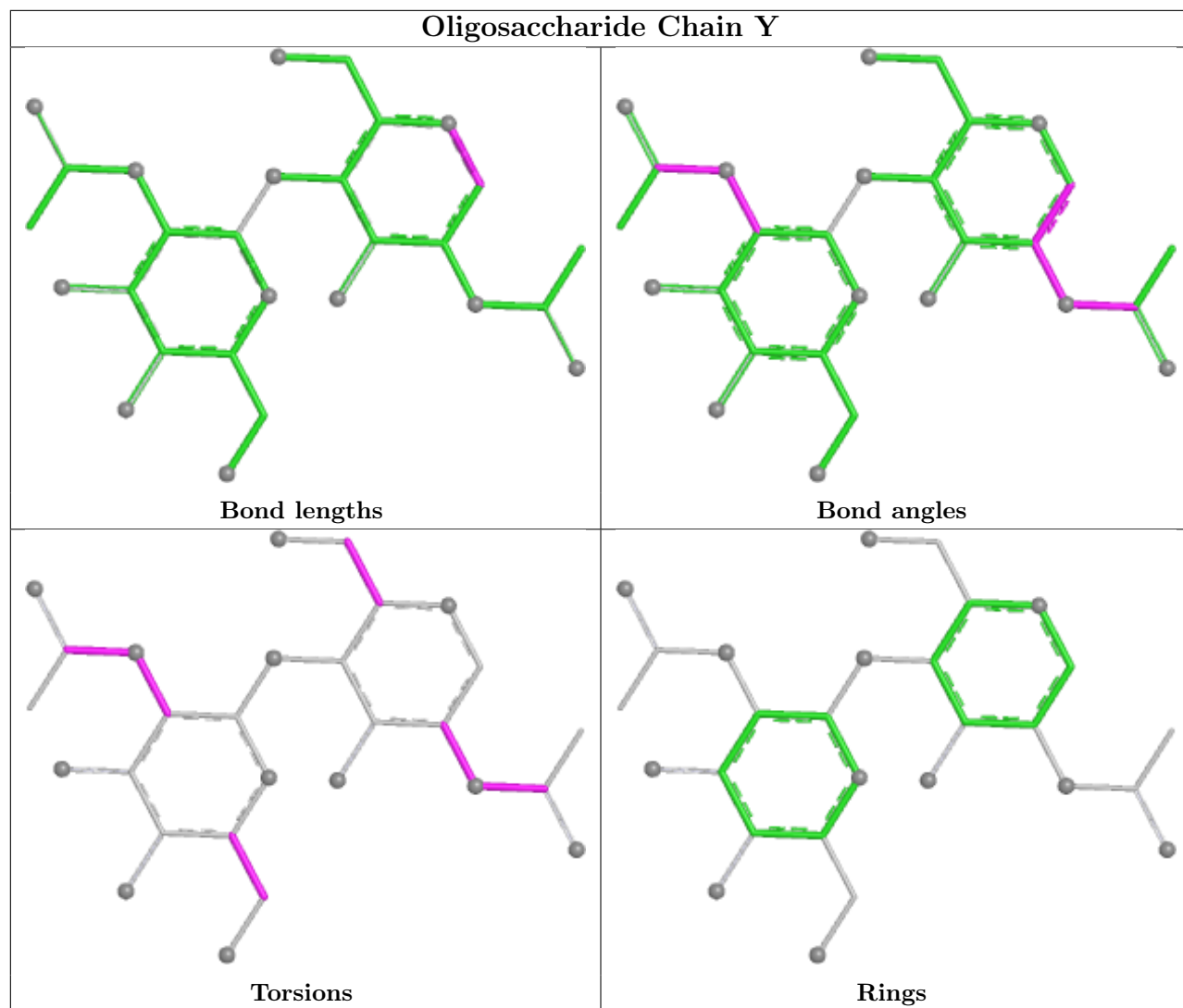


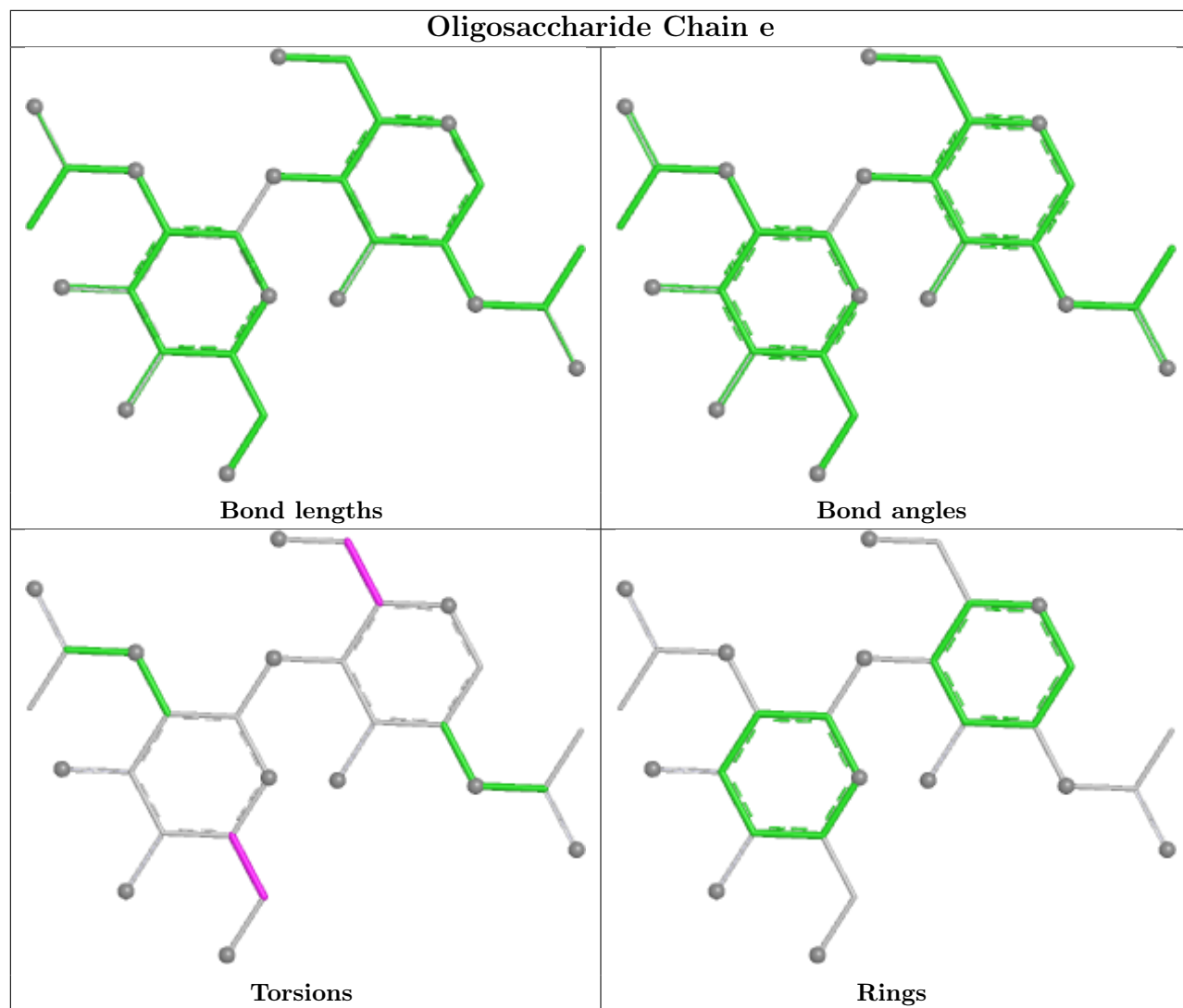


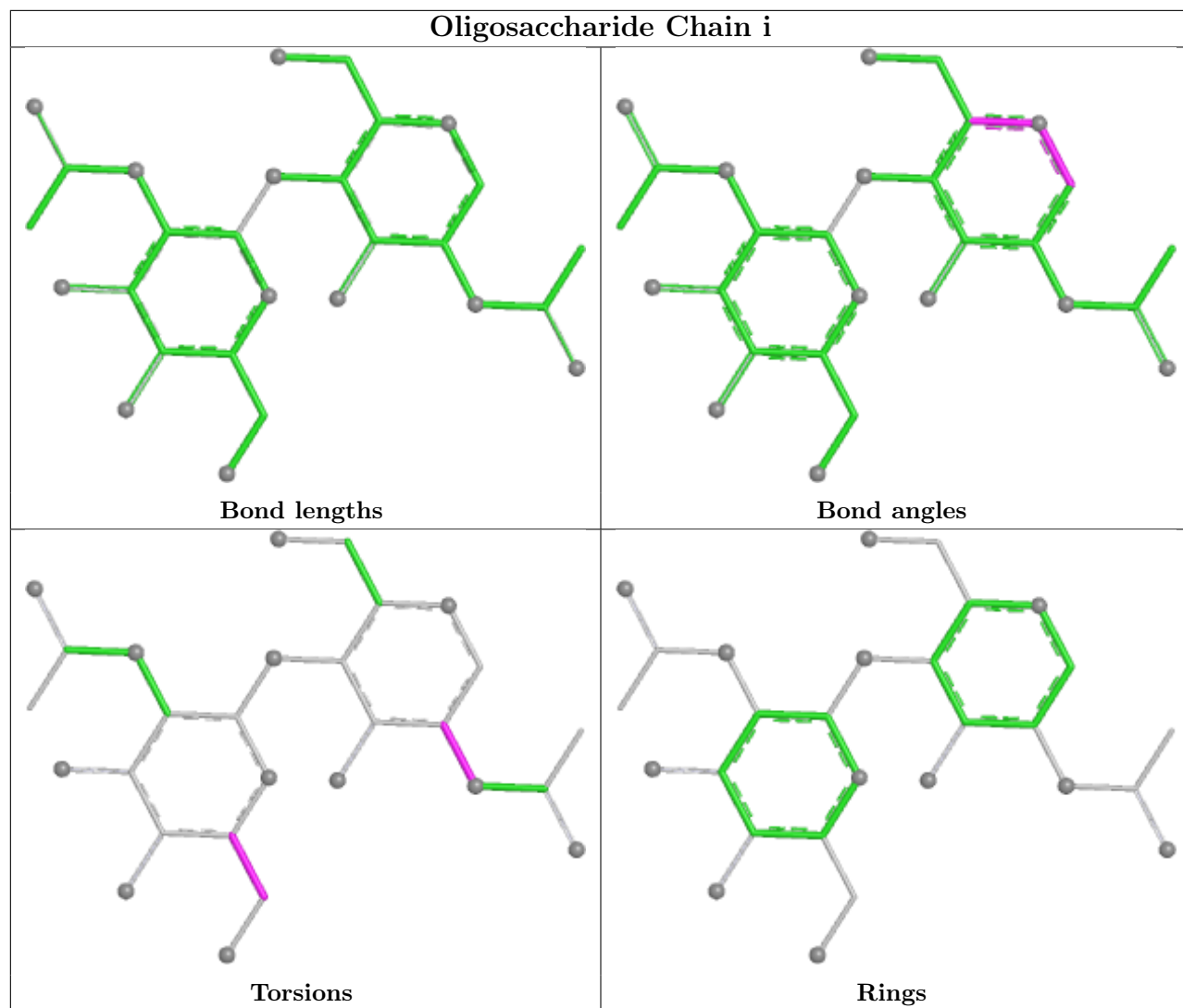


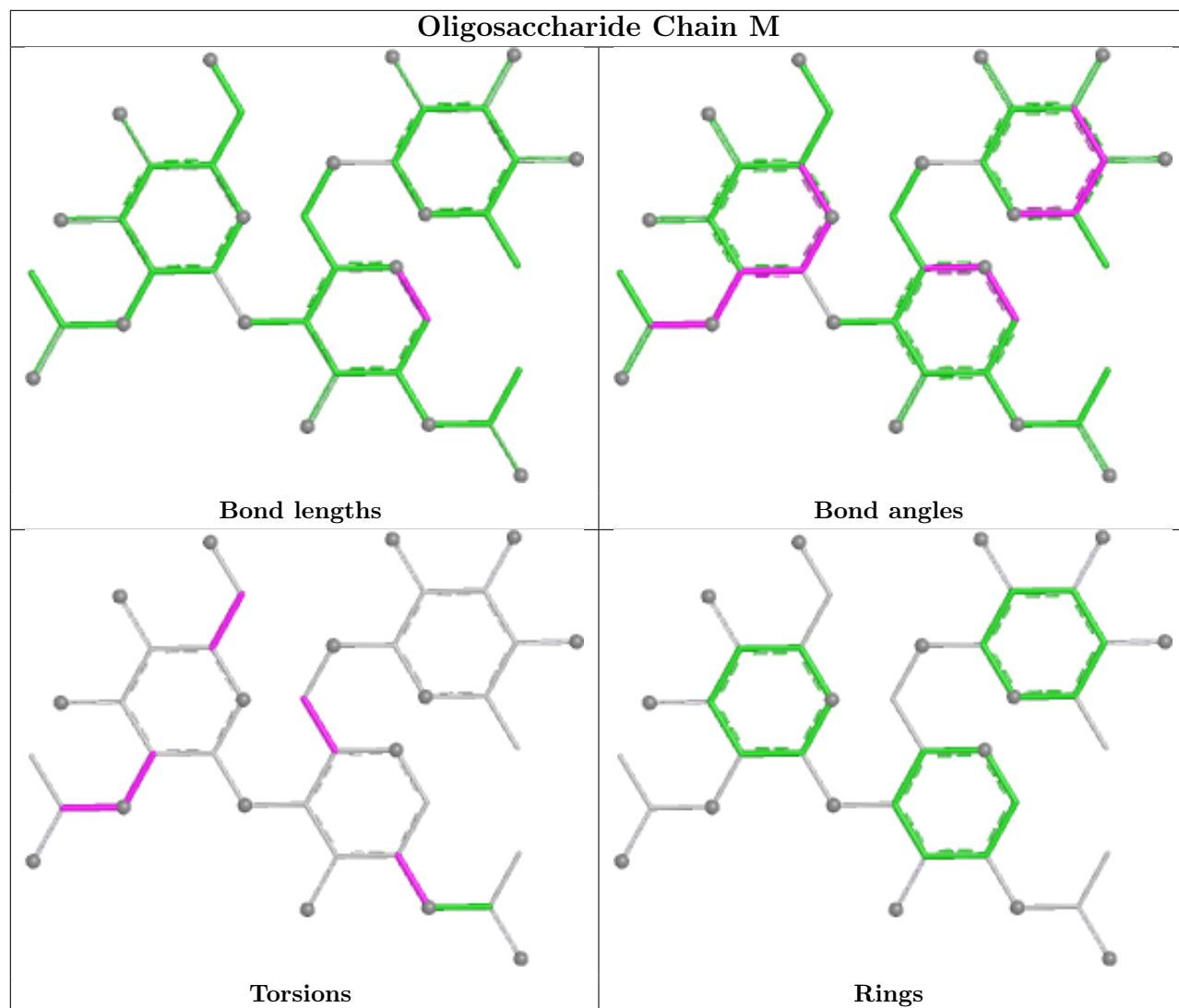


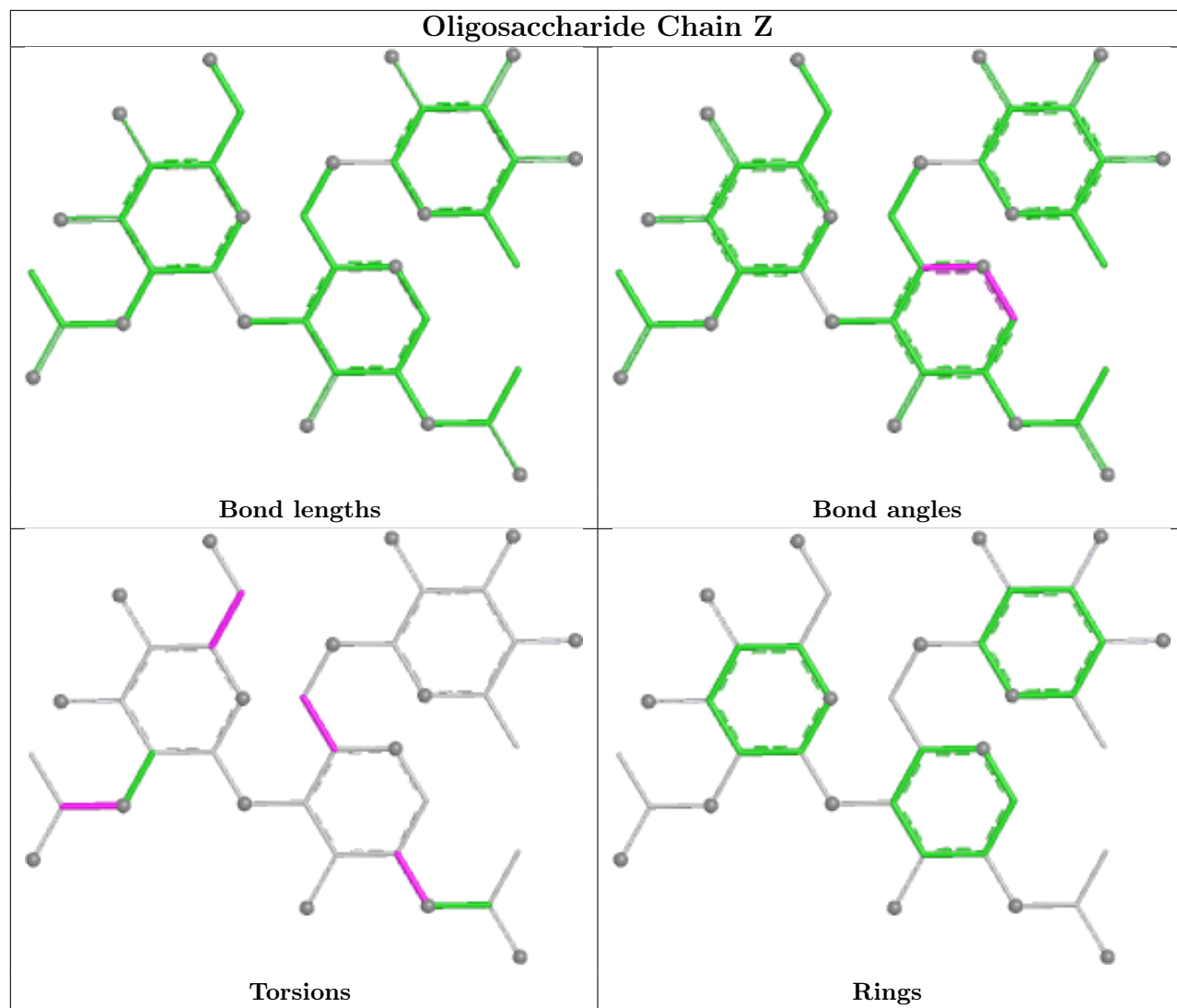


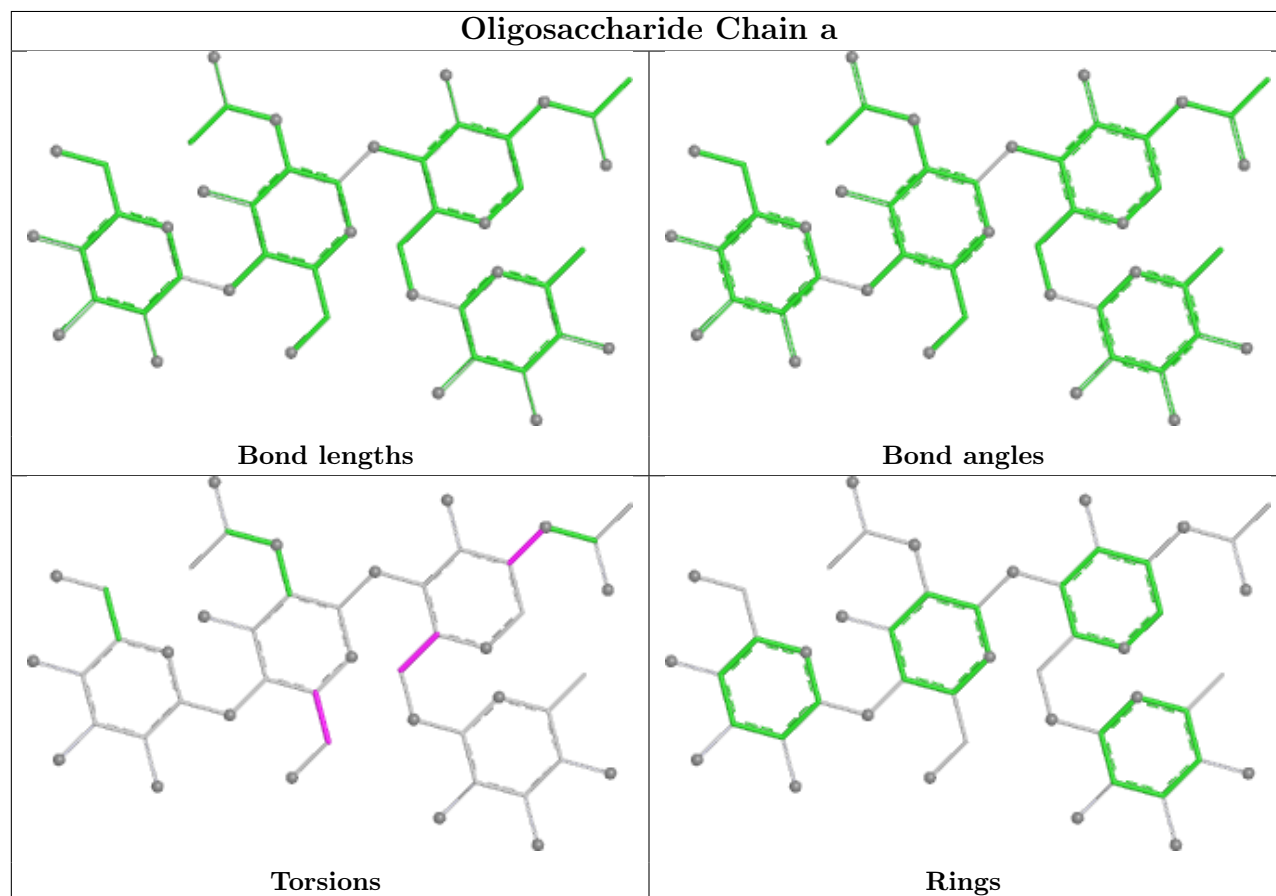
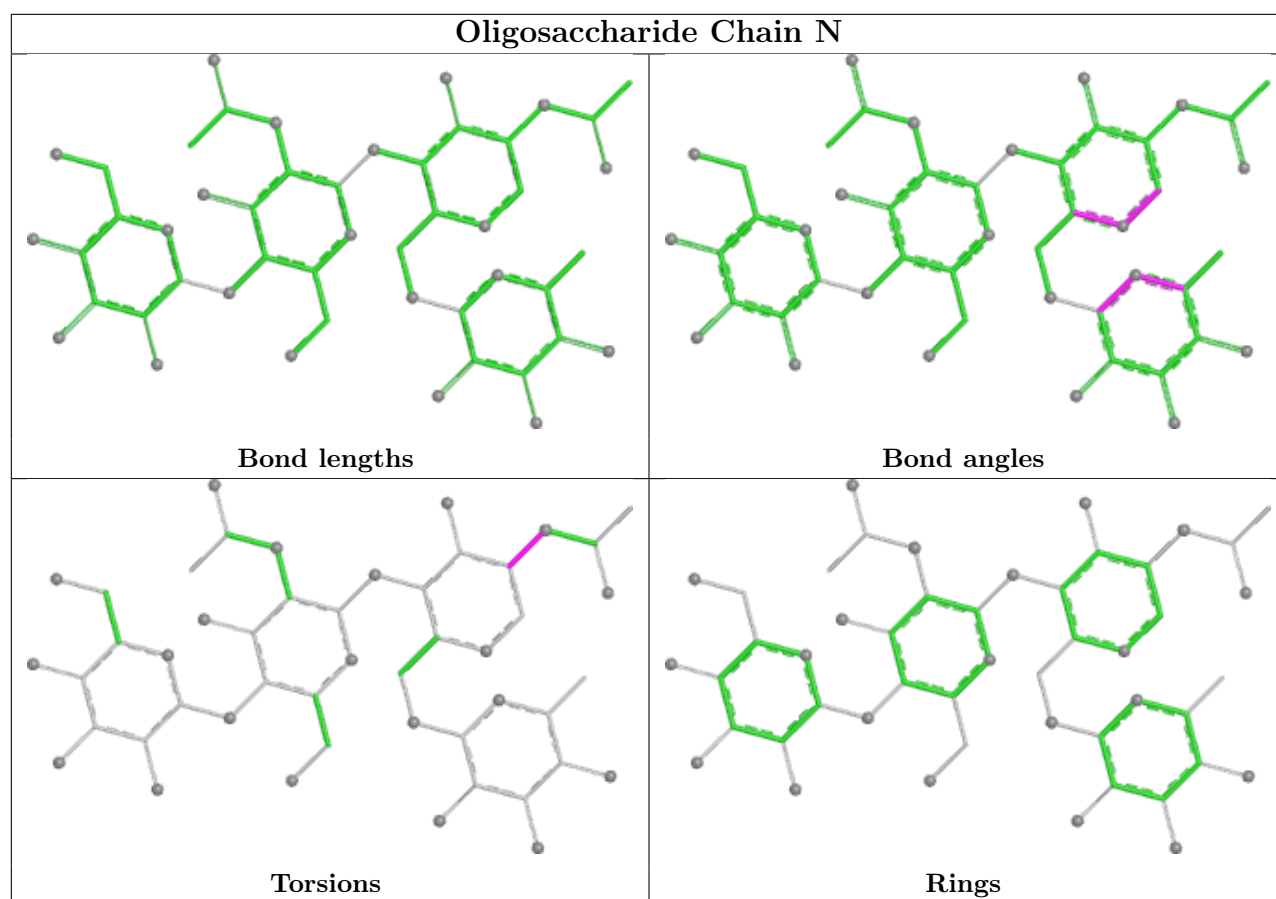


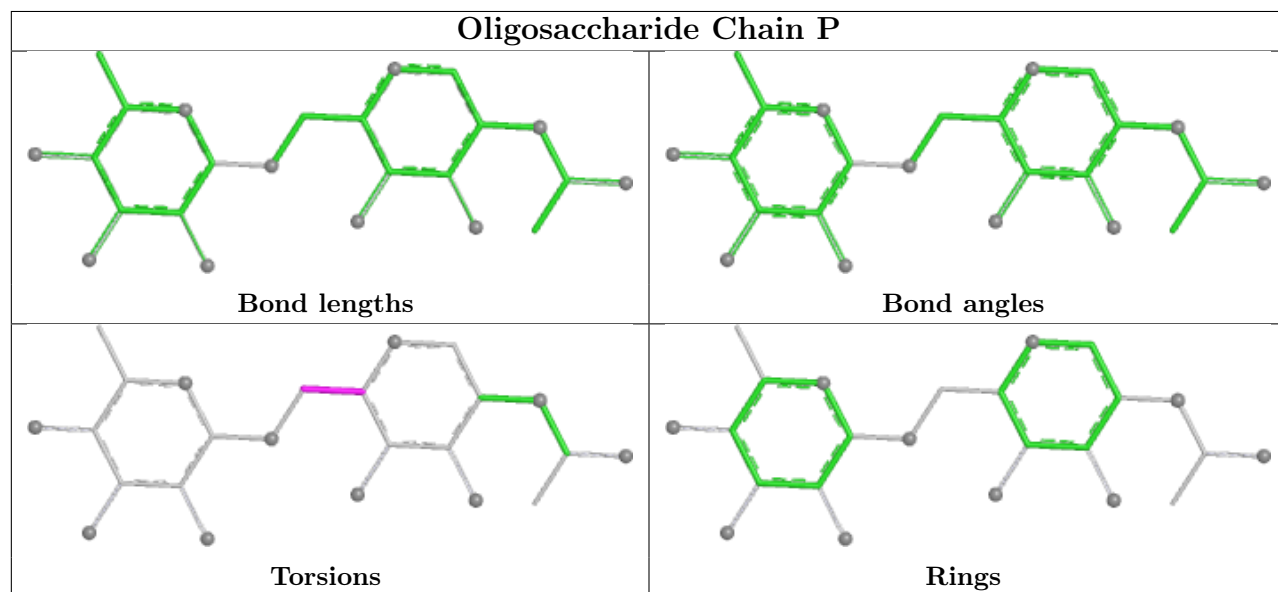
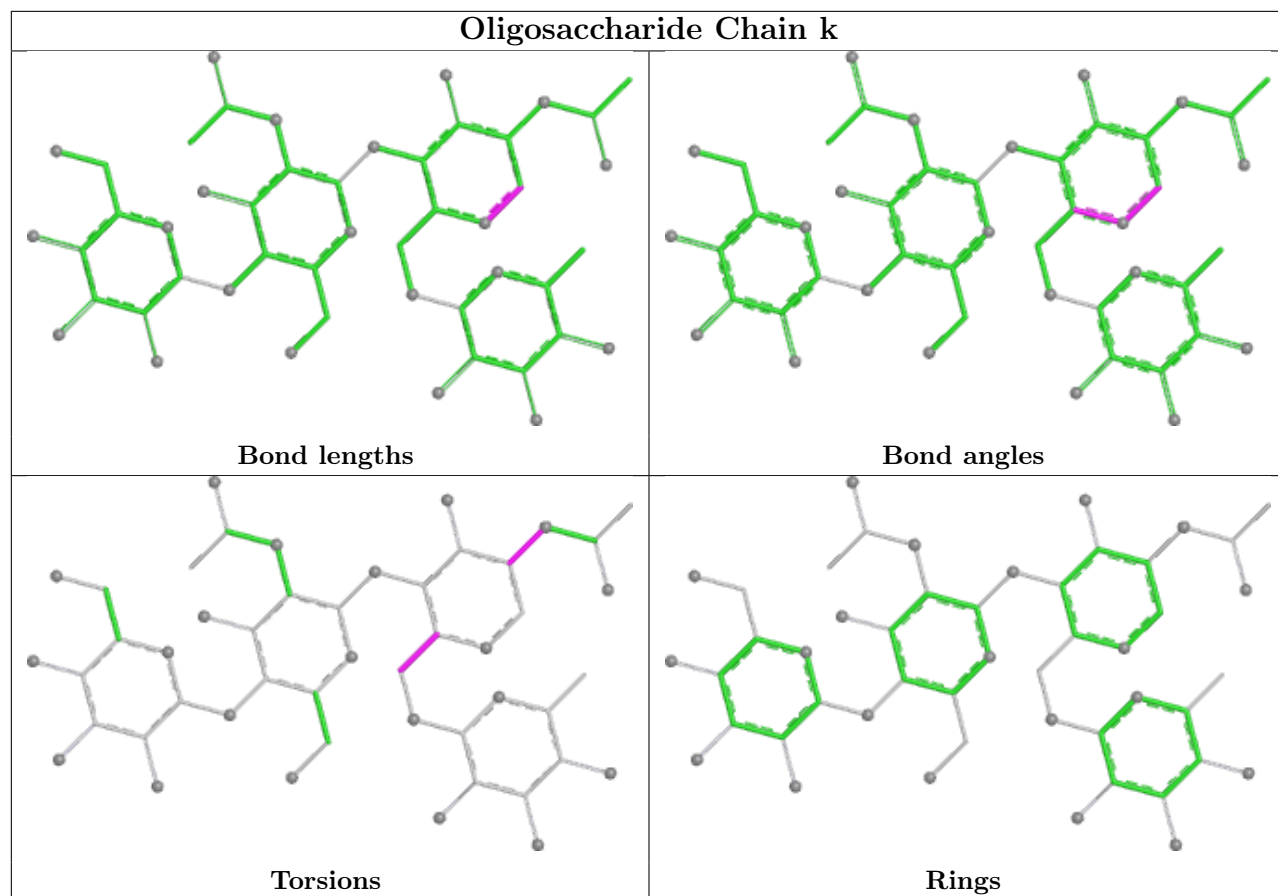


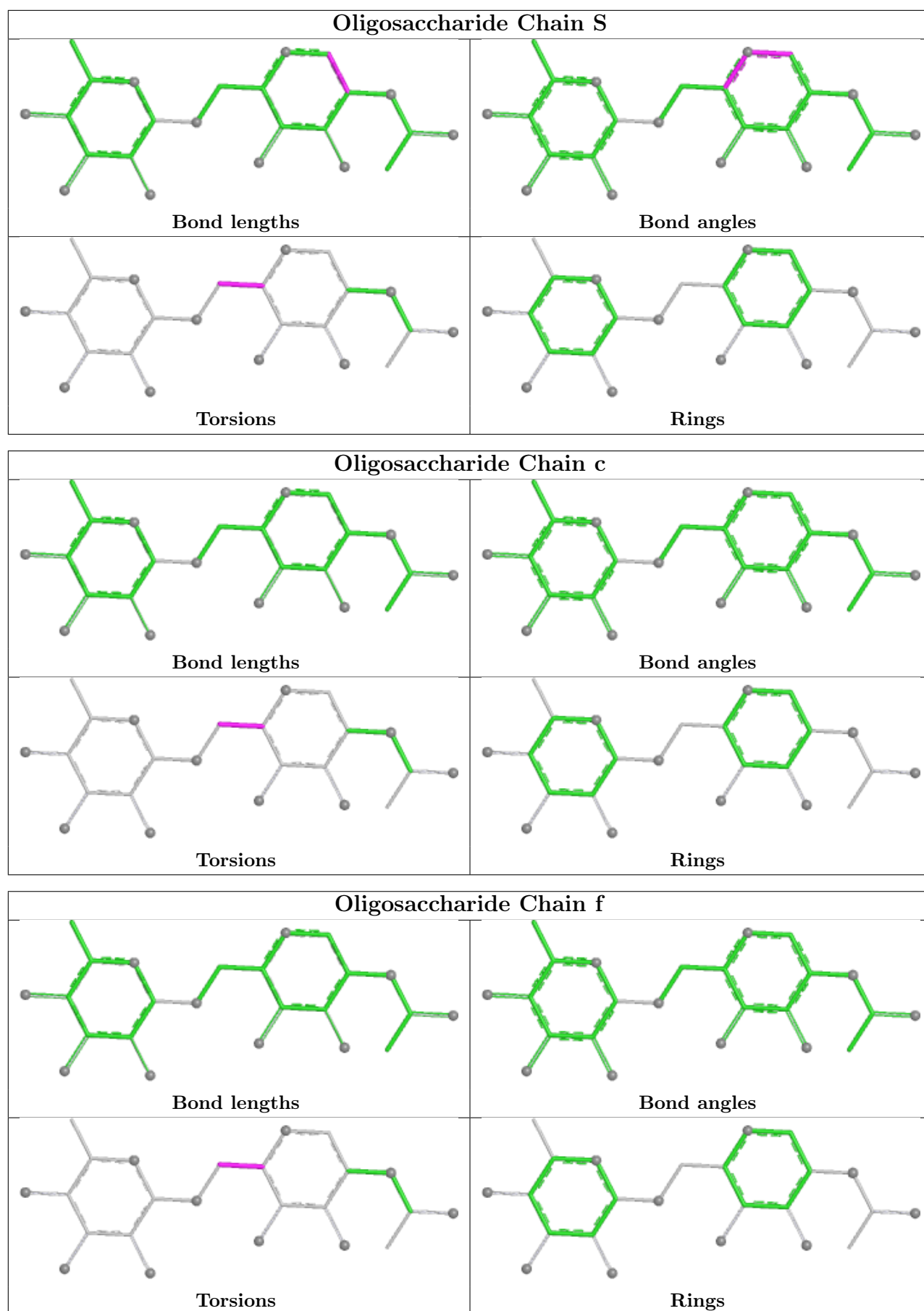












5.6 Ligand geometry

18 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	A	1502	1	14,14,15	0.51	0	17,19,21	0.59	0
8	NAG	A	1503	1	14,14,15	0.37	0	17,19,21	0.57	0
8	NAG	C	1504	1	14,14,15	0.24	0	17,19,21	0.51	0
8	NAG	A	1501	1	14,14,15	0.17	0	17,19,21	0.55	0
8	NAG	B	1505	1	14,14,15	0.31	0	17,19,21	0.52	0
8	NAG	B	1507	1	14,14,15	0.21	0	17,19,21	0.43	0
8	NAG	B	1503	1	14,14,15	0.24	0	17,19,21	0.40	0
8	NAG	A	1504	1	14,14,15	0.19	0	17,19,21	0.43	0
8	NAG	A	1506	1	14,14,15	0.48	0	17,19,21	0.61	0
8	NAG	C	1505	1	14,14,15	0.93	1 (7%)	17,19,21	0.60	0
8	NAG	B	1502	1	14,14,15	0.30	0	17,19,21	0.43	0
8	NAG	B	1506	1	14,14,15	0.26	0	17,19,21	0.41	0
8	NAG	B	1504	1	14,14,15	0.31	0	17,19,21	0.47	0
8	NAG	C	1502	1	14,14,15	0.22	0	17,19,21	0.45	0
8	NAG	A	1505	1	14,14,15	0.70	0	17,19,21	1.17	1 (5%)
8	NAG	B	1501	1	14,14,15	0.27	0	17,19,21	0.40	0
8	NAG	C	1501	1	14,14,15	0.28	0	17,19,21	0.40	0
8	NAG	C	1503	1	14,14,15	0.29	0	17,19,21	0.64	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1502	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1503	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1504	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1501	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1505	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	1507	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1503	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1504	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1506	1	-	4/6/23/26	0/1/1/1
8	NAG	C	1505	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1502	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1506	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1504	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1502	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1505	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1501	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1501	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1503	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1505	NAG	O5-C1	-3.13	1.38	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1505	NAG	C1-O5-C5	4.44	118.14	112.19
8	C	1503	NAG	C1-O5-C5	2.09	114.98	112.19

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1503	NAG	O5-C5-C6-O6
8	B	1503	NAG	O5-C5-C6-O6
8	B	1505	NAG	C4-C5-C6-O6
8	A	1506	NAG	C4-C5-C6-O6
8	C	1504	NAG	O5-C5-C6-O6
8	B	1507	NAG	O5-C5-C6-O6
8	C	1505	NAG	C4-C5-C6-O6
8	B	1503	NAG	C4-C5-C6-O6
8	A	1506	NAG	O5-C5-C6-O6
8	C	1502	NAG	O5-C5-C6-O6
8	B	1505	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	1503	NAG	C4-C5-C6-O6
8	A	1501	NAG	O5-C5-C6-O6
8	B	1507	NAG	C4-C5-C6-O6
8	C	1504	NAG	C4-C5-C6-O6
8	A	1501	NAG	C4-C5-C6-O6
8	C	1501	NAG	C4-C5-C6-O6
8	A	1506	NAG	C8-C7-N2-C2
8	A	1506	NAG	O7-C7-N2-C2
8	C	1505	NAG	O5-C5-C6-O6
8	C	1503	NAG	O5-C5-C6-O6
8	C	1503	NAG	C4-C5-C6-O6
8	A	1502	NAG	O5-C5-C6-O6
8	C	1502	NAG	C4-C5-C6-O6
8	C	1501	NAG	O5-C5-C6-O6
8	C	1504	NAG	C1-C2-N2-C7
8	A	1502	NAG	C4-C5-C6-O6
8	A	1502	NAG	C3-C2-N2-C7
8	C	1504	NAG	C3-C2-N2-C7
8	A	1502	NAG	C1-C2-N2-C7
8	B	1506	NAG	C1-C2-N2-C7
8	B	1502	NAG	O5-C5-C6-O6

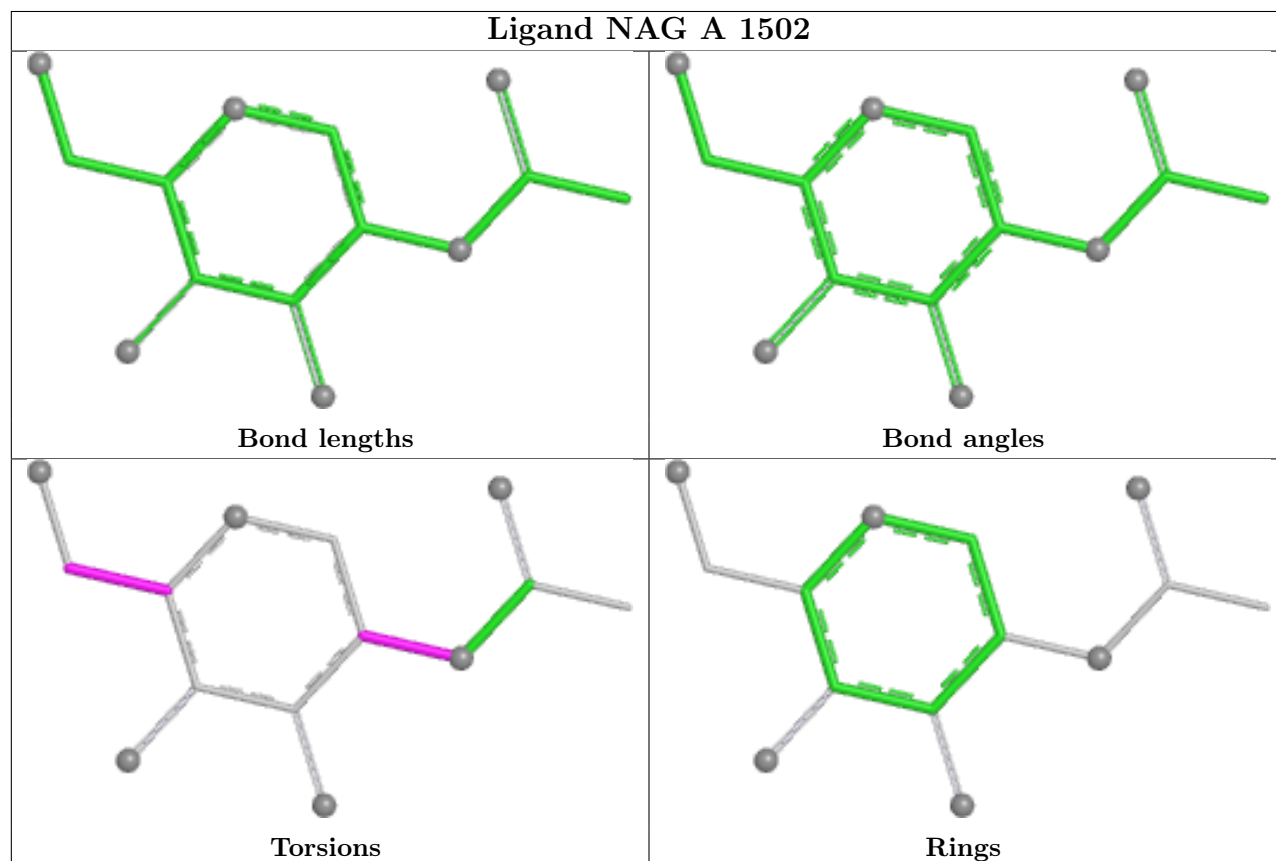
There are no ring outliers.

10 monomers are involved in 11 short contacts:

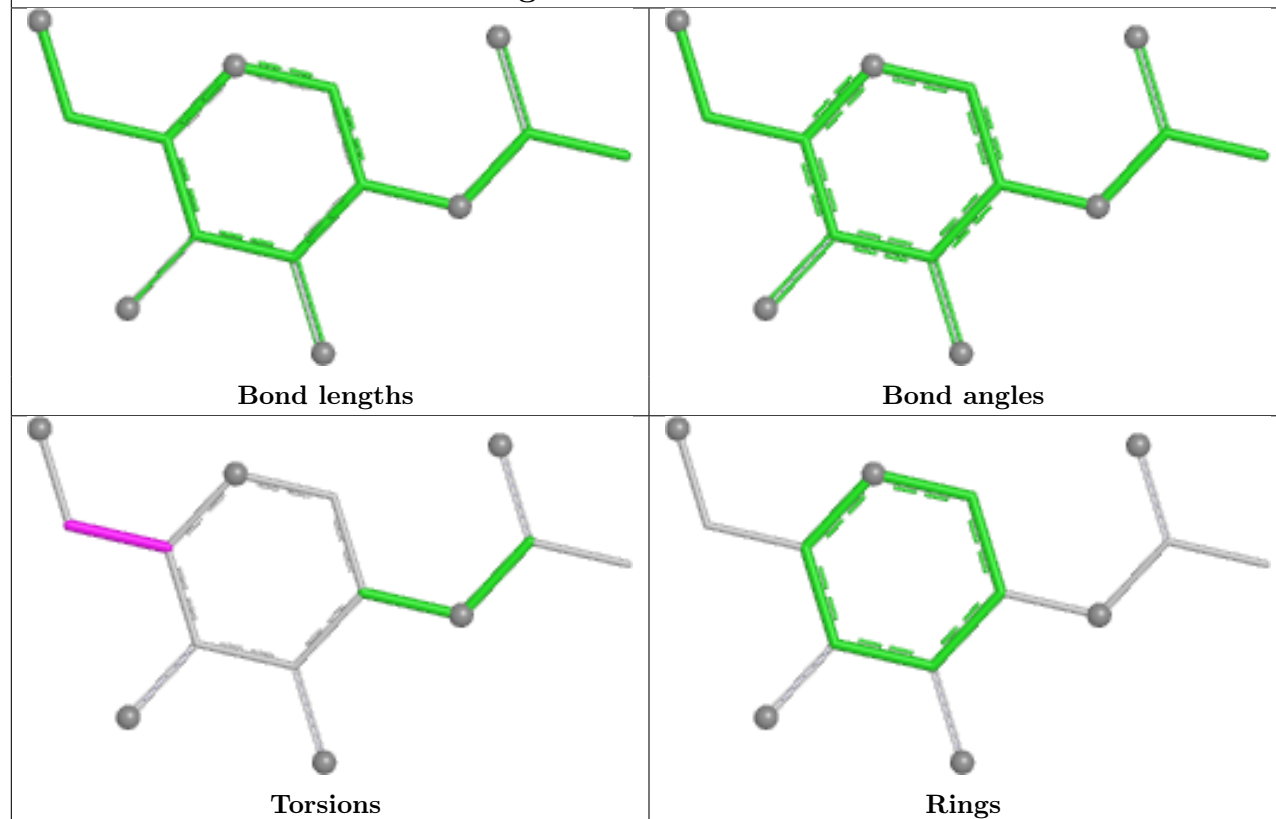
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1502	NAG	1	0
8	A	1501	NAG	1	0
8	B	1505	NAG	1	0
8	B	1503	NAG	1	0
8	A	1506	NAG	2	0
8	B	1502	NAG	1	0
8	A	1505	NAG	1	0
8	B	1501	NAG	1	0
8	C	1501	NAG	1	0
8	C	1503	NAG	1	0

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.

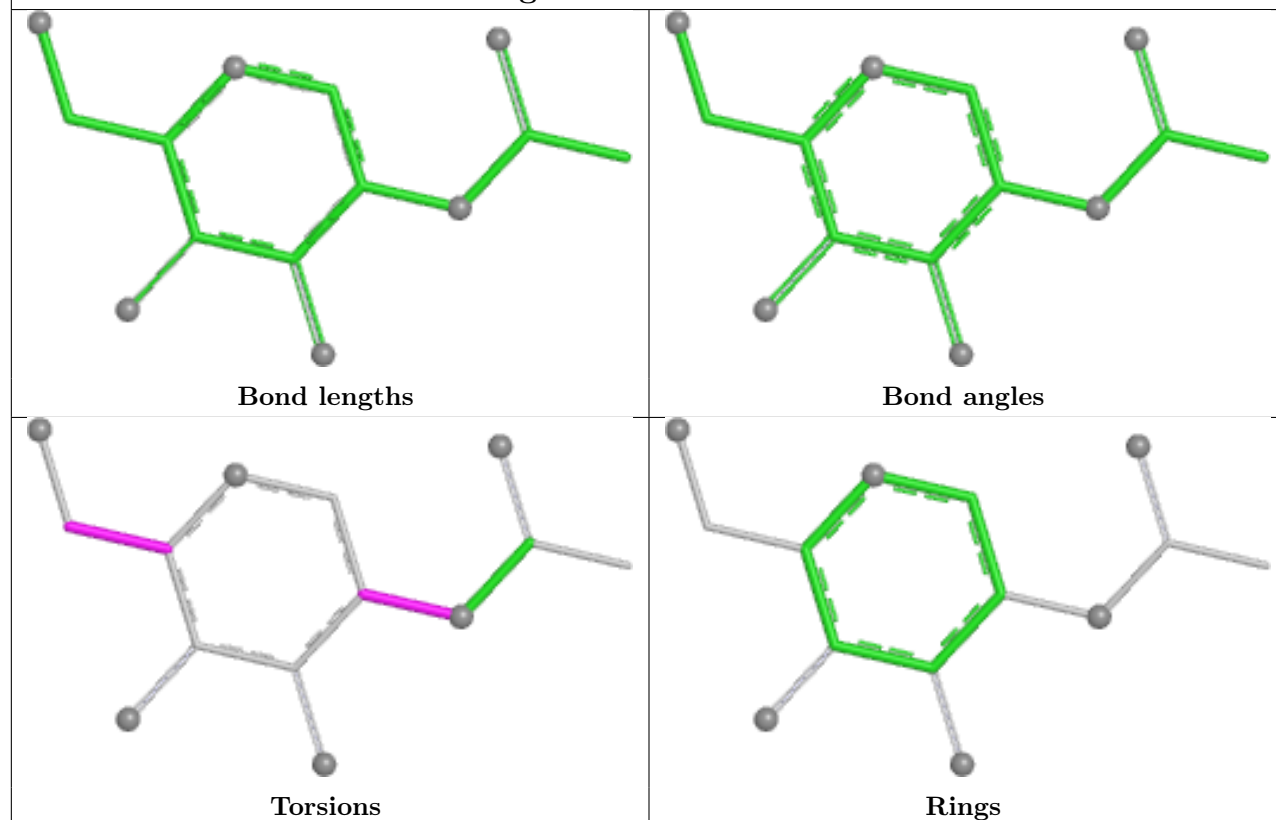
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



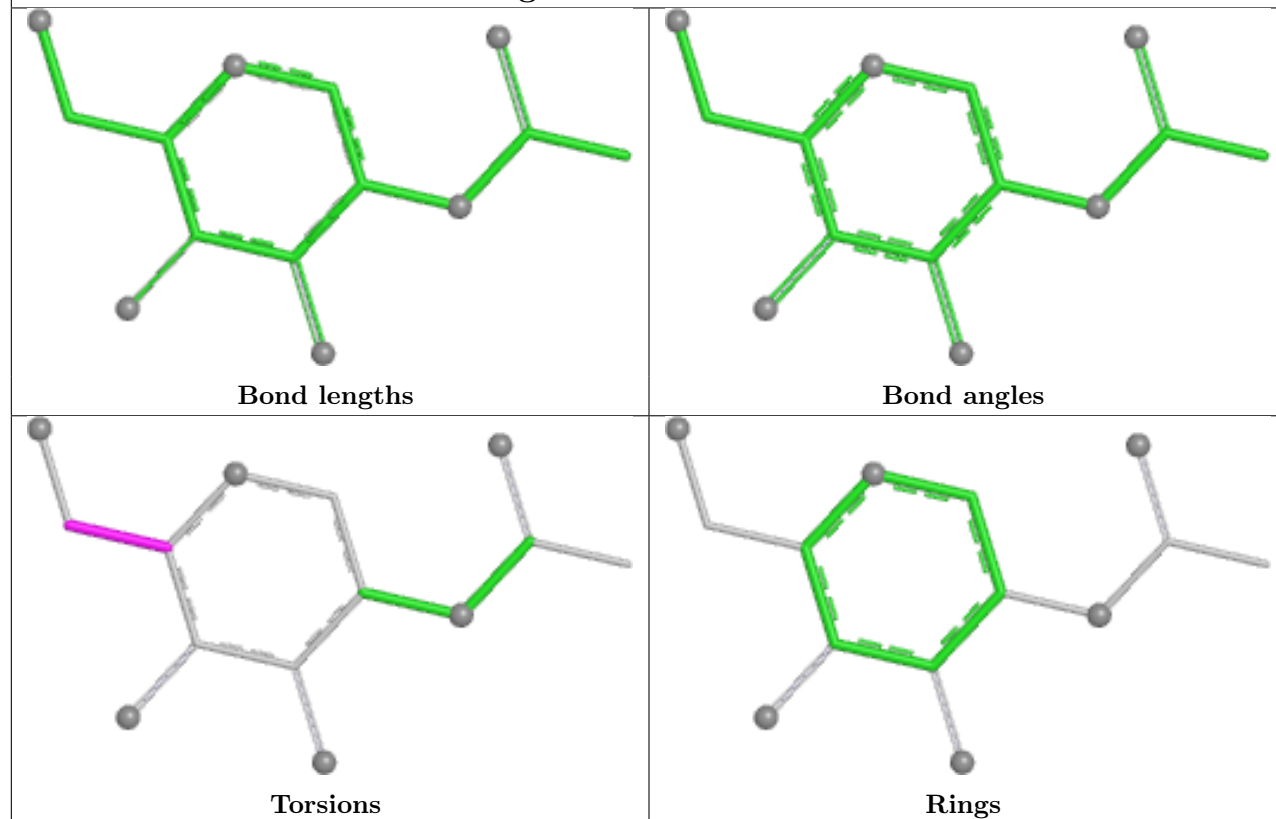
Ligand NAG A 1503



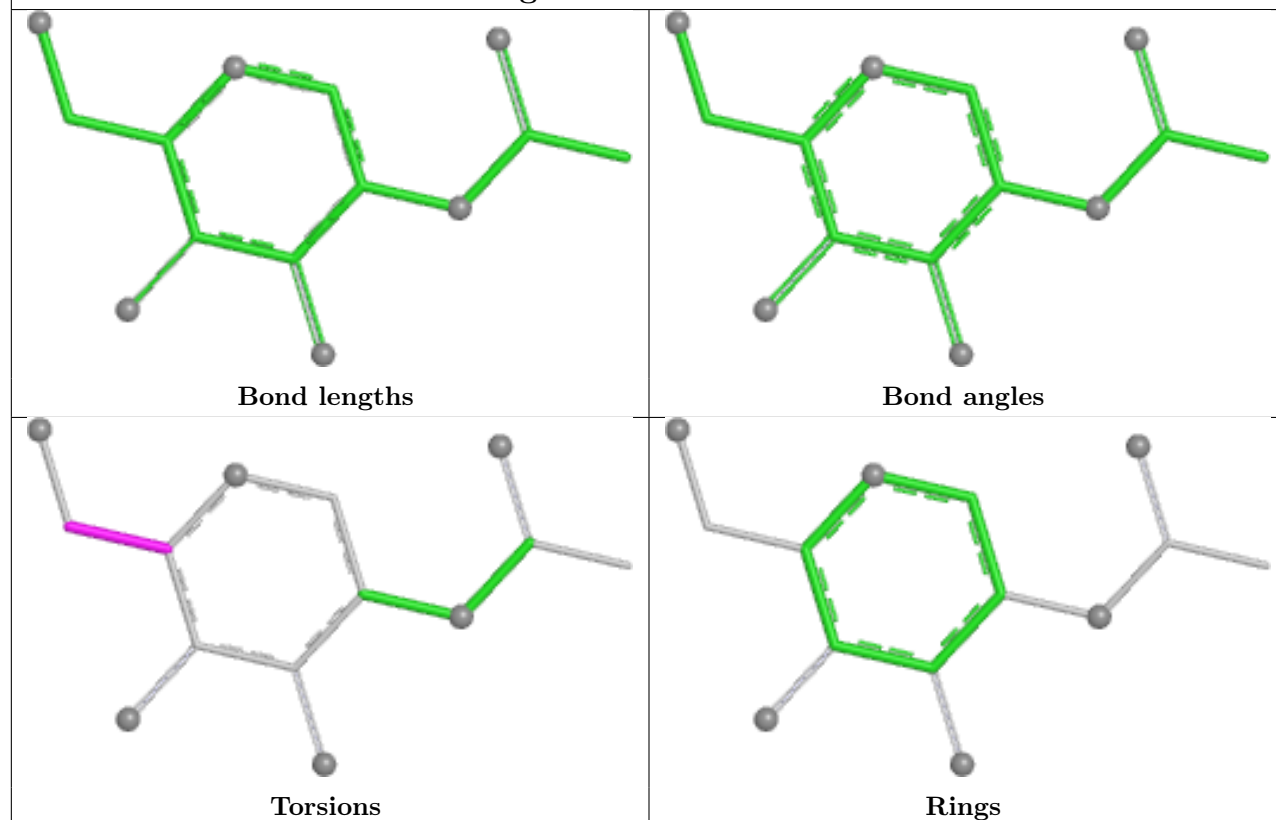
Ligand NAG C 1504

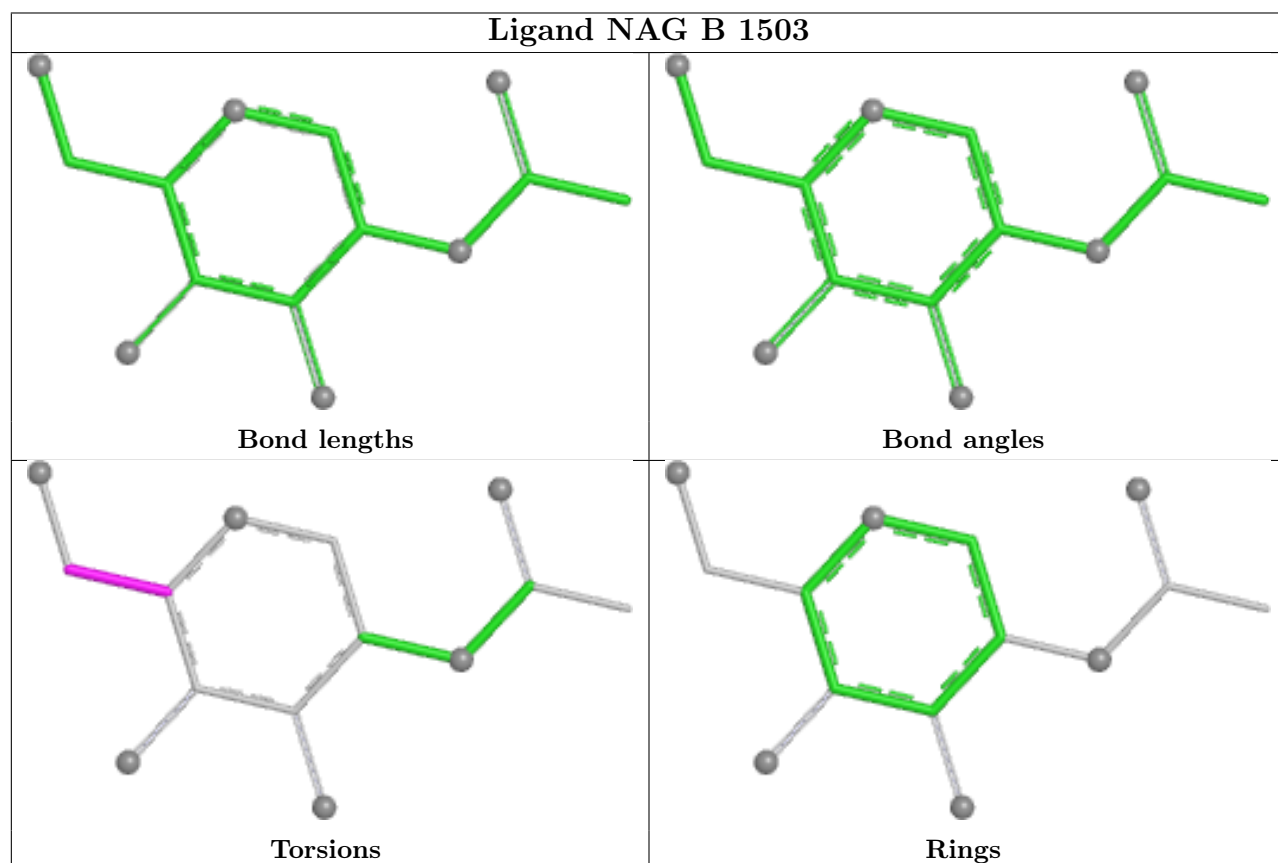
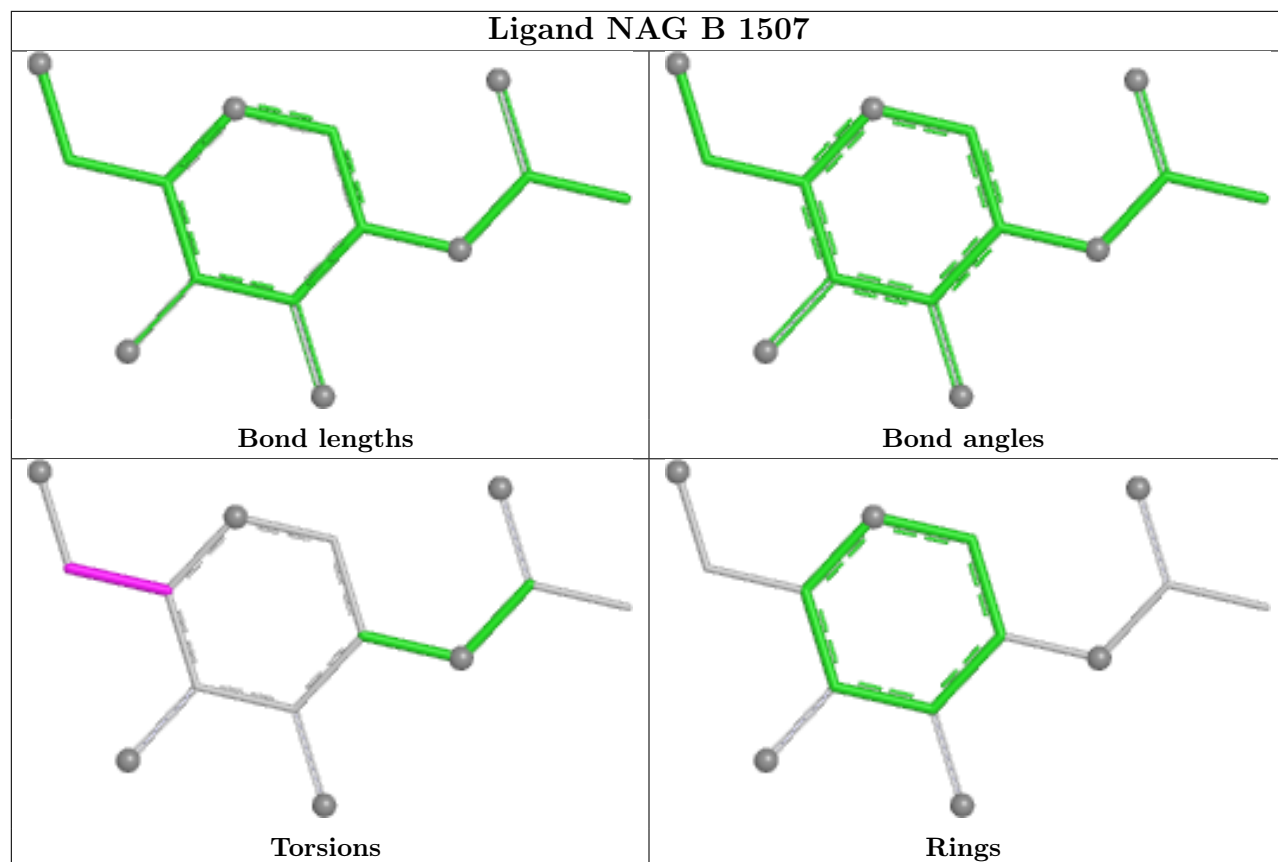


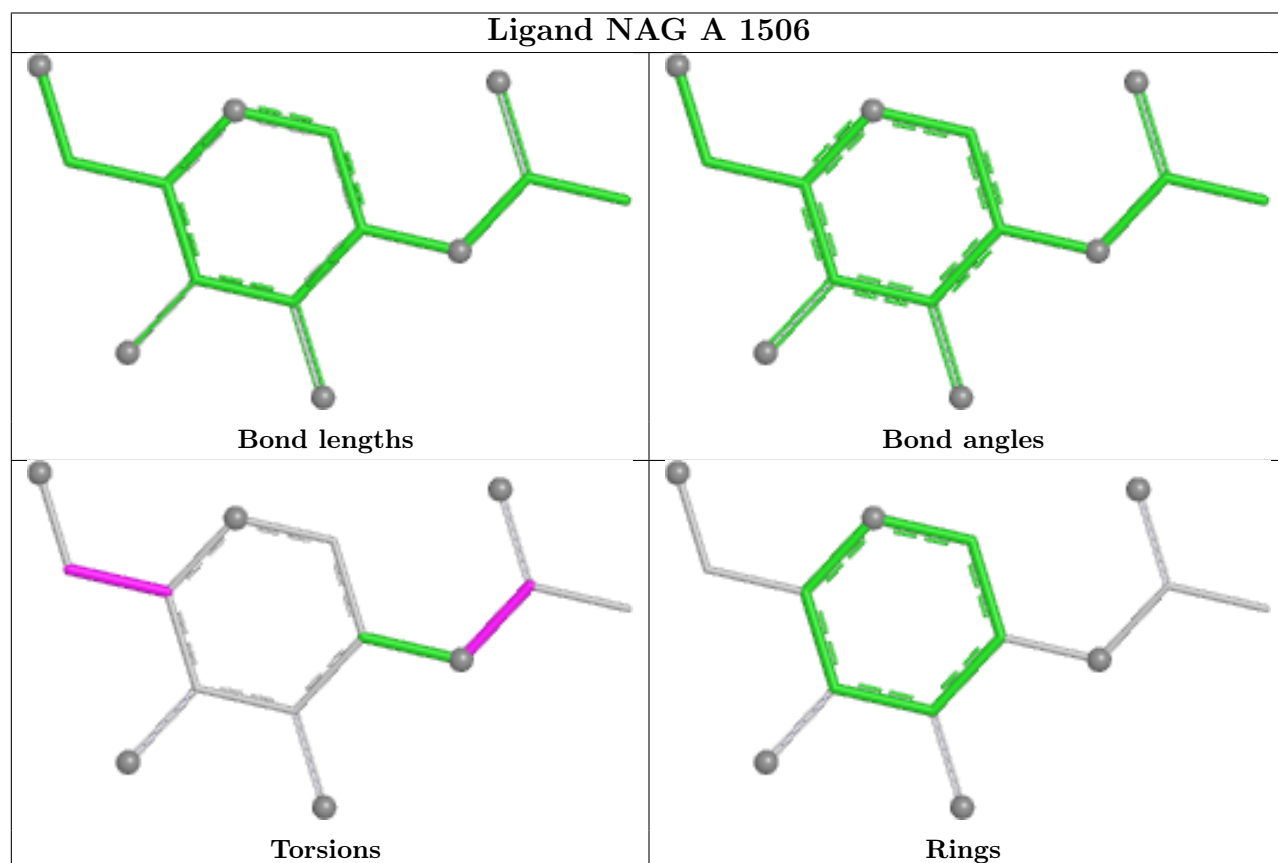
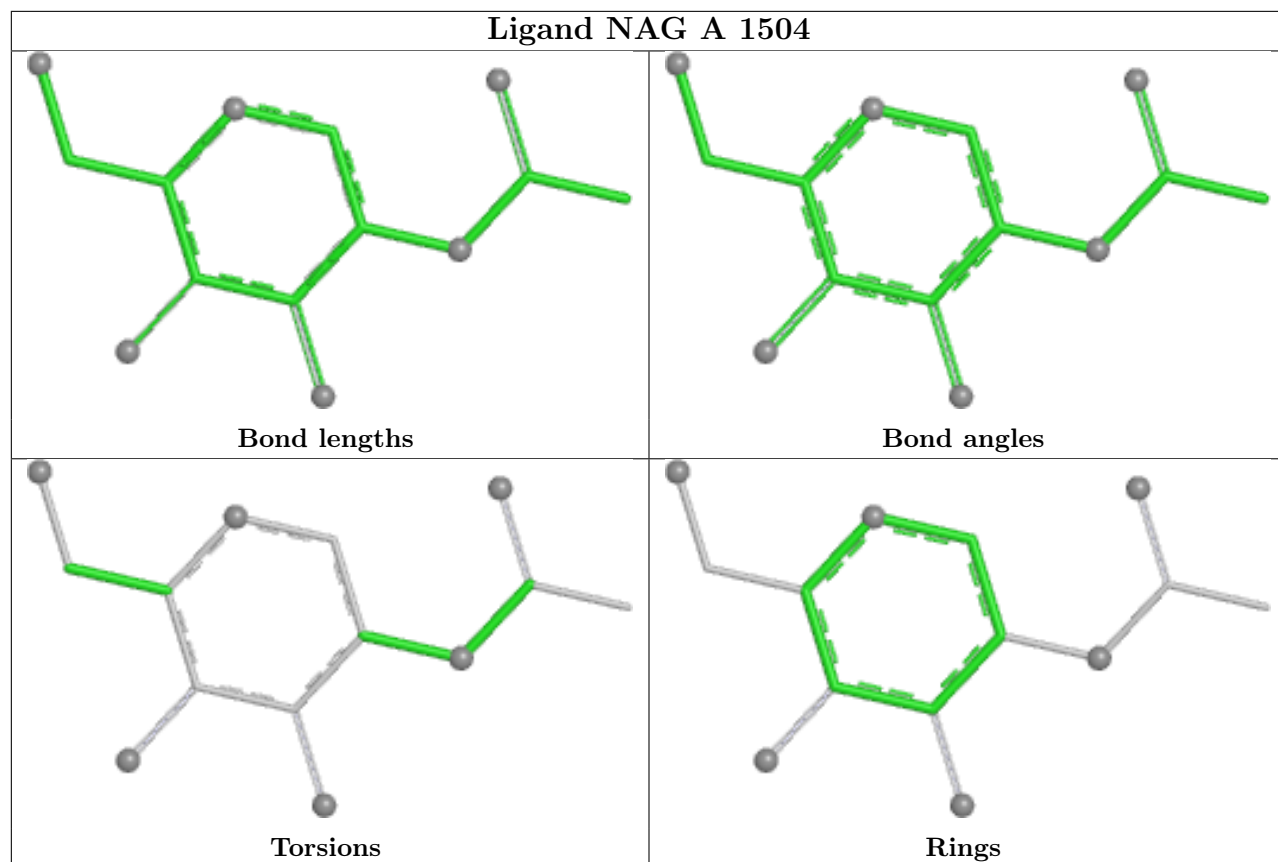
Ligand NAG A 1501



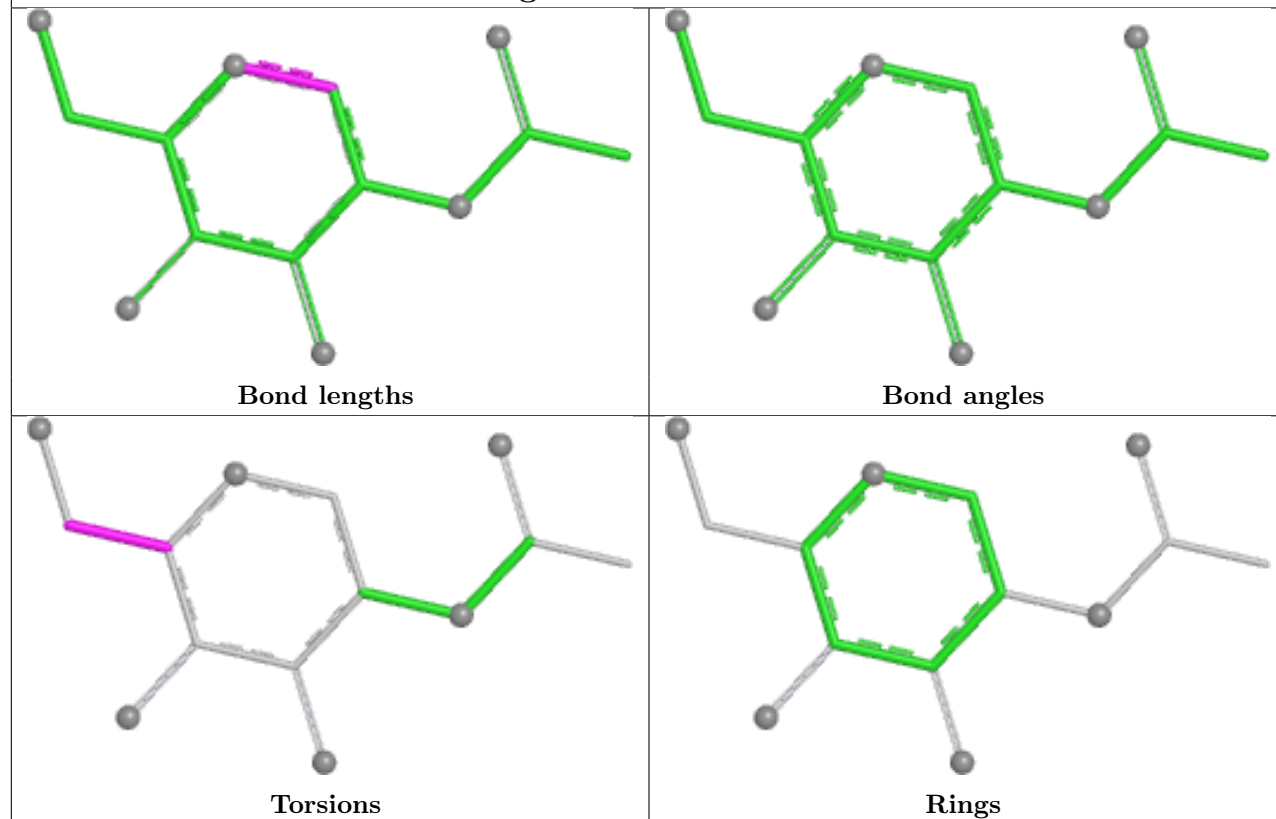
Ligand NAG B 1505



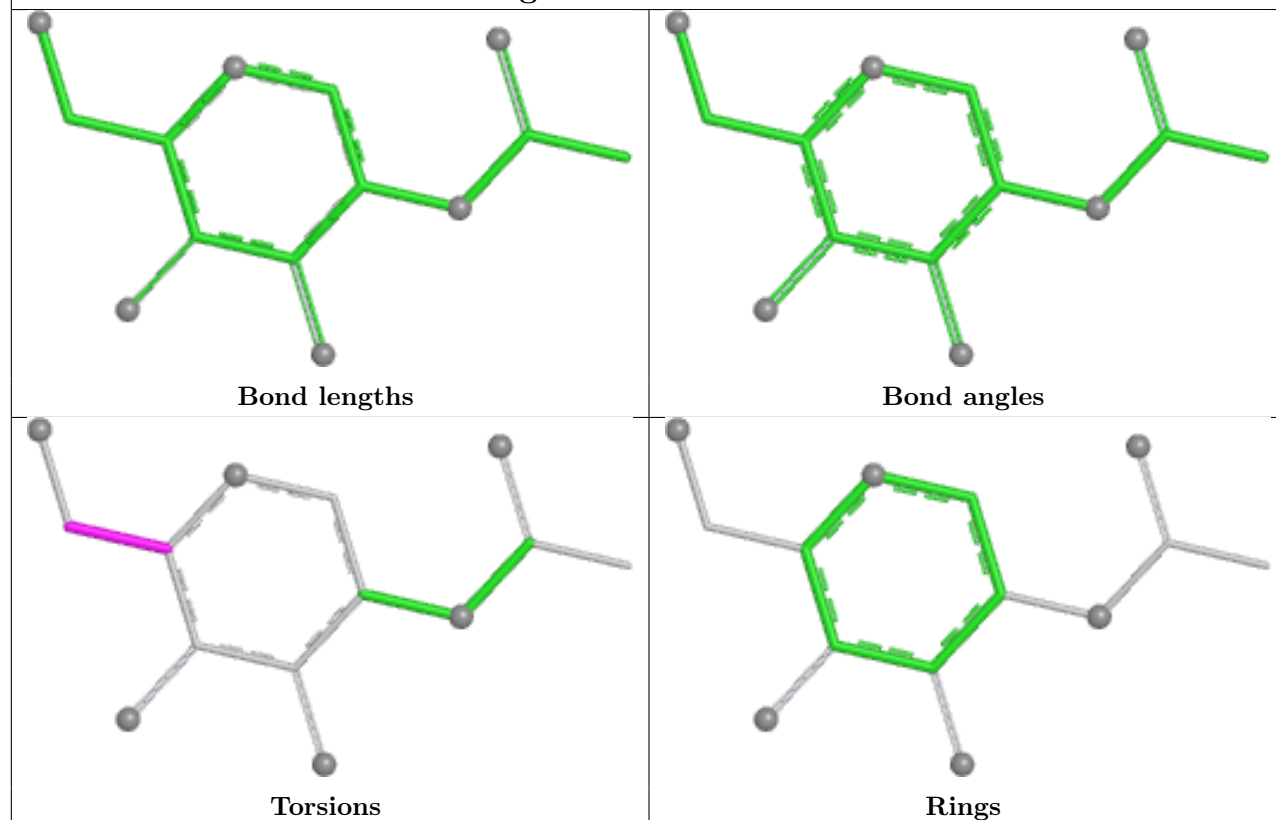




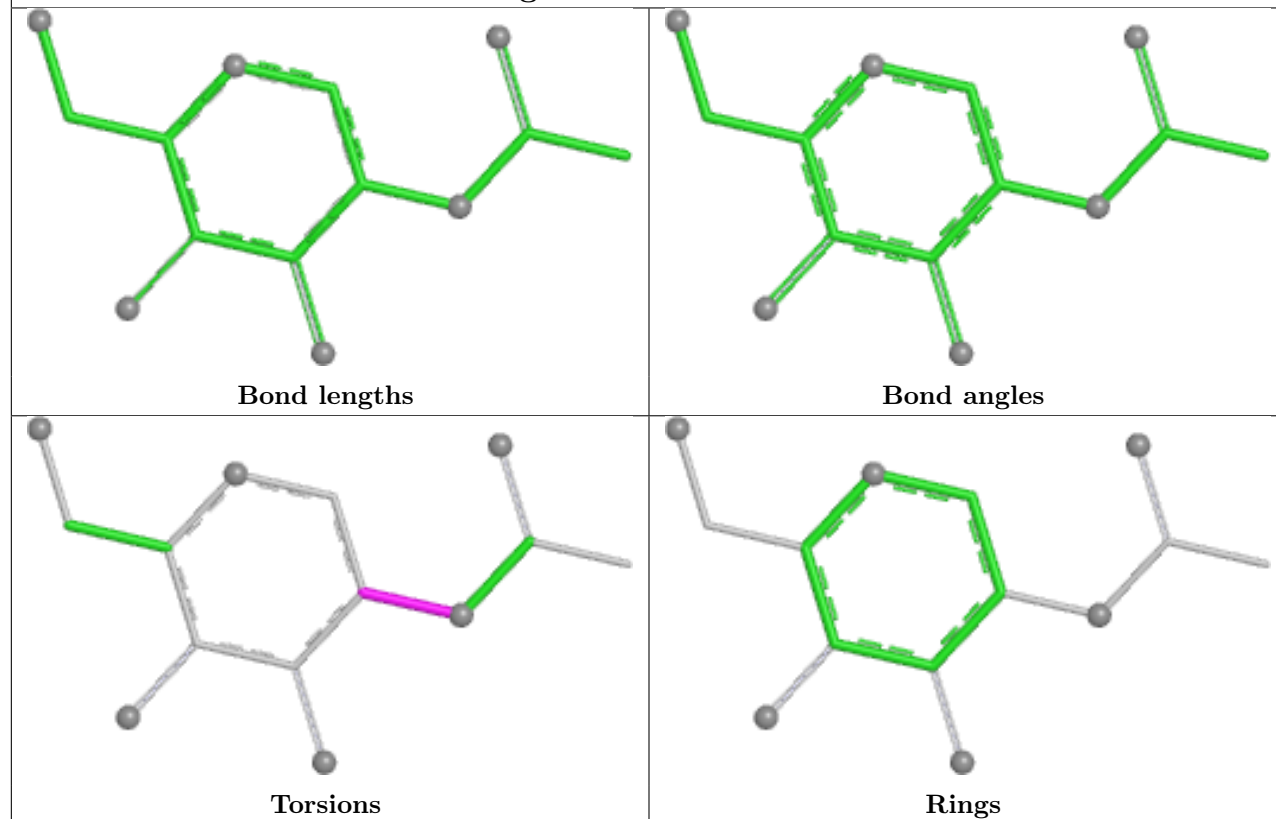
Ligand NAG C 1505



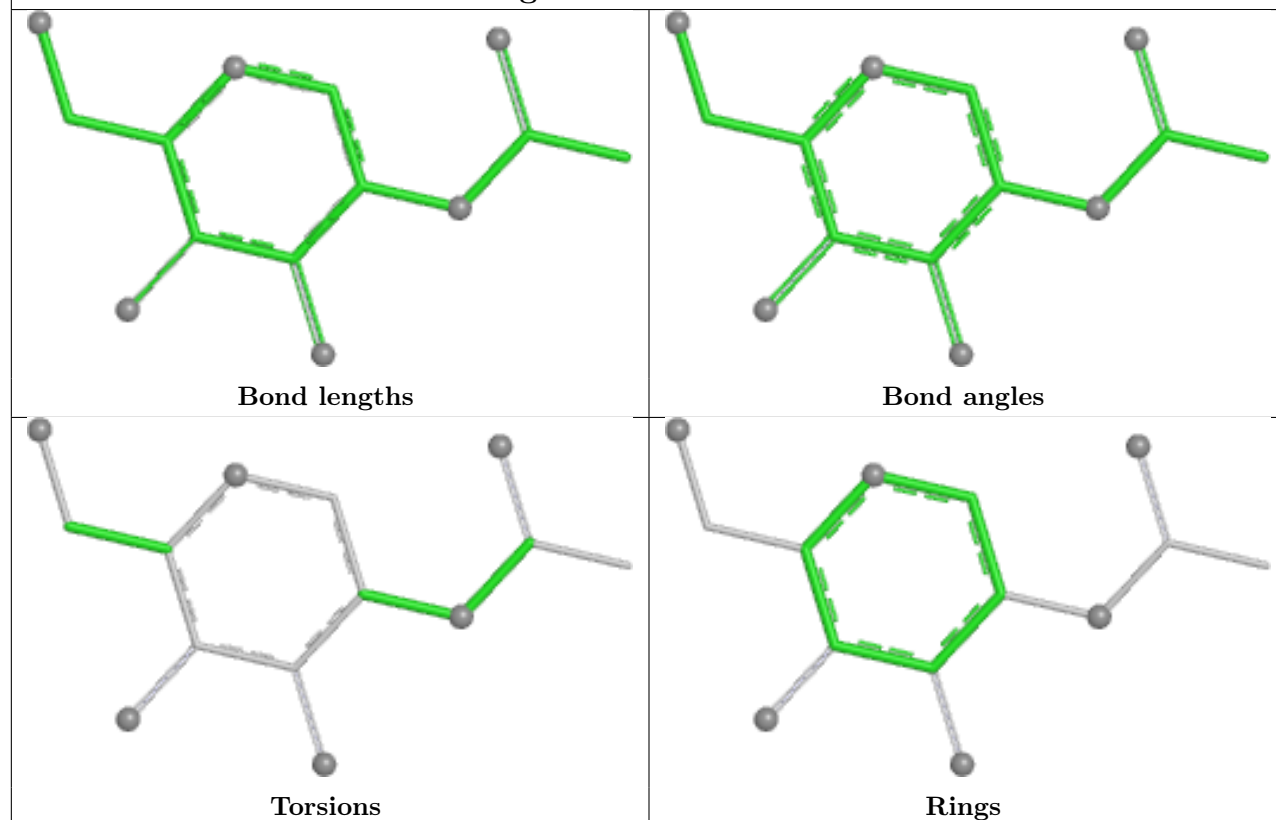
Ligand NAG B 1502



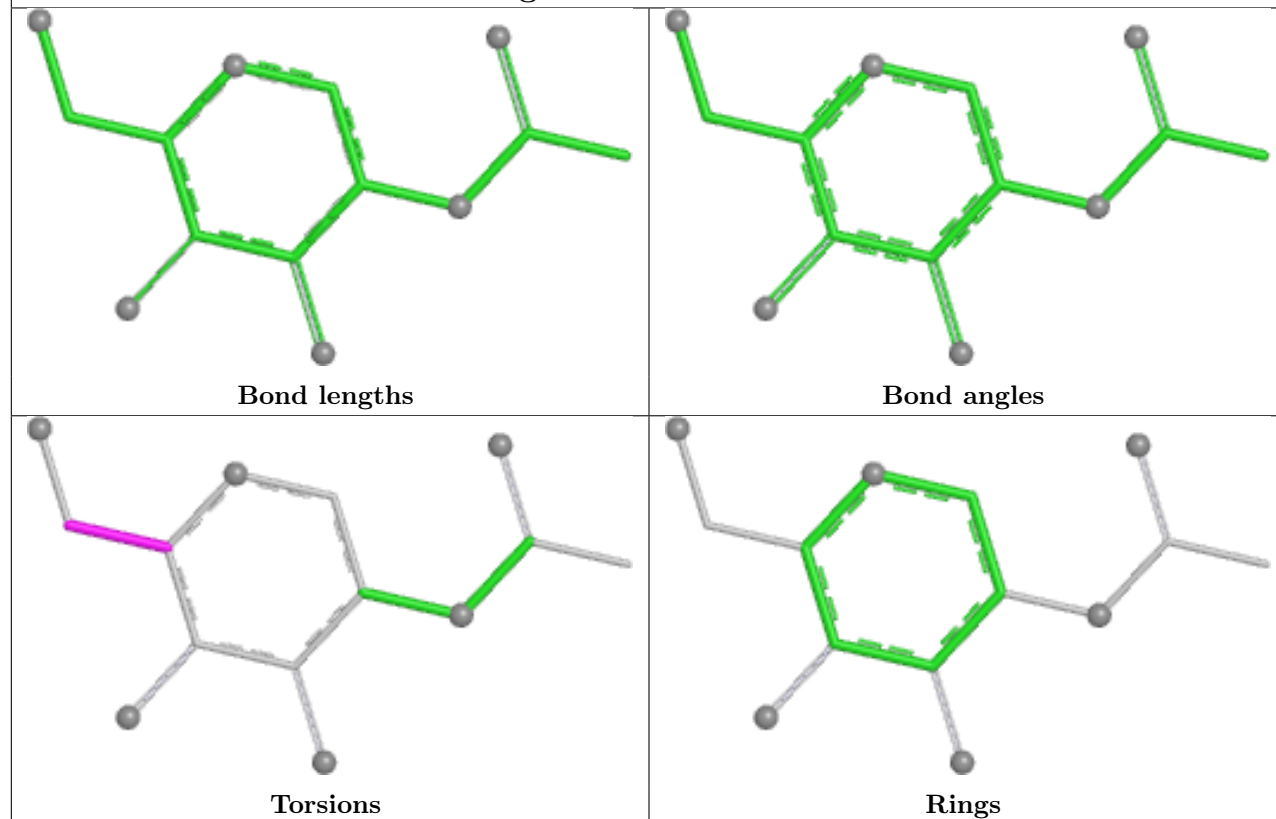
Ligand NAG B 1506



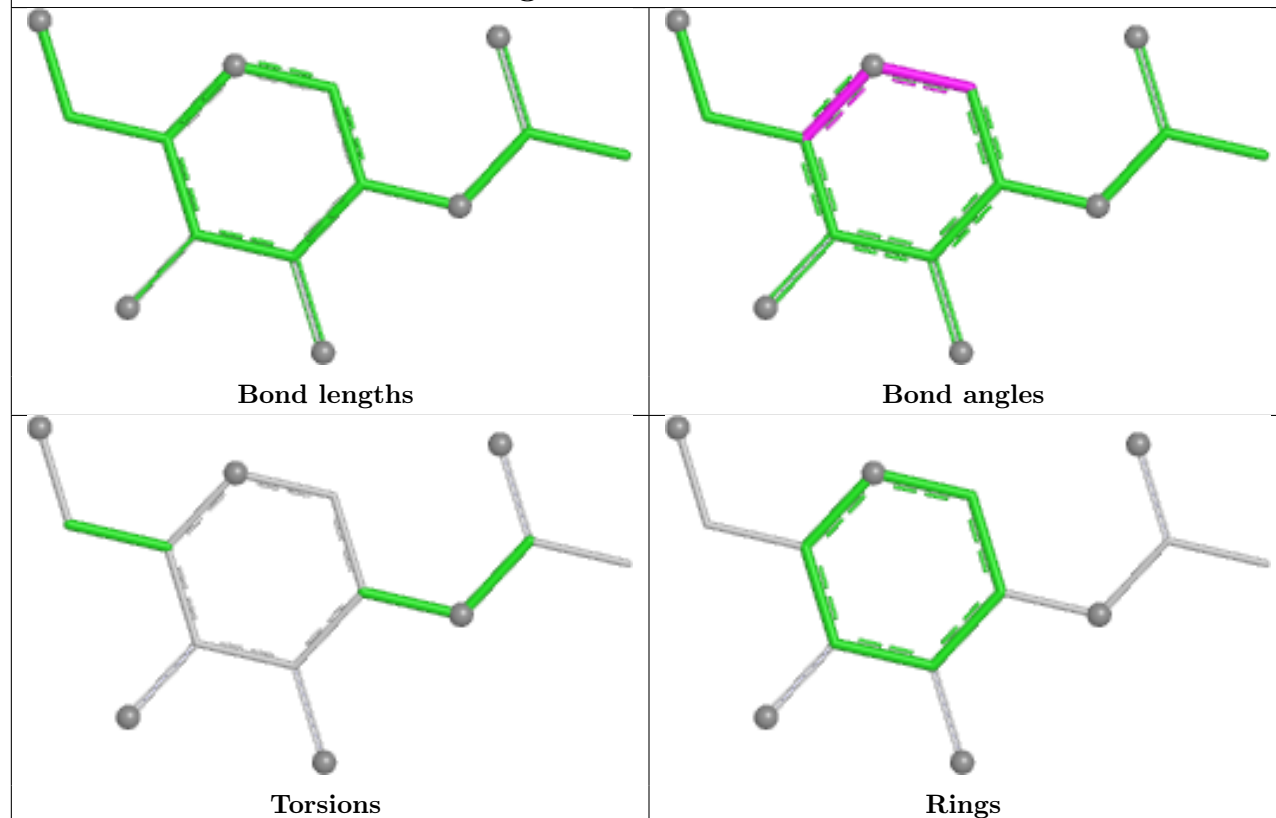
Ligand NAG B 1504



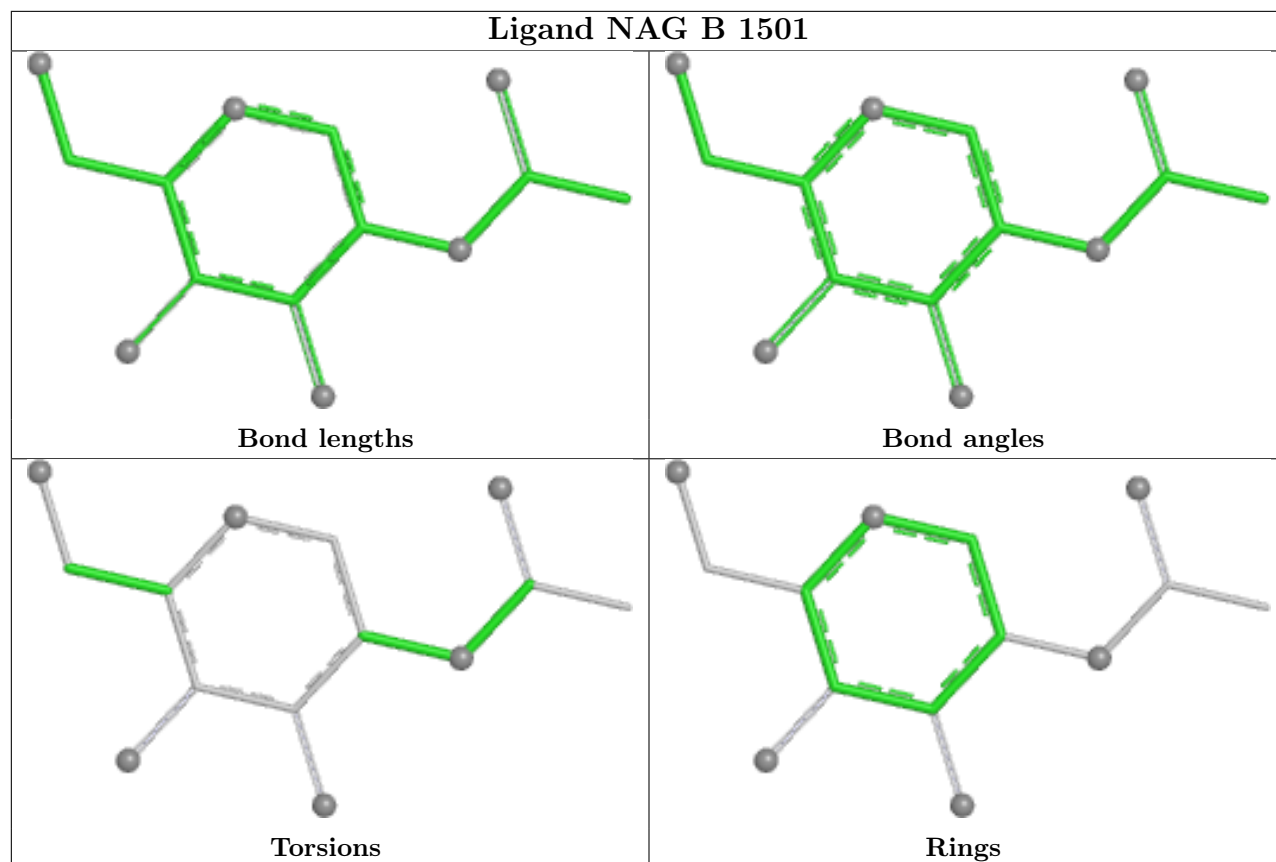
Ligand NAG C 1502



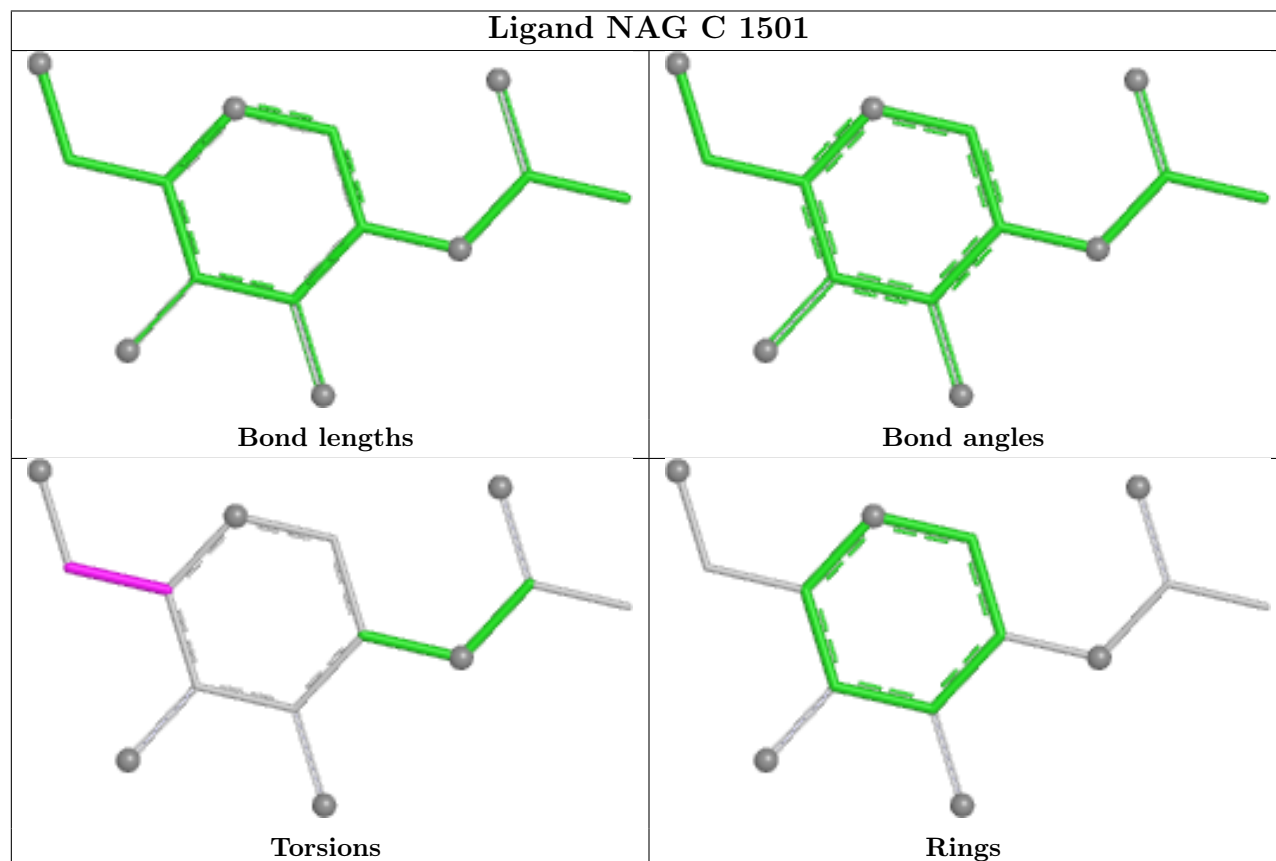
Ligand NAG A 1505

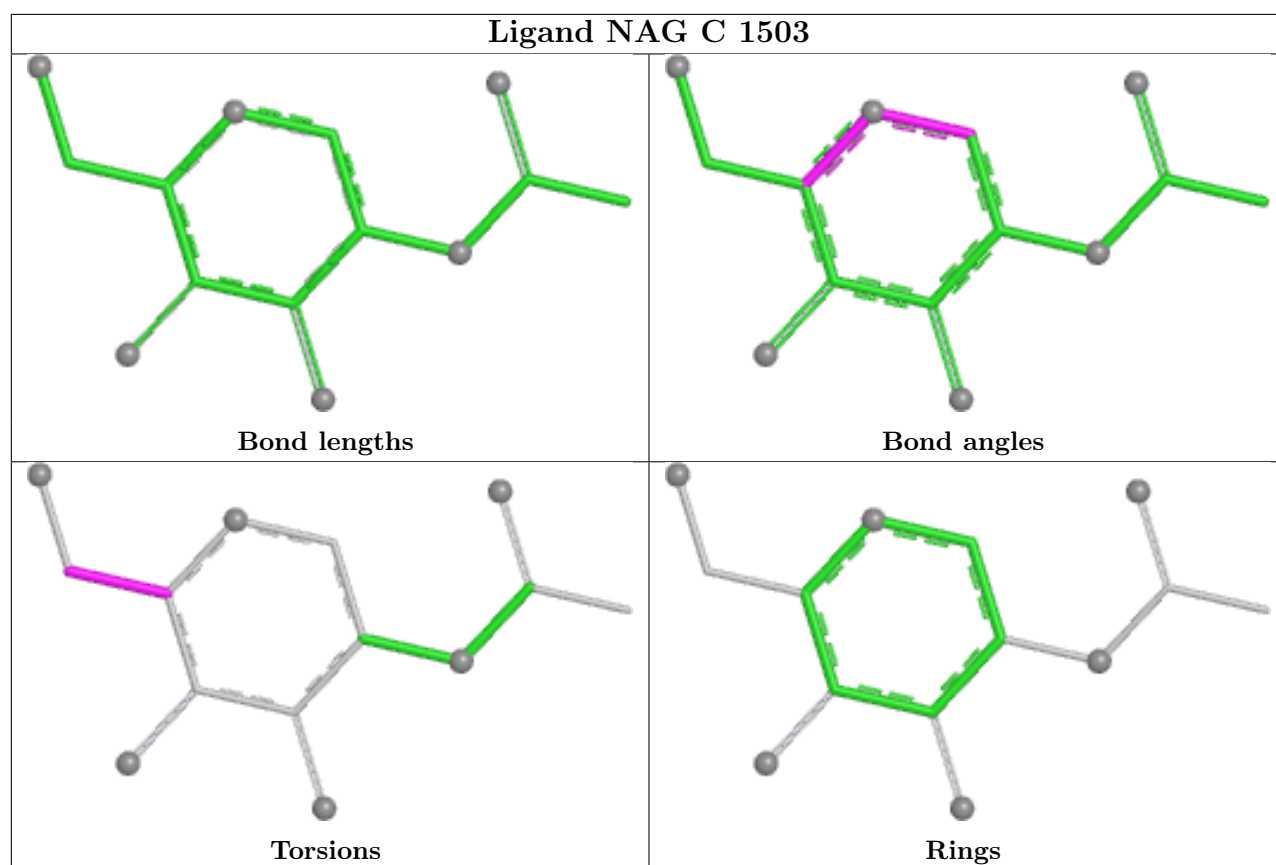


Ligand NAG B 1501



Ligand NAG C 1501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

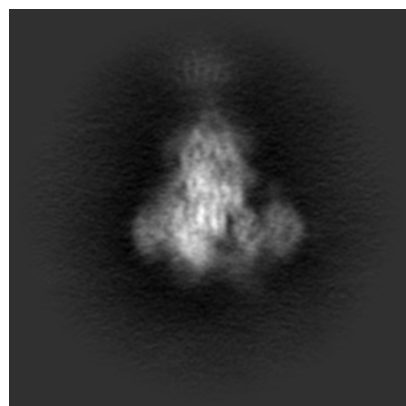
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33647. These allow visual inspection of the internal detail of the map and identification of artifacts.

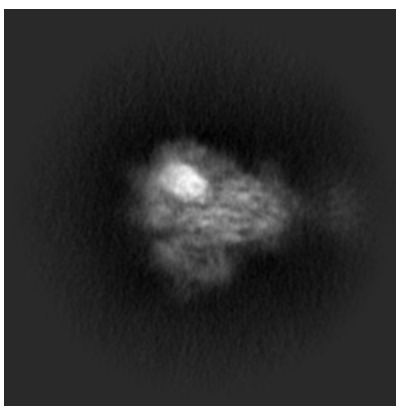
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

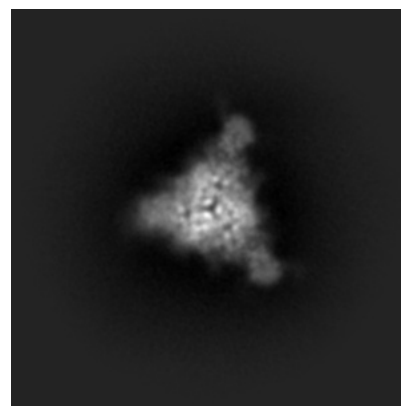
6.1.1 Primary map



X

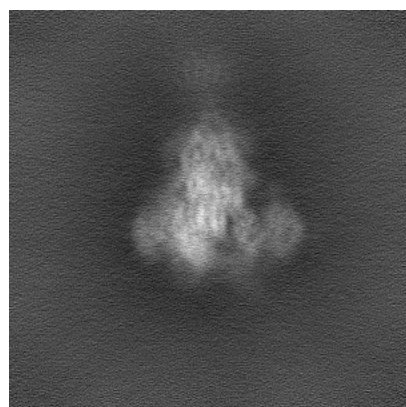


Y

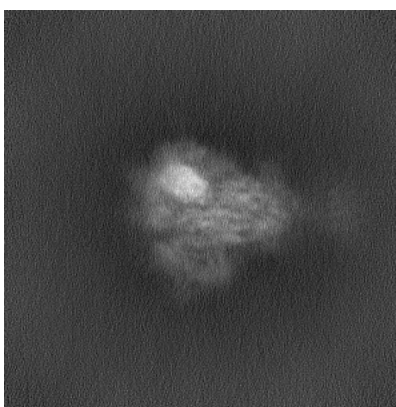


Z

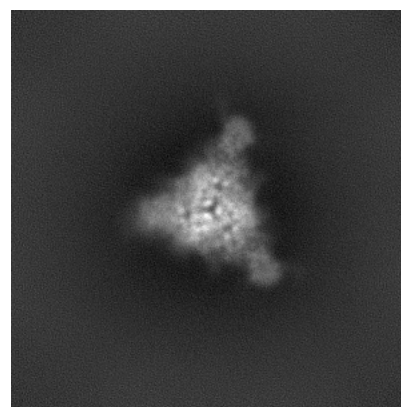
6.1.2 Raw map



X



Y

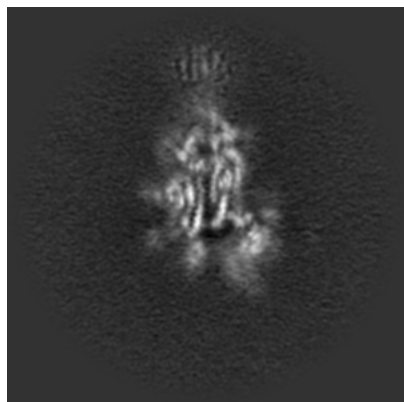


Z

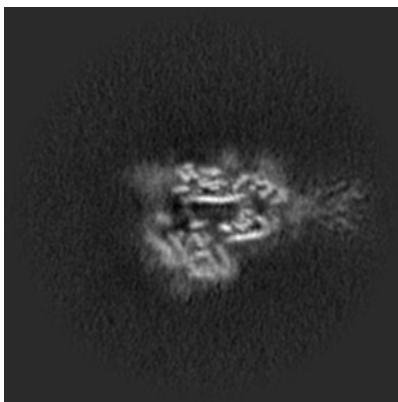
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

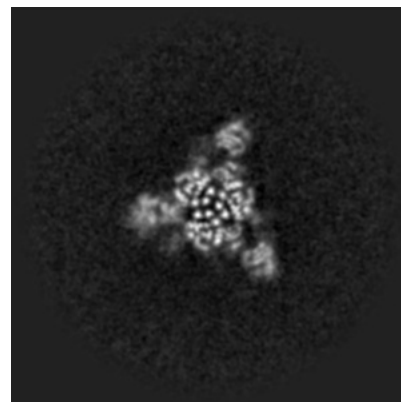
6.2.1 Primary map



X Index: 182

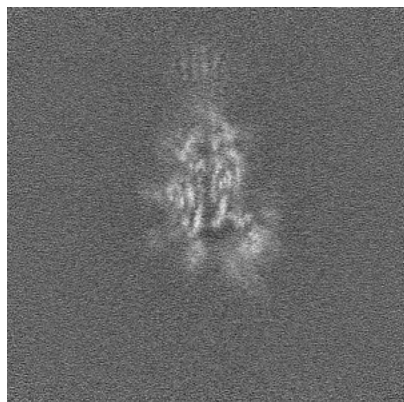


Y Index: 182



Z Index: 182

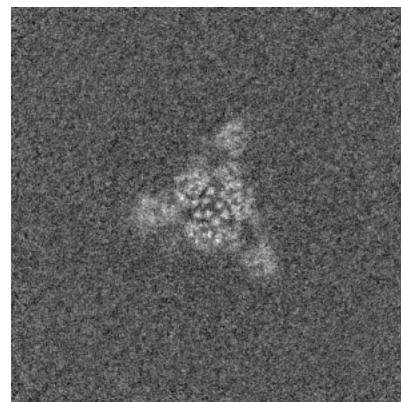
6.2.2 Raw map



X Index: 182



Y Index: 182

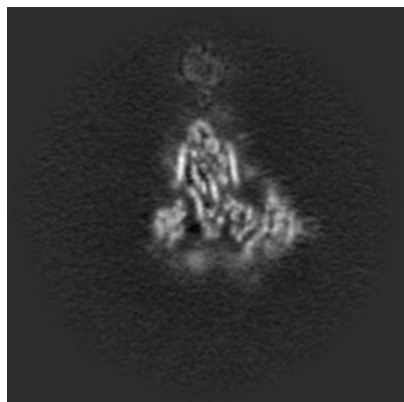


Z Index: 182

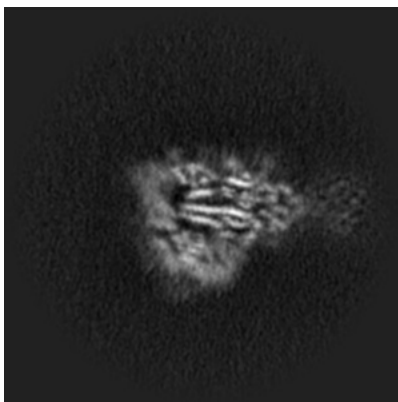
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

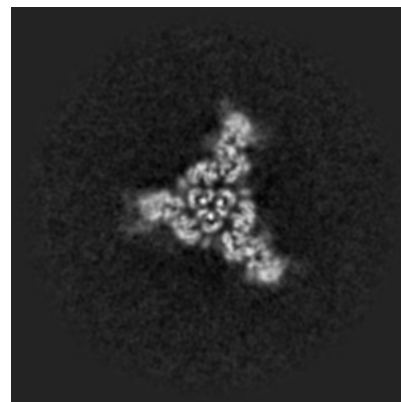
6.3.1 Primary map



X Index: 196

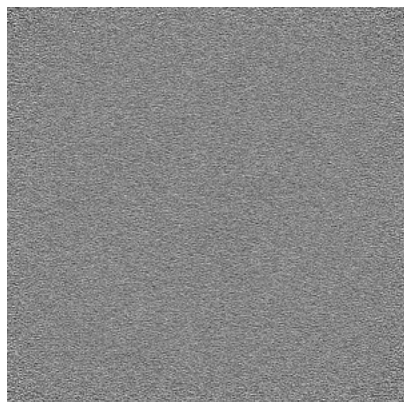


Y Index: 175

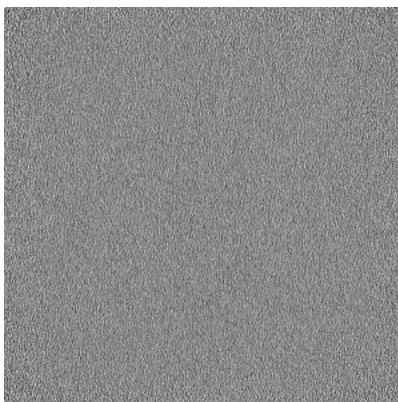


Z Index: 170

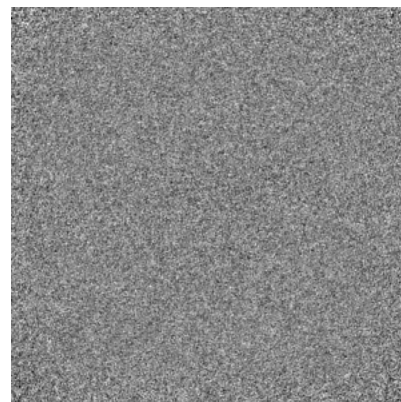
6.3.2 Raw map



X Index: 0



Y Index: 0

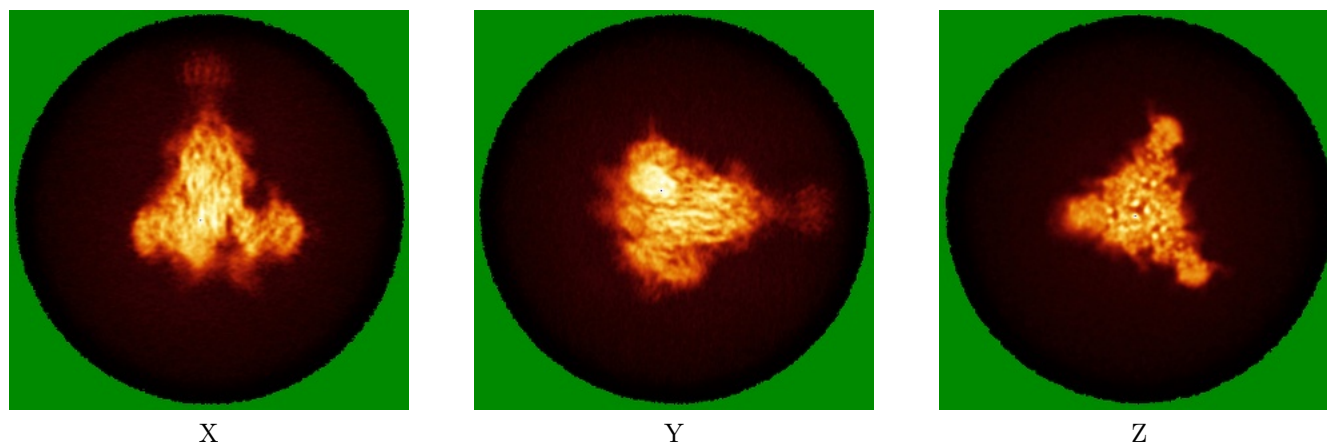


Z Index: 0

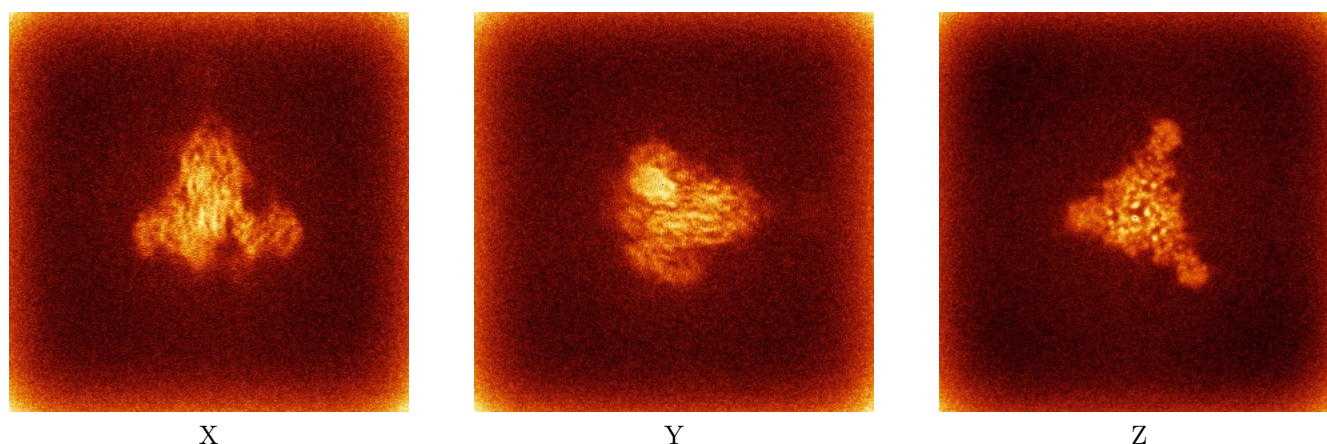
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

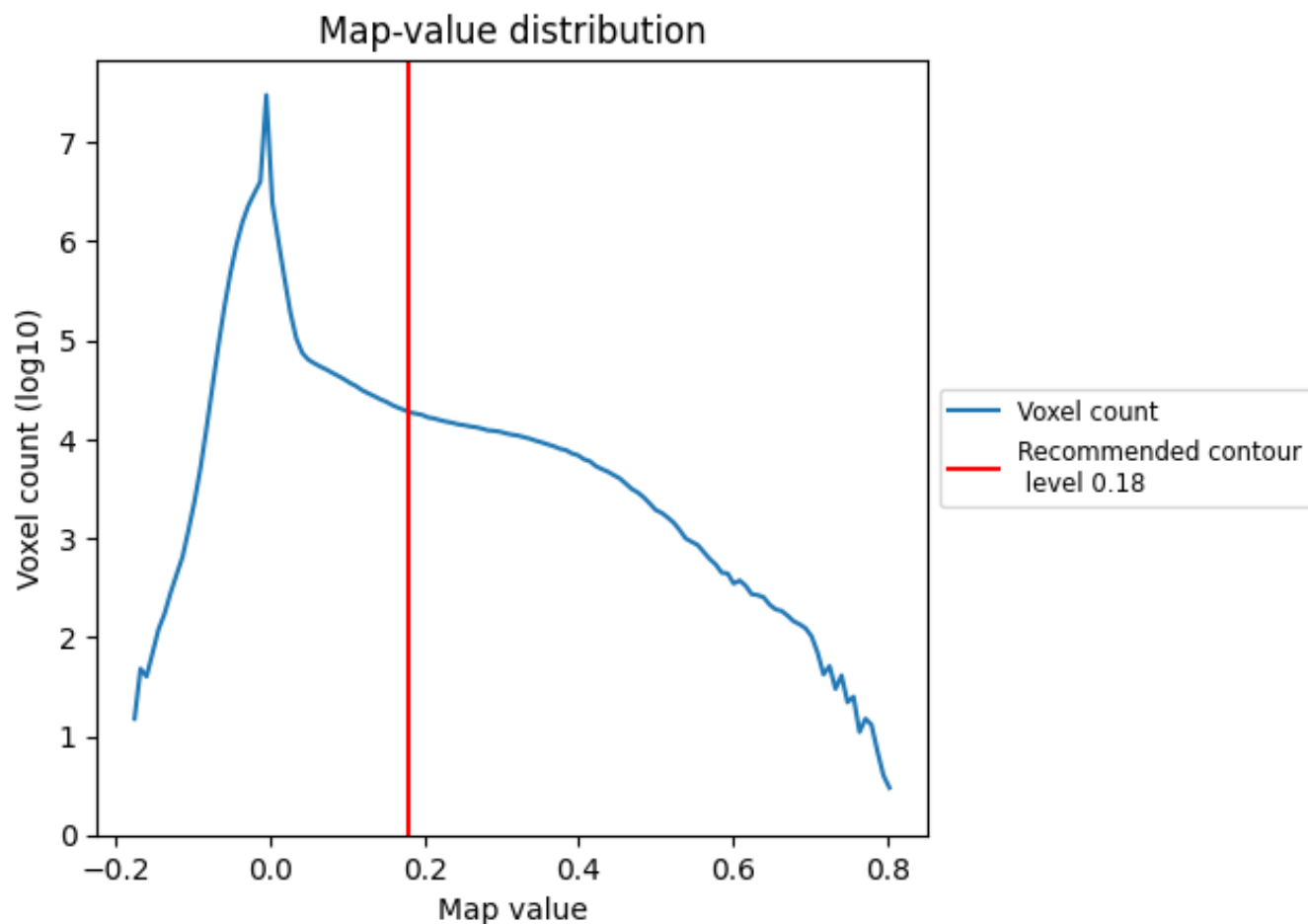
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

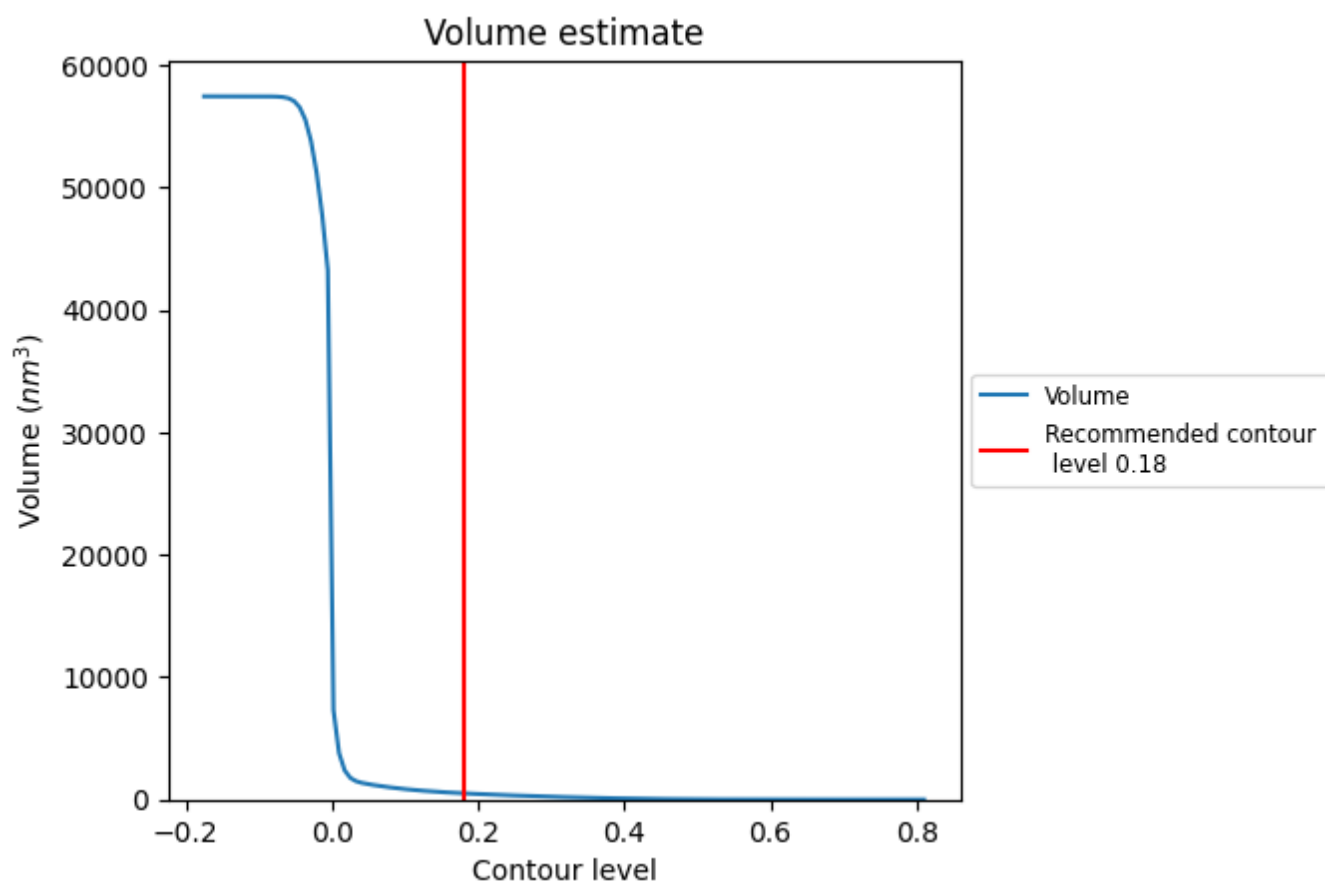
This section contains the results of statistical analysis of the map.

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.

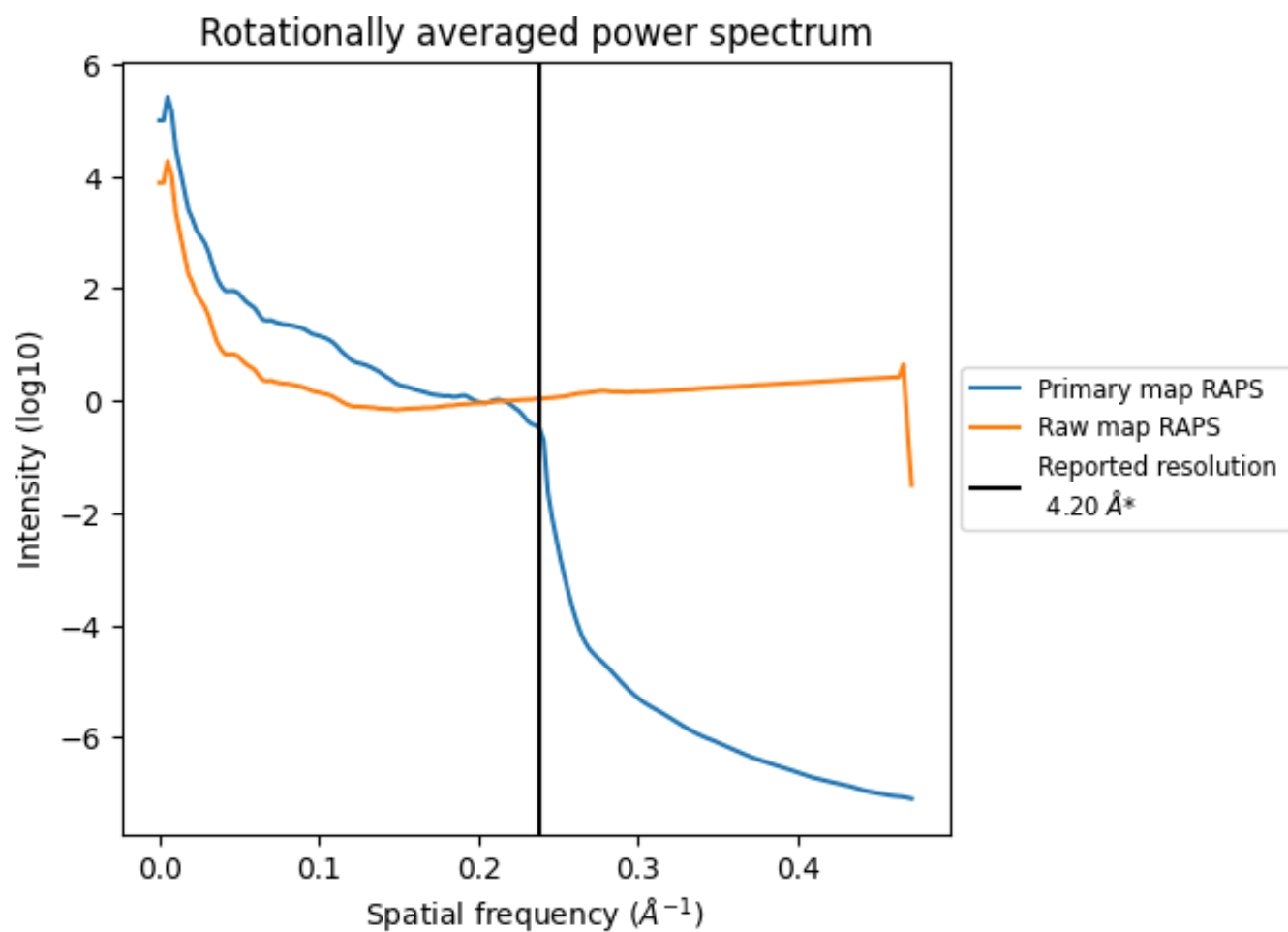
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 511 nm³; this corresponds to an approximate mass of 461 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 ⓘ

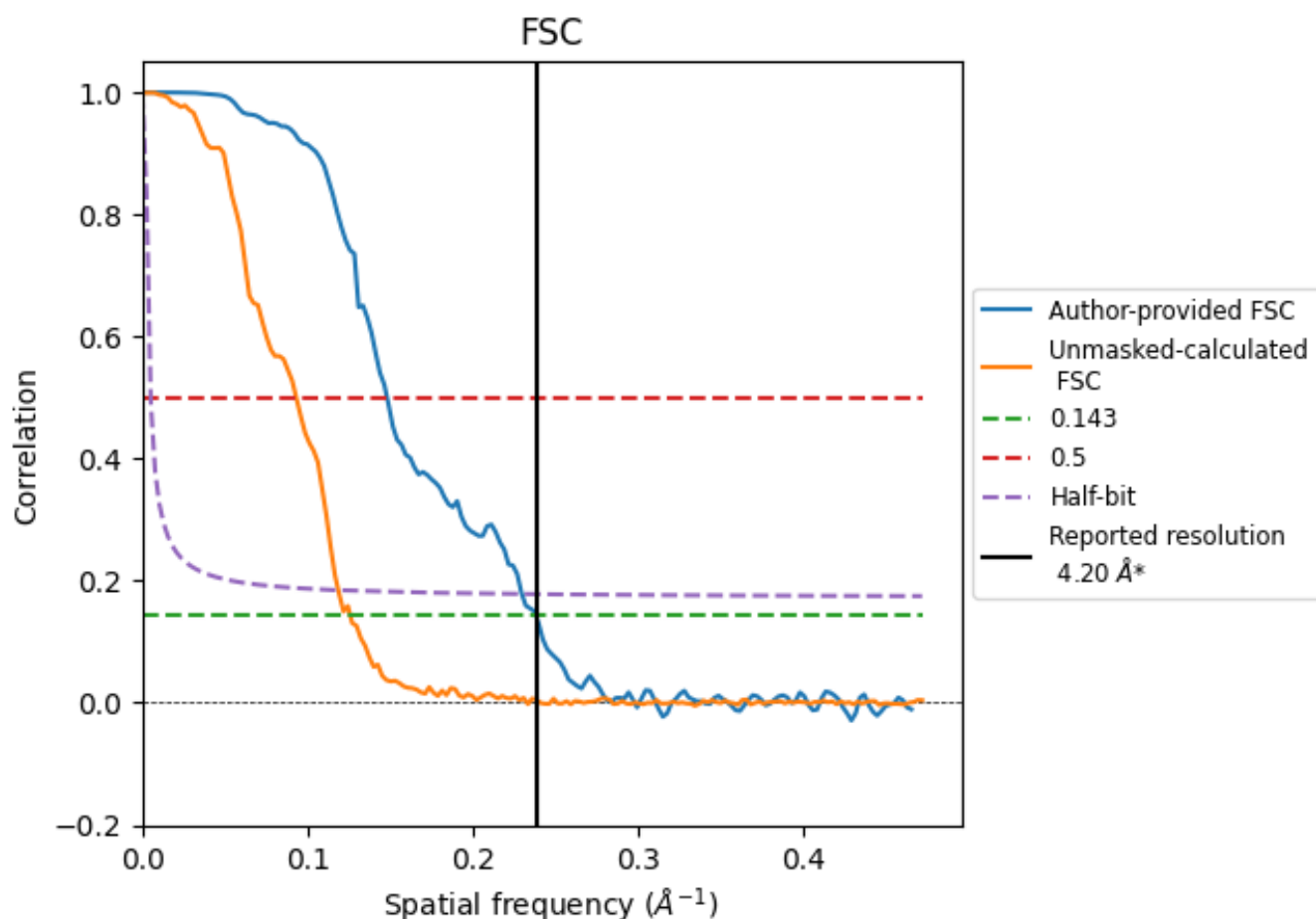


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

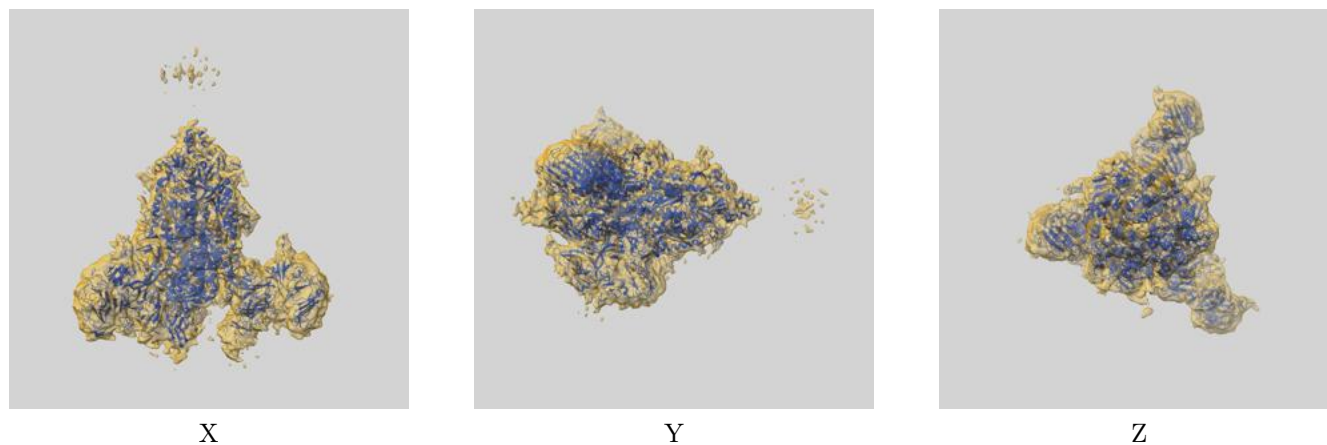
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	6.75	4.36
Unmasked-calculated*	7.95	10.74	8.43

*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 7.95 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

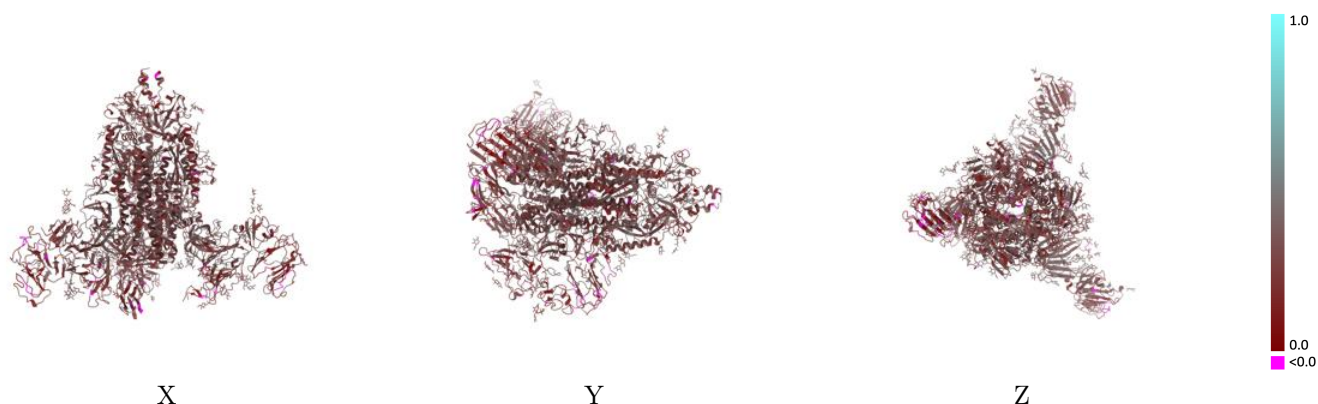
This section contains information regarding the fit between EMDB map EMD-33647 and PDB model 7Y6T. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.18 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](#)



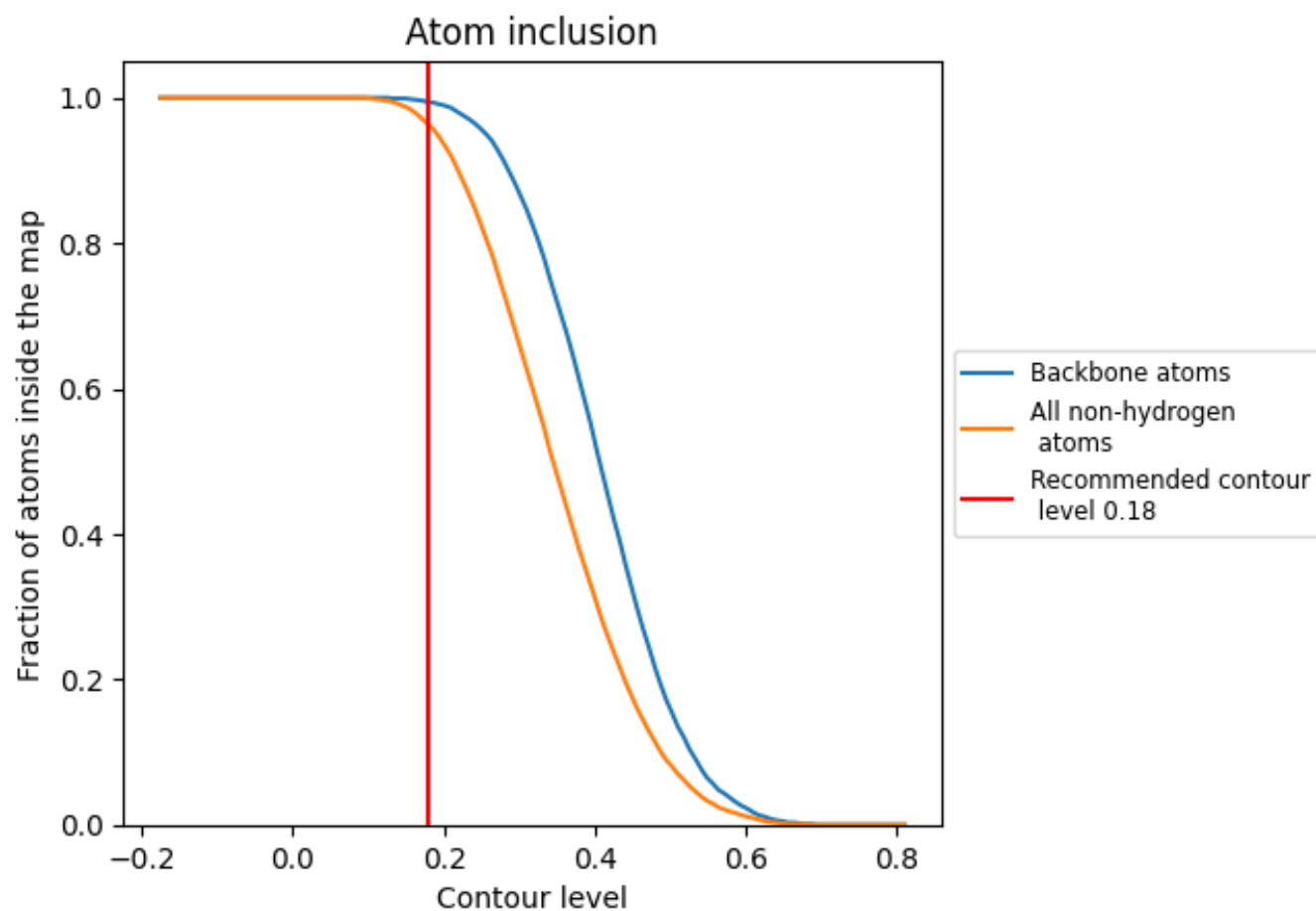
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.2640
A	 0.9590	 0.2440
B	 0.9670	 0.2670
C	 0.9650	 0.2740
D	 0.9840	 0.3490
E	 0.9490	 0.2130
F	 1.0000	 0.3190
G	 0.9740	 0.3540
H	 0.7860	 0.3230
I	 0.9640	 0.3110
J	 0.9290	 0.3290
K	 0.9740	 0.3700
L	 0.7860	 0.2950
M	 0.9740	 0.2390
N	 0.9390	 0.3040
O	 1.0000	 0.3950
P	 0.8750	 0.1870
Q	 0.9490	 0.3760
R	 0.9640	 0.3060
S	 0.9580	 0.2530
T	 0.9740	 0.3620
U	 1.0000	 0.3300
V	 0.9740	 0.3270
W	 0.8930	 0.3130
X	 0.9230	 0.2980
Y	 0.9640	 0.3150
Z	 0.8680	 0.3110
a	 0.9590	 0.3200
b	 1.0000	 0.4180
c	 0.7920	 0.2190
d	 0.9740	 0.3350
e	 0.9290	 0.2700
f	 0.8750	 0.2570
g	 0.9740	 0.3680
h	 1.0000	 0.3410



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 1.0000	 0.3800
j	 0.9740	 0.3870
k	 0.8160	 0.2890