



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 07:48 PM JST

PDB ID : 7WUH
EMDB ID : EMD-32832
Title : SARS-CoV-2 Spike in complex with Fab of m31A7
Authors : Chen, X.; Wu, Y.-M.
Deposited on : 2022-02-08
Resolution : 4.70 Å (reported)
Based on initial model : 7CN9

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:

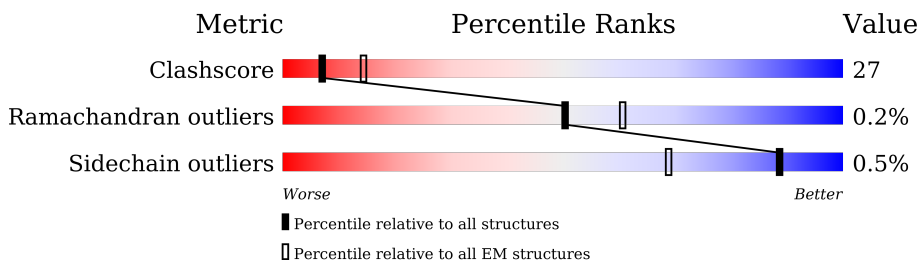
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1242	
1	C	1242	
1	E	1242	
2	D	239	
2	H	239	
2	K	239	
3	F	240	
3	I	240	

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Mol	Chain	Length	Quality of chain
3	L	240	
4	B	3	
4	b	3	
5	G	2	
5	N	2	
5	O	2	
5	P	2	
5	R	2	
5	T	2	
5	V	2	
5	X	2	
6	J	4	
6	Y	4	
7	M	3	
7	Q	3	
7	Z	3	
7	e	3	
8	S	5	
8	W	5	
9	U	5	
10	a	4	
10	g	4	
11	c	2	
12	d	6	
13	f	6	

2 Entry composition i

There are 14 unique types of molecules in this entry. The entry contains 35569 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1038	8062	5137	1354	1535	36	0	0
1	C	1038	8072	5145	1353	1538	36	0	0
1	E	1044	8123	5177	1361	1549	36	0	0

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	GLY	ARG	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	ASP	-	expression tag	UNP P0DTC2
A	1210	ILE	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	LEU	-	expression tag	UNP P0DTC2
A	1214	VAL	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	SER	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	SER	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	ILE	-	expression tag	UNP P0DTC2
A	1225	PRO	-	expression tag	UNP P0DTC2
A	1226	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ALA	-	expression tag	UNP P0DTC2
A	1228	PRO	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLN	-	expression tag	UNP P0DTC2
A	1233	ALA	-	expression tag	UNP P0DTC2
A	1234	TYR	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	ARG	-	expression tag	UNP P0DTC2
A	1237	LYS	-	expression tag	UNP P0DTC2
A	1238	ASP	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLU	-	expression tag	UNP P0DTC2
A	1241	TRP	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	THR	-	expression tag	UNP P0DTC2
A	1247	PHE	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	GLY	ARG	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	ASP	-	expression tag	UNP P0DTC2
C	1210	ILE	-	expression tag	UNP P0DTC2
C	1211	ARG	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	LEU	-	expression tag	UNP P0DTC2
C	1214	VAL	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	SER	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	SER	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	ILE	-	expression tag	UNP P0DTC2
C	1225	PRO	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	ALA	-	expression tag	UNP P0DTC2
C	1228	PRO	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLN	-	expression tag	UNP P0DTC2
C	1233	ALA	-	expression tag	UNP P0DTC2
C	1234	TYR	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	LYS	-	expression tag	UNP P0DTC2
C	1238	ASP	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	GLU	-	expression tag	UNP P0DTC2
C	1241	TRP	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	THR	-	expression tag	UNP P0DTC2
C	1247	PHE	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
E	614	GLY	ASP	engineered mutation	UNP P0DTC2
E	682	GLY	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	683	SER	ARG	variant	UNP P0DTC2
E	685	GLY	ARG	variant	UNP P0DTC2
E	986	PRO	LYS	variant	UNP P0DTC2
E	987	PRO	VAL	variant	UNP P0DTC2
E	1209	ASP	-	expression tag	UNP P0DTC2
E	1210	ILE	-	expression tag	UNP P0DTC2
E	1211	ARG	-	expression tag	UNP P0DTC2
E	1212	SER	-	expression tag	UNP P0DTC2
E	1213	LEU	-	expression tag	UNP P0DTC2
E	1214	VAL	-	expression tag	UNP P0DTC2
E	1215	PRO	-	expression tag	UNP P0DTC2
E	1216	ARG	-	expression tag	UNP P0DTC2
E	1217	GLY	-	expression tag	UNP P0DTC2
E	1218	SER	-	expression tag	UNP P0DTC2
E	1219	PRO	-	expression tag	UNP P0DTC2
E	1220	GLY	-	expression tag	UNP P0DTC2
E	1221	SER	-	expression tag	UNP P0DTC2
E	1222	GLY	-	expression tag	UNP P0DTC2
E	1223	TYR	-	expression tag	UNP P0DTC2
E	1224	ILE	-	expression tag	UNP P0DTC2
E	1225	PRO	-	expression tag	UNP P0DTC2
E	1226	GLU	-	expression tag	UNP P0DTC2
E	1227	ALA	-	expression tag	UNP P0DTC2
E	1228	PRO	-	expression tag	UNP P0DTC2
E	1229	ARG	-	expression tag	UNP P0DTC2
E	1230	ASP	-	expression tag	UNP P0DTC2
E	1231	GLY	-	expression tag	UNP P0DTC2
E	1232	GLN	-	expression tag	UNP P0DTC2
E	1233	ALA	-	expression tag	UNP P0DTC2
E	1234	TYR	-	expression tag	UNP P0DTC2
E	1235	VAL	-	expression tag	UNP P0DTC2
E	1236	ARG	-	expression tag	UNP P0DTC2
E	1237	LYS	-	expression tag	UNP P0DTC2
E	1238	ASP	-	expression tag	UNP P0DTC2
E	1239	GLY	-	expression tag	UNP P0DTC2
E	1240	GLU	-	expression tag	UNP P0DTC2
E	1241	TRP	-	expression tag	UNP P0DTC2
E	1242	VAL	-	expression tag	UNP P0DTC2
E	1243	LEU	-	expression tag	UNP P0DTC2
E	1244	LEU	-	expression tag	UNP P0DTC2
E	1245	SER	-	expression tag	UNP P0DTC2
E	1246	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1247	PHE	-	expression tag	UNP P0DTC2
E	1248	LEU	-	expression tag	UNP P0DTC2
E	1249	GLY	-	expression tag	UNP P0DTC2
E	1250	HIS	-	expression tag	UNP P0DTC2
E	1251	HIS	-	expression tag	UNP P0DTC2
E	1252	HIS	-	expression tag	UNP P0DTC2
E	1253	HIS	-	expression tag	UNP P0DTC2
E	1254	HIS	-	expression tag	UNP P0DTC2
E	1255	HIS	-	expression tag	UNP P0DTC2

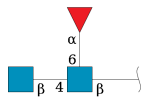
- Molecule 2 is a protein called m31A7 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	218	Total	C	N	O	S	0	0
			1641	1039	265	331	6		
2	H	218	Total	C	N	O	S	0	0
			1641	1039	265	331	6		
2	K	218	Total	C	N	O	S	0	0
			1641	1039	265	331	6		

- Molecule 3 is a protein called m31A7 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	219	Total	C	N	O	S	0	0
			1705	1073	283	343	6		
3	I	219	Total	C	N	O	S	0	0
			1705	1073	283	343	6		
3	L	219	Total	C	N	O	S	0	0
			1705	1073	283	343	6		

- Molecule 4 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.



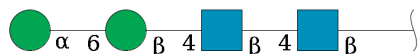
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	B	3	Total	C	N	O	0	0
			38	22	2	14		
4	b	3	Total	C	N	O	0	0
			38	22	2	14		

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



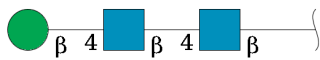
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	2	28	16	2	10	0	0
5	N	2	28	16	2	10	0	0
5	O	2	28	16	2	10	0	0
5	P	2	28	16	2	10	0	0
5	R	2	28	16	2	10	0	0
5	T	2	28	16	2	10	0	0
5	V	2	28	16	2	10	0	0
5	X	2	28	16	2	10	0	0

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



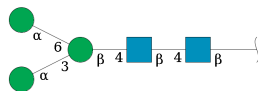
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	J	4	50	28	2	20	0	0
6	Y	4	50	28	2	20	0	0

- Molecule 7 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.



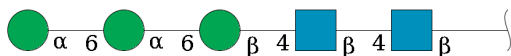
Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	3	Total	C	N	O	0	0
			39	22	2	15		
7	Q	3	Total	C	N	O	0	0
			39	22	2	15		
7	Z	3	Total	C	N	O	0	0
			39	22	2	15		
7	e	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 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.



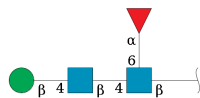
Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	5	Total	C	N	O	0	0
			61	34	2	25		
8	W	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
9	U	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



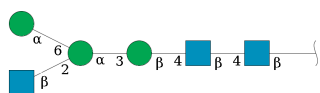
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	a	4	49	28	2	19	0	0
10	g	4	49	28	2	19	0	0

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



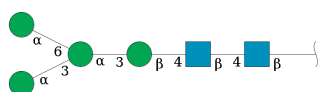
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	c	2	24	14	1	9	0	0

- Molecule 12 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O		
12	d	6	75	42	3	30	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O		
13	f	6	72	40	2	30	0	0

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
14	A	1	Total	C	N	O	0
			70	40	5	25	
14	A	1	Total	C	N	O	0
			70	40	5	25	
14	A	1	Total	C	N	O	0
			70	40	5	25	
14	A	1	Total	C	N	O	0
			70	40	5	25	
14	A	1	Total	C	N	O	0
			70	40	5	25	
14	C	1	Total	C	N	O	0
			112	64	8	40	
14	C	1	Total	C	N	O	0
			112	64	8	40	
14	C	1	Total	C	N	O	0
			112	64	8	40	
14	C	1	Total	C	N	O	0
			112	64	8	40	
14	C	1	Total	C	N	O	0
			112	64	8	40	

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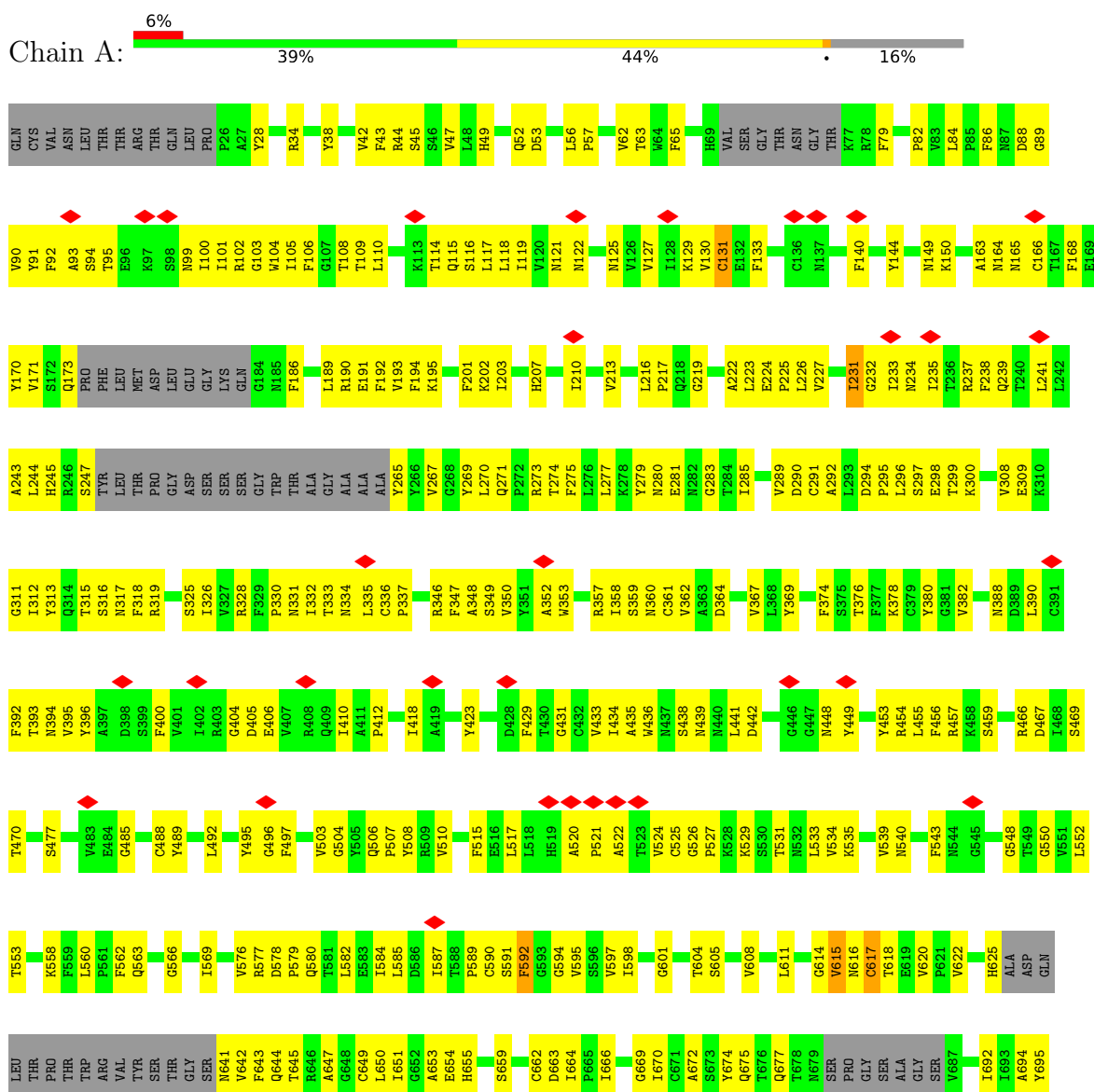
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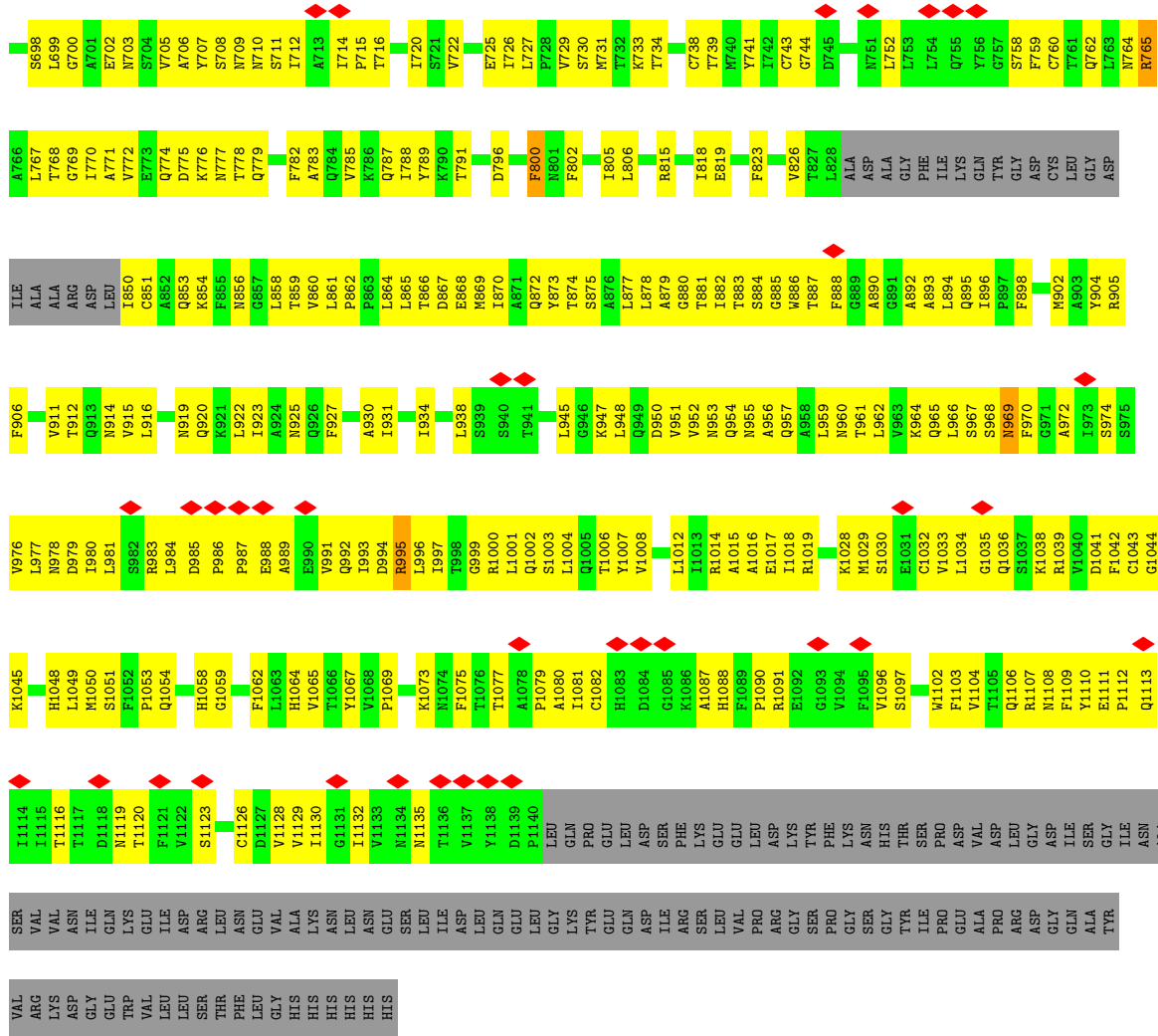
Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	N	O	0
			112	64	8	40	
14	C	1	Total	C	N	O	0
			112	64	8	40	
14	C	1	Total	C	N	O	0
			112	64	8	40	
14	E	1	Total	C	N	O	0
			70	40	5	25	
14	E	1	Total	C	N	O	0
			70	40	5	25	
14	E	1	Total	C	N	O	0
			70	40	5	25	
14	E	1	Total	C	N	O	0
			70	40	5	25	
14	E	1	Total	C	N	O	0
			70	40	5	25	
14	K	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots [i](#)

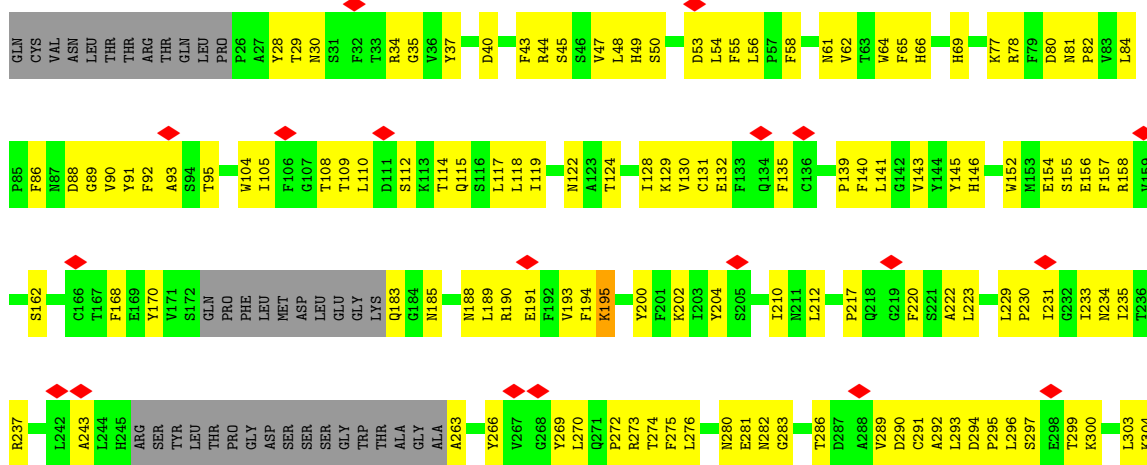
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein

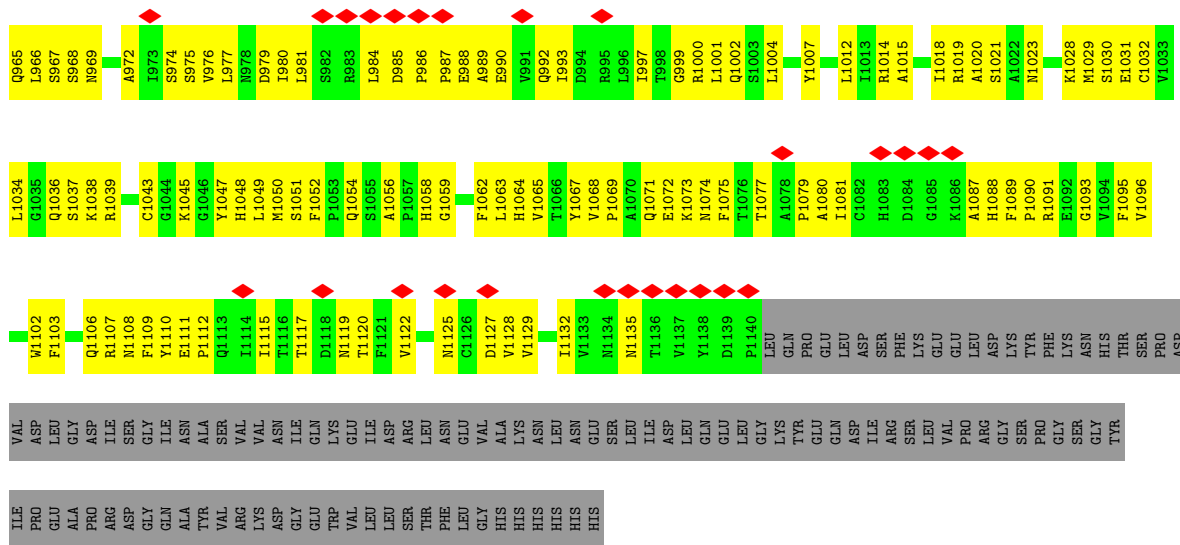


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GLY	Q1106	G1035	V963	ASP	Y756	ALA	S689	F543	I468	C391	I312
ILE	Q1036	K964	ALA	GLY	G757	Q690	Q690	T549	S469	F392	S316
ALA	S1037	Q965	GLY	PHE	S758	Q901	A623	T549	T470	T393	N317
TYR	F1042	S968	ILE	LYS	F759	N902	I1E	G480	N994	N994	F318
VAL	C1043	N969	LYS	GLN	C760	N903	HIS	M481	V396	V396	R319
ARG	Y1047	N970	GLN	TYR	T761	G904	ALA	M482	Y397	Y397	T323
LYS	H1048	G971	TYR	ASP	Q762	V995	ASP	G482	A397	A397	I326
ASP	L1049	F906	GLY	TYR	L763	T696	GLN	V483	D398	D398	R328
GLU	M1050	N907	ASP	ASP	N764	M697	THR	F484	S399	S399	M331
TRP	S1051	G908	CYS	CYS	N765	M697	THR	G485	F400	F400	I332
VAL	F1052	I909	LEU	LEU	A766	S898	THR	G486	I401	I401	T333
LEU	F1053	G910	GLY	GLY	L767	L699	THR	M487	I402	I402	
LEU	V1121	V911	ASP	ASP	I770	G700	TRP	C488	R403	R403	
SER	V1122	T912	ILE	ASP	E773	A701	ARG	P491	G404	G404	
THR	S1123	Q913	ALA	ALA	O774	E702	VAL	L492	D405	D405	
PHE	G1124	N914	ARG	ASP	O775	N703	VAL	L492	E406	E406	
LEU	N1125	V915	ASP	ASP	A706	V705	VAL	Q493	V407	V407	
GLY	C1126	K776	ASP	ASP	E776	V706	VAL	G496	R408	R408	
HIS	D1127	K776	LEU	ASP	I777	Y707	VAL	P499	A411	A411	
HIS	V1128	N777	LEU	ILE	O778	Y707	VAL	T500	P412	P412	
HIS	V1129	E918	ILE	CYS	I778	Y707	VAL	R577	G413	G413	
HIS	I1130	N819	ALA	ALA	Q779	M710	VAL	N501	Q414	Q414	
HIS	N1134	Q920	GLN	GLN	E780	I712	VAL	G502	I418	I418	
GLY	ASN	L922	R654	R654	F781	I714	VAL	G503	M222	M222	
SER	THR	I923	F855	F855	A783	P715	VAL	G504	P426	P426	
LEU	THR	A924	N856	N856	Q784	L582	VAL	Y505	D427	D427	
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LEU	E1072	G932	M869	M869	T791	V729	VAL	Y511	V436	V436	
PRO	K1073	G933	M869	M869	I791	V729	VAL	Y511	M437	M437	
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GLY	Q1002	Q935	T874	T874	D796	V729	VAL	Y511	S443	S443	
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ASP	L1006	L938	A876	A876	N801	T732	VAL	Y511	G447	G447	
GLY	Y1007	S939	L877	L877	F802	T734	VAL	Y511	M448	M448	
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LEU	T1009	T941	A879	A879	Q804	T736	VAL	Y511	M450	M450	
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ARG	L1012	G947	T882	T882	K811	T739	VAL	Y511	F456	F456	
GLY	H1088	L948	T883	T883	P812	M740	VAL	Y511	K378	K378	
GLY	F1089	Q949	S884	S884	S816	M740	VAL	Y511	C379	C379	
PRO	P1090	Q950	G885	G885	F817	I742	VAL	Y511	Y380	Y380	
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SER	T1093	N953	T887	T887	C744	C744	VAL	Y511	K386	K386	
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ASP	V1096	Q957	G889	G889	S746	S746	VAL	Y511	E465	E465	
VAL	M1097	A958	A890	A890	C749	C749	VAL	Y511			
GLU	M1098	Q957	G891	G891	S750	S750	VAL	Y511			
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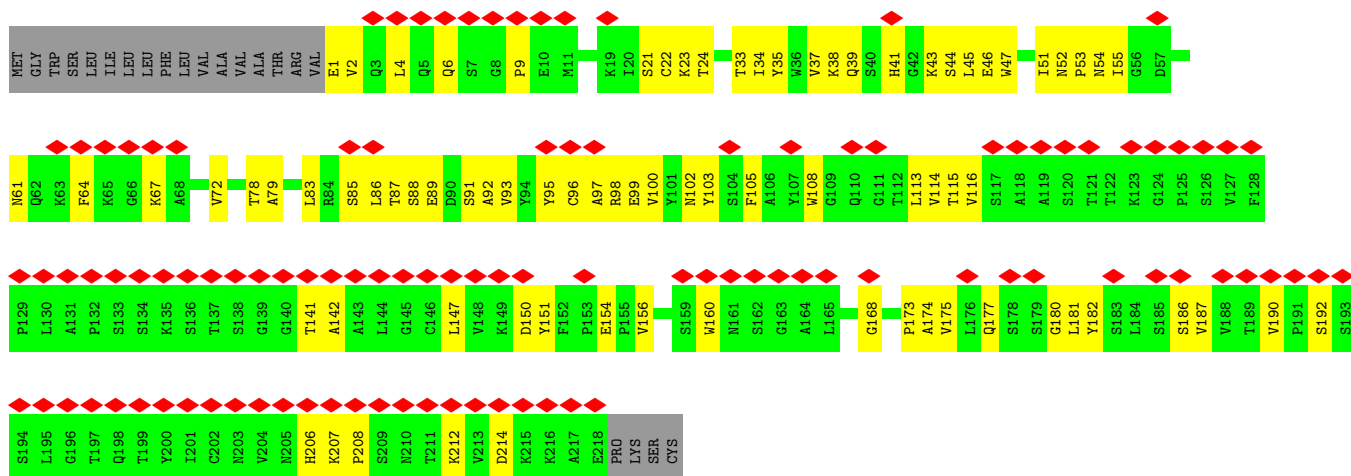
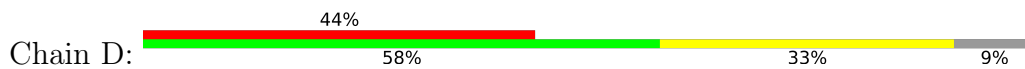
• Molecule 1: Spike glycoprotein



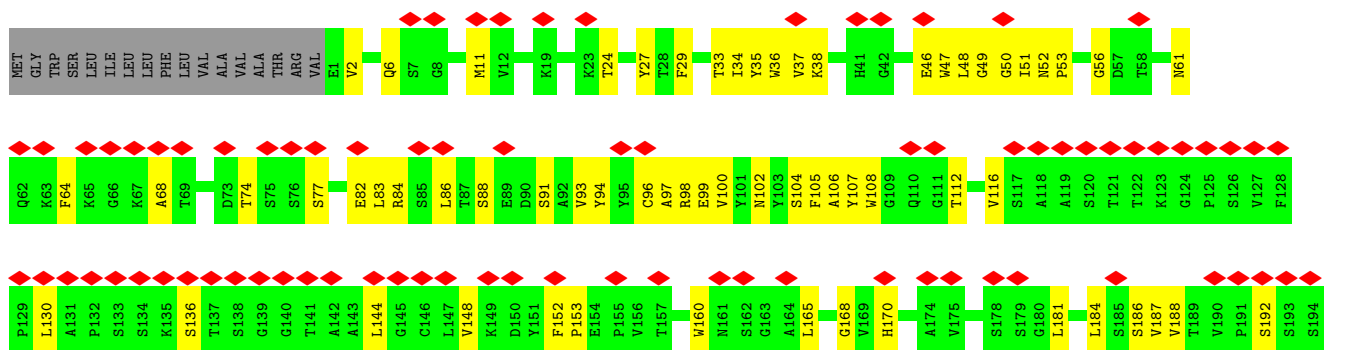
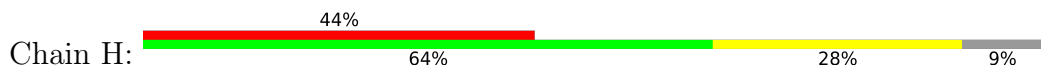
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T95	E96	K97	S98	R99	I100	I101	R102	SER	G103	LEU	W104	T33	LEU	W105	R34	F106	G107	T108	Y37	Y38	F43	R44	V47	L48	H49	S50	T51	G52	D53	L54	F55	L56	P57	F58	W64	I128	P65	H66	A67	H68	V70	S71	GLY	THR	THR	THR	LYS	R78	F79	D80	N81	P82	P85	P86	V90	Y91	N165	F92	A93	S94					
Y170	V171	S172	GLN	PRO	PHE	LEU	MET	ASP	F400	GLU	LEU	GLY	F106	G107	T108	Q183	L189	R190	E191	F192	V193	F194	K195	D198	G199	Y200	K201	L203	Y204	K206	S205	Y206	Q271	K272	R273	T274	F275	P269	I210	ASN	LEU	VAL	R214	D215	Q218	G219	F220	S221	A222	L223	E224	P225	D228	L229	P295	D294	L296	S297	I231	G232	I233	N234	K300	L303	T236
R237	F238	L241	L242	H245	ARG	SER	TYR	LEU	THR	THR	GLY	Q183	L189	R190	E191	F192	V193	F194	K195	D198	G199	Y200	K201	L203	Y204	K206	S205	Y206	Q271	K272	R273	T274	F275	P269	I210	ASN	LEU	VAL	R214	D215	Q218	G219	F220	S221	A222	L223	E224	P225	D228	L229	P295	D294	L296	S297	I231	G232	I233	N234	K300	L303	T236				
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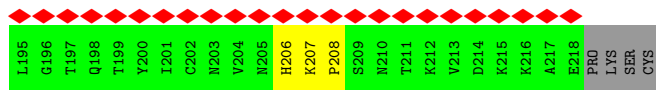


• Molecule 2: m31A7 Fab heavy chain

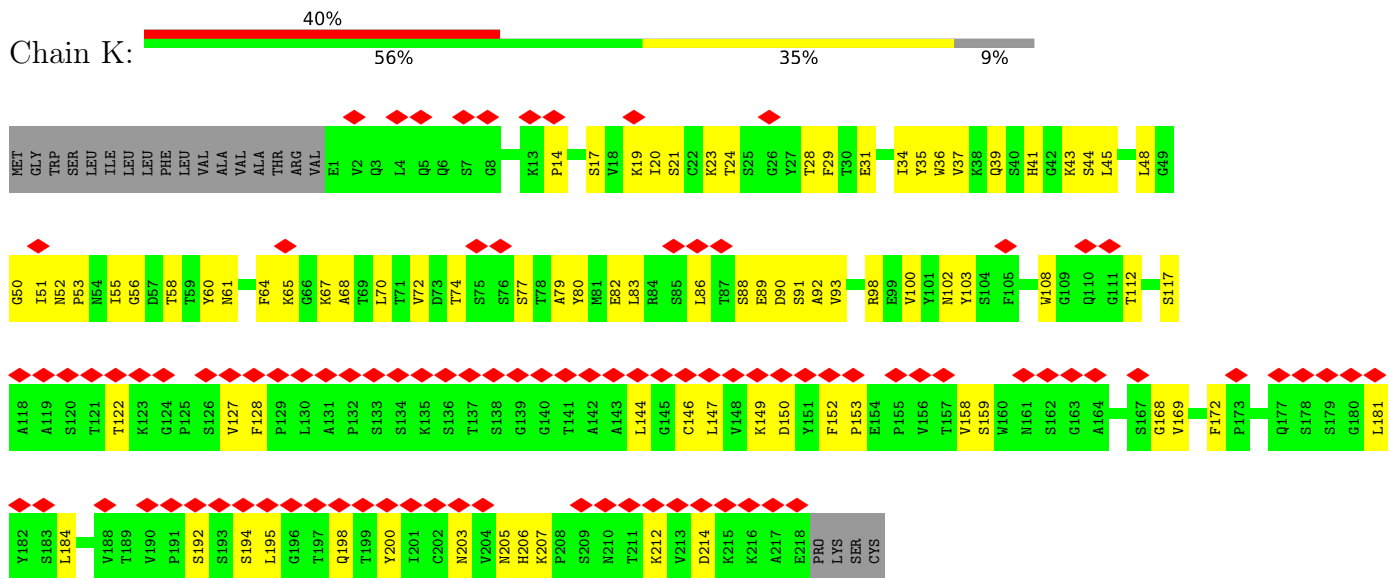


• Molecule 2: m31A7 Fab heavy chain

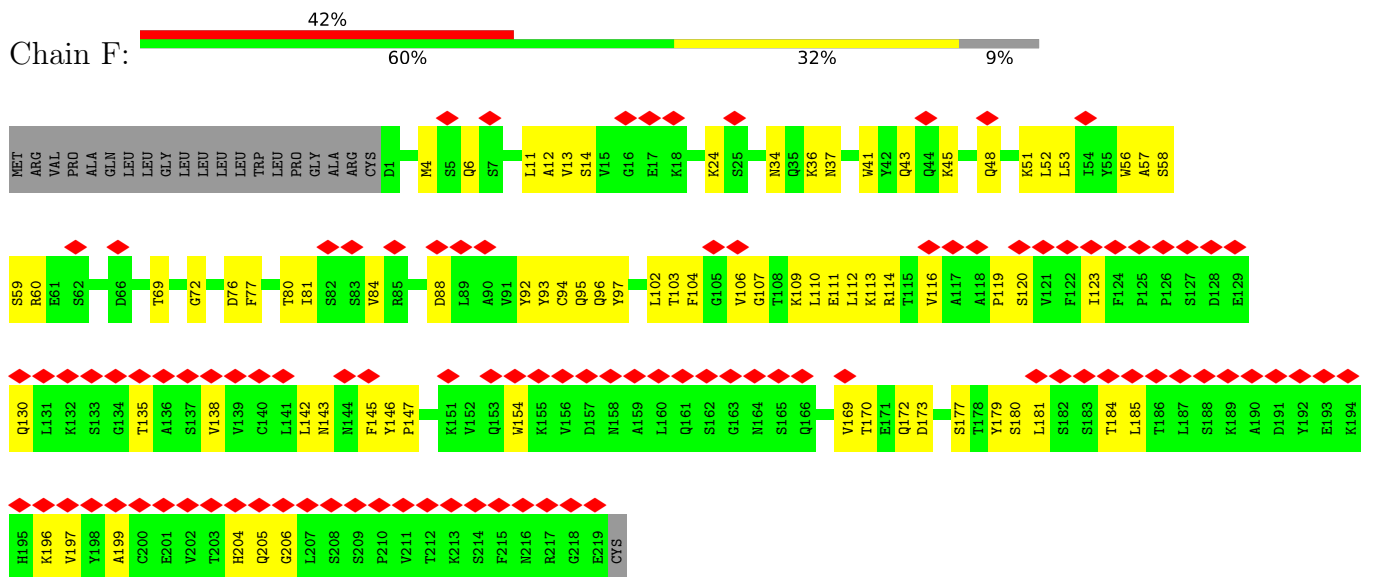




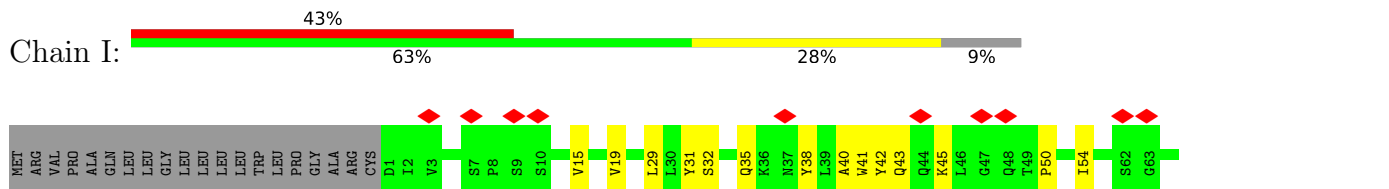
• Molecule 2: m31A7 Fab heavy chain

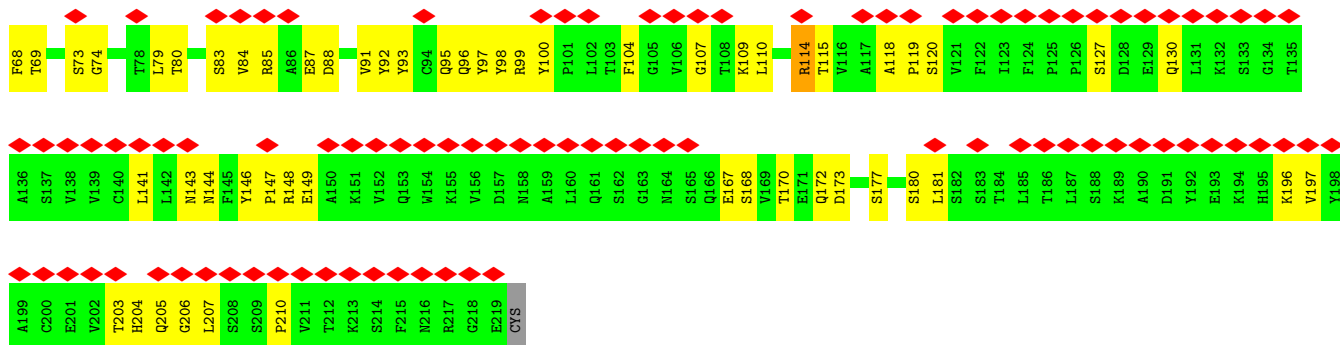


• Molecule 3: m31A7 Fab light chain

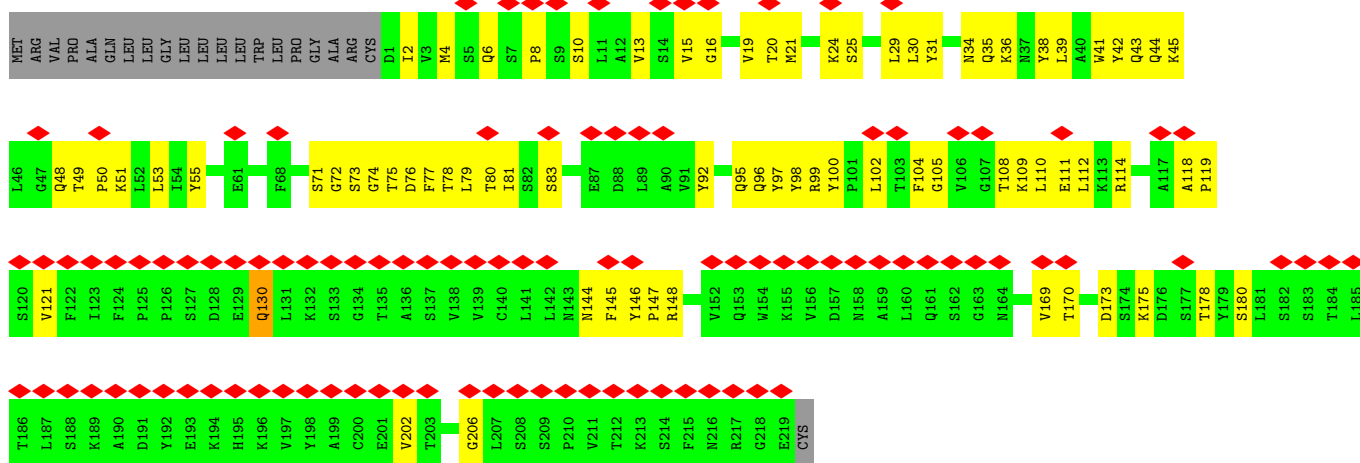
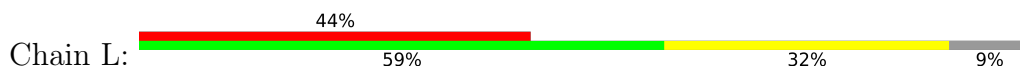


• Molecule 3: m31A7 Fab light chain





- Molecule 3: m31A7 Fab light chain



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



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



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





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

Chain N:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  100%



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

Chain R:  50% 50%

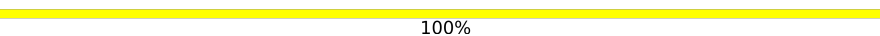


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



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

Chain V:  100%

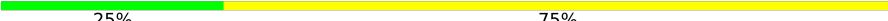


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1
MAG2

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

Chain J:  25% 75%

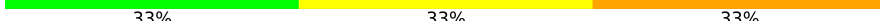
MAG1
MAG2
BMA3
MAN4

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

Chain Y:  50% 50%

MAG1
MAG2
BMA3
MAN4

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 33% 33%

MAG1
MAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  67% 33%

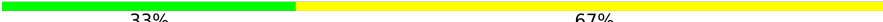
MAG1
MAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

MAG1
MAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  33% 67%




- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  60% 40%

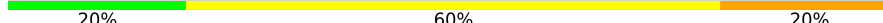


- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  20% 40% 40%



- Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  20% 60% 20%



- Molecule 10: 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:  50% 50%



- Molecule 10: 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 g:  75% 25%

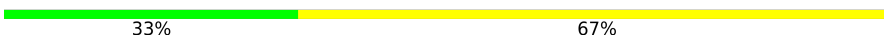


- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%

MAG1
FUC2

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  33% 67%

MAG1
MAG2
BMA3
MAN4
MAG5
MAN6

- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  17% 83%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108565	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 ($e^-/\text{\AA}^2$)	1.1	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	11.642	Depositor
Minimum map value	-3.915	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.385	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	315.4, 315.4, 315.4	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: BMA, NAG, MAN, FUC

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	0.31	0/8245	0.56	0/11227
1	C	0.31	0/8256	0.57	1/11234 (0.0%)
1	E	0.30	0/8308	0.55	1/11306 (0.0%)
2	D	0.26	0/1681	0.51	0/2292
2	H	0.27	0/1681	0.51	0/2292
2	K	0.26	0/1681	0.50	0/2292
3	F	0.26	0/1741	0.52	0/2361
3	I	0.26	0/1741	0.55	0/2361
3	L	0.27	0/1741	0.51	0/2361
All	All	0.29	0/35075	0.55	2/47726 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	995	ARG	CA-CB-CG	5.79	126.15	113.40
1	E	571	ASP	CB-CG-OD1	5.12	122.90	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	CYS	Peptide
1	A	800	PHE	Peptide

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	8062	0	7808	563	0
1	C	8072	0	7852	528	0
1	E	8123	0	7890	537	0
2	D	1641	0	1604	69	0
2	H	1641	0	1603	56	0
2	K	1641	0	1603	59	0
3	F	1705	0	1669	71	0
3	I	1705	0	1669	56	0
3	L	1705	0	1669	67	0
4	B	38	0	32	3	0
4	b	38	0	34	0	0
5	G	28	0	25	0	0
5	N	28	0	25	2	0
5	O	28	0	25	1	0
5	P	28	0	25	5	0
5	R	28	0	25	0	0
5	T	28	0	25	1	0
5	V	28	0	25	2	0
5	X	28	0	25	2	0
6	J	50	0	43	1	0
6	Y	50	0	43	6	0
7	M	39	0	34	2	0
7	Q	39	0	34	1	0
7	Z	39	0	34	0	0
7	e	39	0	34	0	0
8	S	61	0	52	3	0
8	W	61	0	52	2	0
9	U	61	0	52	2	0
10	a	49	0	43	0	0
10	g	49	0	43	0	0
11	c	24	0	22	0	0
12	d	75	0	63	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	f	72	0	61	0	0
14	A	70	0	65	1	0
14	C	112	0	104	5	0
14	E	70	0	65	4	0
14	K	14	0	13	0	0
All	All	35569	0	34490	1880	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 27.

All (1880) 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:591:SER:O	1:A:615:VAL:HG13	1.48	1.12
1:A:591:SER:C	1:A:615:VAL:HG13	1.77	1.04
1:C:866:THR:H	1:C:869:MET:HE2	1.31	0.96
1:A:591:SER:CA	1:A:615:VAL:HG13	1.96	0.95
1:C:1028:LYS:O	1:C:1032:CYS:HB3	1.68	0.93
1:A:591:SER:CA	1:A:615:VAL:CG1	2.47	0.92
1:A:591:SER:HA	1:A:615:VAL:CG1	2.01	0.90
1:A:659:SER:HA	1:A:695:TYR:HB2	1.50	0.90
2:D:6:GLN:NE2	2:D:22:CYS:SG	2.47	0.87
2:H:100:VAL:HG12	2:H:102:ASN:H	1.41	0.86
1:A:350:VAL:HG21	1:A:418:ILE:HD12	1.57	0.86
1:C:882:ILE:HG23	1:C:883:THR:HG23	1.56	0.86
1:A:712:ILE:HG13	1:E:896:ILE:HG22	1.58	0.85
1:A:865:LEU:HA	1:A:869:MET:HE3	1.57	0.84
1:A:1087:ALA:HB2	1:A:1126:CYS:HB3	1.57	0.84
1:E:710:ASN:HD21	1:E:1077:THR:H	1.23	0.83
1:C:80:ASP:OD1	1:C:81:ASN:N	2.12	0.83
1:E:396:TYR:H	1:E:514:SER:HB3	1.41	0.83
1:E:883:THR:O	1:E:896:ILE:N	2.10	0.83
1:C:1028:LYS:HE3	1:C:1043:CYS:HA	1.61	0.82
1:E:388:ASN:HD21	1:E:528:LYS:HG3	1.45	0.82
1:A:782:PHE:HA	1:A:877:LEU:HD11	1.61	0.82
1:C:1002:GLN:OE1	1:C:1005:GLN:NE2	2.13	0.82
1:A:969:ASN:HB2	1:A:972:ALA:HB3	1.62	0.82
1:C:576:VAL:HG22	1:C:587:ILE:HD11	1.62	0.81
1:A:42:VAL:O	1:A:44:ARG:NH1	2.13	0.81
1:A:330:PRO:HG3	1:A:579:PRO:HB2	1.62	0.81
2:D:23:LYS:HA	2:D:78:THR:HG21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:SER:HA	1:A:1034:LEU:HD13	1.63	0.80
1:C:438:SER:HB2	1:C:507:PRO:HB2	1.64	0.80
3:F:45:LYS:HB2	3:F:48:GLN:HB2	1.63	0.80
1:C:650:LEU:HD21	1:C:653:ALA:HB3	1.64	0.80
1:A:591:SER:HA	1:A:615:VAL:HG13	1.61	0.80
1:C:296:LEU:HD23	1:C:608:VAL:HG12	1.64	0.79
1:A:916:LEU:O	1:A:920:GLN:HB3	1.83	0.79
3:L:2:ILE:HD11	3:L:25:SER:HB2	1.65	0.79
1:C:1073:LYS:NZ	1:C:1097:SER:O	2.14	0.78
1:A:708:SER:HB2	1:E:796:ASP:HB3	1.65	0.78
1:E:937:SER:HA	1:E:941:THR:HB	1.66	0.78
1:E:598:ILE:HG12	1:E:672:ALA:HB3	1.64	0.78
3:F:72:GLY:HA3	3:F:77:PHE:HA	1.65	0.78
1:A:861:LEU:HD12	1:A:862:PRO:HD2	1.66	0.78
1:A:895:GLN:NE2	1:C:711:SER:OG	2.14	0.77
1:E:941:THR:HG22	1:E:943:SER:H	1.49	0.77
1:A:106:PHE:HB2	1:A:117:LEU:HD13	1.67	0.77
1:A:193:VAL:HG12	1:A:223:LEU:HD23	1.65	0.77
1:E:866:THR:H	1:E:869:MET:HE2	1.50	0.76
1:E:577:ARG:NH1	1:E:583:GLU:O	2.18	0.76
2:K:24:THR:OG1	2:K:77:SER:O	2.04	0.76
1:E:729:VAL:H	1:E:1059:GLY:HA2	1.51	0.76
3:I:29:LEU:O	3:I:35:GLN:NE2	2.18	0.76
1:A:984:LEU:HD23	1:A:988:GLU:HB3	1.68	0.76
1:A:739:THR:O	1:A:743:CYS:N	2.18	0.76
1:E:100:ILE:HA	1:E:102:ARG:HH21	1.50	0.75
1:E:273:ARG:NH2	1:E:290:ASP:OD2	2.19	0.75
3:L:43:GLN:HG3	3:L:53:LEU:HD11	1.66	0.75
1:C:758:SER:O	1:C:762:GLN:NE2	2.19	0.75
1:E:277:LEU:HB3	1:E:279:TYR:HE1	1.51	0.75
1:A:226:LEU:HD23	1:A:227:VAL:HG23	1.68	0.75
1:A:598:ILE:HG12	1:A:672:ALA:HB3	1.68	0.75
1:C:779:GLN:NE2	1:C:783:ALA:O	2.20	0.75
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	1.69	0.74
1:C:739:THR:HA	1:C:753:LEU:HD23	1.70	0.74
1:C:977:LEU:HD13	1:C:996:LEU:HB3	1.68	0.74
1:E:55:PHE:O	1:E:271:GLN:N	2.20	0.74
1:E:1028:LYS:O	1:E:1032:CYS:HB3	1.87	0.74
1:A:864:LEU:HD11	1:C:665:PRO:HB2	1.69	0.74
1:C:355:ARG:NH2	1:C:464:PHE:O	2.21	0.74
3:I:45:LYS:NZ	3:I:87:GLU:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:44:GLN:NE2	3:L:48:GLN:O	2.19	0.74
1:A:977:LEU:O	1:A:981:LEU:N	2.19	0.73
1:A:1036:GLN:NE2	1:A:1048:HIS:O	2.21	0.73
1:E:330:PRO:HB3	1:E:580:GLN:HB3	1.69	0.73
1:A:168:PHE:HA	1:C:357:ARG:HH22	1.53	0.73
1:C:294:ASP:OD1	1:C:297:SER:N	2.21	0.73
3:F:109:LYS:NZ	3:F:111:GLU:OE2	2.21	0.73
1:A:591:SER:HA	1:A:615:VAL:HG12	1.71	0.73
1:A:1039:ARG:NH1	1:E:1031:GLU:OE2	2.20	0.73
1:C:779:GLN:O	1:C:783:ALA:N	2.22	0.73
1:C:969:ASN:ND2	1:C:974:SER:O	2.21	0.73
3:I:114:ARG:NH1	3:I:115:THR:OG1	2.21	0.73
3:L:29:LEU:H	3:L:74:GLY:HA2	1.52	0.73
1:A:1107:ARG:HB3	1:E:886:TRP:HZ2	1.53	0.73
1:C:115:GLN:NE2	9:U:1:NAG:O7	2.21	0.73
2:H:47:TRP:O	2:H:61:ASN:ND2	2.21	0.72
1:E:1091:ARG:NH1	1:E:1119:ASN:O	2.21	0.72
2:K:108:TRP:HB2	3:L:49:THR:HB	1.72	0.72
1:A:34:ARG:NH2	1:A:217:PRO:O	2.22	0.72
3:F:146:TYR:HD1	3:F:179:TYR:HE2	1.37	0.72
1:A:887:THR:HG21	1:A:894:LEU:HB2	1.71	0.72
1:E:779:GLN:NE2	1:E:783:ALA:O	2.22	0.72
2:H:35:TYR:HD1	2:H:50:GLY:HA3	1.54	0.72
1:C:117:LEU:HA	1:C:130:VAL:HA	1.70	0.72
1:E:676:THR:HA	1:E:690:GLN:HA	1.70	0.72
1:E:980:ILE:O	1:E:992:GLN:NE2	2.22	0.72
2:D:83:LEU:HD23	2:D:86:LEU:HD21	1.69	0.72
1:A:707:TYR:HD2	1:E:792:PRO:HB3	1.55	0.71
1:E:1019:ARG:HD3	1:E:1023:ASN:HD21	1.54	0.71
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.72	0.71
2:H:105:PHE:O	3:I:42:TYR:OH	2.07	0.71
3:I:43:GLN:NE2	3:I:91:VAL:O	2.21	0.71
1:C:767:LEU:HA	1:C:770:ILE:HD12	1.71	0.71
1:C:140:PHE:HB2	1:C:243:ALA:HA	1.70	0.71
1:C:984:LEU:HD22	1:C:992:GLN:HG2	1.71	0.71
1:C:1106:GLN:NE2	1:C:1111:GLU:OE1	2.23	0.71
2:H:53:PRO:HB2	2:H:74:THR:HG22	1.72	0.71
3:L:15:VAL:HG13	3:L:83:SER:HA	1.73	0.71
1:E:200:TYR:HB3	1:E:230:PRO:HA	1.72	0.71
1:C:861:LEU:HD12	1:C:862:PRO:HD2	1.71	0.71
1:C:391:CYS:HB3	1:C:525:CYS:HA	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:TYR:HA	1:E:461:LEU:HD12	1.73	0.71
1:A:644:GLN:NE2	1:A:645:THR:O	2.24	0.71
1:A:1036:GLN:HE21	1:A:1049:LEU:HA	1.55	0.71
1:C:1036:GLN:NE2	1:C:1048:HIS:O	2.23	0.71
2:D:4:LEU:HD11	2:D:24:THR:HG22	1.73	0.71
1:C:356:LYS:HB3	1:C:397:ALA:HB3	1.70	0.70
1:A:729:VAL:H	1:A:1059:GLY:HA2	1.57	0.70
1:A:952:VAL:HA	1:A:955:ASN:HD22	1.54	0.70
1:C:326:ILE:HG23	1:C:532:ASN:HB2	1.73	0.70
1:C:598:ILE:HG12	1:C:672:ALA:HB3	1.73	0.70
1:C:884:SER:HA	1:C:895:GLN:HA	1.74	0.70
1:E:676:THR:OG1	1:E:690:GLN:NE2	2.25	0.70
1:C:84:LEU:HB3	1:C:269:TYR:CE1	2.27	0.70
1:C:200:TYR:HE1	1:C:202:LYS:HE3	1.54	0.70
1:E:193:VAL:HB	1:E:223:LEU:HD11	1.71	0.70
3:F:111:GLU:HB3	3:F:146:TYR:HE1	1.56	0.70
3:I:167:GLU:HB2	3:I:181:LEU:HD11	1.74	0.70
1:A:669:GLY:HA3	1:E:869:MET:HE3	1.73	0.70
1:A:711:SER:OG	1:E:895:GLN:NE2	2.25	0.70
1:C:44:ARG:HE	1:C:49:HIS:CE1	2.10	0.70
2:H:36:TRP:HB2	2:H:48:LEU:HD11	1.74	0.70
1:E:533:LEU:HD22	1:E:539:VAL:HG21	1.73	0.69
1:A:331:ASN:OD1	1:A:332:ILE:N	2.25	0.69
1:A:525:CYS:SG	1:A:526:GLY:N	2.64	0.69
1:A:563:GLN:HB3	1:A:577:ARG:CZ	2.23	0.69
2:D:177:GLN:HG3	2:D:180:GLY:H	1.57	0.69
1:A:591:SER:C	1:A:615:VAL:CG1	2.60	0.69
1:C:379:CYS:H	1:C:384:PRO:HD3	1.58	0.69
1:E:189:LEU:HB3	1:E:208:THR:HG23	1.73	0.69
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.73	0.69
1:C:958:ALA:O	1:C:961:THR:OG1	2.10	0.69
1:E:905:ARG:HH21	1:E:1036:GLN:HB2	1.57	0.69
1:A:604:THR:HG22	1:A:605:SER:H	1.57	0.69
1:A:978:ASN:HA	1:A:981:LEU:HD12	1.73	0.69
1:C:782:PHE:HA	1:C:877:LEU:HD21	1.73	0.69
1:E:328:ARG:NH1	1:E:528:LYS:O	2.25	0.69
1:A:887:THR:OG1	1:A:892:ALA:O	2.10	0.69
1:C:880:GLY:O	1:C:885:GLY:N	2.20	0.69
2:D:4:LEU:HD23	2:D:22:CYS:HB3	1.75	0.69
1:A:992:GLN:HG3	1:A:993:ILE:HD12	1.75	0.69
1:C:715:PRO:HG3	1:C:1069:PRO:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:HD11	1:A:585:LEU:HD21	1.75	0.69
1:E:993:ILE:O	1:E:997:ILE:HG12	1.93	0.69
1:A:819:GLU:OE2	1:A:1054:GLN:NE2	2.26	0.68
1:E:706:ALA:O	1:E:711:SER:OG	2.08	0.68
2:D:9:PRO:HB3	2:D:113:LEU:HB3	1.75	0.68
1:A:295:PRO:HB3	1:A:597:VAL:HG21	1.74	0.68
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.74	0.68
1:E:350:VAL:HA	1:E:400:PHE:HB2	1.74	0.68
2:D:6:GLN:NE2	2:D:21:SER:O	2.26	0.68
1:A:550:GLY:HA2	1:A:587:ILE:HG23	1.74	0.68
3:F:119:PRO:HG3	3:F:143:ASN:H	1.58	0.68
1:A:309:GLU:O	1:A:313:TYR:OH	2.10	0.68
1:A:109:THR:O	1:A:237:ARG:NH2	2.27	0.68
1:C:885:GLY:HA3	1:C:896:ILE:HD11	1.76	0.68
1:E:64:TRP:NE1	1:E:262:ALA:O	2.27	0.68
2:D:51:ILE:HD11	2:D:72:VAL:HG23	1.76	0.68
2:K:17:SER:HA	2:K:86:LEU:HD12	1.75	0.68
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.27	0.68
1:A:105:ILE:HG23	1:A:116:SER:HB2	1.75	0.68
1:A:883:THR:O	1:A:896:ILE:N	2.16	0.68
1:C:779:GLN:HG2	1:C:783:ALA:HB3	1.75	0.68
1:C:903:ALA:HB1	1:C:913:GLN:HG2	1.75	0.68
1:E:710:ASN:OD1	1:E:1077:THR:OG1	2.12	0.68
1:C:736:VAL:O	1:C:764:ASN:ND2	2.25	0.67
2:H:36:TRP:HZ3	2:H:94:TYR:HB3	1.59	0.67
1:A:140:PHE:HA	1:A:241:LEU:HB2	1.75	0.67
1:E:644:GLN:NE2	1:E:645:THR:O	2.27	0.67
1:A:715:PRO:HG3	1:A:1069:PRO:HB3	1.76	0.67
1:A:315:THR:HG21	1:A:597:VAL:HG23	1.77	0.67
1:A:325:SER:HA	1:A:539:VAL:HB	1.76	0.67
1:E:34:ARG:HH22	1:E:191:GLU:HB3	1.59	0.67
1:A:726:ILE:HB	1:A:948:LEU:HG	1.76	0.67
1:A:1128:VAL:HG22	1:E:921:LYS:H	1.58	0.67
1:C:883:THR:O	1:C:896:ILE:N	2.19	0.67
1:E:66:HIS:O	1:E:78:ARG:NH1	2.28	0.67
3:L:41:TRP:CZ3	3:L:79:LEU:HB2	2.30	0.67
1:A:591:SER:HB3	1:A:615:VAL:HG11	1.76	0.67
1:C:438:SER:N	1:C:507:PRO:O	2.27	0.67
1:C:549:THR:HG23	1:C:589:PRO:HA	1.76	0.67
1:E:439:ASN:HD22	1:E:506:GLN:HG2	1.60	0.67
1:E:112:SER:HA	1:E:132:GLU:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:LYS:HE2	1:A:1043:CYS:HA	1.77	0.67
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.75	0.67
1:E:907:ASN:ND2	1:E:913:GLN:OE1	2.27	0.66
1:A:611:LEU:HD22	1:A:666:ILE:HB	1.77	0.66
1:A:318:PHE:HZ	1:A:615:VAL:HG21	1.59	0.66
1:A:349:SER:HB2	1:A:352:ALA:HB3	1.78	0.66
1:E:985:ASP:O	1:E:989:ALA:N	2.23	0.66
2:K:43:LYS:HG2	2:K:44:SER:H	1.59	0.66
1:A:44:ARG:NH2	1:A:279:TYR:OH	2.25	0.66
1:A:591:SER:HB3	1:A:615:VAL:CG1	2.26	0.66
1:A:992:GLN:HA	1:A:995:ARG:NH1	2.10	0.66
1:A:1129:VAL:O	1:E:921:LYS:NZ	2.27	0.66
2:D:88:SER:O	2:D:91:SER:OG	2.13	0.66
1:C:788:ILE:N	1:E:699:LEU:O	2.22	0.66
1:C:803:SER:HB3	5:X:1:NAG:HN2	1.60	0.66
1:E:393:THR:HA	1:E:522:ALA:HA	1.78	0.66
1:A:591:SER:CB	1:A:615:VAL:CG1	2.73	0.66
1:A:650:LEU:HD21	1:A:653:ALA:HB3	1.77	0.66
1:C:358:ILE:HD11	1:C:397:ALA:HB2	1.76	0.66
3:I:31:TYR:HB3	3:I:35:GLN:HA	1.78	0.66
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.78	0.66
1:E:568:ASP:HB2	1:E:574:ASP:HB2	1.77	0.66
1:E:457:ARG:NH1	1:E:459:SER:O	2.29	0.65
1:E:816:SER:OG	1:E:819:GLU:OE1	2.14	0.65
2:K:52:ASN:O	2:K:56:GLY:N	2.18	0.65
1:A:902:MET:HA	1:A:905:ARG:HG2	1.79	0.65
1:E:133:PHE:HD2	1:E:161:SER:H	1.44	0.65
1:C:726:ILE:HG23	1:C:1061:VAL:HA	1.77	0.65
1:C:981:LEU:HD12	1:C:989:ALA:HB1	1.76	0.65
2:D:38:LYS:HB3	2:D:46:GLU:HB2	1.78	0.65
2:D:43:LYS:HG3	2:D:44:SER:H	1.61	0.65
1:A:882:ILE:HG23	1:A:898:PHE:CD1	2.31	0.65
3:F:43:GLN:HG2	3:F:53:LEU:HD21	1.77	0.65
2:K:153:PRO:O	2:K:206:HIS:NE2	2.28	0.65
1:C:1015:ALA:O	1:C:1019:ARG:HB2	1.97	0.65
1:C:1103:PHE:HB3	1:C:1112:PRO:HB3	1.79	0.65
1:C:352:ALA:HA	1:C:466:ARG:HH11	1.62	0.65
1:A:503:VAL:HA	1:A:506:GLN:HB2	1.78	0.65
1:A:641:ASN:N	1:A:654:GLU:OE1	2.29	0.65
1:A:789:TYR:OH	1:C:705:VAL:N	2.30	0.65
1:C:35:GLY:HA3	1:C:56:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:N	1:A:239:GLN:O	2.29	0.65
1:A:969:ASN:ND2	1:A:969:ASN:O	2.28	0.64
1:C:609:ALA:HB2	1:C:692:ILE:HD13	1.77	0.64
1:C:921:LYS:NZ	1:E:1128:VAL:O	2.20	0.64
1:A:787:GLN:NE2	1:C:701:ALA:O	2.30	0.64
1:C:1029:MET:O	1:C:1034:LEU:N	2.29	0.64
1:A:722:VAL:HG21	1:A:934:ILE:HD11	1.78	0.64
1:A:118:LEU:N	1:A:129:LYS:O	2.29	0.64
1:C:64:TRP:NE1	1:C:263:ALA:O	2.30	0.64
1:E:78:ARG:NH1	1:E:80:ASP:OD1	2.25	0.64
1:E:141:LEU:HD21	1:E:150:LYS:HD2	1.80	0.64
1:E:611:LEU:HD22	1:E:666:ILE:HB	1.77	0.64
3:F:170:THR:OG1	3:F:180:SER:N	2.26	0.64
1:E:1073:LYS:HD3	1:E:1075:PHE:HB2	1.78	0.64
1:E:329:PHE:HB2	1:E:527:PRO:HA	1.78	0.64
1:A:364:ASP:OD1	1:A:388:ASN:ND2	2.31	0.64
1:C:805:ILE:HG22	1:C:818:ILE:HD13	1.79	0.64
1:E:323:THR:H	1:E:539:VAL:HG12	1.61	0.64
1:A:726:ILE:HG13	1:A:947:LYS:HG2	1.78	0.64
1:A:758:SER:HB2	1:A:762:GLN:HE22	1.61	0.64
1:A:882:ILE:HG23	1:A:898:PHE:HD1	1.63	0.64
1:A:912:THR:O	1:A:915:VAL:HG12	1.98	0.64
1:C:886:TRP:HZ2	1:E:1107:ARG:HB3	1.63	0.64
1:E:128:ILE:HG21	1:E:170:TYR:HD2	1.63	0.64
1:E:473:TYR:HB2	1:E:491:PRO:HB3	1.80	0.64
2:K:39:GLN:O	2:K:93:VAL:N	2.29	0.64
1:A:374:PHE:HA	1:A:436:TRP:HB2	1.80	0.64
1:A:388:ASN:ND2	1:A:527:PRO:O	2.31	0.64
1:C:55:PHE:HE1	1:C:275:PHE:H	1.46	0.64
1:C:886:TRP:HH2	1:E:1107:ARG:HH11	1.46	0.64
1:C:568:ASP:HB2	1:C:574:ASP:HB2	1.80	0.63
1:A:716:THR:HA	1:A:1110:TYR:HB3	1.80	0.63
1:A:888:PHE:HD1	1:A:893:ALA:HB2	1.63	0.63
1:A:966:LEU:HD23	1:A:976:VAL:HG22	1.79	0.63
1:E:294:ASP:OD1	1:E:297:SER:N	2.29	0.63
1:A:1128:VAL:HG13	1:E:920:GLN:HG2	1.79	0.63
1:C:727:LEU:HB2	1:C:1062:PHE:HE2	1.64	0.63
1:E:206:LYS:HE3	1:E:222:ALA:H	1.63	0.63
1:E:614:GLY:N	1:E:647:ALA:O	2.26	0.63
1:A:442:ASP:HB3	1:A:507:PRO:HG2	1.80	0.63
1:A:393:THR:HA	1:A:522:ALA:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:THR:HG21	2:H:29:PHE:HE1	1.63	0.63
1:A:920:GLN:HA	1:A:923:ILE:HB	1.81	0.63
1:A:318:PHE:CZ	1:A:615:VAL:HG21	2.33	0.63
1:A:328:ARG:NH1	1:A:531:THR:O	2.32	0.63
1:C:961:THR:HA	1:C:964:LYS:HG2	1.80	0.62
1:E:604:THR:HG22	1:E:605:SER:H	1.62	0.62
1:A:733:LYS:NZ	1:A:771:ALA:O	2.28	0.62
2:D:91:SER:HB2	2:D:116:VAL:H	1.64	0.62
1:C:716:THR:HA	1:C:1110:TYR:HB3	1.81	0.62
1:A:577:ARG:HG2	1:A:584:ILE:HD12	1.80	0.62
1:E:562:PHE:O	1:E:564:GLN:NE2	2.33	0.62
1:A:726:ILE:HD12	1:A:948:LEU:H	1.65	0.62
1:C:332:ILE:HG22	1:C:333:THR:H	1.64	0.62
1:E:300:LYS:NZ	1:E:306:PHE:O	2.32	0.62
2:D:141:THR:O	3:F:120:SER:OG	2.17	0.62
3:I:83:SER:OG	3:I:85:ARG:NH2	2.32	0.62
1:A:189:LEU:HD22	1:A:210:ILE:HD13	1.81	0.62
1:C:168:PHE:HE2	1:C:229:LEU:HD22	1.64	0.62
1:E:897:PRO:HB2	1:E:900:MET:HG2	1.80	0.62
2:D:34:ILE:HG22	2:D:51:ILE:HG22	1.81	0.62
1:A:767:LEU:HA	1:A:770:ILE:HD12	1.82	0.62
1:C:338:PHE:HZ	1:C:513:LEU:HD11	1.65	0.62
1:C:1006:THR:O	1:C:1009:THR:OG1	2.14	0.62
1:E:1037:SER:HB3	1:E:1039:ARG:HG3	1.81	0.62
3:F:58:SER:O	3:F:60:ARG:NH1	2.32	0.62
1:A:116:SER:OG	1:A:131:CYS:O	2.13	0.62
1:A:953:ASN:O	1:A:956:ALA:N	2.32	0.62
1:C:276:LEU:N	1:C:289:VAL:O	2.30	0.62
1:C:200:TYR:CE1	1:C:202:LYS:HE3	2.33	0.62
1:E:401:VAL:HG13	1:E:507:PRO:HB3	1.82	0.62
1:E:883:THR:HB	1:E:895:GLN:HB2	1.82	0.62
2:K:100:VAL:HG12	2:K:102:ASN:H	1.63	0.62
1:A:290:ASP:O	1:A:297:SER:HB2	1.99	0.62
1:A:957:GLN:HA	1:A:960:ASN:HB2	1.82	0.62
1:A:1091:ARG:O	1:E:907:ASN:ND2	2.33	0.62
1:C:437:ASN:ND2	1:C:507:PRO:O	2.33	0.62
1:C:438:SER:HB3	1:C:442:ASP:HB2	1.82	0.62
1:A:42:VAL:HG13	1:A:44:ARG:NH1	2.14	0.61
1:A:775:ASP:OD1	1:A:776:LYS:N	2.33	0.61
1:C:289:VAL:HG11	1:C:300:LYS:HD2	1.82	0.61
3:L:144:ASN:ND2	3:L:173:ASP:OD2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:PRO:HA	1:E:237:ARG:HA	1.81	0.61
1:E:1049:LEU:HD12	1:E:1065:VAL:HG12	1.82	0.61
6:Y:2:NAG:H83	6:Y:2:NAG:O3	2.00	0.61
2:H:68:ALA:HB2	2:H:84:ARG:HG3	1.82	0.61
1:C:30:ASN:HA	1:C:62:VAL:H	1.66	0.61
1:C:674:TYR:HE2	1:C:690:GLN:HE21	1.48	0.61
1:C:1043:CYS:HB2	1:C:1048:HIS:HB2	1.82	0.61
1:E:86:PHE:N	1:E:236:THR:O	2.34	0.61
1:E:825:LYS:HG2	1:E:945:LEU:HG	1.83	0.61
1:A:1097:SER:HB2	1:A:1102:TRP:HA	1.83	0.61
1:C:557:LYS:H	1:C:584:ILE:HG21	1.65	0.61
1:A:563:GLN:OE1	1:A:577:ARG:NH2	2.34	0.61
1:C:825:LYS:NZ	1:C:938:LEU:O	2.28	0.61
1:C:961:THR:HB	1:C:965:GLN:HE22	1.65	0.61
1:E:1091:ARG:HH22	1:E:1119:ASN:HA	1.65	0.61
2:H:2:VAL:HB	2:H:98:ARG:HD2	1.80	0.61
1:A:317:ASN:ND2	1:E:737:ASP:OD2	2.34	0.61
1:A:712:ILE:N	1:A:1075:PHE:O	2.27	0.61
1:C:591:SER:HB3	1:C:615:VAL:HG11	1.83	0.61
2:D:91:SER:HB2	2:D:115:THR:HA	1.82	0.61
6:Y:2:NAG:H83	6:Y:2:NAG:C3	2.30	0.61
1:A:931:ILE:HA	1:A:934:ILE:HD12	1.83	0.61
1:C:140:PHE:O	1:C:158:ARG:NE	2.33	0.61
1:C:212:LEU:HD11	1:C:217:PRO:HG3	1.83	0.61
1:A:985:ASP:O	1:A:989:ALA:N	2.20	0.60
1:C:670:ILE:HD13	1:C:696:THR:HA	1.82	0.60
1:C:907:ASN:ND2	1:C:911:VAL:O	2.34	0.60
1:E:1090:PRO:HB3	1:E:1120:THR:HA	1.83	0.60
1:E:541:PHE:HB3	1:E:552:LEU:HD21	1.82	0.60
1:E:753:LEU:HA	1:E:756:TYR:HD2	1.66	0.60
1:A:725:GLU:OE2	1:A:1064:HIS:NE2	2.34	0.60
1:C:906:PHE:HB3	1:C:911:VAL:HB	1.83	0.60
1:E:327:VAL:O	1:E:529:LYS:NZ	2.27	0.60
1:A:1080:ALA:HB1	1:A:1087:ALA:HB1	1.84	0.60
1:C:131:CYS:SG	1:C:132:GLU:N	2.75	0.60
1:C:663:ASP:OD1	1:C:664:ILE:N	2.34	0.60
1:E:1051:SER:OG	1:E:1062:PHE:HB3	2.01	0.60
3:F:11:LEU:HG	3:F:13:VAL:HB	1.83	0.60
1:A:881:THR:HG21	1:A:1033:VAL:HG12	1.84	0.60
1:C:109:THR:H	1:C:114:THR:HG21	1.66	0.60
1:E:172:SER:HB3	14:E:1304:NAG:H4	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:966:LEU:HD23	1:E:1000:ARG:HH22	1.66	0.60
3:L:25:SER:OG	3:L:74:GLY:O	2.19	0.60
1:C:890:ALA:HB1	1:E:1068:VAL:HG13	1.83	0.60
1:E:350:VAL:HG22	1:E:422:ASN:HB3	1.83	0.60
1:E:954:GLN:HA	1:E:957:GLN:HG3	1.84	0.60
1:A:319:ARG:NH2	1:E:739:THR:O	2.35	0.60
1:C:669:GLY:O	1:C:697:MET:N	2.30	0.60
2:D:91:SER:HB3	2:D:116:VAL:HG23	1.83	0.60
1:C:758:SER:OG	1:C:762:GLN:NE2	2.34	0.60
1:C:937:SER:O	1:C:941:THR:N	2.31	0.60
1:E:457:ARG:NH1	1:E:459:SER:OG	2.35	0.60
1:A:560:LEU:HD12	1:A:562:PHE:HE2	1.67	0.60
1:C:735:SER:HA	1:C:767:LEU:HD13	1.84	0.60
1:E:164:ASN:HA	14:E:1303:NAG:H82	1.84	0.60
2:H:48:LEU:HD12	2:H:49:GLY:N	2.17	0.60
2:H:51:ILE:HD11	2:H:56:GLY:HA2	1.84	0.60
1:A:779:GLN:O	1:A:783:ALA:N	2.35	0.59
1:A:961:THR:O	1:A:965:GLN:HB2	2.02	0.59
1:C:920:GLN:OE1	1:C:920:GLN:N	2.29	0.59
1:E:403:ARG:H	1:E:406:GLU:HB2	1.66	0.59
2:D:93:VAL:HA	2:D:113:LEU:HA	1.84	0.59
1:C:726:ILE:HD12	1:C:1061:VAL:HG23	1.82	0.59
1:E:342:PHE:HB3	1:E:374:PHE:HZ	1.67	0.59
1:A:622:VAL:HB	1:A:642:VAL:HG23	1.83	0.59
1:E:172:SER:O	14:E:1304:NAG:O3	2.20	0.59
1:A:364:ASP:O	1:A:367:VAL:HG22	2.01	0.59
1:A:894:LEU:HA	1:C:713:ALA:HB3	1.84	0.59
1:A:1090:PRO:HD3	1:A:1120:THR:HG22	1.83	0.59
1:C:44:ARG:HH21	1:C:49:HIS:CG	2.20	0.59
1:C:905:ARG:NH1	1:C:1050:MET:HA	2.16	0.59
1:E:715:PRO:HG3	1:E:1069:PRO:HB3	1.85	0.59
1:E:322:PRO:HB3	1:E:539:VAL:HA	1.84	0.59
3:F:116:VAL:HB	3:F:206:GLY:HA3	1.83	0.59
2:K:19:LYS:HD2	2:K:80:TYR:HB3	1.84	0.59
1:A:850:ILE:HG13	1:A:851:CYS:H	1.66	0.59
1:C:331:ASN:HA	1:C:580:GLN:HB2	1.84	0.59
1:E:310:LYS:HG2	1:E:601:GLY:H	1.67	0.59
2:H:206:HIS:CD2	2:H:208:PRO:HD2	2.37	0.59
1:E:56:LEU:HD12	1:E:57:PRO:HD2	1.85	0.59
2:D:67:LYS:NZ	2:D:85:SER:O	2.34	0.59
3:F:114:ARG:NH2	3:F:177:SER:HB2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:172:PHE:HB2	2:K:184:LEU:HG	1.85	0.59
1:A:456:PHE:CE2	1:A:489:TYR:HB3	2.37	0.59
7:Q:2:NAG:H83	7:Q:2:NAG:H3	1.84	0.59
1:A:674:TYR:HA	1:A:692:ILE:HA	1.84	0.59
1:A:738:CYS:SG	1:A:739:THR:N	2.76	0.59
1:C:326:ILE:HD12	1:C:532:ASN:HB3	1.83	0.59
1:E:131:CYS:HA	1:E:166:CYS:HB3	1.83	0.59
2:D:37:VAL:HG11	2:D:108:TRP:HZ3	1.68	0.59
1:A:91:TYR:OH	1:A:191:GLU:OE2	2.13	0.59
1:A:698:SER:OG	1:A:700:GLY:O	2.21	0.59
1:C:212:LEU:HD21	1:C:217:PRO:HB3	1.84	0.59
3:I:68:PHE:HD1	3:I:79:LEU:HD11	1.68	0.59
1:A:326:ILE:HD12	1:A:534:VAL:HG23	1.85	0.58
1:C:816:SER:H	1:C:819:GLU:CD	2.05	0.58
1:C:1010:GLN:O	1:C:1014:ARG:HG2	2.03	0.58
1:C:1088:HIS:HD2	1:C:1122:VAL:HG22	1.68	0.58
1:E:871:ALA:O	1:E:874:THR:OG1	2.18	0.58
1:A:1049:LEU:HD12	1:A:1065:VAL:HG12	1.85	0.58
1:C:145:TYR:HD1	1:C:146:HIS:HB2	1.67	0.58
1:C:549:THR:OG1	1:C:590:CYS:SG	2.51	0.58
1:C:611:LEU:HD22	1:C:666:ILE:HB	1.84	0.58
1:E:916:LEU:O	1:E:920:GLN:HB3	2.02	0.58
1:E:1052:PHE:HB2	1:E:1063:LEU:HD12	1.85	0.58
3:L:34:ASN:HB3	3:L:36:LYS:HE3	1.84	0.58
1:A:312:ILE:HD13	1:A:666:ILE:HA	1.84	0.58
1:A:348:ALA:HB3	1:A:400:PHE:HB3	1.83	0.58
1:E:1106:GLN:HE22	1:E:1108:ASN:HB2	1.69	0.58
1:A:110:LEU:HB2	1:A:237:ARG:HH21	1.68	0.58
1:A:521:PRO:HD2	1:E:230:PRO:HB3	1.84	0.58
1:C:1030:SER:HA	1:C:1034:LEU:HB2	1.84	0.58
1:E:557:LYS:H	1:E:584:ILE:HG21	1.69	0.58
1:A:1107:ARG:HG3	1:E:904:TYR:CE1	2.39	0.58
1:C:550:GLY:HA3	1:C:588:THR:O	2.03	0.58
1:E:962:LEU:HD13	1:E:1007:TYR:CG	2.39	0.58
2:H:187:VAL:HG23	3:I:141:LEU:HD21	1.86	0.58
1:E:1106:GLN:OE1	1:E:1109:PHE:N	2.37	0.58
5:O:2:NAG:H3	5:O:2:NAG:H83	1.86	0.58
1:A:457:ARG:NH1	1:A:459:SER:O	2.34	0.58
1:C:281:GLU:H	1:C:281:GLU:CD	2.05	0.58
1:C:386:LYS:HG2	1:C:390:LEU:HD13	1.85	0.58
2:D:212:LYS:NZ	2:D:214:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASN:HD21	4:B:3:FUC:H3	1.68	0.58
1:A:273:ARG:HG3	1:A:274:THR:H	1.69	0.58
1:C:354:ASN:OD1	1:C:355:ARG:N	2.36	0.58
1:C:895:GLN:NE2	1:E:712:ILE:O	2.37	0.58
1:C:1096:VAL:O	1:C:1103:PHE:HB2	2.04	0.58
1:E:716:THR:H	1:E:1071:GLN:HB3	1.69	0.58
2:H:91:SER:HB2	2:H:116:VAL:HB	1.86	0.58
3:L:31:TYR:HB2	3:L:98:TYR:HE1	1.69	0.58
5:P:1:NAG:H83	5:P:2:NAG:H62	1.84	0.58
1:A:669:GLY:HA3	1:E:869:MET:CE	2.34	0.57
1:A:979:ASP:N	1:A:979:ASP:OD1	2.37	0.57
1:C:118:LEU:HD13	1:C:129:LYS:HE2	1.86	0.57
1:C:501:ASN:HB3	1:C:505:TYR:HB2	1.86	0.57
1:C:1060:VAL:HG13	1:C:1062:PHE:CZ	2.39	0.57
1:C:1080:ALA:HB1	1:C:1088:HIS:H	1.69	0.57
1:E:126:VAL:HB	14:E:1304:NAG:HN2	1.68	0.57
1:E:733:LYS:NZ	1:E:862:PRO:O	2.27	0.57
3:I:95:GLN:NE2	3:I:96:GLN:O	2.37	0.57
1:A:99:ASN:O	1:A:102:ARG:NH1	2.38	0.57
1:A:884:SER:HB2	1:C:707:TYR:HE1	1.69	0.57
1:A:1036:GLN:HE22	1:A:1049:LEU:HD23	1.69	0.57
1:C:47:VAL:HG13	1:C:49:HIS:HE1	1.68	0.57
1:C:1024:LEU:O	1:C:1028:LYS:HG2	2.03	0.57
1:E:914:ASN:OD1	1:E:915:VAL:N	2.37	0.57
3:F:173:ASP:H	3:F:177:SER:HA	1.67	0.57
1:E:576:VAL:HG22	1:E:587:ILE:HD11	1.86	0.57
1:E:738:CYS:HB2	1:E:753:LEU:HD21	1.86	0.57
1:C:43:PHE:HZ	1:E:558:LYS:HZ2	1.52	0.57
1:C:712:ILE:HB	1:C:1077:THR:HG21	1.87	0.57
1:C:920:GLN:HG2	1:C:921:LYS:HD2	1.85	0.57
1:E:92:PHE:HB3	1:E:192:PHE:H	1.69	0.57
1:E:647:ALA:HB2	1:E:668:ALA:HB3	1.86	0.57
2:D:206:HIS:CD2	2:D:208:PRO:HD2	2.39	0.57
1:C:961:THR:O	1:C:964:LYS:N	2.36	0.57
1:E:984:LEU:HD23	1:E:988:GLU:HB3	1.86	0.57
1:A:435:ALA:HA	1:A:510:VAL:HA	1.86	0.57
1:A:906:PHE:CE2	1:A:916:LEU:HB2	2.38	0.57
1:A:705:VAL:HB	1:A:707:TYR:CE1	2.40	0.57
1:E:456:PHE:HB3	1:E:473:TYR:CD1	2.39	0.57
2:D:97:ALA:HB3	2:D:105:PHE:HD1	1.70	0.57
1:A:84:LEU:HD13	1:A:267:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ASN:O	1:A:707:TYR:OH	2.15	0.57
1:A:866:THR:HG22	1:A:869:MET:HG2	1.85	0.57
1:C:404:GLY:HA3	1:C:504:GLY:HA2	1.85	0.57
1:C:972:ALA:HB1	1:C:980:ILE:HG12	1.85	0.57
1:E:710:ASN:HD21	1:E:1077:THR:N	2.00	0.57
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.39	0.57
3:L:19:VAL:HB	3:L:80:THR:HA	1.86	0.57
3:L:29:LEU:N	3:L:74:GLY:HA2	2.19	0.57
1:A:920:GLN:NE2	1:C:1129:VAL:HA	2.19	0.57
1:E:231:ILE:HG13	1:E:232:GLY:H	1.69	0.57
1:A:106:PHE:HD1	1:A:238:PHE:HB2	1.70	0.57
1:E:802:PHE:CD1	1:E:805:ILE:HD11	2.39	0.57
1:C:737:ASP:HB2	1:C:740:MET:HB2	1.87	0.56
1:E:422:ASN:OD1	1:E:454:ARG:N	2.32	0.56
1:A:666:ILE:HG12	1:A:670:ILE:O	2.06	0.56
1:C:37:TYR:CZ	1:C:195:LYS:HG2	2.41	0.56
1:E:710:ASN:ND2	1:E:1077:THR:H	2.00	0.56
1:A:800:PHE:HZ	1:C:1130:ILE:HD13	1.70	0.56
1:A:970:PHE:HE1	1:E:759:PHE:HE2	1.53	0.56
1:C:43:PHE:CZ	1:C:45:SER:HB2	2.40	0.56
1:C:367:VAL:HA	1:C:370:ASN:ND2	2.20	0.56
1:C:968:SER:O	1:C:968:SER:OG	2.22	0.56
1:C:1049:LEU:HB2	1:C:1065:VAL:HG12	1.86	0.56
3:F:57:ALA:HB1	3:F:77:PHE:CE1	2.40	0.56
5:T:2:NAG:H83	5:T:2:NAG:H3	1.87	0.56
1:A:369:TYR:HA	1:A:374:PHE:HE2	1.70	0.56
1:A:752:LEU:HD21	1:A:994:ASP:HA	1.86	0.56
1:A:912:THR:HG22	1:A:914:ASN:H	1.69	0.56
1:A:1116:THR:O	1:A:1120:THR:OG1	2.21	0.56
1:A:1128:VAL:HG11	1:E:919:ASN:N	2.20	0.56
1:C:906:PHE:CD1	1:C:1049:LEU:HD22	2.40	0.56
1:E:316:SER:OG	1:E:317:ASN:N	2.37	0.56
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.40	0.56
1:A:906:PHE:HB3	1:A:911:VAL:HB	1.86	0.56
1:C:902:MET:SD	1:C:916:LEU:HD21	2.44	0.56
1:C:1033:VAL:HG22	1:C:1051:SER:HB3	1.88	0.56
1:E:815:ARG:HE	1:E:819:GLU:HB3	1.71	0.56
1:A:336:CYS:HA	1:A:358:ILE:HD11	1.88	0.56
1:A:706:ALA:HB3	1:A:711:SER:HB2	1.87	0.56
1:C:503:VAL:HA	1:C:506:GLN:HB2	1.87	0.56
1:C:742:ILE:HD12	1:C:1000:ARG:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:128:PHE:HE2	2:K:149:LYS:HB3	1.69	0.56
1:A:44:ARG:HG2	1:A:49:HIS:CD2	2.40	0.56
1:A:783:ALA:HB2	1:A:873:TYR:CZ	2.41	0.56
1:C:393:THR:HG21	1:C:518:LEU:HB3	1.87	0.56
1:C:914:ASN:ND2	1:C:1111:GLU:OE2	2.39	0.56
1:E:64:TRP:HD1	1:E:65:PHE:N	2.03	0.56
1:E:481:ASN:OD1	3:I:32:SER:OG	2.22	0.56
3:L:13:VAL:HB	3:L:110:LEU:HD22	1.88	0.56
1:A:715:PRO:HD3	1:E:894:LEU:HD13	1.88	0.56
1:A:190:ARG:HH22	1:A:207:HIS:HA	1.69	0.56
1:A:938:LEU:HD22	1:A:945:LEU:HB3	1.87	0.56
1:C:34:ARG:HH21	1:C:217:PRO:HB2	1.71	0.56
1:C:726:ILE:CD1	1:C:1061:VAL:HG23	2.36	0.56
1:E:984:LEU:HB2	1:E:992:GLN:NE2	2.20	0.56
1:A:296:LEU:O	1:A:299:THR:OG1	2.19	0.56
1:C:739:THR:O	1:C:743:CYS:N	2.36	0.56
1:C:784:GLN:O	1:E:1045:LYS:NZ	2.39	0.56
1:E:672:ALA:HA	1:E:694:ALA:HA	1.88	0.56
2:H:108:TRP:NE1	3:I:50:PRO:O	2.38	0.56
3:L:92:TYR:O	3:L:108:THR:OG1	2.23	0.56
1:A:404:GLY:HA2	1:A:508:TYR:HB2	1.87	0.55
1:A:767:LEU:HD23	1:A:770:ILE:HD12	1.88	0.55
1:A:1073:LYS:HE2	1:A:1075:PHE:HD2	1.70	0.55
1:E:577:ARG:HH12	1:E:585:LEU:N	2.03	0.55
1:E:722:VAL:HG22	1:E:1065:VAL:HA	1.88	0.55
1:E:981:LEU:HD23	1:E:989:ALA:HB1	1.88	0.55
3:F:130:GLN:NE2	3:F:135:THR:O	2.39	0.55
1:A:364:ASP:HB2	1:A:527:PRO:HG2	1.87	0.55
1:A:457:ARG:NE	1:A:467:ASP:OD2	2.39	0.55
1:A:699:LEU:H	1:E:788:ILE:CG1	2.19	0.55
1:A:972:ALA:HB2	1:A:996:LEU:HD12	1.87	0.55
1:C:312:ILE:HG23	1:C:664:ILE:HG22	1.88	0.55
1:A:800:PHE:CZ	1:C:1130:ILE:HD13	2.40	0.55
1:C:200:TYR:HA	1:C:230:PRO:HA	1.88	0.55
1:C:280:ASN:HD21	1:C:282:ASN:HB3	1.71	0.55
1:C:456:PHE:HB2	1:C:491:PRO:HB3	1.87	0.55
1:C:773:GLU:HA	1:C:776:LYS:HE3	1.89	0.55
1:C:890:ALA:HB3	1:E:1069:PRO:HD2	1.89	0.55
3:F:96:GLN:HE21	3:F:103:THR:H	1.53	0.55
1:A:42:VAL:HA	1:C:565:PHE:HB2	1.87	0.55
1:A:1107:ARG:HB3	1:E:886:TRP:CZ2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:TYR:HB3	1:C:61:ASN:HD21	1.72	0.55
1:C:791:THR:HG22	1:C:879:ALA:HB2	1.87	0.55
1:E:485:GLY:H	1:E:488:CYS:HB2	1.70	0.55
1:E:934:ILE:O	1:E:938:LEU:HG	2.06	0.55
1:A:125:ASN:ND2	5:P:1:NAG:O5	2.39	0.55
1:C:1105:THR:HB	1:C:1112:PRO:HA	1.89	0.55
1:E:905:ARG:HG2	1:E:905:ARG:HH11	1.71	0.55
1:A:195:LYS:HG3	1:A:202:LYS:HZ3	1.70	0.55
1:A:331:ASN:HD21	7:M:1:NAG:H62	1.71	0.55
1:A:886:TRP:O	1:A:890:ALA:N	2.40	0.55
1:E:122:ASN:HB2	1:E:190:ARG:HH12	1.72	0.55
1:E:710:ASN:ND2	1:E:1077:THR:O	2.39	0.55
1:E:989:ALA:O	1:E:993:ILE:HG12	2.06	0.55
2:H:148:VAL:HB	2:H:184:LEU:HB3	1.89	0.55
5:X:2:NAG:H3	5:X:2:NAG:H83	1.86	0.55
1:A:709:ASN:OD1	1:A:710:ASN:ND2	2.40	0.55
1:A:993:ILE:HG23	1:A:997:ILE:CG1	2.36	0.55
1:E:611:LEU:HD13	1:E:666:ILE:HD12	1.87	0.55
2:D:2:VAL:HG21	2:D:98:ARG:HH21	1.71	0.55
3:L:2:ILE:HD12	3:L:29:LEU:HD21	1.88	0.55
1:A:566:GLY:HA2	1:E:43:PHE:O	2.07	0.55
1:A:614:GLY:N	1:A:647:ALA:O	2.24	0.55
1:A:743:CYS:O	1:C:319:ARG:NH2	2.39	0.55
1:A:782:PHE:HB3	1:A:873:TYR:HB3	1.87	0.55
1:C:422:ASN:ND2	1:C:454:ARG:O	2.40	0.55
1:C:1086:LYS:HA	1:C:1126:CYS:HB2	1.87	0.55
1:E:48:LEU:HD21	1:E:276:LEU:HD21	1.87	0.55
1:E:904:TYR:HD2	1:E:905:ARG:HH22	1.55	0.55
2:K:72:VAL:HG23	2:K:79:ALA:HA	1.87	0.55
1:E:280:ASN:HD21	1:E:282:ASN:HB2	1.71	0.55
1:E:779:GLN:HA	1:E:783:ALA:HB3	1.89	0.55
3:I:29:LEU:HD11	3:I:73:SER:HB2	1.88	0.55
1:C:811:LYS:HE3	1:C:812:PRO:HD2	1.89	0.55
1:E:931:ILE:HA	1:E:934:ILE:HD12	1.89	0.55
3:I:119:PRO:HD2	3:I:207:LEU:HG	1.88	0.55
1:A:1029:MET:HE2	1:A:1029:MET:HA	1.89	0.54
1:E:107:GLY:HA3	1:E:110:LEU:HD12	1.89	0.54
2:D:168:GLY:HA2	2:D:187:VAL:H	1.71	0.54
2:K:60:TYR:H	2:K:65:LYS:HE2	1.72	0.54
3:L:25:SER:OG	3:L:75:THR:HA	2.07	0.54
1:C:323:THR:HG1	1:C:539:VAL:HG12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ILE:HG12	1:C:540:ASN:O	2.08	0.54
1:C:403:ARG:HE	1:C:405:ASP:HB2	1.72	0.54
1:C:738:CYS:SG	1:C:739:THR:N	2.80	0.54
1:E:865:LEU:HD12	1:E:873:TYR:HE2	1.71	0.54
3:I:119:PRO:HA	3:I:143:ASN:O	2.08	0.54
1:A:297:SER:HA	1:A:300:LYS:HD3	1.89	0.54
1:A:965:GLN:O	1:A:968:SER:OG	2.25	0.54
1:C:616:ASN:HA	1:C:644:GLN:HE22	1.72	0.54
1:C:1097:SER:OG	1:C:1098:ASN:N	2.40	0.54
6:Y:2:NAG:C3	6:Y:2:NAG:C8	2.85	0.54
1:C:466:ARG:HH22	1:C:468:ILE:HB	1.72	0.54
1:C:957:GLN:O	1:C:961:THR:HG23	2.08	0.54
1:E:300:LYS:HG2	1:E:308:VAL:HG21	1.88	0.54
1:E:767:LEU:HA	1:E:770:ILE:HD12	1.90	0.54
3:L:39:LEU:O	3:L:55:TYR:HA	2.07	0.54
1:A:28:TYR:HB2	14:A:1304:NAG:H62	1.89	0.54
1:A:105:ILE:HD12	1:A:133:PHE:HB2	1.89	0.54
1:A:984:LEU:HD13	1:A:992:GLN:HE22	1.71	0.54
1:A:988:GLU:HA	1:A:991:VAL:HG22	1.89	0.54
1:C:643:PHE:CG	1:C:655:HIS:HB2	2.43	0.54
1:E:96:GLU:HG2	1:E:100:ILE:H	1.73	0.54
1:E:330:PRO:HG3	1:E:579:PRO:HG2	1.89	0.54
3:I:29:LEU:HG	3:I:74:GLY:HA2	1.89	0.54
1:A:986:PRO:HA	1:A:989:ALA:HB3	1.88	0.54
1:C:948:LEU:HA	1:C:951:VAL:HG22	1.89	0.54
1:E:145:TYR:O	1:E:146:HIS:ND1	2.40	0.54
1:E:202:LYS:HE3	1:E:228:ASP:OD1	2.08	0.54
1:C:140:PHE:H	1:C:158:ARG:HH21	1.54	0.54
1:C:338:PHE:CZ	1:C:513:LEU:HD11	2.43	0.54
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.89	0.54
5:V:1:NAG:O3	5:V:2:NAG:O7	2.22	0.54
1:A:280:ASN:OD1	1:A:281:GLU:N	2.41	0.54
1:A:970:PHE:HE1	1:E:759:PHE:CE2	2.25	0.54
1:A:1067:TYR:OH	1:A:1108:ASN:O	2.15	0.54
1:C:422:ASN:OD1	1:C:454:ARG:N	2.34	0.54
1:E:908:GLY:HA2	1:E:1038:LYS:HE3	1.90	0.54
1:E:960:ASN:HB3	1:E:964:LYS:HE3	1.90	0.54
2:H:98:ARG:HG3	2:H:106:ALA:HB3	1.90	0.54
1:A:894:LEU:HD23	1:C:1072:GLU:HG3	1.90	0.54
1:A:1081:ILE:HB	1:A:1088:HIS:HB2	1.89	0.54
1:C:887:THR:HB	1:C:894:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:901:GLN:HE22	1:C:905:ARG:HE	1.54	0.54
1:E:101:ILE:HD12	1:E:242:LEU:HD21	1.90	0.54
1:C:122:ASN:O	1:C:124:THR:N	2.40	0.54
1:E:726:ILE:HG13	1:E:948:LEU:HG	1.89	0.54
2:H:97:ALA:HB3	2:H:105:PHE:HD1	1.73	0.54
1:A:103:GLY:HA3	1:A:241:LEU:HG	1.89	0.53
1:A:905:ARG:HD2	1:A:1050:MET:SD	2.48	0.53
1:E:280:ASN:OD1	1:E:284:THR:N	2.38	0.53
3:I:196:LYS:HG3	3:I:197:VAL:HG23	1.89	0.53
1:C:104:TRP:HB2	1:C:119:ILE:HB	1.90	0.53
1:C:726:ILE:HB	1:C:948:LEU:HD23	1.88	0.53
1:E:573:THR:HG22	1:E:587:ILE:HD13	1.90	0.53
3:L:121:VAL:HG21	3:L:202:VAL:HG11	1.90	0.53
1:A:535:LYS:HD3	1:A:553:THR:HA	1.90	0.53
1:A:1001:LEU:HD13	1:A:1004:LEU:HD12	1.89	0.53
1:C:920:GLN:NE2	1:E:1128:VAL:O	2.41	0.53
3:F:69:THR:HG22	3:F:80:THR:HB	1.90	0.53
3:I:144:ASN:ND2	3:I:177:SER:O	2.41	0.53
1:C:91:TYR:CZ	1:C:93:ALA:HB2	2.43	0.53
1:C:600:PRO:HG3	1:C:674:TYR:CG	2.43	0.53
1:C:716:THR:H	1:C:1071:GLN:HB3	1.73	0.53
1:E:157:PHE:CE2	1:E:160:TYR:HB3	2.43	0.53
1:E:818:ILE:O	1:E:822:LEU:HD23	2.08	0.53
3:F:142:LEU:HD23	3:F:145:PHE:HZ	1.73	0.53
1:A:552:LEU:HD23	1:A:585:LEU:HD13	1.90	0.53
1:A:590:CYS:SG	1:A:591:SER:N	2.82	0.53
1:A:1014:ARG:O	1:A:1018:ILE:HG13	2.08	0.53
1:C:84:LEU:HB3	1:C:269:TYR:HE1	1.72	0.53
1:C:274:THR:HG23	1:C:291:CYS:SG	2.48	0.53
1:E:319:ARG:NH2	1:E:591:SER:OG	2.41	0.53
1:E:877:LEU:HD23	1:E:1029:MET:SD	2.48	0.53
1:E:1001:LEU:HA	1:E:1004:LEU:HD12	1.91	0.53
2:D:214:ASP:OD2	2:K:122:THR:OG1	2.27	0.53
3:F:41:TRP:CZ3	3:F:94:CYS:HB2	2.44	0.53
3:L:30:LEU:HD11	3:L:35:GLN:HG3	1.90	0.53
1:A:225:PRO:HG2	1:C:562:PHE:HB2	1.90	0.53
1:A:1062:PHE:HB3	1:A:1064:HIS:CE1	2.44	0.53
1:E:295:PRO:HD2	1:E:608:VAL:HG21	1.89	0.53
1:E:344:ALA:HB3	1:E:347:PHE:HE1	1.74	0.53
1:C:350:VAL:HG21	1:C:418:ILE:HG23	1.91	0.53
1:E:351:TYR:CE1	1:E:452:LEU:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:TYR:CD1	2:H:50:GLY:HA3	2.41	0.53
1:A:102:ARG:HH11	1:A:102:ARG:HG3	1.74	0.53
1:A:611:LEU:HD13	1:A:666:ILE:HD12	1.89	0.53
1:A:789:TYR:CE2	1:C:707:TYR:HE2	2.27	0.53
1:E:967:SER:HA	1:E:975:SER:HA	1.90	0.53
2:K:35:TYR:CD1	2:K:50:GLY:HA3	2.43	0.53
2:K:67:LYS:HB2	2:K:83:LEU:HD22	1.90	0.53
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.90	0.53
1:A:854:LYS:HB2	1:C:588:THR:HG23	1.90	0.53
1:A:1107:ARG:NH2	1:E:904:TYR:HB2	2.24	0.53
1:E:342:PHE:HZ	1:E:513:LEU:HD21	1.74	0.53
2:D:173:PRO:HD2	3:F:169:VAL:O	2.08	0.53
3:I:43:GLN:HG2	3:I:92:TYR:HA	1.90	0.53
1:A:622:VAL:HA	1:A:651:ILE:HD11	1.90	0.53
1:C:380:TYR:HE2	1:C:433:VAL:HG23	1.73	0.53
1:C:616:ASN:HA	1:C:644:GLN:NE2	2.24	0.53
1:C:1075:PHE:CE2	1:C:1076:THR:HG22	2.44	0.53
1:C:1091:ARG:HD2	1:C:1092:GLU:N	2.23	0.53
1:E:818:ILE:HD11	1:E:1054:GLN:HG2	1.91	0.53
1:E:905:ARG:HA	1:E:1036:GLN:OE1	2.09	0.53
1:A:186:PHE:HE2	1:A:210:ILE:HG13	1.72	0.52
1:A:244:LEU:HD11	1:A:247:SER:HA	1.91	0.52
1:A:617:CYS:SG	1:A:644:GLN:OE1	2.67	0.52
1:A:733:LYS:HB2	1:A:861:LEU:HB3	1.91	0.52
1:E:201:PHE:HB2	1:E:231:ILE:HD13	1.91	0.52
1:E:919:ASN:OD1	1:E:923:ILE:HG13	2.09	0.52
2:H:152:PHE:H	2:H:206:HIS:CE1	2.27	0.52
1:A:699:LEU:H	1:E:788:ILE:HG12	1.73	0.52
1:E:725:GLU:O	1:E:726:ILE:HD13	2.09	0.52
1:E:800:PHE:HB3	1:E:802:PHE:CZ	2.44	0.52
1:E:1018:ILE:O	1:E:1021:SER:OG	2.20	0.52
2:D:43:LYS:HA	3:F:106:VAL:HG12	1.91	0.52
1:A:962:LEU:HD13	1:A:1007:TYR:CD2	2.44	0.52
1:C:61:ASN:HB3	14:C:1301:NAG:HN2	1.73	0.52
1:E:1001:LEU:O	1:E:1004:LEU:HB2	2.09	0.52
3:F:96:GLN:NE2	3:F:103:THR:H	2.06	0.52
3:F:116:VAL:HG13	3:F:145:PHE:HB2	1.92	0.52
3:I:84:VAL:HG13	3:I:88:ASP:HB2	1.92	0.52
3:L:29:LEU:HD12	3:L:77:PHE:HZ	1.74	0.52
3:L:39:LEU:HD21	3:L:41:TRP:HE1	1.75	0.52
1:A:1016:ALA:HA	1:A:1019:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:SER:N	1:C:584:ILE:O	2.37	0.52
1:C:770:ILE:O	1:C:773:GLU:HG2	2.10	0.52
1:E:594:GLY:HA3	1:E:613:GLN:HB2	1.92	0.52
2:K:34:ILE:HD12	2:K:98:ARG:HA	1.92	0.52
2:K:37:VAL:HG21	2:K:45:LEU:HB3	1.91	0.52
3:L:81:ILE:HG13	3:L:92:TYR:HE2	1.74	0.52
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.45	0.52
1:A:231:ILE:HG13	1:A:232:GLY:H	1.74	0.52
1:A:1028:LYS:O	1:A:1032:CYS:HB3	2.10	0.52
1:C:65:PHE:HB3	1:C:82:PRO:HG3	1.92	0.52
1:C:985:ASP:O	1:C:989:ALA:N	2.23	0.52
1:E:289:VAL:HG11	1:E:300:LYS:HD2	1.90	0.52
1:E:766:ALA:HB1	1:E:1012:LEU:HD21	1.91	0.52
1:E:1089:PHE:O	1:E:1091:ARG:N	2.43	0.52
1:A:291:CYS:O	1:A:297:SER:OG	2.26	0.52
1:A:357:ARG:HE	1:A:394:ASN:CG	2.13	0.52
1:A:905:ARG:HB2	1:A:1036:GLN:NE2	2.25	0.52
1:A:1081:ILE:HD12	1:A:1135:ASN:HB3	1.90	0.52
1:C:900:MET:SD	1:C:917:TYR:OH	2.62	0.52
1:C:918:GLU:OE2	1:E:1125:ASN:N	2.24	0.52
1:C:1118:ASP:OD1	1:C:1119:ASN:N	2.43	0.52
1:E:1088:HIS:CE1	1:E:1122:VAL:HG22	2.44	0.52
3:F:81:ILE:HB	3:F:84:VAL:HG22	1.90	0.52
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.91	0.52
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.45	0.52
1:C:1031:GLU:OE2	1:E:1039:ARG:NE	2.42	0.52
1:E:221:SER:OG	1:E:222:ALA:N	2.42	0.52
1:E:935:GLN:HA	1:E:938:LEU:HD12	1.92	0.52
2:K:39:GLN:HB3	2:K:93:VAL:HB	1.91	0.52
1:A:418:ILE:O	1:A:423:TYR:N	2.30	0.52
1:A:752:LEU:HD13	1:A:993:ILE:HG22	1.91	0.52
1:C:367:VAL:HA	1:C:370:ASN:HD21	1.75	0.52
1:C:48:LEU:HD23	1:C:276:LEU:HD21	1.90	0.52
1:C:110:LEU:HD22	1:C:237:ARG:HH21	1.75	0.52
1:C:152:TRP:C	1:C:154:GLU:H	2.14	0.52
1:C:802:PHE:HB3	1:C:805:ILE:HG13	1.91	0.52
1:E:909:ILE:HG23	1:E:1036:GLN:HE21	1.75	0.52
3:L:10:SER:HB3	3:L:111:GLU:OE2	2.10	0.52
1:A:762:GLN:HA	1:A:765:ARG:CD	2.39	0.51
1:C:455:LEU:HD12	1:C:456:PHE:CD1	2.46	0.51
1:C:641:ASN:HD21	1:C:654:GLU:N	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:770:ILE:O	1:E:773:GLU:HG3	2.10	0.51
2:D:151:TYR:OH	2:D:154:GLU:OE2	2.22	0.51
2:H:82:GLU:N	2:H:82:GLU:OE1	2.43	0.51
2:H:130:LEU:HD22	3:I:127:SER:H	1.75	0.51
5:N:2:NAG:H83	5:N:2:NAG:H3	1.91	0.51
1:C:140:PHE:H	1:C:158:ARG:NH2	2.08	0.51
1:C:412:PRO:HB3	1:C:429:PHE:CD2	2.45	0.51
1:C:661:GLU:O	1:C:695:TYR:OH	2.27	0.51
1:C:712:ILE:O	1:C:1074:ASN:HA	2.10	0.51
1:C:1054:GLN:HB3	1:C:1061:VAL:CG1	2.41	0.51
1:E:578:ASP:HB3	1:E:581:THR:O	2.10	0.51
1:E:913:GLN:HG3	1:E:917:TYR:CE2	2.45	0.51
1:E:1093:GLY:H	1:E:1107:ARG:HE	1.57	0.51
1:A:533:LEU:HD22	1:A:535:LYS:HE3	1.92	0.51
1:A:953:ASN:HB3	1:A:957:GLN:HE22	1.75	0.51
1:C:300:LYS:O	1:C:304:LYS:N	2.42	0.51
1:E:34:ARG:HD3	1:E:91:TYR:OH	2.11	0.51
1:E:92:PHE:HE1	1:E:265:TYR:HB2	1.75	0.51
2:D:72:VAL:HA	2:D:79:ALA:HB2	1.92	0.51
2:D:147:LEU:HD21	3:F:184:THR:HG23	1.91	0.51
1:A:920:GLN:OE1	1:A:920:GLN:N	2.36	0.51
1:E:909:ILE:HG23	1:E:1036:GLN:NE2	2.25	0.51
1:E:1036:GLN:NE2	1:E:1049:LEU:HA	2.24	0.51
1:E:1047:TYR:OH	1:E:1108:ASN:OD1	2.18	0.51
1:A:291:CYS:O	1:A:298:GLU:N	2.44	0.51
1:A:295:PRO:O	1:A:299:THR:HG23	2.10	0.51
1:A:962:LEU:HD13	1:A:1007:TYR:CG	2.45	0.51
1:A:993:ILE:HG23	1:A:997:ILE:HG13	1.93	0.51
1:C:426:PRO:HG3	1:C:463:PRO:HB3	1.92	0.51
1:C:612:TYR:HD2	1:C:649:CYS:HB3	1.74	0.51
1:C:729:VAL:HG12	1:C:1059:GLY:HA2	1.92	0.51
1:C:895:GLN:O	1:E:713:ALA:N	2.43	0.51
1:E:303:LEU:HD12	1:E:308:VAL:HG13	1.93	0.51
1:A:744:GLY:HA2	1:C:319:ARG:HH21	1.75	0.51
1:C:622:VAL:HG22	1:C:651:ILE:HD11	1.93	0.51
1:E:741:TYR:HD1	1:E:857:GLY:HA3	1.75	0.51
3:I:69:THR:OG1	3:I:80:THR:HB	2.10	0.51
3:I:167:GLU:HA	3:I:181:LEU:HD21	1.93	0.51
3:I:173:ASP:OD2	3:I:177:SER:N	2.44	0.51
1:A:116:SER:O	1:A:131:CYS:N	2.44	0.51
1:A:382:VAL:HG21	1:A:390:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.76	0.51
1:A:962:LEU:HD22	1:A:1007:TYR:CZ	2.46	0.51
1:A:974:SER:OG	1:A:976:VAL:O	2.26	0.51
1:C:275:PHE:HD1	1:C:290:ASP:HA	1.76	0.51
1:E:94:SER:OG	1:E:190:ARG:N	2.39	0.51
1:E:901:GLN:HE22	1:E:905:ARG:HD2	1.76	0.51
2:H:152:PHE:HB2	2:H:181:LEU:HD22	1.93	0.51
1:A:319:ARG:NH2	1:E:743:CYS:O	2.44	0.51
1:A:1028:LYS:HD3	1:A:1042:PHE:CE2	2.46	0.51
1:C:732:THR:O	1:C:734:THR:N	2.42	0.51
1:C:895:GLN:NE2	1:E:1074:ASN:OD1	2.44	0.51
1:C:1104:VAL:N	1:C:1113:GLN:O	2.27	0.51
1:E:804:GLN:O	1:E:816:SER:OG	2.28	0.51
1:E:977:LEU:HD21	1:E:1000:ARG:HH12	1.76	0.51
2:D:141:THR:OG1	2:D:190:VAL:O	2.29	0.51
3:L:99:ARG:HH21	3:L:100:TYR:HD2	1.59	0.51
1:A:86:PHE:CE1	1:A:90:VAL:HG22	2.45	0.51
1:A:102:ARG:HG2	1:A:121:ASN:HB3	1.93	0.51
1:A:1036:GLN:NE2	1:A:1049:LEU:HA	2.25	0.51
1:A:1129:VAL:HG21	1:A:1132:ILE:HB	1.91	0.51
1:C:231:ILE:HD11	1:C:235:ILE:HD11	1.93	0.51
1:C:789:TYR:HE1	1:E:703:ASN:HB2	1.75	0.51
1:C:1084:ASP:H	1:C:1088:HIS:HE1	1.59	0.51
1:C:1104:VAL:O	1:C:1113:GLN:N	2.42	0.51
1:E:192:PHE:HD1	1:E:205:SER:HB2	1.76	0.51
1:E:310:LYS:HG2	1:E:601:GLY:N	2.25	0.51
1:E:766:ALA:O	1:E:770:ILE:HG13	2.11	0.51
1:A:43:PHE:HE1	1:A:283:GLY:HA3	1.75	0.51
1:A:104:TRP:CE3	1:A:119:ILE:HG13	2.46	0.51
1:C:316:SER:OG	1:C:317:ASN:N	2.44	0.51
1:C:800:PHE:HD1	1:C:924:ALA:HB2	1.76	0.51
1:E:66:HIS:CE1	1:E:262:ALA:HA	2.45	0.51
1:E:307:THR:O	1:E:602:THR:OG1	2.23	0.51
1:E:705:VAL:HB	1:E:707:TYR:CE1	2.46	0.51
2:D:47:TRP:CD1	3:F:102:LEU:HD12	2.46	0.51
3:F:110:LEU:O	3:F:172:GLN:NE2	2.43	0.51
2:K:158:VAL:H	2:K:169:VAL:HG21	1.76	0.51
1:C:281:GLU:OE1	1:C:281:GLU:N	2.22	0.50
1:C:539:VAL:N	1:C:550:GLY:O	2.26	0.50
1:E:97:LYS:HZ3	1:E:261:GLY:N	2.10	0.50
1:E:473:TYR:HB3	1:E:489:TYR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1103:PHE:HD1	1:E:1112:PRO:HB2	1.76	0.50
2:D:150:ASP:HA	2:D:181:LEU:HB3	1.94	0.50
3:F:138:VAL:HB	3:F:185:LEU:HD23	1.93	0.50
2:K:212:LYS:NZ	2:K:214:ASP:OD1	2.37	0.50
3:L:121:VAL:HG11	3:L:202:VAL:HG21	1.94	0.50
1:A:894:LEU:HB3	1:C:713:ALA:O	2.11	0.50
1:C:191:GLU:HG2	1:C:223:LEU:HD21	1.94	0.50
1:C:774:GLN:HA	1:C:777:ASN:OD1	2.12	0.50
1:E:453:TYR:HD1	1:E:495:TYR:HH	1.59	0.50
1:E:486:PHE:HZ	2:H:50:GLY:H	1.60	0.50
2:D:39:GLN:NE2	2:D:43:LYS:O	2.40	0.50
1:A:92:PHE:CZ	1:A:94:SER:HB3	2.46	0.50
1:A:591:SER:CA	1:A:615:VAL:HG12	2.35	0.50
1:A:914:ASN:OD1	1:A:915:VAL:N	2.44	0.50
1:A:1077:THR:HG21	1:E:897:PRO:HG2	1.92	0.50
1:C:969:ASN:ND2	1:C:974:SER:H	2.09	0.50
1:A:101:ILE:HG21	1:A:265:TYR:CE1	2.47	0.50
1:A:333:THR:OG1	1:A:361:CYS:HB2	2.11	0.50
1:A:569:ILE:HG23	1:E:47:VAL:HG21	1.92	0.50
1:A:1036:GLN:NE2	1:A:1049:LEU:HD23	2.27	0.50
1:C:29:THR:HG22	1:C:64:TRP:HB2	1.94	0.50
1:C:437:ASN:HA	1:C:508:TYR:HA	1.94	0.50
1:C:873:TYR:O	1:C:876:ALA:N	2.44	0.50
1:E:214:ARG:HG3	1:E:215:ASP:H	1.76	0.50
1:E:293:LEU:HB3	1:E:297:SER:OG	2.10	0.50
1:E:666:ILE:HG12	1:E:670:ILE:O	2.11	0.50
1:E:1109:PHE:CD1	1:E:1111:GLU:HB2	2.47	0.50
1:A:617:CYS:N	1:A:649:CYS:SG	2.84	0.50
1:A:805:ILE:HG22	1:A:818:ILE:HD13	1.92	0.50
1:A:884:SER:HB2	1:C:707:TYR:CE1	2.46	0.50
1:A:920:GLN:HA	1:A:923:ILE:HD12	1.94	0.50
1:C:1088:HIS:CD2	1:C:1122:VAL:HG22	2.46	0.50
1:E:589:PRO:HG2	1:E:592:PHE:CE1	2.46	0.50
1:E:642:VAL:HG22	1:E:651:ILE:HG22	1.93	0.50
1:E:805:ILE:HG22	1:E:818:ILE:HD13	1.94	0.50
1:A:985:ASP:OD1	1:A:986:PRO:HD2	2.12	0.50
1:C:555:SER:OG	1:C:584:ILE:HG22	2.11	0.50
1:E:37:TYR:CD2	1:E:223:LEU:HB2	2.47	0.50
1:E:805:ILE:HG13	1:E:806:LEU:N	2.26	0.50
1:A:720:ILE:HG21	1:A:1065:VAL:HG13	1.93	0.50
1:C:403:ARG:HD2	1:C:505:TYR:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:802:PHE:HB3	1:C:805:ILE:CG1	2.41	0.50
1:C:1031:GLU:O	1:C:1037:SER:N	2.45	0.50
3:F:4:MET:HE3	3:F:24:LYS:O	2.12	0.50
3:L:119:PRO:HG3	3:L:145:PHE:HA	1.94	0.50
1:C:273:ARG:HH21	1:C:292:ALA:HB3	1.77	0.50
1:C:901:GLN:OE1	1:C:1050:MET:HE1	2.12	0.50
1:C:909:ILE:HG13	1:C:911:VAL:HG23	1.93	0.50
1:E:195:LYS:HB3	1:E:204:TYR:HE2	1.77	0.50
1:E:720:ILE:HG12	1:E:722:VAL:HG23	1.93	0.50
1:C:816:SER:OG	1:C:819:GLU:OE1	2.22	0.49
1:E:886:TRP:H	1:E:886:TRP:HE3	1.60	0.49
1:A:369:TYR:HA	1:A:374:PHE:CE2	2.47	0.49
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.45	0.49
1:A:1015:ALA:O	1:A:1019:ARG:HG3	2.12	0.49
1:C:326:ILE:HB	1:C:541:PHE:HA	1.94	0.49
1:E:822:LEU:O	1:E:826:VAL:HG22	2.12	0.49
1:E:930:ALA:O	1:E:934:ILE:HG13	2.13	0.49
1:E:985:ASP:OD2	1:E:987:PRO:HD2	2.12	0.49
3:I:204:HIS:CG	3:I:205:GLN:H	2.30	0.49
1:A:662:CYS:SG	1:A:663:ASP:N	2.85	0.49
1:A:888:PHE:CD1	1:A:893:ALA:HB2	2.46	0.49
1:A:920:GLN:HE21	1:C:1130:ILE:HD12	1.77	0.49
1:A:1123:SER:OG	1:E:914:ASN:ND2	2.40	0.49
1:C:866:THR:N	1:C:869:MET:HE2	2.14	0.49
1:C:901:GLN:HE22	1:C:905:ARG:NE	2.09	0.49
1:C:1010:GLN:HA	1:C:1013:ILE:HG12	1.94	0.49
1:E:58:PHE:HE2	1:E:289:VAL:HA	1.77	0.49
3:F:154:TRP:CH2	3:F:185:LEU:HD22	2.47	0.49
2:H:108:TRP:HE1	3:I:42:TYR:HE1	1.60	0.49
3:L:99:ARG:HG3	3:L:100:TYR:O	2.13	0.49
1:A:65:PHE:CE2	1:A:82:PRO:HG3	2.47	0.49
1:A:733:LYS:HD2	1:A:771:ALA:HA	1.95	0.49
1:A:870:ILE:O	1:A:874:THR:HG23	2.12	0.49
1:C:427:ASP:HA	1:C:429:PHE:CE1	2.47	0.49
1:E:721:SER:O	1:E:723:THR:HG23	2.12	0.49
1:A:380:TYR:HE2	1:A:412:PRO:HD2	1.77	0.49
1:C:792:PRO:HG2	1:E:707:TYR:CE2	2.47	0.49
3:F:111:GLU:HB3	3:F:146:TYR:CE1	2.44	0.49
2:K:29:PHE:CZ	2:K:74:THR:HA	2.47	0.49
2:K:45:LEU:HG	2:K:108:TRP:CH2	2.47	0.49
1:C:40:ASP:OD1	1:C:202:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:ASP:OD1	1:C:737:ASP:N	2.45	0.49
1:C:1101:HIS:HB2	1:C:1103:PHE:CE1	2.48	0.49
1:E:104:TRP:HE3	1:E:106:PHE:HE1	1.60	0.49
2:D:142:ALA:HB2	2:D:192:SER:HA	1.95	0.49
1:C:47:VAL:HG13	1:C:49:HIS:CE1	2.47	0.49
1:C:462:LYS:HD3	1:C:462:LYS:N	2.26	0.49
1:C:951:VAL:HA	1:C:954:GLN:OE1	2.13	0.49
1:C:1056:ALA:HB3	1:C:1059:GLY:C	2.33	0.49
1:E:805:ILE:HD12	1:E:1052:PHE:HD2	1.77	0.49
2:D:33:THR:HG22	2:D:53:PRO:HD3	1.93	0.49
1:A:764:ASN:O	1:A:768:THR:HG23	2.12	0.49
1:A:964:LYS:O	1:A:967:SER:OG	2.16	0.49
1:C:426:PRO:HB2	1:C:428:ASP:OD1	2.13	0.49
1:C:578:ASP:HB3	1:C:581:THR:O	2.12	0.49
1:C:920:GLN:HA	1:C:923:ILE:HD12	1.95	0.49
3:F:112:LEU:HD23	3:F:114:ARG:CZ	2.43	0.49
2:K:108:TRP:CD2	3:L:50:PRO:HD2	2.47	0.49
2:K:153:PRO:HD2	2:K:206:HIS:CE1	2.48	0.49
3:L:73:SER:N	3:L:76:ASP:O	2.46	0.49
1:A:378:LYS:HB2	1:A:433:VAL:HG13	1.95	0.49
1:A:934:ILE:HG23	1:A:938:LEU:HD12	1.94	0.49
1:E:131:CYS:CA	1:E:166:CYS:HB3	2.43	0.49
1:E:905:ARG:HH21	1:E:1036:GLN:CB	2.25	0.49
1:E:969:ASN:ND2	1:E:974:SER:HB3	2.28	0.49
2:H:207:LYS:HB2	2:H:208:PRO:HD3	1.94	0.49
1:A:93:ALA:HA	1:A:191:GLU:HA	1.95	0.49
1:A:931:ILE:HD13	1:A:934:ILE:HD12	1.94	0.49
1:A:1079:PRO:HB3	1:E:900:MET:HE2	1.95	0.49
1:C:401:VAL:O	1:C:402:ILE:HD13	2.12	0.49
1:C:725:GLU:HA	1:C:947:LYS:HZ1	1.76	0.49
1:C:905:ARG:CZ	1:C:1050:MET:HG3	2.43	0.49
1:E:402:ILE:O	1:E:508:TYR:N	2.46	0.49
1:A:190:ARG:NH2	1:A:207:HIS:HA	2.26	0.48
1:A:312:ILE:HG21	1:A:666:ILE:HG22	1.94	0.48
1:A:727:LEU:HD11	1:A:1028:LYS:HG3	1.95	0.48
1:A:1130:ILE:HD13	1:E:798:GLY:HA3	1.95	0.48
1:E:598:ILE:O	1:E:609:ALA:HB3	2.13	0.48
1:A:34:ARG:NH2	1:A:219:GLY:O	2.38	0.48
1:A:105:ILE:HB	1:A:239:GLN:HB3	1.95	0.48
1:A:1041:ASP:OD1	1:E:1030:SER:HB3	2.13	0.48
1:C:326:ILE:O	1:C:542:ASN:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:932:GLY:O	1:C:935:GLN:HG2	2.13	0.48
3:I:88:ASP:O	3:I:92:TYR:OH	2.28	0.48
1:A:380:TYR:CE2	1:A:412:PRO:HD2	2.48	0.48
1:A:867:ASP:N	1:A:867:ASP:OD1	2.46	0.48
1:A:880:GLY:O	1:A:885:GLY:N	2.44	0.48
1:A:906:PHE:HE2	1:A:916:LEU:HB2	1.78	0.48
1:A:1033:VAL:HG22	1:A:1051:SER:HB2	1.95	0.48
1:C:183:GLN:HG3	1:C:185:ASN:H	1.77	0.48
1:C:645:THR:HG23	1:C:647:ALA:H	1.78	0.48
1:C:1110:TYR:OH	14:C:1308:NAG:O7	2.32	0.48
1:E:132:GLU:HG2	1:E:164:ASN:HB2	1.94	0.48
1:E:346:ARG:HB3	1:E:346:ARG:NH1	2.28	0.48
1:E:805:ILE:HG13	1:E:806:LEU:H	1.78	0.48
1:E:920:GLN:HA	1:E:923:ILE:HD12	1.95	0.48
1:E:1109:PHE:HD1	1:E:1111:GLU:HB2	1.77	0.48
3:F:14:SER:HA	3:F:112:LEU:HD13	1.95	0.48
3:F:37:ASN:O	3:F:56:TRP:HA	2.14	0.48
3:F:57:ALA:HB1	3:F:77:PHE:CD1	2.48	0.48
1:A:895:GLN:NE2	1:C:712:ILE:O	2.46	0.48
1:A:977:LEU:HD11	1:A:996:LEU:HB3	1.96	0.48
1:A:1128:VAL:HG12	1:E:917:TYR:O	2.14	0.48
1:C:752:LEU:HD22	1:C:997:ILE:HG21	1.95	0.48
1:C:894:LEU:HD23	1:E:1072:GLU:HG3	1.94	0.48
1:E:91:TYR:HA	1:E:193:VAL:HG13	1.94	0.48
3:I:68:PHE:CD1	3:I:79:LEU:HD11	2.46	0.48
1:C:69:HIS:CE1	1:C:143:VAL:HG21	2.48	0.48
1:C:578:ASP:OD2	1:C:581:THR:HG22	2.13	0.48
1:C:710:ASN:O	1:C:1077:THR:N	2.44	0.48
1:C:1028:LYS:O	1:C:1032:CYS:CB	2.53	0.48
1:E:107:GLY:HA2	1:E:114:THR:OG1	2.13	0.48
1:E:353:TRP:CZ3	1:E:355:ARG:HB2	2.49	0.48
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.48	0.48
1:C:954:GLN:HA	1:C:957:GLN:HB3	1.94	0.48
1:E:771:ALA:O	1:E:774:GLN:HG3	2.14	0.48
3:L:95:GLN:HG3	3:L:104:PHE:CZ	2.48	0.48
1:A:295:PRO:HD2	1:A:608:VAL:HG21	1.96	0.48
1:A:951:VAL:HA	1:A:954:GLN:OE1	2.13	0.48
1:C:979:ASP:OD1	1:C:980:ILE:HD12	2.13	0.48
3:F:114:ARG:NH1	3:F:177:SER:O	2.46	0.48
1:A:130:VAL:O	1:A:166:CYS:HA	2.12	0.48
1:A:275:PHE:HA	1:A:289:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ALA:O	1:A:883:THR:OG1	2.21	0.48
1:C:441:LEU:HD13	1:C:509:ARG:CZ	2.44	0.48
1:C:877:LEU:HD23	1:C:1029:MET:SD	2.54	0.48
1:C:950:ASP:O	1:C:953:ASN:HB2	2.13	0.48
1:E:581:THR:HG23	1:E:583:GLU:OE1	2.14	0.48
1:E:905:ARG:CD	1:E:1050:MET:HB3	2.43	0.48
3:L:43:GLN:O	3:L:51:LYS:HG2	2.14	0.48
1:A:802:PHE:O	1:A:805:ILE:HG12	2.14	0.48
1:C:34:ARG:NH2	1:C:217:PRO:HB2	2.28	0.48
1:C:155:SER:OG	1:C:156:GLU:N	2.47	0.48
1:C:883:THR:HG21	1:E:707:TYR:CE2	2.49	0.48
1:E:92:PHE:CG	1:E:104:TRP:HZ2	2.32	0.48
1:E:309:GLU:O	1:E:313:TYR:OH	2.23	0.48
1:E:553:THR:O	1:E:585:LEU:HD12	2.14	0.48
2:D:92:ALA:N	2:D:114:VAL:O	2.47	0.48
2:H:29:PHE:CD1	2:H:77:SER:HA	2.48	0.48
1:A:86:PHE:HE1	1:A:90:VAL:HG22	1.79	0.48
1:A:95:THR:HG21	1:A:186:PHE:CE1	2.49	0.48
1:A:785:VAL:HG11	1:A:888:PHE:CZ	2.49	0.48
1:A:1008:VAL:O	1:A:1012:LEU:HG	2.13	0.48
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.33	0.48
1:E:764:ASN:O	1:E:767:LEU:HG	2.14	0.48
3:I:43:GLN:O	3:I:50:PRO:HB3	2.14	0.48
2:K:150:ASP:HB3	2:K:181:LEU:HD12	1.96	0.48
1:A:578:ASP:OD1	1:A:580:GLN:HG3	2.14	0.47
1:A:672:ALA:HA	1:A:694:ALA:HA	1.96	0.47
1:C:666:ILE:HG12	1:C:670:ILE:O	2.14	0.47
1:C:897:PRO:HB2	1:C:900:MET:HE1	1.96	0.47
1:C:917:TYR:OH	1:E:1079:PRO:O	2.32	0.47
1:E:362:VAL:HA	1:E:525:CYS:O	2.12	0.47
8:S:1:NAG:O3	8:S:2:NAG:O5	2.32	0.47
1:A:294:ASP:O	1:A:297:SER:N	2.39	0.47
1:E:474:GLN:HE21	1:E:479:PRO:HA	1.77	0.47
1:E:523:THR:HG22	1:E:523:THR:O	2.14	0.47
2:K:168:GLY:HA3	3:L:175:LYS:HE3	1.95	0.47
1:A:497:PHE:CE1	1:A:507:PRO:HG3	2.49	0.47
1:A:722:VAL:O	1:A:722:VAL:HG13	2.13	0.47
1:C:403:ARG:HD2	1:C:505:TYR:HD1	1.79	0.47
1:C:787:GLN:OE1	1:E:701:ALA:N	2.47	0.47
1:C:905:ARG:HH12	1:C:1048:HIS:HE1	1.61	0.47
1:E:51:THR:O	1:E:274:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:803:SER:OG	1:E:804:GLN:OE1	2.32	0.47
3:I:168:SER:H	3:I:181:LEU:HG	1.79	0.47
1:A:331:ASN:H	1:A:580:GLN:HA	1.80	0.47
1:A:702:GLU:HG2	1:E:789:TYR:CD2	2.50	0.47
1:C:275:PHE:CD1	1:C:290:ASP:HA	2.48	0.47
1:C:276:LEU:HD13	1:C:300:LYS:HB3	1.97	0.47
1:C:486:PHE:HA	2:D:52:ASN:HD22	1.80	0.47
2:D:87:THR:HG23	2:D:89:GLU:HG2	1.97	0.47
3:F:12:ALA:HB1	3:F:113:LYS:N	2.29	0.47
2:K:103:TYR:HA	3:L:97:TYR:OH	2.14	0.47
3:L:6:GLN:HB2	3:L:105:GLY:HA3	1.96	0.47
3:L:21:MET:HE1	3:L:79:LEU:HD13	1.96	0.47
1:A:101:ILE:HG21	1:A:265:TYR:HE1	1.78	0.47
1:A:895:GLN:HB2	1:C:707:TYR:CD1	2.49	0.47
1:C:449:TYR:HB3	1:C:496:GLY:HA2	1.95	0.47
1:C:567:ARG:NH1	1:C:571:ASP:OD1	2.38	0.47
1:C:783:ALA:HB2	1:C:873:TYR:CZ	2.49	0.47
1:C:930:ALA:O	1:C:934:ILE:HG13	2.15	0.47
1:E:82:PRO:HD2	1:E:265:TYR:CE1	2.49	0.47
1:E:114:THR:OG1	1:E:115:GLN:N	2.47	0.47
1:E:274:THR:HG23	1:E:291:CYS:CB	2.44	0.47
1:E:349:SER:OG	1:E:451:TYR:HA	2.15	0.47
1:E:395:VAL:HG13	1:E:514:SER:H	1.80	0.47
1:E:552:LEU:HD23	1:E:585:LEU:HD21	1.96	0.47
1:E:738:CYS:HB3	1:E:760:CYS:HB2	1.73	0.47
2:K:51:ILE:HD12	2:K:58:THR:HG22	1.97	0.47
2:K:128:PHE:HB2	2:K:147:LEU:HB3	1.96	0.47
3:L:99:ARG:NH2	3:L:100:TYR:HD2	2.13	0.47
1:C:44:ARG:HH21	1:C:49:HIS:CD2	2.33	0.47
1:E:56:LEU:HD13	1:E:269:TYR:O	2.15	0.47
1:E:882:ILE:HA	1:E:898:PHE:HD1	1.80	0.47
1:E:969:ASN:ND2	1:E:972:ALA:HB3	2.28	0.47
2:K:44:SER:HB2	3:L:104:PHE:HB3	1.95	0.47
1:A:52:GLN:NE2	1:A:273:ARG:O	2.47	0.47
1:A:122:ASN:HB3	5:P:1:NAG:C2	2.44	0.47
1:A:127:VAL:HG23	1:A:171:VAL:HA	1.97	0.47
1:A:164:ASN:ND2	4:B:3:FUC:H3	2.30	0.47
1:A:201:PHE:HD2	1:A:235:ILE:HD13	1.79	0.47
1:A:222:ALA:HB2	1:A:285:ILE:HB	1.97	0.47
1:A:289:VAL:HG21	1:A:300:LYS:HE3	1.97	0.47
1:A:796:ASP:OD2	5:V:1:NAG:O6	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:GLN:CD	1:A:1108:ASN:H	2.17	0.47
1:A:1109:PHE:CE2	1:A:1111:GLU:HB2	2.50	0.47
1:C:92:PHE:CG	1:C:104:TRP:HH2	2.32	0.47
1:C:643:PHE:HD2	1:C:650:LEU:HD22	1.80	0.47
1:C:781:VAL:HG13	1:C:782:PHE:CD1	2.50	0.47
1:C:866:THR:HG22	1:C:869:MET:HG2	1.96	0.47
1:C:993:ILE:HG13	1:C:997:ILE:HG12	1.97	0.47
1:E:64:TRP:CD1	1:E:65:PHE:N	2.82	0.47
1:E:986:PRO:HA	1:E:989:ALA:HB3	1.97	0.47
1:E:1115:ILE:HG23	1:E:1120:THR:HG21	1.95	0.47
2:H:98:ARG:HG2	2:H:107:TYR:HB2	1.96	0.47
1:A:769:GLY:HA2	1:A:772:VAL:HG12	1.97	0.47
1:A:961:THR:HG1	1:E:758:SER:HG	1.63	0.47
1:A:984:LEU:HB2	1:A:992:GLN:NE2	2.30	0.47
1:C:887:THR:OG1	1:C:894:LEU:HB2	2.14	0.47
1:E:778:THR:O	1:E:782:PHE:N	2.33	0.47
1:E:1028:LYS:O	1:E:1032:CYS:CB	2.61	0.47
1:A:190:ARG:HH12	1:A:207:HIS:HA	1.80	0.47
1:A:477:SER:HB2	3:L:97:TYR:HE2	1.79	0.47
1:A:895:GLN:O	1:C:712:ILE:HA	2.15	0.47
1:C:927:PHE:O	1:C:931:ILE:HG12	2.15	0.47
1:C:1008:VAL:O	1:C:1012:LEU:HD23	2.15	0.47
1:E:21:ARG:NH1	1:E:71:SER:OG	2.48	0.47
1:E:974:SER:OG	1:E:976:VAL:O	2.33	0.47
2:K:20:ILE:HG13	2:K:112:THR:HG21	1.97	0.47
1:A:82:PRO:HG2	1:A:265:TYR:CD2	2.50	0.47
1:A:455:LEU:HD22	1:A:456:PHE:CE2	2.50	0.47
1:A:774:GLN:HA	1:A:777:ASN:OD1	2.15	0.47
1:A:1003:SER:O	1:A:1006:THR:OG1	2.27	0.47
1:C:135:PHE:CD1	1:C:139:PRO:HD3	2.50	0.47
1:C:438:SER:OG	1:C:509:ARG:HG3	2.16	0.47
1:C:578:ASP:OD2	1:C:580:GLN:HG3	2.15	0.47
1:C:645:THR:OG1	1:C:646:ARG:N	2.46	0.47
1:C:726:ILE:O	1:C:947:LYS:HE2	2.15	0.47
1:C:773:GLU:O	1:C:776:LYS:HG2	2.14	0.47
1:C:819:GLU:OE1	1:C:819:GLU:N	2.37	0.47
1:C:1075:PHE:HD1	14:C:1307:NAG:H81	1.79	0.47
1:E:37:TYR:OH	1:E:195:LYS:HE3	2.15	0.47
1:E:410:ILE:HD11	1:E:418:ILE:HG22	1.97	0.47
1:E:1032:CYS:SG	1:E:1048:HIS:NE2	2.88	0.47
2:H:33:THR:OG1	2:H:99:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:194:SER:HB2	2:K:198:GLN:HB2	1.97	0.47
3:L:170:THR:OG1	3:L:180:SER:N	2.48	0.47
1:A:57:PRO:HG3	1:A:271:GLN:OE1	2.15	0.46
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.50	0.46
1:A:388:ASN:HA	1:A:526:GLY:HA3	1.96	0.46
1:A:439:ASN:ND2	1:A:506:GLN:OE1	2.48	0.46
1:A:591:SER:O	1:A:615:VAL:CG1	2.41	0.46
1:A:904:TYR:CD1	1:C:1107:ARG:HD3	2.50	0.46
1:E:92:PHE:H	1:E:193:VAL:HG22	1.80	0.46
1:E:724:THR:HG21	1:E:944:ALA:HA	1.96	0.46
1:E:1043:CYS:HB2	1:E:1048:HIS:HB2	1.98	0.46
1:E:1081:ILE:O	1:E:1087:ALA:HA	2.14	0.46
1:E:1093:GLY:H	1:E:1107:ARG:NE	2.12	0.46
3:I:91:VAL:HG13	3:I:109:LYS:HG2	1.97	0.46
1:A:131:CYS:HB3	1:A:165:ASN:O	2.15	0.46
1:A:149:ASN:O	1:A:150:LYS:NZ	2.34	0.46
1:A:308:VAL:O	1:A:601:GLY:HA3	2.16	0.46
1:C:900:MET:HE3	1:E:1079:PRO:HA	1.98	0.46
1:C:1091:ARG:HH11	1:C:1092:GLU:HB3	1.80	0.46
1:E:518:LEU:HG	1:E:519:HIS:H	1.81	0.46
1:E:962:LEU:HD22	1:E:1007:TYR:CE2	2.50	0.46
2:D:6:GLN:NE2	2:D:96:CYS:SG	2.88	0.46
2:H:6:GLN:HE22	2:H:93:VAL:CG1	2.29	0.46
2:H:144:LEU:O	2:H:188:VAL:HG12	2.14	0.46
2:K:68:ALA:HB2	2:K:83:LEU:HD23	1.98	0.46
2:K:172:PHE:H	2:K:184:LEU:HD21	1.79	0.46
3:L:16:GLY:H	3:L:83:SER:H	1.64	0.46
1:A:404:GLY:HA2	1:A:508:TYR:H	1.80	0.46
1:A:722:VAL:HG11	1:A:934:ILE:HG13	1.97	0.46
1:A:1043:CYS:HB2	1:A:1048:HIS:HB2	1.97	0.46
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.97	0.46
1:E:408:ARG:HH11	1:E:408:ARG:HG3	1.80	0.46
1:E:411:ALA:HB3	1:E:414:GLN:HG3	1.98	0.46
1:E:656:VAL:HG12	1:E:658:ASN:N	2.31	0.46
1:A:82:PRO:HG2	1:A:265:TYR:HD2	1.80	0.46
1:E:1088:HIS:ND1	1:E:1122:VAL:HA	2.31	0.46
2:D:33:THR:OG1	2:D:99:GLU:OE1	2.21	0.46
3:F:24:LYS:HA	3:F:76:ASP:OD1	2.15	0.46
2:K:52:ASN:HB3	2:K:55:ILE:HB	1.97	0.46
8:S:2:NAG:H61	8:S:3:BMA:O2	2.15	0.46
1:A:274:THR:O	1:A:290:ASP:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:TYR:HB3	1:A:496:GLY:HA2	1.98	0.46
1:C:646:ARG:HG2	1:C:668:ALA:HB1	1.97	0.46
1:C:879:ALA:HA	1:C:882:ILE:HG22	1.98	0.46
2:K:53:PRO:HB3	2:K:72:VAL:HG13	1.97	0.46
1:A:895:GLN:HE22	1:C:1074:ASN:HB2	1.80	0.46
1:C:86:PHE:CZ	1:C:89:GLY:HA2	2.50	0.46
1:C:95:THR:OG1	1:C:189:LEU:HD13	2.16	0.46
1:C:105:ILE:HG21	1:C:110:LEU:HD21	1.97	0.46
1:C:188:ASN:OD1	1:C:189:LEU:N	2.48	0.46
1:C:210:ILE:HG13	1:C:210:ILE:O	2.15	0.46
1:C:303:LEU:HD12	1:C:308:VAL:HG13	1.97	0.46
1:E:90:VAL:HG12	1:E:194:PHE:HB2	1.98	0.46
1:E:103:GLY:HA3	1:E:241:LEU:HB2	1.96	0.46
1:E:279:TYR:CZ	1:E:285:ILE:HG12	2.51	0.46
1:E:468:ILE:HG23	9:U:5:MAN:H61	1.98	0.46
1:E:726:ILE:C	1:E:727:LEU:HD12	2.36	0.46
2:K:89:GLU:HG3	2:K:90:ASP:OD1	2.15	0.46
3:L:109:LYS:HZ3	3:L:148:ARG:NE	2.14	0.46
8:W:2:NAG:H4	8:W:3:BMA:H2	1.69	0.46
1:A:38:TYR:HE2	1:A:224:GLU:HG3	1.81	0.46
1:A:125:ASN:ND2	5:P:1:NAG:O6	2.48	0.46
1:A:362:VAL:HB	1:A:527:PRO:HD3	1.98	0.46
1:A:589:PRO:HB2	1:A:592:PHE:HE2	1.80	0.46
1:A:788:ILE:HG12	1:C:699:LEU:CB	2.45	0.46
1:A:866:THR:H	1:A:869:MET:HE3	1.79	0.46
1:A:922:LEU:O	1:A:925:ASN:N	2.48	0.46
1:C:58:PHE:HE2	1:C:290:ASP:N	2.13	0.46
1:C:726:ILE:HB	1:C:948:LEU:CD2	2.46	0.46
1:C:1005:GLN:O	1:C:1009:THR:HG23	2.16	0.46
1:E:720:ILE:HD11	1:E:1065:VAL:HG13	1.98	0.46
2:D:103:TYR:CD2	3:F:52:LEU:HD13	2.50	0.46
2:K:14:PRO:HG3	2:K:117:SER:O	2.15	0.46
1:A:79:PHE:HA	1:A:244:LEU:HD11	1.97	0.46
1:A:394:ASN:OD1	1:A:524:VAL:HG21	2.16	0.46
1:A:485:GLY:H	1:A:488:CYS:HB2	1.80	0.46
1:A:914:ASN:HB3	1:C:1089:PHE:HZ	1.80	0.46
1:E:1028:LYS:NZ	1:E:1043:CYS:HA	2.30	0.46
2:D:23:LYS:HD2	2:D:78:THR:HG21	1.98	0.46
3:F:93:TYR:HD1	3:F:107:GLY:HA3	1.81	0.46
2:K:21:SER:OG	2:K:23:LYS:NZ	2.44	0.46
1:A:163:ALA:HB1	1:A:166:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:CYS:HB2	1:A:760:CYS:HB2	1.39	0.46
1:C:90:VAL:HG23	1:C:194:PHE:HD2	1.80	0.46
1:C:118:LEU:HB3	1:C:129:LYS:HG3	1.97	0.46
1:C:729:VAL:HB	1:C:1060:VAL:HG12	1.97	0.46
1:C:766:ALA:O	1:C:770:ILE:HG13	2.16	0.46
1:C:994:ASP:O	1:C:998:THR:HG23	2.16	0.46
1:E:948:LEU:O	1:E:952:VAL:HG22	2.16	0.46
2:H:24:THR:OG1	2:H:77:SER:HB3	2.15	0.46
1:A:334:ASN:O	1:A:361:CYS:HB3	2.15	0.46
1:A:360:ASN:H	1:A:524:VAL:HG22	1.81	0.46
1:A:734:THR:HG21	1:A:959:LEU:HD21	1.98	0.46
1:C:152:TRP:HZ2	1:C:157:PHE:CD2	2.33	0.46
1:E:296:LEU:HD21	1:E:300:LYS:HE2	1.98	0.46
1:E:906:PHE:HB3	1:E:911:VAL:HG13	1.98	0.46
2:D:1:GLU:OE1	2:D:2:VAL:N	2.49	0.46
2:D:23:LYS:HB3	2:D:23:LYS:HE3	1.77	0.46
3:I:118:ALA:HA	3:I:206:GLY:HA3	1.97	0.46
1:A:328:ARG:HB2	1:A:543:PHE:HE1	1.81	0.45
1:C:643:PHE:CZ	1:C:645:THR:HB	2.51	0.45
1:C:727:LEU:HB2	1:C:1062:PHE:CE2	2.47	0.45
1:C:1047:TYR:N	1:C:1066:THR:OG1	2.49	0.45
1:E:110:LEU:HD13	1:E:237:ARG:NH2	2.31	0.45
1:E:475:ALA:HB1	2:H:52:ASN:ND2	2.30	0.45
3:F:196:LYS:HG3	3:F:197:VAL:HG23	1.98	0.45
1:A:895:GLN:HB2	1:C:707:TYR:HD1	1.81	0.45
1:A:905:ARG:HB2	1:A:1036:GLN:CD	2.36	0.45
1:A:983:ARG:HB3	1:A:984:LEU:HD12	1.98	0.45
1:C:656:VAL:HG12	1:C:658:ASN:H	1.82	0.45
1:C:906:PHE:CE1	1:C:1049:LEU:HD22	2.51	0.45
1:E:214:ARG:HD3	1:E:214:ARG:HA	1.81	0.45
1:E:393:THR:HG21	1:E:520:ALA:HB3	1.98	0.45
1:E:951:VAL:O	1:E:954:GLN:HG3	2.16	0.45
1:E:1106:GLN:CD	1:E:1108:ASN:H	2.20	0.45
2:D:160:TRP:HE1	2:D:186:SER:HB3	1.80	0.45
2:H:136:SER:HB3	2:H:192:SER:HB2	1.98	0.45
3:I:120:SER:H	3:I:143:ASN:H	1.64	0.45
1:A:762:GLN:HA	1:A:765:ARG:NE	2.31	0.45
1:A:1111:GLU:O	1:A:1113:GLN:NE2	2.50	0.45
1:C:299:THR:HG22	1:C:308:VAL:HG11	1.98	0.45
1:E:320:VAL:HG21	1:E:538:CYS:SG	2.56	0.45
1:E:438:SER:HB2	1:E:509:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:737:ASP:OD2	1:E:740:MET:HB3	2.16	0.45
2:D:41:HIS:HB2	2:D:174:ALA:O	2.16	0.45
2:K:108:TRP:CG	3:L:50:PRO:HD2	2.51	0.45
1:A:328:ARG:HB2	1:A:543:PHE:CE1	2.51	0.45
1:A:560:LEU:HB2	1:A:563:GLN:HG3	1.98	0.45
1:C:789:TYR:CE1	1:E:703:ASN:HB2	2.51	0.45
1:C:1092:GLU:HA	1:C:1092:GLU:OE1	2.16	0.45
1:E:927:PHE:O	1:E:931:ILE:HG12	2.17	0.45
2:D:45:LEU:HB2	3:F:104:PHE:CG	2.51	0.45
3:F:146:TYR:CE2	3:F:147:PRO:HB3	2.50	0.45
3:L:4:MET:SD	3:L:96:GLN:N	2.89	0.45
1:A:675:GLN:NE2	1:A:677:GLN:OE1	2.50	0.45
1:A:711:SER:C	1:E:895:GLN:HE21	2.20	0.45
1:A:883:THR:HB	1:C:707:TYR:CD1	2.51	0.45
1:A:1045:LYS:HE3	1:E:784:GLN:HE21	1.80	0.45
1:C:528:LYS:HD2	1:C:530:SER:CB	2.47	0.45
1:C:855:PHE:HD1	1:E:589:PRO:HD3	1.82	0.45
1:C:947:LYS:O	1:C:951:VAL:HG13	2.16	0.45
1:E:104:TRP:CE3	1:E:106:PHE:HE1	2.34	0.45
1:E:316:SER:O	1:E:595:VAL:HB	2.16	0.45
1:E:656:VAL:HG12	1:E:658:ASN:H	1.82	0.45
3:F:204:HIS:CG	3:F:205:GLN:H	2.35	0.45
2:K:36:TRP:HB2	2:K:48:LEU:HD21	1.98	0.45
2:K:205:ASN:O	2:K:207:LYS:HG3	2.17	0.45
1:A:731:MET:HB2	1:A:1018:ILE:HD13	1.99	0.45
1:A:1029:MET:HE1	1:A:1053:PRO:HG3	1.99	0.45
1:C:816:SER:N	1:C:819:GLU:OE2	2.50	0.45
1:E:86:PHE:HB2	1:E:238:PHE:HD1	1.82	0.45
1:E:105:ILE:HD11	1:E:241:LEU:HD11	1.98	0.45
1:E:535:LYS:HB3	1:E:553:THR:HA	1.98	0.45
1:E:675:GLN:N	1:E:691:SER:O	2.50	0.45
1:E:742:ILE:HG22	1:E:749:CYS:SG	2.56	0.45
2:K:37:VAL:CG2	2:K:45:LEU:HB3	2.47	0.45
1:A:273:ARG:HH22	1:A:292:ALA:HB3	1.81	0.45
1:A:290:ASP:CG	1:A:291:CYS:H	2.19	0.45
1:C:54:LEU:HB3	1:C:270:LEU:HD21	1.99	0.45
1:C:112:SER:O	1:C:112:SER:OG	2.34	0.45
1:C:485:GLY:N	1:C:488:CYS:O	2.47	0.45
1:C:828:LEU:HD11	1:C:949:GLN:HB2	1.98	0.45
1:C:886:TRP:CZ2	1:E:1107:ARG:HB3	2.48	0.45
1:E:37:TYR:CG	1:E:223:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ASP:OD2	1:E:293:LEU:N	2.50	0.45
1:E:295:PRO:HB2	1:E:608:VAL:HB	1.99	0.45
1:E:740:MET:HA	1:E:743:CYS:O	2.16	0.45
1:A:346:ARG:NH1	1:A:347:PHE:O	2.50	0.45
1:A:759:PHE:CZ	1:C:970:PHE:HE1	2.35	0.45
1:A:858:LEU:HD22	1:A:959:LEU:HD22	1.98	0.45
1:A:1029:MET:CE	1:A:1053:PRO:HG3	2.46	0.45
1:C:726:ILE:H	1:C:947:LYS:NZ	2.15	0.45
1:E:1014:ARG:HH12	1:E:1018:ILE:HG13	1.82	0.45
1:E:1029:MET:HA	1:E:1029:MET:HE2	1.98	0.45
3:I:38:TYR:HB3	3:I:97:TYR:CD1	2.51	0.45
2:K:61:ASN:O	2:K:65:LYS:HB2	2.17	0.45
1:A:165:ASN:HB2	4:B:1:NAG:O5	2.17	0.45
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.82	0.45
1:A:759:PHE:CE2	1:C:970:PHE:HE1	2.35	0.45
1:C:43:PHE:HZ	1:E:558:LYS:NZ	2.14	0.45
1:C:308:VAL:N	1:C:602:THR:OG1	2.50	0.45
1:C:312:ILE:HB	1:C:596:SER:OG	2.17	0.45
1:C:790:LYS:N	1:E:702:GLU:OE1	2.48	0.45
1:C:882:ILE:HG13	1:C:898:PHE:CE1	2.52	0.45
1:E:105:ILE:HG21	1:E:110:LEU:HD21	1.99	0.45
1:E:322:PRO:HG2	1:E:540:ASN:CG	2.38	0.45
1:E:342:PHE:CZ	1:E:513:LEU:HD21	2.52	0.45
1:E:360:ASN:HA	1:E:523:THR:O	2.16	0.45
1:E:757:GLY:O	1:E:761:THR:HG23	2.17	0.45
3:F:4:MET:SD	3:F:96:GLN:HG2	2.57	0.45
3:F:93:TYR:CD1	3:F:107:GLY:HA3	2.52	0.45
3:I:146:TYR:CD1	3:I:147:PRO:HA	2.52	0.45
3:I:203:THR:HG22	3:I:210:PRO:HG3	1.98	0.45
1:A:108:THR:OG1	1:A:234:ASN:OD1	2.35	0.45
1:C:326:ILE:N	1:C:540:ASN:O	2.47	0.45
1:C:338:PHE:HE1	1:C:513:LEU:HD21	1.81	0.45
1:C:1049:LEU:HD11	1:C:1067:TYR:HD1	1.82	0.45
1:E:53:ASP:HB3	1:E:55:PHE:CZ	2.52	0.45
1:E:220:PHE:HZ	1:E:285:ILE:HB	1.82	0.45
1:E:705:VAL:HB	1:E:707:TYR:HE1	1.81	0.45
1:E:878:LEU:O	1:E:882:ILE:HG13	2.17	0.45
1:E:1067:TYR:OH	1:E:1108:ASN:O	2.22	0.45
1:E:1081:ILE:HG22	1:E:1135:ASN:HB3	1.97	0.45
1:E:1093:GLY:HA2	1:E:1107:ARG:HG3	1.99	0.45
3:L:112:LEU:O	3:L:146:TYR:OH	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HH12	1:A:216:LEU:HD12	1.81	0.44
1:A:84:LEU:HB3	1:A:269:TYR:OH	2.17	0.44
1:A:535:LYS:HB3	1:A:553:THR:HG22	1.98	0.44
1:A:872:GLN:O	1:A:875:SER:OG	2.31	0.44
1:C:923:ILE:HA	1:C:926:GLN:NE2	2.32	0.44
1:E:905:ARG:HG2	1:E:905:ARG:NH1	2.32	0.44
3:F:146:TYR:CD1	3:F:147:PRO:HA	2.53	0.44
2:H:88:SER:O	2:H:91:SER:OG	2.19	0.44
3:L:13:VAL:HG11	3:L:110:LEU:HD13	1.98	0.44
1:A:190:ARG:HH12	1:A:207:HIS:CG	2.35	0.44
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.50	0.44
1:E:401:VAL:HG21	1:E:451:TYR:CD1	2.52	0.44
1:E:986:PRO:O	1:E:990:GLU:HG2	2.17	0.44
1:E:1020:ALA:HA	1:E:1023:ASN:HD22	1.82	0.44
1:A:108:THR:H	1:A:114:THR:HG21	1.82	0.44
1:A:741:TYR:OH	1:A:962:LEU:O	2.34	0.44
1:C:535:LYS:HD3	1:C:535:LYS:HA	1.65	0.44
1:E:274:THR:HG23	1:E:291:CYS:HB2	1.99	0.44
1:E:870:ILE:O	1:E:874:THR:HG23	2.16	0.44
1:E:1079:PRO:HG2	1:E:1132:ILE:HA	2.00	0.44
3:F:6:GLN:NE2	3:F:94:CYS:SG	2.90	0.44
1:A:357:ARG:HD3	1:A:359:SER:HB2	2.00	0.44
1:A:529:LYS:HD2	1:A:529:LYS:HA	1.87	0.44
1:A:589:PRO:HB2	1:A:592:PHE:CE2	2.52	0.44
1:C:886:TRP:CH2	1:E:1107:ARG:HD3	2.52	0.44
1:C:909:ILE:HG23	1:C:1036:GLN:HE21	1.81	0.44
1:E:316:SER:C	1:E:595:VAL:HB	2.38	0.44
1:E:329:PHE:HB2	1:E:527:PRO:CA	2.44	0.44
1:E:759:PHE:O	1:E:763:LEU:HD23	2.18	0.44
1:E:903:ALA:HB1	1:E:913:GLN:OE1	2.18	0.44
2:D:174:ALA:HB1	2:D:182:TYR:OH	2.17	0.44
3:L:148:ARG:NH2	3:L:169:VAL:HB	2.32	0.44
1:A:192:PHE:HB3	1:A:194:PHE:CZ	2.53	0.44
1:A:1038:LYS:HB2	1:A:1038:LYS:HE3	1.78	0.44
1:C:50:SER:HB3	1:C:304:LYS:NZ	2.32	0.44
1:C:392:PHE:CD2	1:C:515:PHE:HB3	2.52	0.44
1:E:86:PHE:HB2	1:E:238:PHE:CD1	2.53	0.44
1:E:412:PRO:HB3	1:E:427:ASP:HA	1.99	0.44
1:E:750:SER:O	1:E:754:LEU:HD23	2.18	0.44
1:E:806:LEU:HG	1:E:807:PRO:HD2	1.99	0.44
2:D:37:VAL:HG13	2:D:95:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:THR:HG21	2:H:29:PHE:CE1	2.48	0.44
2:K:192:SER:O	2:K:195:LEU:HD13	2.18	0.44
1:A:45:SER:O	1:A:47:VAL:HG13	2.18	0.44
1:A:203:ILE:HD11	1:A:226:LEU:HD22	1.99	0.44
1:A:892:ALA:HB1	1:C:1072:GLU:OE2	2.17	0.44
1:A:1128:VAL:O	1:E:921:LYS:HG3	2.18	0.44
1:C:117:LEU:HD13	1:C:130:VAL:HG12	1.99	0.44
1:C:141:LEU:HD23	1:C:157:PHE:HA	2.00	0.44
1:C:577:ARG:NH2	1:C:584:ILE:HA	2.32	0.44
1:C:888:PHE:HB3	1:C:1034:LEU:HD22	1.99	0.44
1:E:296:LEU:HD13	1:E:606:ASN:CG	2.38	0.44
1:E:332:ILE:O	1:E:333:THR:OG1	2.29	0.44
1:E:773:GLU:O	1:E:777:ASN:ND2	2.50	0.44
3:F:146:TYR:HD1	3:F:179:TYR:CE2	2.26	0.44
3:F:147:PRO:HD2	3:F:204:HIS:CE1	2.52	0.44
2:K:48:LEU:HA	2:K:64:PHE:HD2	1.82	0.44
3:L:4:MET:HA	3:L:24:LYS:O	2.18	0.44
1:C:347:PHE:HB3	1:C:400:PHE:HA	2.00	0.44
1:C:368:LEU:HB3	1:C:374:PHE:CE2	2.53	0.44
1:E:50:SER:H	1:E:304:LYS:NZ	2.16	0.44
1:E:55:PHE:HB3	1:E:275:PHE:CZ	2.53	0.44
1:E:388:ASN:ND2	1:E:528:LYS:HG3	2.23	0.44
1:E:801:ASN:HB2	1:E:928:ASN:OD1	2.18	0.44
1:E:1077:THR:HG22	1:E:1096:VAL:HG22	2.00	0.44
1:E:1102:TRP:HB3	1:E:1115:ILE:HD11	1.98	0.44
2:H:38:LYS:HE2	2:H:46:GLU:OE1	2.18	0.44
3:L:45:LYS:HE3	3:L:48:GLN:HG3	1.99	0.44
1:A:100:ILE:C	1:A:102:ARG:HH12	2.21	0.44
1:A:985:ASP:CG	1:A:987:PRO:HD2	2.38	0.44
1:A:1081:ILE:O	1:A:1087:ALA:HA	2.18	0.44
1:C:378:LYS:HA	1:C:384:PRO:HG3	2.00	0.44
1:C:567:ARG:HD3	1:C:567:ARG:HA	1.75	0.44
2:D:175:VAL:N	2:D:182:TYR:OH	2.50	0.44
2:K:144:LEU:HD11	2:K:200:TYR:CD1	2.53	0.44
6:Y:2:NAG:C8	6:Y:2:NAG:H3	2.48	0.44
1:A:315:THR:OG1	1:A:316:SER:N	2.51	0.44
1:A:1129:VAL:HG11	1:A:1132:ILE:HB	2.00	0.44
1:C:455:LEU:HG	1:C:491:PRO:O	2.18	0.44
1:C:557:LYS:O	1:C:584:ILE:HG12	2.18	0.44
1:C:902:MET:HA	1:C:905:ARG:HB2	1.99	0.44
1:E:92:PHE:CD1	1:E:104:TRP:HZ2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:GLU:OE2	1:E:225:PRO:HD2	2.18	0.44
1:E:804:GLN:O	1:E:818:ILE:HG12	2.17	0.44
1:E:807:PRO:HA	1:E:815:ARG:O	2.18	0.44
1:E:867:ASP:O	1:E:870:ILE:HG22	2.17	0.44
2:D:156:VAL:HG12	2:D:206:HIS:CD2	2.53	0.44
2:K:39:GLN:O	2:K:92:ALA:HB1	2.17	0.44
3:L:173:ASP:HB3	3:L:178:THR:H	1.83	0.44
1:A:376:THR:O	1:A:434:ILE:HG23	2.18	0.43
1:A:431:GLY:HA2	1:A:515:PHE:CE2	2.52	0.43
1:A:438:SER:HB3	1:A:441:LEU:HB2	2.00	0.43
1:A:868:GLU:HG2	1:A:869:MET:N	2.33	0.43
1:A:947:LYS:O	1:A:951:VAL:HG23	2.18	0.43
1:C:77:LYS:HG3	1:C:78:ARG:N	2.33	0.43
1:C:89:GLY:HA3	1:C:270:LEU:HD13	1.99	0.43
1:C:356:LYS:O	1:C:397:ALA:N	2.29	0.43
1:C:869:MET:SD	1:E:669:GLY:HA3	2.59	0.43
1:C:974:SER:HB3	1:C:980:ILE:HD11	2.00	0.43
1:C:1036:GLN:HE22	1:C:1049:LEU:HA	1.83	0.43
1:E:1117:THR:HA	1:E:1120:THR:O	2.18	0.43
2:D:47:TRP:CG	3:F:102:LEU:HB2	2.53	0.43
2:H:47:TRP:HD1	3:I:104:PHE:CZ	2.35	0.43
1:A:299:THR:HB	1:A:313:TYR:CD2	2.52	0.43
1:A:326:ILE:HG12	1:A:328:ARG:HG2	2.01	0.43
1:A:454:ARG:NH2	1:A:469:SER:O	2.51	0.43
1:A:997:ILE:HG22	1:A:1001:LEU:HD23	2.00	0.43
1:C:47:VAL:CG1	1:C:49:HIS:HE1	2.31	0.43
1:C:132:GLU:O	1:C:162:SER:OG	2.28	0.43
1:C:411:ALA:HB3	1:C:414:GLN:HG3	2.00	0.43
1:C:1051:SER:HA	1:C:1063:LEU:O	2.18	0.43
1:E:471:GLU:O	1:E:491:PRO:HG3	2.18	0.43
1:E:526:GLY:HA2	1:E:527:PRO:HD3	1.77	0.43
1:E:966:LEU:HD23	1:E:1000:ARG:NH2	2.32	0.43
2:H:11:MET:HA	2:H:116:VAL:HG13	2.01	0.43
2:H:165:LEU:HD12	2:H:165:LEU:HA	1.89	0.43
3:L:13:VAL:N	3:L:111:GLU:O	2.35	0.43
1:A:767:LEU:O	1:A:770:ILE:HB	2.17	0.43
1:A:789:TYR:OH	1:C:705:VAL:O	2.35	0.43
1:A:887:THR:HG21	1:A:894:LEU:CB	2.45	0.43
1:A:927:PHE:O	1:A:931:ILE:HG12	2.18	0.43
1:C:55:PHE:C	1:C:270:LEU:HG	2.38	0.43
1:C:995:ARG:HA	1:C:998:THR:OG1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:VAL:H	1:E:245:HIS:N	2.16	0.43
2:D:207:LYS:HB2	2:D:208:PRO:HD3	2.00	0.43
2:H:36:TRP:CB	2:H:48:LEU:HD11	2.46	0.43
2:H:36:TRP:CZ3	2:H:94:TYR:HB3	2.47	0.43
3:I:114:ARG:HD3	3:I:115:THR:O	2.17	0.43
2:K:52:ASN:ND2	2:K:55:ILE:HG12	2.32	0.43
3:L:38:TYR:HB3	3:L:97:TYR:CE2	2.53	0.43
1:A:117:LEU:HA	1:A:130:VAL:HA	1.99	0.43
1:A:979:ASP:OD1	1:A:980:ILE:HD12	2.18	0.43
1:E:403:ARG:HD2	1:E:504:GLY:O	2.18	0.43
1:E:498:GLN:HB2	1:E:501:ASN:OD1	2.18	0.43
1:E:980:ILE:HD12	1:E:980:ILE:H	1.83	0.43
2:D:47:TRP:NE1	3:F:102:LEU:HD12	2.34	0.43
1:A:102:ARG:O	1:A:119:ILE:HB	2.19	0.43
1:A:110:LEU:H	1:A:114:THR:HG22	1.84	0.43
1:A:333:THR:OG1	1:A:336:CYS:SG	2.75	0.43
1:A:335:LEU:C	1:A:337:PRO:HD3	2.38	0.43
1:A:950:ASP:O	1:A:954:GLN:OE1	2.37	0.43
1:C:28:TYR:CE1	14:C:1301:NAG:H83	2.53	0.43
1:C:643:PHE:CD2	1:C:655:HIS:HB2	2.54	0.43
1:E:580:GLN:NE2	1:E:581:THR:HG22	2.33	0.43
1:E:867:ASP:HA	1:E:870:ILE:HG22	2.00	0.43
1:E:964:LYS:O	1:E:967:SER:OG	2.28	0.43
2:D:54:ASN:HB3	2:D:55:ILE:HD12	1.99	0.43
3:F:123:ILE:HD13	3:F:199:ALA:HA	2.00	0.43
2:H:36:TRP:HA	2:H:96:CYS:HA	2.01	0.43
3:I:110:LEU:HB3	3:I:172:GLN:HE22	1.84	0.43
3:I:168:SER:O	3:I:181:LEU:HA	2.18	0.43
1:A:63:THR:HG1	1:A:65:PHE:HE1	1.67	0.43
1:A:919:ASN:OD1	1:A:922:LEU:HB2	2.19	0.43
1:A:1050:MET:O	1:A:1064:HIS:HA	2.19	0.43
1:A:1128:VAL:HG11	1:E:920:GLN:H	1.82	0.43
1:C:347:PHE:CE1	1:C:399:SER:HB2	2.54	0.43
1:E:1050:MET:HE1	1:E:1052:PHE:CE1	2.54	0.43
2:D:98:ARG:HD2	2:D:99:GLU:O	2.19	0.43
3:F:173:ASP:O	3:F:177:SER:OG	2.17	0.43
2:H:83:LEU:HB2	2:H:86:LEU:HD21	1.99	0.43
2:H:160:TRP:HD1	2:H:168:GLY:O	2.02	0.43
2:K:41:HIS:ND1	2:K:41:HIS:O	2.52	0.43
2:K:159:SER:O	2:K:203:ASN:HB2	2.18	0.43
8:S:2:NAG:H4	8:S:3:BMA:H2	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD12	1:A:57:PRO:HD2	2.01	0.43
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.99	0.43
1:A:905:ARG:HD3	1:A:1049:LEU:O	2.18	0.43
1:A:1077:THR:OG1	1:E:900:MET:SD	2.76	0.43
1:C:435:ALA:HB2	1:C:510:VAL:HG13	2.00	0.43
1:C:821:LEU:HD23	1:C:821:LEU:O	2.19	0.43
1:E:55:PHE:HB3	1:E:275:PHE:CE2	2.53	0.43
1:E:425:LEU:HD11	1:E:429:PHE:CD2	2.54	0.43
1:E:503:VAL:HA	1:E:506:GLN:HB2	2.00	0.43
1:E:713:ALA:HA	1:E:1073:LYS:O	2.19	0.43
3:F:114:ARG:CZ	3:F:177:SER:HB2	2.48	0.43
3:I:93:TYR:CD2	3:I:107:GLY:HA3	2.53	0.43
1:A:331:ASN:ND2	7:M:1:NAG:H62	2.33	0.43
1:A:392:PHE:CD1	1:A:517:LEU:HD11	2.53	0.43
1:A:520:ALA:HA	1:E:200:TYR:CZ	2.53	0.43
1:A:859:THR:O	1:A:859:THR:OG1	2.32	0.43
1:A:997:ILE:HD13	1:A:1000:ARG:HG3	2.00	0.43
1:E:578:ASP:OD1	1:E:580:GLN:HG3	2.19	0.43
1:A:823:PHE:HA	1:A:826:VAL:HG22	2.01	0.43
1:A:930:ALA:O	1:A:934:ILE:HG13	2.19	0.43
1:A:977:LEU:HD23	1:A:980:ILE:HD13	2.01	0.43
1:A:1082:CYS:SG	1:A:1132:ILE:HD13	2.59	0.43
1:C:763:LEU:HD23	1:C:1008:VAL:HG11	2.00	0.43
1:C:789:TYR:HH	1:E:707:TYR:HH	1.51	0.43
1:C:811:LYS:HA	1:C:811:LYS:HD2	1.70	0.43
1:E:276:LEU:HD22	1:E:300:LYS:HB3	2.00	0.43
1:E:417:LYS:HE2	1:E:417:LYS:HB2	1.85	0.43
1:E:418:ILE:HA	1:E:422:ASN:ND2	2.34	0.43
2:H:24:THR:HG22	2:H:34:ILE:HD11	2.01	0.43
1:A:576:VAL:HG13	1:A:587:ILE:HD11	2.01	0.43
1:C:117:LEU:HD11	1:C:128:ILE:HD12	1.99	0.43
1:C:337:PRO:HG2	1:C:358:ILE:HD12	2.01	0.43
1:C:358:ILE:HB	1:C:395:VAL:HB	2.01	0.43
1:C:993:ILE:O	1:C:997:ILE:HG12	2.18	0.43
1:A:316:SER:OG	1:A:317:ASN:N	2.52	0.42
1:C:534:VAL:HG22	1:C:537:LYS:HE3	2.00	0.42
1:C:784:GLN:NE2	1:C:889:GLY:O	2.32	0.42
1:E:557:LYS:HD3	1:E:557:LYS:HA	1.91	0.42
1:E:743:CYS:HB3	1:E:749:CYS:HB3	1.79	0.42
2:D:35:TYR:CZ	3:F:102:LEU:HD11	2.54	0.42
2:D:160:TRP:NE1	2:D:186:SER:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:99:ARG:HG2	3:I:100:TYR:H	1.84	0.42
1:A:540:ASN:HA	1:A:548:GLY:O	2.19	0.42
1:A:886:TRP:HB3	1:A:1034:LEU:O	2.19	0.42
1:A:920:GLN:NE2	1:C:1128:VAL:HG13	2.34	0.42
1:C:88:ASP:O	1:C:270:LEU:HD22	2.18	0.42
1:C:280:ASN:OD1	1:C:283:GLY:N	2.52	0.42
1:C:312:ILE:HA	1:C:597:VAL:O	2.19	0.42
1:C:617:CYS:N	1:C:644:GLN:OE1	2.45	0.42
1:C:712:ILE:HG21	1:C:1096:VAL:CG2	2.49	0.42
1:C:714:ILE:HG22	1:C:1110:TYR:HB2	2.00	0.42
1:C:757:GLY:O	1:C:761:THR:HG23	2.19	0.42
2:H:170:HIS:HB2	2:H:186:SER:OG	2.18	0.42
3:L:6:GLN:HB3	3:L:108:THR:HG23	2.01	0.42
1:E:94:SER:O	1:E:189:LEU:HA	2.18	0.42
1:E:108:THR:HG22	1:E:236:THR:HG23	2.01	0.42
1:E:396:TYR:N	1:E:514:SER:HB3	2.20	0.42
1:E:776:LYS:HE3	1:E:776:LYS:HB3	1.88	0.42
1:E:920:GLN:HA	1:E:923:ILE:HB	2.00	0.42
1:E:947:LYS:HA	1:E:950:ASP:OD2	2.19	0.42
2:K:127:VAL:HG13	2:K:146:CYS:HB2	2.02	0.42
3:L:71:SER:OG	3:L:72:GLY:N	2.52	0.42
3:L:96:GLN:O	3:L:102:LEU:HD22	2.20	0.42
1:A:100:ILE:HD12	1:A:243:ALA:O	2.20	0.42
1:A:144:TYR:HA	1:A:245:HIS:HD2	1.84	0.42
1:A:722:VAL:HB	1:A:930:ALA:HB1	2.00	0.42
1:A:791:THR:OG1	1:A:806:LEU:HD11	2.20	0.42
1:A:997:ILE:O	1:A:1001:LEU:HD23	2.19	0.42
1:A:1103:PHE:HD2	1:A:1112:PRO:HB2	1.85	0.42
1:C:661:GLU:HB3	1:C:700:GLY:HA2	2.02	0.42
1:E:64:TRP:HD1	1:E:65:PHE:H	1.65	0.42
1:E:117:LEU:C	1:E:129:LYS:HE3	2.38	0.42
1:E:774:GLN:HA	1:E:777:ASN:HD22	1.84	0.42
1:E:1081:ILE:HG12	1:E:1095:PHE:CZ	2.54	0.42
3:F:142:LEU:HB3	3:F:181:LEU:HD12	2.01	0.42
3:L:45:LYS:HB3	3:L:48:GLN:HG3	2.01	0.42
1:A:38:TYR:HB2	1:A:225:PRO:HD3	2.01	0.42
1:A:203:ILE:HG12	1:A:227:VAL:O	2.19	0.42
1:A:714:ILE:HD12	1:A:1096:VAL:HG21	2.01	0.42
1:A:772:VAL:HA	1:A:775:ASP:OD2	2.20	0.42
1:A:1044:GLY:HA3	1:A:1064:HIS:CD2	2.54	0.42
1:A:1079:PRO:HB3	1:E:900:MET:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:GLU:OE1	1:A:1111:GLU:HA	2.20	0.42
1:C:28:TYR:HE1	14:C:1301:NAG:H83	1.84	0.42
1:C:777:ASN:HA	1:C:780:GLU:HG3	2.01	0.42
1:C:894:LEU:CD2	1:E:1072:GLU:HG3	2.49	0.42
1:E:96:GLU:HG3	1:E:98:SER:H	1.84	0.42
1:E:462:LYS:HE3	1:E:463:PRO:HD2	2.01	0.42
1:E:677:GLN:HB2	1:E:691:SER:OG	2.20	0.42
3:L:42:TYR:HE2	3:L:95:GLN:HB3	1.84	0.42
1:A:186:PHE:HB2	1:A:213:VAL:HG23	2.02	0.42
1:A:311:GLY:HA2	1:A:664:ILE:HD13	2.01	0.42
1:A:325:SER:HB3	1:A:540:ASN:HB2	2.02	0.42
1:A:643:PHE:CG	1:A:655:HIS:HB2	2.55	0.42
1:A:782:PHE:HB3	1:A:873:TYR:CB	2.50	0.42
1:A:856:ASN:C	1:A:858:LEU:H	2.22	0.42
1:A:947:LYS:HA	1:A:950:ASP:HB2	2.00	0.42
1:C:872:GLN:O	1:C:875:SER:OG	2.36	0.42
1:E:326:ILE:HG13	1:E:533:LEU:HD11	2.00	0.42
1:E:346:ARG:HB3	1:E:346:ARG:CZ	2.49	0.42
1:E:477:SER:OG	2:H:104:SER:HB3	2.19	0.42
1:E:879:ALA:HA	1:E:882:ILE:HD12	2.00	0.42
1:E:906:PHE:CD2	1:E:916:LEU:HB2	2.53	0.42
1:E:945:LEU:O	1:E:949:GLN:HG3	2.20	0.42
1:E:969:ASN:HD22	1:E:974:SER:HB3	1.84	0.42
1:E:1056:ALA:HB3	1:E:1059:GLY:C	2.40	0.42
2:D:2:VAL:HG11	2:D:98:ARG:HH21	1.85	0.42
3:I:31:TYR:HD1	3:I:98:TYR:HE1	1.68	0.42
1:A:56:LEU:HB2	1:A:270:LEU:HD22	2.01	0.42
1:A:100:ILE:HD13	1:A:100:ILE:HA	1.90	0.42
1:A:353:TRP:CZ2	1:A:466:ARG:HB2	2.53	0.42
1:A:999:GLY:O	1:A:1002:GLN:HG3	2.20	0.42
1:C:58:PHE:HD2	1:C:293:LEU:HD22	1.84	0.42
1:C:66:HIS:HE2	1:C:77:LYS:HE3	1.83	0.42
1:C:328:ARG:HD2	1:C:543:PHE:CE1	2.55	0.42
1:C:388:ASN:HB3	1:C:527:PRO:HG3	2.02	0.42
1:E:730:SER:O	1:E:1058:HIS:HB3	2.20	0.42
1:E:731:MET:HE3	1:E:1015:ALA:HA	2.02	0.42
2:D:61:ASN:OD1	2:D:64:PHE:N	2.43	0.42
3:F:36:LYS:HD3	3:F:56:TRP:NE1	2.35	0.42
2:H:6:GLN:HB2	2:H:112:THR:HG23	2.01	0.42
2:H:48:LEU:HD22	2:H:64:PHE:CD1	2.54	0.42
3:L:20:THR:HA	3:L:78:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HG2	1:A:191:GLU:OE2	2.20	0.42
1:C:528:LYS:HD2	1:C:530:SER:HB3	2.01	0.42
1:C:604:THR:HG22	1:C:605:SER:H	1.85	0.42
1:C:767:LEU:O	1:C:770:ILE:HB	2.20	0.42
1:C:785:VAL:HG22	1:C:891:GLY:HA2	2.02	0.42
1:C:1002:GLN:O	1:C:1005:GLN:HG3	2.19	0.42
1:E:85:PRO:HG2	1:E:269:TYR:OH	2.19	0.42
1:E:655:HIS:CG	1:E:656:VAL:N	2.88	0.42
1:E:1019:ARG:HD3	1:E:1023:ASN:ND2	2.29	0.42
2:K:70:LEU:HD21	2:K:82:GLU:H	1.85	0.42
1:A:470:THR:HG21	1:A:492:LEU:HD11	2.02	0.42
1:A:970:PHE:CE1	1:E:759:PHE:CE2	3.07	0.42
1:C:364:ASP:HA	1:C:527:PRO:HB3	2.00	0.42
1:C:782:PHE:O	1:C:877:LEU:HD11	2.19	0.42
1:C:913:GLN:HB2	1:E:1089:PHE:HB3	2.01	0.42
1:C:1073:LYS:NZ	1:C:1075:PHE:HB3	2.34	0.42
1:E:739:THR:O	1:E:743:CYS:HB2	2.20	0.42
1:E:968:SER:O	1:E:968:SER:OG	2.37	0.42
2:D:175:VAL:O	2:D:182:TYR:CZ	2.73	0.42
2:H:2:VAL:HG22	2:H:27:TYR:HB3	2.01	0.42
2:K:122:THR:HA	2:K:152:PHE:HD2	1.84	0.42
1:A:110:LEU:HD12	1:A:237:ARG:NE	2.34	0.42
1:A:376:THR:HB	1:A:435:ALA:H	1.84	0.42
1:A:620:VAL:HG11	1:A:625:HIS:CG	2.55	0.42
1:A:853:GLN:HA	1:A:860:VAL:HB	2.02	0.42
1:A:878:LEU:HD12	1:A:879:ALA:N	2.34	0.42
1:A:1090:PRO:HB3	1:A:1119:ASN:O	2.19	0.42
1:C:312:ILE:HG23	1:C:664:ILE:CG2	2.49	0.42
1:C:436:TRP:O	1:C:509:ARG:N	2.42	0.42
1:C:449:TYR:HB3	1:C:496:GLY:H	1.85	0.42
1:C:1052:PHE:O	1:C:1062:PHE:HA	2.20	0.42
1:E:32:PHE:CD2	1:E:218:GLN:HG3	2.55	0.42
1:E:192:PHE:CD1	1:E:205:SER:HB2	2.55	0.42
1:E:303:LEU:HD23	1:E:303:LEU:HA	1.86	0.42
1:E:889:GLY:HA3	1:E:1034:LEU:HD23	2.02	0.42
1:E:1096:VAL:N	1:E:1103:PHE:O	2.49	0.42
1:A:334:ASN:O	1:A:335:LEU:HB2	2.20	0.41
1:A:730:SER:C	1:A:1058:HIS:HB3	2.39	0.41
1:A:883:THR:HB	1:C:707:TYR:CG	2.55	0.41
1:A:951:VAL:HA	1:A:954:GLN:CD	2.41	0.41
1:A:1033:VAL:C	1:A:1035:GLY:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:GLY:HA2	1:C:664:ILE:HD13	2.02	0.41
1:C:356:LYS:HD3	1:C:356:LYS:HA	1.79	0.41
1:E:105:ILE:HG23	1:E:116:SER:OG	2.19	0.41
1:E:215:ASP:OD1	1:E:215:ASP:N	2.45	0.41
1:E:348:ALA:O	1:E:401:VAL:HG23	2.20	0.41
1:E:720:ILE:HG23	1:E:720:ILE:O	2.20	0.41
3:I:38:TYR:HD1	3:I:97:TYR:HE1	1.68	0.41
3:L:39:LEU:HD21	3:L:41:TRP:NE1	2.35	0.41
5:N:1:NAG:O3	5:N:2:NAG:O5	2.38	0.41
1:A:558:LYS:HZ2	1:A:560:LEU:HD11	1.85	0.41
1:A:622:VAL:HG11	1:A:641:ASN:HB3	2.02	0.41
1:A:730:SER:OG	1:A:1058:HIS:ND1	2.41	0.41
1:C:220:PHE:HB3	1:C:286:THR:O	2.20	0.41
1:C:913:GLN:OE1	1:E:1089:PHE:HB3	2.20	0.41
1:C:1106:GLN:HE22	1:C:1111:GLU:HB3	1.85	0.41
1:E:403:ARG:NH1	1:E:406:GLU:OE2	2.53	0.41
3:I:148:ARG:HD3	3:I:149:GLU:OE2	2.20	0.41
1:A:102:ARG:NH1	1:A:102:ARG:HG3	2.35	0.41
1:A:299:THR:HB	1:A:313:TYR:HD2	1.85	0.41
1:A:453:TYR:HB3	1:A:495:TYR:HE1	1.85	0.41
1:C:448:ASN:ND2	1:C:450:ASN:OD1	2.46	0.41
1:C:984:LEU:HD23	1:C:988:GLU:HG2	2.02	0.41
1:C:1024:LEU:HD22	1:C:1042:PHE:CZ	2.54	0.41
1:E:616:ASN:OD1	1:E:617:CYS:N	2.53	0.41
1:E:645:THR:HG23	1:E:647:ALA:H	1.86	0.41
1:E:666:ILE:HD11	1:E:670:ILE:HB	2.01	0.41
1:E:909:ILE:HB	1:E:1047:TYR:CD2	2.55	0.41
1:E:1043:CYS:HB2	1:E:1048:HIS:CB	2.51	0.41
3:F:51:LYS:HA	3:F:51:LYS:HD3	1.96	0.41
3:F:146:TYR:CZ	3:F:147:PRO:HB3	2.54	0.41
3:F:169:VAL:HA	3:F:181:LEU:HD23	2.01	0.41
3:I:19:VAL:HG21	3:I:84:VAL:HG21	2.02	0.41
2:K:28:THR:OG1	2:K:31:GLU:HB2	2.20	0.41
3:L:118:ALA:HB2	3:L:206:GLY:HA3	2.02	0.41
1:A:84:LEU:HB2	1:A:238:PHE:CE1	2.55	0.41
1:A:115:GLN:NE2	1:A:233:ILE:O	2.54	0.41
1:A:170:TYR:OH	1:A:173:GLN:NE2	2.52	0.41
1:A:195:LYS:HD2	1:A:202:LYS:HD2	2.02	0.41
1:A:707:TYR:CD2	1:E:792:PRO:HB3	2.46	0.41
1:C:412:PRO:HB3	1:C:429:PHE:CG	2.55	0.41
1:C:746:SER:OG	1:C:749:CYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:ASP:O	1:E:368:LEU:HG	2.20	0.41
1:E:408:ARG:HG3	1:E:408:ARG:NH1	2.35	0.41
1:E:591:SER:O	1:E:615:VAL:HG22	2.20	0.41
1:E:715:PRO:O	1:E:1110:TYR:HB2	2.20	0.41
3:I:40:ALA:HB2	3:I:97:TYR:CE2	2.55	0.41
3:L:170:THR:HG21	3:L:180:SER:HB3	2.02	0.41
1:A:190:ARG:NH1	1:A:207:HIS:HA	2.34	0.41
1:A:710:ASN:HA	1:A:1077:THR:HG22	2.03	0.41
1:A:787:GLN:NE2	1:C:703:ASN:OD1	2.54	0.41
1:C:117:LEU:HG	1:C:119:ILE:HD11	2.02	0.41
1:C:393:THR:HA	1:C:522:ALA:HA	2.01	0.41
1:C:470:THR:HG22	1:C:470:THR:O	2.19	0.41
1:E:108:THR:HA	1:E:236:THR:OG1	2.21	0.41
1:E:541:PHE:O	1:E:547:THR:HA	2.21	0.41
1:E:1019:ARG:O	1:E:1023:ASN:ND2	2.53	0.41
3:F:95:GLN:HE22	3:F:97:TYR:HD2	1.69	0.41
1:A:122:ASN:HB3	5:P:1:NAG:H2	2.02	0.41
1:A:194:PHE:HE1	1:A:203:ILE:HG22	1.86	0.41
1:A:616:ASN:O	1:A:618:THR:N	2.53	0.41
1:A:997:ILE:HA	1:A:1000:ARG:HB2	2.02	0.41
1:A:1028:LYS:HB3	1:A:1062:PHE:CE2	2.55	0.41
1:C:54:LEU:HD13	1:C:272:PRO:HA	2.02	0.41
1:C:231:ILE:HD12	1:C:233:ILE:HG13	2.02	0.41
1:C:408:ARG:NH1	1:C:414:GLN:HE22	2.19	0.41
1:C:716:THR:HG22	1:C:1110:TYR:CD2	2.55	0.41
1:C:818:ILE:O	1:C:822:LEU:HD23	2.20	0.41
1:E:322:PRO:HG2	1:E:540:ASN:ND2	2.36	0.41
1:E:577:ARG:HD3	1:E:577:ARG:HA	1.68	0.41
1:E:643:PHE:CG	1:E:655:HIS:HB2	2.56	0.41
1:E:733:LYS:HZ1	1:E:862:PRO:C	2.18	0.41
3:F:88:ASP:HB3	3:F:92:TYR:OH	2.20	0.41
3:I:170:THR:HB	3:I:180:SER:H	1.86	0.41
2:K:88:SER:O	2:K:91:SER:OG	2.30	0.41
3:L:112:LEU:HD22	3:L:114:ARG:HE	1.86	0.41
3:L:130:GLN:HE21	3:L:130:GLN:HB3	1.74	0.41
1:A:783:ALA:HB2	1:A:873:TYR:CE2	2.55	0.41
1:A:802:PHE:HE2	1:A:806:LEU:HD12	1.86	0.41
1:A:950:ASP:O	1:A:953:ASN:HB2	2.20	0.41
1:A:966:LEU:HG	1:A:1000:ARG:NH1	2.36	0.41
1:A:984:LEU:HD13	1:A:992:GLN:NE2	2.35	0.41
1:A:1033:VAL:CG2	1:A:1051:SER:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:CYS:O	1:C:483:VAL:N	2.45	0.41
1:C:541:PHE:CE2	1:C:587:ILE:HG12	2.55	0.41
1:C:750:SER:O	1:C:754:LEU:HD23	2.20	0.41
1:C:828:LEU:HB3	1:C:953:ASN:ND2	2.35	0.41
1:C:886:TRP:HB3	1:C:1035:GLY:HA2	2.03	0.41
1:E:418:ILE:HA	1:E:422:ASN:HD22	1.86	0.41
1:E:725:GLU:OE2	1:E:1064:HIS:N	2.54	0.41
1:E:856:ASN:C	1:E:858:LEU:H	2.23	0.41
1:E:1038:LYS:HD3	1:E:1038:LYS:HA	1.88	0.41
3:F:34:ASN:OD1	3:F:36:LYS:HE3	2.21	0.41
3:F:59:SER:C	3:F:60:ARG:HD3	2.41	0.41
2:K:43:LYS:HG2	2:K:44:SER:N	2.29	0.41
3:L:95:GLN:NE2	3:L:96:GLN:O	2.43	0.41
6:Y:1:NAG:H83	6:Y:1:NAG:H2	1.95	0.41
1:A:316:SER:O	1:A:595:VAL:N	2.49	0.41
1:A:802:PHE:CE2	1:A:806:LEU:HD12	2.56	0.41
1:C:195:LYS:HE3	1:C:202:LYS:HD2	2.03	0.41
1:C:283:GLY:HA3	1:E:558:LYS:HZ1	1.86	0.41
1:C:728:PRO:HG3	1:C:951:VAL:HG21	2.01	0.41
1:C:1090:PRO:HG2	1:C:1092:GLU:C	2.41	0.41
1:E:332:ILE:HG22	1:E:333:THR:N	2.35	0.41
1:E:774:GLN:NE2	1:E:775:ASP:HB3	2.36	0.41
1:E:1080:ALA:HB1	1:E:1087:ALA:HB1	2.03	0.41
2:D:100:VAL:HG12	2:D:102:ASN:H	1.84	0.41
3:F:36:LYS:HD3	3:F:56:TRP:CD1	2.55	0.41
2:H:37:VAL:HG23	2:H:105:PHE:CE1	2.56	0.41
3:I:43:GLN:OE1	3:I:45:LYS:HE2	2.21	0.41
1:A:294:ASP:O	1:A:297:SER:OG	2.31	0.41
1:A:726:ILE:HD11	1:A:947:LYS:H	1.85	0.41
1:A:778:THR:O	1:A:782:PHE:HB2	2.20	0.41
1:C:128:ILE:HB	1:C:170:TYR:HB3	2.02	0.41
1:C:189:LEU:HG	1:C:191:GLU:OE1	2.20	0.41
1:C:530:SER:O	1:C:531:THR:OG1	2.28	0.41
1:C:656:VAL:HG21	1:C:693:ILE:HB	2.03	0.41
1:C:961:THR:CB	1:C:965:GLN:HE22	2.32	0.41
1:C:1005:GLN:HA	1:C:1008:VAL:HG22	2.01	0.41
1:E:67:ALA:HB1	1:E:69:HIS:CD2	2.56	0.41
1:E:203:ILE:O	1:E:225:PRO:HA	2.21	0.41
1:E:355:ARG:HH22	1:E:464:PHE:HD1	1.69	0.41
1:E:360:ASN:H	1:E:524:VAL:HG22	1.85	0.41
1:E:391:CYS:O	1:E:517:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:VAL:HG13	1:E:514:SER:N	2.36	0.41
1:E:671:CYS:SG	1:E:697:MET:HG2	2.61	0.41
1:E:725:GLU:CG	1:E:1062:PHE:HB2	2.51	0.41
1:E:878:LEU:HG	1:E:882:ILE:HD11	2.02	0.41
2:D:2:VAL:HG11	2:D:98:ARG:NH2	2.35	0.41
2:D:38:LYS:O	2:D:46:GLU:N	2.51	0.41
2:D:39:GLN:HA	2:D:45:LEU:HD23	2.02	0.41
2:D:177:GLN:HG3	2:D:180:GLY:N	2.30	0.41
3:F:110:LEU:HD23	3:F:110:LEU:HA	1.92	0.41
2:H:6:GLN:NE2	2:H:112:THR:OG1	2.54	0.41
3:I:38:TYR:HD1	3:I:97:TYR:CE1	2.39	0.41
3:I:41:TRP:HD1	3:I:54:ILE:HB	1.86	0.41
2:K:128:PHE:CE2	2:K:149:LYS:HB3	2.54	0.41
3:L:146:TYR:CD1	3:L:147:PRO:HA	2.55	0.41
6:J:2:NAG:H4	6:J:3:BMA:H2	1.80	0.41
1:A:980:ILE:HG23	1:A:983:ARG:NH1	2.36	0.41
1:C:108:THR:HG23	1:C:234:ASN:HB2	2.02	0.41
1:C:403:ARG:CZ	1:C:406:GLU:HG3	2.51	0.41
1:C:605:SER:OG	1:C:606:ASN:N	2.54	0.41
1:C:764:ASN:HA	1:C:767:LEU:HG	2.03	0.41
1:C:796:ASP:N	1:C:796:ASP:OD1	2.52	0.41
1:E:275:PHE:CD1	1:E:290:ASP:HA	2.56	0.41
1:E:419:ALA:O	1:E:424:LYS:HG2	2.20	0.41
1:A:104:TRP:HE3	1:A:119:ILE:HG13	1.84	0.40
1:A:992:GLN:HG3	1:A:993:ILE:H	1.85	0.40
1:C:732:THR:HG22	1:C:1058:HIS:CE1	2.55	0.40
1:C:920:GLN:NE2	1:E:1129:VAL:HA	2.36	0.40
1:C:962:LEU:HD13	1:C:1007:TYR:CG	2.56	0.40
1:E:100:ILE:HA	1:E:102:ARG:NH2	2.28	0.40
1:E:819:GLU:OE1	1:E:819:GLU:N	2.52	0.40
1:E:965:GLN:OE1	1:E:968:SER:OG	2.36	0.40
1:E:999:GLY:HA2	1:E:1002:GLN:HG2	2.03	0.40
1:E:1037:SER:HB3	1:E:1039:ARG:CG	2.50	0.40
2:D:47:TRP:CD2	3:F:102:LEU:HB2	2.56	0.40
3:L:8:PRO:HD2	3:L:21:MET:HB2	2.03	0.40
8:W:3:BMA:H3	8:W:4:MAN:H2	1.35	0.40
1:A:88:ASP:O	1:A:270:LEU:HB2	2.21	0.40
1:A:89:GLY:HA3	1:A:270:LEU:HD12	2.04	0.40
1:A:405:ASP:OD1	1:A:504:GLY:HA2	2.22	0.40
1:C:222:ALA:C	1:C:223:LEU:HD12	2.41	0.40
1:C:283:GLY:HA3	1:E:558:LYS:NZ	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:TYR:O	1:C:466:ARG:HG2	2.21	0.40
1:C:577:ARG:HH11	1:C:582:LEU:HG	1.85	0.40
1:C:804:GLN:HG3	1:C:817:PHE:HB3	2.01	0.40
1:E:38:TYR:CE1	1:E:285:ILE:HG13	2.56	0.40
1:E:351:TYR:HB2	1:E:454:ARG:HB2	2.02	0.40
1:E:398:ASP:HB2	1:E:512:VAL:HB	2.03	0.40
1:E:777:ASN:O	1:E:781:VAL:HB	2.21	0.40
2:H:152:PHE:HA	2:H:153:PRO:HA	1.90	0.40
3:I:31:TYR:CD1	3:I:98:TYR:HE1	2.39	0.40
1:A:52:GLN:NE2	1:A:53:ASP:O	2.55	0.40
1:A:308:VAL:HG12	1:A:309:GLU:O	2.22	0.40
1:A:406:GLU:O	1:A:410:ILE:HG12	2.21	0.40
1:A:582:LEU:HG	1:A:582:LEU:O	2.22	0.40
1:A:759:PHE:CZ	1:C:970:PHE:CE1	3.09	0.40
1:A:770:ILE:O	1:A:774:GLN:OE1	2.38	0.40
1:A:815:ARG:HD3	1:A:819:GLU:HB3	2.04	0.40
1:A:1014:ARG:O	1:A:1017:GLU:HG3	2.22	0.40
1:C:86:PHE:HE1	1:C:194:PHE:HB2	1.86	0.40
1:C:403:ARG:O	1:C:407:VAL:HG23	2.21	0.40
1:C:447:GLY:HA2	1:C:499:PRO:HD3	2.03	0.40
1:C:539:VAL:O	1:C:550:GLY:N	2.42	0.40
1:C:620:VAL:HG13	1:C:622:VAL:HG23	2.03	0.40
1:C:732:THR:HA	1:C:1058:HIS:NE2	2.36	0.40
1:E:752:LEU:O	1:E:755:GLN:HG3	2.21	0.40
1:E:764:ASN:O	1:E:768:THR:HG23	2.21	0.40
1:E:974:SER:OG	1:E:979:ASP:OD2	2.32	0.40
3:F:119:PRO:HG3	3:F:143:ASN:N	2.31	0.40
1:A:1079:PRO:HG2	1:A:1132:ILE:HG13	2.04	0.40
1:A:1104:VAL:HG23	1:A:1113:GLN:HB2	2.04	0.40
1:C:295:PRO:HG3	1:C:610:VAL:HG22	2.04	0.40
1:C:670:ILE:HA	1:C:695:TYR:O	2.22	0.40
1:C:738:CYS:HB2	1:C:760:CYS:HB2	1.55	0.40
1:C:933:LYS:HA	1:C:933:LYS:HD2	1.82	0.40
1:E:277:LEU:HB3	1:E:279:TYR:CE1	2.41	0.40
1:E:953:ASN:O	1:E:957:GLN:HG3	2.22	0.40
3:F:36:LYS:HD3	3:F:56:TRP:CE2	2.56	0.40
3:I:204:HIS:CG	3:I:205:GLN:N	2.88	0.40
3:L:146:TYR:CG	3:L:147:PRO:HA	2.57	0.40
6:Y:2:NAG:H83	6:Y:2:NAG:H3	2.03	0.40
1:A:277:LEU:HD22	1:A:279:TYR:OH	2.22	0.40
1:A:922:LEU:HD23	1:A:922:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:ARG:O	1:A:1003:SER:OG	2.19	0.40
1:C:740:MET:HA	1:C:743:CYS:O	2.22	0.40
1:E:347:PHE:CG	1:E:509:ARG:HD2	2.57	0.40
1:E:753:LEU:O	1:E:753:LEU:HD12	2.21	0.40
1:E:807:PRO:HG3	1:E:875:SER:HB3	2.03	0.40
3:I:15:VAL:HG13	3:I:84:VAL:HG11	2.04	0.40
3:I:40:ALA:HA	3:I:54:ILE:O	2.22	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	1024/1242 (82%)	873 (85%)	148 (14%)	3 (0%)	41	76
1	C	1026/1242 (83%)	870 (85%)	156 (15%)	0	100	100
1	E	1028/1242 (83%)	884 (86%)	140 (14%)	4 (0%)	34	72
2	D	216/239 (90%)	202 (94%)	14 (6%)	0	100	100
2	H	216/239 (90%)	198 (92%)	18 (8%)	0	100	100
2	K	216/239 (90%)	206 (95%)	10 (5%)	0	100	100
3	F	217/240 (90%)	203 (94%)	14 (6%)	0	100	100
3	I	217/240 (90%)	202 (93%)	15 (7%)	0	100	100
3	L	217/240 (90%)	201 (93%)	16 (7%)	0	100	100
All	All	4377/5163 (85%)	3839 (88%)	531 (12%)	7 (0%)	50	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	592	PHE

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Mol	Chain	Res	Type
1	A	617	CYS
1	A	231	ILE
1	E	153	MET
1	E	1127	ASP
1	E	308	VAL
1	E	121	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	894/1077 (83%)	889 (99%)	5 (1%)	86	92
1	C	898/1077 (83%)	891 (99%)	7 (1%)	81	89
1	E	903/1077 (84%)	897 (99%)	6 (1%)	84	90
2	D	186/204 (91%)	186 (100%)	0	100	100
2	H	186/204 (91%)	186 (100%)	0	100	100
2	K	186/204 (91%)	186 (100%)	0	100	100
3	F	195/212 (92%)	195 (100%)	0	100	100
3	I	195/212 (92%)	193 (99%)	2 (1%)	76	86
3	L	195/212 (92%)	194 (100%)	1 (0%)	88	93
All	All	3838/4479 (86%)	3817 (100%)	21 (0%)	89	93

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	615	VAL
1	A	765	ARG
1	A	969	ASN
1	A	995	ARG
1	C	190	ARG
1	C	195	LYS
1	C	558	LYS

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Mol	Chain	Res	Type
1	C	765	ARG
1	C	856	ASN
1	C	995	ARG
1	C	1019	ARG
1	E	34	ARG
1	E	44	ARG
1	E	129	LYS
1	E	195	LYS
1	E	558	LYS
1	E	928	ASN
3	I	114	ARG
3	I	130	GLN
3	L	130	GLN

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

Mol	Chain	Res	Type
1	A	115	GLN
1	A	644	GLN
1	A	787	GLN
1	A	901	GLN
1	A	955	ASN
1	A	969	ASN
1	A	992	GLN
1	A	1036	GLN
1	A	1054	GLN
1	C	49	HIS
1	C	498	GLN
1	C	540	ASN
1	C	762	GLN
1	C	965	GLN
1	C	1036	GLN
1	C	1058	HIS
1	E	121	ASN
1	E	439	ASN
1	E	644	GLN
1	E	690	GLN
1	E	777	ASN
1	E	895	GLN
1	E	1023	ASN
3	F	96	GLN
2	H	6	GLN

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Mol	Chain	Res	Type
3	I	35	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

79 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1	1,4	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	B	2	4	14,14,15	0.24	0	17,19,21	0.59	0
4	FUC	B	3	4	10,10,11	0.63	0	14,14,16	0.88	0
5	NAG	G	1	5,1	14,14,15	0.29	0	17,19,21	0.46	0
5	NAG	G	2	5	14,14,15	0.30	0	17,19,21	0.39	0
6	NAG	J	1	6,1	14,14,15	0.23	0	17,19,21	0.36	0
6	NAG	J	2	6	14,14,15	0.19	0	17,19,21	0.46	0
6	BMA	J	3	6	11,11,12	0.47	0	15,15,17	0.82	0
6	MAN	J	4	6	11,11,12	0.77	1 (9%)	15,15,17	1.25	2 (13%)
7	NAG	M	1	7,1	14,14,15	0.92	1 (7%)	17,19,21	1.29	1 (5%)
7	NAG	M	2	7	14,14,15	0.90	1 (7%)	17,19,21	1.25	1 (5%)
7	BMA	M	3	7	11,11,12	0.53	0	15,15,17	0.86	0
5	NAG	N	1	5,1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	N	2	5	14,14,15	0.32	0	17,19,21	1.32	2 (11%)
5	NAG	O	1	5,1	14,14,15	0.77	1 (7%)	17,19,21	0.66	0
5	NAG	O	2	5	14,14,15	0.40	0	17,19,21	1.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	P	1	5,1	14,14,15	0.44	0	17,19,21	0.45	0
5	NAG	P	2	5	14,14,15	0.23	0	17,19,21	0.52	0
7	NAG	Q	1	7,1	14,14,15	0.37	0	17,19,21	0.61	0
7	NAG	Q	2	7	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
7	BMA	Q	3	7	11,11,12	0.59	0	15,15,17	0.74	0
5	NAG	R	1	5,1	14,14,15	0.47	0	17,19,21	0.94	1 (5%)
5	NAG	R	2	5	14,14,15	0.26	0	17,19,21	0.43	0
8	NAG	S	1	1,8	14,14,15	0.28	0	17,19,21	0.49	0
8	NAG	S	2	8	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
8	BMA	S	3	8	11,11,12	0.65	0	15,15,17	0.80	1 (6%)
8	MAN	S	4	8	11,11,12	0.57	0	15,15,17	1.07	2 (13%)
8	MAN	S	5	8	11,11,12	0.61	0	15,15,17	1.10	2 (13%)
5	NAG	T	1	5,1	14,14,15	0.36	0	17,19,21	0.39	0
5	NAG	T	2	5	14,14,15	0.41	0	17,19,21	1.24	1 (5%)
9	NAG	U	1	9,1	14,14,15	0.30	0	17,19,21	0.64	0
9	NAG	U	2	9	14,14,15	0.26	0	17,19,21	0.59	0
9	BMA	U	3	9	11,11,12	0.61	0	15,15,17	0.98	1 (6%)
9	MAN	U	4	9	11,11,12	0.61	0	15,15,17	1.19	2 (13%)
9	MAN	U	5	9	11,11,12	0.62	0	15,15,17	1.61	5 (33%)
5	NAG	V	1	5,1	14,14,15	0.56	0	17,19,21	0.53	0
5	NAG	V	2	5	14,14,15	0.24	0	17,19,21	0.41	0
8	NAG	W	1	1,8	14,14,15	0.16	0	17,19,21	0.69	0
8	NAG	W	2	8	14,14,15	0.26	0	17,19,21	0.39	0
8	BMA	W	3	8	11,11,12	0.74	1 (9%)	15,15,17	1.19	1 (6%)
8	MAN	W	4	8	11,11,12	0.94	1 (9%)	15,15,17	1.09	3 (20%)
8	MAN	W	5	8	11,11,12	0.64	0	15,15,17	0.93	1 (6%)
5	NAG	X	1	5,1	14,14,15	0.66	1 (7%)	17,19,21	0.60	0
5	NAG	X	2	5	14,14,15	0.42	0	17,19,21	1.24	1 (5%)
6	NAG	Y	1	6,1	14,14,15	0.69	0	17,19,21	1.22	3 (17%)
6	NAG	Y	2	6	14,14,15	0.90	0	17,19,21	2.81	8 (47%)
6	BMA	Y	3	6	11,11,12	0.62	0	15,15,17	2.15	7 (46%)
6	MAN	Y	4	6	11,11,12	0.56	0	15,15,17	1.21	2 (13%)
7	NAG	Z	1	7,1	14,14,15	0.54	0	17,19,21	0.60	0
7	NAG	Z	2	7	14,14,15	0.23	0	17,19,21	0.62	0
7	BMA	Z	3	7	11,11,12	0.61	0	15,15,17	0.74	0
10	NAG	a	1	1,10	14,14,15	0.30	0	17,19,21	0.64	1 (5%)
10	NAG	a	2	10	14,14,15	0.55	0	17,19,21	1.31	1 (5%)
10	BMA	a	3	10	11,11,12	0.49	0	15,15,17	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FUC	a	4	10	10,10,11	0.64	0	14,14,16	0.79	0
4	NAG	b	1	1,4	14,14,15	0.87	1 (7%)	17,19,21	0.80	0
4	NAG	b	2	4	14,14,15	0.19	0	17,19,21	0.47	0
4	FUC	b	3	4	10,10,11	0.75	0	14,14,16	1.00	0
11	NAG	c	1	11,1	14,14,15	0.20	0	17,19,21	0.48	0
11	FUC	c	2	11	10,10,11	0.65	0	14,14,16	0.82	0
12	NAG	d	1	12,1	14,14,15	0.49	0	17,19,21	0.87	1 (5%)
12	NAG	d	2	12	14,14,15	0.28	0	17,19,21	0.50	0
12	BMA	d	3	12	11,11,12	0.95	0	15,15,17	1.19	2 (13%)
12	MAN	d	4	12	11,11,12	1.06	2 (18%)	15,15,17	1.63	2 (13%)
12	NAG	d	5	12	14,14,15	0.25	0	17,19,21	0.36	0
12	MAN	d	6	12	11,11,12	0.60	0	15,15,17	1.17	2 (13%)
7	NAG	e	1	7,1	14,14,15	0.64	0	17,19,21	1.01	1 (5%)
7	NAG	e	2	7	14,14,15	0.29	0	17,19,21	0.41	0
7	BMA	e	3	7	11,11,12	0.50	0	15,15,17	0.96	1 (6%)
13	NAG	f	1	13,1	14,14,15	0.43	0	17,19,21	0.95	2 (11%)
13	NAG	f	2	13	14,14,15	0.27	0	17,19,21	0.52	0
13	BMA	f	3	13	11,11,12	1.22	2 (18%)	15,15,17	1.61	3 (20%)
13	MAN	f	4	13	11,11,12	0.83	0	15,15,17	1.07	1 (6%)
13	MAN	f	5	13	11,11,12	0.53	0	15,15,17	1.03	2 (13%)
13	MAN	f	6	13	11,11,12	0.88	0	15,15,17	0.98	1 (6%)
10	NAG	g	1	2,10	14,14,15	0.20	0	17,19,21	0.54	0
10	NAG	g	2	10	14,14,15	0.21	0	17,19,21	0.41	0
10	BMA	g	3	10	11,11,12	0.77	1 (9%)	15,15,17	0.91	1 (6%)
10	FUC	g	4	10	10,10,11	0.71	0	14,14,16	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	B	2	4	-	3/6/23/26	0/1/1/1
4	FUC	B	3	4	-	-	0/1/1/1
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
6	NAG	J	1	6,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	J	2	6	-	4/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
7	NAG	M	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
7	BMA	M	3	7	-	0/2/19/22	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	5/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	5/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
7	NAG	Q	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	5/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	4/6/23/26	0/1/1/1
8	NAG	S	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	S	2	8	-	2/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	0/2/19/22	0/1/1/1
8	MAN	S	5	8	-	1/2/19/22	0/1/1/1
5	NAG	T	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	3/6/23/26	0/1/1/1
9	NAG	U	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	U	2	9	-	2/6/23/26	0/1/1/1
9	BMA	U	3	9	-	2/2/19/22	0/1/1/1
9	MAN	U	4	9	-	2/2/19/22	0/1/1/1
9	MAN	U	5	9	-	2/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
8	NAG	W	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	1/6/23/26	0/1/1/1
8	BMA	W	3	8	-	1/2/19/22	0/1/1/1
8	MAN	W	4	8	-	1/2/19/22	0/1/1/1
8	MAN	W	5	8	-	0/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	X	2	5	-	4/6/23/26	0/1/1/1
6	NAG	Y	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	5/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Y	4	6	-	0/2/19/22	0/1/1/1
7	NAG	Z	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	0/2/19/22	0/1/1/1
10	NAG	a	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	a	2	10	-	5/6/23/26	0/1/1/1
10	BMA	a	3	10	-	1/2/19/22	0/1/1/1
10	FUC	a	4	10	-	-	0/1/1/1
4	NAG	b	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	FUC	b	3	4	-	-	0/1/1/1
11	NAG	c	1	11,1	-	4/6/23/26	0/1/1/1
11	FUC	c	2	11	-	-	0/1/1/1
12	NAG	d	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	d	2	12	-	3/6/23/26	0/1/1/1
12	BMA	d	3	12	-	2/2/19/22	0/1/1/1
12	MAN	d	4	12	-	1/2/19/22	1/1/1/1
12	NAG	d	5	12	-	1/6/23/26	0/1/1/1
12	MAN	d	6	12	-	0/2/19/22	0/1/1/1
7	NAG	e	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	e	2	7	-	2/6/23/26	0/1/1/1
7	BMA	e	3	7	-	2/2/19/22	0/1/1/1
13	NAG	f	1	13,1	-	2/6/23/26	0/1/1/1
13	NAG	f	2	13	-	2/6/23/26	0/1/1/1
13	BMA	f	3	13	-	0/2/19/22	0/1/1/1
13	MAN	f	4	13	-	2/2/19/22	0/1/1/1
13	MAN	f	5	13	-	1/2/19/22	0/1/1/1
13	MAN	f	6	13	-	2/2/19/22	0/1/1/1
10	NAG	g	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	g	2	10	-	2/6/23/26	0/1/1/1
10	BMA	g	3	10	-	2/2/19/22	0/1/1/1
10	FUC	g	4	10	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1	NAG	O5-C1	3.32	1.49	1.43
7	M	2	NAG	O5-C1	3.20	1.48	1.43
4	b	1	NAG	O5-C1	-3.00	1.38	1.43
13	f	3	BMA	C1-C2	2.77	1.58	1.52
12	d	4	MAN	C1-C2	2.65	1.58	1.52
5	O	1	NAG	O5-C1	-2.64	1.39	1.43
13	f	3	BMA	C2-C3	2.61	1.56	1.52
8	W	4	MAN	C1-C2	2.58	1.58	1.52
6	J	4	MAN	C1-C2	2.36	1.57	1.52
10	g	3	BMA	C1-C2	2.34	1.57	1.52
8	W	3	BMA	C1-C2	2.12	1.57	1.52
12	d	4	MAN	O5-C5	2.10	1.47	1.43
5	X	1	NAG	O5-C1	-2.06	1.40	1.43

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	2	NAG	C1-C2-N2	-6.05	100.15	110.49
6	Y	2	NAG	O3-C3-C2	-5.46	98.16	109.47
7	M	1	NAG	C1-O5-C5	5.09	119.09	112.19
7	M	2	NAG	C1-O5-C5	4.87	118.79	112.19
12	d	4	MAN	C1-O5-C5	4.54	118.35	112.19
5	N	2	NAG	C2-N2-C7	4.42	129.19	122.90
6	Y	3	BMA	O5-C5-C6	4.38	114.06	107.20
5	T	2	NAG	C2-N2-C7	4.30	129.03	122.90
5	X	2	NAG	C2-N2-C7	4.30	129.02	122.90
7	Q	2	NAG	C2-N2-C7	4.29	129.01	122.90
10	a	2	NAG	C2-N2-C7	4.25	128.95	122.90
5	O	2	NAG	C2-N2-C7	4.22	128.92	122.90
13	f	3	BMA	C1-C2-C3	4.14	114.75	109.67
6	Y	3	BMA	C1-O5-C5	-3.44	107.53	112.19
6	Y	2	NAG	O5-C5-C6	3.39	112.53	107.20
7	e	1	NAG	C1-O5-C5	3.37	116.76	112.19
6	Y	2	NAG	C2-N2-C7	3.31	127.61	122.90
6	Y	3	BMA	C2-C3-C4	-3.12	105.50	110.89
12	d	6	MAN	C1-O5-C5	3.06	116.34	112.19
5	R	1	NAG	C1-O5-C5	2.95	116.19	112.19
6	Y	2	NAG	C3-C4-C5	-2.93	105.02	110.24
9	U	5	MAN	C2-C3-C4	-2.87	105.92	110.89
12	d	1	NAG	C1-O5-C5	2.84	116.03	112.19
9	U	4	MAN	C2-C3-C4	-2.75	106.13	110.89
6	Y	3	BMA	C6-C5-C4	-2.72	106.64	113.00
9	U	5	MAN	O4-C4-C3	-2.71	104.09	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	1	NAG	C4-C3-C2	-2.70	107.06	111.02
8	S	4	MAN	C1-O5-C5	2.69	115.83	112.19
12	d	4	MAN	O2-C2-C3	-2.65	104.82	110.14
6	Y	2	NAG	C4-C3-C2	2.63	114.88	111.02
6	Y	1	NAG	C1-C2-N2	2.63	114.98	110.49
6	J	4	MAN	C1-O5-C5	2.60	115.71	112.19
8	S	2	NAG	C1-O5-C5	2.57	115.67	112.19
6	Y	4	MAN	O2-C2-C3	-2.56	105.00	110.14
9	U	5	MAN	C6-C5-C4	-2.55	107.04	113.00
13	f	1	NAG	C1-O5-C5	2.54	115.63	112.19
6	Y	3	BMA	O2-C2-C3	-2.53	105.07	110.14
13	f	5	MAN	C1-O5-C5	2.51	115.59	112.19
8	S	4	MAN	O2-C2-C3	-2.45	105.23	110.14
12	d	6	MAN	O2-C2-C3	-2.44	105.25	110.14
6	J	4	MAN	O2-C2-C3	-2.42	105.30	110.14
8	W	5	MAN	O2-C2-C3	-2.41	105.31	110.14
8	S	5	MAN	C1-O5-C5	2.40	115.45	112.19
6	Y	2	NAG	C1-O5-C5	2.40	115.44	112.19
8	W	3	BMA	O2-C2-C3	-2.39	105.36	110.14
6	Y	3	BMA	O6-C6-C5	-2.38	103.12	111.29
13	f	3	BMA	O5-C5-C4	-2.31	105.20	110.83
13	f	1	NAG	C3-C4-C5	2.30	114.34	110.24
7	e	3	BMA	O2-C2-C3	-2.29	105.55	110.14
9	U	5	MAN	O2-C2-C3	-2.29	105.55	110.14
8	S	5	MAN	O2-C2-C3	-2.29	105.55	110.14
6	Y	2	NAG	O7-C7-N2	-2.28	117.76	121.95
8	S	3	BMA	O2-C2-C3	-2.25	105.64	110.14
13	f	5	MAN	O2-C2-C3	-2.24	105.64	110.14
13	f	4	MAN	O2-C2-C3	-2.22	105.69	110.14
9	U	4	MAN	O5-C5-C6	2.20	110.65	107.20
13	f	6	MAN	O2-C2-C3	-2.18	105.76	110.14
6	Y	1	NAG	O5-C1-C2	-2.18	107.85	111.29
13	f	3	BMA	C2-C3-C4	2.15	114.62	110.89
6	Y	3	BMA	C3-C4-C5	-2.14	106.42	110.24
5	N	2	NAG	C1-C2-N2	2.14	114.14	110.49
9	U	5	MAN	O5-C5-C6	-2.11	103.89	107.20
12	d	3	BMA	O2-C2-C3	-2.11	105.91	110.14
5	O	2	NAG	C1-C2-N2	2.09	114.06	110.49
8	W	4	MAN	C1-O5-C5	2.07	114.99	112.19
10	g	3	BMA	O2-C2-C3	-2.06	106.00	110.14
8	W	4	MAN	C1-C2-C3	2.06	112.20	109.67
8	W	4	MAN	O2-C2-C3	-2.06	106.02	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	4	MAN	C2-C3-C4	-2.04	107.36	110.89
10	a	1	NAG	C1-O5-C5	2.04	114.95	112.19
9	U	3	BMA	C2-C3-C4	-2.03	107.39	110.89
12	d	3	BMA	O5-C1-C2	-2.01	107.67	110.77

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Y	1	NAG	C8-C7-N2-C2
6	Y	1	NAG	O7-C7-N2-C2
6	Y	2	NAG	C8-C7-N2-C2
6	Y	2	NAG	O7-C7-N2-C2
7	Z	1	NAG	C4-C5-C6-O6
9	U	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
10	a	1	NAG	O5-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
8	S	2	NAG	O5-C5-C6-O6
12	d	3	BMA	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
9	U	4	MAN	C4-C5-C6-O6
9	U	2	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
7	M	1	NAG	C4-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
12	d	1	NAG	O5-C5-C6-O6
8	S	2	NAG	C4-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
12	d	3	BMA	C4-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
9	U	5	MAN	O5-C5-C6-O6
13	f	6	MAN	O5-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
10	a	1	NAG	C4-C5-C6-O6
10	g	2	NAG	C4-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	M	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
9	U	5	MAN	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	Y	3	BMA	O5-C5-C6-O6
9	U	4	MAN	O5-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
10	g	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
8	S	3	BMA	C4-C5-C6-O6
6	Y	2	NAG	C1-C2-N2-C7
7	e	3	BMA	O5-C5-C6-O6
8	W	1	NAG	O5-C5-C6-O6
9	U	1	NAG	O5-C5-C6-O6
7	Q	2	NAG	C4-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
13	f	4	MAN	C4-C5-C6-O6
9	U	3	BMA	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
6	Y	3	BMA	C4-C5-C6-O6
9	U	1	NAG	C4-C5-C6-O6
7	Z	2	NAG	O5-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
12	d	1	NAG	C4-C5-C6-O6
13	f	6	MAN	C4-C5-C6-O6
4	b	1	NAG	C8-C7-N2-C2
4	b	1	NAG	O7-C7-N2-C2
5	N	2	NAG	C8-C7-N2-C2
5	N	2	NAG	O7-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
5	X	2	NAG	C8-C7-N2-C2
5	X	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
7	Q	2	NAG	C8-C7-N2-C2
7	Q	2	NAG	O7-C7-N2-C2
7	e	1	NAG	C8-C7-N2-C2
7	e	1	NAG	O7-C7-N2-C2
10	a	2	NAG	C8-C7-N2-C2
10	a	2	NAG	O7-C7-N2-C2
11	c	1	NAG	C8-C7-N2-C2
11	c	1	NAG	O7-C7-N2-C2
8	S	3	BMA	O5-C5-C6-O6
13	f	4	MAN	O5-C5-C6-O6
8	W	1	NAG	C4-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
10	a	3	BMA	O5-C5-C6-O6
12	d	2	NAG	O5-C5-C6-O6
7	Q	3	BMA	C4-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
8	W	3	BMA	O5-C5-C6-O6
9	U	3	BMA	O5-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
13	f	5	MAN	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
10	g	3	BMA	O5-C5-C6-O6
12	d	2	NAG	C4-C5-C6-O6
11	c	1	NAG	O5-C5-C6-O6
13	f	1	NAG	C4-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
10	a	2	NAG	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
6	J	3	BMA	C4-C5-C6-O6
11	c	1	NAG	C4-C5-C6-O6
13	f	1	NAG	O5-C5-C6-O6
8	W	4	MAN	O5-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
6	Y	2	NAG	O5-C5-C6-O6
12	d	5	NAG	O5-C5-C6-O6
7	e	1	NAG	O5-C5-C6-O6
12	d	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	2	NAG	C4-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
8	W	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
8	S	5	MAN	O5-C5-C6-O6
12	d	2	NAG	C1-C2-N2-C7
6	Y	1	NAG	C4-C5-C6-O6
10	a	2	NAG	C4-C5-C6-O6
10	g	3	BMA	C4-C5-C6-O6
13	f	2	NAG	C4-C5-C6-O6
4	B	1	NAG	C3-C2-N2-C7
6	Y	2	NAG	C3-C2-N2-C7
9	U	1	NAG	C3-C2-N2-C7
13	f	2	NAG	O5-C5-C6-O6
6	Y	1	NAG	O5-C5-C6-O6
7	e	3	BMA	C4-C5-C6-O6
5	V	1	NAG	C1-C2-N2-C7
4	B	2	NAG	C3-C2-N2-C7
5	N	2	NAG	C3-C2-N2-C7
5	O	2	NAG	C3-C2-N2-C7
5	T	2	NAG	C3-C2-N2-C7
5	V	1	NAG	C3-C2-N2-C7
5	X	2	NAG	C3-C2-N2-C7
7	Q	2	NAG	C3-C2-N2-C7
10	a	2	NAG	C3-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	d	4	MAN	C1-C2-C3-C4-C5-O5

26 monomers are involved in 33 short contacts:

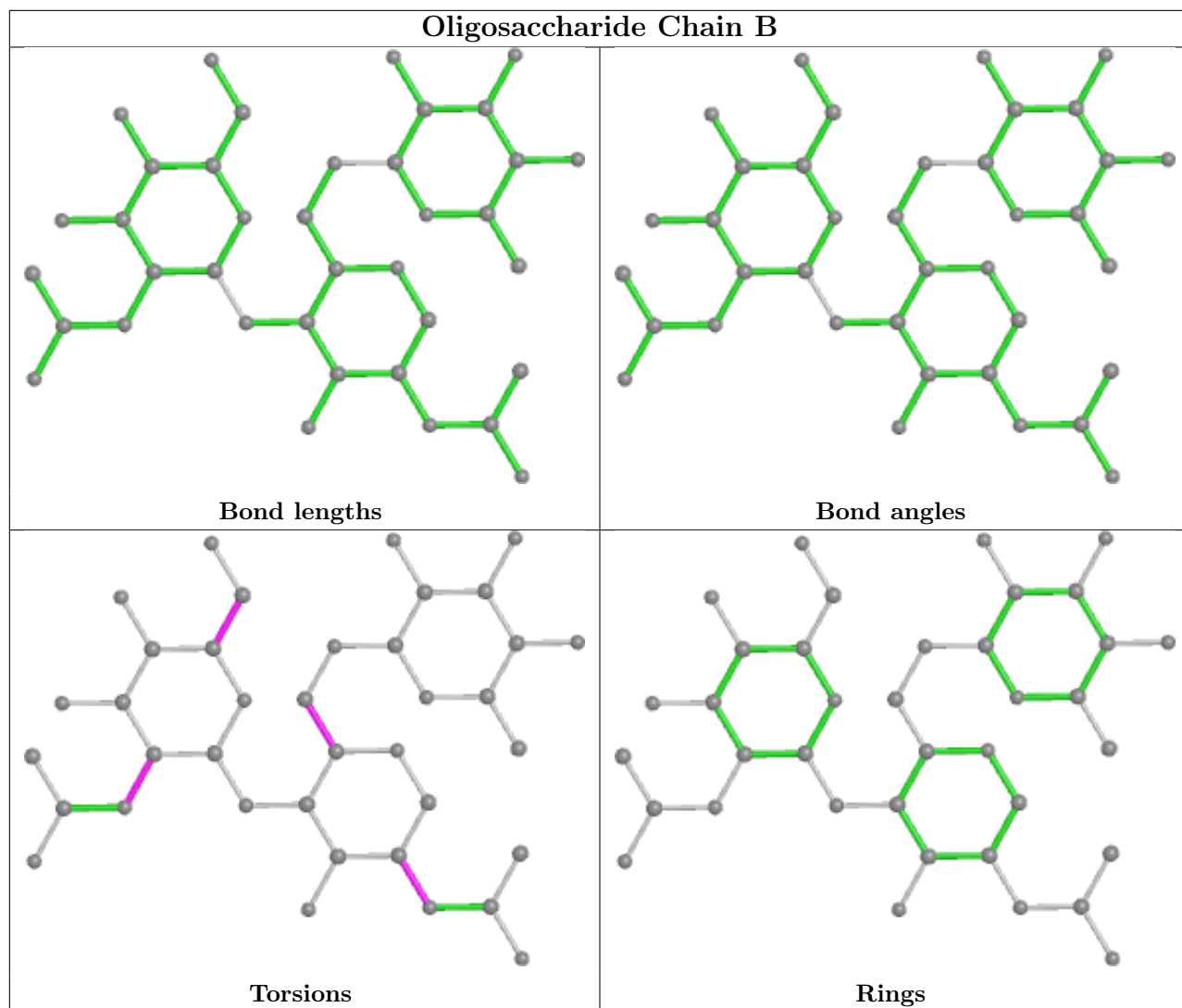
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	2	NAG	2	0
4	B	1	NAG	1	0
8	W	2	NAG	1	0
5	V	1	NAG	2	0
5	N	1	NAG	1	0

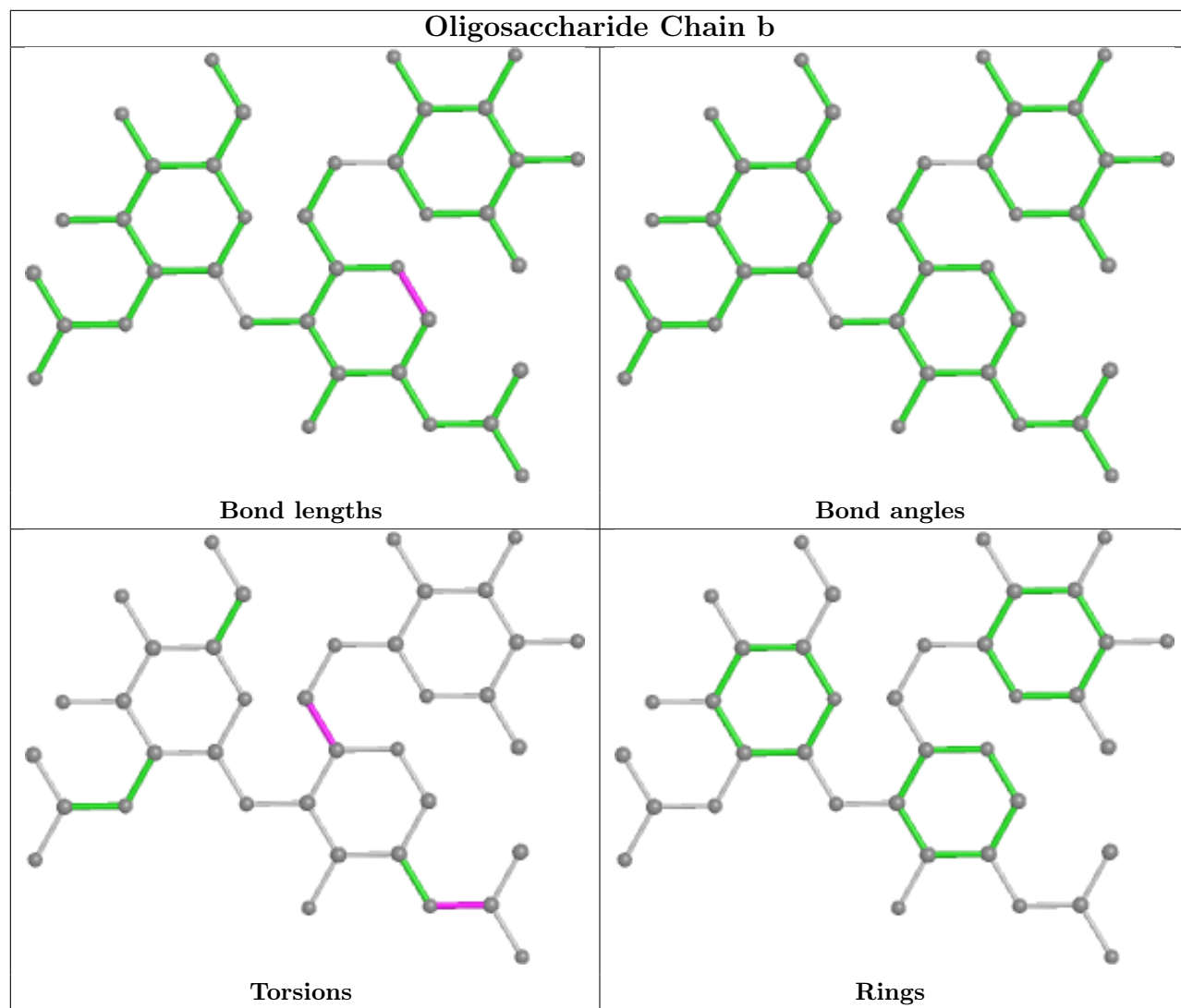
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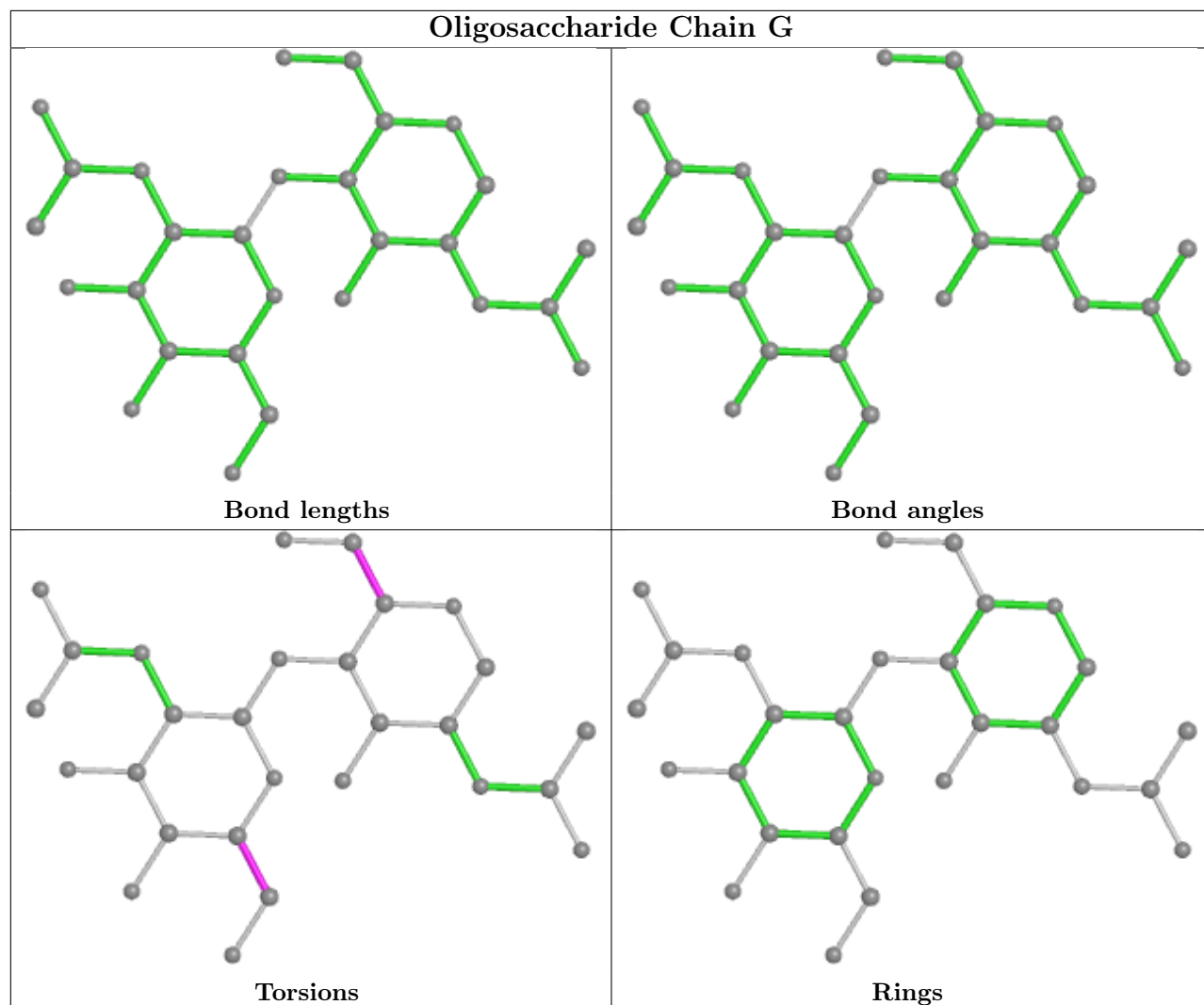
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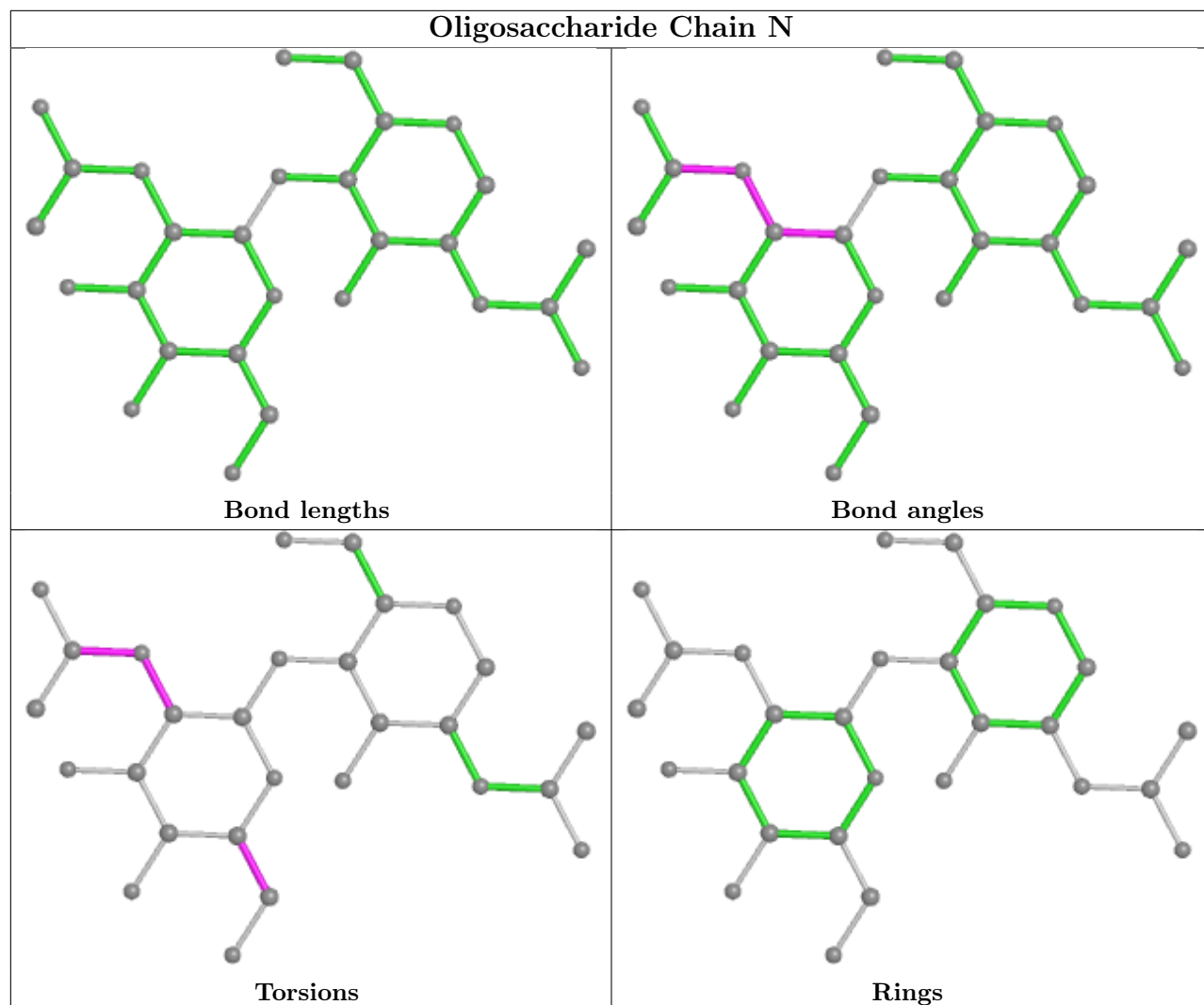
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Y	1	NAG	1	0
5	V	2	NAG	1	0
8	W	3	BMA	2	0
7	Q	2	NAG	1	0
5	O	2	NAG	1	0
6	J	3	BMA	1	0
7	M	1	NAG	2	0
9	U	5	MAN	1	0
4	B	3	FUC	2	0
6	Y	2	NAG	5	0
5	X	2	NAG	1	0
5	P	1	NAG	5	0
8	S	2	NAG	3	0
5	P	2	NAG	1	0
8	W	4	MAN	1	0
5	X	1	NAG	1	0
9	U	1	NAG	1	0
8	S	1	NAG	1	0
8	S	3	BMA	2	0
5	T	2	NAG	1	0
6	J	2	NAG	1	0

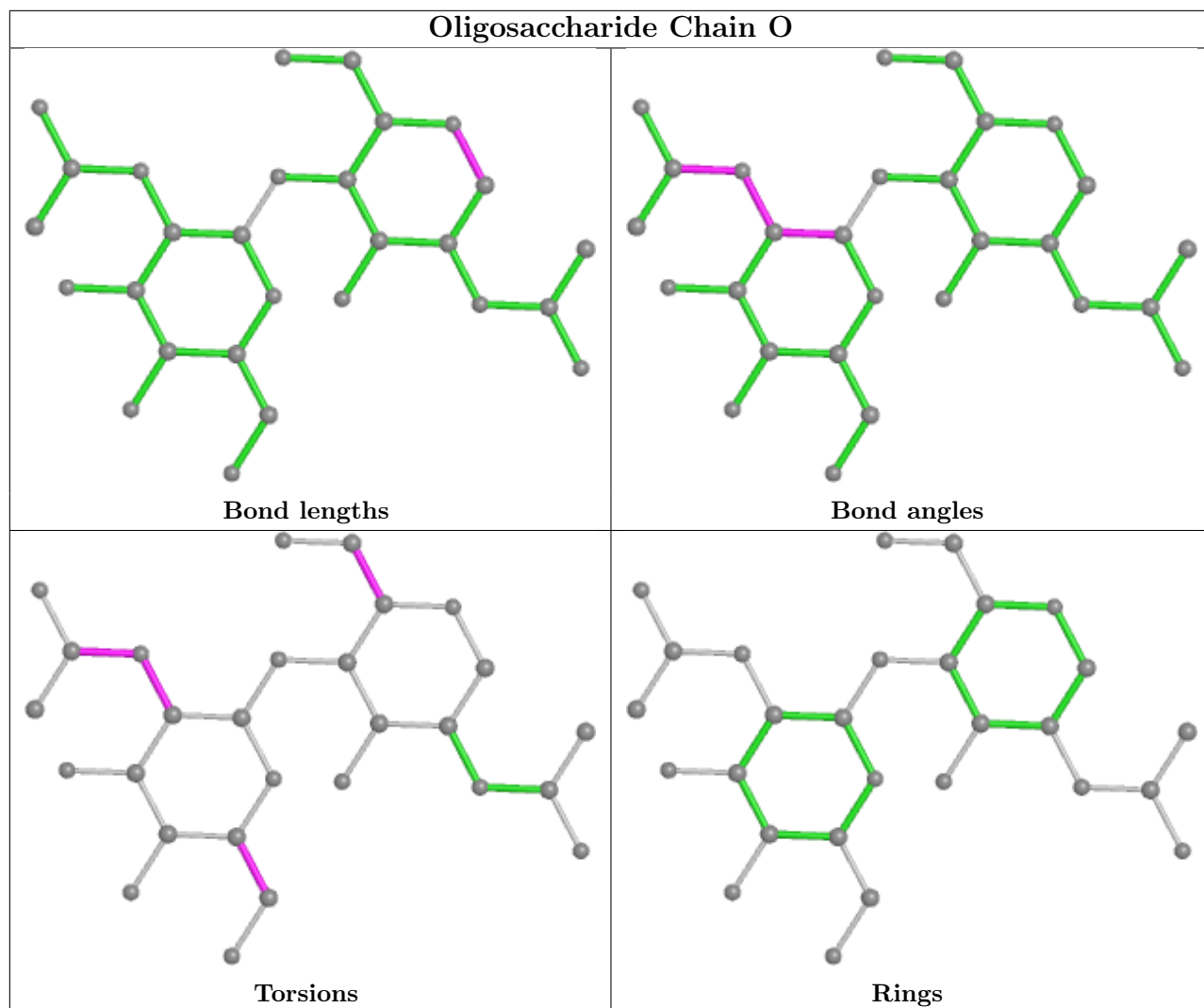
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

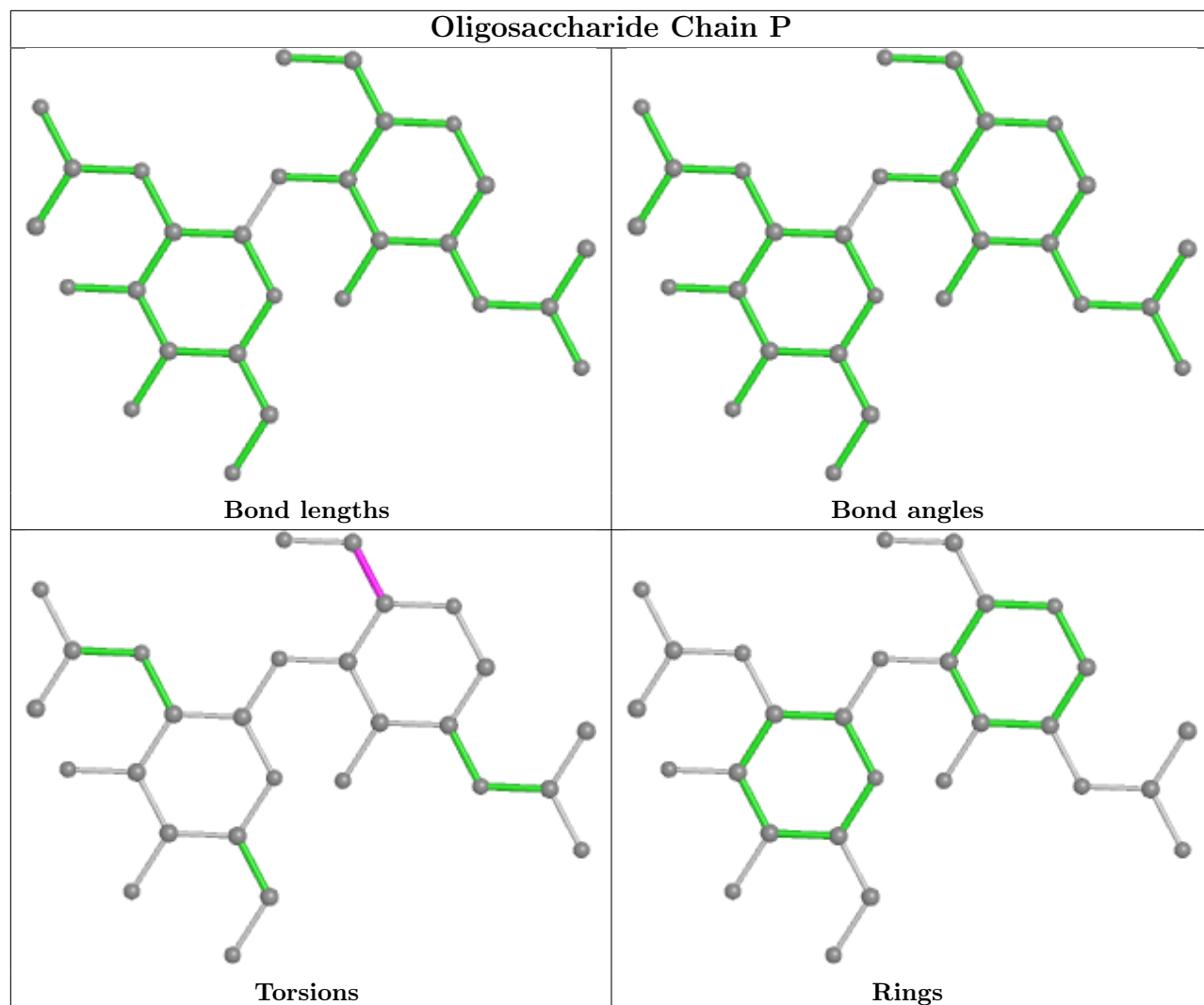


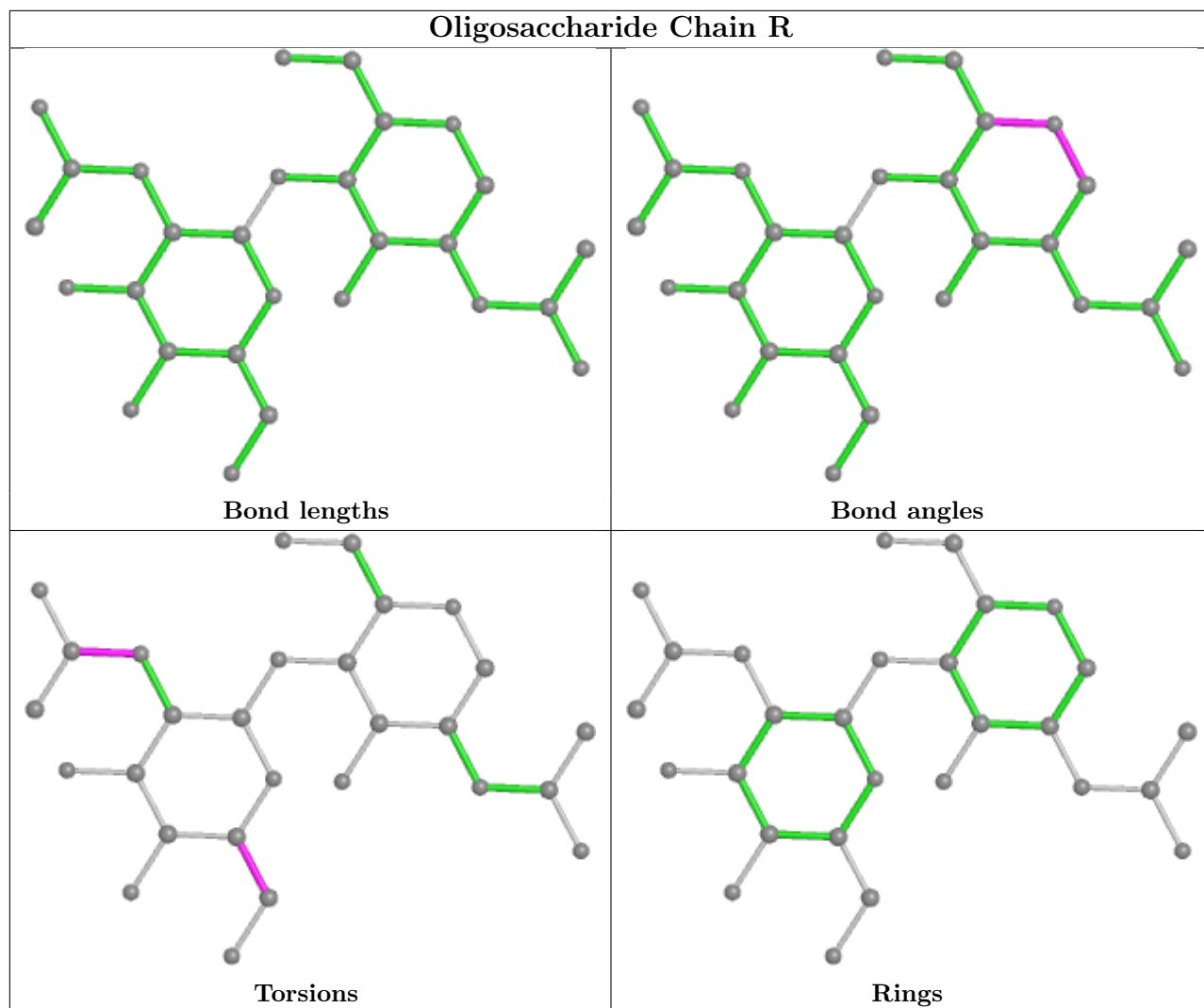


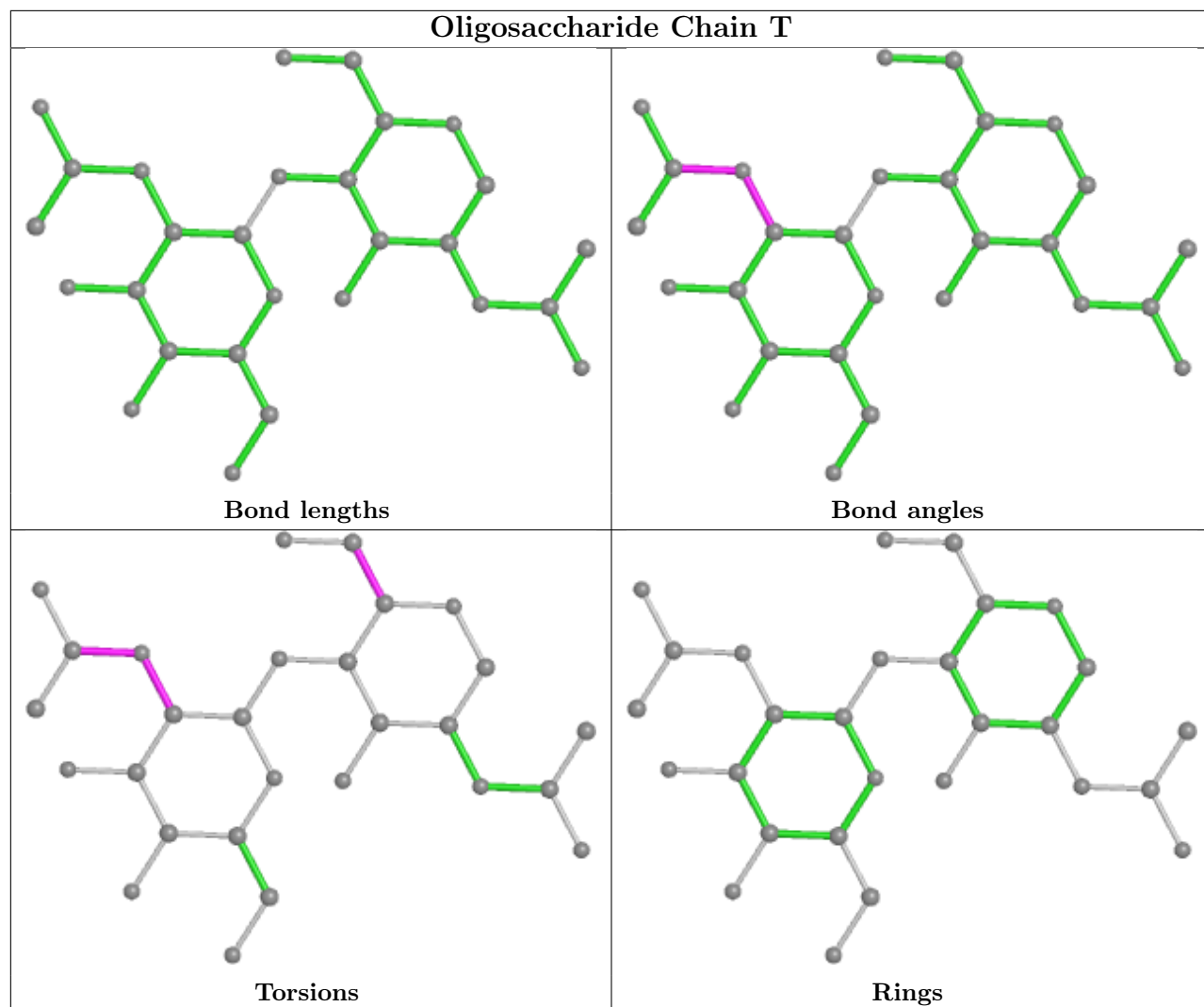


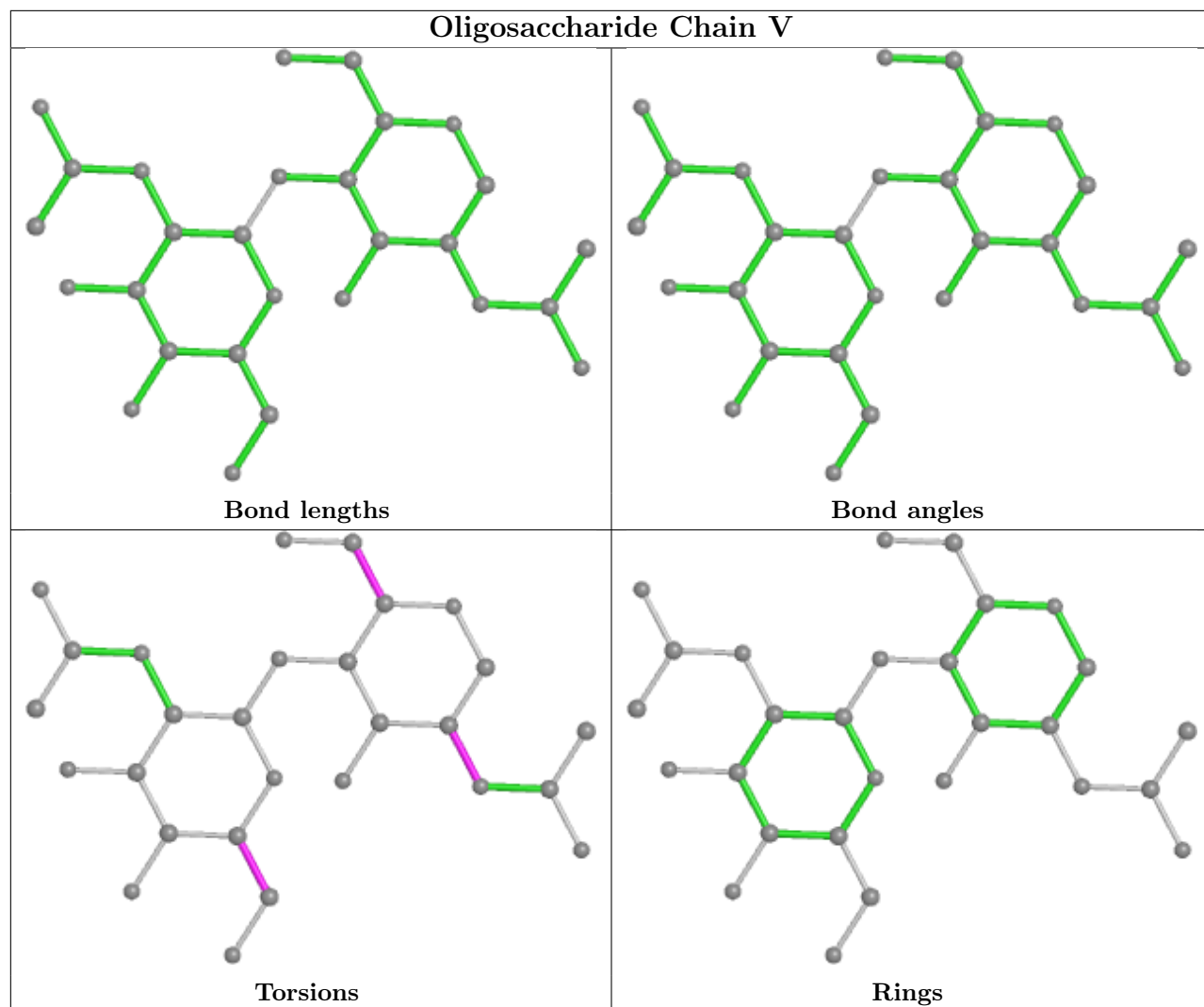


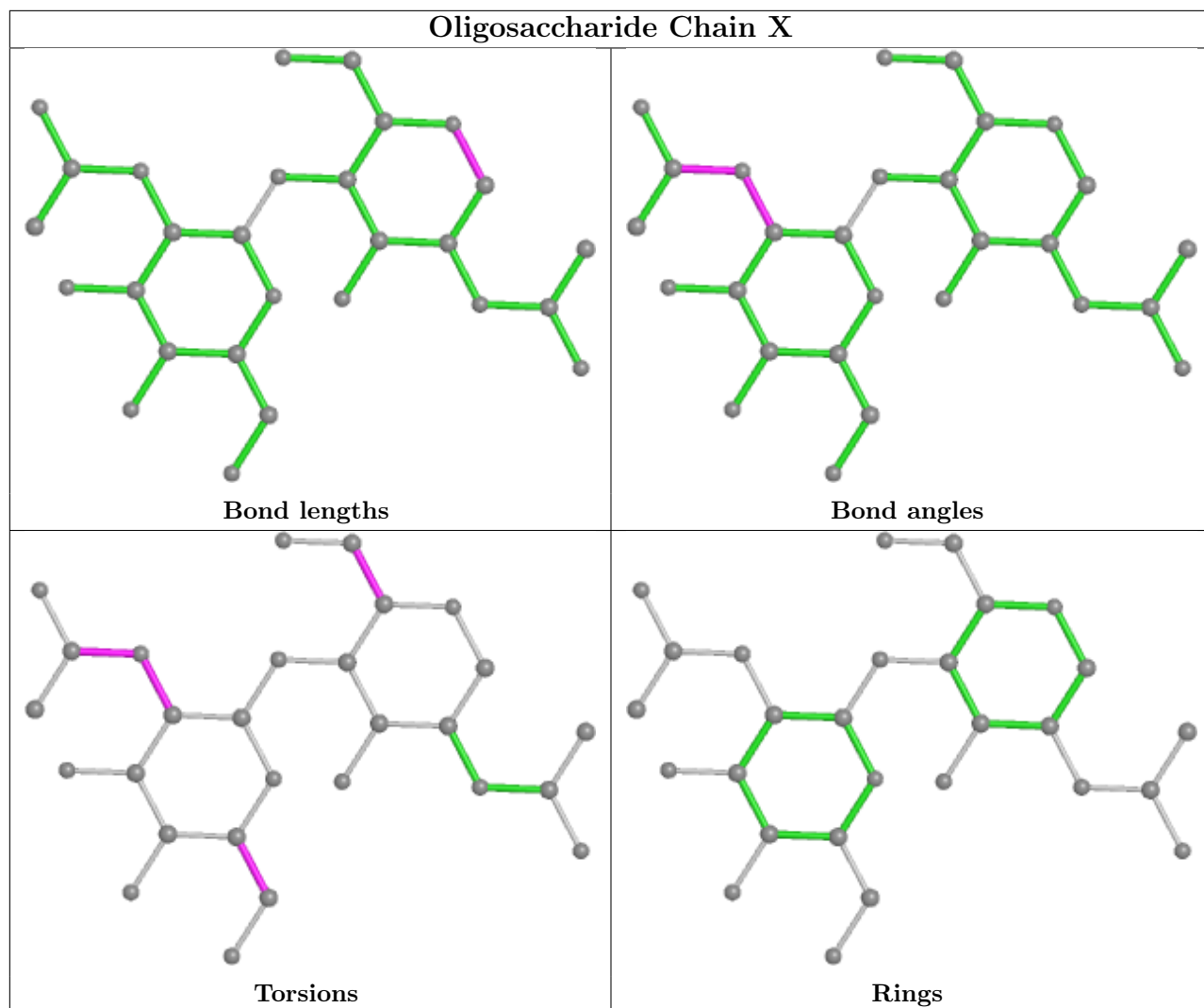


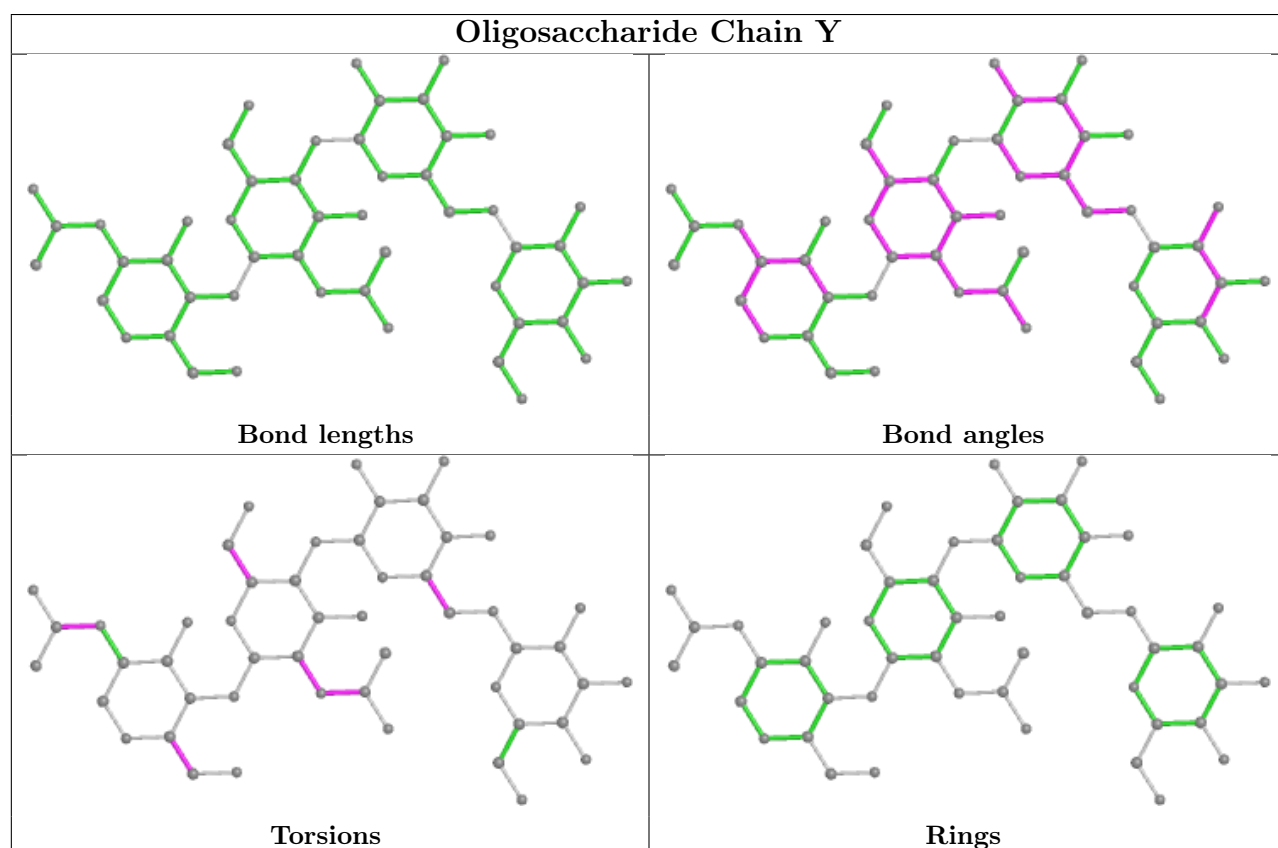
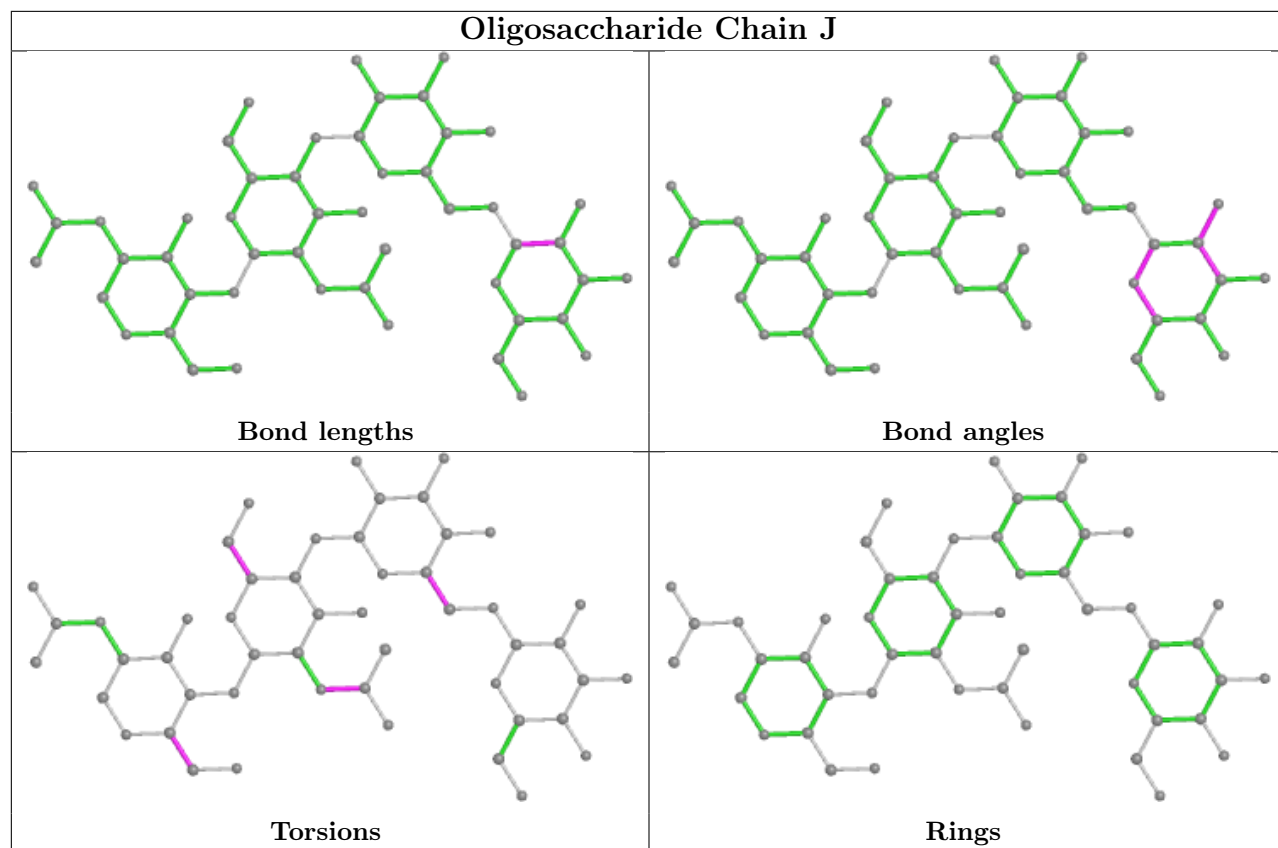


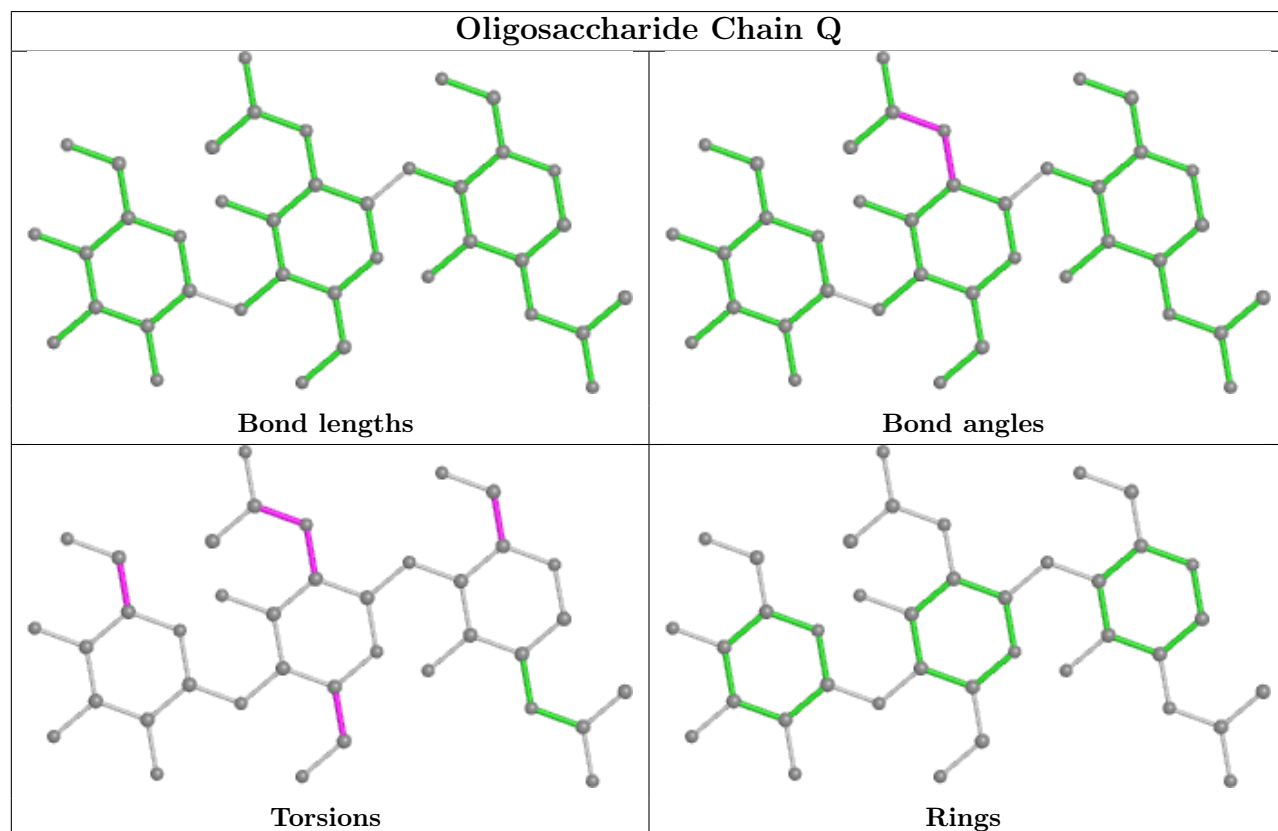
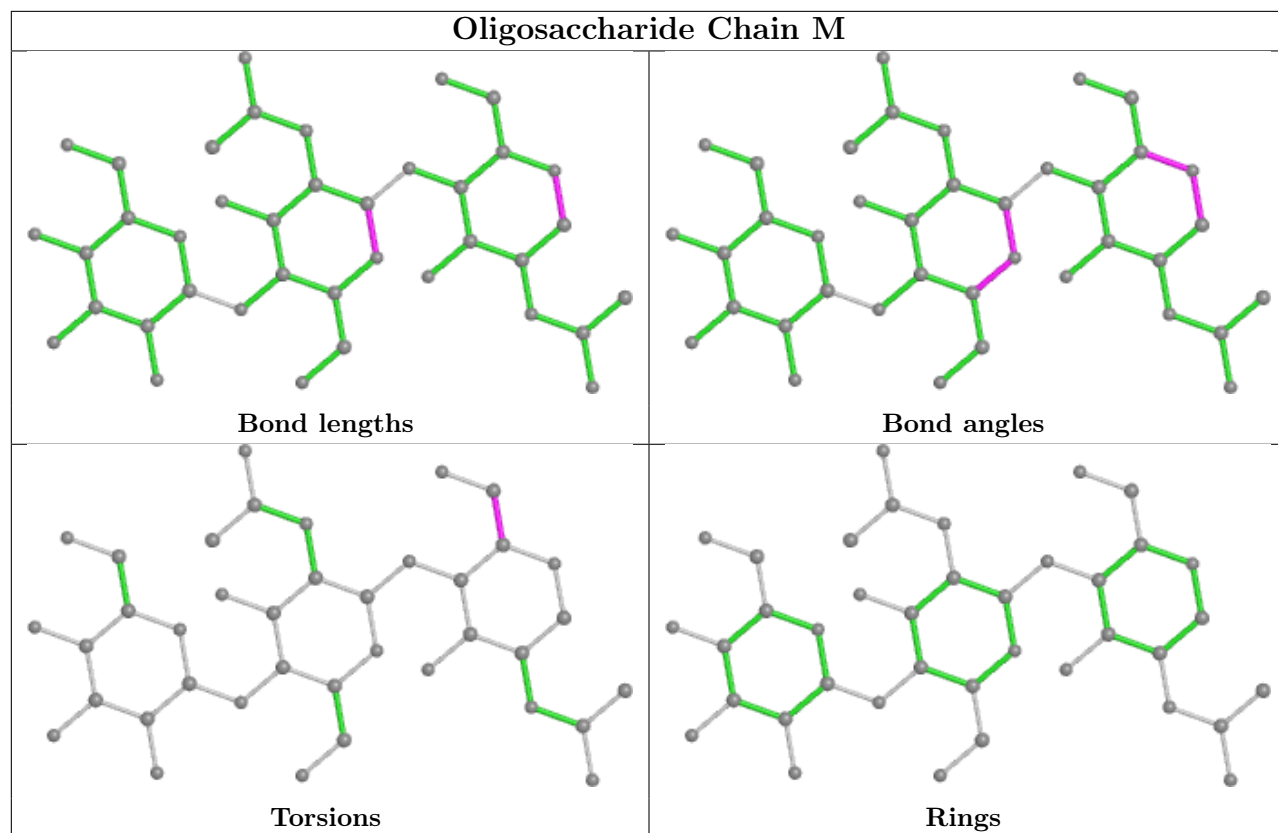


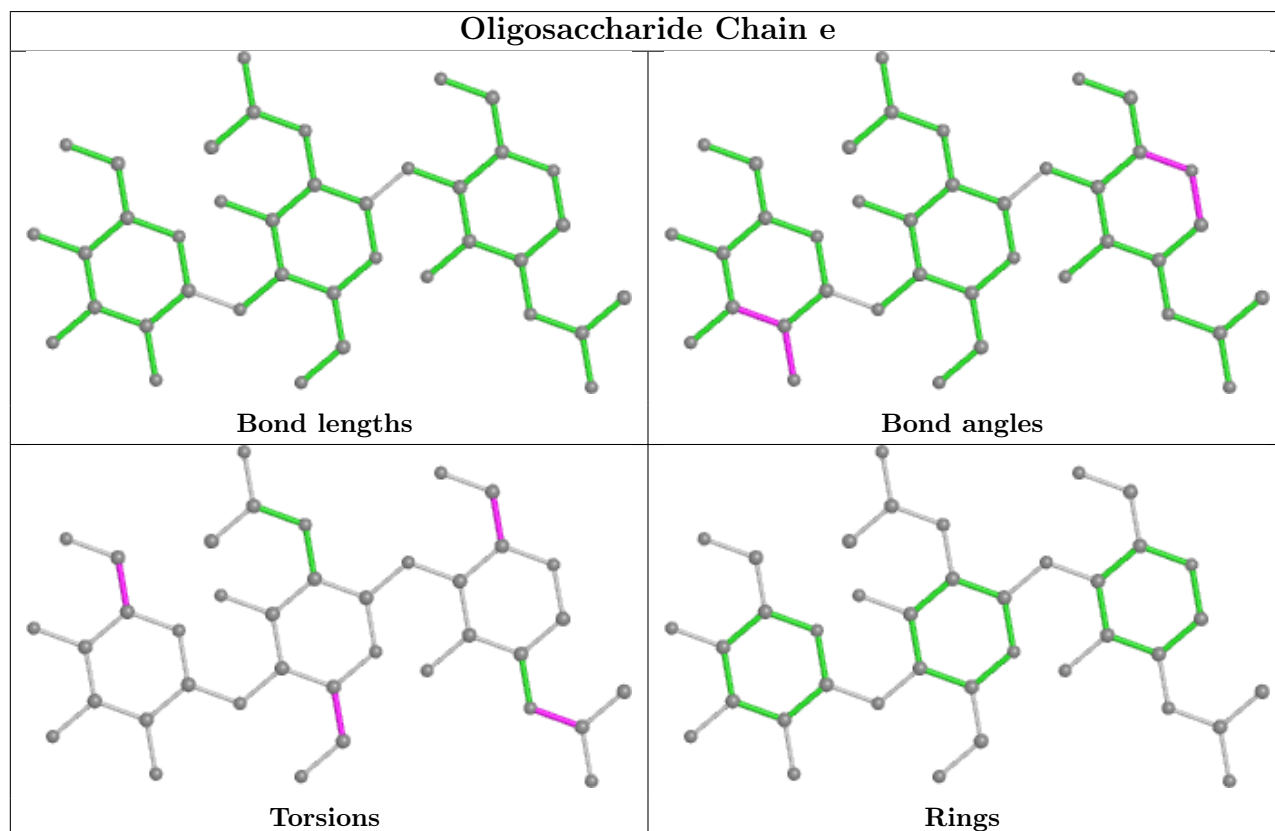
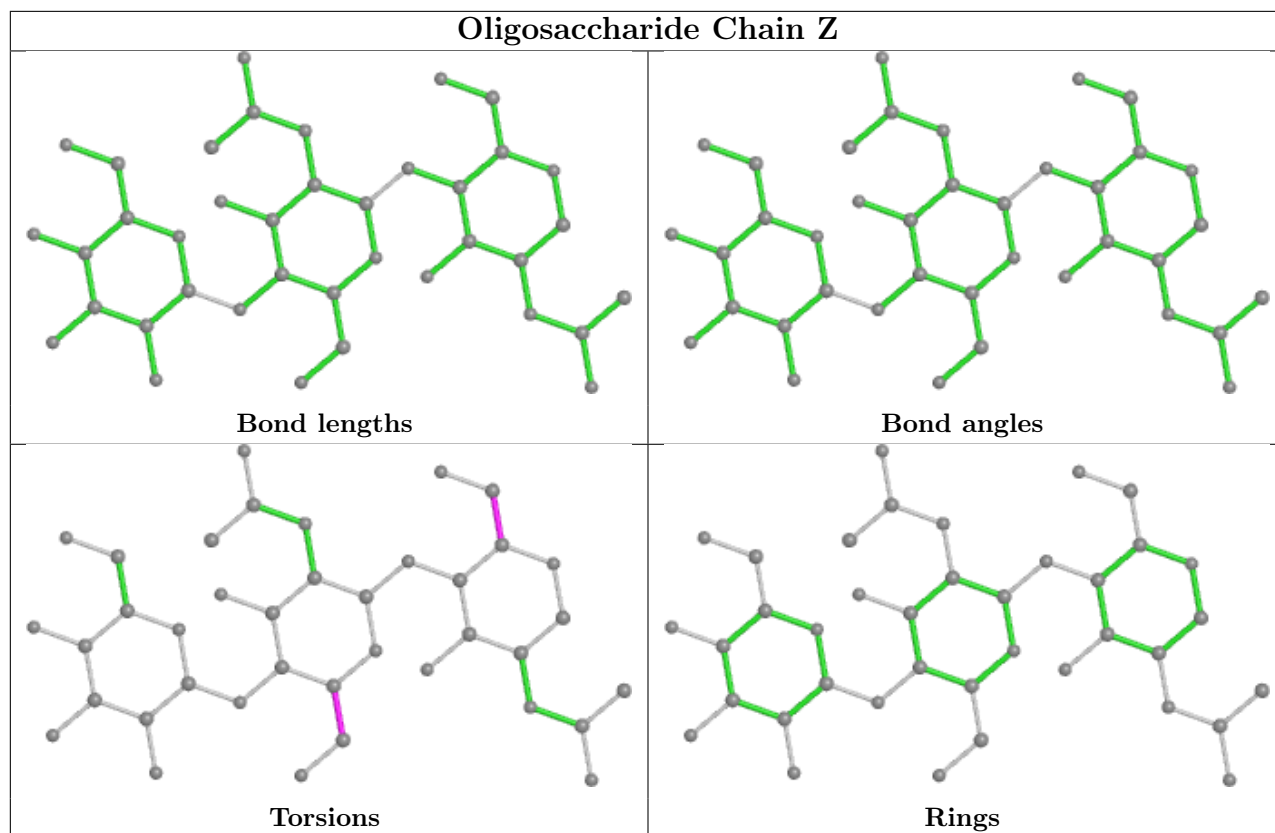


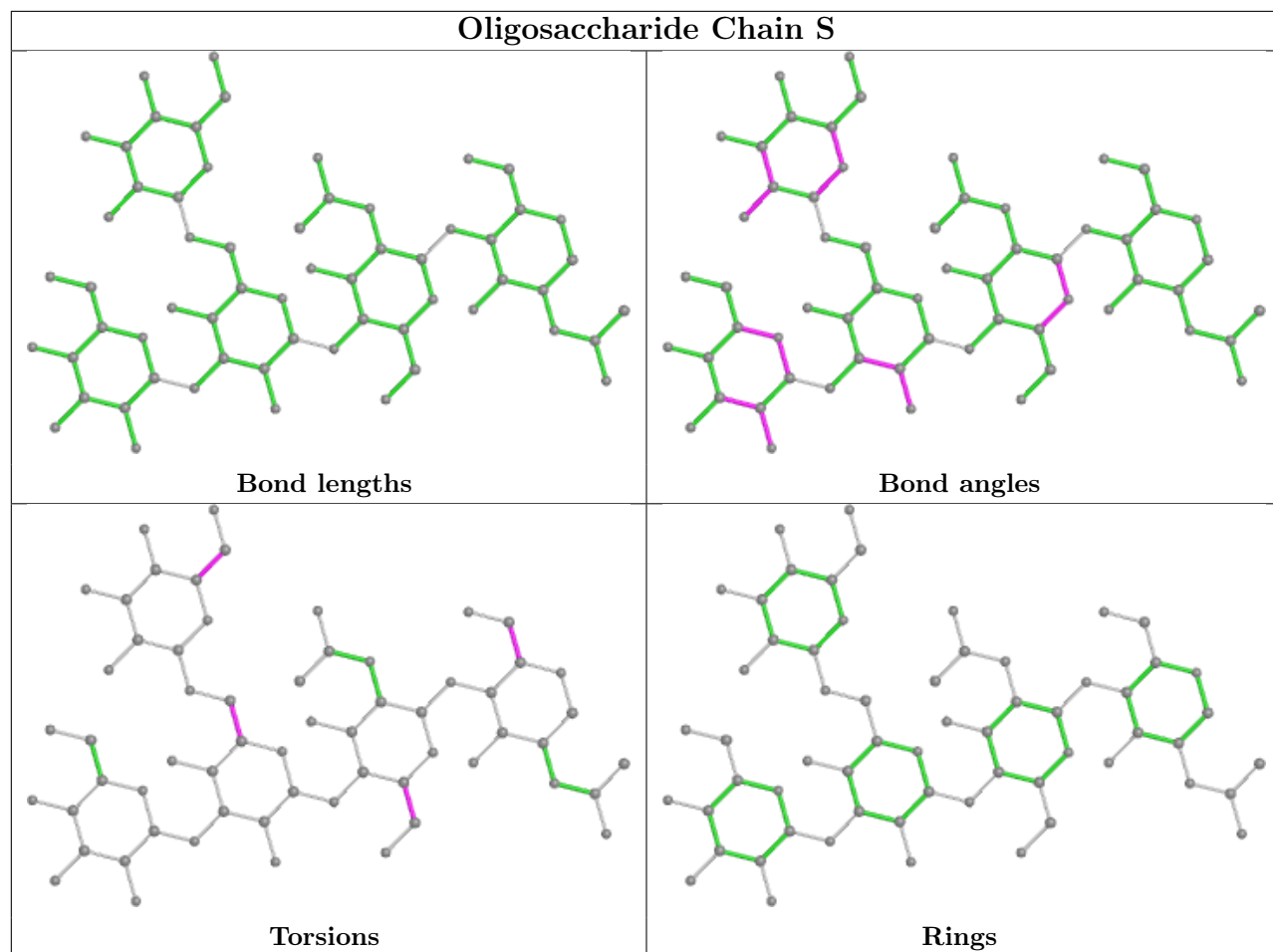


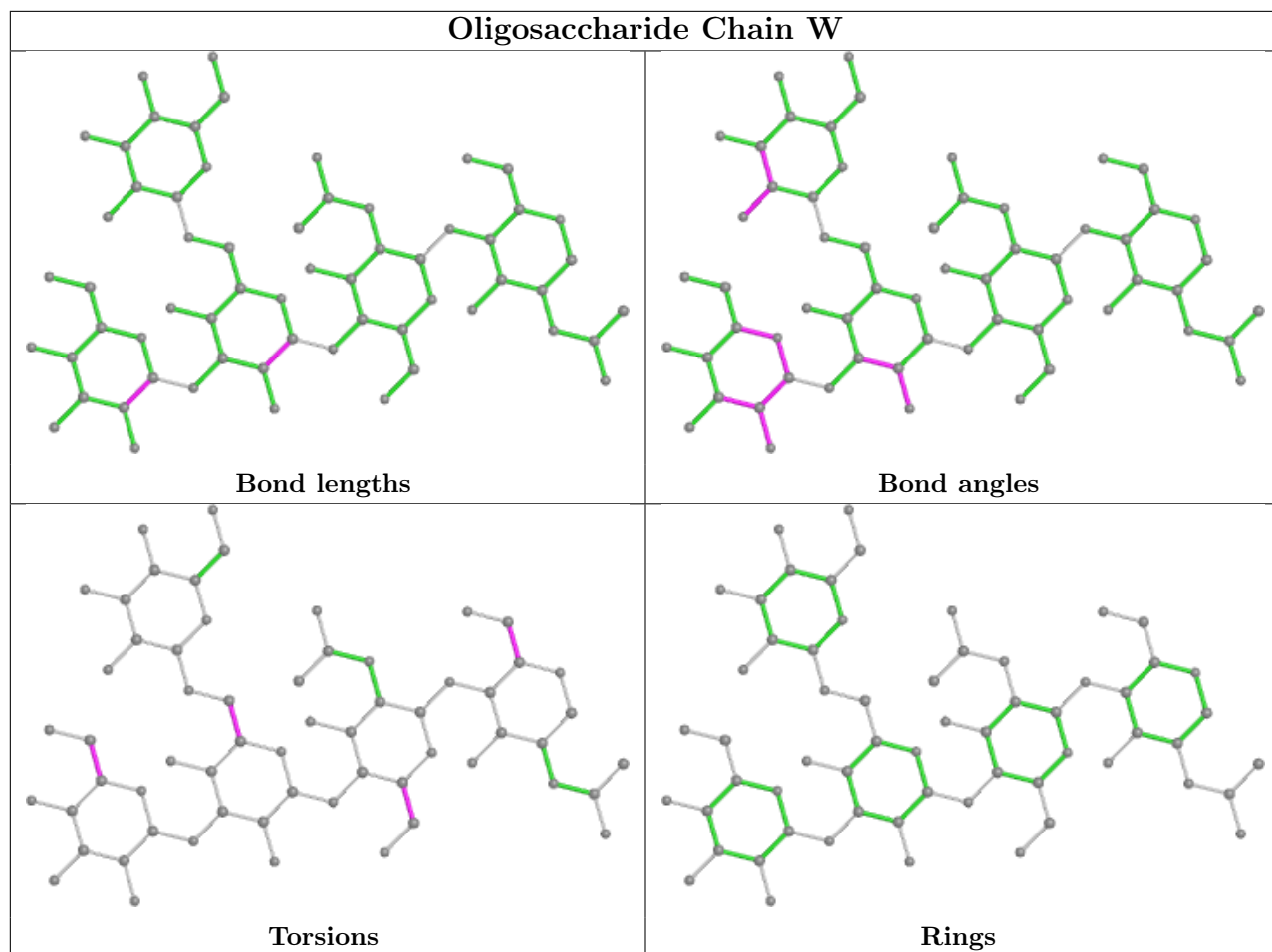


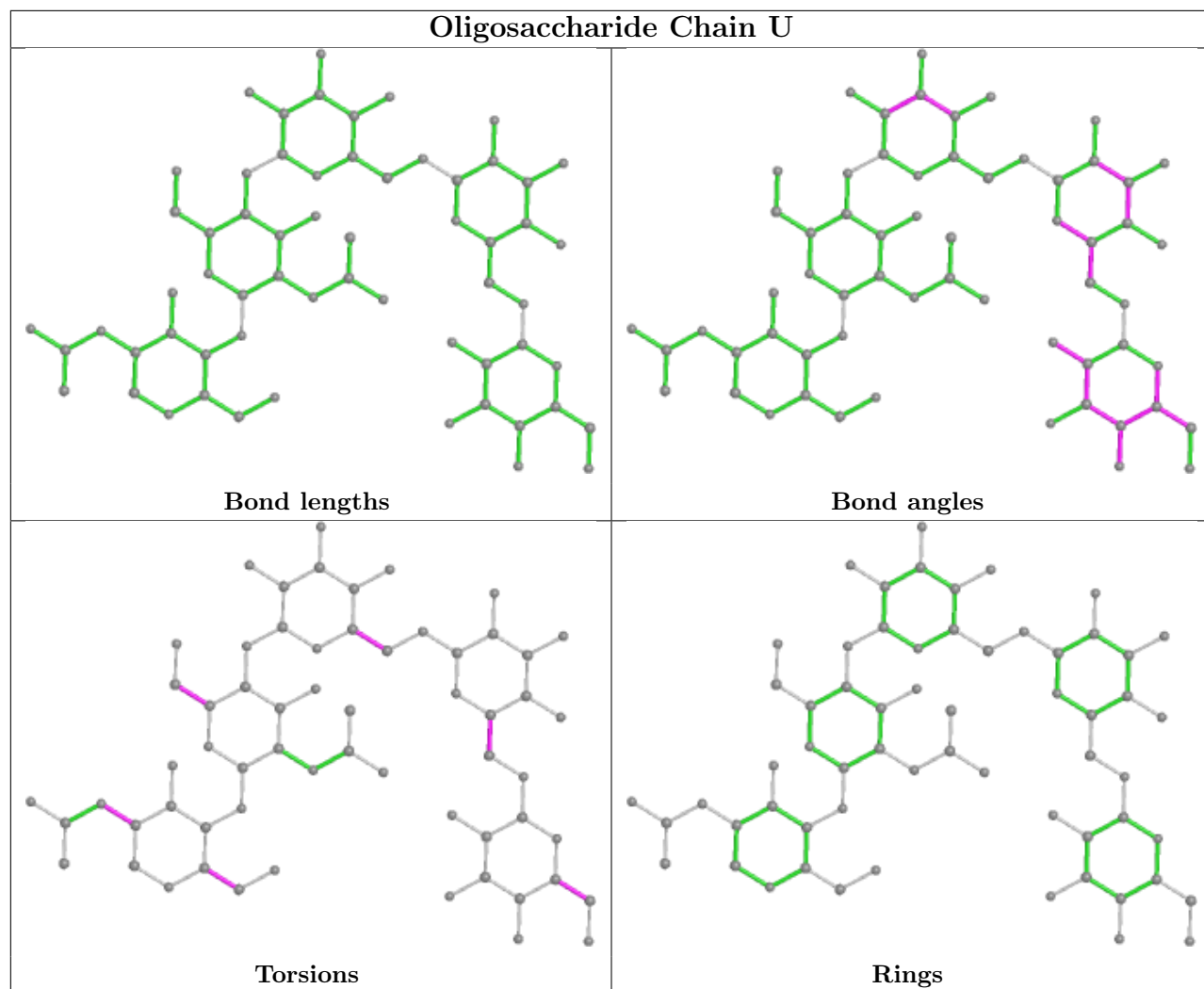


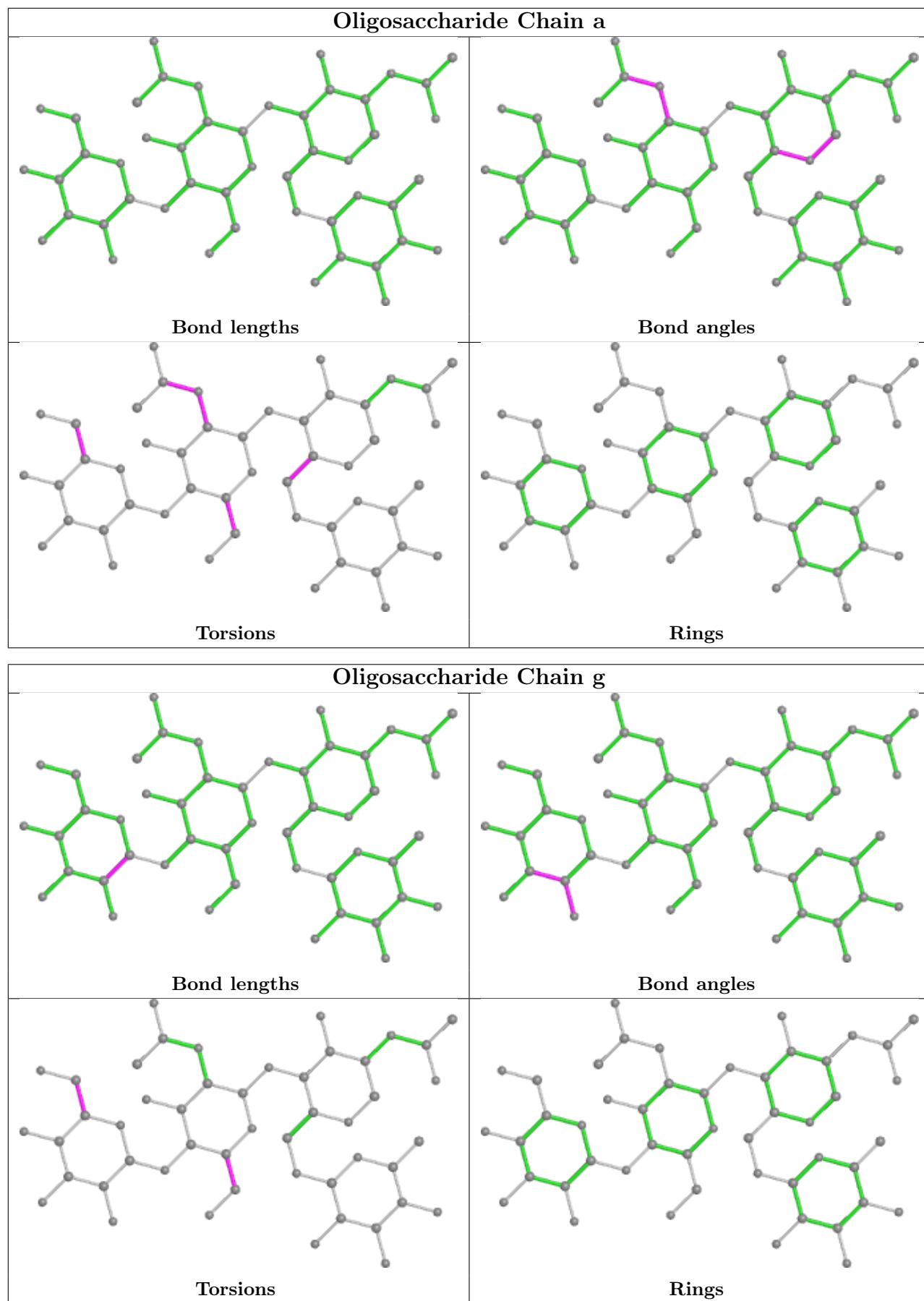


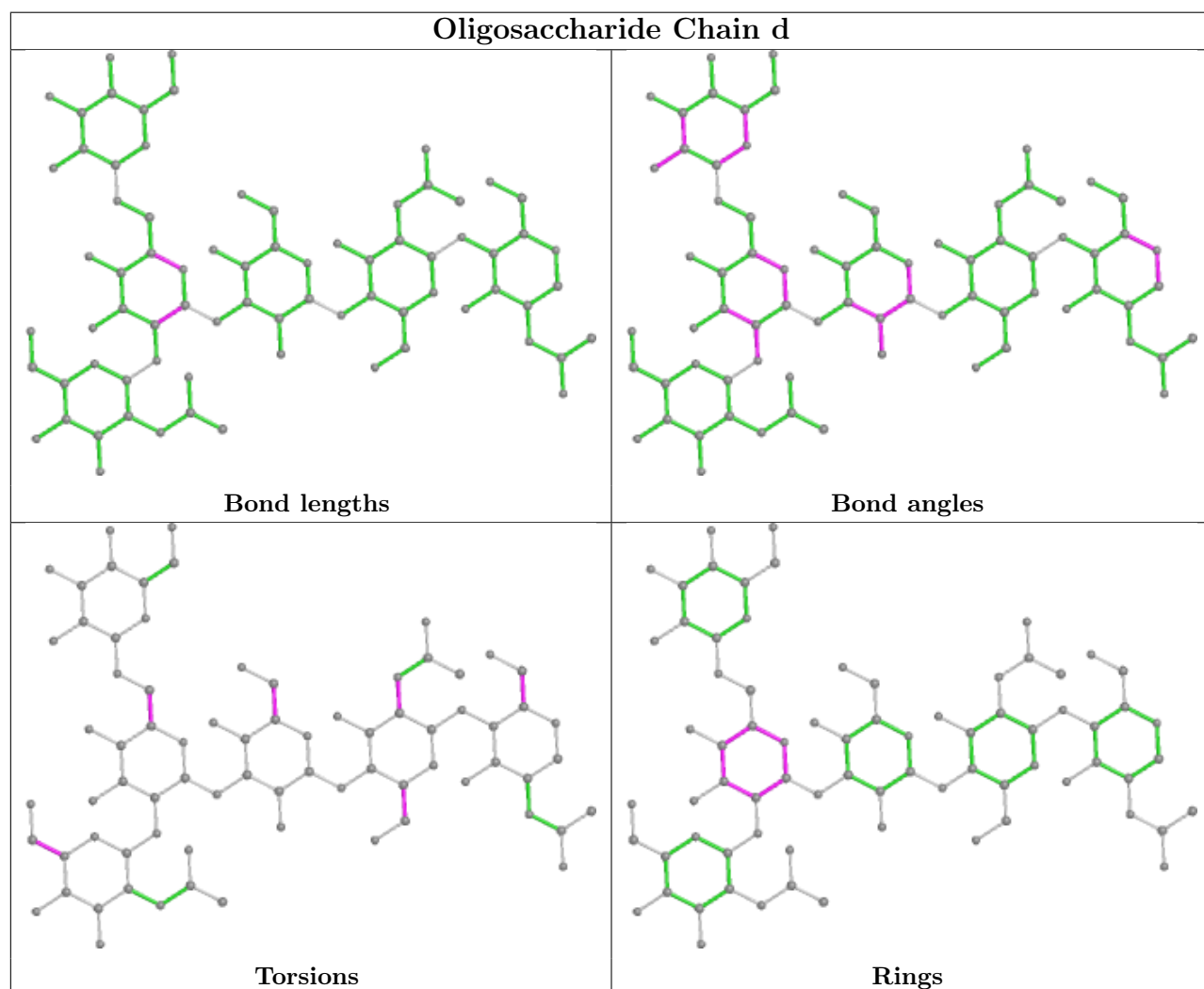
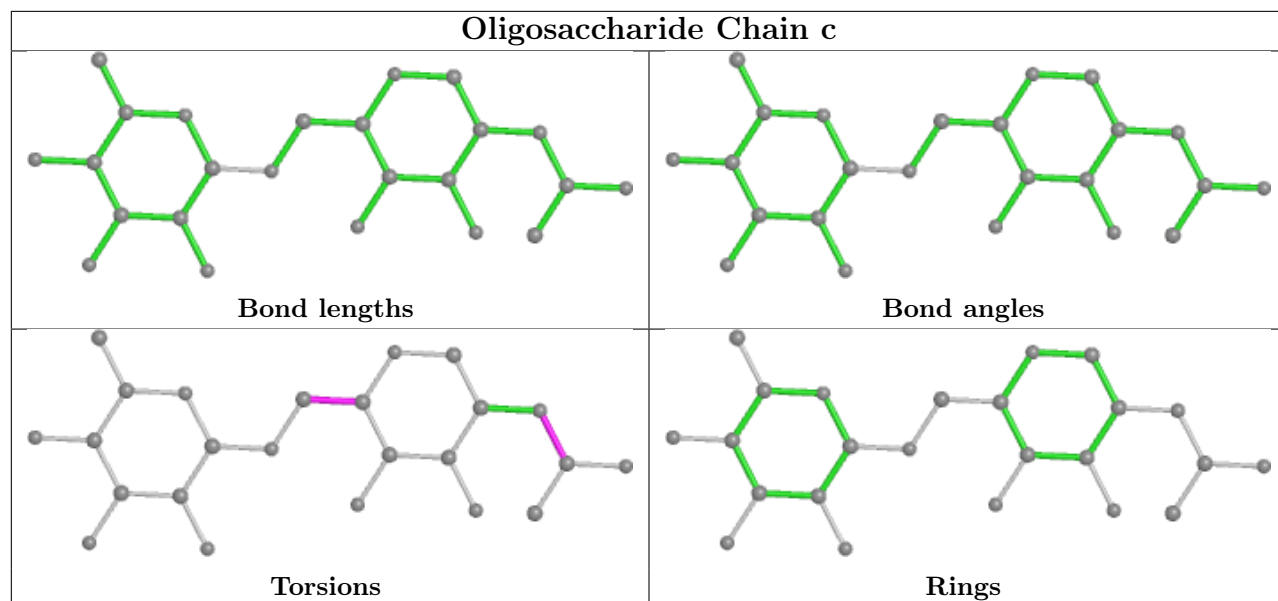


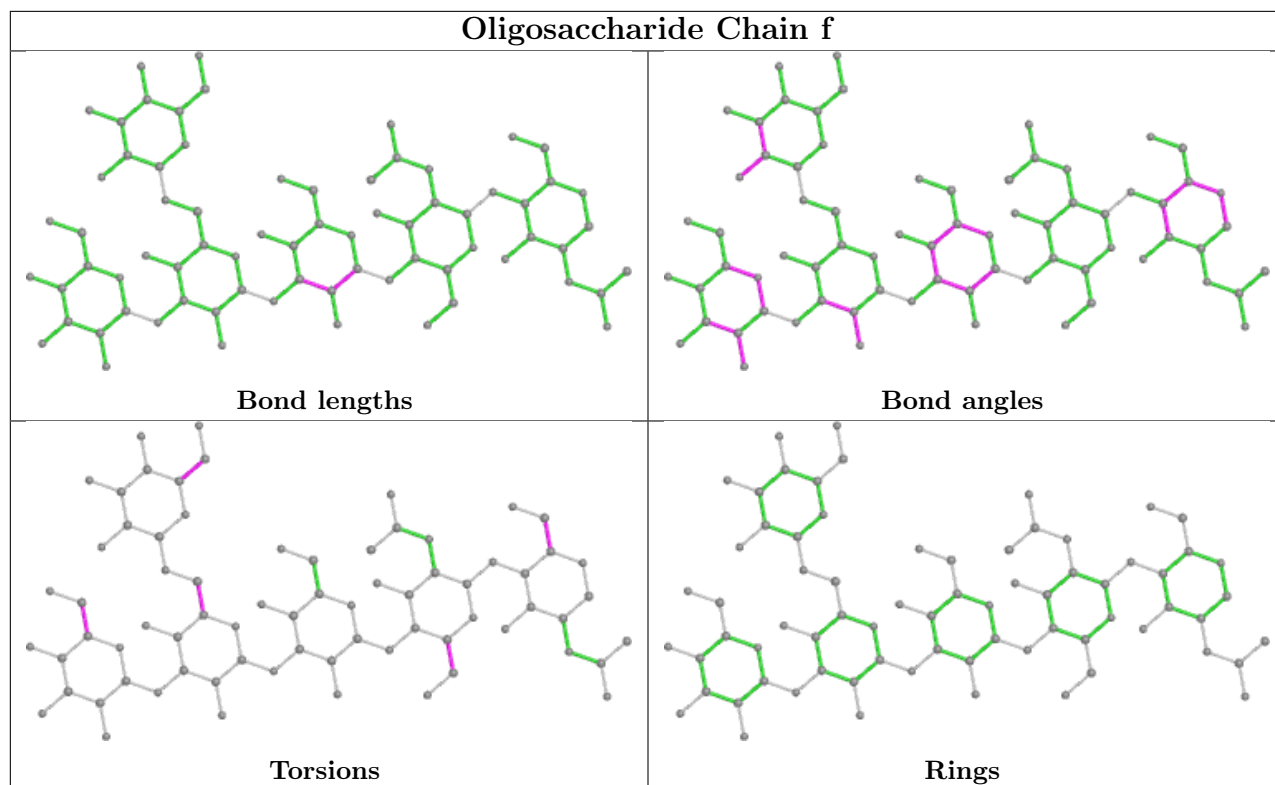












5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	NAG	E	1304	1	14,14,15	0.17	0	17,19,21	0.58	0
14	NAG	K	301	2	14,14,15	0.19	0	17,19,21	0.39	0
14	NAG	E	1301	1	14,14,15	0.35	0	17,19,21	0.41	0
14	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.35	0
14	NAG	E	1305	1	14,14,15	0.25	0	17,19,21	0.43	0
14	NAG	E	1303	1	14,14,15	0.51	0	17,19,21	0.65	1 (5%)
14	NAG	C	1302	1	14,14,15	0.44	0	17,19,21	0.68	1 (5%)
14	NAG	E	1302	1	14,14,15	0.25	0	17,19,21	0.36	0
14	NAG	C	1301	1	14,14,15	0.25	0	17,19,21	0.57	0
14	NAG	A	1304	1	14,14,15	0.48	0	17,19,21	1.16	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	C	1305	1	14,14,15	0.29	0	17,19,21	0.50	0
14	NAG	C	1307	1	14,14,15	0.24	0	17,19,21	0.51	0
14	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.40	0
14	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.51	0
14	NAG	A	1303	1	14,14,15	0.47	0	17,19,21	0.44	0
14	NAG	C	1308	1	14,14,15	0.85	1 (7%)	17,19,21	0.96	1 (5%)
14	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.32	0
14	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.71	0
14	NAG	C	1306	1	14,14,15	0.32	0	17,19,21	0.37	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	E	1304	1	-	2/6/23/26	0/1/1/1
14	NAG	K	301	2	-	2/6/23/26	0/1/1/1
14	NAG	E	1301	1	-	2/6/23/26	0/1/1/1
14	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
14	NAG	E	1305	1	-	2/6/23/26	0/1/1/1
14	NAG	E	1303	1	-	4/6/23/26	0/1/1/1
14	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
14	NAG	E	1302	1	-	2/6/23/26	0/1/1/1
14	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1304	1	-	4/6/23/26	0/1/1/1
14	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
14	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
14	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
14	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
14	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
14	NAG	C	1306	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)
14	C	1308	NAG	O5-C1	2.61	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	1308	NAG	C1-O5-C5	3.55	117.00	112.19
14	A	1304	NAG	O5-C5-C6	2.26	110.75	107.20
14	A	1304	NAG	C6-C5-C4	-2.19	107.87	113.00
14	E	1303	NAG	C1-O5-C5	2.16	115.12	112.19
14	A	1304	NAG	C2-N2-C7	2.09	125.88	122.90
14	C	1302	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	1304	NAG	C8-C7-N2-C2
14	A	1304	NAG	O7-C7-N2-C2
14	A	1305	NAG	C8-C7-N2-C2
14	A	1305	NAG	O7-C7-N2-C2
14	E	1303	NAG	C4-C5-C6-O6
14	A	1303	NAG	O5-C5-C6-O6
14	E	1305	NAG	O5-C5-C6-O6
14	E	1303	NAG	O5-C5-C6-O6
14	C	1305	NAG	C4-C5-C6-O6
14	C	1306	NAG	C4-C5-C6-O6
14	E	1302	NAG	O5-C5-C6-O6
14	E	1305	NAG	C4-C5-C6-O6
14	K	301	NAG	O5-C5-C6-O6
14	E	1302	NAG	C4-C5-C6-O6
14	C	1304	NAG	O5-C5-C6-O6
14	C	1305	NAG	O5-C5-C6-O6
14	A	1303	NAG	C4-C5-C6-O6
14	C	1304	NAG	C4-C5-C6-O6
14	C	1301	NAG	C8-C7-N2-C2
14	C	1301	NAG	O7-C7-N2-C2
14	K	301	NAG	C4-C5-C6-O6
14	A	1304	NAG	O5-C5-C6-O6
14	C	1303	NAG	O5-C5-C6-O6
14	C	1306	NAG	O5-C5-C6-O6
14	A	1301	NAG	O5-C5-C6-O6
14	A	1302	NAG	O5-C5-C6-O6

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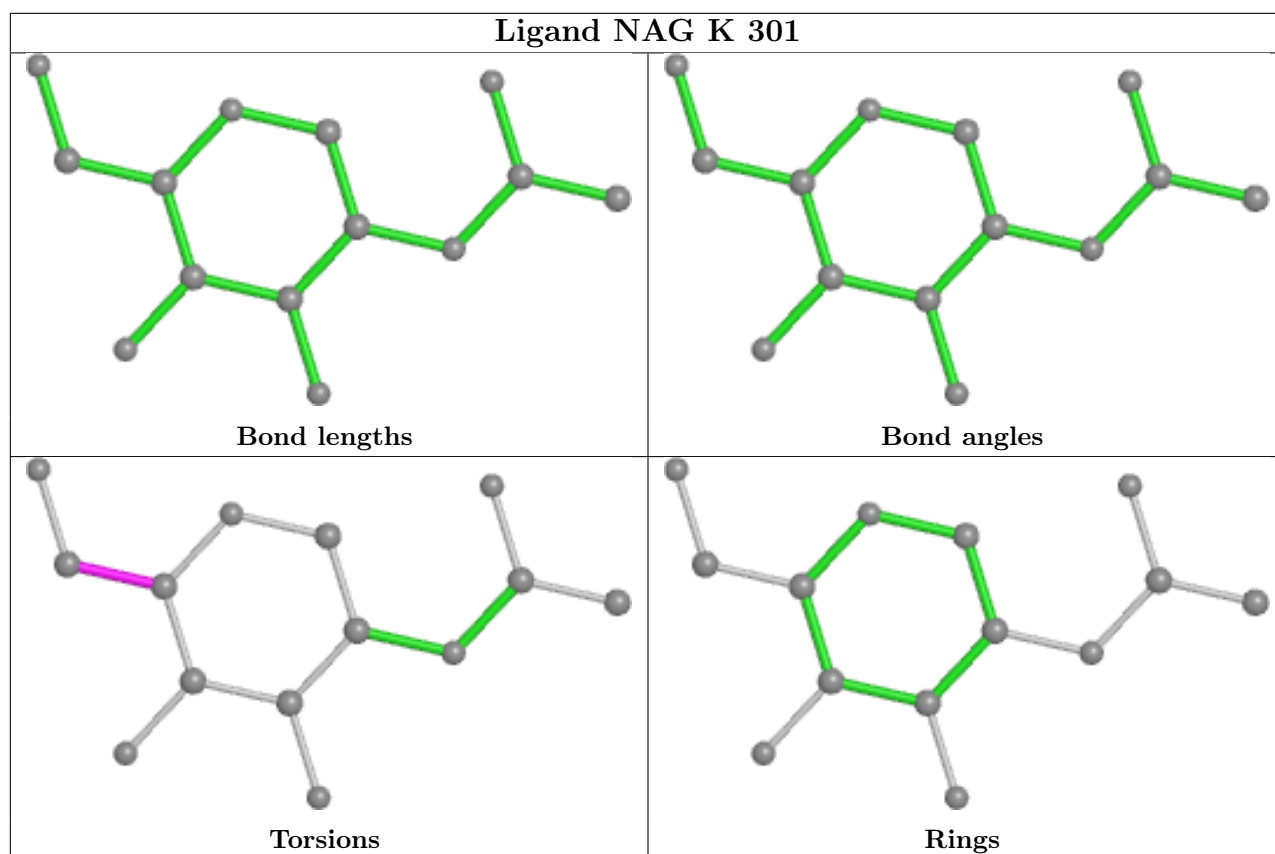
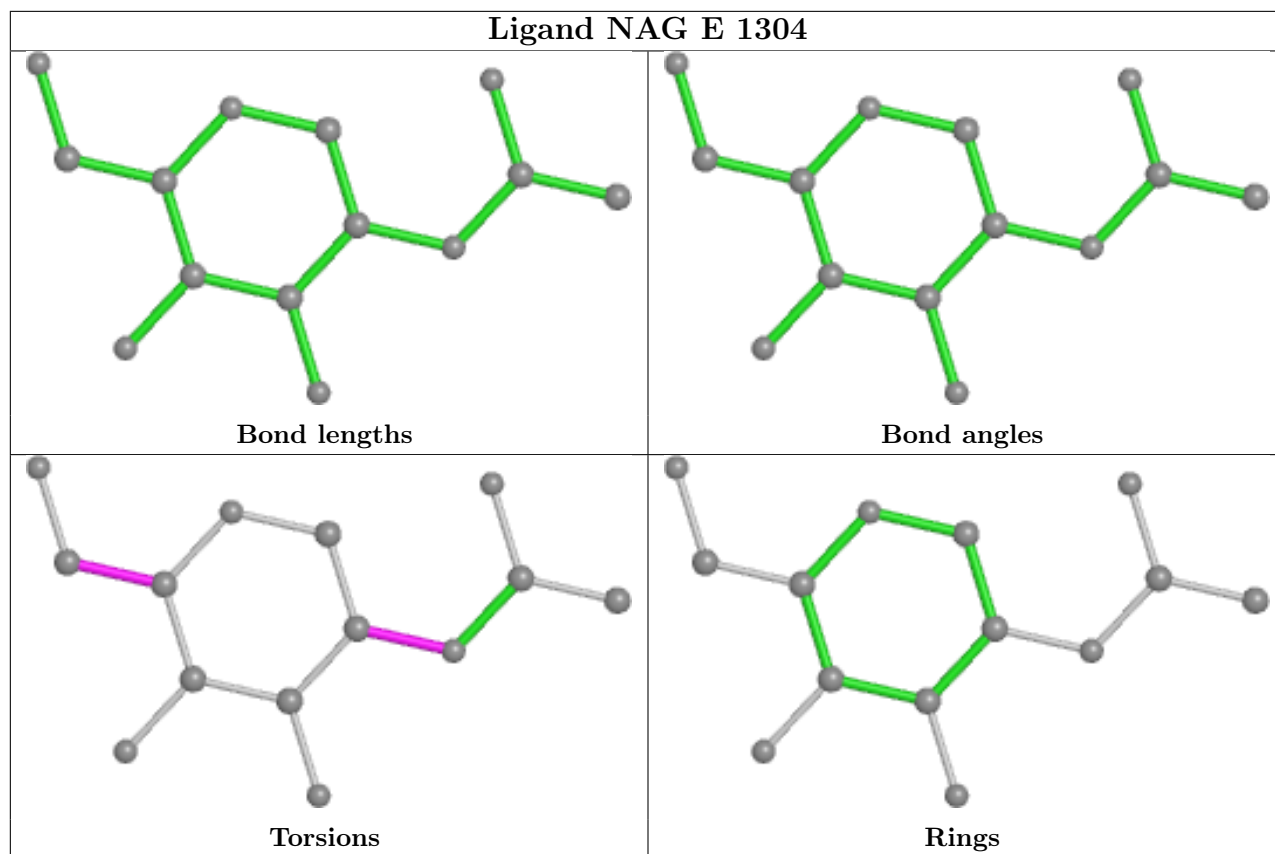
Mol	Chain	Res	Type	Atoms
14	A	1302	NAG	C4-C5-C6-O6
14	E	1303	NAG	C1-C2-N2-C7
14	C	1303	NAG	C4-C5-C6-O6
14	C	1307	NAG	C4-C5-C6-O6
14	E	1304	NAG	O5-C5-C6-O6
14	E	1301	NAG	O5-C5-C6-O6
14	A	1305	NAG	O5-C5-C6-O6
14	C	1302	NAG	O5-C5-C6-O6
14	C	1307	NAG	O5-C5-C6-O6
14	E	1303	NAG	C3-C2-N2-C7
14	E	1304	NAG	C3-C2-N2-C7
14	E	1301	NAG	C1-C2-N2-C7
14	A	1304	NAG	C4-C5-C6-O6

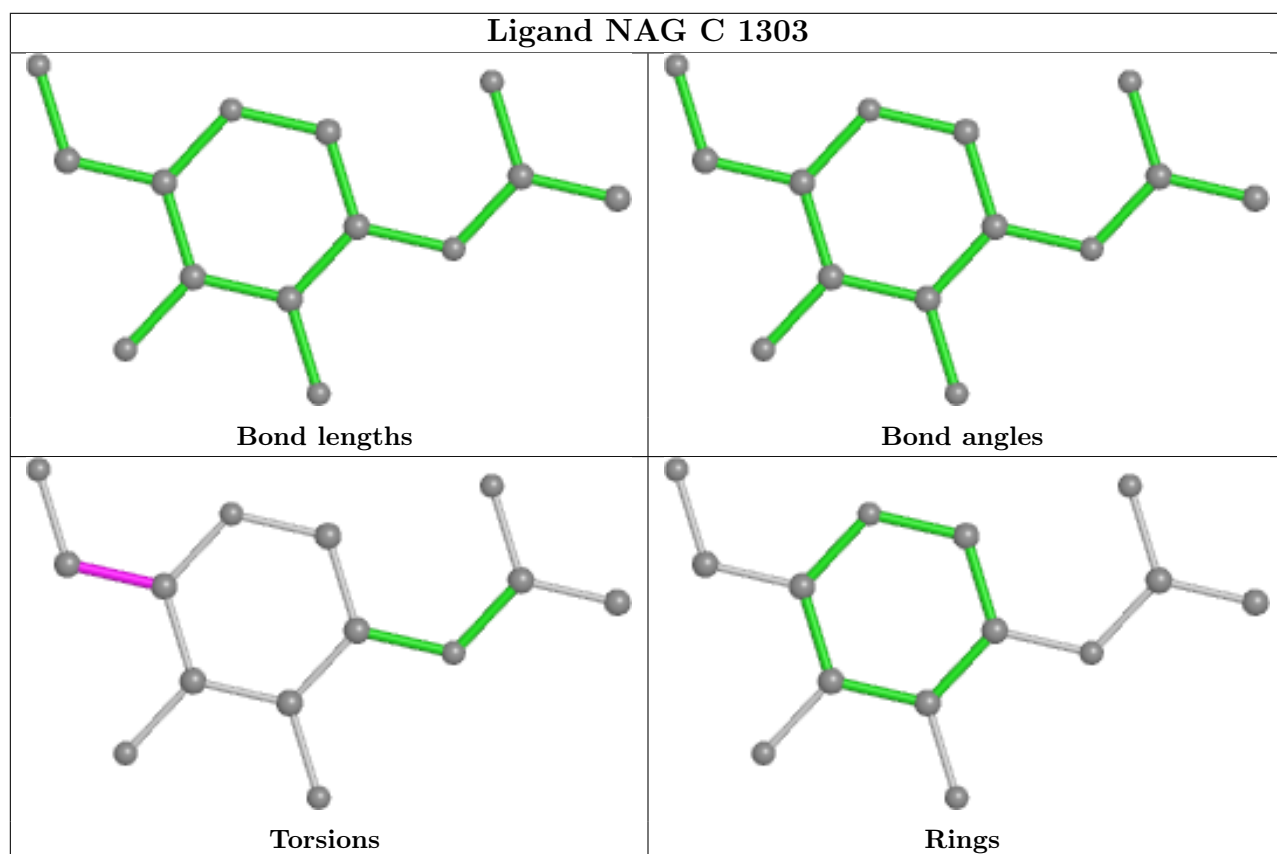
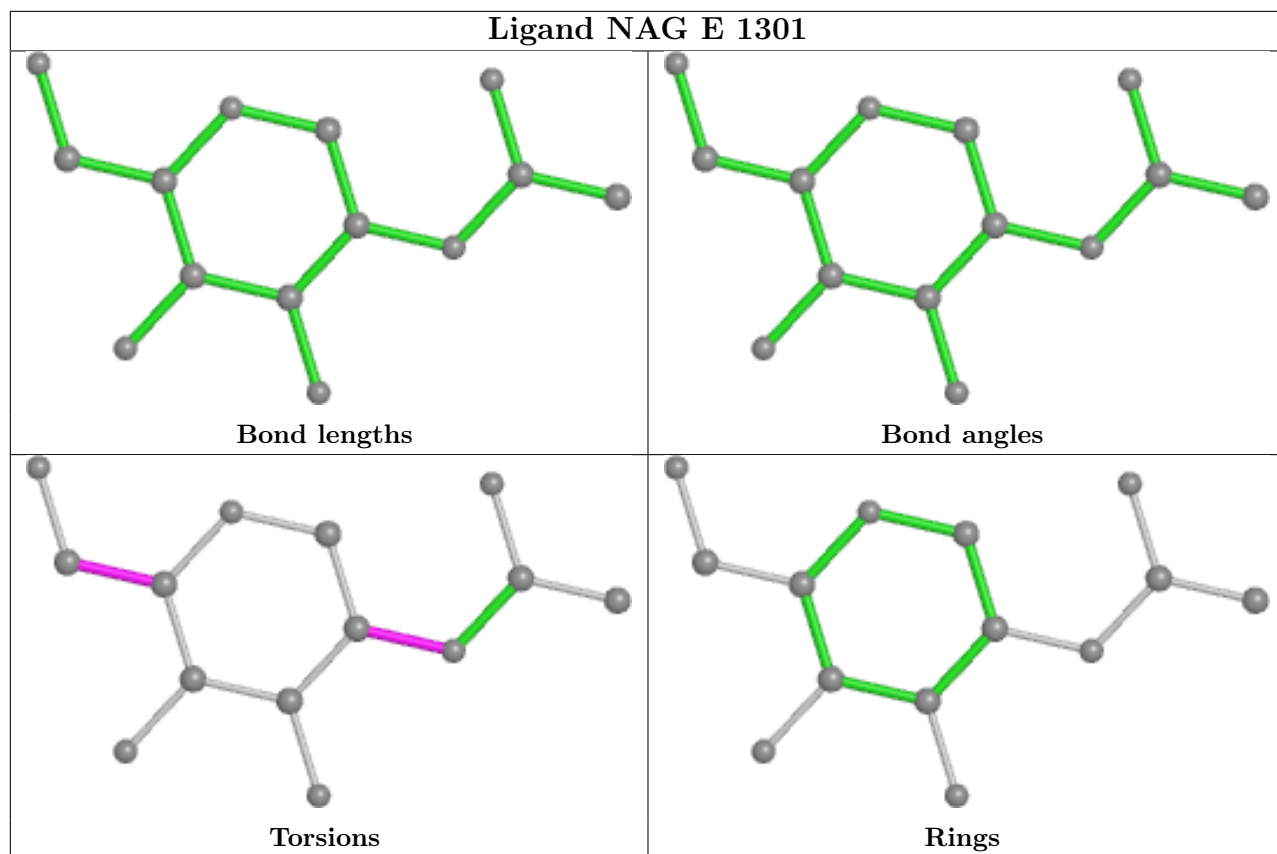
There are no ring outliers.

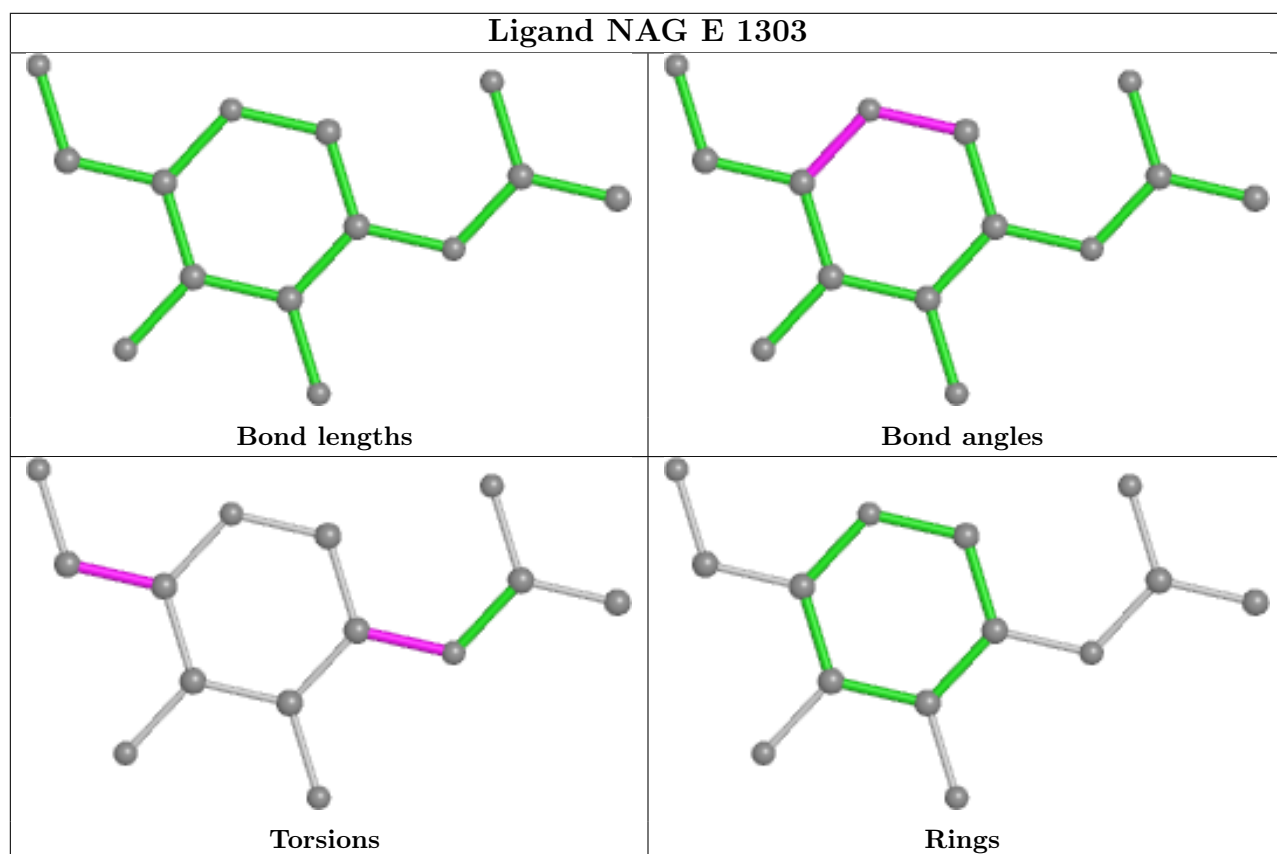
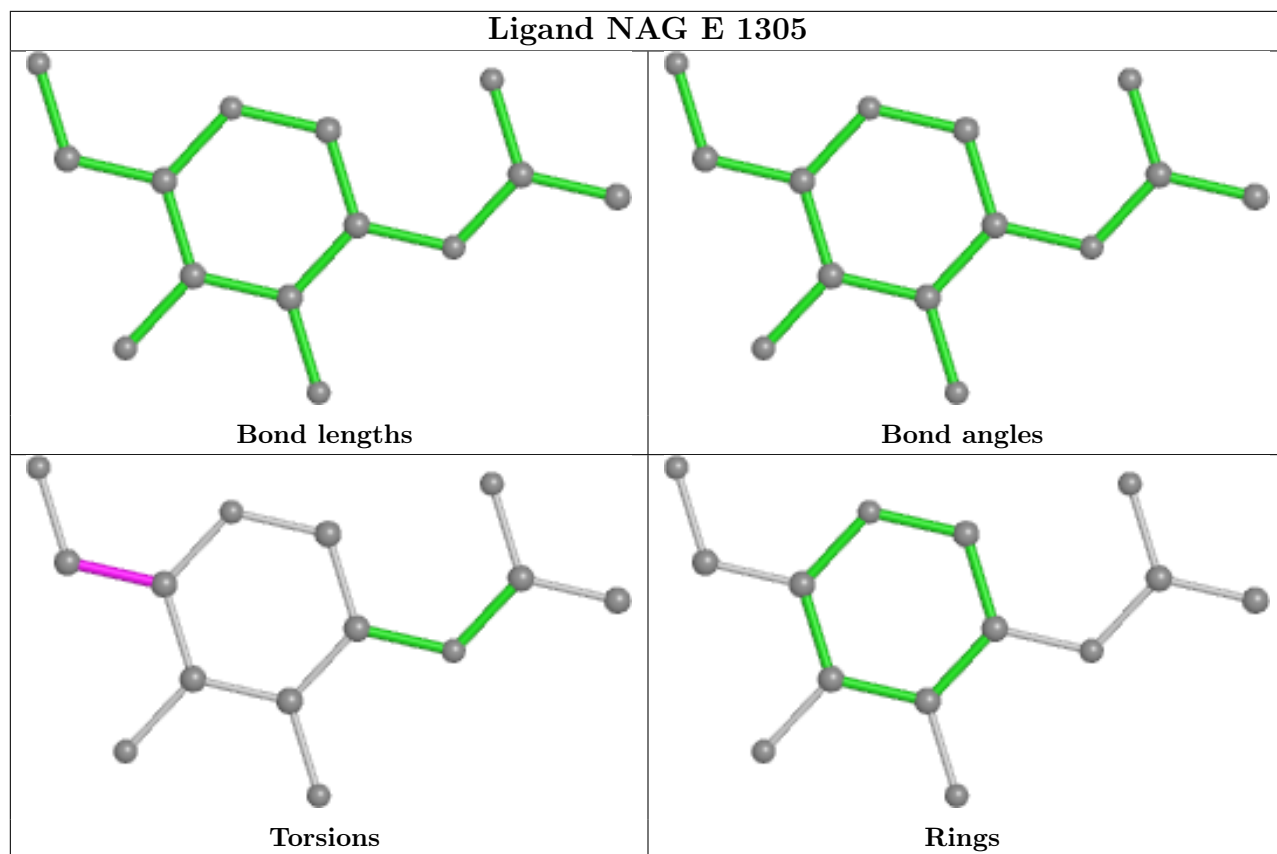
6 monomers are involved in 10 short contacts:

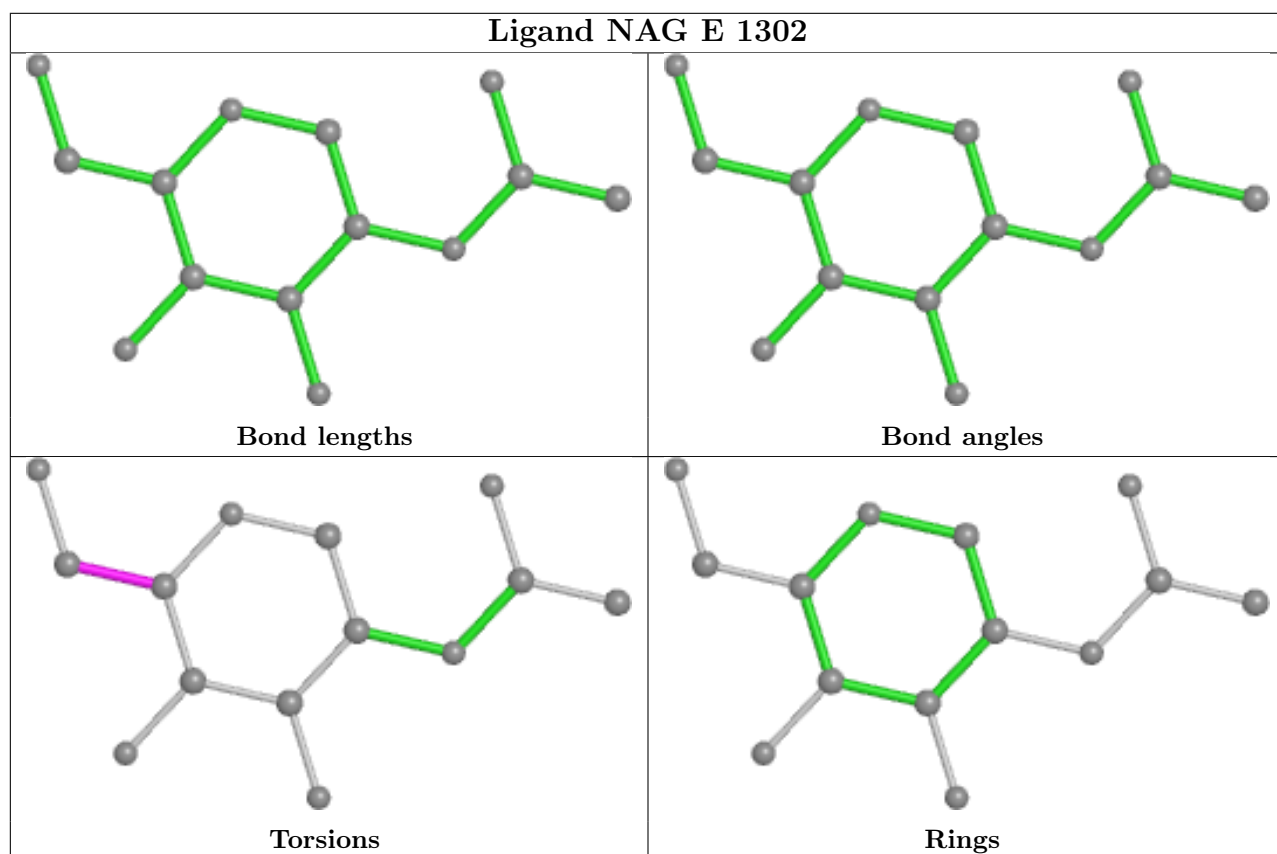
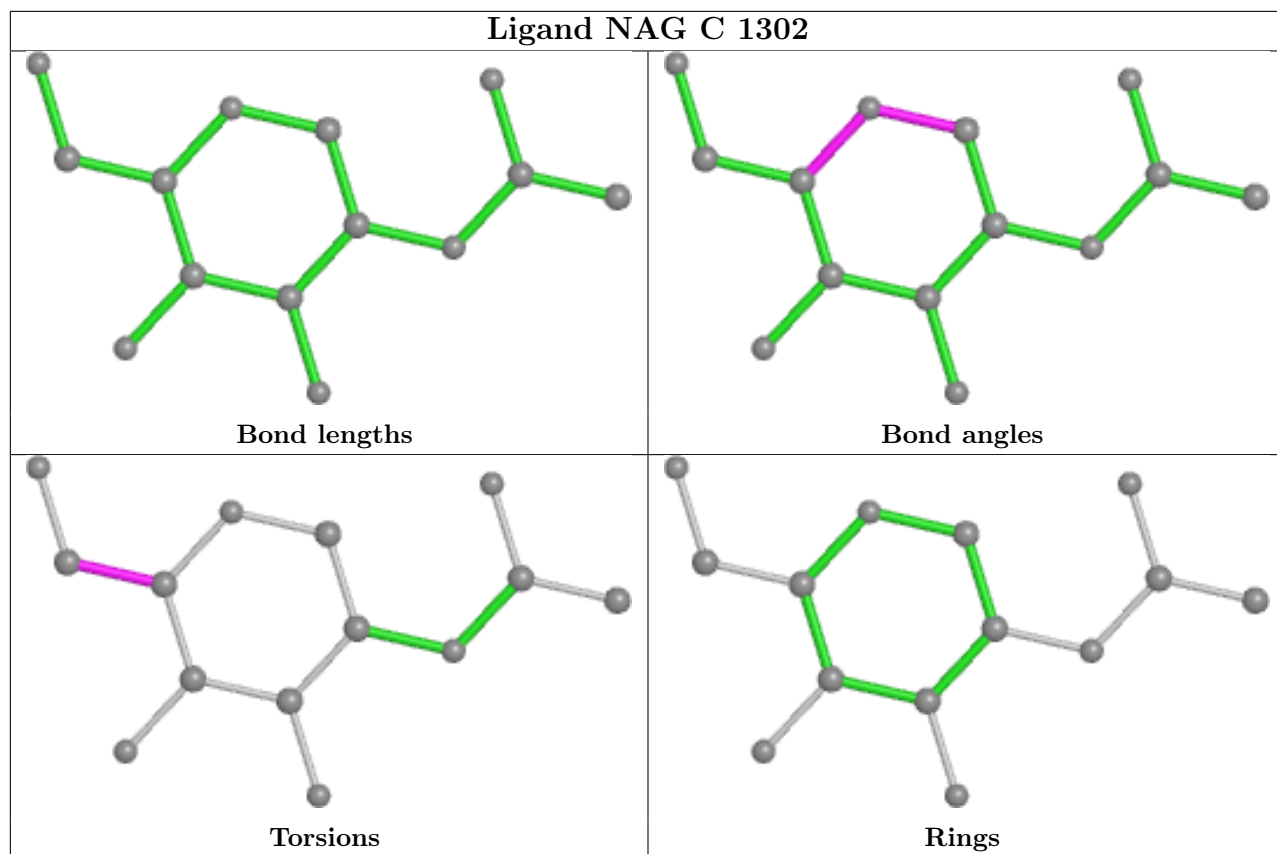
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	E	1304	NAG	3	0
14	E	1303	NAG	1	0
14	C	1301	NAG	3	0
14	A	1304	NAG	1	0
14	C	1307	NAG	1	0
14	C	1308	NAG	1	0

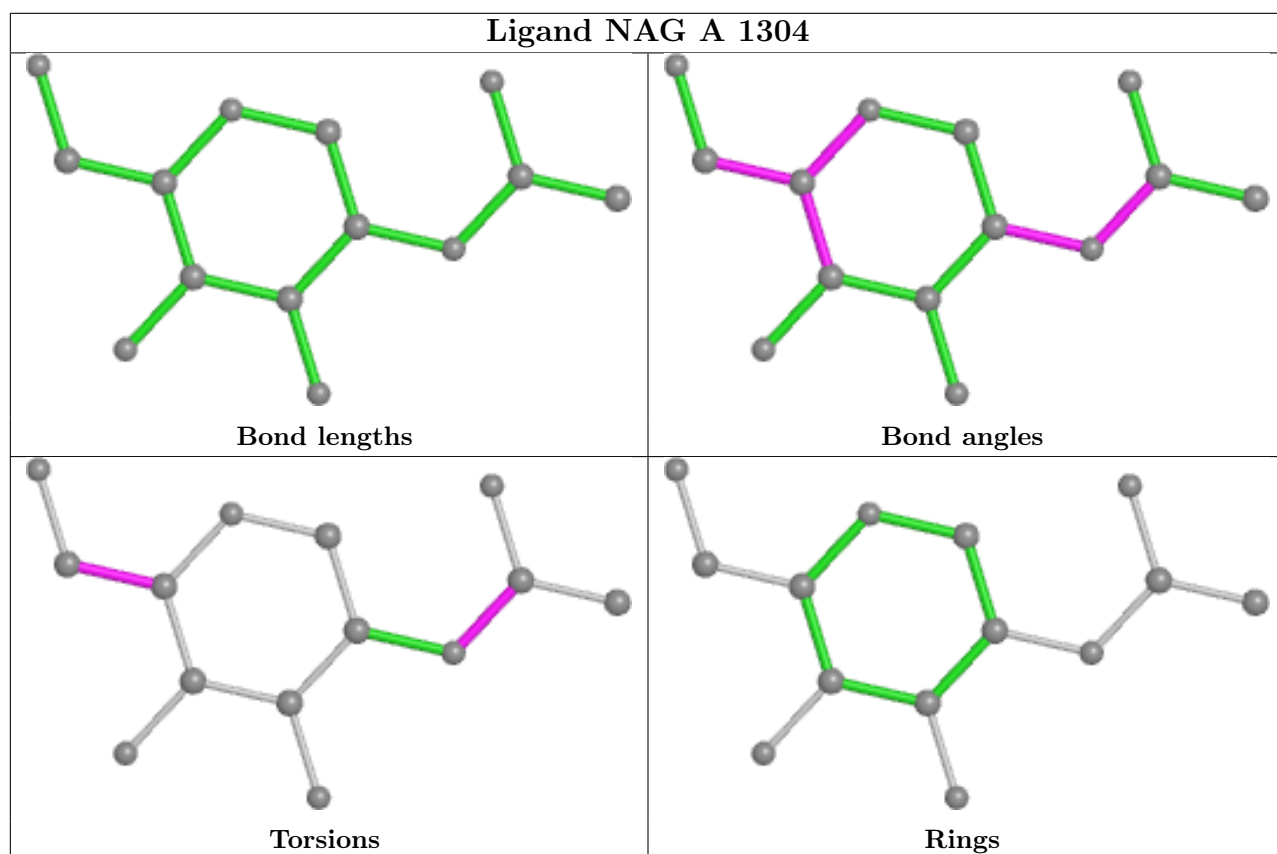
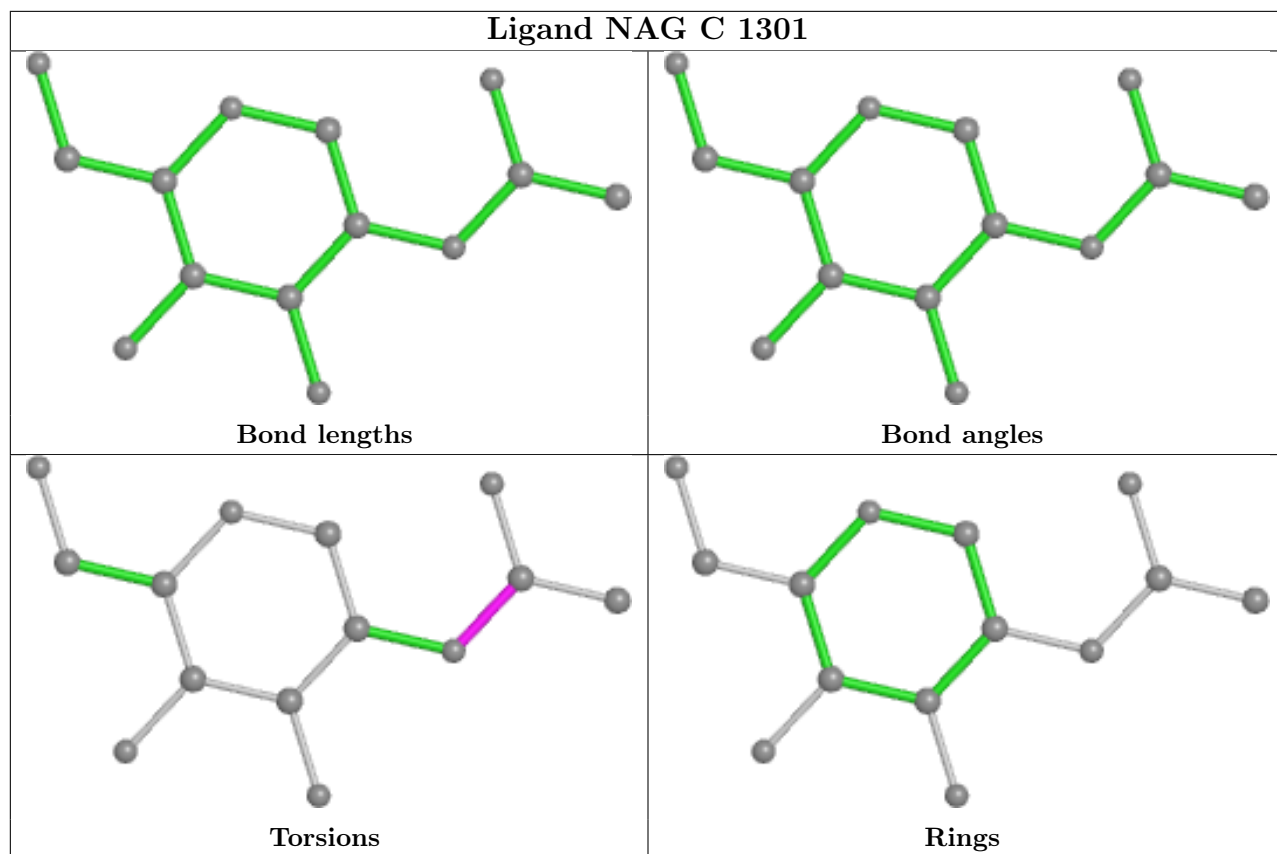
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

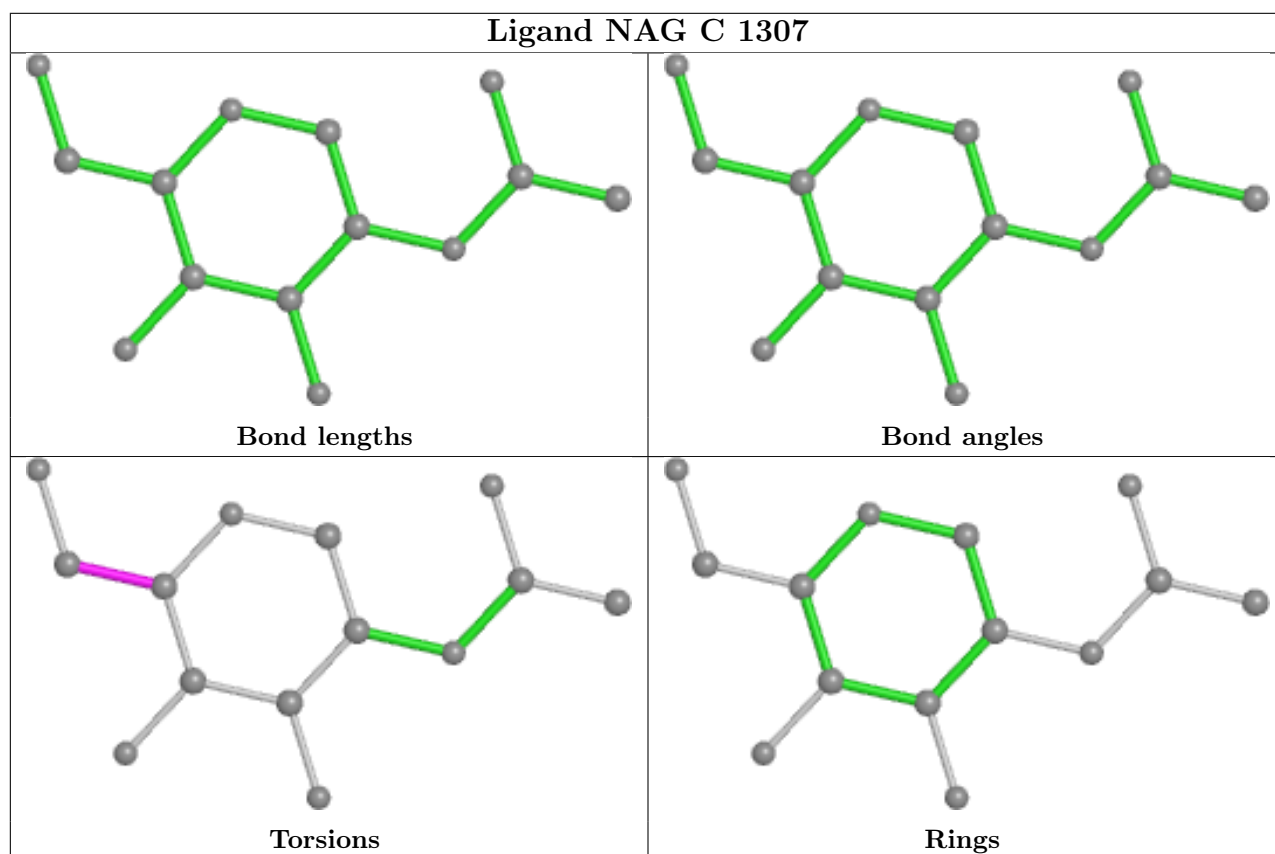
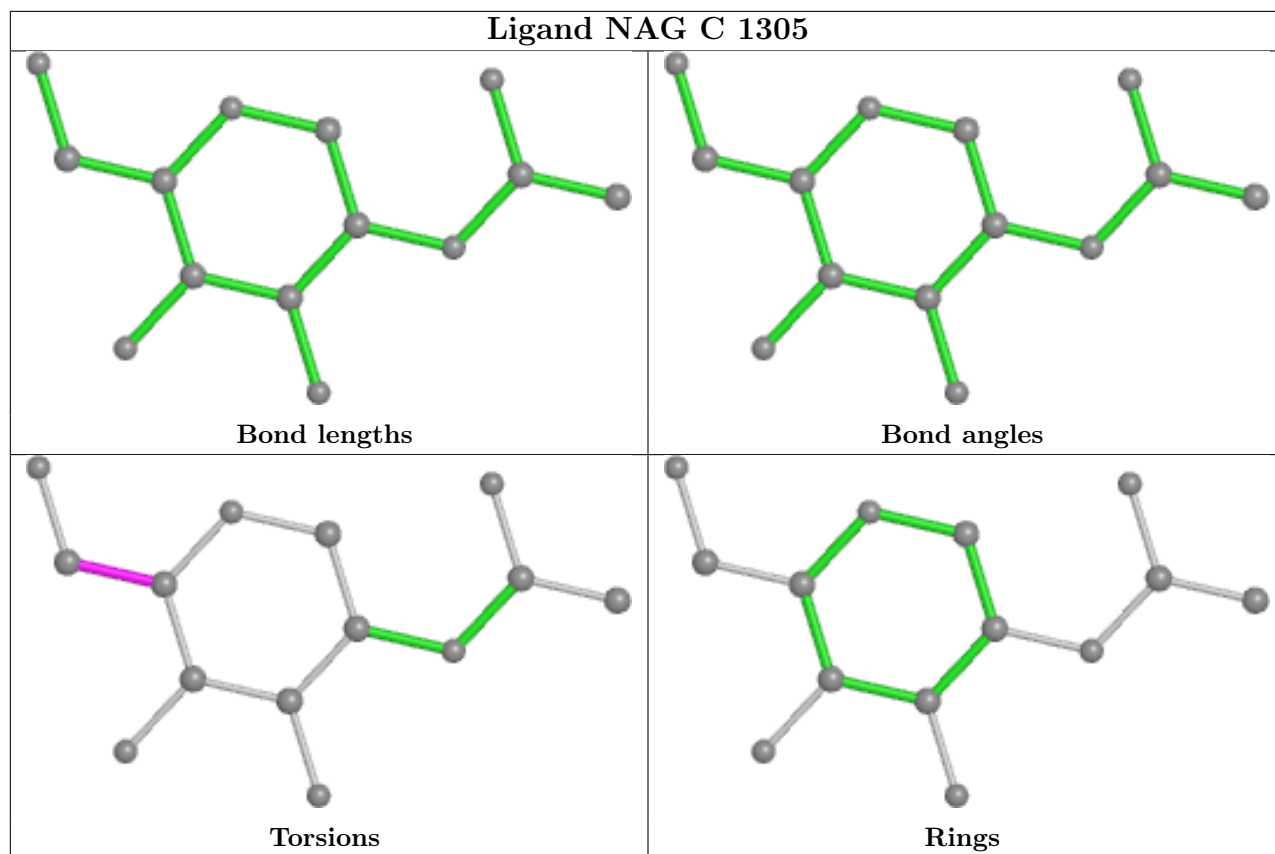


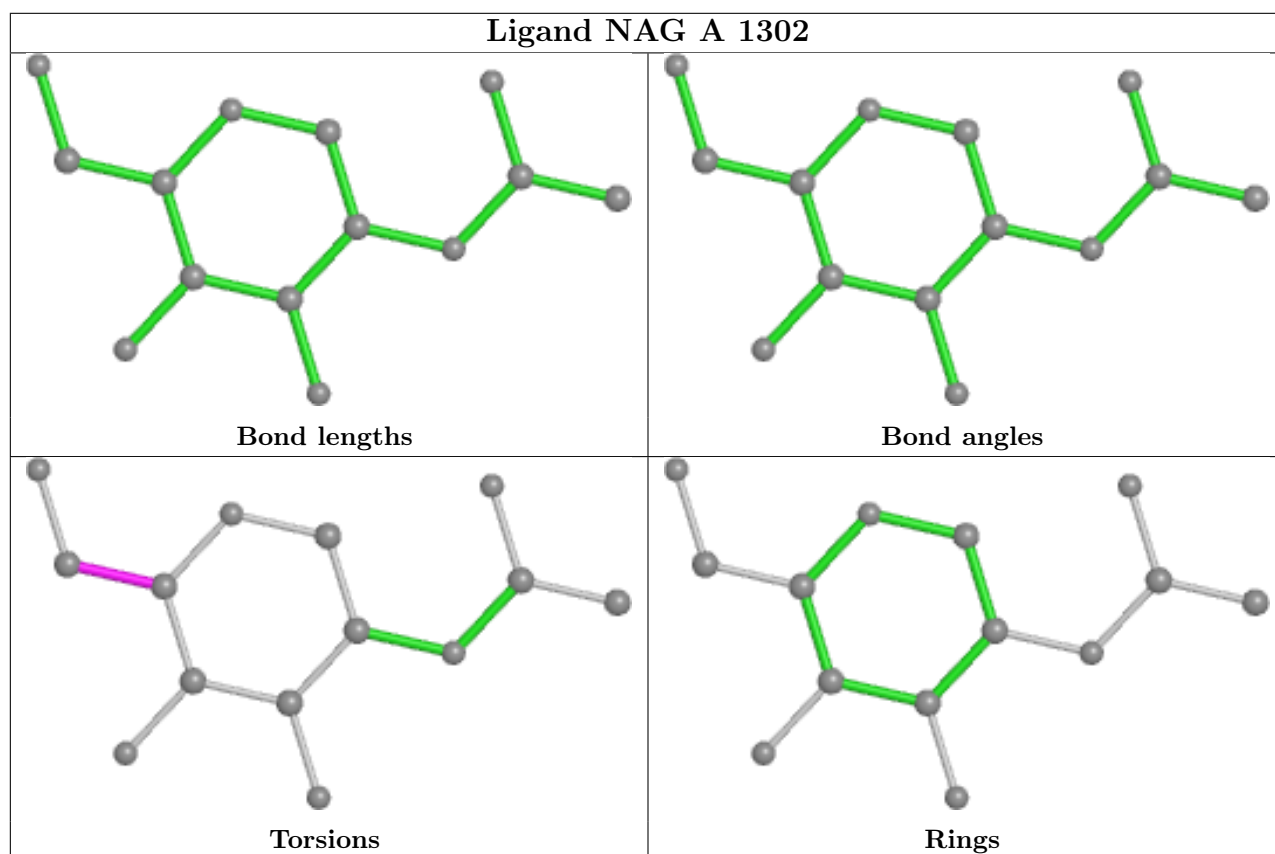
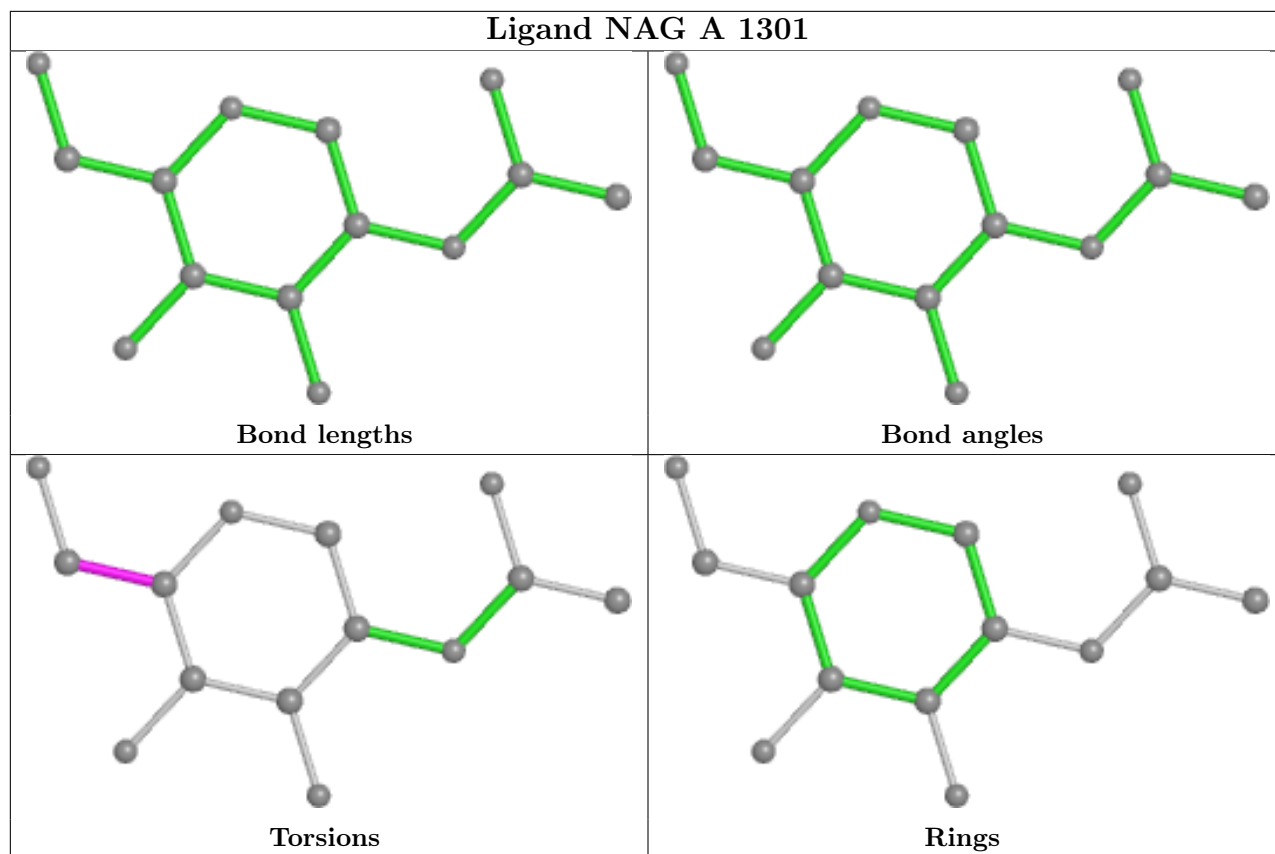


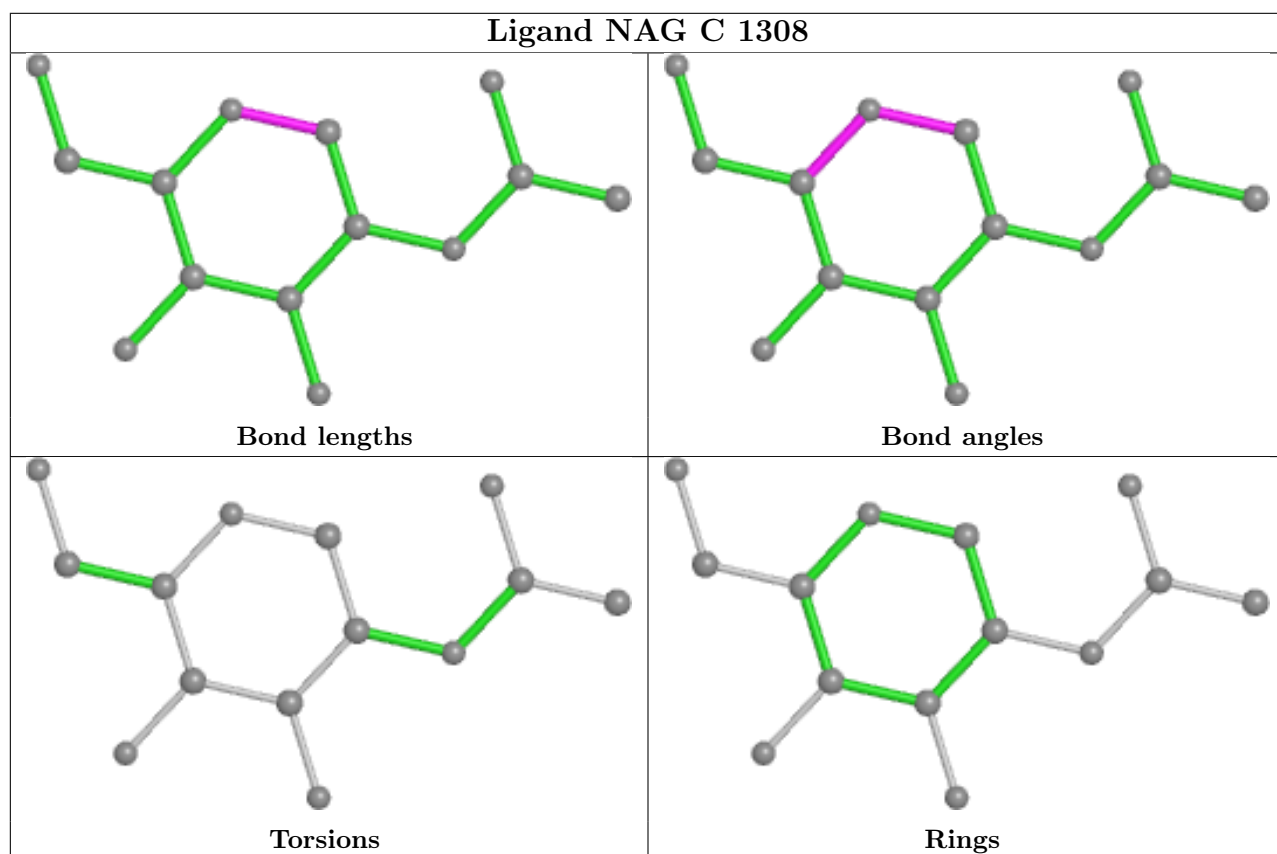
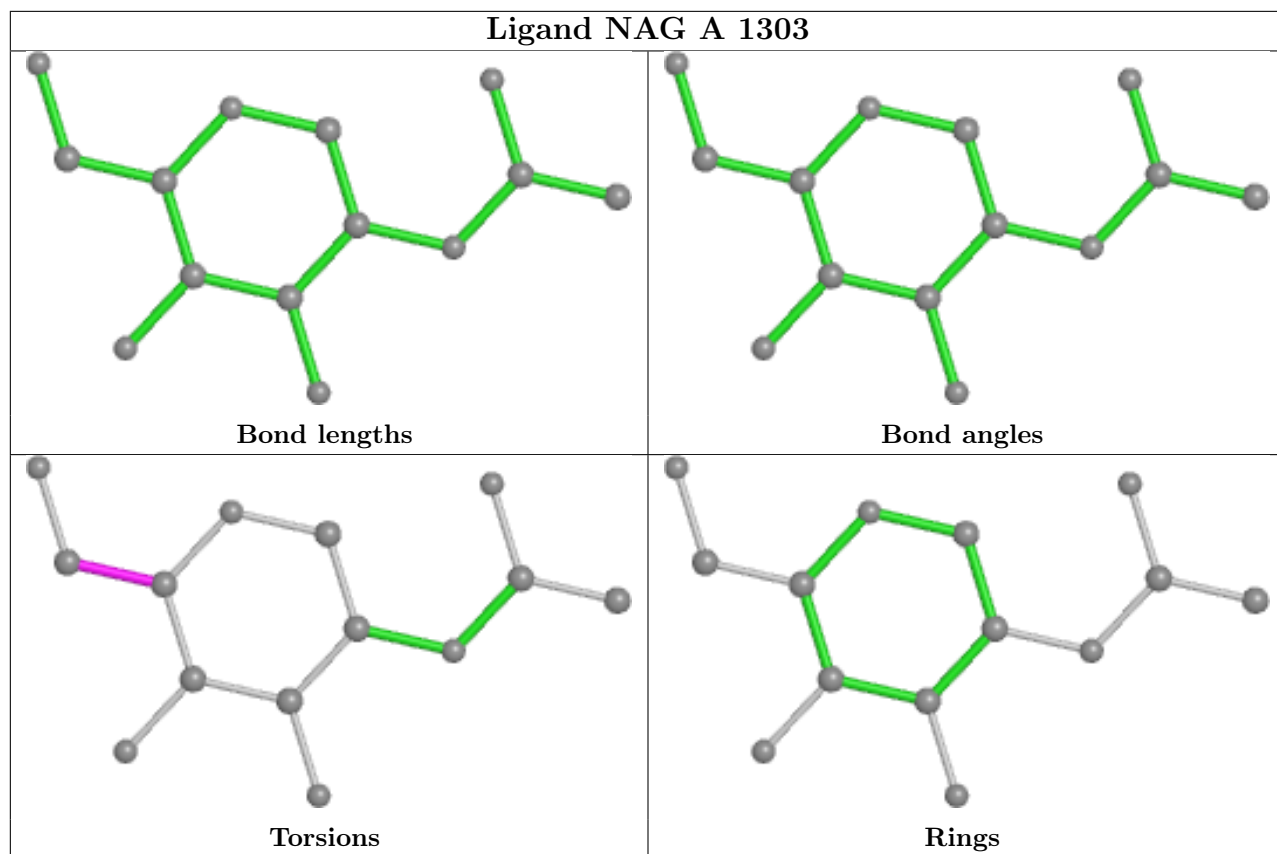


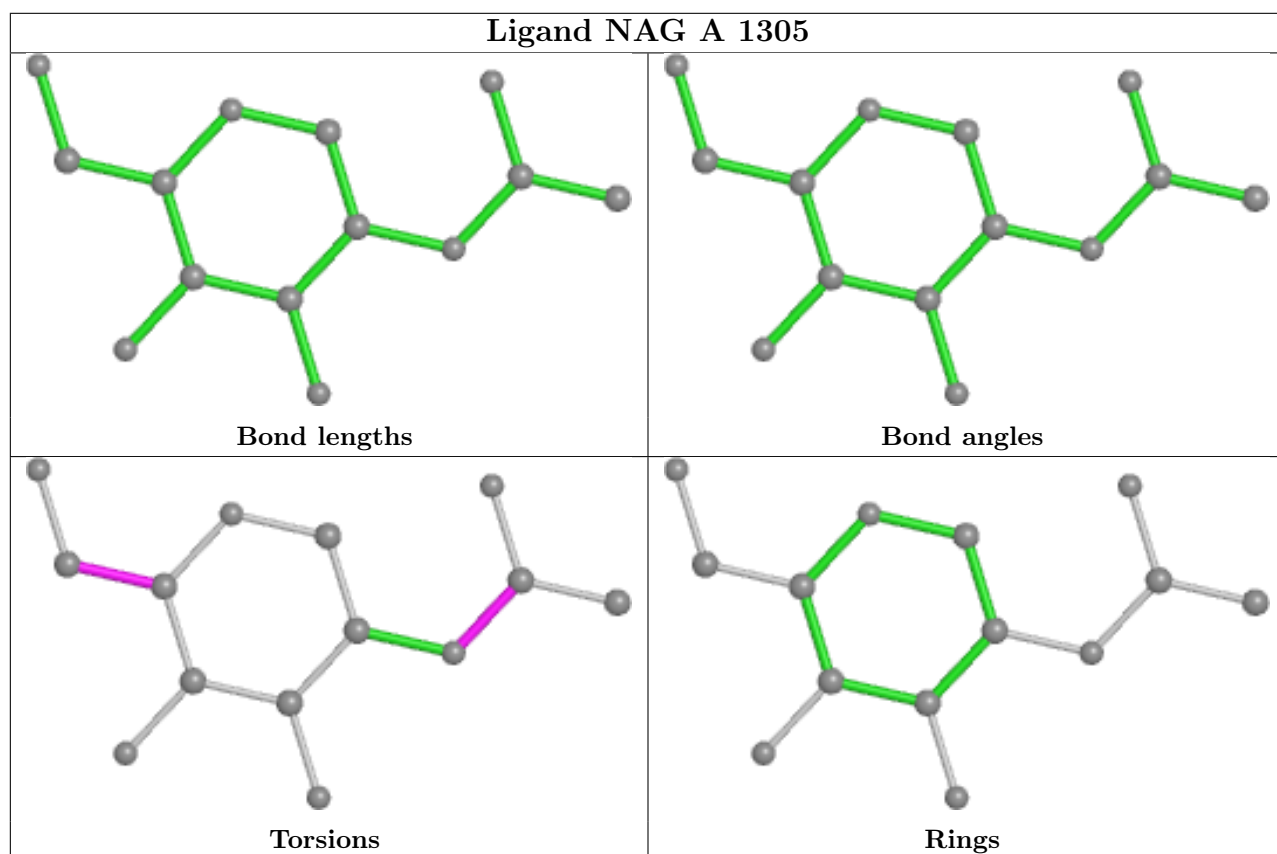
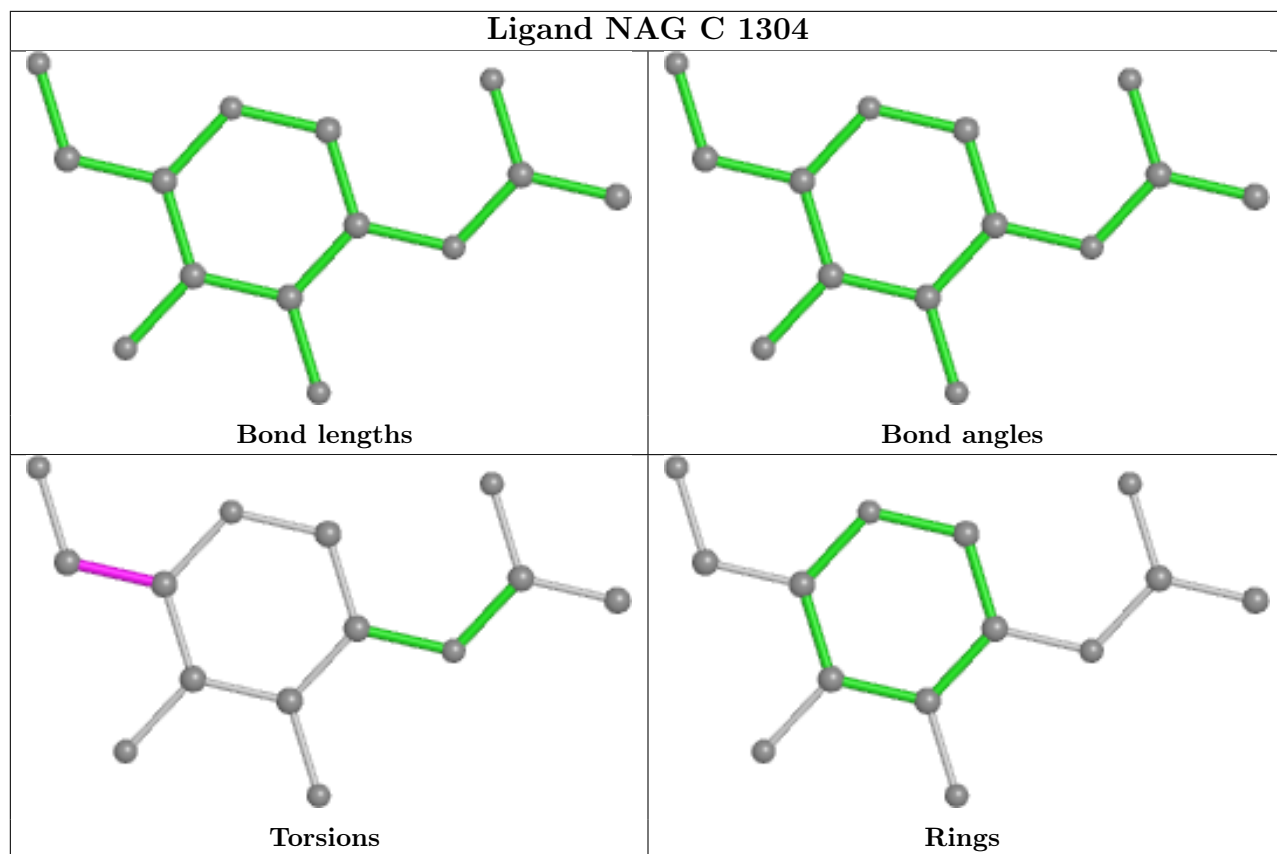


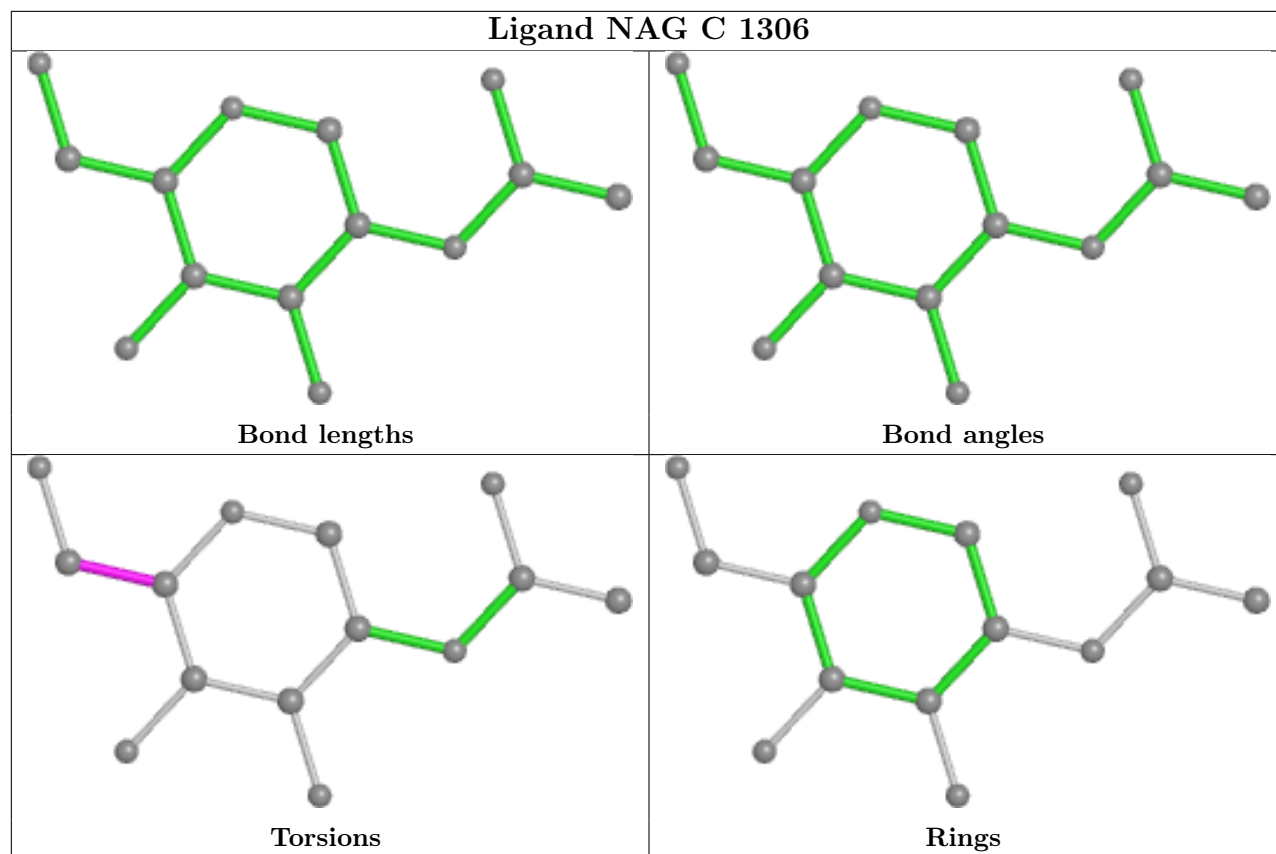












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

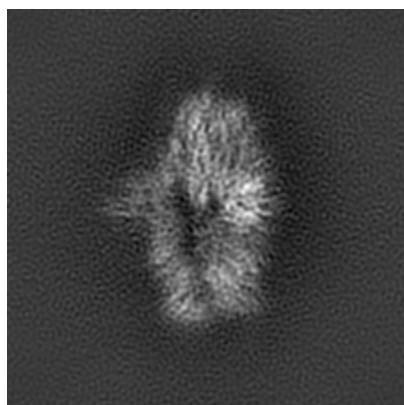
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32832. These allow visual inspection of the internal detail of the map and identification of artifacts.

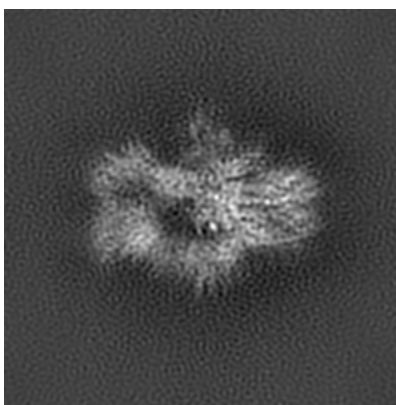
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

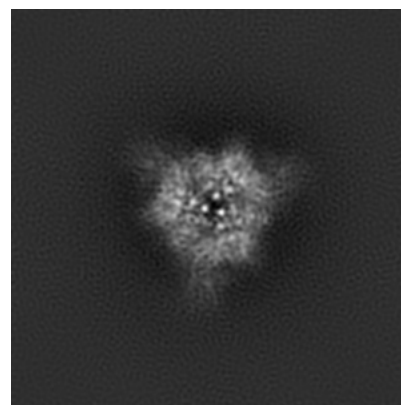
6.1.1 Primary map



X



Y

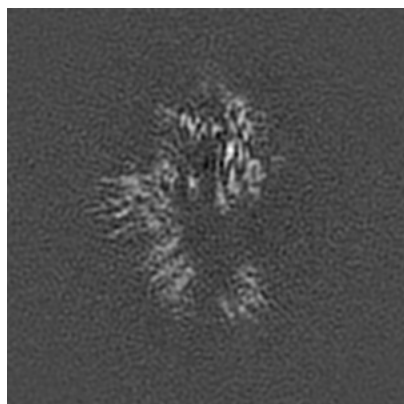


Z

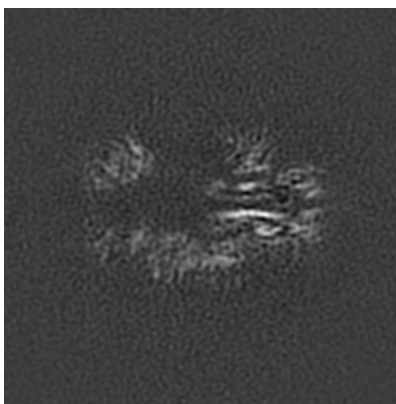
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

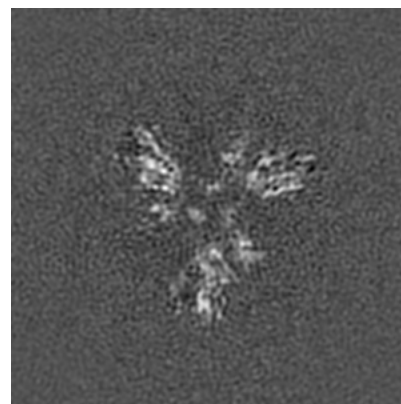
6.2.1 Primary map



X Index: 190



Y Index: 190

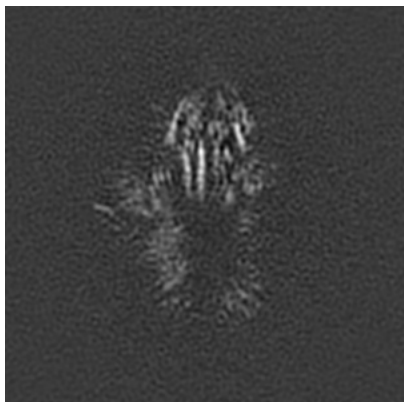


Z Index: 190

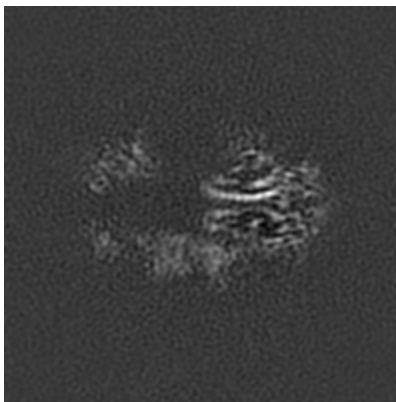
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

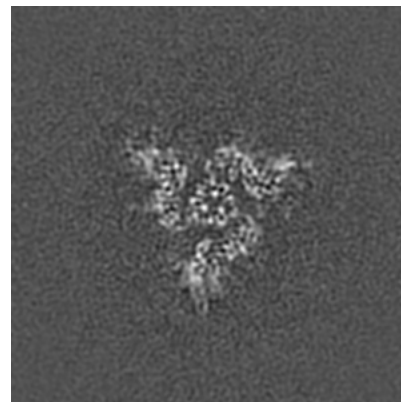
6.3.1 Primary map



X Index: 198



Y Index: 186



Z Index: 211

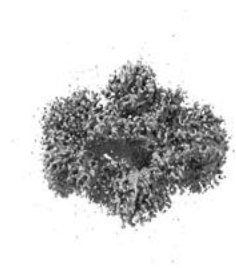
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

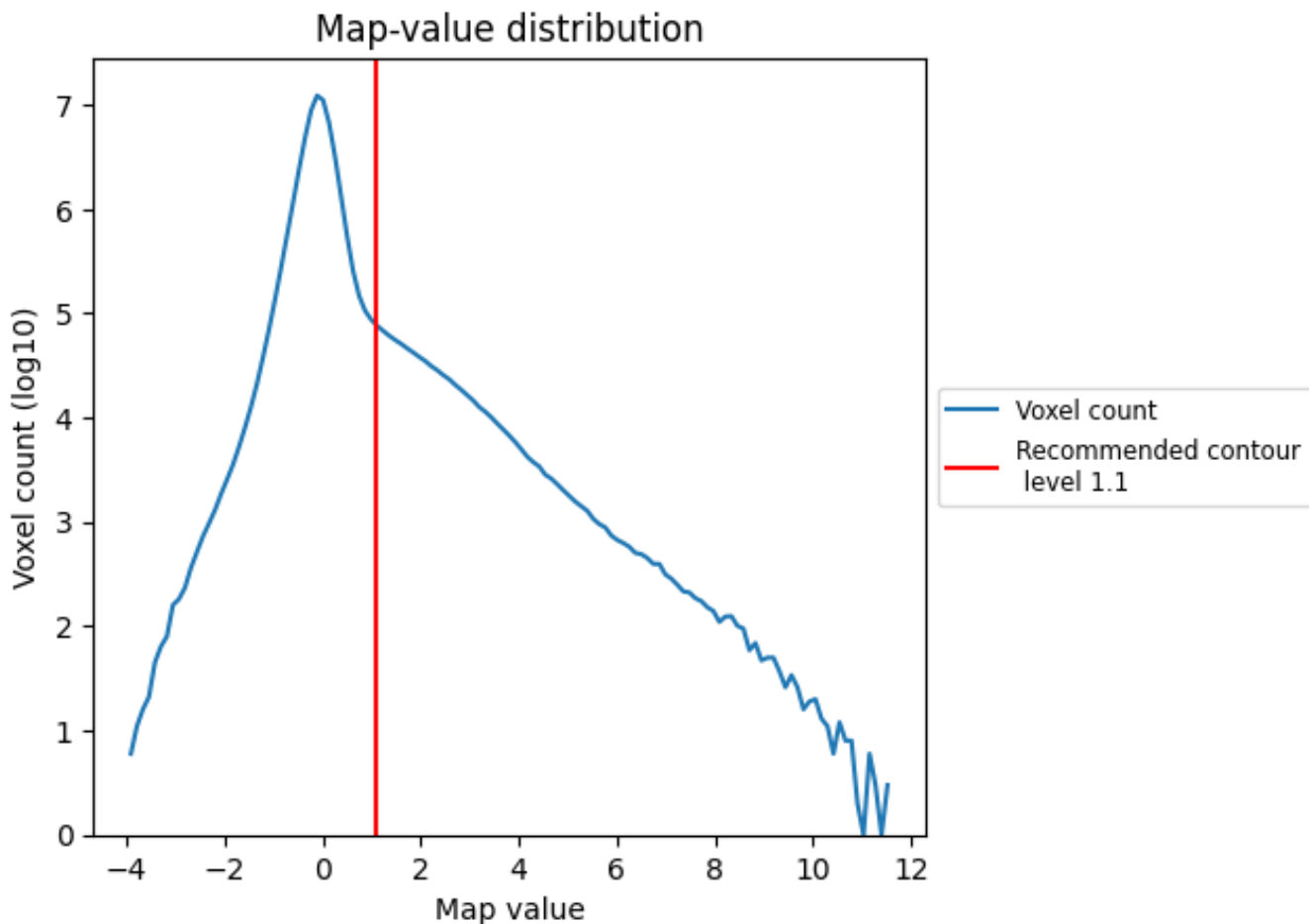
6.5 Mask visualisation

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

7 Map analysis [i](#)

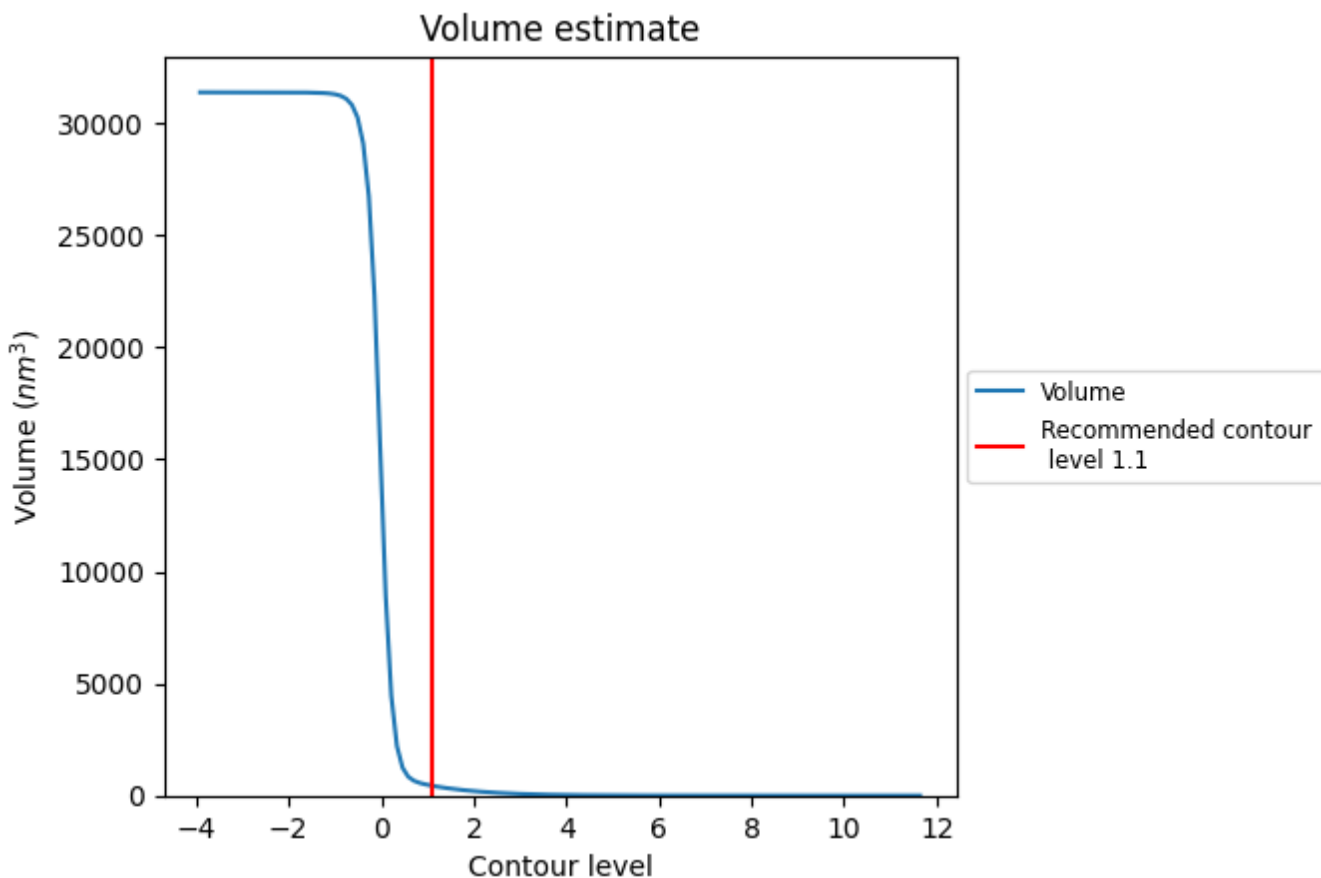
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

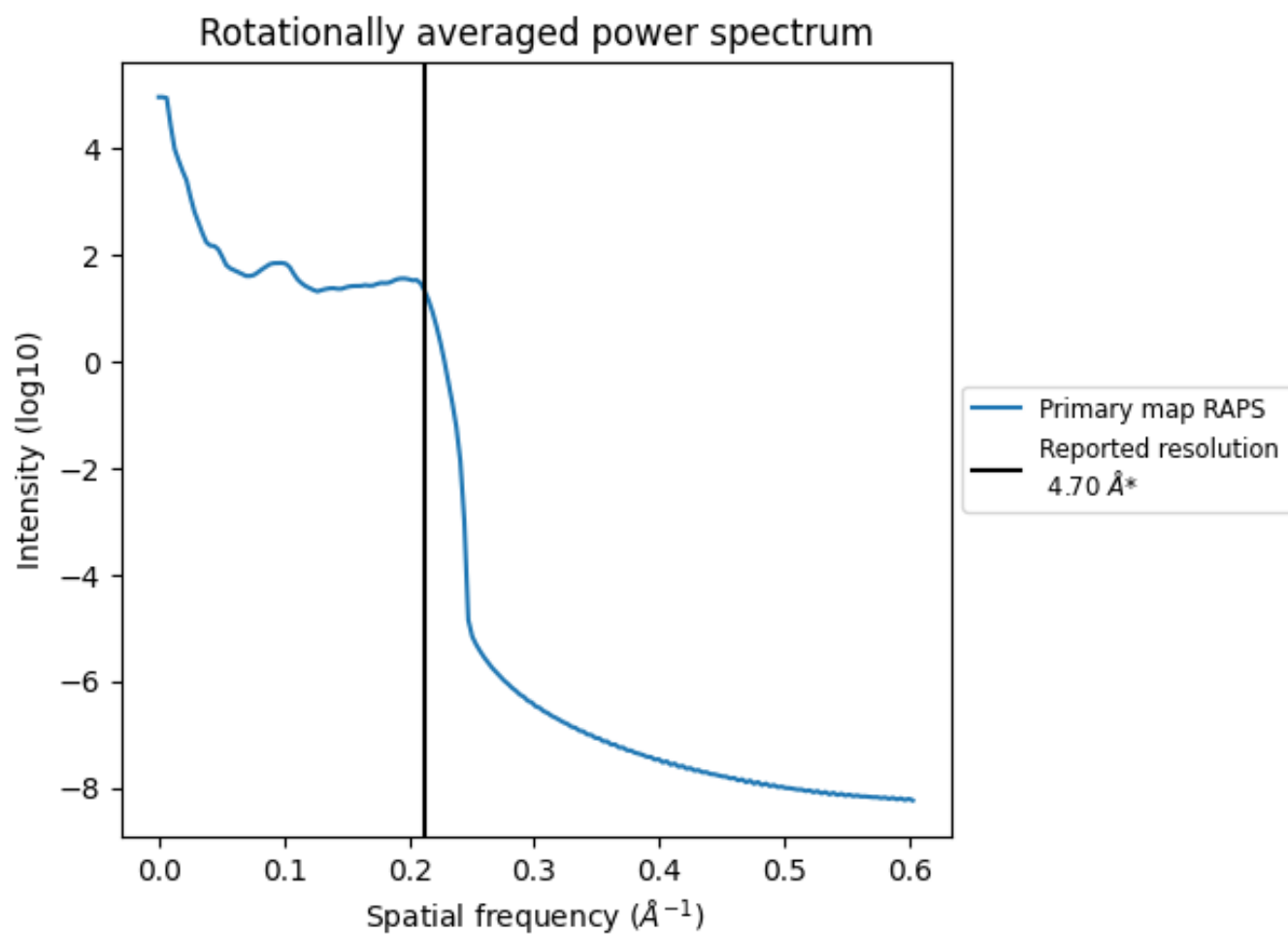
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 438 nm³; this corresponds to an approximate mass of 395 kDa.

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

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

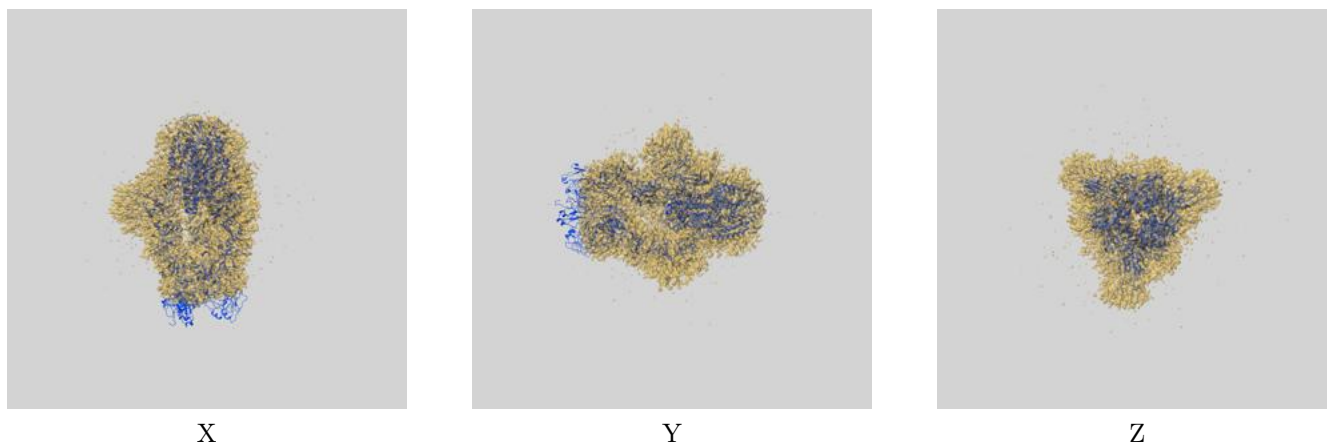
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

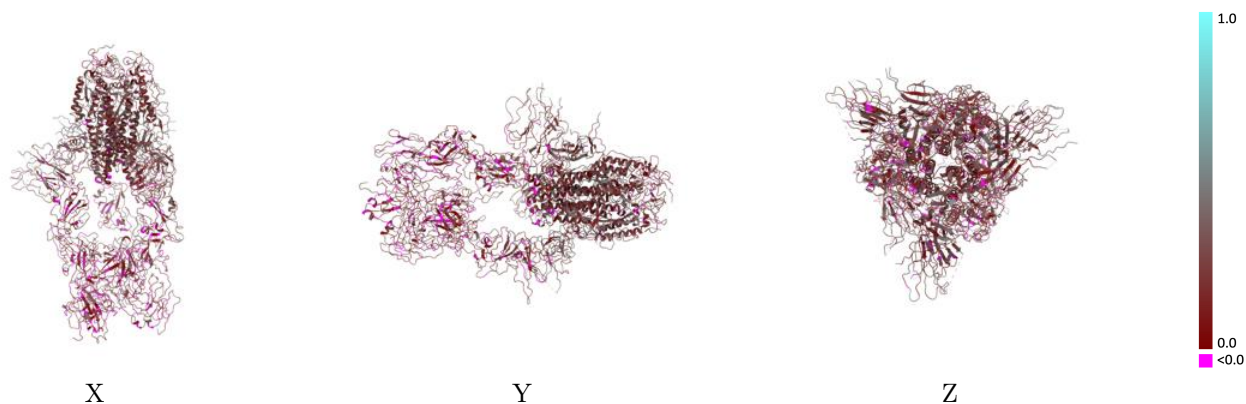
This section contains information regarding the fit between EMDB map EMD-32832 and PDB model 7WUH. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



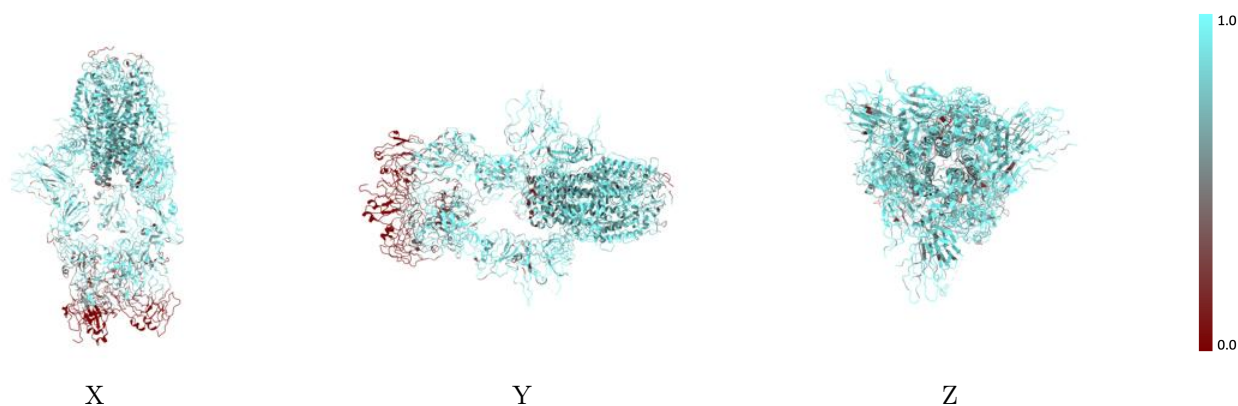
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



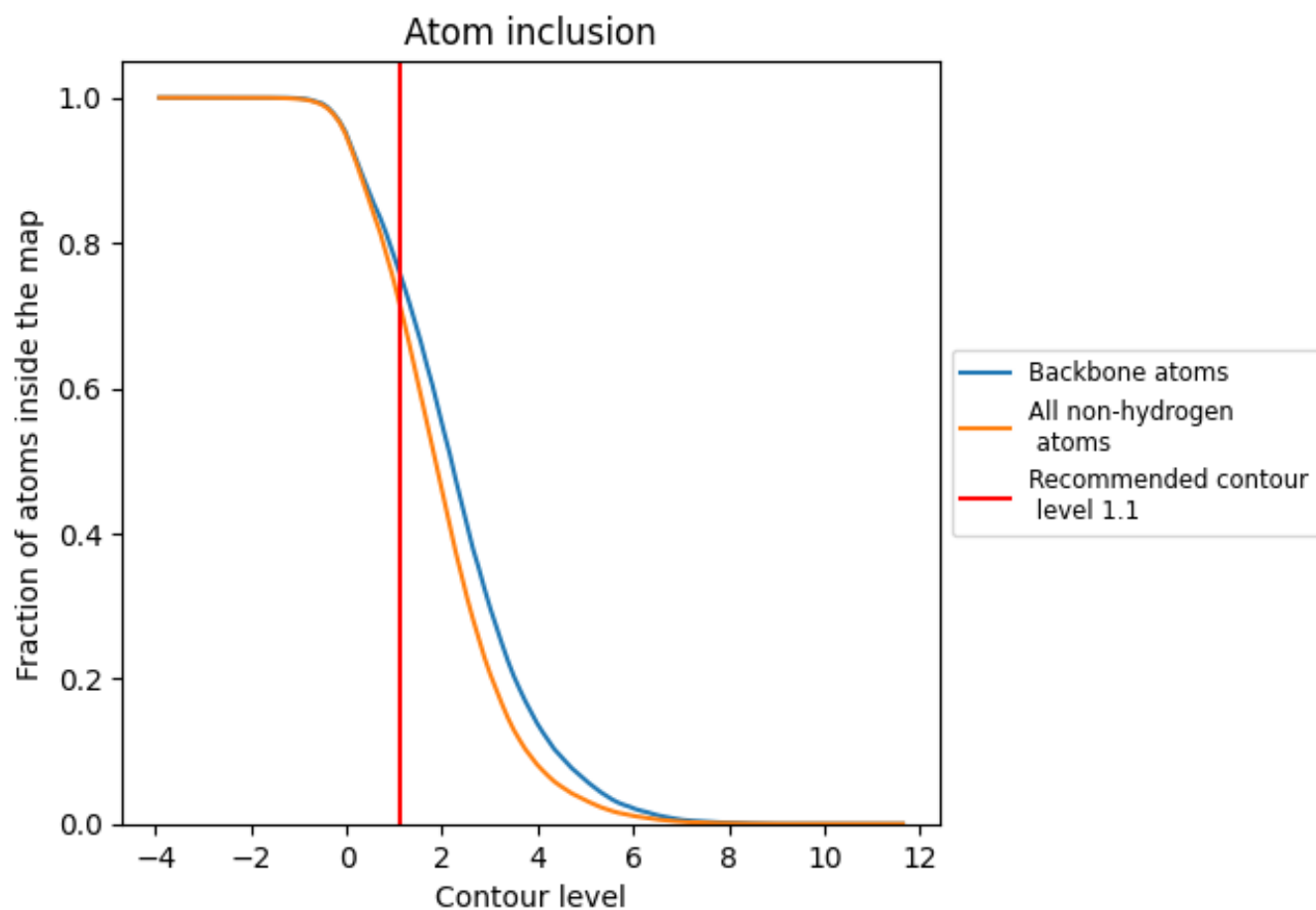
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7194	 0.2450
A	 0.8206	 0.2660
B	 0.7895	 0.3650
C	 0.8186	 0.2670
D	 0.4648	 0.1830
E	 0.8105	 0.2630
F	 0.4722	 0.1970
G	 0.5357	 0.3740
H	 0.4747	 0.1840
I	 0.4693	 0.1820
J	 0.8400	 0.3700
K	 0.5012	 0.1850
L	 0.4436	 0.1560
M	 0.9487	 0.3480
N	 0.9286	 0.4250
O	 0.8929	 0.3810
P	 0.9643	 0.4010
Q	 0.7949	 0.2830
R	 0.7500	 0.4520
S	 0.9016	 0.4280
T	 1.0000	 0.4440
U	 0.8852	 0.4100
V	 0.7143	 0.3780
W	 0.7377	 0.4040
X	 0.7500	 0.3580
Y	 0.8600	 0.3810
Z	 0.7949	 0.4160
a	 0.8367	 0.4420
b	 0.7368	 0.3940
c	 0.7500	 0.3630
d	 0.9467	 0.4620
e	 0.9487	 0.4430
f	 0.7500	 0.4300
g	 0.8367	 0.3510

