



Full wwPDB EM Validation Report ⓘ

Jul 8, 2024 – 02:49 PM JST

PDB ID : 8WLZ
EMDB ID : EMD-37636
Title : Cryo-EM structure of the WIV1 S-hACE2 complex
Authors : Wang, X.; Qiao, S.
Deposited on : 2023-10-01
Resolution : 4.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

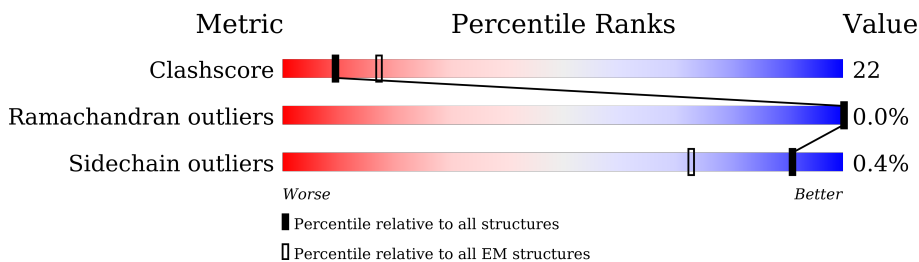
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.45 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	1271	 42% 41% 16%
1	B	1271	 45% 38% 16%
1	C	1271	 47% 37% 16%
2	D	603	 23% 66% 33% 16%
2	G	603	 17% 63% 36% 16%
3	E	2	 100%
3	F	2	 100%
3	H	2	 50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	2	 100%
3	J	2	 100%
3	K	2	 50% 50%
3	L	2	 50% 50%
3	O	2	 50% 50%
3	P	2	 50% 50%
3	Q	2	 50% 50%
3	R	2	 100%
3	T	2	 50% 50%
3	U	2	 100%
4	M	3	 100%
4	N	3	 100%
4	S	3	 67% 33%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 35498 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1068	8332	5317	1387	1587	41	0	0
1	B	1067	8319	5309	1383	1586	41	0	0
1	C	1068	8332	5317	1387	1587	41	0	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	969	PRO	LYS	conflict	UNP U5WI05
A	970	PRO	VAL	conflict	UNP U5WI05
A	1192	GLY	-	linker	UNP U5WI05
A	1193	SER	-	linker	UNP U5WI05
A	1220	LEU	-	expression tag	UNP A0A346FJN8
A	1221	GLY	-	expression tag	UNP A0A346FJN8
A	1222	ARG	-	expression tag	UNP A0A346FJN8
A	1223	SER	-	expression tag	UNP A0A346FJN8
A	1224	LEU	-	expression tag	UNP A0A346FJN8
A	1225	GLU	-	expression tag	UNP A0A346FJN8
A	1226	VAL	-	expression tag	UNP A0A346FJN8
A	1227	LEU	-	expression tag	UNP A0A346FJN8
A	1228	PHE	-	expression tag	UNP A0A346FJN8
A	1229	GLN	-	expression tag	UNP A0A346FJN8
A	1230	GLY	-	expression tag	UNP A0A346FJN8
A	1231	PRO	-	expression tag	UNP A0A346FJN8
A	1232	GLY	-	expression tag	UNP A0A346FJN8
A	1233	HIS	-	expression tag	UNP A0A346FJN8
A	1234	HIS	-	expression tag	UNP A0A346FJN8
A	1235	HIS	-	expression tag	UNP A0A346FJN8
A	1236	HIS	-	expression tag	UNP A0A346FJN8
A	1237	HIS	-	expression tag	UNP A0A346FJN8
A	1238	HIS	-	expression tag	UNP A0A346FJN8
A	1239	HIS	-	expression tag	UNP A0A346FJN8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	HIS	-	expression tag	UNP A0A346FJN8
A	1241	SER	-	expression tag	UNP A0A346FJN8
A	1242	ALA	-	expression tag	UNP A0A346FJN8
A	1243	TRP	-	expression tag	UNP A0A346FJN8
A	1244	SER	-	expression tag	UNP A0A346FJN8
A	1245	HIS	-	expression tag	UNP A0A346FJN8
A	1246	PRO	-	expression tag	UNP A0A346FJN8
A	1247	GLN	-	expression tag	UNP A0A346FJN8
A	1248	PHE	-	expression tag	UNP A0A346FJN8
A	1249	GLU	-	expression tag	UNP A0A346FJN8
A	1250	LYS	-	expression tag	UNP A0A346FJN8
A	1251	GLY	-	expression tag	UNP A0A346FJN8
A	1252	GLY	-	expression tag	UNP A0A346FJN8
A	1253	GLY	-	expression tag	UNP A0A346FJN8
A	1254	SER	-	expression tag	UNP A0A346FJN8
A	1255	GLY	-	expression tag	UNP A0A346FJN8
A	1256	GLY	-	expression tag	UNP A0A346FJN8
A	1257	GLY	-	expression tag	UNP A0A346FJN8
A	1258	GLY	-	expression tag	UNP A0A346FJN8
A	1259	SER	-	expression tag	UNP A0A346FJN8
A	1260	GLY	-	expression tag	UNP A0A346FJN8
A	1261	GLY	-	expression tag	UNP A0A346FJN8
A	1262	SER	-	expression tag	UNP A0A346FJN8
A	1263	ALA	-	expression tag	UNP A0A346FJN8
A	1264	TRP	-	expression tag	UNP A0A346FJN8
A	1265	SER	-	expression tag	UNP A0A346FJN8
A	1266	HIS	-	expression tag	UNP A0A346FJN8
A	1267	PRO	-	expression tag	UNP A0A346FJN8
A	1268	GLN	-	expression tag	UNP A0A346FJN8
A	1269	PHE	-	expression tag	UNP A0A346FJN8
A	1270	GLU	-	expression tag	UNP A0A346FJN8
A	1271	LYS	-	expression tag	UNP A0A346FJN8
B	969	PRO	LYS	conflict	UNP U5WI05
B	970	PRO	VAL	conflict	UNP U5WI05
B	1192	GLY	-	linker	UNP U5WI05
B	1193	SER	-	linker	UNP U5WI05
B	1220	LEU	-	expression tag	UNP A0A346FJN8
B	1221	GLY	-	expression tag	UNP A0A346FJN8
B	1222	ARG	-	expression tag	UNP A0A346FJN8
B	1223	SER	-	expression tag	UNP A0A346FJN8
B	1224	LEU	-	expression tag	UNP A0A346FJN8
B	1225	GLU	-	expression tag	UNP A0A346FJN8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1226	VAL	-	expression tag	UNP A0A346FJN8
B	1227	LEU	-	expression tag	UNP A0A346FJN8
B	1228	PHE	-	expression tag	UNP A0A346FJN8
B	1229	GLN	-	expression tag	UNP A0A346FJN8
B	1230	GLY	-	expression tag	UNP A0A346FJN8
B	1231	PRO	-	expression tag	UNP A0A346FJN8
B	1232	GLY	-	expression tag	UNP A0A346FJN8
B	1233	HIS	-	expression tag	UNP A0A346FJN8
B	1234	HIS	-	expression tag	UNP A0A346FJN8
B	1235	HIS	-	expression tag	UNP A0A346FJN8
B	1236	HIS	-	expression tag	UNP A0A346FJN8
B	1237	HIS	-	expression tag	UNP A0A346FJN8
B	1238	HIS	-	expression tag	UNP A0A346FJN8
B	1239	HIS	-	expression tag	UNP A0A346FJN8
B	1240	HIS	-	expression tag	UNP A0A346FJN8
B	1241	SER	-	expression tag	UNP A0A346FJN8
B	1242	ALA	-	expression tag	UNP A0A346FJN8
B	1243	TRP	-	expression tag	UNP A0A346FJN8
B	1244	SER	-	expression tag	UNP A0A346FJN8
B	1245	HIS	-	expression tag	UNP A0A346FJN8
B	1246	PRO	-	expression tag	UNP A0A346FJN8
B	1247	GLN	-	expression tag	UNP A0A346FJN8
B	1248	PHE	-	expression tag	UNP A0A346FJN8
B	1249	GLU	-	expression tag	UNP A0A346FJN8
B	1250	LYS	-	expression tag	UNP A0A346FJN8
B	1251	GLY	-	expression tag	UNP A0A346FJN8
B	1252	GLY	-	expression tag	UNP A0A346FJN8
B	1253	GLY	-	expression tag	UNP A0A346FJN8
B	1254	SER	-	expression tag	UNP A0A346FJN8
B	1255	GLY	-	expression tag	UNP A0A346FJN8
B	1256	GLY	-	expression tag	UNP A0A346FJN8
B	1257	GLY	-	expression tag	UNP A0A346FJN8
B	1258	GLY	-	expression tag	UNP A0A346FJN8
B	1259	SER	-	expression tag	UNP A0A346FJN8
B	1260	GLY	-	expression tag	UNP A0A346FJN8
B	1261	GLY	-	expression tag	UNP A0A346FJN8
B	1262	SER	-	expression tag	UNP A0A346FJN8
B	1263	ALA	-	expression tag	UNP A0A346FJN8
B	1264	TRP	-	expression tag	UNP A0A346FJN8
B	1265	SER	-	expression tag	UNP A0A346FJN8
B	1266	HIS	-	expression tag	UNP A0A346FJN8
B	1267	PRO	-	expression tag	UNP A0A346FJN8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1268	GLN	-	expression tag	UNP A0A346FJN8
B	1269	PHE	-	expression tag	UNP A0A346FJN8
B	1270	GLU	-	expression tag	UNP A0A346FJN8
B	1271	LYS	-	expression tag	UNP A0A346FJN8
C	969	PRO	LYS	conflict	UNP U5WI05
C	970	PRO	VAL	conflict	UNP U5WI05
C	1192	GLY	-	linker	UNP U5WI05
C	1193	SER	-	linker	UNP U5WI05
C	1220	LEU	-	expression tag	UNP A0A346FJN8
C	1221	GLY	-	expression tag	UNP A0A346FJN8
C	1222	ARG	-	expression tag	UNP A0A346FJN8
C	1223	SER	-	expression tag	UNP A0A346FJN8
C	1224	LEU	-	expression tag	UNP A0A346FJN8
C	1225	GLU	-	expression tag	UNP A0A346FJN8
C	1226	VAL	-	expression tag	UNP A0A346FJN8
C	1227	LEU	-	expression tag	UNP A0A346FJN8
C	1228	PHE	-	expression tag	UNP A0A346FJN8
C	1229	GLN	-	expression tag	UNP A0A346FJN8
C	1230	GLY	-	expression tag	UNP A0A346FJN8
C	1231	PRO	-	expression tag	UNP A0A346FJN8
C	1232	GLY	-	expression tag	UNP A0A346FJN8
C	1233	HIS	-	expression tag	UNP A0A346FJN8
C	1234	HIS	-	expression tag	UNP A0A346FJN8
C	1235	HIS	-	expression tag	UNP A0A346FJN8
C	1236	HIS	-	expression tag	UNP A0A346FJN8
C	1237	HIS	-	expression tag	UNP A0A346FJN8
C	1238	HIS	-	expression tag	UNP A0A346FJN8
C	1239	HIS	-	expression tag	UNP A0A346FJN8
C	1240	HIS	-	expression tag	UNP A0A346FJN8
C	1241	SER	-	expression tag	UNP A0A346FJN8
C	1242	ALA	-	expression tag	UNP A0A346FJN8
C	1243	TRP	-	expression tag	UNP A0A346FJN8
C	1244	SER	-	expression tag	UNP A0A346FJN8
C	1245	HIS	-	expression tag	UNP A0A346FJN8
C	1246	PRO	-	expression tag	UNP A0A346FJN8
C	1247	GLN	-	expression tag	UNP A0A346FJN8
C	1248	PHE	-	expression tag	UNP A0A346FJN8
C	1249	GLU	-	expression tag	UNP A0A346FJN8
C	1250	LYS	-	expression tag	UNP A0A346FJN8
C	1251	GLY	-	expression tag	UNP A0A346FJN8
C	1252	GLY	-	expression tag	UNP A0A346FJN8
C	1253	GLY	-	expression tag	UNP A0A346FJN8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1254	SER	-	expression tag	UNP A0A346FJN8
C	1255	GLY	-	expression tag	UNP A0A346FJN8
C	1256	GLY	-	expression tag	UNP A0A346FJN8
C	1257	GLY	-	expression tag	UNP A0A346FJN8
C	1258	GLY	-	expression tag	UNP A0A346FJN8
C	1259	SER	-	expression tag	UNP A0A346FJN8
C	1260	GLY	-	expression tag	UNP A0A346FJN8
C	1261	GLY	-	expression tag	UNP A0A346FJN8
C	1262	SER	-	expression tag	UNP A0A346FJN8
C	1263	ALA	-	expression tag	UNP A0A346FJN8
C	1264	TRP	-	expression tag	UNP A0A346FJN8
C	1265	SER	-	expression tag	UNP A0A346FJN8
C	1266	HIS	-	expression tag	UNP A0A346FJN8
C	1267	PRO	-	expression tag	UNP A0A346FJN8
C	1268	GLN	-	expression tag	UNP A0A346FJN8
C	1269	PHE	-	expression tag	UNP A0A346FJN8
C	1270	GLU	-	expression tag	UNP A0A346FJN8
C	1271	LYS	-	expression tag	UNP A0A346FJN8

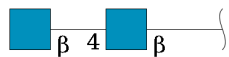
- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	597	4870	3115	806	920	29	0	0
2	G	597	4870	3115	806	920	29	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1
G	616	HIS	-	expression tag	UNP Q9BYF1
G	617	HIS	-	expression tag	UNP Q9BYF1
G	618	HIS	-	expression tag	UNP Q9BYF1
G	619	HIS	-	expression tag	UNP Q9BYF1
G	620	HIS	-	expression tag	UNP Q9BYF1
G	621	HIS	-	expression tag	UNP Q9BYF1

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



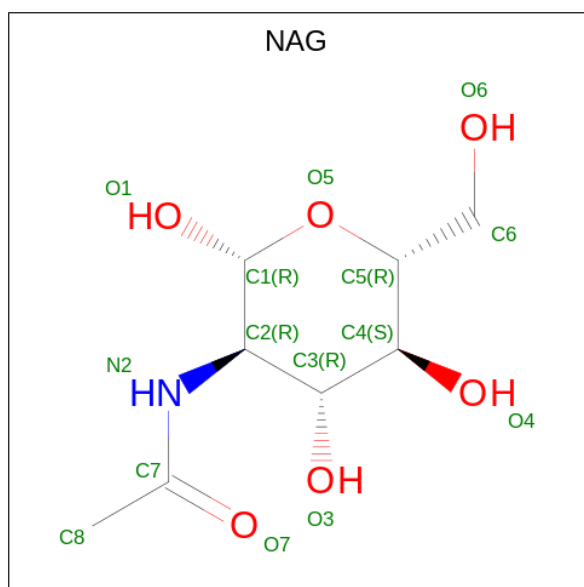
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	2	28	16	2	10	0	0
3	F	2	28	16	2	10	0	0
3	H	2	28	16	2	10	0	0
3	I	2	28	16	2	10	0	0
3	J	2	28	16	2	10	0	0
3	K	2	28	16	2	10	0	0
3	L	2	28	16	2	10	0	0
3	O	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0
3	Q	2	28	16	2	10	0	0
3	R	2	28	16	2	10	0	0
3	T	2	28	16	2	10	0	0
3	U	2	28	16	2	10	0	0

- Molecule 4 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
4	M	3	Total	C	N	O	0	0
			39	22	2	15		
4	N	3	Total	C	N	O	0	0
			39	22	2	15		
4	S	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

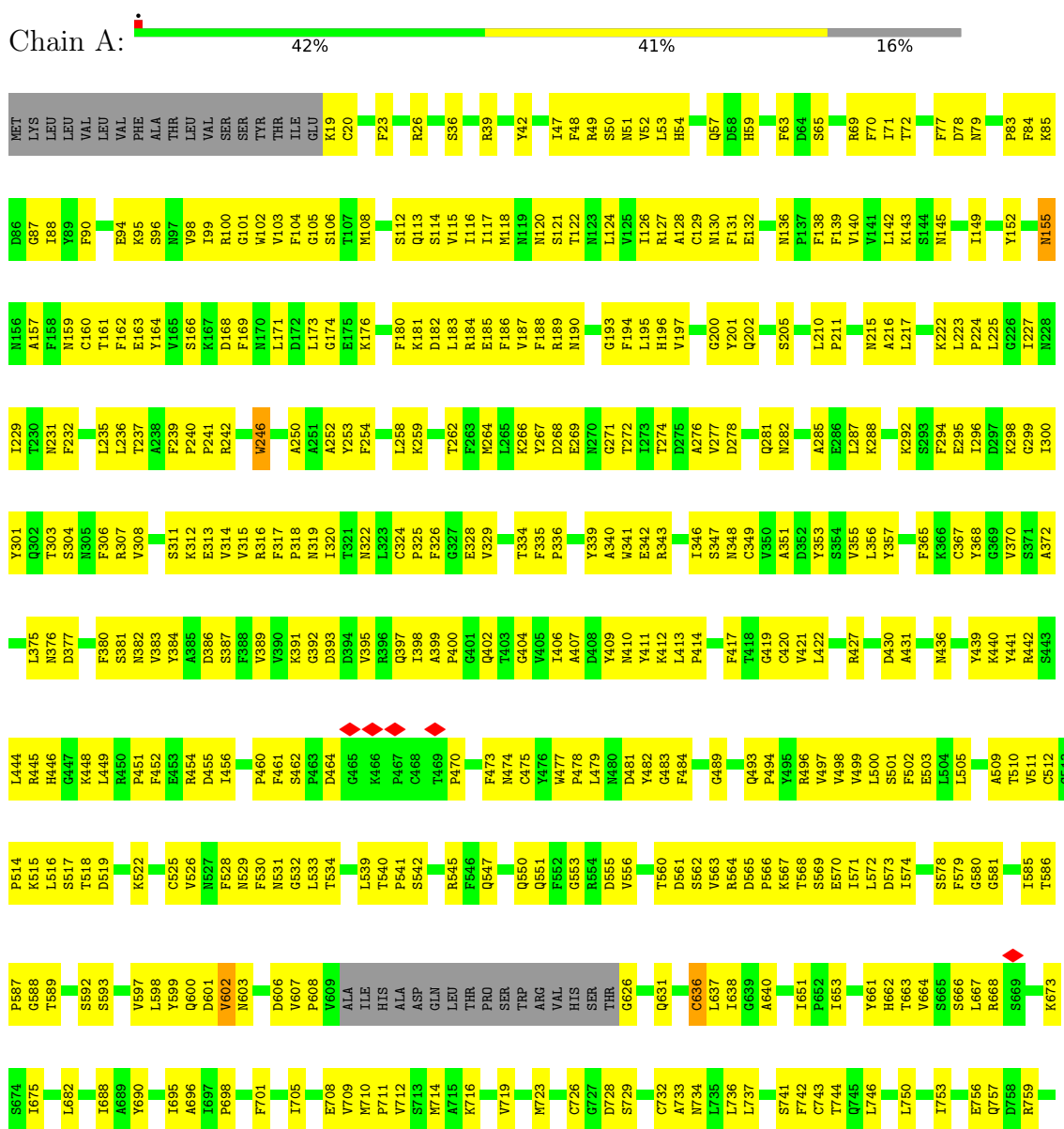
Continued from previous page...

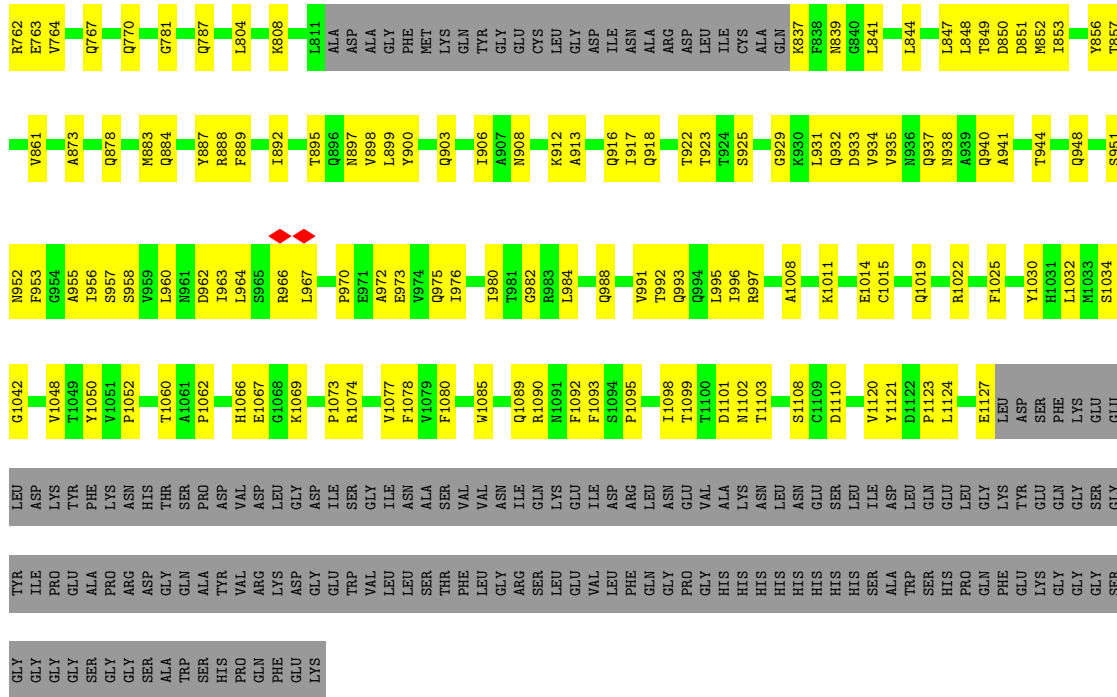
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	Total 14	8	1	5	0
5	B	1	Total 14	8	1	5	0
5	B	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1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

3 Residue-property plots

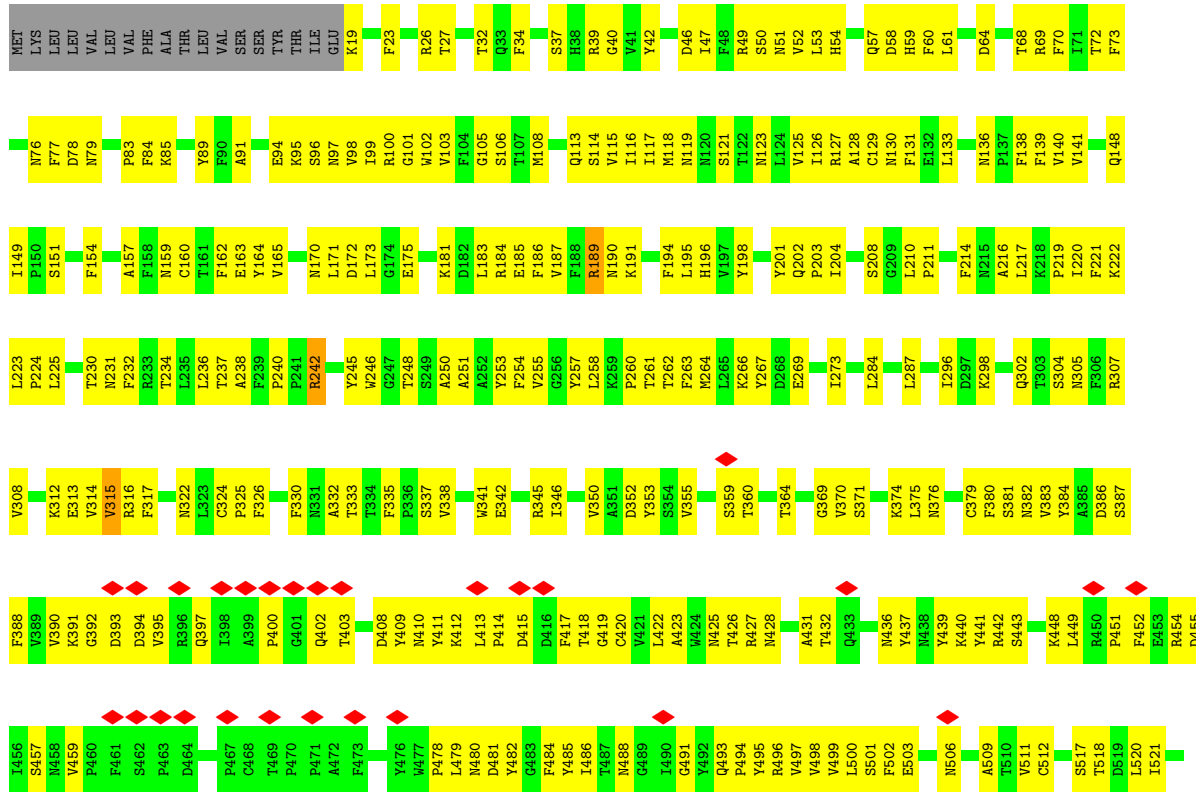
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

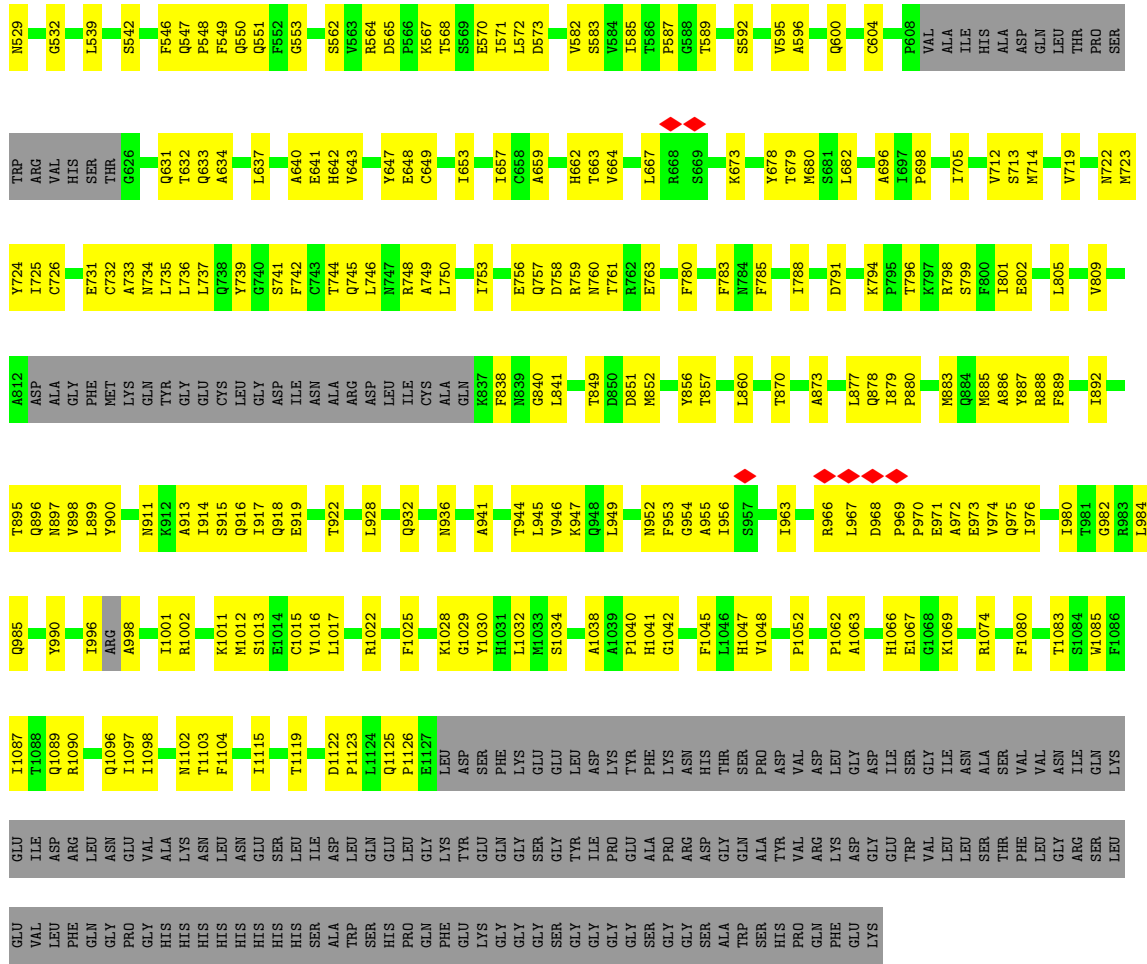
• Molecule 1: Spike glycoprotein,Fibrin



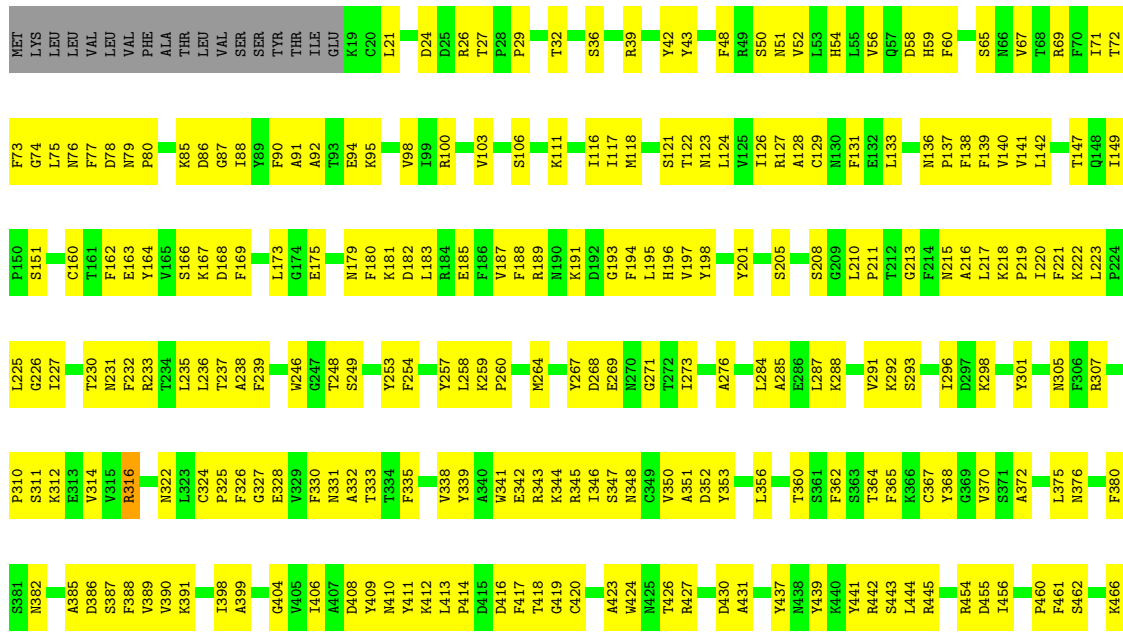


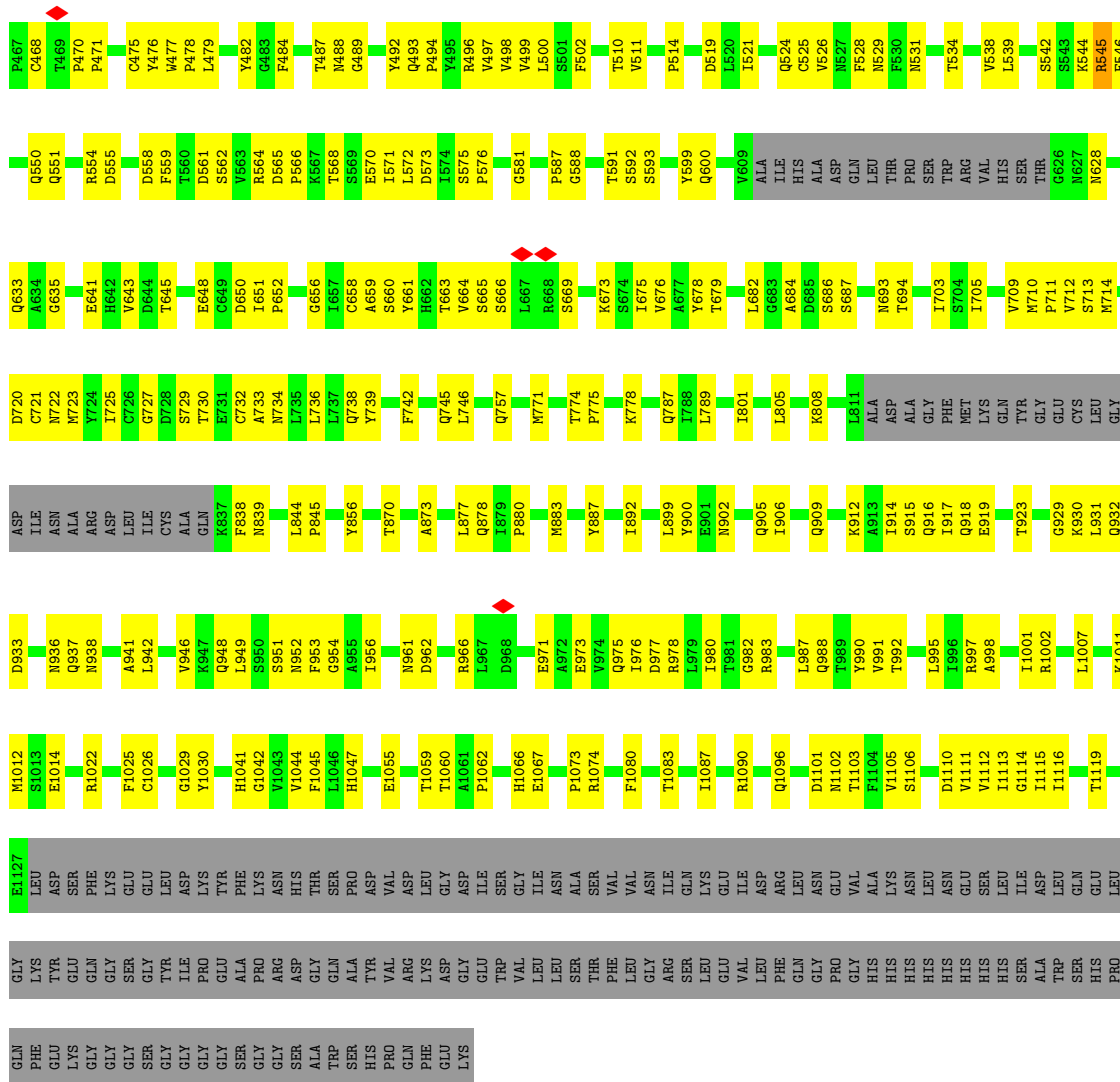
● Molecule 1: Spike glycoprotein, Fibrin



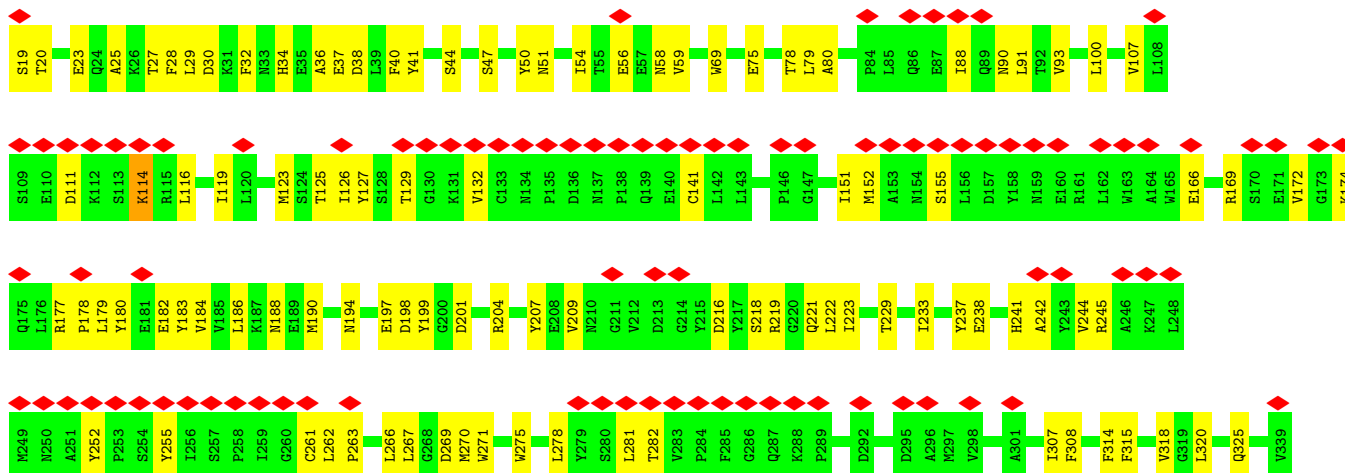


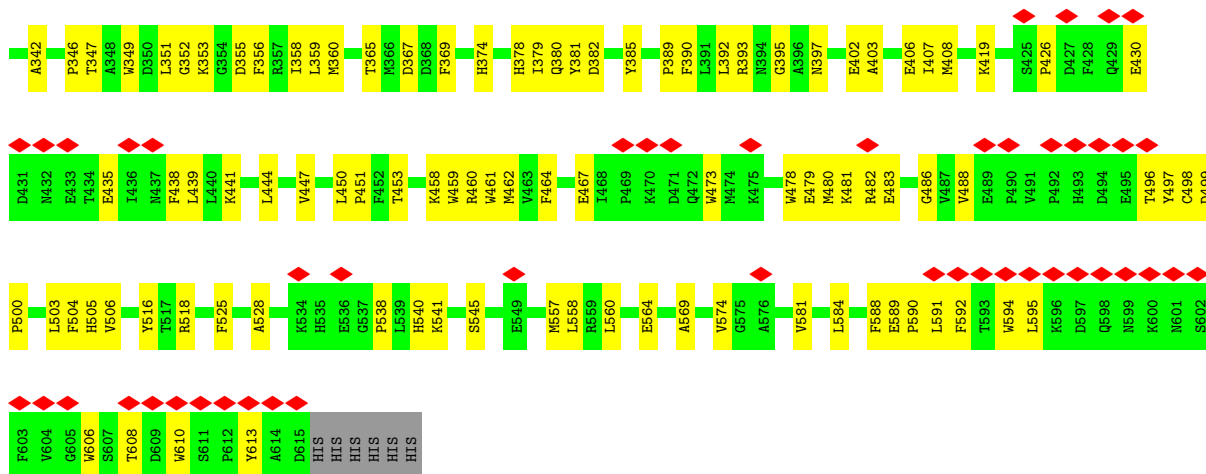
• Molecule 1: Spike glycoprotein, Fibrin



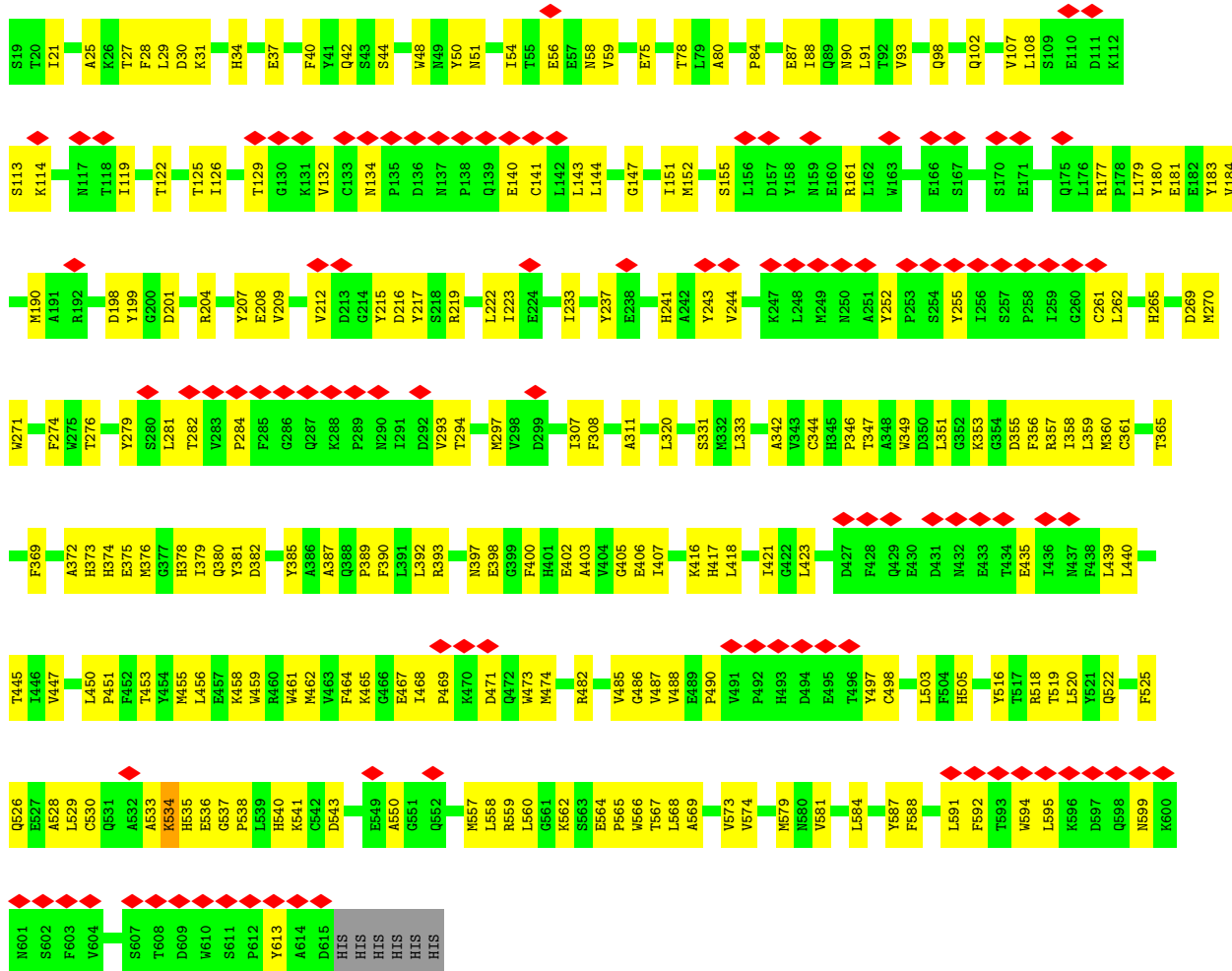


• Molecule 2: Processed angiotensin-converting enzyme 2





• Molecule 2: Processed angiotensin-converting enzyme 2



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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

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

Chain H:  50% 50%


MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

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

Chain L:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  50% 50%



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

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain T:  50% 50%



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

Chain U:  100%



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

Chain M:  100%

MAG1
MAG2
BMA3

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

Chain N:  100%

MAG1
MAG2
BMA3

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

Chain S:  67% 33%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.957	Depositor
Minimum map value	-0.509	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.0601	Depositor
Map size (\AA)	446.2, 446.2, 446.2	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.97, 0.97, 0.97	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/8534	0.56	1/11621 (0.0%)
1	B	0.35	0/8520	0.54	0/11601
1	C	0.35	0/8534	0.55	0/11621
2	D	0.27	0/5007	0.49	0/6803
2	G	0.25	0/5007	0.47	0/6803
All	All	0.33	0/35602	0.53	1/48449 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	CYS	CA-CB-SG	6.15	125.07	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	602	VAL	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	8332	0	8098	471	0
1	B	8319	0	8076	439	0
1	C	8332	0	8091	396	0
2	D	4870	0	4643	158	0
2	G	4870	0	4643	162	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	0	0
3	J	28	0	25	2	0
3	K	28	0	25	0	0
3	L	28	0	25	1	0
3	O	28	0	25	1	0
3	P	28	0	25	1	0
3	Q	28	0	25	1	0
3	R	28	0	25	0	0
3	T	28	0	25	1	0
3	U	28	0	25	0	0
4	M	39	0	34	0	0
4	N	39	0	34	0	0
4	S	39	0	34	1	0
5	A	56	0	52	0	0
5	B	98	0	91	2	0
5	C	140	0	130	4	0
All	All	35498	0	34251	1568	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 22.

All (1568) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HB3	1:B:202:GLN:O	1.65	0.96
1:A:128:ALA:HB3	1:A:162:PHE:HB3	1.51	0.93
1:B:103:VAL:HG22	1:B:116:ILE:HG12	1.53	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:ILE:H	1:A:975:GLN:HE22	1.21	0.88
1:B:189:ARG:NH1	1:B:190:ASN:O	2.07	0.87
1:C:427:ARG:HA	1:C:494:PRO:HG2	1.56	0.87
1:A:59:HIS:HB3	1:A:258:LEU:HB3	1.55	0.87
1:B:662:HIS:O	1:B:673:LYS:HA	1.74	0.86
1:B:799:SER:HB2	1:B:802:GLU:HG3	1.58	0.85
1:A:298:LYS:HG2	1:A:651:ILE:HD11	1.57	0.84
1:A:741:SER:O	1:A:744:THR:OG1	1.95	0.84
2:D:346:PRO:HA	2:D:359:LEU:O	1.76	0.84
1:B:73:PHE:H	1:B:76:ASN:HB3	1.40	0.83
1:A:343:ARG:HB2	1:A:384:TYR:HB3	1.61	0.82
1:A:39:ARG:HE	1:A:210:LEU:HD21	1.44	0.82
1:C:932:GLN:OE1	1:C:936:ASN:ND2	2.14	0.81
1:A:585:ILE:HD11	1:A:653:ILE:HD11	1.60	0.81
1:A:346:ILE:HB	1:A:383:VAL:HG13	1.63	0.80
1:A:960:LEU:HD11	1:A:976:ILE:HG12	1.63	0.80
1:B:562:SER:HA	1:B:572:LEU:O	1.81	0.80
1:B:996:ILE:O	1:B:998:ALA:N	2.15	0.80
1:C:380:PHE:HB2	1:C:511:VAL:HB	1.64	0.80
1:A:522:LYS:HD2	1:A:541:PRO:HD3	1.62	0.80
1:C:87:GLY:HA2	1:C:188:PHE:O	1.83	0.79
1:C:545:ARG:NH1	1:C:546:PHE:O	2.14	0.79
1:A:100:ARG:HH21	1:A:237:THR:HG21	1.48	0.79
1:B:121:SER:O	1:B:170:ASN:ND2	2.16	0.79
1:B:953:PHE:HD2	1:B:982:GLY:HA3	1.48	0.79
1:A:298:LYS:HG3	1:A:587:PRO:HA	1.65	0.79
1:B:77:PHE:HE2	1:B:136:ASN:HD21	1.25	0.79
1:A:278:ASP:HB2	1:A:281:GLN:HB2	1.65	0.79
1:A:662:HIS:O	1:A:673:LYS:HA	1.84	0.78
1:B:956:ILE:HD12	1:B:966:ARG:HH11	1.50	0.77
1:A:883:MET:SD	1:A:900:TYR:OH	2.43	0.77
1:A:712:VAL:HG21	1:A:764:VAL:HG11	1.67	0.76
1:C:347:SER:HA	1:C:510:THR:HB	1.67	0.76
1:C:938:ASN:HB3	1:C:997:ARG:HH22	1.50	0.75
1:C:330:PHE:HB2	1:C:360:THR:HG21	1.68	0.75
1:A:316:ARG:HH21	1:A:517:SER:HB2	1.51	0.74
1:A:753:ILE:O	1:A:757:GLN:NE2	2.20	0.74
1:A:756:GLU:OE1	1:A:759:ARG:NH2	2.20	0.74
1:C:59:HIS:HB2	1:C:189:ARG:HH22	1.52	0.74
1:A:53:LEU:HD13	1:A:292:LYS:HG2	1.70	0.74
1:B:106:SER:HA	1:B:231:ASN:H	1.53	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PHE:H	1:A:136:ASN:HD22	1.34	0.74
1:B:1011:LYS:NZ	1:B:1025:PHE:O	2.21	0.74
1:B:194:PHE:HD1	1:B:224:PRO:HA	1.53	0.74
1:A:753:ILE:HG22	1:A:757:GLN:HE22	1.53	0.73
1:A:95:LYS:NZ	1:A:250:ALA:O	2.20	0.73
1:A:329:VAL:HG22	1:A:498:VAL:HG21	1.71	0.73
1:B:731:GLU:O	1:B:734:ASN:ND2	2.21	0.73
1:C:181:LYS:HA	1:C:205:SER:HB3	1.71	0.73
1:B:140:VAL:HG23	1:B:151:SER:HB3	1.70	0.73
1:A:631:GLN:HA	1:A:636:CYS:HB3	1.70	0.73
1:A:421:VAL:HG22	1:A:499:VAL:HG12	1.71	0.73
1:B:101:GLY:HA2	1:B:118:MET:HA	1.70	0.73
1:B:953:PHE:CD2	1:B:982:GLY:HA3	2.23	0.72
2:G:406:GLU:HG3	2:G:518:ARG:HD3	1.71	0.72
1:A:300:ILE:HG12	1:A:585:ILE:HG12	1.71	0.72
1:A:849:THR:H	1:A:852:MET:HE3	1.54	0.72
1:B:419:GLY:HA2	1:B:502:PHE:HD2	1.51	0.72
2:D:528:ALA:HB2	2:D:574:VAL:HG12	1.72	0.72
1:A:113:GLN:HB3	1:A:227:ILE:HG21	1.72	0.72
1:A:712:VAL:HG12	1:A:1042:GLY:HA2	1.72	0.72
1:C:892:ILE:HD12	1:C:1030:TYR:HB3	1.72	0.71
1:A:84:PHE:H	1:A:231:ASN:HA	1.53	0.71
1:A:550:GLN:O	1:A:564:ARG:NH2	2.18	0.71
1:B:1029:GLY:HA2	1:C:873:ALA:HB1	1.72	0.71
1:A:427:ARG:HA	1:A:494:PRO:HG2	1.70	0.71
2:G:261:CYS:HB2	2:G:488:VAL:HG13	1.70	0.71
1:A:531:ASN:ND2	1:A:566:PRO:HB3	2.05	0.71
1:A:306:PHE:HZ	1:A:608:PRO:HD2	1.56	0.71
1:A:115:VAL:HG21	1:A:225:LEU:HD13	1.73	0.71
1:A:688:ILE:HD11	1:B:878:GLN:HB3	1.70	0.71
2:D:406:GLU:HG3	2:D:518:ARG:HD3	1.71	0.71
1:B:130:ASN:OD1	1:B:159:ASN:ND2	2.15	0.70
2:G:389:PRO:HG2	2:G:392:LEU:HB2	1.73	0.70
2:D:177:ARG:HH12	2:D:473:TRP:HE3	1.40	0.70
2:G:462:MET:HB2	2:G:467:GLU:HB2	1.74	0.70
1:B:353:TYR:HB2	1:B:375:LEU:HB3	1.74	0.70
1:C:316:ARG:HH12	1:C:529:ASN:H	1.37	0.70
1:A:96:SER:HB2	1:A:98:VAL:HG23	1.72	0.70
1:B:952:ASN:ND2	1:B:955:ALA:O	2.24	0.70
1:B:885:MET:HG3	1:B:899:LEU:HD11	1.74	0.70
1:B:895:THR:HG23	1:B:1089:GLN:HE22	1.55	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:GLN:HE22	1:C:742:PHE:HE1	1.37	0.70
1:A:952:ASN:HB2	1:A:955:ALA:HB3	1.74	0.70
1:B:437:TYR:O	1:B:440:LYS:NZ	2.25	0.70
2:G:209:VAL:HG11	2:G:565:PRO:HB3	1.73	0.70
1:C:142:LEU:HD12	1:C:147:THR:HB	1.72	0.69
1:A:287:LEU:HD11	1:A:301:TYR:HD2	1.56	0.69
1:A:311:SER:N	1:A:525:CYS:O	2.21	0.69
1:A:398:ILE:HG21	1:A:497:VAL:HG11	1.74	0.69
1:B:127:ARG:NH2	1:B:160:CYS:SG	2.61	0.69
1:C:103:VAL:HG22	1:C:116:ILE:HG22	1.74	0.69
1:A:420:CYS:HB3	1:A:500:LEU:HD12	1.75	0.69
1:C:42:TYR:OH	1:C:189:ARG:NH2	2.26	0.69
1:C:269:GLU:OE1	3:Q:1:NAG:N2	2.26	0.69
1:C:732:CYS:SG	1:C:733:ALA:N	2.66	0.69
2:G:320:LEU:HD13	2:G:380:GLN:HG2	1.74	0.69
1:A:349:CYS:H	1:A:511:VAL:HA	1.58	0.69
1:B:565:ASP:HB3	1:B:568:THR:O	1.93	0.69
1:A:1098:ILE:HG22	1:A:1120:VAL:HG23	1.75	0.69
1:A:714:MET:HB3	1:A:757:GLN:HG2	1.75	0.69
1:B:69:ARG:NH1	1:B:208:SER:OG	2.26	0.69
1:B:269:GLU:OE2	3:P:1:NAG:N2	2.22	0.69
2:D:389:PRO:HG2	2:D:392:LEU:HB2	1.74	0.69
1:A:726:CYS:SG	1:A:729:SER:OG	2.51	0.68
1:C:185:GLU:OE2	1:C:215:ASN:ND2	2.26	0.68
1:B:637:LEU:HD21	1:B:640:ALA:HB3	1.73	0.68
1:A:729:SER:OG	1:A:732:CYS:SG	2.52	0.68
1:B:195:LEU:HD23	1:B:223:LEU:HD12	1.73	0.68
1:B:488:ASN:O	1:B:493:GLN:NE2	2.26	0.68
1:C:1073:PRO:HA	1:C:1103:THR:HG22	1.75	0.68
1:B:113:GLN:NE2	1:B:114:SER:O	2.26	0.68
1:B:352:ASP:OD1	1:B:376:ASN:ND2	2.26	0.68
1:C:546:PHE:CE2	1:C:571:ILE:HG21	2.28	0.68
1:B:897:ASN:OD1	1:B:898:VAL:N	2.27	0.68
1:C:90:PHE:HE1	1:C:92:ALA:HB2	1.58	0.68
1:C:348:ASN:N	1:C:510:THR:O	2.26	0.68
2:D:30:ASP:O	2:D:34:HIS:ND1	2.26	0.68
2:G:503:LEU:HD23	2:G:505:HIS:H	1.58	0.68
1:A:312:LYS:H	1:A:526:VAL:HG12	1.58	0.68
1:B:187:VAL:HG23	1:B:217:LEU:HD12	1.74	0.68
1:A:626:GLY:HA2	1:A:638:ILE:HG23	1.75	0.68
1:B:653:ILE:HD11	1:B:659:ALA:HB2	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:ILE:HG12	1:B:913:ALA:HB1	1.76	0.68
1:A:129:CYS:SG	1:A:160:CYS:N	2.67	0.67
1:C:426:THR:HG21	1:C:496:ARG:HD2	1.76	0.67
1:A:39:ARG:NH2	1:A:211:PRO:O	2.27	0.67
1:B:126:ILE:HB	1:B:164:TYR:HB3	1.76	0.67
1:B:449:LEU:HD11	1:B:455:ASP:HB3	1.77	0.67
1:A:484:PHE:CE1	1:A:494:PRO:HB3	2.29	0.67
1:C:58:ASP:OD1	1:C:59:HIS:N	2.26	0.67
2:D:263:PRO:HB2	2:D:266:LEU:HD23	1.75	0.67
1:B:1074:ARG:NH2	1:B:1103:THR:O	2.27	0.67
1:B:431:ALA:HA	1:B:484:PHE:HB3	1.77	0.67
1:B:604:CYS:SG	1:B:631:GLN:NE2	2.68	0.67
1:A:411:TYR:HA	1:A:449:LEU:HD12	1.77	0.67
1:A:282:ASN:H	1:A:285:ALA:HB3	1.60	0.67
1:C:314:VAL:O	1:C:316:ARG:NH1	2.28	0.67
1:A:441:TYR:HE2	2:D:34:HIS:HB3	1.61	0.66
1:C:977:ASP:OD2	1:C:978:ARG:N	2.28	0.66
1:C:551:GLN:HG3	1:C:564:ARG:HE	1.59	0.66
1:C:633:GLN:OE1	1:C:633:GLN:N	2.24	0.66
1:B:129:CYS:SG	1:B:160:CYS:N	2.68	0.66
1:C:531:ASN:HB2	1:C:566:PRO:HG3	1.78	0.66
1:C:562:SER:OG	1:C:573:ASP:OD1	2.13	0.66
1:C:665:SER:HA	1:C:669:SER:HA	1.77	0.66
1:A:743:CYS:HA	1:A:746:LEU:HB2	1.77	0.66
1:A:1067:GLU:O	1:A:1069:LYS:NZ	2.28	0.66
1:A:682:LEU:HD22	1:B:856:TYR:HE2	1.60	0.66
1:A:663:THR:HA	1:A:673:LYS:HA	1.78	0.66
2:D:320:LEU:HD13	2:D:380:GLN:HG2	1.77	0.66
1:A:414:PRO:HG3	1:A:452:PHE:H	1.61	0.65
1:B:436:ASN:HB2	1:B:484:PHE:HD2	1.60	0.65
1:C:325:PRO:HG2	1:C:344:LYS:HZ3	1.61	0.65
1:C:344:LYS:HB3	1:C:385:ALA:HB3	1.78	0.65
1:C:973:GLU:HA	1:C:976:ILE:HG12	1.78	0.65
1:B:364:THR:HB	1:B:423:ALA:HB3	1.79	0.65
1:C:305:ASN:HA	1:C:581:GLY:HA2	1.77	0.65
1:C:343:ARG:HE	1:C:454:ARG:HH12	1.44	0.65
1:A:464:ASP:OD2	1:A:474:ASN:ND2	2.29	0.65
1:A:414:PRO:HB3	1:A:451:PRO:HB3	1.79	0.65
1:A:142:LEU:HB3	1:A:145:ASN:HB3	1.78	0.65
1:B:1122:ASP:HB3	1:B:1125:GLN:HG2	1.77	0.65
1:C:332:ALA:HB3	1:C:335:PHE:HE1	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:LYS:O	1:C:292:LYS:HG2	1.96	0.65
1:C:79:ASN:HB3	1:C:233:ARG:HH11	1.62	0.65
1:A:759:ARG:HG3	1:A:762:ARG:HH22	1.62	0.64
1:A:115:VAL:HG23	1:A:227:ILE:HD11	1.80	0.64
1:A:343:ARG:HD3	1:A:384:TYR:CG	2.33	0.64
1:B:386:ASP:HB2	1:B:499:VAL:HB	1.79	0.64
1:B:725:ILE:HG21	1:B:736:LEU:HD21	1.80	0.64
1:A:381:SER:HB3	1:A:509:ALA:HA	1.79	0.64
1:C:196:HIS:HE1	1:C:222:LYS:HE2	1.63	0.64
1:C:550:GLN:O	1:C:564:ARG:NH2	2.31	0.64
1:A:336:PRO:HD2	1:A:387:SER:HB2	1.78	0.64
1:C:949:LEU:HB2	1:C:983:ARG:HH22	1.63	0.64
2:D:453:THR:HG21	2:D:516:TYR:HB2	1.80	0.64
1:B:550:GLN:O	1:B:564:ARG:NH2	2.23	0.64
1:C:316:ARG:NH1	1:C:529:ASN:H	1.96	0.64
1:C:367:CYS:HA	1:C:420:CYS:HA	1.80	0.64
1:C:468:CYS:N	1:C:475:CYS:SG	2.67	0.64
1:A:414:PRO:HD2	1:A:417:PHE:HD2	1.62	0.63
1:C:746:LEU:HD13	1:C:987:LEU:HD22	1.80	0.63
1:A:368:TYR:HB2	1:A:400:PRO:HB2	1.80	0.63
1:A:399:ALA:HB3	1:A:402:GLN:HB2	1.81	0.63
1:C:58:ASP:HB3	1:C:60:PHE:CZ	2.34	0.63
1:B:1074:ARG:HG2	1:B:1102:ASN:O	1.99	0.63
1:B:326:PHE:HZ	1:B:383:VAL:HG11	1.64	0.63
1:A:194:PHE:HA	1:A:223:LEU:O	1.99	0.62
1:A:419:GLY:HA3	1:A:500:LEU:O	1.99	0.62
1:A:578:SER:HB2	1:A:601:ASP:HB3	1.79	0.62
1:A:984:LEU:HG	1:A:988:GLN:HE22	1.64	0.62
2:G:482:ARG:HG2	2:G:488:VAL:HG12	1.81	0.62
1:A:850:ASP:OD1	1:A:851:ASP:N	2.32	0.62
1:A:1011:LYS:HD3	1:A:1025:PHE:CE2	2.34	0.62
1:A:95:LYS:HB3	1:A:180:PHE:HA	1.80	0.62
1:A:126:ILE:HB	1:A:164:TYR:HB3	1.81	0.62
1:A:318:PRO:HA	1:A:566:PRO:HB2	1.81	0.62
1:B:759:ARG:NH1	1:B:763:GLU:OE2	2.31	0.62
1:A:131:PHE:HB3	1:A:157:ALA:HA	1.80	0.62
1:A:933:ASP:OD1	1:A:934:VAL:N	2.33	0.62
2:G:557:MET:SD	2:G:569:ALA:HB1	2.39	0.62
1:A:460:PRO:HA	1:A:478:PRO:HD3	1.80	0.62
1:B:553:GLY:HA2	1:C:48:PHE:HB3	1.82	0.62
1:C:353:TYR:HA	1:C:356:LEU:HD12	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:929:GLY:O	1:C:932:GLN:NE2	2.33	0.62
1:C:956:ILE:N	1:C:975:GLN:OE1	2.25	0.62
1:A:427:ARG:HG3	1:A:493:GLN:HG2	1.80	0.62
1:B:27:THR:OG1	1:B:77:PHE:N	2.32	0.62
1:B:442:ARG:NH2	1:B:457:SER:O	2.33	0.62
1:C:291:VAL:HG13	1:C:293:SER:H	1.65	0.62
1:A:441:TYR:HB3	1:A:482:TYR:CE1	2.35	0.62
1:C:1105:VAL:HG13	1:C:1106:SER:H	1.64	0.62
2:D:459:TRP:HZ2	2:D:473:TRP:HB3	1.65	0.62
1:A:36:SER:HB3	1:A:65:SER:H	1.65	0.62
1:A:389:VAL:HG22	1:A:496:ARG:HG2	1.80	0.62
1:A:409:TYR:HB3	1:A:445:ARG:HB2	1.80	0.62
1:C:1066:HIS:CD2	1:C:1067:GLU:HG2	2.35	0.62
2:G:402:GLU:HG3	2:G:518:ARG:HG3	1.81	0.62
1:B:314:VAL:O	1:B:518:THR:OG1	2.15	0.61
1:A:705:ILE:HG22	1:A:1048:VAL:HA	1.81	0.61
1:C:953:PHE:CD1	1:C:982:GLY:HA3	2.34	0.61
1:A:662:HIS:O	1:A:673:LYS:CA	2.48	0.61
1:B:91:ALA:HB3	1:B:254:PHE:HB2	1.82	0.61
1:C:350:VAL:HG12	1:C:514:PRO:HD2	1.82	0.61
2:D:459:TRP:HB2	2:D:480:MET:HE3	1.82	0.61
1:B:968:ASP:HB3	1:B:971:GLU:HG2	1.82	0.61
2:G:528:ALA:HB2	2:G:574:VAL:HG12	1.81	0.61
1:A:322:ASN:ND2	1:A:348:ASN:O	2.34	0.61
1:C:460:PRO:HA	1:C:477:TRP:HA	1.82	0.61
1:A:288:LYS:HE3	1:A:294:PHE:HA	1.82	0.61
1:A:452:PHE:CD1	1:A:501:SER:HB2	2.36	0.61
1:A:966:ARG:HH22	1:A:975:GLN:HE21	1.49	0.61
1:B:191:LYS:HB3	1:B:196:HIS:CD2	2.36	0.61
1:B:963:ILE:HG23	1:B:975:GLN:HE21	1.65	0.61
2:D:119:ILE:HG23	2:D:179:LEU:HD22	1.82	0.61
2:G:281:LEU:HD12	2:G:282:THR:HG23	1.83	0.61
1:B:59:HIS:ND1	1:B:258:LEU:O	2.28	0.61
1:B:417:PHE:HE2	1:B:501:SER:HA	1.66	0.61
1:C:419:GLY:CA	1:C:500:LEU:O	2.49	0.61
1:A:316:ARG:NH1	1:A:519:ASP:HA	2.15	0.60
1:A:929:GLY:HA2	1:A:932:GLN:HB3	1.82	0.60
1:B:139:PHE:HB2	1:B:237:THR:HB	1.83	0.60
2:G:208:GLU:OE2	2:G:219:ARG:NH1	2.33	0.60
1:A:462:SER:HB2	1:A:475:CYS:HB3	1.83	0.60
2:G:215:TYR:CE2	2:G:568:LEU:HD12	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:HE1	1:A:235:LEU:HB3	1.65	0.60
1:A:473:PHE:HB3	2:D:79:LEU:HD11	1.82	0.60
1:A:952:ASN:HB3	1:A:958:SER:HA	1.82	0.60
2:G:265:HIS:CD2	2:G:490:PRO:HG2	2.36	0.60
2:G:588:PHE:O	2:G:592:PHE:N	2.34	0.60
1:A:319:ASN:HB2	1:A:567:LYS:HA	1.83	0.60
1:A:95:LYS:HG3	1:A:176:LYS:HB2	1.84	0.60
1:C:51:ASN:HA	1:C:267:TYR:O	2.02	0.60
1:C:722:ASN:O	1:C:727:GLY:N	2.35	0.60
2:G:212:VAL:HG11	2:G:215:TYR:HB2	1.82	0.60
1:A:114:SER:HB2	1:A:131:PHE:CZ	2.36	0.60
1:A:603:ASN:O	1:A:606:ASP:N	2.30	0.60
1:B:84:PHE:H	1:B:231:ASN:HA	1.66	0.60
1:C:311:SER:HB2	1:C:526:VAL:HG12	1.82	0.60
1:B:99:ILE:HG12	1:B:236:LEU:HB3	1.83	0.60
1:C:324:CYS:HB2	1:C:326:PHE:CE1	2.37	0.60
1:B:307:ARG:NH1	1:B:308:VAL:H	1.99	0.60
1:C:420:CYS:O	1:C:499:VAL:HA	2.01	0.60
1:B:441:TYR:HE2	1:B:443:SER:HB3	1.67	0.60
1:B:1097:ILE:O	1:B:1102:ASN:ND2	2.34	0.60
1:B:58:ASP:HB3	1:B:60:PHE:CE1	2.37	0.60
1:B:97:ASN:HD22	1:B:171:LEU:HD11	1.66	0.60
2:D:50:TYR:HA	2:D:58:ASN:HB3	1.82	0.60
1:C:175:GLU:OE2	1:C:249:SER:OG	2.19	0.59
1:B:745:GLN:OE1	1:B:748:ARG:NH2	2.35	0.59
3:H:2:NAG:H3	3:H:2:NAG:H83	1.84	0.59
1:A:325:PRO:HD2	1:A:346:ILE:HG23	1.84	0.59
1:A:530:PHE:HD1	1:A:566:PRO:HD2	1.67	0.59
1:B:946:VAL:O	1:B:949:LEU:HB3	2.01	0.59
2:G:207:TYR:CE1	2:G:397:ASN:HB2	2.37	0.59
1:B:1098:ILE:HA	1:B:1102:ASN:HD22	1.67	0.59
1:C:87:GLY:CA	1:C:188:PHE:O	2.49	0.59
1:C:129:CYS:HB3	1:C:131:PHE:CE1	2.37	0.59
1:C:343:ARG:NE	1:C:454:ARG:HH12	2.00	0.59
1:C:1011:LYS:NZ	1:C:1025:PHE:O	2.35	0.59
2:D:174:LYS:HG2	2:D:496:THR:HG22	1.84	0.59
1:B:427:ARG:HD3	1:B:486:ILE:HA	1.83	0.59
1:C:386:ASP:O	1:C:498:VAL:HA	2.02	0.59
1:C:1055:GLU:OE1	1:C:1055:GLU:N	2.34	0.59
1:A:547:GLN:HB2	1:A:550:GLN:HB2	1.84	0.59
1:B:83:PRO:HB2	1:B:85:LYS:HE3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLY:N	1:B:491:GLY:O	2.36	0.59
1:C:962:ASP:O	1:C:966:ARG:N	2.36	0.59
1:B:972:ALA:HA	1:B:975:GLN:NE2	2.18	0.59
1:C:79:ASN:O	1:C:233:ARG:NH1	2.36	0.59
2:D:252:TYR:HB3	2:D:255:TYR:HD2	1.67	0.59
1:C:100:ARG:HH21	1:C:237:THR:HG21	1.67	0.58
1:C:123:ASN:HD21	5:C:1309:NAG:H5	1.67	0.58
1:C:988:GLN:O	1:C:992:THR:HG23	2.03	0.58
2:D:125:THR:O	2:D:129:THR:OG1	2.17	0.58
2:D:480:MET:HA	2:D:483:GLU:HB3	1.85	0.58
2:G:482:ARG:NH2	2:G:613:TYR:OH	2.34	0.58
1:A:439:TYR:HB2	1:A:484:PHE:HE2	1.68	0.58
2:D:37:GLU:OE1	2:D:393:ARG:NH1	2.35	0.58
1:A:215:ASN:OD1	1:A:216:ALA:N	2.36	0.58
1:B:34:PHE:HE2	1:B:69:ARG:HD2	1.67	0.58
1:B:442:ARG:NH1	1:B:455:ASP:HB2	2.18	0.58
2:D:459:TRP:CD1	2:D:480:MET:HE1	2.39	0.58
1:A:542:SER:HB3	1:A:571:ILE:HG13	1.85	0.58
1:C:32:THR:HG23	1:C:69:ARG:HB3	1.85	0.58
1:C:370:VAL:HG13	1:C:418:THR:HB	1.84	0.58
1:C:948:GLN:O	1:C:951:SER:OG	2.21	0.58
2:G:216:ASP:OD1	2:G:217:TYR:N	2.36	0.58
1:B:796:THR:HG23	1:B:798:ARG:H	1.69	0.58
1:C:264:MET:O	1:C:276:ALA:HA	2.04	0.58
1:C:962:ASP:HA	1:C:966:ARG:HH11	1.68	0.58
2:D:169:ARG:NH2	2:D:270:MET:O	2.35	0.58
1:A:49:ARG:HB2	1:A:267:TYR:CD1	2.38	0.58
1:C:1066:HIS:CE1	1:C:1119:THR:HG23	2.39	0.58
2:D:177:ARG:CD	2:D:498:CYS:HB2	2.34	0.58
2:D:233:ILE:HD11	2:D:581:VAL:HG21	1.86	0.58
1:A:122:THR:O	1:A:168:ASP:HA	2.03	0.58
1:B:849:THR:HG22	1:B:852:MET:CE	2.33	0.58
2:D:347:THR:HG1	2:D:349:TRP:HE1	1.51	0.58
2:G:233:ILE:HD11	2:G:581:VAL:HG21	1.85	0.58
1:A:42:TYR:HA	1:A:217:LEU:H	1.68	0.58
1:A:953:PHE:HD2	1:A:982:GLY:HA3	1.68	0.58
1:B:918:GLN:O	1:B:922:THR:OG1	2.12	0.58
1:A:1077:VAL:HG23	1:A:1090:ARG:NH1	2.19	0.58
1:B:391:LYS:HB3	1:B:482:TYR:CE2	2.39	0.58
1:C:387:SER:HA	1:C:498:VAL:HG22	1.86	0.58
1:C:742:PHE:O	1:C:745:GLN:HG2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:GLY:O	1:C:978:ARG:NH2	2.29	0.58
2:D:588:PHE:O	2:D:592:PHE:N	2.34	0.58
1:A:528:PHE:O	1:A:534:THR:HA	2.03	0.58
1:A:568:THR:O	1:A:570:GLU:N	2.35	0.58
1:B:106:SER:OG	1:B:230:THR:N	2.35	0.58
1:A:316:ARG:NH2	1:A:517:SER:HB2	2.18	0.57
1:C:437:TYR:OH	2:G:42:GLN:OE1	2.19	0.57
2:D:184:VAL:HG12	2:D:464:PHE:HE1	1.69	0.57
1:A:42:TYR:OH	1:A:59:HIS:O	2.21	0.57
1:A:103:VAL:HG22	1:A:116:ILE:HG12	1.87	0.57
1:C:709:VAL:HG22	1:C:1044:VAL:HG22	1.85	0.57
2:G:403:ALA:O	2:G:407:ILE:HG12	2.04	0.57
1:B:338:VAL:HA	1:B:388:PHE:HB2	1.86	0.57
2:G:453:THR:HG21	2:G:516:TYR:HB2	1.85	0.57
1:A:440:LYS:HE3	1:A:479:LEU:HD12	1.87	0.57
2:G:237:TYR:OH	2:G:485:VAL:O	2.15	0.57
1:B:181:LYS:HA	1:B:204:ILE:H	1.70	0.57
1:A:115:VAL:HG22	1:A:128:ALA:HB2	1.85	0.57
1:A:367:CYS:SG	1:A:372:ALA:N	2.78	0.57
1:B:129:CYS:SG	1:B:157:ALA:HB1	2.45	0.57
2:D:307:ILE:HG23	2:D:369:PHE:HD1	1.70	0.57
2:D:352:GLY:H	2:D:356:PHE:HE1	1.53	0.57
1:A:988:GLN:HA	1:A:991:VAL:HG12	1.86	0.57
1:B:380:PHE:N	1:B:511:VAL:O	2.19	0.57
1:B:391:LYS:NZ	1:B:394:ASP:OD2	2.38	0.57
1:B:849:THR:HG23	1:B:851:ASP:H	1.70	0.57
1:C:442:ARG:HG3	1:C:478:PRO:HB2	1.86	0.57
1:C:521:ILE:HG21	1:C:526:VAL:HG21	1.86	0.57
1:A:391:LYS:O	1:A:395:VAL:N	2.36	0.57
1:C:325:PRO:HD2	1:C:346:ILE:HG23	1.86	0.57
1:C:581:GLY:H	1:C:600:GLN:HG2	1.69	0.57
1:A:716:LYS:HG2	1:A:844:LEU:HB2	1.87	0.56
1:B:649:CYS:HB2	1:B:680:MET:HG3	1.85	0.56
1:B:838:PHE:HB2	1:B:841:LEU:HD12	1.87	0.56
2:D:281:LEU:HD12	2:D:282:THR:HG23	1.87	0.56
1:C:122:THR:O	1:C:169:PHE:N	2.35	0.56
1:C:412:LYS:HG3	1:C:414:PRO:HD3	1.86	0.56
1:C:648:GLU:O	1:C:678:TYR:OH	2.16	0.56
1:C:733:ALA:HA	1:C:736:LEU:HB3	1.87	0.56
1:A:391:LYS:HB3	1:A:482:TYR:HE2	1.69	0.56
1:A:763:GLU:OE1	1:A:767:GLN:NE2	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLY:HA3	1:B:418:THR:HG23	1.87	0.56
1:B:889:PHE:CD2	1:B:899:LEU:HD12	2.40	0.56
1:C:69:ARG:NH2	1:C:208:SER:O	2.38	0.56
2:G:416:LYS:HB3	2:G:543:ASP:HB2	1.88	0.56
1:B:412:LYS:HZ3	1:B:413:LEU:H	1.52	0.56
1:C:419:GLY:HA2	1:C:500:LEU:O	2.06	0.56
1:C:1074:ARG:NH1	1:C:1101:ASP:O	2.39	0.56
2:D:238:GLU:HA	2:D:606:TRP:HZ3	1.69	0.56
2:G:307:ILE:HG23	2:G:369:PHE:HD1	1.71	0.56
1:A:182:ASP:OD1	1:A:201:TYR:OH	2.23	0.56
1:A:640:ALA:HB2	1:A:675:ILE:HG23	1.88	0.56
1:A:743:CYS:HA	1:A:746:LEU:HD12	1.88	0.56
1:B:390:VAL:HG22	1:B:497:VAL:HG21	1.87	0.56
1:B:895:THR:HG23	1:B:1089:GLN:NE2	2.19	0.56
1:A:132:GLU:HB3	1:A:155:ASN:HB3	1.88	0.56
1:A:441:TYR:CE2	2:D:34:HIS:HB3	2.41	0.56
1:B:392:GLY:HA3	1:B:491:GLY:HA2	1.86	0.56
2:D:261:CYS:HB2	2:D:488:VAL:HG13	1.87	0.56
1:A:83:PRO:HB2	1:A:85:LYS:HE3	1.88	0.56
1:B:662:HIS:O	1:B:673:LYS:CA	2.52	0.56
1:B:945:LEU:HD21	1:B:990:TYR:HB2	1.88	0.56
1:B:976:ILE:O	1:B:980:ILE:HD12	2.05	0.56
1:B:1062:PRO:HB3	1:C:900:TYR:CZ	2.41	0.56
1:C:54:HIS:HE2	1:C:56:VAL:HB	1.71	0.56
1:A:386:ASP:HB2	1:A:499:VAL:HG22	1.88	0.56
1:A:561:ASP:OD1	1:A:562:SER:N	2.39	0.56
1:C:187:VAL:O	1:C:197:VAL:HA	2.06	0.56
1:C:191:LYS:HB3	1:C:196:HIS:CD2	2.40	0.56
1:A:106:SER:HB3	1:A:112:SER:OG	2.05	0.56
1:A:349:CYS:O	1:A:512:CYS:N	2.39	0.56
1:A:698:PRO:HD3	1:B:877:LEU:HD22	1.88	0.56
1:C:71:ILE:HG22	1:C:73:PHE:H	1.71	0.56
1:A:94:GLU:HA	1:A:180:PHE:HB2	1.88	0.55
1:B:722:ASN:OD1	1:B:723:MET:N	2.37	0.55
2:D:278:LEU:O	2:D:282:THR:N	2.39	0.55
1:A:340:ALA:HB1	1:A:456:ILE:HD12	1.88	0.55
1:B:216:ALA:HB1	1:B:273:ILE:HD12	1.89	0.55
1:C:77:PHE:CG	1:C:246:TRP:HZ2	2.24	0.55
1:C:352:ASP:OD1	1:C:376:ASN:ND2	2.39	0.55
2:D:478:TRP:NE1	2:D:499:ASP:OD2	2.37	0.55
2:G:381:TYR:HD1	2:G:558:LEU:HD12	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:534:LYS:HD2	2:G:534:LYS:O	2.06	0.55
1:A:682:LEU:HD21	1:B:852:MET:HG2	1.87	0.55
1:C:124:LEU:HB3	1:C:166:SER:HB3	1.87	0.55
1:A:143:LYS:HG2	1:A:241:PRO:HG3	1.88	0.55
1:B:53:LEU:HB3	1:B:264:MET:CE	2.37	0.55
1:B:972:ALA:HA	1:B:975:GLN:HE22	1.71	0.55
1:C:51:ASN:CA	1:C:267:TYR:O	2.55	0.55
1:A:564:ARG:HD3	1:A:569:SER:HB3	1.88	0.55
1:B:37:SER:H	1:B:64:ASP:H	1.53	0.55
1:C:67:VAL:HG21	1:C:254:PHE:HB3	1.89	0.55
2:D:459:TRP:HB2	2:D:480:MET:CE	2.37	0.55
1:A:787:GLN:NE2	1:A:918:GLN:OE1	2.40	0.55
1:A:900:TYR:CZ	1:C:1062:PRO:HB3	2.41	0.55
2:D:54:ILE:HG13	2:D:342:ALA:HA	1.89	0.55
2:G:152:MET:O	2:G:161:ARG:NH2	2.40	0.55
1:A:20:CYS:HB2	1:A:152:TYR:HD2	1.72	0.55
1:A:101:GLY:HA3	1:A:235:LEU:HD12	1.88	0.55
2:G:378:HIS:HE1	2:G:402:GLU:HA	1.70	0.55
1:A:708:GLU:OE2	1:A:1011:LYS:NZ	2.38	0.55
1:C:139:PHE:O	1:C:238:ALA:N	2.33	0.55
2:D:241:HIS:HA	2:D:244:VAL:HG22	1.87	0.55
1:A:322:ASN:ND2	1:A:348:ASN:HD22	2.05	0.55
1:A:682:LEU:HD11	1:B:852:MET:HG3	1.88	0.55
1:A:1099:THR:OG1	1:A:1101:ASP:OD1	2.17	0.55
1:B:49:ARG:HH12	1:B:54:HIS:CE1	2.25	0.55
1:B:181:LYS:O	1:B:203:PRO:HA	2.07	0.55
1:C:899:LEU:HD12	1:C:906:ILE:HD12	1.89	0.55
2:G:387:ALA:HB3	2:G:559:ARG:HH21	1.70	0.55
1:A:202:GLN:OE1	1:A:215:ASN:ND2	2.39	0.54
1:A:372:ALA:HB2	1:A:420:CYS:SG	2.46	0.54
1:B:325:PRO:HG2	1:B:346:ILE:HD12	1.89	0.54
1:C:36:SER:N	1:C:65:SER:O	2.39	0.54
2:D:378:HIS:HE1	2:D:402:GLU:HA	1.71	0.54
2:G:51:ASN:HB3	2:G:359:LEU:CD1	2.37	0.54
1:B:568:THR:O	1:B:570:GLU:N	2.38	0.54
1:C:339:TYR:HD2	1:C:456:ILE:HA	1.72	0.54
1:C:431:ALA:HB2	1:C:494:PRO:HG3	1.88	0.54
2:G:30:ASP:O	2:G:34:HIS:ND1	2.41	0.54
2:G:360:MET:HE3	2:G:372:ALA:HA	1.89	0.54
1:C:106:SER:O	1:C:231:ASN:ND2	2.37	0.54
1:C:127:ARG:NH2	1:C:160:CYS:SG	2.79	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:729:SER:OG	1:C:732:CYS:HB3	2.07	0.54
1:C:732:CYS:C	1:C:734:ASN:H	2.11	0.54
2:D:123:MET:HA	2:D:126:ILE:HG12	1.88	0.54
2:D:169:ARG:NH1	2:D:270:MET:SD	2.70	0.54
2:D:180:TYR:HA	2:D:183:TYR:HB3	1.90	0.54
2:D:482:ARG:HG2	2:D:488:VAL:HG12	1.88	0.54
1:A:317:PHE:CD2	1:A:515:LYS:HB2	2.42	0.54
1:A:404:GLY:H	1:A:407:ALA:HB3	1.71	0.54
1:A:562:SER:HA	1:A:572:LEU:O	2.07	0.54
1:A:565:ASP:HB3	1:A:568:THR:O	2.07	0.54
1:B:34:PHE:CE2	1:B:69:ARG:HD2	2.42	0.54
1:B:352:ASP:HB3	1:B:355:VAL:HG22	1.89	0.54
1:C:362:PHE:HB2	1:C:365:PHE:HB2	1.90	0.54
2:G:75:GLU:O	2:G:78:THR:OG1	2.23	0.54
1:A:100:ARG:HD2	1:A:120:ASN:HB3	1.89	0.54
1:B:379:CYS:HB3	1:B:509:ALA:CB	2.38	0.54
1:B:485:TYR:H	1:B:488:ASN:ND2	2.06	0.54
1:A:287:LEU:HD11	1:A:301:TYR:CD2	2.41	0.54
1:A:662:HIS:O	1:A:673:LYS:C	2.46	0.54
1:A:993:GLN:HE22	1:A:997:ARG:NH1	2.05	0.54
1:B:333:THR:O	1:B:496:ARG:NH2	2.40	0.54
1:C:117:ILE:HG13	1:C:126:ILE:HG23	1.90	0.54
1:A:957:SER:HB3	1:A:963:ILE:HG13	1.88	0.54
1:B:757:GLN:HE22	1:B:1001:ILE:HG21	1.72	0.54
1:C:59:HIS:HB2	1:C:189:ARG:HH12	1.72	0.54
1:C:116:ILE:HB	1:C:118:MET:HE3	1.88	0.54
1:B:116:ILE:HG13	1:B:131:PHE:CE2	2.43	0.54
1:B:345:ARG:HG3	1:B:382:ASN:OD1	2.08	0.54
1:C:72:THR:HG21	1:C:236:LEU:HG	1.90	0.54
2:G:108:LEU:HB2	2:G:113:SER:HB3	1.90	0.54
1:A:317:PHE:HE1	1:A:532:GLY:HA2	1.73	0.54
1:A:441:TYR:CE1	1:A:482:TYR:HA	2.43	0.54
1:A:449:LEU:HD21	1:A:455:ASP:HB3	1.89	0.54
1:A:57:GLN:HB2	1:A:262:THR:HG22	1.88	0.54
1:A:183:LEU:HB3	1:A:202:GLN:HB2	1.90	0.54
1:B:198:TYR:HA	1:B:219:PRO:HA	1.89	0.54
2:D:40:PHE:HB2	2:D:69:TRP:CZ3	2.43	0.54
1:A:804:LEU:HD11	1:A:922:THR:HA	1.90	0.53
1:A:993:GLN:HE22	1:A:997:ARG:HH11	1.55	0.53
1:B:49:ARG:HH21	1:B:267:TYR:HE2	1.54	0.53
1:B:51:ASN:N	1:B:267:TYR:O	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ARG:HG3	1:B:478:PRO:HB2	1.89	0.53
1:A:36:SER:HB3	1:A:65:SER:N	2.23	0.53
1:A:129:CYS:HB3	1:A:131:PHE:HD2	1.73	0.53
1:B:98:VAL:HG12	1:B:236:LEU:HB2	1.91	0.53
1:A:94:GLU:OE1	1:A:99:ILE:HG13	2.08	0.53
1:A:555:ASP:CG	1:A:556:VAL:H	2.11	0.53
1:A:696:ALA:HB2	1:B:878:GLN:HG2	1.90	0.53
1:B:72:THR:OG1	1:B:77:PHE:HA	2.09	0.53
1:B:130:ASN:O	1:B:157:ALA:HA	2.09	0.53
1:B:181:LYS:HG2	1:B:203:PRO:HB3	1.91	0.53
1:C:121:SER:HB3	5:C:1309:NAG:H82	1.90	0.53
1:A:556:VAL:HG22	1:B:52:VAL:HG11	1.91	0.53
1:A:852:MET:SD	1:C:682:LEU:HD21	2.48	0.53
2:G:573:VAL:HG12	2:G:574:VAL:HG13	1.90	0.53
1:B:941:ALA:O	1:B:944:THR:OG1	2.16	0.53
1:C:71:ILE:HB	1:C:76:ASN:HD21	1.74	0.53
1:A:72:THR:HG21	1:A:236:LEU:HD23	1.89	0.53
2:G:346:PRO:HA	2:G:359:LEU:O	2.09	0.53
1:A:597:VAL:O	1:A:598:LEU:HD22	2.09	0.53
1:B:59:HIS:CE1	1:B:260:PRO:HD3	2.44	0.53
1:B:547:GLN:HG2	1:B:549:PHE:CE1	2.44	0.53
1:B:307:ARG:NH2	1:B:308:VAL:O	2.42	0.53
1:B:408:ASP:HB3	1:B:448:LYS:HD3	1.89	0.53
1:C:587:PRO:HG3	1:C:661:TYR:CD1	2.43	0.53
1:A:956:ILE:H	1:A:975:GLN:NE2	2.00	0.53
1:C:128:ALA:HB3	1:C:162:PHE:HB3	1.90	0.53
1:C:367:CYS:SG	1:C:372:ALA:HA	2.49	0.53
1:C:546:PHE:HE2	1:C:571:ILE:HG21	1.73	0.53
2:D:351:LEU:HB2	2:D:355:ASP:O	2.09	0.53
2:D:403:ALA:O	2:D:407:ILE:HG12	2.09	0.53
1:B:72:THR:HB	1:B:78:ASP:OD1	2.09	0.52
1:C:94:GLU:O	1:C:182:ASP:HB2	2.09	0.52
2:D:402:GLU:HG3	2:D:518:ARG:HG3	1.91	0.52
1:A:397:GLN:HB3	1:A:404:GLY:HA3	1.91	0.52
1:B:296:ILE:H	1:B:589:THR:HG22	1.74	0.52
1:B:302:GLN:HE22	1:B:582:VAL:N	2.07	0.52
1:B:648:GLU:O	1:B:678:TYR:OH	2.23	0.52
1:B:972:ALA:O	1:B:976:ILE:HG13	2.10	0.52
1:C:129:CYS:HB3	1:C:131:PHE:CZ	2.45	0.52
1:B:184:ARG:HG2	1:B:201:TYR:CD1	2.44	0.52
1:B:390:VAL:HB	1:B:394:ASP:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLY:HA2	1:B:395:VAL:HG13	1.91	0.52
1:B:485:TYR:HD2	1:B:488:ASN:HD21	1.57	0.52
1:B:952:ASN:OD1	1:B:953:PHE:N	2.43	0.52
2:G:108:LEU:HD11	2:G:190:MET:HB2	1.91	0.52
1:A:174:GLY:HA2	1:A:239:PHE:HE2	1.75	0.52
1:B:210:LEU:HD12	1:B:211:PRO:HD2	1.90	0.52
1:B:322:ASN:O	1:B:350:VAL:N	2.40	0.52
1:B:600:GLN:HG2	1:C:844:LEU:HD11	1.92	0.52
2:G:374:HIS:CE1	2:G:406:GLU:HG2	2.44	0.52
1:A:586:THR:HG22	1:A:587:PRO:O	2.10	0.52
1:B:23:PHE:CD2	1:B:246:TRP:HB3	2.44	0.52
1:B:379:CYS:HA	1:B:512:CYS:HA	1.92	0.52
1:B:750:LEU:HA	1:B:753:ILE:HD12	1.91	0.52
1:C:322:ASN:HB2	1:C:348:ASN:O	2.09	0.52
1:A:105:GLY:H	1:A:108:MET:HE1	1.73	0.52
1:A:932:GLN:O	1:A:935:VAL:HG12	2.09	0.52
1:B:742:PHE:O	1:B:746:LEU:HG	2.10	0.52
1:B:947:LYS:HD3	1:B:947:LYS:N	2.24	0.52
1:A:139:PHE:CE1	1:A:235:LEU:HB3	2.44	0.52
1:B:314:VAL:HG22	1:B:521:ILE:HD12	1.92	0.52
1:C:778:LYS:HG2	1:C:789:LEU:HD23	1.90	0.52
1:C:912:LYS:NZ	1:C:916:GLN:OE1	2.43	0.52
1:C:930:LYS:HA	1:C:933:ASP:OD2	2.10	0.52
2:G:358:ILE:HD12	2:G:376:MET:HE1	1.92	0.52
1:A:295:GLU:OE2	1:A:589:THR:OG1	2.28	0.52
1:A:377:ASP:O	1:A:515:LYS:HD3	2.10	0.52
1:A:853:ILE:HA	1:A:856:TYR:HD1	1.74	0.52
1:B:27:THR:OG1	1:B:76:ASN:OD1	2.16	0.52
1:B:314:VAL:HG13	1:B:520:LEU:HA	1.92	0.52
1:B:315:VAL:HG12	1:B:517:SER:HA	1.91	0.52
2:D:19:SER:N	2:D:23:GLU:OE1	2.43	0.52
2:G:241:HIS:NE2	2:G:486:GLY:O	2.42	0.52
1:A:83:PRO:O	1:A:85:LYS:NZ	2.40	0.52
1:A:196:HIS:HB3	1:A:222:LYS:HZ1	1.75	0.52
1:A:392:GLY:HA2	1:A:395:VAL:HB	1.90	0.52
1:C:342:GLU:O	1:C:386:ASP:HA	2.10	0.52
1:C:484:PHE:CE2	1:C:494:PRO:HB3	2.45	0.52
2:D:177:ARG:HD3	2:D:497:TYR:O	2.09	0.52
2:D:482:ARG:NH2	2:D:613:TYR:OH	2.35	0.52
2:G:252:TYR:HB3	2:G:255:TYR:HD2	1.73	0.52
2:G:276:THR:O	2:G:279:TYR:HD1	1.93	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LYS:HG2	1:A:481:ASP:HA	1.90	0.52
1:B:99:ILE:HD13	1:B:234:THR:HB	1.91	0.52
1:B:304:SER:HB2	1:B:582:VAL:HB	1.92	0.52
1:B:788:ILE:O	1:B:799:SER:OG	2.18	0.52
1:B:1090:ARG:NH2	1:C:887:TYR:HB2	2.25	0.52
1:C:341:TRP:CE2	1:C:454:ARG:HG2	2.45	0.52
1:C:787:GLN:OE1	4:S:1:NAG:H62	2.10	0.52
1:A:317:PHE:CE2	1:A:515:LYS:HB2	2.45	0.51
1:A:382:ASN:HB2	1:A:503:GLU:HB2	1.91	0.51
1:A:1080:PHE:HB2	1:A:1085:TRP:CD2	2.46	0.51
1:B:96:SER:HB2	1:B:98:VAL:HG22	1.92	0.51
1:C:285:ALA:HA	1:C:288:LYS:HD2	1.91	0.51
1:C:380:PHE:HE2	1:C:502:PHE:CE1	2.28	0.51
2:D:358:ILE:HG13	2:D:379:ILE:HG13	1.93	0.51
1:B:982:GLY:O	1:B:985:GLN:HG3	2.10	0.51
2:G:294:THR:HG23	2:G:365:THR:HA	1.92	0.51
1:A:240:PRO:HA	1:A:246:TRP:HA	1.92	0.51
1:B:305:ASN:ND2	1:C:720:ASP:OD1	2.43	0.51
2:G:351:LEU:HB2	2:G:355:ASP:O	2.10	0.51
1:A:122:THR:O	1:A:124:LEU:N	2.41	0.51
1:A:439:TYR:HB2	1:A:484:PHE:CE2	2.45	0.51
1:A:728:ASP:OD2	1:C:307:ARG:NH2	2.44	0.51
1:A:918:GLN:O	1:A:922:THR:OG1	2.10	0.51
1:A:1101:ASP:OD1	1:A:1102:ASN:N	2.44	0.51
1:B:394:ASP:HA	1:B:397:GLN:HG3	1.91	0.51
1:B:756:GLU:OE2	1:B:1002:ARG:HD2	2.10	0.51
1:C:138:PHE:O	1:C:151:SER:OG	2.20	0.51
1:C:314:VAL:HG23	1:C:316:ARG:NH1	2.25	0.51
2:D:75:GLU:O	2:D:78:THR:OG1	2.25	0.51
1:A:381:SER:OG	1:A:505:LEU:HA	2.11	0.51
1:A:562:SER:OG	1:A:573:ASP:OD1	2.29	0.51
1:B:261:THR:HG22	1:B:262:THR:H	1.75	0.51
1:B:422:LEU:HD13	1:B:500:LEU:HD13	1.92	0.51
1:C:555:ASP:OD1	1:C:561:ASP:HB2	2.10	0.51
1:C:942:LEU:O	1:C:946:VAL:HG12	2.10	0.51
2:G:360:MET:HE1	2:G:375:GLU:HB2	1.92	0.51
1:A:102:TRP:HE3	1:A:117:ILE:HD13	1.76	0.51
1:B:315:VAL:HG22	1:B:529:ASN:HD22	1.76	0.51
1:B:719:VAL:HG22	1:B:841:LEU:HD23	1.93	0.51
1:B:758:ASP:O	1:B:761:THR:OG1	2.25	0.51
1:C:1062:PRO:HD2	1:C:1114:GLY:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:THR:HB	1:B:69:ARG:HB3	1.92	0.51
1:B:181:LYS:O	1:B:183:LEU:N	2.44	0.51
1:B:885:MET:CG	1:B:899:LEU:HD11	2.40	0.51
1:C:324:CYS:HB3	1:C:346:ILE:HG21	1.93	0.51
1:C:352:ASP:HA	1:C:376:ASN:HB3	1.92	0.51
2:D:557:MET:HG2	2:D:569:ALA:HB1	1.93	0.51
1:A:367:CYS:HA	1:A:420:CYS:HA	1.93	0.51
1:A:503:GLU:O	1:A:505:LEU:N	2.40	0.51
1:C:54:HIS:NE2	1:C:56:VAL:HB	2.25	0.51
2:D:241:HIS:O	2:D:245:ARG:HG3	2.11	0.51
1:A:664:VAL:HG21	1:A:667:LEU:HG	1.93	0.51
1:B:370:VAL:HA	1:C:966:ARG:O	2.11	0.51
1:B:402:GLN:NE2	1:B:403:THR:O	2.43	0.51
1:B:539:LEU:HD12	1:B:572:LEU:HB3	1.93	0.51
1:C:703:ILE:HG13	1:C:906:ILE:HG23	1.92	0.51
2:D:245:ARG:HA	2:D:262:LEU:HD21	1.92	0.51
1:A:132:GLU:O	1:A:155:ASN:N	2.41	0.51
1:A:314:VAL:HB	1:A:528:PHE:HA	1.93	0.51
1:C:141:VAL:HG13	1:C:173:LEU:HD12	1.93	0.51
1:C:1026:CYS:HB2	1:C:1047:HIS:CE1	2.45	0.51
2:G:207:TYR:HE1	2:G:398:GLU:HG2	1.76	0.51
2:G:223:ILE:HG12	2:G:461:TRP:CZ3	2.46	0.51
1:A:50:SER:O	1:A:52:VAL:HG23	2.10	0.50
1:A:187:VAL:HG11	1:A:189:ARG:NH2	2.26	0.50
1:A:336:PRO:HG2	1:A:342:GLU:HB3	1.93	0.50
1:C:444:LEU:HD11	2:G:27:THR:HG23	1.93	0.50
1:C:565:ASP:HB3	1:C:568:THR:O	2.11	0.50
1:C:730:THR:O	1:C:734:ASN:ND2	2.44	0.50
1:A:129:CYS:HA	1:A:160:CYS:HA	1.93	0.50
1:B:314:VAL:HG12	1:B:316:ARG:HG2	1.92	0.50
1:B:662:HIS:CE1	1:B:664:VAL:HG22	2.46	0.50
1:B:744:THR:HB	1:B:748:ARG:HH12	1.76	0.50
1:C:991:VAL:O	1:C:995:LEU:HD23	2.11	0.50
1:A:599:TYR:HB2	1:A:602:VAL:CG2	2.41	0.50
1:B:76:ASN:O	1:B:248:THR:OG1	2.27	0.50
2:D:438:PHE:HA	2:D:441:LYS:HG2	1.93	0.50
1:A:121:SER:HB3	1:A:173:LEU:HD11	1.94	0.50
1:B:105:GLY:HA2	1:B:114:SER:OG	2.11	0.50
1:C:492:TYR:CD2	2:G:353:LYS:HG2	2.47	0.50
1:A:116:ILE:HD11	1:A:131:PHE:CZ	2.46	0.50
1:A:124:LEU:HG	1:A:166:SER:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:GLY:HA3	1:C:226:GLY:HA2	1.94	0.50
2:D:51:ASN:O	2:D:342:ALA:HB1	2.11	0.50
2:D:177:ARG:HD3	2:D:498:CYS:HB2	1.92	0.50
1:A:104:PHE:HB3	1:A:229:ILE:HG21	1.94	0.50
1:A:1019:GLN:HE21	1:A:1032:LEU:HA	1.76	0.50
1:B:648:GLU:OE1	1:B:648:GLU:N	2.41	0.50
1:B:952:ASN:C	1:B:953:PHE:HD1	2.15	0.50
2:D:209:VAL:HG23	2:D:216:ASP:HA	1.93	0.50
2:D:503:LEU:HD23	2:D:505:HIS:H	1.76	0.50
2:G:243:TYR:HA	2:G:599:ASN:HD21	1.75	0.50
1:A:70:PHE:HB2	1:A:253:TYR:CE2	2.47	0.50
1:A:326:PHE:HZ	1:A:500:LEU:HD21	1.77	0.50
1:A:522:LYS:HZ3	1:A:539:LEU:HB3	1.76	0.50
1:A:903:GLN:HA	1:A:906:ILE:HG22	1.94	0.50
1:B:220:ILE:HD12	1:B:221:PHE:HD2	1.77	0.50
1:C:1007:LEU:O	1:C:1011:LYS:HG2	2.12	0.50
1:C:1059:THR:HG23	1:C:1080:PHE:HB3	1.92	0.50
1:A:592:SER:OG	1:A:593:SER:N	2.44	0.50
1:B:51:ASN:CA	1:B:267:TYR:O	2.60	0.50
1:B:330:PHE:CE1	1:B:498:VAL:HG21	2.47	0.50
1:B:412:LYS:NZ	1:B:413:LEU:H	2.09	0.50
1:B:714:MET:H	1:B:757:GLN:NE2	2.10	0.50
1:C:215:ASN:OD1	1:C:216:ALA:N	2.45	0.50
1:C:713:SER:O	1:C:1041:HIS:HB3	2.11	0.50
1:C:949:LEU:HB2	1:C:983:ARG:NH2	2.26	0.50
1:B:39:ARG:HH21	1:B:211:PRO:HG2	1.76	0.50
1:B:870:THR:O	1:B:873:ALA:N	2.45	0.50
1:C:59:HIS:CE1	1:C:86:ASP:HB2	2.47	0.50
1:C:188:PHE:HB3	1:C:195:LEU:HD11	1.94	0.50
1:C:739:TYR:HB3	1:C:742:PHE:CE2	2.46	0.50
2:G:184:VAL:HG12	2:G:464:PHE:HE1	1.77	0.50
2:G:435:GLU:O	2:G:439:LEU:HD23	2.12	0.50
2:G:526:GLN:NE2	2:G:530:CYS:SG	2.81	0.50
1:A:296:ILE:HD11	1:A:586:THR:HG21	1.93	0.49
1:A:847:LEU:HD12	1:C:652:PRO:HB3	1.92	0.49
1:C:21:LEU:HB2	1:C:138:PHE:CZ	2.46	0.49
1:C:100:ARG:NH2	1:C:237:THR:HG21	2.27	0.49
2:G:108:LEU:HD21	2:G:190:MET:HA	1.94	0.49
2:G:455:MET:SD	2:G:456:LEU:N	2.84	0.49
1:A:196:HIS:HB3	1:A:222:LYS:NZ	2.27	0.49
1:A:853:ILE:O	1:A:857:THR:HG23	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:ARG:HH21	1:B:887:TYR:HD1	1.58	0.49
1:B:102:TRP:CD1	1:B:232:PHE:HZ	2.31	0.49
1:A:48:PHE:HD2	1:C:550:GLN:NE2	2.10	0.49
1:A:889:PHE:HE1	1:A:1032:LEU:HD11	1.76	0.49
1:A:895:THR:OG1	1:A:897:ASN:OD1	2.24	0.49
1:B:392:GLY:O	1:B:395:VAL:HG22	2.12	0.49
1:B:714:MET:HG3	1:B:757:GLN:HE21	1.77	0.49
1:C:43:TYR:CE1	1:C:216:ALA:HB1	2.47	0.49
1:C:714:MET:N	1:C:757:GLN:OE1	2.37	0.49
1:C:946:VAL:O	1:C:949:LEU:HG	2.12	0.49
2:D:174:LYS:HA	2:D:496:THR:O	2.12	0.49
2:D:223:ILE:HG12	2:D:461:TRP:CZ3	2.47	0.49
2:G:215:TYR:HE2	2:G:568:LEU:HD12	1.75	0.49
2:G:237:TYR:HD1	2:G:447:VAL:HG12	1.77	0.49
1:B:102:TRP:HD1	1:B:232:PHE:HZ	1.59	0.49
1:B:332:ALA:HB3	1:B:335:PHE:CE1	2.47	0.49
1:B:549:PHE:CE1	1:C:218:LYS:HB3	2.47	0.49
1:B:712:VAL:HG12	1:B:1042:GLY:HA2	1.93	0.49
1:C:163:GLU:OE1	1:C:164:TYR:N	2.46	0.49
1:C:528:PHE:O	1:C:534:THR:HA	2.11	0.49
1:A:71:ILE:HG23	1:A:252:ALA:HB2	1.93	0.49
1:A:391:LYS:HE3	1:A:393:ASP:HB3	1.95	0.49
1:B:100:ARG:HD3	1:B:171:LEU:HD23	1.95	0.49
1:B:108:MET:HB3	1:B:133:LEU:HB2	1.95	0.49
1:B:1011:LYS:HG3	1:B:1045:PHE:CE1	2.47	0.49
1:C:568:THR:O	1:C:570:GLU:N	2.45	0.49
2:D:439:LEU:HD21	2:D:540:HIS:HB2	1.94	0.49
1:B:100:ARG:O	1:B:119:ASN:N	2.32	0.49
1:B:381:SER:HB2	1:B:506:ASN:H	1.77	0.49
1:B:441:TYR:O	1:B:480:ASN:N	2.42	0.49
1:C:310:PRO:HA	1:C:525:CYS:O	2.11	0.49
1:C:915:SER:O	1:C:918:GLN:HG2	2.13	0.49
1:C:962:ASP:HA	1:C:966:ARG:NH1	2.28	0.49
2:D:244:VAL:HG23	2:D:262:LEU:HD11	1.95	0.49
2:G:403:ALA:HA	2:G:518:ARG:HG2	1.93	0.49
1:B:97:ASN:HB2	1:B:172:ASP:OD1	2.12	0.49
1:B:384:TYR:HB2	1:B:501:SER:HB2	1.95	0.49
1:B:886:ALA:HB1	1:B:896:GLN:HB3	1.93	0.49
1:B:1087:ILE:HG23	1:B:1096:GLN:HB2	1.95	0.49
1:A:804:LEU:O	1:A:808:LYS:HG2	2.12	0.49
1:A:1022:ARG:HH22	1:A:1025:PHE:HD1	1.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:SER:O	1:B:100:ARG:NH1	2.46	0.49
1:B:196:HIS:CE1	1:B:222:LYS:HG3	2.48	0.49
1:B:236:LEU:HD23	1:B:236:LEU:H	1.77	0.49
1:B:1062:PRO:HB3	1:C:900:TYR:CE1	2.48	0.49
1:C:660:SER:O	1:C:676:VAL:HG22	2.13	0.49
1:A:48:PHE:O	1:C:554:ARG:HG2	2.13	0.49
1:A:460:PRO:HG3	1:A:477:TRP:CD1	2.47	0.49
1:A:781:GLY:O	1:A:903:GLN:NE2	2.42	0.49
1:A:908:ASN:O	1:A:912:LYS:HD3	2.13	0.49
1:B:51:ASN:HA	1:B:267:TYR:O	2.13	0.49
1:B:115:VAL:HA	1:B:128:ALA:HA	1.95	0.49
1:B:892:ILE:HD12	1:B:1030:TYR:HB3	1.95	0.49
1:C:660:SER:O	1:C:675:ILE:HD12	2.13	0.49
1:A:1089:GLN:HE21	1:A:1092:PHE:HB3	1.77	0.49
1:A:1121:TYR:CZ	1:A:1123:PRO:HA	2.48	0.49
1:B:60:PHE:HD2	1:B:263:PHE:CG	2.31	0.49
1:B:647:TYR:HB2	1:B:678:TYR:CZ	2.47	0.49
1:B:888:ARG:NH1	1:B:1032:LEU:O	2.46	0.49
2:D:318:VAL:HG12	2:D:545:SER:HA	1.94	0.49
1:C:196:HIS:CE1	1:C:222:LYS:HG3	2.48	0.48
2:G:37:GLU:OE1	2:G:393:ARG:NH1	2.46	0.48
1:A:563:VAL:HG12	1:A:574:ILE:HD11	1.95	0.48
1:A:673:LYS:HB3	1:A:673:LYS:HE2	1.69	0.48
1:B:968:ASP:OD2	1:B:970:PRO:HD2	2.14	0.48
2:D:197:GLU:HB2	2:D:201:ASP:HB2	1.94	0.48
1:B:391:LYS:HE3	1:B:482:TYR:CD2	2.49	0.48
1:B:714:MET:HG3	1:B:757:GLN:NE2	2.29	0.48
1:C:686:SER:OG	1:C:687:SER:N	2.45	0.48
2:G:276:THR:HB	2:G:445:THR:OG1	2.13	0.48
2:G:358:ILE:HG13	2:G:379:ILE:HG13	1.94	0.48
1:A:184:ARG:HB3	1:A:186:PHE:CZ	2.48	0.48
1:A:547:GLN:O	1:A:564:ARG:NH2	2.46	0.48
1:B:546:PHE:HZ	1:B:553:GLY:HA3	1.78	0.48
1:B:589:THR:HA	1:B:592:SER:O	2.13	0.48
1:C:325:PRO:HG2	1:C:344:LYS:NZ	2.28	0.48
1:C:368:TYR:CZ	1:C:399:ALA:HB1	2.48	0.48
1:C:641:GLU:OE2	1:C:676:VAL:HG12	2.13	0.48
2:D:308:PHE:HZ	2:D:360:MET:HG2	1.77	0.48
1:A:269:GLU:HG2	3:J:1:NAG:H82	1.94	0.48
1:A:441:TYR:HD1	1:A:482:TYR:CD1	2.32	0.48
1:A:701:PHE:HB2	1:A:1050:TYR:CE1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ARG:HB2	1:B:245:TYR:CE2	2.48	0.48
1:B:1001:ILE:HD12	1:B:1001:ILE:H	1.79	0.48
1:C:388:PHE:CE2	1:C:497:VAL:HB	2.48	0.48
1:C:476:TYR:HB3	2:G:31:LYS:HD2	1.95	0.48
1:A:315:VAL:HA	1:A:529:ASN:HB3	1.95	0.48
1:A:412:LYS:HG2	1:A:448:LYS:HB3	1.96	0.48
1:B:53:LEU:HD13	1:B:266:LYS:HA	1.95	0.48
1:B:744:THR:HB	1:B:748:ARG:NH1	2.28	0.48
1:B:138:PHE:CZ	1:B:140:VAL:HG22	2.49	0.48
1:B:298:LYS:HG3	1:B:587:PRO:HA	1.95	0.48
1:B:337:SER:OG	1:B:439:TYR:HA	2.13	0.48
1:B:412:LYS:NZ	1:B:413:LEU:O	2.45	0.48
1:B:653:ILE:HD12	1:B:657:ILE:HG22	1.96	0.48
2:G:51:ASN:O	2:G:342:ALA:HB1	2.14	0.48
1:A:316:ARG:HH11	1:A:519:ASP:HA	1.78	0.48
1:A:878:GLN:HE22	1:C:694:THR:C	2.17	0.48
1:B:39:ARG:HD2	1:B:210:LEU:HD21	1.95	0.48
1:B:40:GLY:HA2	1:B:89:TYR:CD1	2.49	0.48
1:C:427:ARG:HG2	1:C:494:PRO:HD2	1.95	0.48
2:D:307:ILE:HG23	2:D:369:PHE:CD1	2.49	0.48
2:D:499:ASP:N	2:D:500:PRO:HD2	2.29	0.48
2:G:44:SER:HB3	2:G:351:LEU:HG	1.95	0.48
2:G:269:ASP:OD2	2:G:274:PHE:N	2.43	0.48
1:A:493:GLN:NE2	2:D:325:GLN:OE1	2.40	0.48
1:A:937:GLN:HB3	1:A:997:ARG:HH12	1.78	0.48
1:B:439:TYR:HD2	1:B:484:PHE:HE2	1.62	0.48
1:C:59:HIS:HE1	1:C:86:ASP:HB2	1.79	0.48
2:D:594:TRP:HE3	2:D:595:LEU:HD22	1.79	0.48
2:G:382:ASP:HA	2:G:385:TYR:CZ	2.49	0.48
2:G:450:LEU:HB2	2:G:451:PRO:HD3	1.95	0.48
1:A:303:THR:O	1:A:304:SER:OG	2.32	0.48
1:A:664:VAL:HG11	1:A:667:LEU:HB2	1.96	0.48
1:A:1124:LEU:HD23	1:A:1124:LEU:H	1.79	0.48
1:B:547:GLN:HG2	1:B:549:PHE:CZ	2.49	0.48
1:B:967:LEU:HD12	1:B:975:GLN:NE2	2.29	0.48
1:B:969:PRO:HB2	1:B:970:PRO:HD3	1.96	0.48
1:C:327:GLY:O	1:C:331:ASN:N	2.47	0.48
1:C:386:ASP:OD2	1:C:411:TYR:OH	2.23	0.48
1:C:460:PRO:HA	1:C:478:PRO:HD3	1.95	0.48
2:D:460:ARG:CZ	2:D:506:VAL:HG13	2.43	0.48
1:B:296:ILE:H	1:B:589:THR:CG2	2.26	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:ARG:NH2	1:B:1104:PHE:HB3	2.29	0.47
1:C:29:PRO:HG3	1:C:78:ASP:HB3	1.96	0.47
1:C:59:HIS:HB2	1:C:189:ARG:NH2	2.24	0.47
1:C:333:THR:O	1:C:496:ARG:NH1	2.44	0.47
1:C:345:ARG:HD2	1:C:382:ASN:HA	1.96	0.47
1:C:1111:VAL:HG23	1:C:1112:VAL:HG23	1.96	0.47
2:G:98:GLN:O	2:G:102:GLN:HG2	2.14	0.47
2:G:540:HIS:HA	2:G:587:TYR:CE1	2.49	0.47
1:A:383:VAL:HG23	1:A:502:PHE:CE1	2.49	0.47
1:A:1066:HIS:CE1	1:A:1120:VAL:H	2.32	0.47
1:A:1074:ARG:HG2	1:A:1102:ASN:O	2.15	0.47
1:C:364:THR:HB	1:C:423:ALA:HB3	1.94	0.47
1:C:462:SER:OG	1:C:466:LYS:N	2.47	0.47
2:D:56:GLU:HA	2:D:59:VAL:HG12	1.97	0.47
1:A:336:PRO:HB2	1:A:341:TRP:HA	1.96	0.47
1:B:26:ARG:HD2	1:B:79:ASN:H	1.79	0.47
1:B:391:LYS:HD2	1:B:393:ASP:HB2	1.94	0.47
1:B:696:ALA:HB2	1:C:878:GLN:OE1	2.14	0.47
1:B:1123:PRO:O	1:B:1126:PRO:HD2	2.15	0.47
1:C:291:VAL:HG13	1:C:293:SER:N	2.29	0.47
1:C:328:GLU:OE1	1:C:328:GLU:N	2.46	0.47
1:C:404:GLY:O	1:C:408:ASP:N	2.35	0.47
2:D:169:ARG:HH22	2:D:270:MET:HG3	1.79	0.47
1:A:129:CYS:HB3	1:A:131:PHE:CD2	2.48	0.47
1:A:343:ARG:HE	1:A:454:ARG:NH1	2.12	0.47
1:A:347:SER:HA	1:A:511:VAL:HG23	1.95	0.47
1:B:139:PHE:HB3	1:B:148:GLN:OE1	2.14	0.47
1:C:332:ALA:HB3	1:C:335:PHE:CE1	2.46	0.47
1:C:542:SER:HB2	1:C:573:ASP:N	2.29	0.47
1:C:705:ILE:HD12	1:C:1047:HIS:O	2.13	0.47
1:A:122:THR:HB	1:A:168:ASP:HB3	1.97	0.47
1:A:1062:PRO:HB3	1:B:900:TYR:CZ	2.50	0.47
1:B:371:SER:HB3	1:B:374:LYS:HE2	1.95	0.47
1:B:802:GLU:OE1	1:B:1038:ALA:HB3	2.14	0.47
1:C:26:ARG:HD2	1:C:77:PHE:HD2	1.80	0.47
1:C:746:LEU:HD22	1:C:991:VAL:HG21	1.96	0.47
2:D:36:ALA:HB1	2:D:69:TRP:HZ3	1.80	0.47
2:D:374:HIS:CE1	2:D:406:GLU:HG2	2.49	0.47
2:G:518:ARG:O	2:G:522:GLN:HB2	2.14	0.47
1:A:105:GLY:HA3	1:A:108:MET:SD	2.54	0.47
1:B:51:ASN:HA	1:B:266:LYS:NZ	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:HIS:ND1	1:B:664:VAL:HG22	2.30	0.47
1:B:1066:HIS:ND1	1:B:1119:THR:HA	2.29	0.47
2:D:41:TYR:CG	2:D:353:LYS:HD2	2.49	0.47
2:D:116:LEU:HD13	2:D:186:LEU:HB2	1.96	0.47
2:D:207:TYR:CE1	2:D:397:ASN:HB2	2.49	0.47
3:J:1:NAG:H61	3:J:2:NAG:C7	2.44	0.47
1:A:84:PHE:HB2	1:A:232:PHE:HB2	1.95	0.47
1:A:266:LYS:NZ	1:A:274:THR:OG1	2.43	0.47
1:A:551:GLN:N	1:B:46:ASP:OD1	2.40	0.47
1:B:162:PHE:CZ	1:B:164:TYR:HB2	2.49	0.47
1:B:459:VAL:H	1:B:478:PRO:HG3	1.78	0.47
1:B:780:PHE:HE2	1:B:785:PHE:HD2	1.61	0.47
1:B:791:ASP:O	1:B:794:LYS:HG2	2.15	0.47
1:C:27:THR:HB	1:C:76:ASN:HB3	1.96	0.47
1:C:116:ILE:HD12	1:C:118:MET:HE1	1.96	0.47
1:C:140:VAL:O	1:C:149:ILE:N	2.47	0.47
1:C:182:ASP:HB3	1:C:201:TYR:HE2	1.79	0.47
1:C:628:ASN:ND2	1:C:641:GLU:HB3	2.30	0.47
1:C:709:VAL:HB	1:C:930:LYS:NZ	2.30	0.47
2:D:237:TYR:CG	2:D:451:PRO:HG2	2.50	0.47
2:G:207:TYR:CE1	2:G:398:GLU:HG2	2.50	0.47
2:G:241:HIS:HA	2:G:244:VAL:HG22	1.96	0.47
2:G:560:LEU:HD23	2:G:564:GLU:HB2	1.95	0.47
1:A:84:PHE:CE1	1:A:88:ILE:HG12	2.50	0.47
1:A:531:ASN:HD21	1:A:566:PRO:HB3	1.76	0.47
1:A:937:GLN:HA	1:A:940:GLN:HB3	1.96	0.47
1:C:126:ILE:HG21	1:C:223:LEU:HD11	1.96	0.47
2:G:134:ASN:HB2	2:G:140:GLU:HB3	1.97	0.47
1:A:319:ASN:HA	1:A:567:LYS:NZ	2.29	0.47
1:A:753:ILE:HG22	1:A:757:GLN:NE2	2.25	0.47
1:B:267:TYR:CE1	1:B:273:ILE:HG12	2.50	0.47
1:B:342:GLU:HA	1:B:454:ARG:NH1	2.30	0.47
1:B:801:ILE:O	1:B:805:LEU:HD23	2.14	0.47
1:C:312:LYS:NZ	1:C:524:GLN:OE1	2.48	0.47
1:C:391:LYS:HB2	1:C:492:TYR:HA	1.96	0.47
1:C:430:ASP:OD1	1:C:439:TYR:OH	2.29	0.47
1:C:953:PHE:CE1	1:C:982:GLY:HA3	2.50	0.47
2:D:28:PHE:CE2	2:D:80:ALA:HB2	2.50	0.47
2:D:28:PHE:HE2	2:D:80:ALA:HB2	1.79	0.47
1:A:324:CYS:HB3	1:A:346:ILE:HG23	1.97	0.47
1:A:723:MET:SD	1:C:307:ARG:NH1	2.87	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:LEU:HD21	1:A:856:TYR:CE1	2.50	0.47
1:B:37:SER:H	1:B:64:ASP:N	2.13	0.47
1:B:140:VAL:O	1:B:149:ILE:N	2.35	0.47
1:B:261:THR:HG22	1:B:262:THR:N	2.29	0.47
1:B:1015:CYS:HB3	1:B:1034:SER:OG	2.14	0.47
1:C:220:ILE:HG22	1:C:221:PHE:CD1	2.50	0.47
1:C:389:VAL:HG22	1:C:496:ARG:HG2	1.95	0.47
2:D:152:MET:HE2	2:D:270:MET:SD	2.55	0.47
2:G:204:ARG:NH1	2:G:223:ILE:HD11	2.30	0.47
1:B:420:CYS:HB2	1:B:502:PHE:HE2	1.79	0.46
1:B:427:ARG:NH2	1:B:428:ASN:OD1	2.41	0.46
1:B:857:THR:HG21	1:B:1038:ALA:HB2	1.97	0.46
1:C:116:ILE:HG12	1:C:131:PHE:HE2	1.80	0.46
1:C:230:THR:HG21	5:C:1304:NAG:H83	1.97	0.46
2:D:315:PHE:HD1	2:D:320:LEU:HD12	1.80	0.46
2:D:381:TYR:HD1	2:D:558:LEU:HD12	1.80	0.46
2:G:269:ASP:OD1	2:G:269:ASP:N	2.47	0.46
1:A:900:TYR:CE1	1:C:1062:PRO:HB3	2.51	0.46
1:B:99:ILE:HA	1:B:236:LEU:HA	1.98	0.46
1:B:412:LYS:HB3	1:B:451:PRO:HA	1.97	0.46
1:B:759:ARG:HH22	1:B:763:GLU:CD	2.18	0.46
1:C:656:GLY:O	1:C:679:THR:HA	2.15	0.46
2:G:594:TRP:HE3	2:G:595:LEU:HD22	1.80	0.46
1:A:935:VAL:O	1:A:938:ASN:HB2	2.15	0.46
2:D:382:ASP:HA	2:D:385:TYR:CZ	2.50	0.46
2:G:177:ARG:HB2	2:G:498:CYS:HB2	1.97	0.46
1:A:142:LEU:HB2	1:A:149:ILE:HD11	1.96	0.46
1:A:663:THR:HA	1:A:673:LYS:HG2	1.96	0.46
1:C:971:GLU:OE1	1:C:971:GLU:N	2.48	0.46
2:D:127:TYR:HA	2:D:172:VAL:HG21	1.98	0.46
2:G:122:THR:O	2:G:126:ILE:HG12	2.15	0.46
2:G:435:GLU:OE2	2:G:540:HIS:NE2	2.48	0.46
1:A:39:ARG:HG2	1:A:210:LEU:HD11	1.97	0.46
1:A:49:ARG:HH12	1:A:54:HIS:CD2	2.34	0.46
1:A:127:ARG:NH1	1:A:160:CYS:SG	2.89	0.46
1:A:143:LYS:HB2	1:A:239:PHE:HB3	1.98	0.46
1:A:753:ILE:C	1:A:757:GLN:HE22	2.19	0.46
1:B:97:ASN:HB3	1:B:171:LEU:HD21	1.97	0.46
1:C:284:LEU:O	1:C:288:LYS:HG3	2.15	0.46
1:C:482:TYR:HD2	1:C:484:PHE:CE2	2.33	0.46
1:C:652:PRO:HA	1:C:658:CYS:SG	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:143:LEU:H	2:G:143:LEU:HD23	1.81	0.46
2:G:297:MET:HG3	2:G:423:LEU:HD11	1.96	0.46
1:A:277:VAL:HG21	1:A:288:LYS:HE2	1.96	0.46
1:A:326:PHE:CZ	1:A:500:LEU:HD21	2.50	0.46
1:A:889:PHE:CD2	1:A:899:LEU:HB2	2.50	0.46
1:B:312:LYS:HG3	1:B:521:ILE:HD13	1.96	0.46
1:C:24:ASP:OD1	1:C:24:ASP:N	2.47	0.46
1:C:326:PHE:HE1	1:C:351:ALA:HA	1.81	0.46
1:C:430:ASP:OD1	1:C:496:ARG:NH2	2.49	0.46
1:C:1113:ILE:HD12	1:C:1113:ILE:H	1.81	0.46
2:D:204:ARG:HG2	2:D:222:LEU:HD23	1.96	0.46
2:D:419:LYS:HE3	2:D:426:PRO:O	2.16	0.46
1:A:365:PHE:CD1	1:A:422:LEU:HA	2.51	0.46
1:B:317:PHE:HE1	1:B:532:GLY:H	1.62	0.46
1:B:791:ASP:H	1:B:794:LYS:HD2	1.81	0.46
1:B:971:GLU:O	1:B:974:VAL:HG22	2.15	0.46
1:B:985:GLN:NE2	1:C:742:PHE:HE1	2.07	0.46
2:G:459:TRP:HZ2	2:G:473:TRP:HB3	1.79	0.46
1:A:69:ARG:HB2	1:A:254:PHE:CD2	2.51	0.46
1:A:118:MET:O	1:A:124:LEU:HA	2.16	0.46
1:A:384:TYR:HB2	1:A:501:SER:OG	2.16	0.46
1:A:690:TYR:CE1	1:B:880:PRO:HA	2.50	0.46
1:B:42:TYR:HB3	1:B:187:VAL:HG21	1.98	0.46
1:B:431:ALA:HB2	1:B:494:PRO:CD	2.46	0.46
1:C:51:ASN:N	1:C:268:ASP:O	2.44	0.46
1:C:91:ALA:HB1	1:C:183:LEU:HD11	1.97	0.46
2:D:25:ALA:O	2:D:29:LEU:HD23	2.15	0.46
2:G:346:PRO:HB3	2:G:360:MET:HG2	1.98	0.46
1:B:50:SER:O	1:B:52:VAL:HG13	2.16	0.46
1:C:21:LEU:HB2	1:C:138:PHE:HZ	1.80	0.46
1:A:193:GLY:O	1:A:225:LEU:N	2.47	0.46
1:A:759:ARG:HG3	1:A:762:ARG:NH2	2.31	0.46
1:B:412:LYS:HA	1:B:412:LYS:HD2	1.81	0.46
1:B:911:ASN:O	1:B:914:ILE:HG22	2.15	0.46
1:C:223:LEU:HD22	1:C:225:LEU:HB3	1.98	0.46
1:C:287:LEU:HD21	1:C:296:ILE:HG21	1.98	0.46
1:C:338:VAL:HG13	1:C:410:ASN:HB3	1.97	0.46
1:C:951:SER:OG	1:C:953:PHE:HE2	1.99	0.46
1:A:223:LEU:HA	1:A:224:PRO:HD3	1.78	0.45
1:A:746:LEU:O	1:A:750:LEU:HD13	2.16	0.45
1:B:713:SER:O	1:B:1041:HIS:ND1	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:643:VAL:HG21	1:C:676:VAL:HB	1.98	0.45
1:C:801:ILE:O	1:C:805:LEU:HD23	2.16	0.45
2:D:38:ASP:OD1	2:D:353:LYS:NZ	2.45	0.45
2:D:408:MET:SD	2:D:408:MET:N	2.89	0.45
2:D:459:TRP:HD1	2:D:480:MET:HE1	1.78	0.45
1:A:664:VAL:C	1:A:666:SER:H	2.19	0.45
1:A:966:ARG:HG3	1:A:967:LEU:HG	1.97	0.45
1:B:72:THR:HG23	1:B:251:ALA:HB3	1.98	0.45
1:B:98:VAL:HA	1:B:100:ARG:NH2	2.32	0.45
1:B:126:ILE:HD13	1:B:223:LEU:HD11	1.98	0.45
1:B:190:ASN:HA	1:B:196:HIS:H	1.81	0.45
1:C:51:ASN:N	1:C:267:TYR:O	2.50	0.45
1:C:287:LEU:O	1:C:291:VAL:HG12	2.15	0.45
2:G:356:PHE:HB3	2:G:379:ILE:HD12	1.98	0.45
1:A:69:ARG:HD3	1:A:71:ILE:HD11	1.99	0.45
1:A:550:GLN:HA	1:B:46:ASP:OD2	2.16	0.45
1:A:857:THR:O	1:A:861:VAL:HG23	2.17	0.45
1:B:985:GLN:NE2	1:C:742:PHE:CE1	2.82	0.45
1:B:1012:MET:HE1	1:B:1016:VAL:HG21	1.99	0.45
1:B:1012:MET:O	1:B:1016:VAL:HB	2.17	0.45
1:C:50:SER:O	1:C:52:VAL:HG23	2.16	0.45
1:C:482:TYR:HD2	1:C:484:PHE:CZ	2.35	0.45
1:C:546:PHE:CZ	1:C:562:SER:HB2	2.51	0.45
2:G:147:GLY:O	2:G:151:ILE:HG12	2.16	0.45
2:G:392:LEU:HG	2:G:562:LYS:HB3	1.98	0.45
1:A:78:ASP:OD1	1:A:78:ASP:N	2.50	0.45
1:A:334:THR:HA	1:A:496:ARG:HH21	1.80	0.45
1:C:54:HIS:CD2	1:C:56:VAL:HB	2.52	0.45
1:C:932:GLN:O	1:C:936:ASN:ND2	2.49	0.45
2:G:90:ASN:OD1	2:G:91:LEU:N	2.50	0.45
1:A:663:THR:CA	1:A:673:LYS:HA	2.45	0.45
1:A:1066:HIS:CE1	1:A:1120:VAL:HG12	2.52	0.45
1:B:341:TRP:HA	1:B:387:SER:O	2.17	0.45
1:B:1028:LYS:HE2	1:B:1028:LYS:HA	1.98	0.45
1:C:67:VAL:CG2	1:C:254:PHE:HB3	2.47	0.45
1:C:406:ILE:HD12	1:C:441:TYR:HB2	1.98	0.45
1:C:659:ALA:HA	1:C:676:VAL:O	2.16	0.45
2:D:88:ILE:HG21	2:D:93:VAL:HG23	1.98	0.45
2:D:169:ARG:NH2	2:D:270:MET:HG3	2.31	0.45
2:G:132:VAL:O	2:G:141:CYS:HA	2.16	0.45
1:A:90:PHE:CE1	1:A:253:TYR:HB2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LYS:HZ2	1:A:572:LEU:HD22	1.80	0.45
1:A:695:ILE:HB	1:A:1060:THR:HG21	1.99	0.45
1:B:47:ILE:HG22	1:B:49:ARG:HD2	1.97	0.45
1:B:371:SER:HB3	1:B:374:LYS:NZ	2.32	0.45
1:B:409:TYR:CZ	1:B:448:LYS:HE2	2.51	0.45
1:B:780:PHE:O	1:B:783:PHE:N	2.36	0.45
1:B:856:TYR:O	1:B:860:LEU:HD23	2.16	0.45
1:C:664:VAL:HG13	1:C:666:SER:H	1.82	0.45
1:C:1087:ILE:CG2	1:C:1096:GLN:HB2	2.46	0.45
2:D:237:TYR:HD1	2:D:447:VAL:HG12	1.82	0.45
1:A:298:LYS:NZ	1:A:588:GLY:H	2.15	0.45
1:A:430:ASP:C	1:A:436:ASN:HD22	2.20	0.45
1:A:719:VAL:HG23	1:A:841:LEU:HD12	1.98	0.45
1:A:991:VAL:O	1:A:995:LEU:HD23	2.17	0.45
1:B:1022:ARG:HB2	1:C:1014:GLU:OE2	2.16	0.45
1:C:419:GLY:HA3	1:C:500:LEU:O	2.17	0.45
1:C:441:TYR:HB3	1:C:482:TYR:HE1	1.80	0.45
2:D:47:SER:O	2:D:51:ASN:ND2	2.50	0.45
2:D:177:ARG:HD2	2:D:498:CYS:HB2	1.97	0.45
2:G:91:LEU:HD21	2:G:212:VAL:HG22	1.98	0.45
1:A:127:ARG:HG3	1:A:163:GLU:OE1	2.17	0.45
1:A:839:ASN:HD21	1:C:559:PHE:HZ	1.65	0.45
1:B:315:VAL:HA	1:B:529:ASN:HB2	1.98	0.45
1:B:359:SER:HB3	5:B:1302:NAG:H4	1.99	0.45
1:B:663:THR:HA	1:B:673:LYS:HA	1.98	0.45
1:B:794:LYS:HD3	1:B:798:ARG:O	2.17	0.45
1:C:85:LYS:H	1:C:88:ILE:HD11	1.81	0.45
1:C:441:TYR:HD2	1:C:482:TYR:CD1	2.35	0.45
1:B:547:GLN:HG3	1:B:548:PRO:HD2	1.98	0.45
1:A:325:PRO:HD2	1:A:346:ILE:HA	1.99	0.45
1:B:57:GLN:HE22	1:B:260:PRO:HB2	1.81	0.45
1:B:722:ASN:C	1:B:724:TYR:H	2.20	0.45
1:B:915:SER:O	1:B:919:GLU:HG2	2.17	0.45
1:B:1083:THR:HG23	3:O:1:NAG:HN2	1.81	0.45
1:C:39:ARG:NH2	1:C:211:PRO:O	2.49	0.45
1:C:106:SER:O	1:C:230:THR:OG1	2.35	0.45
2:D:270:MET:HB3	2:D:271:TRP:CE3	2.52	0.45
2:G:51:ASN:HB3	2:G:359:LEU:HD12	1.98	0.45
2:G:307:ILE:HG23	2:G:369:PHE:CD1	2.50	0.45
1:A:19:LYS:HD3	1:A:152:TYR:CE1	2.52	0.44
1:A:365:PHE:CE1	1:A:422:LEU:HA	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:MET:CE	1:A:1008:ALA:HA	2.47	0.44
1:A:770:GLN:HB3	1:C:684:ALA:O	2.17	0.44
1:A:1124:LEU:HA	1:A:1127:GLU:OE2	2.17	0.44
1:B:1067:GLU:O	1:B:1069:LYS:NZ	2.47	0.44
1:C:103:VAL:HG23	1:C:235:LEU:HD21	1.99	0.44
1:C:487:THR:HB	2:G:357:ARG:NH2	2.32	0.44
2:D:119:ILE:HD12	2:D:179:LEU:HD22	1.99	0.44
2:D:430:GLU:OE2	2:D:541:LYS:HD3	2.17	0.44
1:A:84:PHE:CZ	1:A:87:GLY:HA2	2.52	0.44
1:A:1015:CYS:HB3	1:A:1034:SER:OG	2.17	0.44
1:B:346:ILE:HB	1:B:383:VAL:HG13	1.98	0.44
1:B:410:ASN:HD21	1:B:442:ARG:H	1.65	0.44
1:B:705:ILE:HA	1:B:1047:HIS:O	2.18	0.44
1:C:123:ASN:HB3	1:C:168:ASP:OD1	2.16	0.44
2:G:21:ILE:HD12	2:G:87:GLU:HB2	1.99	0.44
1:A:51:ASN:N	1:A:268:ASP:O	2.31	0.44
1:A:99:ILE:HG12	1:A:236:LEU:HG	2.00	0.44
1:A:122:THR:HA	1:A:169:PHE:N	2.32	0.44
1:A:1089:GLN:NE2	1:A:1092:PHE:O	2.50	0.44
1:B:37:SER:H	1:B:64:ASP:HA	1.82	0.44
1:C:48:PHE:CZ	1:C:50:SER:HB3	2.52	0.44
1:C:133:LEU:HD11	1:C:137:PRO:HG3	1.98	0.44
1:C:194:PHE:HA	1:C:223:LEU:O	2.18	0.44
1:C:659:ALA:HB1	1:C:675:ILE:HD11	2.00	0.44
2:D:381:TYR:CD1	2:D:558:LEU:HD12	2.53	0.44
2:D:403:ALA:HA	2:D:518:ARG:HG2	1.98	0.44
2:D:594:TRP:CE3	2:D:595:LEU:HD22	2.53	0.44
2:G:119:ILE:HD12	2:G:179:LEU:HD22	1.98	0.44
1:A:103:VAL:HA	1:A:115:VAL:O	2.17	0.44
1:A:307:ARG:NE	1:A:308:VAL:O	2.51	0.44
1:A:322:ASN:HD22	1:A:348:ASN:HD22	1.64	0.44
1:A:1080:PHE:HB2	1:A:1085:TRP:CE2	2.52	0.44
1:B:49:ARG:HB3	1:B:52:VAL:CG2	2.47	0.44
1:C:411:TYR:CZ	1:C:413:LEU:HD21	2.52	0.44
1:C:723:MET:HA	1:C:727:GLY:HA2	1.99	0.44
2:D:275:TRP:HB3	2:D:444:LEU:HD12	1.99	0.44
2:G:50:TYR:HA	2:G:58:ASN:HB3	2.00	0.44
2:G:380:GLN:HG3	2:G:558:LEU:HD21	1.99	0.44
1:A:264:MET:O	1:A:276:ALA:HA	2.17	0.44
1:A:328:GLU:HB3	1:A:335:PHE:HE1	1.82	0.44
1:A:406:ILE:HG23	1:A:441:TYR:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:LYS:HE2	1:C:576:PRO:HG2	1.99	0.44
1:A:884:GLN:HE21	1:A:888:ARG:HE	1.66	0.44
1:A:892:ILE:HD12	1:A:1030:TYR:HB3	2.00	0.44
1:B:400:PRO:HB3	1:B:415:ASP:HA	1.98	0.44
1:B:642:HIS:NE2	1:B:643:VAL:O	2.51	0.44
1:B:726:CYS:SG	1:B:733:ALA:N	2.91	0.44
1:C:210:LEU:HD22	1:C:254:PHE:CG	2.52	0.44
1:C:316:ARG:HH22	1:C:528:PHE:HB2	1.83	0.44
1:C:562:SER:HA	1:C:572:LEU:O	2.17	0.44
1:C:838:PHE:O	1:C:839:ASN:HB2	2.17	0.44
1:C:1105:VAL:HG13	1:C:1106:SER:N	2.31	0.44
1:C:1115:ILE:O	1:C:1116:ILE:HD13	2.18	0.44
2:D:560:LEU:HD23	2:D:564:GLU:HB2	2.00	0.44
1:A:142:LEU:HD23	1:A:145:ASN:HD22	1.82	0.44
1:A:414:PRO:HD2	1:A:417:PHE:CD2	2.47	0.44
1:A:439:TYR:O	1:A:482:TYR:HB2	2.18	0.44
1:A:873:ALA:HB1	1:C:1029:GLY:HA2	2.00	0.44
1:B:436:ASN:H	1:B:484:PHE:HB2	1.83	0.44
1:B:682:LEU:HB2	1:C:771:MET:HE1	1.99	0.44
1:B:698:PRO:HG2	1:B:1052:PRO:HB3	1.99	0.44
1:B:732:CYS:SG	1:B:733:ALA:N	2.90	0.44
1:B:805:LEU:HD13	1:B:928:LEU:HD21	2.00	0.44
1:C:489:GLY:O	1:C:493:GLN:HG3	2.17	0.44
1:C:592:SER:OG	1:C:593:SER:N	2.51	0.44
1:C:663:THR:HG23	1:C:673:LYS:NZ	2.32	0.44
1:C:998:ALA:HA	1:C:1001:ILE:HG22	1.99	0.44
2:D:237:TYR:CD1	2:D:451:PRO:HG2	2.52	0.44
2:G:88:ILE:HG21	2:G:93:VAL:HG23	2.00	0.44
2:G:485:VAL:HG12	2:G:487:VAL:HG23	1.99	0.44
1:A:389:VAL:HG11	1:A:430:ASP:HB3	2.00	0.44
1:A:941:ALA:O	1:A:944:THR:OG1	2.30	0.44
1:A:966:ARG:HH12	1:A:975:GLN:HE21	1.65	0.44
1:B:195:LEU:HB2	1:B:225:LEU:HD12	2.00	0.44
1:B:633:GLN:OE1	1:B:633:GLN:N	2.43	0.44
2:G:439:LEU:HB3	2:G:591:LEU:HD22	1.99	0.44
1:A:637:LEU:HD13	1:A:640:ALA:HB3	2.00	0.44
1:A:1108:SER:OG	1:A:1110:ASP:OD1	2.27	0.44
1:B:242:ARG:HB2	1:B:245:TYR:CD2	2.53	0.44
1:B:913:ALA:O	1:B:916:GLN:HG2	2.18	0.44
1:B:980:ILE:O	1:B:984:LEU:HD23	2.18	0.44
1:C:111:LYS:HE3	5:C:1302:NAG:H4	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:LYS:HE2	1:C:196:HIS:NE2	2.33	0.44
1:C:225:LEU:HD12	1:C:227:ILE:HG12	1.99	0.44
2:D:37:GLU:HA	2:D:390:PHE:CE1	2.53	0.44
2:G:538:PRO:HD2	2:G:541:LYS:NZ	2.33	0.44
1:A:26:ARG:NH1	1:A:79:ASN:HB3	2.33	0.44
1:B:58:ASP:O	1:B:260:PRO:HA	2.17	0.44
1:B:123:ASN:ND2	1:B:165:VAL:HG13	2.33	0.44
1:B:705:ILE:HG22	1:B:1048:VAL:HG22	2.00	0.44
1:C:470:PRO:N	1:C:471:PRO:HD2	2.33	0.44
1:C:961:ASN:OD1	1:C:962:ASP:N	2.51	0.44
2:D:178:PRO:O	2:D:182:GLU:OE1	2.36	0.44
2:G:406:GLU:HG3	2:G:518:ARG:HH11	1.83	0.44
2:G:450:LEU:HD21	2:G:519:THR:HG21	1.98	0.44
2:G:474:MET:HE1	2:G:497:TYR:HB2	1.99	0.44
1:A:113:GLN:OE1	1:A:161:THR:OG1	2.34	0.43
1:A:190:ASN:HB2	1:A:195:LEU:HD12	1.99	0.43
1:B:238:ALA:O	1:B:240:PRO:HD3	2.18	0.43
1:B:284:LEU:HB2	1:B:595:VAL:HG11	2.00	0.43
1:B:551:GLN:NE2	1:B:564:ARG:HB3	2.33	0.43
1:B:1080:PHE:HB2	1:B:1085:TRP:CE2	2.53	0.43
1:C:870:THR:HG21	1:C:877:LEU:HD12	1.99	0.43
2:G:535:HIS:NE2	2:G:537:GLY:O	2.51	0.43
1:A:298:LYS:CG	1:A:651:ILE:HD11	2.39	0.43
1:B:632:THR:HG23	1:B:634:ALA:N	2.33	0.43
1:B:973:GLU:HA	1:B:976:ILE:HD12	2.00	0.43
1:C:416:ASP:OD1	1:C:417:PHE:N	2.51	0.43
1:A:101:GLY:CA	1:A:235:LEU:HB2	2.48	0.43
1:A:409:TYR:CE2	1:A:444:LEU:HD23	2.53	0.43
1:A:441:TYR:CD1	1:A:482:TYR:HA	2.53	0.43
1:A:470:PRO:HA	1:A:475:CYS:O	2.18	0.43
1:A:1062:PRO:HG3	1:B:883:MET:HE1	2.00	0.43
1:B:102:TRP:CD1	1:B:234:THR:HG22	2.53	0.43
1:B:131:PHE:HD1	1:B:154:PHE:HB3	1.84	0.43
1:B:641:GLU:OE1	1:B:667:LEU:HD13	2.18	0.43
1:C:95:LYS:HB3	1:C:181:LYS:H	1.83	0.43
1:C:284:LEU:HD12	1:C:284:LEU:HA	1.84	0.43
1:C:941:ALA:HB1	1:C:990:TYR:HE1	1.84	0.43
1:C:1110:ASP:OD1	1:C:1111:VAL:N	2.51	0.43
2:G:284:PRO:HG3	2:G:440:LEU:HD13	1.99	0.43
2:G:536:GLU:HG2	2:G:537:GLY:N	2.33	0.43
2:G:581:VAL:HG22	2:G:584:LEU:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:HH21	1:B:520:LEU:N	2.16	0.43
1:C:43:TYR:CE2	1:C:273:ILE:HG13	2.54	0.43
1:C:73:PHE:HD2	1:C:75:LEU:HG	1.84	0.43
1:C:194:PHE:HB2	1:C:196:HIS:NE2	2.32	0.43
1:C:931:LEU:HD13	1:C:931:LEU:HA	1.88	0.43
2:D:190:MET:SD	2:D:194:ASN:ND2	2.92	0.43
2:D:245:ARG:HG2	2:D:262:LEU:HD21	2.00	0.43
2:G:284:PRO:HD3	2:G:440:LEU:HD22	2.01	0.43
2:G:311:ALA:HA	2:G:373:HIS:CE1	2.54	0.43
1:A:47:ILE:CG2	1:C:554:ARG:HD2	2.49	0.43
1:A:581:GLY:HA3	1:A:600:GLN:HE22	1.84	0.43
1:A:733:ALA:O	1:A:737:LEU:HB2	2.18	0.43
1:B:287:LEU:HD21	1:B:296:ILE:HG21	2.01	0.43
1:B:482:TYR:CE2	1:B:484:PHE:CE1	3.07	0.43
1:C:98:VAL:HA	1:C:100:ARG:NH2	2.34	0.43
1:C:599:TYR:O	1:C:635:GLY:HA3	2.18	0.43
1:C:808:LYS:NZ	1:C:923:THR:O	2.49	0.43
2:D:19:SER:OG	2:D:20:THR:N	2.51	0.43
1:A:306:PHE:N	1:A:580:GLY:O	2.27	0.43
1:A:391:LYS:O	1:A:395:VAL:HG23	2.19	0.43
1:A:960:LEU:O	1:A:964:LEU:HG	2.18	0.43
1:B:70:PHE:HD2	1:B:253:TYR:CE2	2.36	0.43
1:B:117:ILE:HG13	1:B:126:ILE:HG12	1.99	0.43
1:B:657:ILE:HD13	1:B:679:THR:HA	2.01	0.43
1:C:39:ARG:N	1:C:213:GLY:O	2.51	0.43
1:C:88:ILE:HG13	1:C:232:PHE:CE1	2.53	0.43
2:D:406:GLU:HG3	2:D:518:ARG:HH11	1.83	0.43
2:G:25:ALA:O	2:G:29:LEU:HD23	2.19	0.43
2:G:344:CYS:HB3	2:G:361:CYS:HB2	1.88	0.43
3:L:1:NAG:H61	3:L:2:NAG:C7	2.49	0.43
1:A:705:ILE:O	1:A:917:ILE:HD11	2.18	0.43
1:A:957:SER:OG	1:A:962:ASP:HB2	2.18	0.43
1:B:425:ASN:HB2	1:B:495:TYR:CZ	2.54	0.43
1:B:725:ILE:HD13	1:B:984:LEU:HD21	2.00	0.43
2:G:308:PHE:HE1	2:G:360:MET:HE3	1.83	0.43
2:G:520:LEU:HD22	2:G:579:MET:HE2	2.00	0.43
1:A:412:LYS:HB3	1:A:449:LEU:H	1.84	0.43
1:A:710:MET:HA	1:A:711:PRO:HD3	1.90	0.43
1:A:1032:LEU:HA	1:A:1032:LEU:HD23	1.80	0.43
1:B:95:LYS:NZ	1:B:250:ALA:HB3	2.33	0.43
1:C:74:GLY:HA2	1:C:248:THR:OG1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:VAL:HG13	1:C:239:PHE:HE2	1.83	0.43
1:C:198:TYR:HA	1:C:219:PRO:HA	2.01	0.43
1:C:588:GLY:O	1:C:591:THR:N	2.51	0.43
2:G:107:VAL:HG13	2:G:107:VAL:O	2.19	0.43
2:G:181:GLU:HA	2:G:473:TRP:HH2	1.84	0.43
2:G:199:TYR:HB3	2:G:464:PHE:CD2	2.54	0.43
1:A:102:TRP:HB3	1:A:232:PHE:HE1	1.84	0.43
1:A:357:TYR:HD1	1:A:365:PHE:CE2	2.36	0.43
1:A:913:ALA:HA	1:A:916:GLN:OE1	2.19	0.43
1:B:85:LYS:HB2	1:B:257:TYR:CE2	2.54	0.43
1:B:141:VAL:HG11	1:B:173:LEU:HD12	2.01	0.43
1:B:195:LEU:HB3	1:B:223:LEU:HB2	2.00	0.43
1:B:913:ALA:HA	1:B:916:GLN:OE1	2.19	0.43
1:C:391:LYS:HD2	1:C:492:TYR:CD1	2.54	0.43
1:C:460:PRO:HB2	1:C:475:CYS:HB3	2.01	0.43
2:D:407:ILE:HD11	2:D:525:PHE:HB2	2.00	0.43
2:G:56:GLU:HA	2:G:59:VAL:HG12	2.01	0.43
1:A:98:VAL:HG22	1:A:239:PHE:HE1	1.84	0.43
1:A:259:LYS:HA	1:A:259:LYS:HD3	1.79	0.43
1:A:320:ILE:O	1:A:514:PRO:HD3	2.19	0.43
1:A:356:LEU:HD13	1:A:422:LEU:HD13	2.00	0.43
1:A:372:ALA:HA	1:A:375:LEU:HB2	2.00	0.43
1:A:753:ILE:HD11	1:A:995:LEU:HD22	2.01	0.43
1:B:19:LYS:HA	1:B:19:LYS:HD3	1.71	0.43
1:B:51:ASN:HA	1:B:266:LYS:HZ2	1.84	0.43
1:B:585:ILE:HB	1:B:596:ALA:HB3	2.01	0.43
1:C:628:ASN:HD22	1:C:641:GLU:HB3	1.82	0.43
1:C:902:ASN:O	1:C:906:ILE:HG13	2.19	0.43
2:D:36:ALA:HB1	2:D:69:TRP:CZ3	2.54	0.43
2:D:450:LEU:HD22	2:D:516:TYR:CD1	2.54	0.43
2:D:462:MET:HB3	2:D:467:GLU:HB3	2.01	0.43
2:D:488:VAL:HG11	2:D:610:TRP:O	2.19	0.43
2:G:144:LEU:HD11	2:G:270:MET:HG3	2.01	0.43
1:A:121:SER:HA	1:A:171:LEU:HB3	2.01	0.42
1:A:130:ASN:HB3	1:A:159:ASN:HB2	2.00	0.42
1:A:181:LYS:HA	1:A:205:SER:HA	2.01	0.42
1:A:382:ASN:HB3	1:A:384:TYR:CZ	2.54	0.42
1:A:528:PHE:CD1	1:A:539:LEU:HD11	2.53	0.42
1:B:37:SER:N	1:B:64:ASP:H	2.15	0.42
1:B:184:ARG:HB3	1:B:186:PHE:CZ	2.54	0.42
1:B:417:PHE:CE2	1:B:501:SER:HA	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:PHE:CE2	1:B:899:LEU:HD12	2.54	0.42
1:C:931:LEU:HD11	1:C:1042:GLY:HA3	2.01	0.42
2:D:450:LEU:HB2	2:D:451:PRO:HD3	2.00	0.42
2:D:482:ARG:HD3	2:D:608:THR:O	2.18	0.42
2:G:155:SER:O	2:G:252:TYR:OH	2.36	0.42
2:G:198:ASP:OD1	2:G:201:ASP:N	2.49	0.42
2:G:237:TYR:CD1	2:G:451:PRO:HG2	2.54	0.42
2:G:270:MET:HB2	2:G:271:TRP:CE3	2.54	0.42
1:A:348:ASN:O	1:A:348:ASN:ND2	2.52	0.42
1:A:446:HIS:HA	1:A:461:PHE:HD1	1.83	0.42
1:A:482:TYR:CD2	1:A:483:GLY:N	2.87	0.42
1:A:1073:PRO:HA	1:A:1103:THR:HG22	2.00	0.42
1:B:60:PHE:HD2	1:B:263:PHE:CD1	2.37	0.42
1:B:371:SER:HB3	1:B:374:LYS:CE	2.49	0.42
1:B:381:SER:O	1:B:503:GLU:HB2	2.19	0.42
1:B:809:VAL:HB	1:B:1040:PRO:HG2	2.01	0.42
1:C:91:ALA:O	1:C:253:TYR:HB2	2.19	0.42
1:C:116:ILE:HB	1:C:118:MET:CE	2.48	0.42
2:D:538:PRO:HD2	2:D:541:LYS:HZ3	1.84	0.42
2:G:458:LYS:O	2:G:462:MET:HG2	2.19	0.42
2:G:462:MET:HA	2:G:465:LYS:HB3	2.00	0.42
1:A:103:VAL:HG23	1:A:235:LEU:HD11	2.01	0.42
1:A:343:ARG:HB3	1:A:386:ASP:OD1	2.20	0.42
1:A:516:LEU:HD23	1:A:516:LEU:O	2.20	0.42
1:A:709:VAL:HG13	1:A:931:LEU:HG	2.01	0.42
1:A:732:CYS:C	1:A:734:ASN:H	2.23	0.42
1:B:302:GLN:OE1	1:B:583:SER:HB3	2.18	0.42
1:B:441:TYR:CE2	1:B:443:SER:HB3	2.51	0.42
1:C:128:ALA:N	1:C:162:PHE:O	2.33	0.42
1:C:933:ASP:O	1:C:937:GLN:HG2	2.19	0.42
2:D:365:THR:HG22	2:D:367:ASP:H	1.83	0.42
2:G:372:ALA:O	2:G:376:MET:HG2	2.19	0.42
1:A:714:MET:SD	1:A:938:ASN:ND2	2.92	0.42
1:B:184:ARG:HE	1:B:186:PHE:HZ	1.66	0.42
1:B:440:LYS:HG2	1:B:481:ASP:HB3	2.01	0.42
1:B:634:ALA:HA	1:C:845:PRO:HG3	2.02	0.42
1:C:441:TYR:HB3	1:C:482:TYR:CE1	2.55	0.42
1:C:712:VAL:HG12	1:C:1042:GLY:HA2	2.01	0.42
2:D:315:PHE:HA	2:D:318:VAL:HG22	2.01	0.42
2:D:381:TYR:OH	2:D:395:GLY:HA2	2.20	0.42
1:A:77:PHE:CE2	1:A:79:ASN:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LYS:NZ	1:A:413:LEU:O	2.50	0.42
1:B:417:PHE:CD2	1:B:452:PHE:HZ	2.38	0.42
1:C:36:SER:OG	1:C:65:SER:N	2.51	0.42
2:G:204:ARG:HG2	2:G:222:LEU:HD23	2.01	0.42
2:G:347:THR:HG1	2:G:349:TRP:HE1	1.67	0.42
2:G:538:PRO:HD2	2:G:541:LYS:HZ3	1.85	0.42
1:A:84:PHE:HE1	1:A:188:PHE:HB2	1.85	0.42
1:A:187:VAL:O	1:A:197:VAL:HA	2.20	0.42
1:A:348:ASN:H	1:A:510:THR:HB	1.85	0.42
1:A:353:TYR:HB3	1:A:376:ASN:HB3	2.02	0.42
1:A:372:ALA:HA	1:A:375:LEU:HD13	2.01	0.42
1:A:522:LYS:NZ	1:A:539:LEU:HB3	2.35	0.42
1:A:682:LEU:HD21	1:B:852:MET:CG	2.49	0.42
1:A:1014:GLU:OE2	1:C:1022:ARG:NE	2.48	0.42
1:B:106:SER:O	1:B:231:ASN:ND2	2.29	0.42
1:B:1063:ALA:C	1:B:1115:ILE:HG13	2.39	0.42
1:C:390:VAL:HG11	1:C:398:ILE:CD1	2.49	0.42
1:C:977:ASP:HA	1:C:980:ILE:HG12	2.02	0.42
2:D:166:GLU:OE2	2:D:497:TYR:OH	2.26	0.42
2:G:308:PHE:CE2	2:G:333:LEU:HD12	2.54	0.42
1:A:328:GLU:HB3	1:A:335:PHE:CE1	2.55	0.42
1:A:410:ASN:CG	1:A:442:ARG:H	2.21	0.42
1:B:59:HIS:CD2	1:B:260:PRO:HB3	2.55	0.42
1:B:125:VAL:HG13	1:B:163:GLU:OE2	2.19	0.42
1:B:189:ARG:O	1:B:196:HIS:HB2	2.20	0.42
1:B:932:GLN:HG3	1:B:936:ASN:OD1	2.19	0.42
1:C:258:LEU:C	1:C:259:LYS:HD2	2.39	0.42
1:C:488:ASN:HD21	2:G:353:LYS:HD3	1.85	0.42
1:C:905:GLN:O	1:C:909:GLN:HG3	2.19	0.42
2:D:252:TYR:HB3	2:D:255:TYR:CD2	2.51	0.42
2:D:589:GLU:HB3	2:D:590:PRO:HD3	2.01	0.42
2:G:270:MET:HB2	2:G:271:TRP:CD2	2.55	0.42
2:G:400:PHE:CE2	2:G:566:TRP:HB2	2.54	0.42
2:G:417:HIS:NE2	2:G:421:ILE:HD11	2.35	0.42
1:A:313:GLU:OE2	1:A:315:VAL:HG23	2.19	0.42
1:A:339:TYR:HB2	1:A:442:ARG:HE	1.84	0.42
1:A:444:LEU:HD12	2:D:27:THR:HG23	2.02	0.42
1:A:551:GLN:HA	1:A:564:ARG:HE	1.84	0.42
1:A:948:GLN:O	1:A:951:SER:OG	2.20	0.42
1:B:196:HIS:HB3	1:B:198:TYR:CE1	2.54	0.42
1:B:313:GLU:N	1:B:313:GLU:OE1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:PRO:HB3	1:B:414:PRO:O	2.20	0.42
1:C:914:ILE:O	1:C:917:ILE:HG22	2.20	0.42
2:G:48:TRP:HZ2	2:G:331:SER:HA	1.83	0.42
1:A:329:VAL:HG11	1:A:422:LEU:HD13	2.00	0.42
1:A:489:GLY:O	1:A:493:GLN:HG3	2.20	0.42
1:B:185:GLU:HB3	1:B:217:LEU:HD11	2.01	0.42
1:B:735:LEU:O	1:B:739:TYR:HD1	2.03	0.42
1:C:140:VAL:HA	1:C:238:ALA:HB3	2.01	0.42
1:C:246:TRP:O	1:C:246:TRP:CG	2.73	0.42
1:C:721:CYS:O	1:C:725:ILE:HG12	2.20	0.42
2:D:356:PHE:HB3	2:D:379:ILE:HD12	2.02	0.42
1:A:540:THR:CG2	1:A:573:ASP:HB2	2.49	0.42
1:A:705:ILE:HG12	1:A:913:ALA:HB1	2.01	0.42
1:A:888:ARG:HB3	1:A:1019:GLN:HE22	1.85	0.42
1:B:23:PHE:CE2	1:B:246:TRP:HB3	2.55	0.42
1:B:129:CYS:HB3	1:B:131:PHE:CE1	2.55	0.42
1:B:139:PHE:HB2	1:B:237:THR:CB	2.50	0.42
1:B:360:THR:HG23	5:B:1302:NAG:O3	2.20	0.42
1:B:443:SER:OG	1:B:480:ASN:ND2	2.53	0.42
1:B:546:PHE:CE1	1:B:571:ILE:HG21	2.55	0.42
2:D:44:SER:HB3	2:D:351:LEU:HG	2.02	0.42
2:D:199:TYR:HB3	2:D:464:PHE:CD2	2.55	0.42
1:A:1011:LYS:HE2	1:A:1025:PHE:O	2.19	0.41
1:B:49:ARG:HH22	1:B:54:HIS:CE1	2.38	0.41
1:B:733:ALA:HA	1:B:736:LEU:HB2	2.01	0.41
1:C:441:TYR:CD1	1:C:443:SER:HB3	2.54	0.41
1:C:544:LYS:HA	1:C:544:LYS:HD3	1.92	0.41
2:D:177:ARG:HD2	2:D:177:ARG:HA	1.86	0.41
2:D:188:ASN:HD21	2:D:464:PHE:HA	1.84	0.41
2:D:229:THR:HG23	2:D:516:TYR:OH	2.20	0.41
2:G:37:GLU:HA	2:G:390:PHE:CE1	2.55	0.41
2:G:54:ILE:HG13	2:G:342:ALA:HA	2.02	0.41
2:G:244:VAL:HG23	2:G:262:LEU:HD11	2.02	0.41
2:G:439:LEU:HD21	2:G:540:HIS:CD2	2.55	0.41
2:G:474:MET:HE1	2:G:497:TYR:CB	2.50	0.41
2:G:533:ALA:O	2:G:534:LYS:HG3	2.20	0.41
1:A:553:GLY:O	1:A:560:THR:HA	2.20	0.41
1:B:94:GLU:HG3	1:B:97:ASN:HA	2.02	0.41
1:B:562:SER:HB3	1:B:571:ILE:HG22	2.01	0.41
1:B:749:ALA:O	1:B:753:ILE:HG13	2.20	0.41
1:C:42:TYR:HA	1:C:217:LEU:H	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:ASP:OD1	1:C:455:ASP:N	2.53	0.41
1:C:917:ILE:HD12	1:C:917:ILE:HA	1.90	0.41
1:C:973:GLU:HA	1:C:976:ILE:CG1	2.47	0.41
2:D:107:VAL:O	2:D:107:VAL:HG13	2.20	0.41
2:D:127:TYR:CE2	2:D:504:PHE:HA	2.56	0.41
2:D:314:PHE:HE2	2:D:408:MET:HB3	1.86	0.41
2:D:591:LEU:O	2:D:595:LEU:HD23	2.20	0.41
2:G:48:TRP:CZ2	2:G:331:SER:HA	2.55	0.41
2:G:180:TYR:HA	2:G:183:TYR:HB3	2.03	0.41
2:G:407:ILE:HD11	2:G:525:PHE:HB2	2.02	0.41
1:A:90:PHE:O	1:A:185:GLU:HA	2.21	0.41
1:A:349:CYS:SG	1:A:511:VAL:HG22	2.60	0.41
1:C:94:GLU:HA	1:C:180:PHE:CD1	2.55	0.41
1:C:409:TYR:CD1	1:C:445:ARG:HB3	2.55	0.41
2:D:32:PHE:CG	2:D:100:LEU:HD21	2.55	0.41
2:G:529:LEU:HG	2:G:550:ALA:HB1	2.02	0.41
1:A:63:PHE:N	1:A:278:ASP:OD2	2.34	0.41
1:A:121:SER:OG	1:A:122:THR:N	2.53	0.41
1:A:138:PHE:CE2	1:A:140:VAL:HG22	2.56	0.41
1:A:272:THR:O	1:A:274:THR:HG23	2.20	0.41
1:A:299:GLY:HA2	1:A:651:ILE:HD13	2.01	0.41
1:B:411:TYR:HE2	1:B:499:VAL:HG21	1.85	0.41
1:B:549:PHE:CE2	1:B:550:GLN:HG3	2.56	0.41
1:B:1013:SER:O	1:B:1017:LEU:HB2	2.20	0.41
1:C:78:ASP:C	1:C:80:PRO:HD3	2.40	0.41
1:C:95:LYS:HD3	1:C:179:ASN:O	2.20	0.41
1:C:312:LYS:O	1:C:526:VAL:HB	2.20	0.41
1:C:325:PRO:HD2	1:C:346:ILE:CG2	2.49	0.41
2:D:90:ASN:OD1	2:D:91:LEU:N	2.54	0.41
2:G:378:HIS:CE1	2:G:405:GLY:HA3	2.56	0.41
2:G:381:TYR:CD1	2:G:558:LEU:HD12	2.53	0.41
1:A:852:MET:HG2	1:C:682:LEU:HD11	2.01	0.41
1:A:976:ILE:O	1:A:980:ILE:HG13	2.20	0.41
1:B:426:THR:HG21	1:B:496:ARG:HD2	2.02	0.41
1:C:116:ILE:O	1:C:126:ILE:HA	2.21	0.41
1:C:539:LEU:HD12	1:C:572:LEU:HD23	2.03	0.41
2:G:84:PRO:HG2	2:G:87:GLU:OE2	2.21	0.41
1:B:741:SER:O	1:B:745:GLN:NE2	2.53	0.41
1:C:916:GLN:O	1:C:919:GLU:HG3	2.21	0.41
1:C:1087:ILE:HG22	1:C:1096:GLN:HB2	2.03	0.41
2:D:269:ASP:OD1	2:D:269:ASP:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:458:LYS:O	2:D:462:MET:HG2	2.20	0.41
1:A:923:THR:HG23	1:A:925:SER:H	1.85	0.41
1:B:324:CYS:HB3	1:B:326:PHE:CD2	2.56	0.41
1:B:414:PRO:O	1:B:417:PHE:HB3	2.20	0.41
1:B:432:THR:O	1:B:485:TYR:HA	2.21	0.41
1:B:917:ILE:HD12	1:B:917:ILE:HA	1.81	0.41
1:C:85:LYS:HD3	1:C:257:TYR:CE2	2.56	0.41
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.93	0.41
1:C:519:ASP:OD1	1:C:519:ASP:N	2.54	0.41
1:C:643:VAL:HG12	1:C:645:THR:H	1.86	0.41
1:C:710:MET:HE1	1:C:1011:LYS:HG3	2.01	0.41
1:C:774:THR:HA	1:C:775:PRO:HD3	1.94	0.41
1:C:952:ASN:C	1:C:953:PHE:HD2	2.24	0.41
1:C:1074:ARG:NH1	1:C:1102:ASN:HA	2.36	0.41
1:C:1083:THR:HG21	3:T:1:NAG:H3	2.03	0.41
1:A:267:TYR:HB3	1:A:271:GLY:HA2	2.03	0.41
1:A:314:VAL:HA	1:A:518:THR:OG1	2.20	0.41
1:A:351:ALA:HB1	1:A:375:LEU:HD23	2.02	0.41
1:A:579:PHE:CE2	1:B:840:GLY:HA2	2.55	0.41
1:B:40:GLY:HA3	1:B:61:LEU:HB3	2.03	0.41
1:B:117:ILE:HG23	1:B:117:ILE:O	2.20	0.41
1:B:410:ASN:ND2	1:B:442:ARG:H	2.19	0.41
1:B:440:LYS:HD3	1:B:479:LEU:HG	2.02	0.41
1:B:493:GLN:HB3	1:B:494:PRO:HD2	2.02	0.41
1:B:954:GLY:H	1:C:738:GLN:NE2	2.19	0.41
1:C:48:PHE:CE2	1:C:271:GLY:HA3	2.56	0.41
1:C:298:LYS:O	1:C:301:TYR:OH	2.30	0.41
1:C:554:ARG:NH1	1:C:558:ASP:HA	2.36	0.41
2:D:111:ASP:O	2:D:114:LYS:HG3	2.21	0.41
1:A:200:GLY:N	1:A:217:LEU:HD22	2.36	0.41
1:A:306:PHE:CZ	1:A:607:VAL:HG23	2.56	0.41
1:A:529:ASN:HA	1:A:533:LEU:O	2.21	0.41
1:A:710:MET:HE1	1:A:1008:ALA:HA	2.03	0.41
1:B:95:LYS:HD2	1:B:175:GLU:OE2	2.21	0.41
1:B:198:TYR:CD1	1:B:219:PRO:HA	2.56	0.41
1:B:214:PHE:HZ	1:B:273:ILE:HG22	1.86	0.41
1:B:353:TYR:HB2	1:B:375:LEU:HD22	2.03	0.41
1:B:542:SER:HB2	1:B:573:ASP:N	2.35	0.41
1:B:780:PHE:CE2	1:B:785:PHE:HD2	2.39	0.41
1:B:879:ILE:HG22	1:B:880:PRO:O	2.21	0.41
2:D:20:THR:O	2:D:23:GLU:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:ILE:HG23	2:D:155:SER:HB2	2.02	0.41
2:D:204:ARG:HD2	2:D:219:ARG:O	2.21	0.41
2:D:267:LEU:HD22	2:D:275:TRP:CZ2	2.56	0.41
2:D:479:GLU:O	2:D:482:ARG:HB2	2.21	0.41
2:D:481:LYS:O	2:D:486:GLY:N	2.54	0.41
2:G:125:THR:O	2:G:129:THR:HG22	2.20	0.41
2:G:468:ILE:HG22	2:G:469:PRO:O	2.21	0.41
2:G:591:LEU:O	2:G:595:LEU:HD23	2.20	0.41
1:A:20:CYS:HB2	1:A:152:TYR:CD2	2.55	0.41
1:A:115:VAL:HA	1:A:128:ALA:HA	2.02	0.41
1:A:306:PHE:CZ	1:A:608:PRO:HD2	2.46	0.41
1:A:1073:PRO:HB3	1:A:1078:PHE:CE1	2.57	0.41
1:C:424:TRP:HH2	1:C:498:VAL:HG23	1.86	0.41
1:C:441:TYR:O	1:C:479:LEU:HA	2.21	0.41
2:D:44:SER:CB	2:D:351:LEU:HG	2.51	0.41
2:D:242:ALA:HA	2:D:245:ARG:CZ	2.51	0.41
2:G:215:TYR:HB3	2:G:567:THR:OG1	2.20	0.41
2:G:471:ASP:OD1	2:G:471:ASP:N	2.50	0.41
1:A:95:LYS:HD2	1:A:176:LYS:O	2.20	0.40
1:A:375:LEU:HG	1:A:380:PHE:HE2	1.87	0.40
1:A:427:ARG:O	1:A:431:ALA:N	2.54	0.40
1:A:653:ILE:HD13	1:A:653:ILE:HA	1.81	0.40
1:A:709:VAL:CG1	1:A:931:LEU:HG	2.51	0.40
1:A:733:ALA:HA	1:A:736:LEU:HB3	2.03	0.40
1:A:887:TYR:HB2	1:C:1090:ARG:NH2	2.37	0.40
1:B:785:PHE:CD1	1:B:788:ILE:HD11	2.56	0.40
1:B:791:ASP:HB2	1:B:794:LYS:HD2	2.03	0.40
1:C:663:THR:HG22	1:C:673:LYS:HG2	2.03	0.40
1:C:710:MET:HA	1:C:711:PRO:HD3	1.97	0.40
2:D:198:ASP:OD1	2:D:201:ASP:N	2.53	0.40
2:D:538:PRO:HB2	2:D:540:HIS:ND1	2.35	0.40
2:D:581:VAL:HG22	2:D:584:LEU:HB3	2.03	0.40
1:A:343:ARG:HD3	1:A:384:TYR:CD2	2.56	0.40
1:A:742:PHE:CD2	1:A:984:LEU:HD21	2.57	0.40
1:A:1050:TYR:HE2	1:A:1052:PRO:HG3	1.86	0.40
1:B:39:ARG:HB3	1:B:89:TYR:OH	2.21	0.40
1:B:68:THR:OG1	1:B:255:VAL:HB	2.21	0.40
1:B:102:TRP:HB3	1:B:232:PHE:CE1	2.57	0.40
1:B:682:LEU:HD22	1:C:856:TYR:CE2	2.56	0.40
1:B:737:LEU:HD12	1:B:737:LEU:HA	1.93	0.40
1:B:760:ASN:HD21	1:B:1002:ARG:HG3	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:VAL:HG21	1:C:502:PHE:HZ	1.85	0.40
1:C:693:ASN:C	1:C:1060:THR:HG22	2.41	0.40
1:C:1012:MET:HG2	1:C:1045:PHE:HZ	1.87	0.40
2:D:132:VAL:O	2:D:141:CYS:HA	2.21	0.40
2:D:435:GLU:O	2:D:439:LEU:HD23	2.21	0.40
2:G:535:HIS:NE2	2:G:538:PRO:O	2.48	0.40
1:A:348:ASN:HA	1:A:510:THR:O	2.21	0.40
1:A:353:TYR:CE2	1:A:355:VAL:HG23	2.56	0.40
1:A:370:VAL:HG11	1:A:502:PHE:CZ	2.56	0.40
1:A:529:ASN:HD22	1:A:534:THR:HB	1.86	0.40
1:A:587:PRO:HG3	1:A:661:TYR:HB2	2.02	0.40
1:A:897:ASN:OD1	1:A:898:VAL:N	2.55	0.40
1:A:952:ASN:ND2	1:A:955:ALA:O	2.54	0.40
1:A:972:ALA:O	1:A:976:ILE:HG13	2.22	0.40
1:A:992:THR:O	1:A:996:ILE:HG12	2.22	0.40
1:A:1093:PHE:CE1	1:A:1095:PRO:HG3	2.56	0.40
1:B:439:TYR:HD2	1:B:484:PHE:CE2	2.38	0.40
1:B:632:THR:HG23	1:B:634:ALA:H	1.85	0.40
1:C:123:ASN:N	1:C:123:ASN:OD1	2.53	0.40
1:C:461:PHE:N	1:C:476:TYR:O	2.54	0.40
1:C:542:SER:HA	1:C:573:ASP:OD2	2.21	0.40
2:G:28:PHE:HE2	2:G:80:ALA:HB2	1.86	0.40
2:G:402:GLU:CG	2:G:518:ARG:HG3	2.50	0.40
1:A:48:PHE:CE1	1:A:50:SER:HB2	2.57	0.40
1:A:71:ILE:HA	1:A:252:ALA:HA	2.04	0.40
1:A:452:PHE:CE1	1:A:501:SER:HB2	2.57	0.40
1:A:522:LYS:NZ	1:A:572:LEU:HD22	2.37	0.40
1:A:540:THR:HG23	1:A:573:ASP:HB2	2.04	0.40
1:A:579:PHE:O	1:A:579:PHE:CD2	2.75	0.40
1:B:113:GLN:HE22	1:B:129:CYS:N	2.19	0.40
1:B:316:ARG:HD2	1:B:567:LYS:NZ	2.35	0.40
1:B:417:PHE:CZ	1:B:419:GLY:HA3	2.56	0.40
1:B:914:ILE:O	1:B:917:ILE:HG22	2.21	0.40
1:C:59:HIS:CD2	1:C:260:PRO:HB3	2.56	0.40
1:C:326:PHE:CE1	1:C:351:ALA:HA	2.57	0.40
1:C:412:LYS:O	1:C:413:LEU:HD23	2.21	0.40
2:D:557:MET:CG	2:D:569:ALA:HB1	2.51	0.40
2:G:293:VAL:HG21	2:G:418:LEU:HD11	2.02	0.40
1:A:77:PHE:HE1	1:A:236:LEU:HB2	1.86	0.40
1:A:140:VAL:O	1:A:149:ILE:N	2.35	0.40
1:A:970:PRO:O	1:A:973:GLU:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:TYR:CD1	1:B:187:VAL:HG21	2.57	0.40
1:C:538:VAL:CG2	1:C:575:SER:HB2	2.52	0.40
1:C:650:ASP:O	1:C:651:ILE:HD13	2.21	0.40
1:C:880:PRO:HD2	1:C:883:MET:SD	2.62	0.40
2:D:218:SER:HB3	2:D:221:GLN:HG3	2.04	0.40
2:G:40:PHE:HB3	2:G:390:PHE:CZ	2.57	0.40
2:G:381:TYR:HA	2:G:558:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1062/1271 (84%)	974 (92%)	87 (8%)	1 (0%)	51	85
1	B	1059/1271 (83%)	998 (94%)	60 (6%)	1 (0%)	51	85
1	C	1062/1271 (84%)	995 (94%)	67 (6%)	0	100	100
2	D	595/603 (99%)	569 (96%)	26 (4%)	0	100	100
2	G	595/603 (99%)	572 (96%)	23 (4%)	0	100	100
All	All	4373/5019 (87%)	4108 (94%)	263 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	TRP
1	B	315	VAL

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	932/1100 (85%)	928 (100%)	4 (0%)	91	94
1	B	930/1100 (84%)	928 (100%)	2 (0%)	93	96
1	C	932/1100 (85%)	927 (100%)	5 (0%)	88	93
2	D	527/533 (99%)	526 (100%)	1 (0%)	93	96
2	G	527/533 (99%)	525 (100%)	2 (0%)	91	94
All	All	3848/4366 (88%)	3834 (100%)	14 (0%)	91	94

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	242	ARG
1	A	545	ARG
1	A	668	ARG
1	B	189	ARG
1	B	242	ARG
1	C	136	ASN
1	C	167	LYS
1	C	316	ARG
1	C	545	ARG
1	C	1002	ARG
2	D	114	LYS
2	G	114	LYS
2	G	534	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	322	ASN
1	A	474	ASN
1	A	531	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	757	GLN
1	A	787	GLN
1	A	878	GLN
1	A	975	GLN
1	A	993	GLN
1	A	1019	GLN
1	B	54	HIS
1	B	57	GLN
1	B	113	GLN
1	B	488	ASN
1	B	662	HIS
1	B	734	ASN
1	B	757	GLN
1	B	1102	ASN
1	C	59	HIS
1	C	1066	HIS
2	G	265	HIS
2	G	401	HIS

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](#)

35 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
3	NAG	E	1	3,1	14,14,15	0.33	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	2	3	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	F	1	3,1	14,14,15	0.24	0	17,19,21	0.35	0
3	NAG	F	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	H	1	3,1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	1.24	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	I	2	3	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	J	1	3,1	14,14,15	0.25	0	17,19,21	0.52	0
3	NAG	J	2	3	14,14,15	0.28	0	17,19,21	0.47	0
3	NAG	K	1	3,1	14,14,15	0.18	0	17,19,21	0.65	1 (5%)
3	NAG	K	2	3	14,14,15	0.19	0	17,19,21	0.39	0
3	NAG	L	1	3,1	14,14,15	0.40	0	17,19,21	1.03	1 (5%)
3	NAG	L	2	3	14,14,15	0.36	0	17,19,21	0.36	0
4	NAG	M	1	4,1	14,14,15	0.43	0	17,19,21	0.36	0
4	NAG	M	2	4	14,14,15	0.20	0	17,19,21	0.45	0
4	BMA	M	3	4	11,11,12	0.52	0	15,15,17	0.78	0
4	NAG	N	1	4,1	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	N	2	4	14,14,15	0.21	0	17,19,21	0.54	0
4	BMA	N	3	4	11,11,12	0.75	0	15,15,17	0.75	0
3	NAG	O	1	3,1	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	O	2	3	14,14,15	0.18	0	17,19,21	0.43	0
3	NAG	P	1	3,1	14,14,15	0.64	1 (7%)	17,19,21	0.63	0
3	NAG	P	2	3	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	Q	1	3,1	14,14,15	0.29	0	17,19,21	0.40	0
3	NAG	Q	2	3	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	R	1	3,1	14,14,15	0.33	0	17,19,21	0.37	0
3	NAG	R	2	3	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	S	1	4,1	14,14,15	0.40	0	17,19,21	0.53	0
4	NAG	S	2	4	14,14,15	0.26	0	17,19,21	0.39	0
4	BMA	S	3	4	11,11,12	0.53	0	15,15,17	0.82	0
3	NAG	T	1	3,1	14,14,15	0.28	0	17,19,21	0.36	0
3	NAG	T	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	U	1	3,1	14,14,15	0.18	0	17,19,21	0.49	0
3	NAG	U	2	3	14,14,15	0.22	0	17,19,21	0.43	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
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	NAG	O5-C1	-2.24	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C2-N2-C7	4.18	128.85	122.90
3	L	1	NAG	C1-O5-C5	3.05	116.33	112.19
3	K	1	NAG	C1-O5-C5	2.24	115.22	112.19

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	J	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

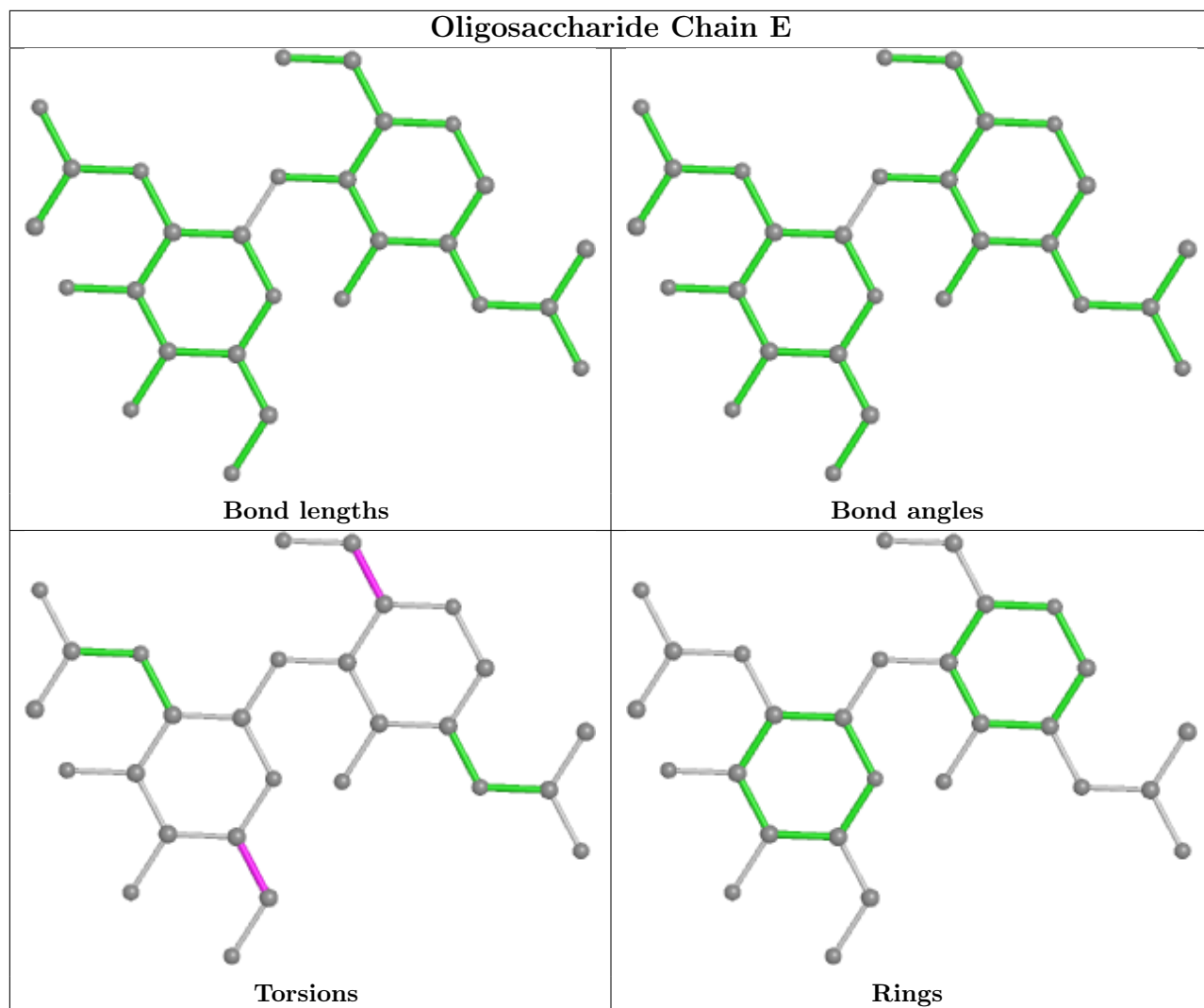
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C3-C2-N2-C7
3	F	1	NAG	C4-C5-C6-O6

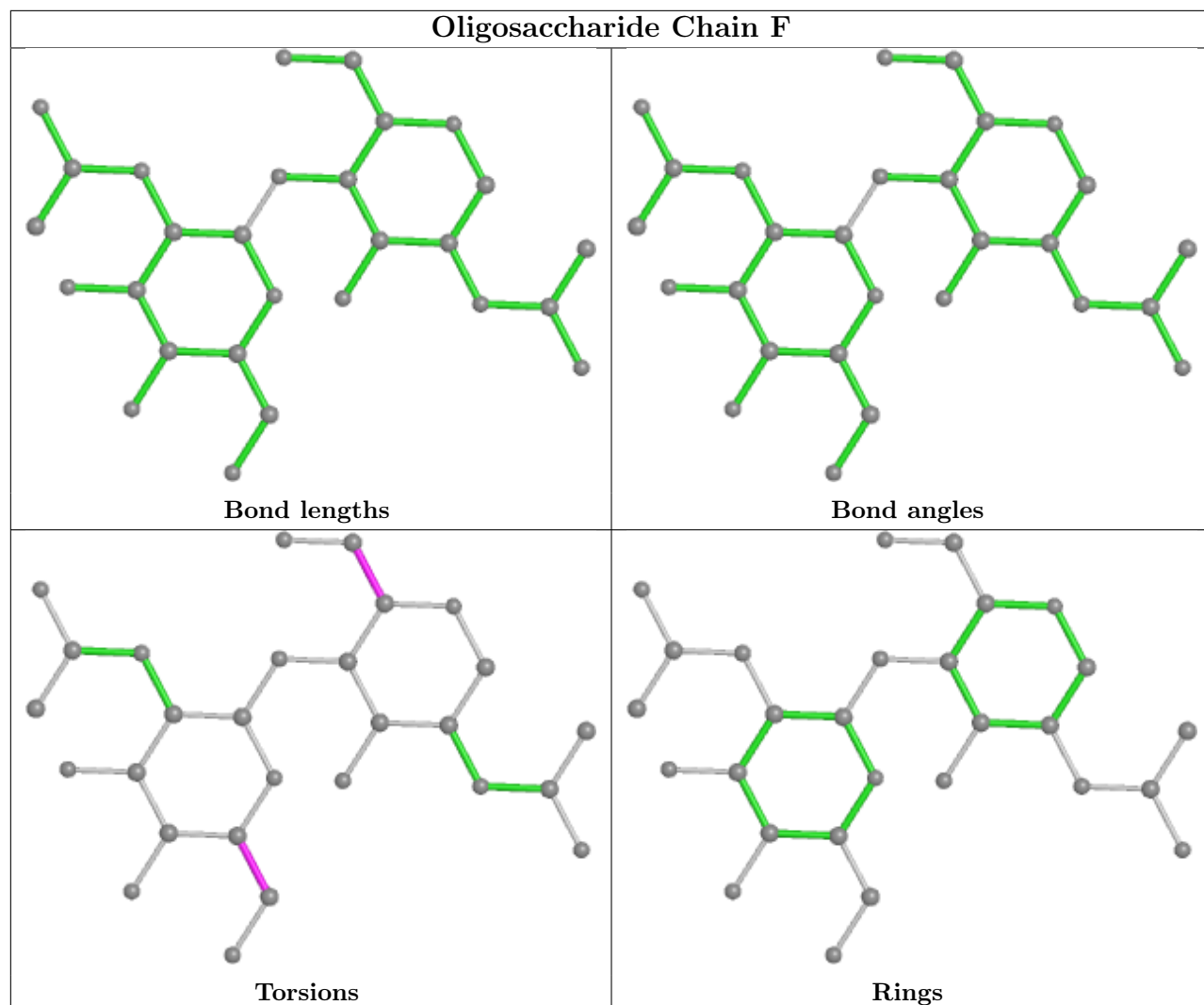
There are no ring outliers.

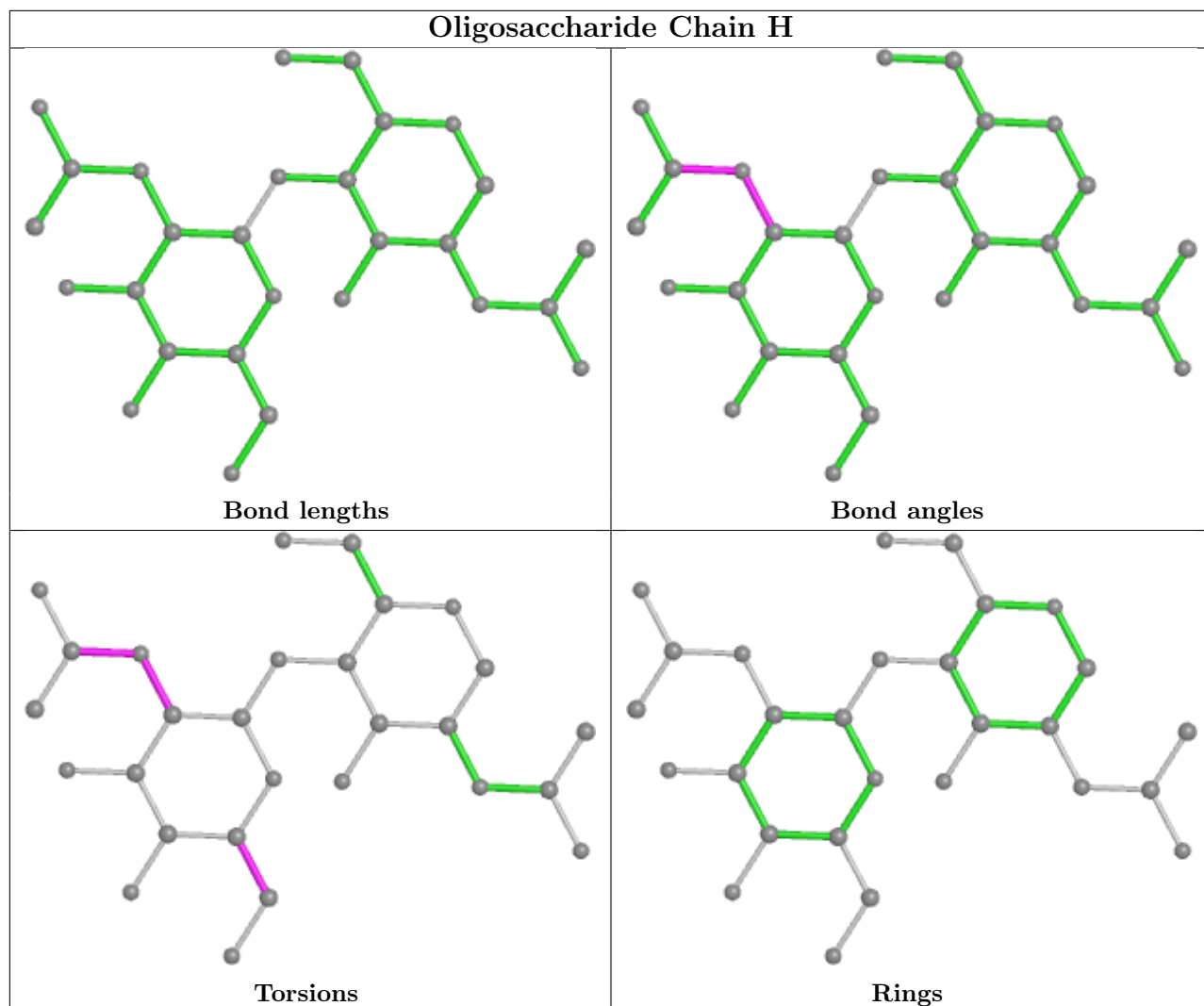
10 monomers are involved in 9 short contacts:

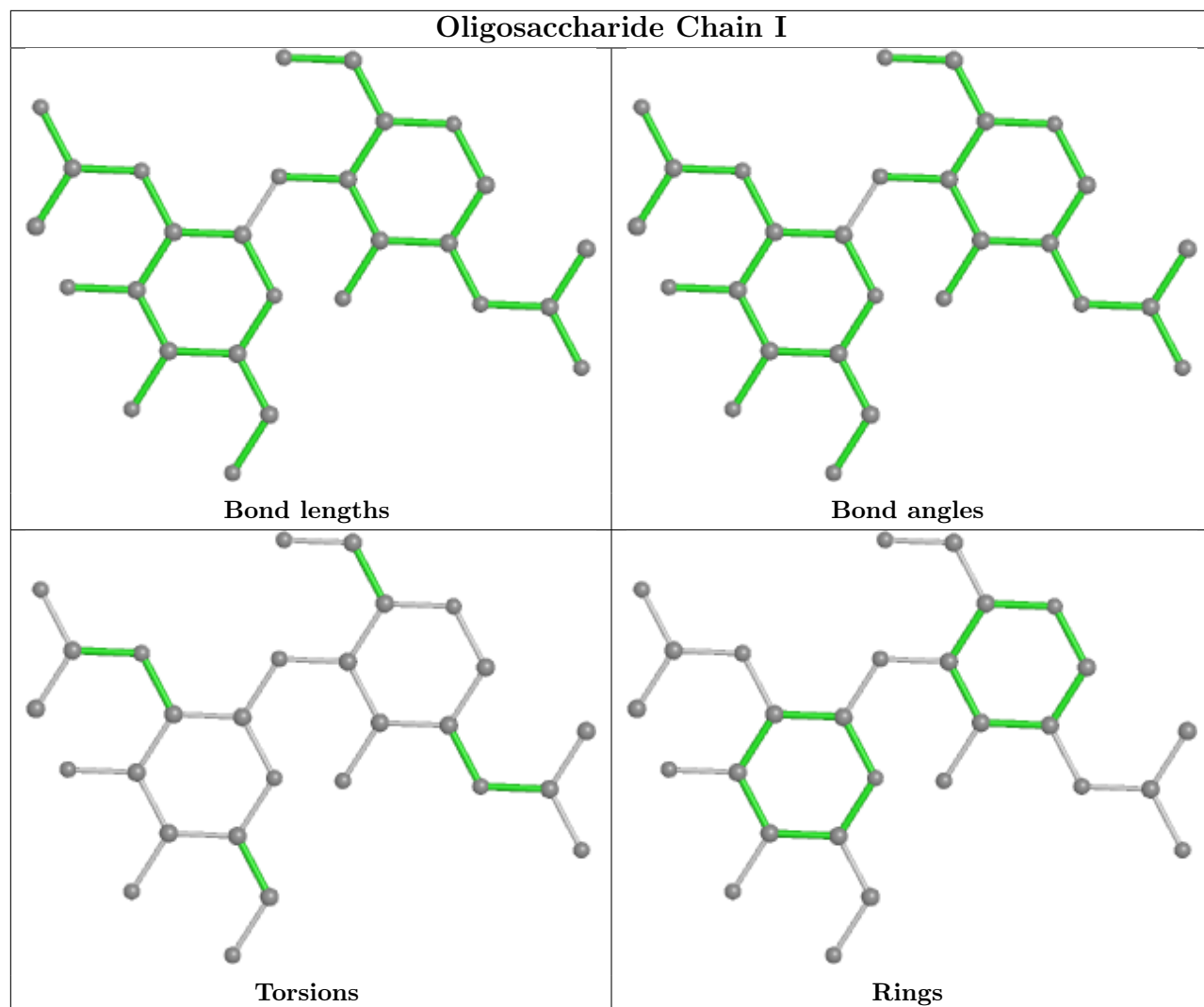
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	1	NAG	1	0
3	L	1	NAG	1	0
4	S	1	NAG	1	0
3	J	1	NAG	2	0
3	H	2	NAG	1	0
3	Q	1	NAG	1	0
3	O	1	NAG	1	0
3	P	1	NAG	1	0
3	J	2	NAG	1	0
3	L	2	NAG	1	0

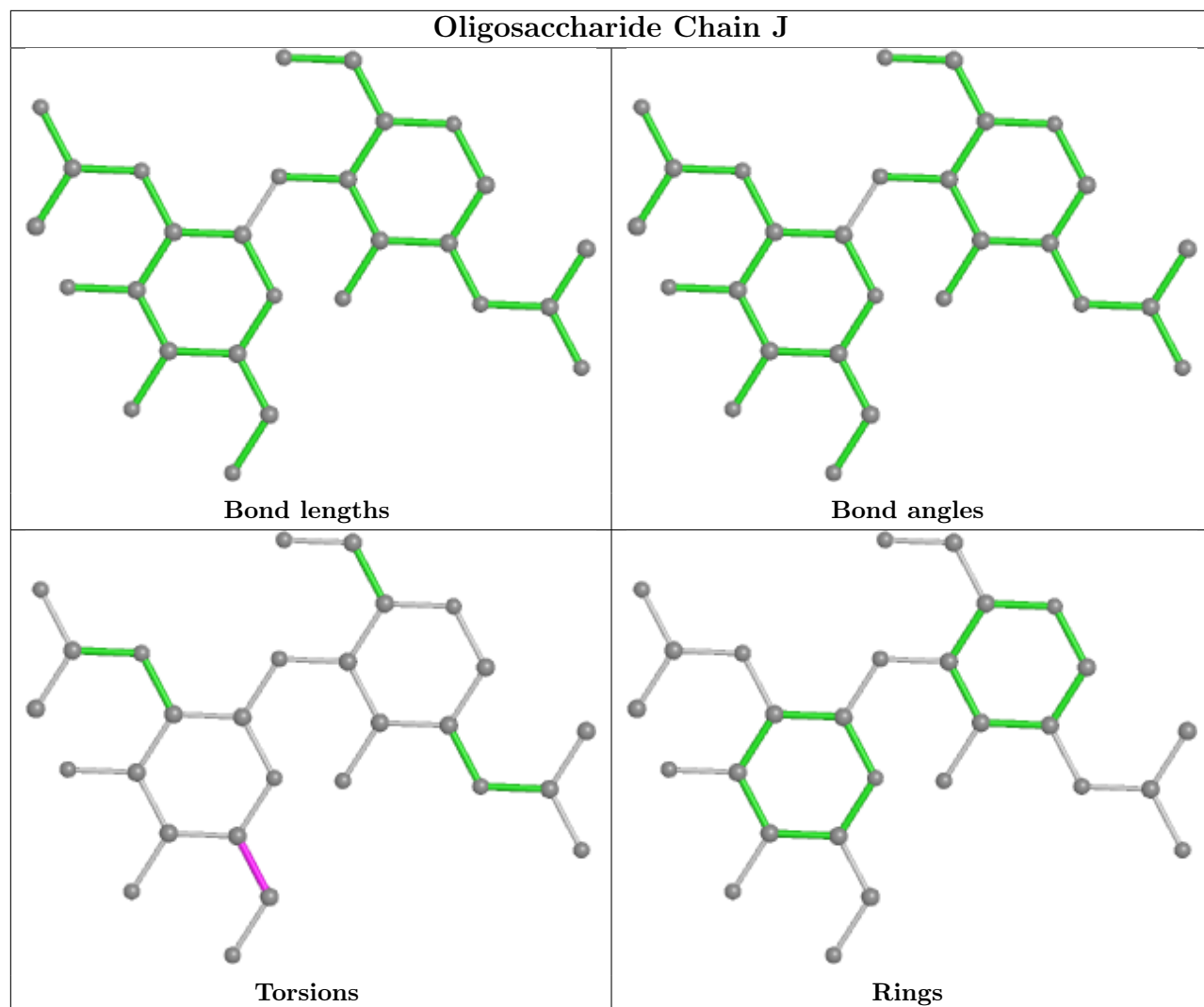
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

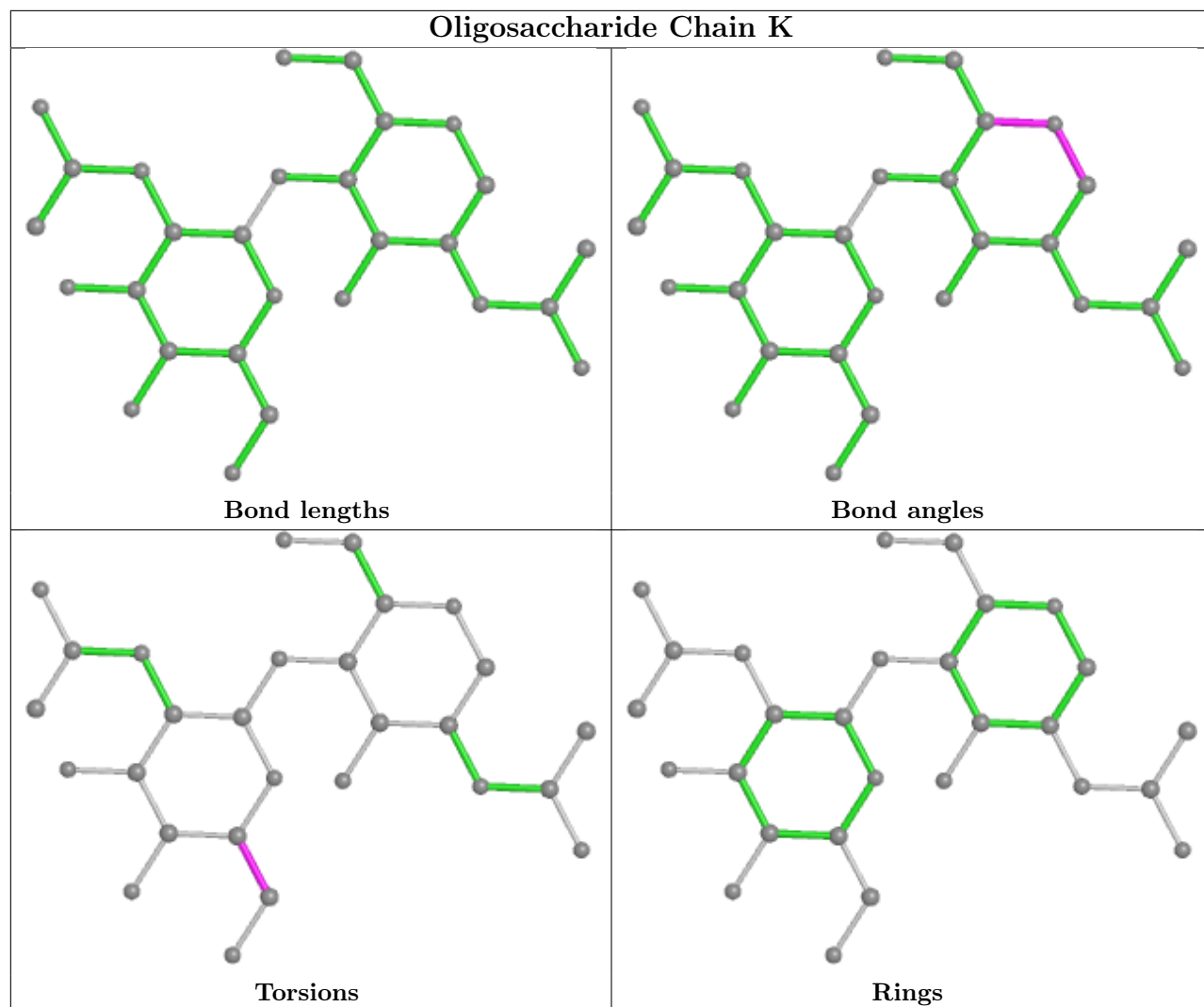


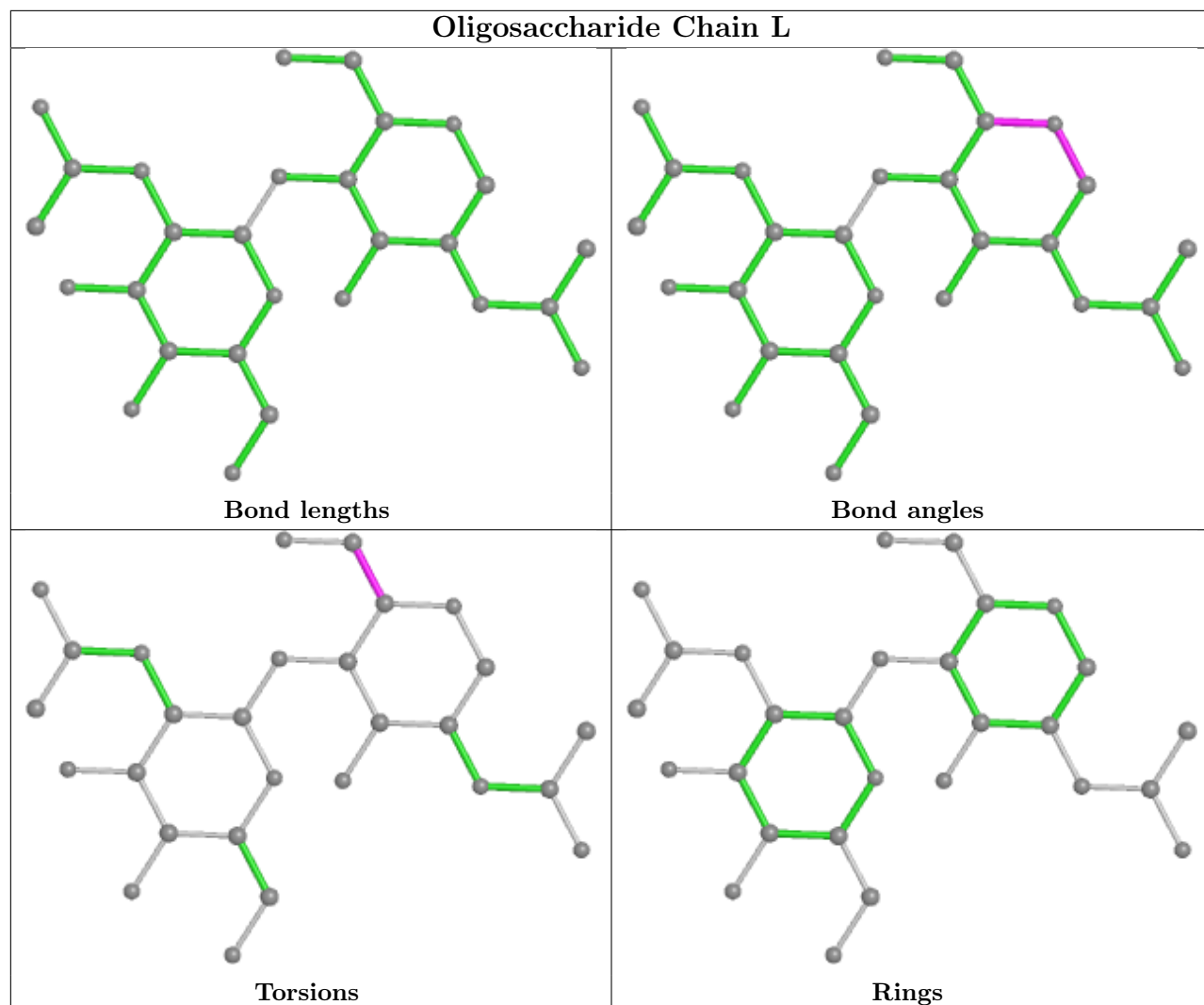


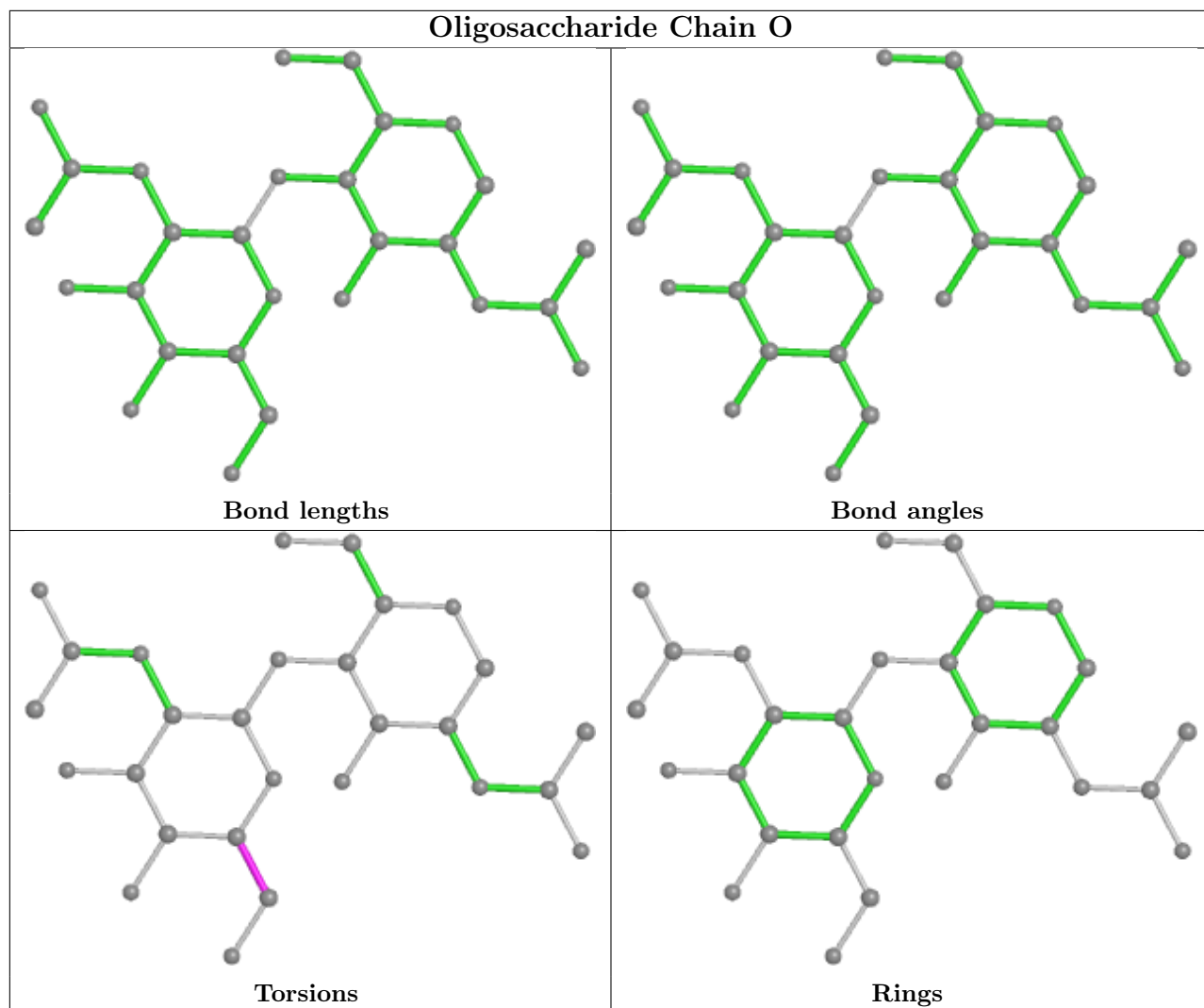


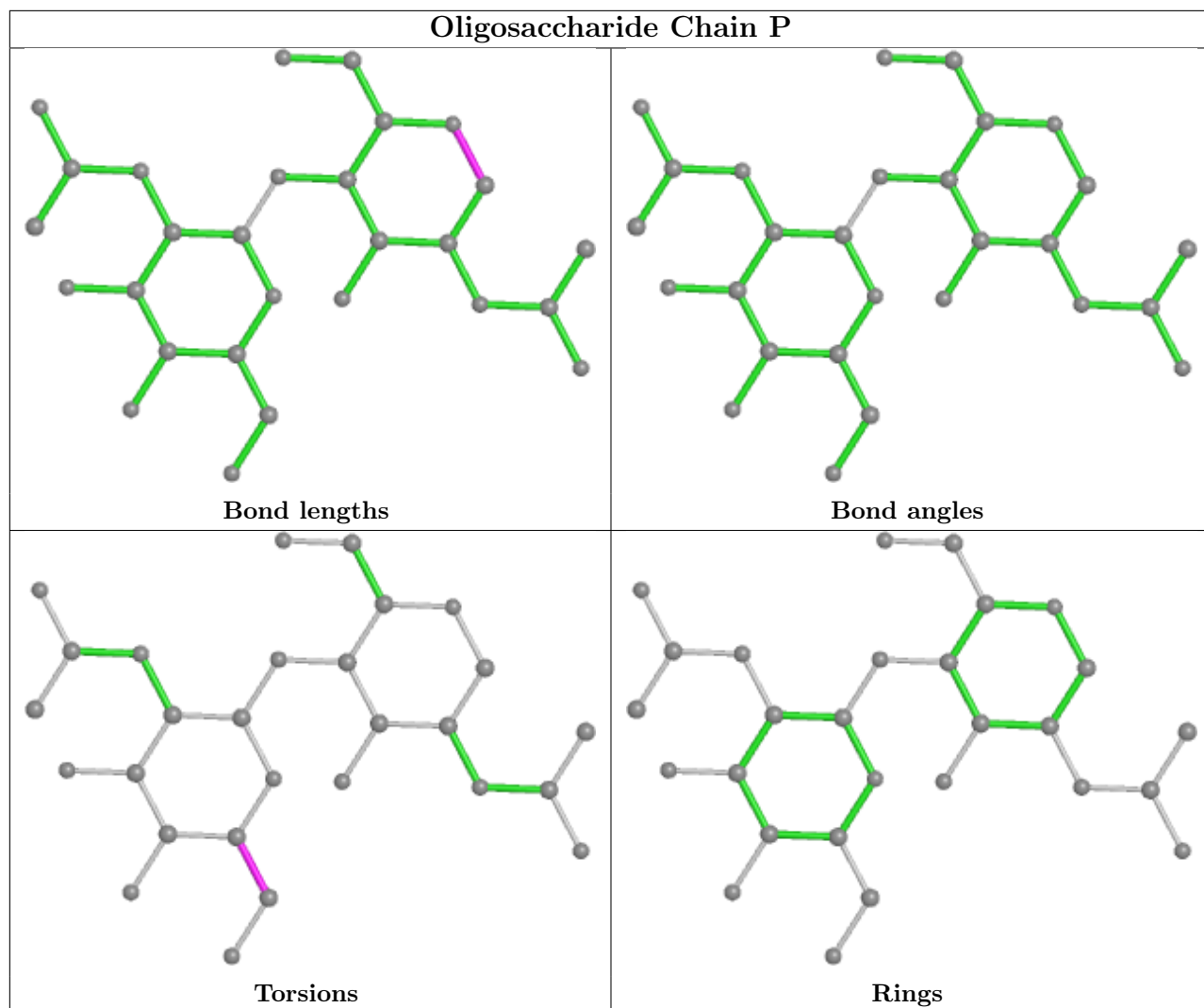


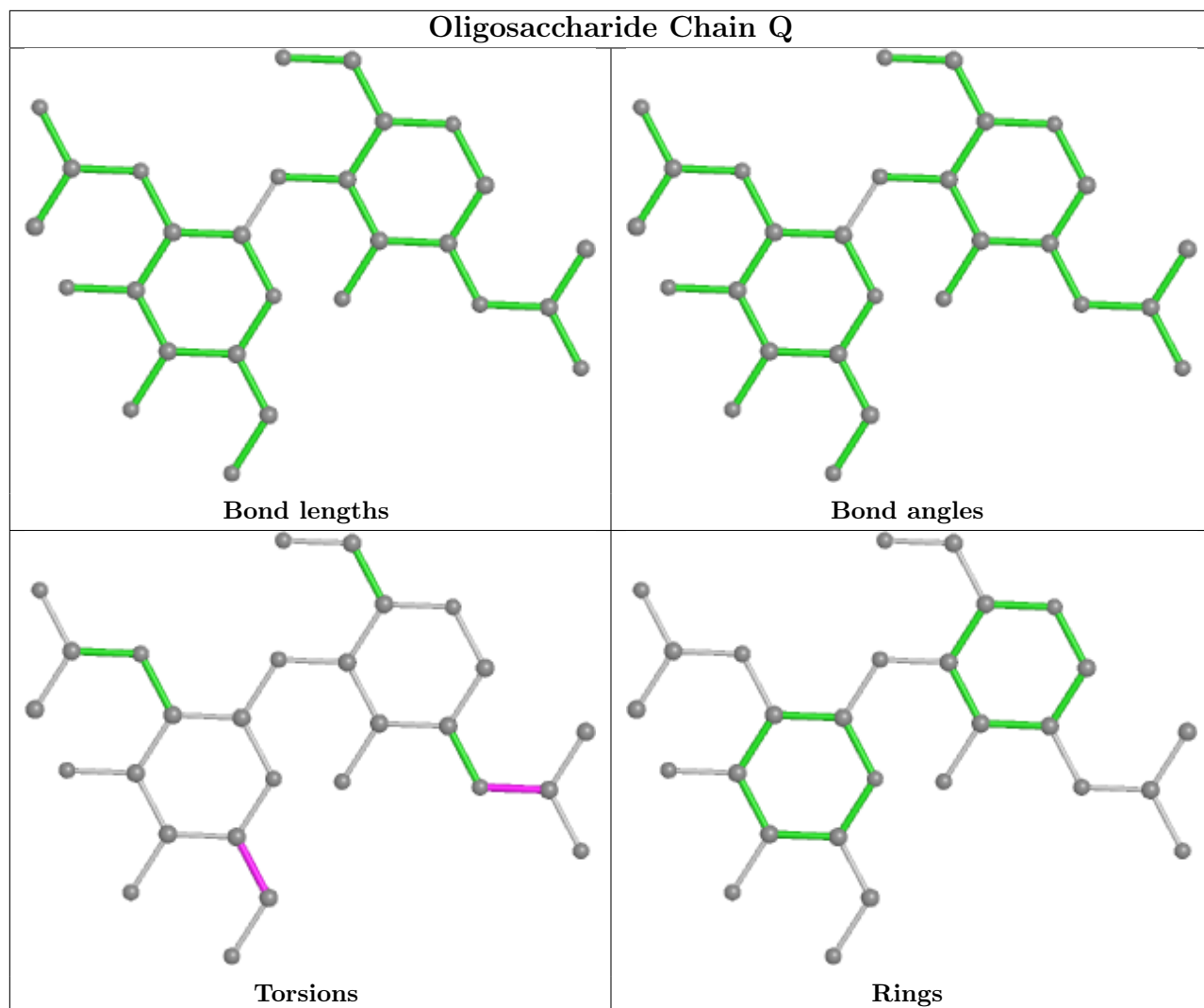


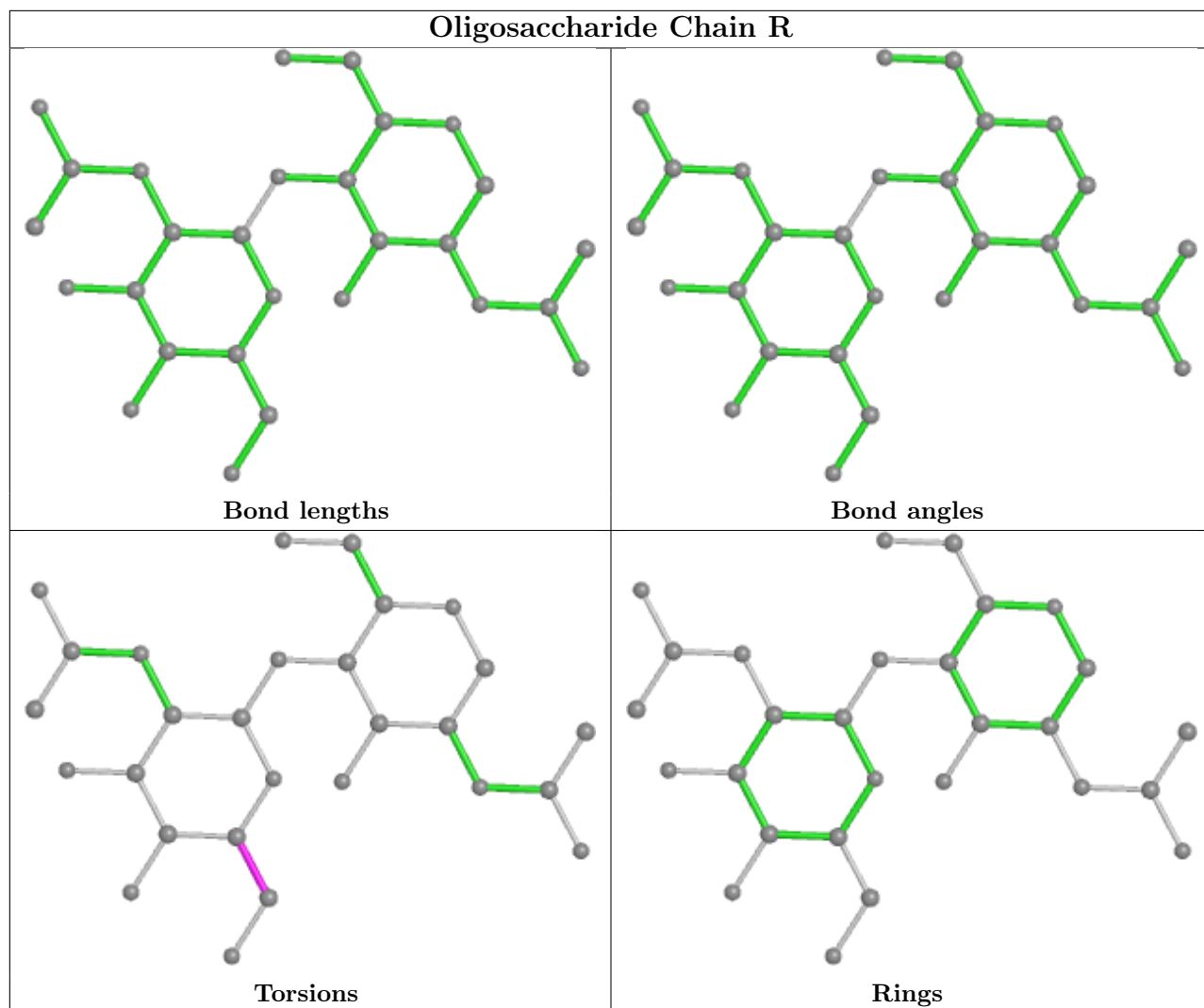


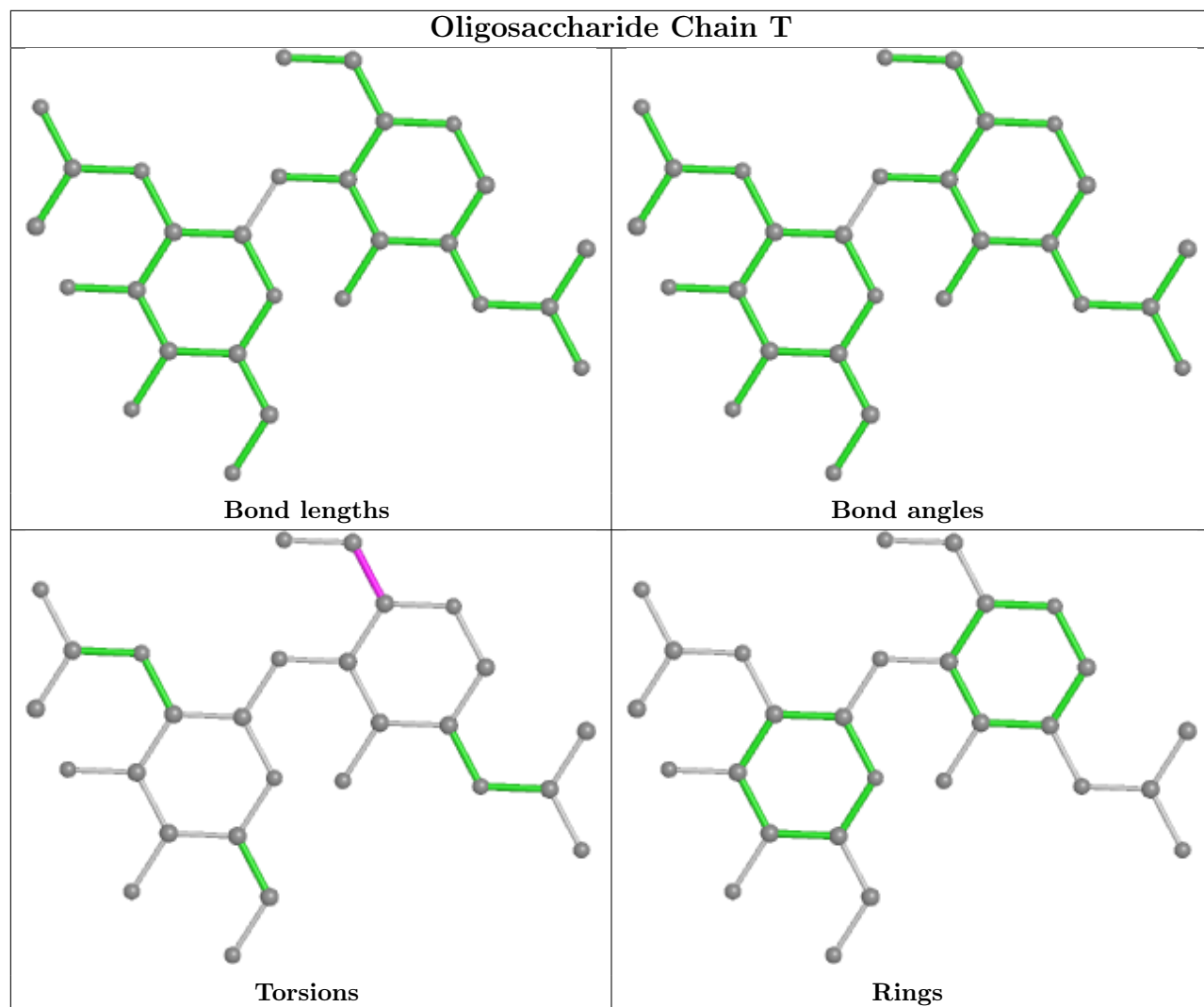


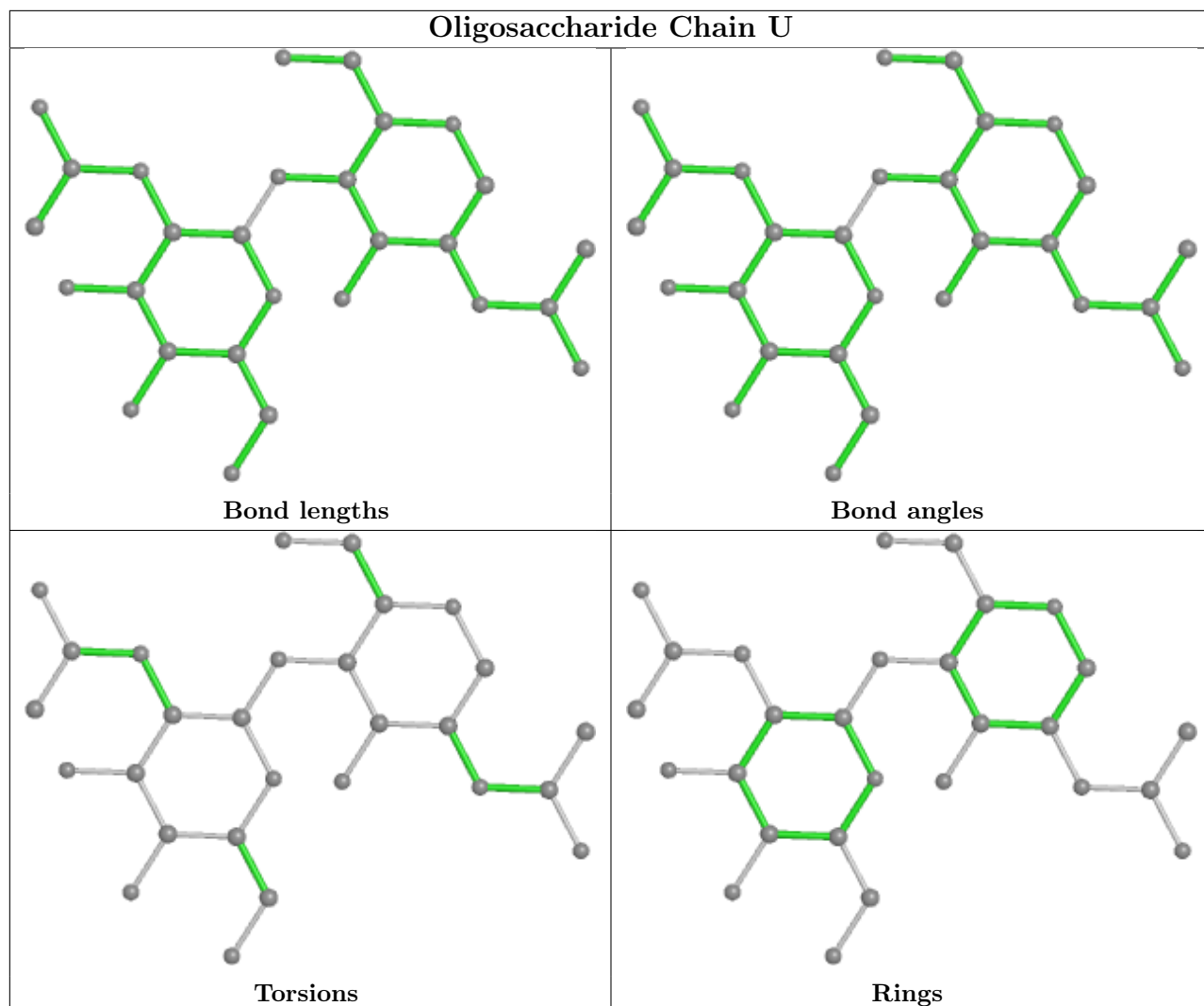


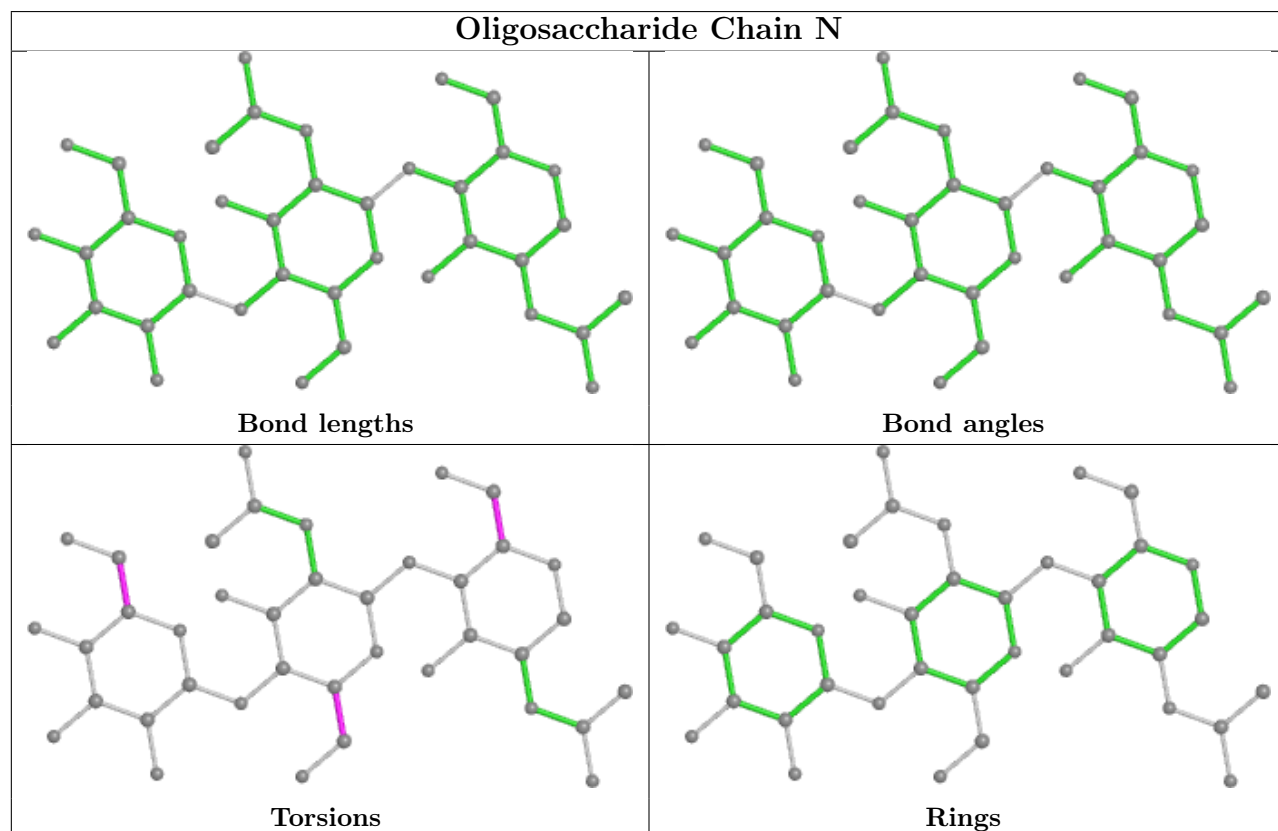
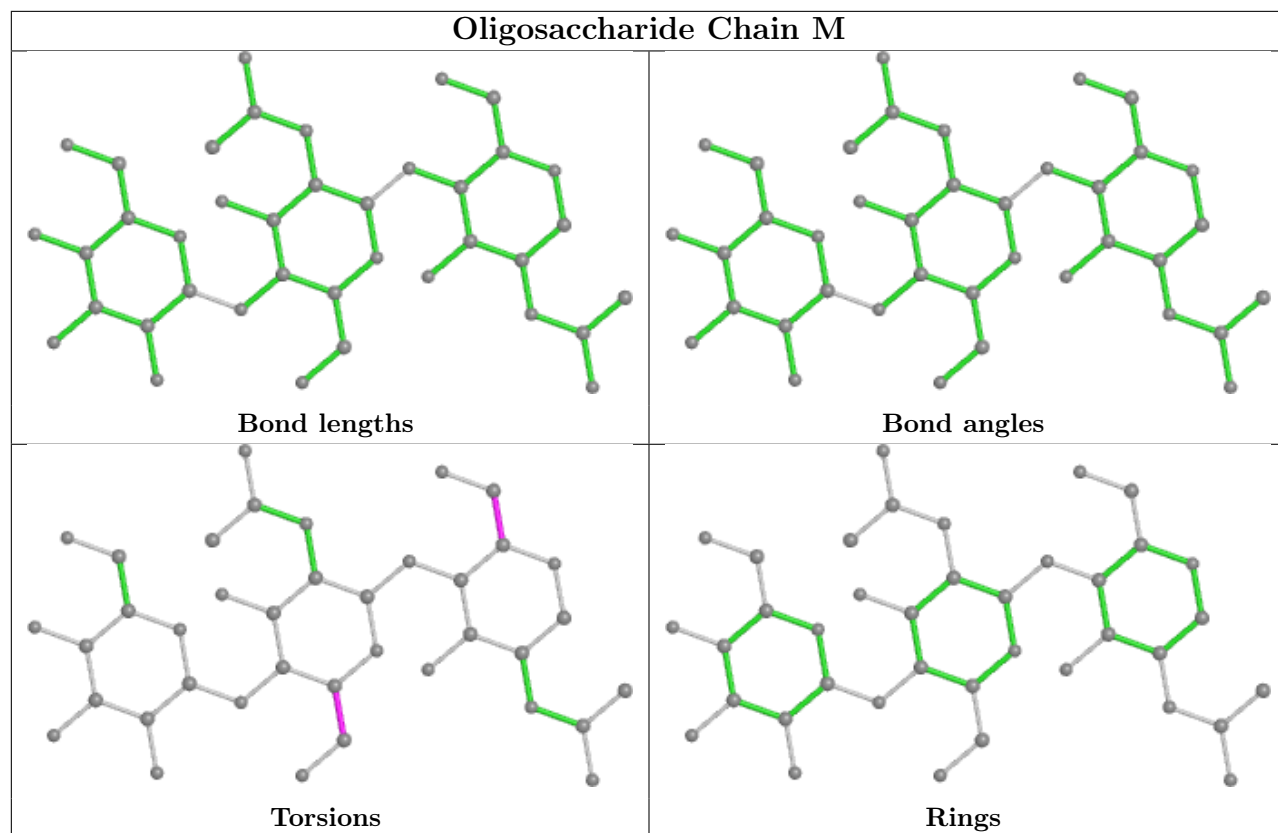


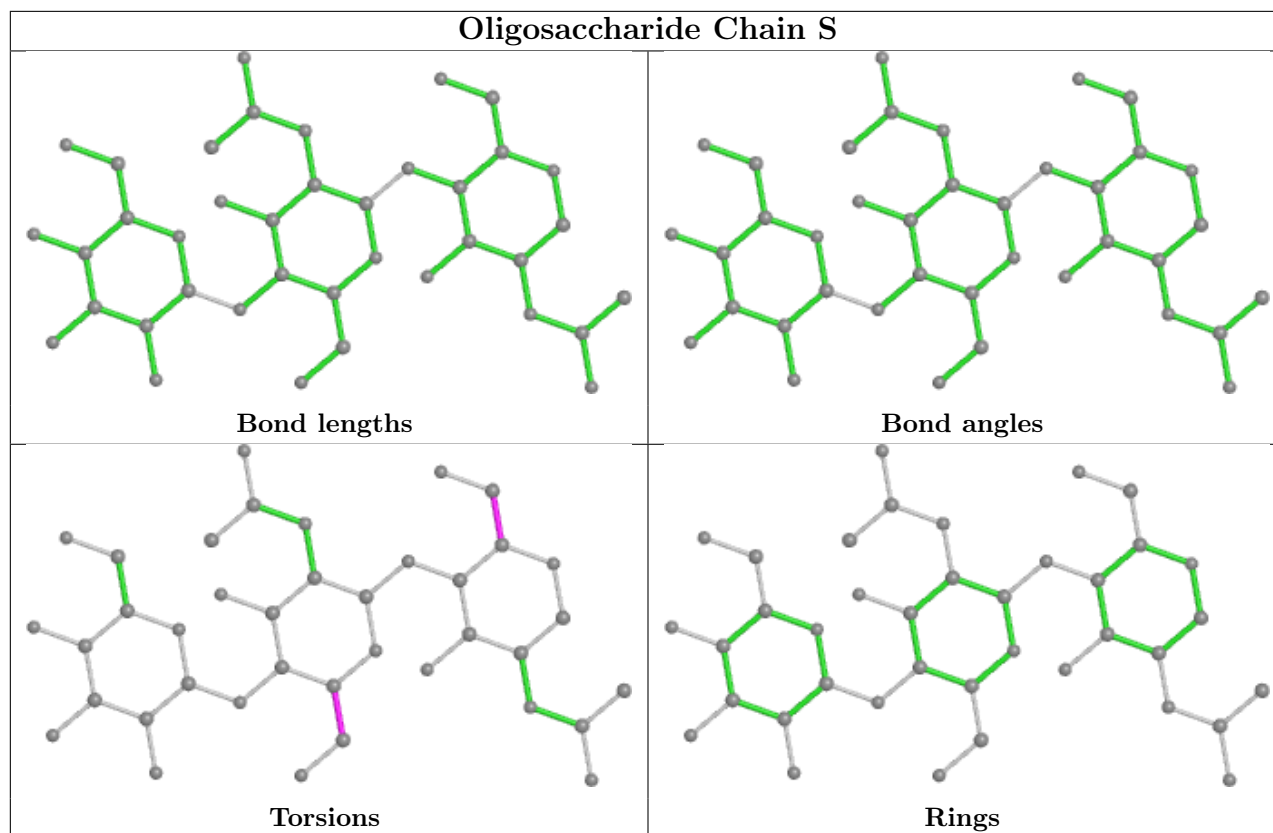












5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	1306	1	14,14,15	0.22	0	17,19,21	0.47	0
5	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.35	0
5	NAG	C	1310	1	14,14,15	0.22	0	17,19,21	0.52	0
5	NAG	C	1305	1	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.41	0
5	NAG	C	1309	1	14,14,15	0.25	0	17,19,21	0.39	0
5	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.38	0
5	NAG	C	1301	1	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	B	1305	1	14,14,15	0.24	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.49	0
5	NAG	C	1302	1	14,14,15	0.30	0	17,19,21	0.32	0
5	NAG	A	1304	1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	A	1302	1	14,14,15	0.31	0	17,19,21	0.44	0
5	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.37	0
5	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.59	0
5	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	B	1302	1	14,14,15	0.18	0	17,19,21	0.41	0
5	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.36	0
5	NAG	C	1308	1	14,14,15	0.31	0	17,19,21	0.34	0
5	NAG	C	1307	1	14,14,15	0.60	0	17,19,21	0.43	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
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1301	NAG	O5-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	A	1301	NAG	C8-C7-N2-C2
5	A	1301	NAG	O7-C7-N2-C2
5	A	1304	NAG	C8-C7-N2-C2
5	A	1304	NAG	O7-C7-N2-C2
5	B	1302	NAG	C8-C7-N2-C2
5	B	1302	NAG	O7-C7-N2-C2
5	C	1301	NAG	C8-C7-N2-C2
5	C	1301	NAG	O7-C7-N2-C2
5	C	1308	NAG	C8-C7-N2-C2
5	C	1308	NAG	O7-C7-N2-C2
5	A	1303	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	C	1310	NAG	C4-C5-C6-O6
5	C	1307	NAG	C1-C2-N2-C7
5	C	1302	NAG	O5-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	C	1310	NAG	O5-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1306	NAG	O5-C5-C6-O6
5	C	1304	NAG	C3-C2-N2-C7
5	C	1307	NAG	C3-C2-N2-C7
5	C	1306	NAG	C1-C2-N2-C7
5	C	1302	NAG	C4-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1309	NAG	2	0
5	C	1304	NAG	1	0
5	C	1302	NAG	1	0
5	B	1302	NAG	2	0

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.

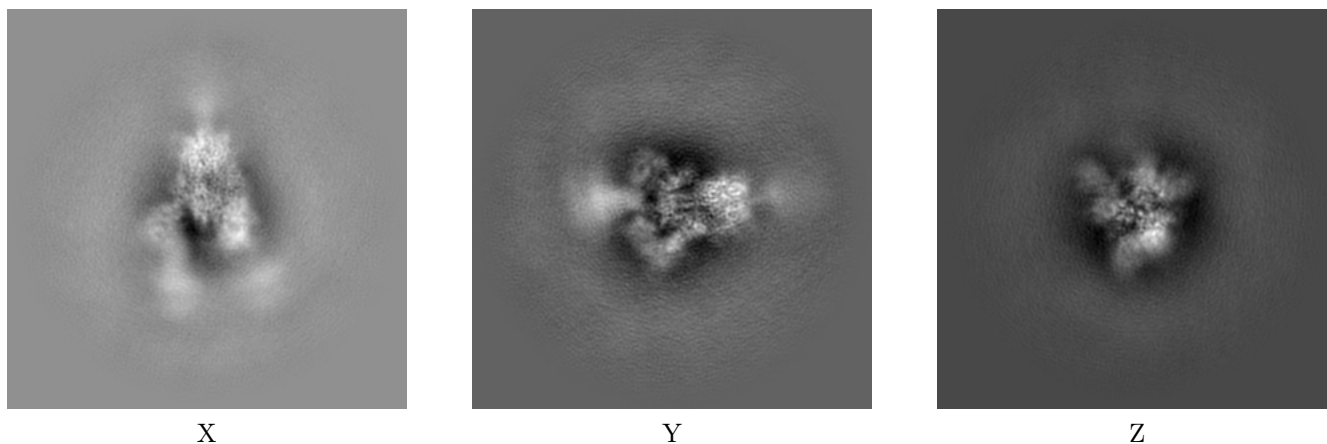
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37636. These allow visual inspection of the internal detail of the map and identification of artifacts.

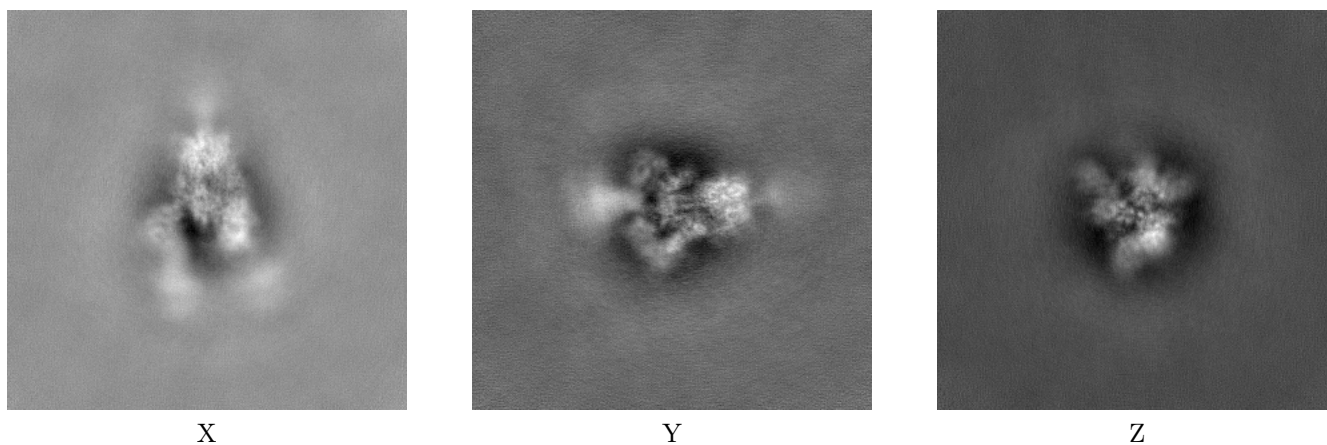
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



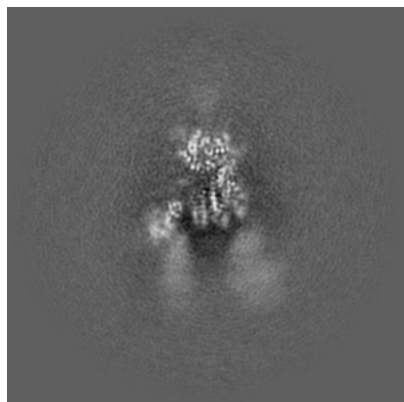
6.1.2 Raw map



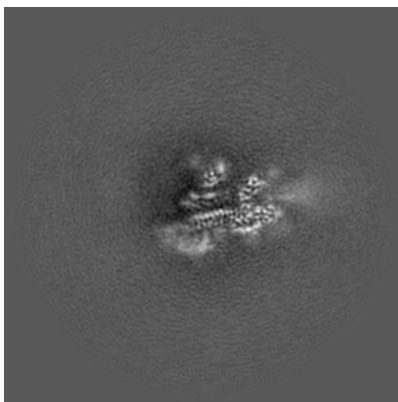
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

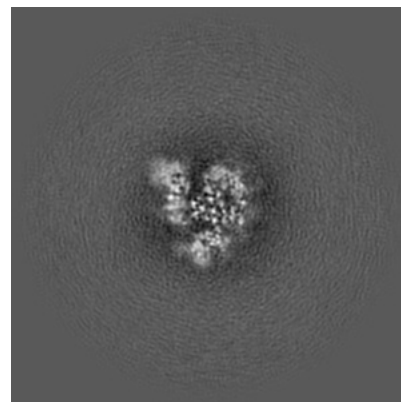
6.2.1 Primary map



X Index: 230

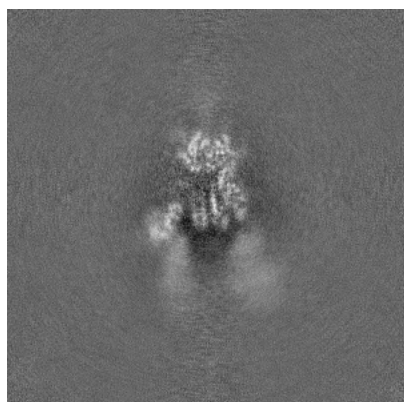


Y Index: 230

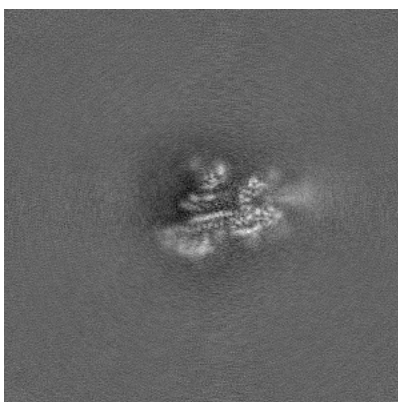


Z Index: 230

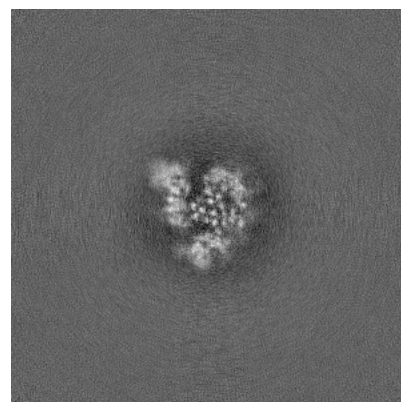
6.2.2 Raw map



X Index: 230



Y Index: 230

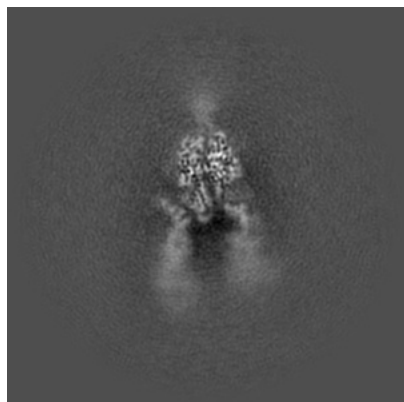


Z Index: 230

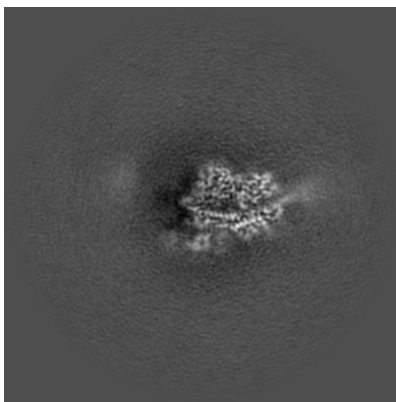
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

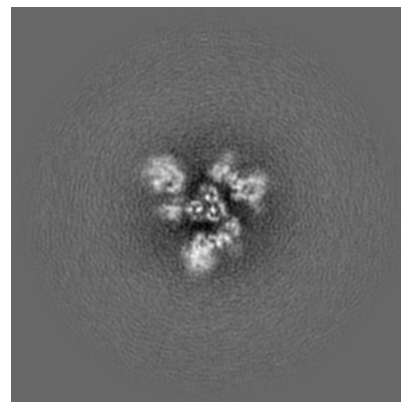
6.3.1 Primary map



X Index: 245

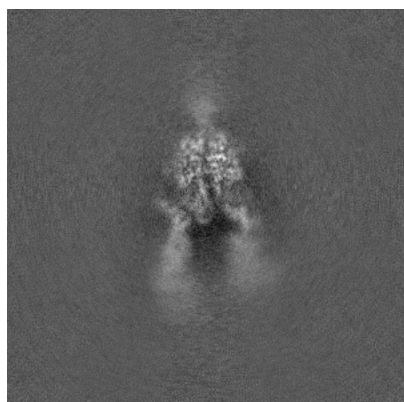


Y Index: 219

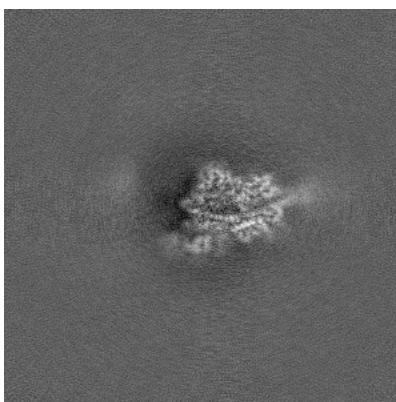


Z Index: 218

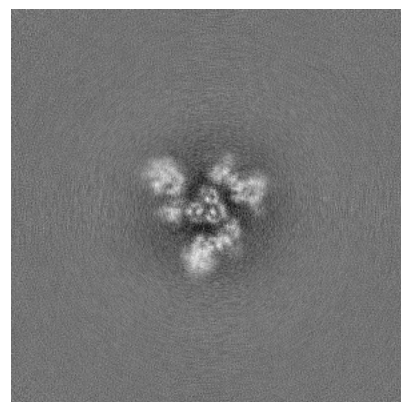
6.3.2 Raw map



X Index: 246



Y Index: 220

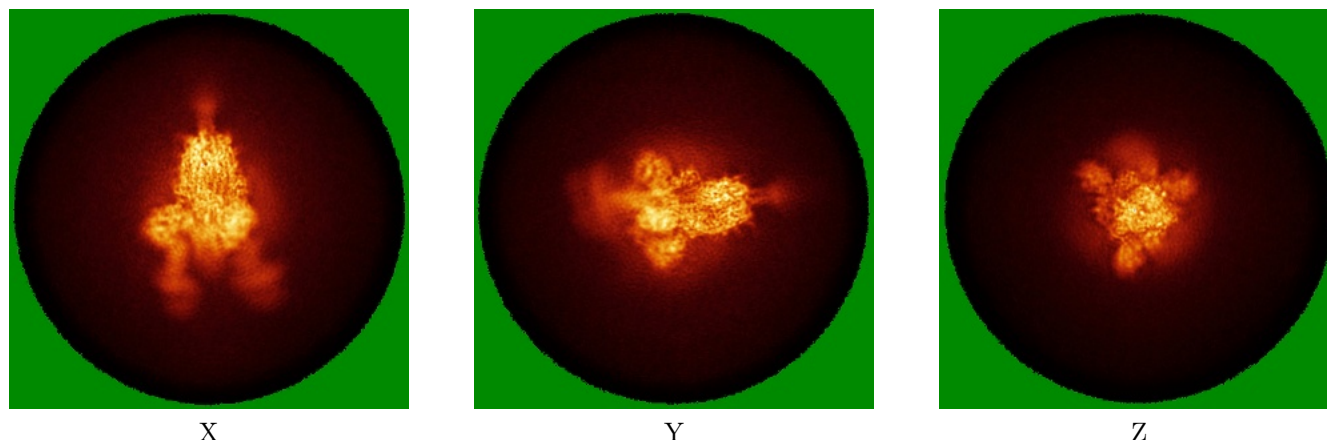


Z Index: 218

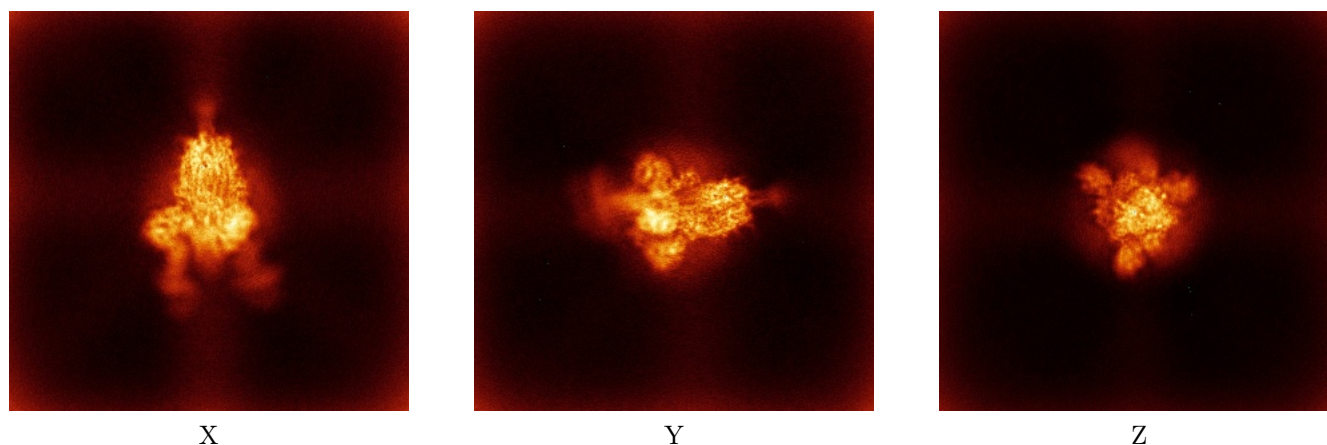
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



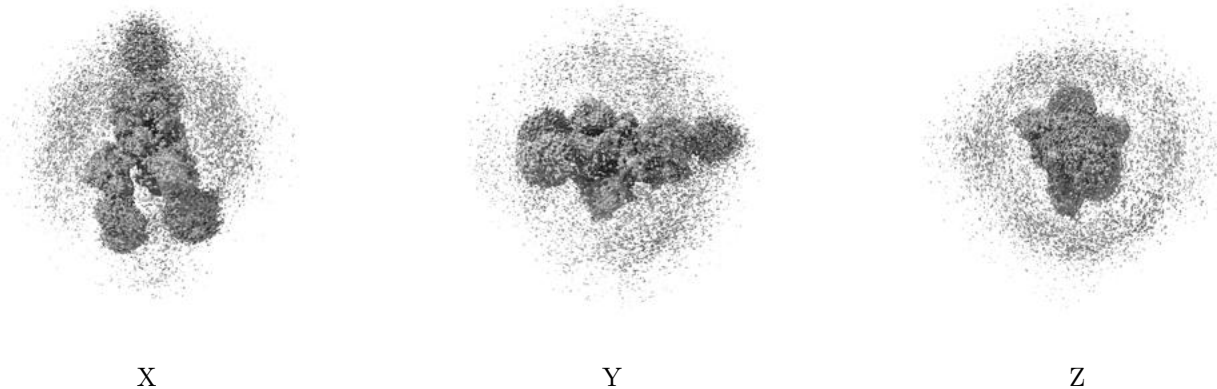
6.4.2 Raw map



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

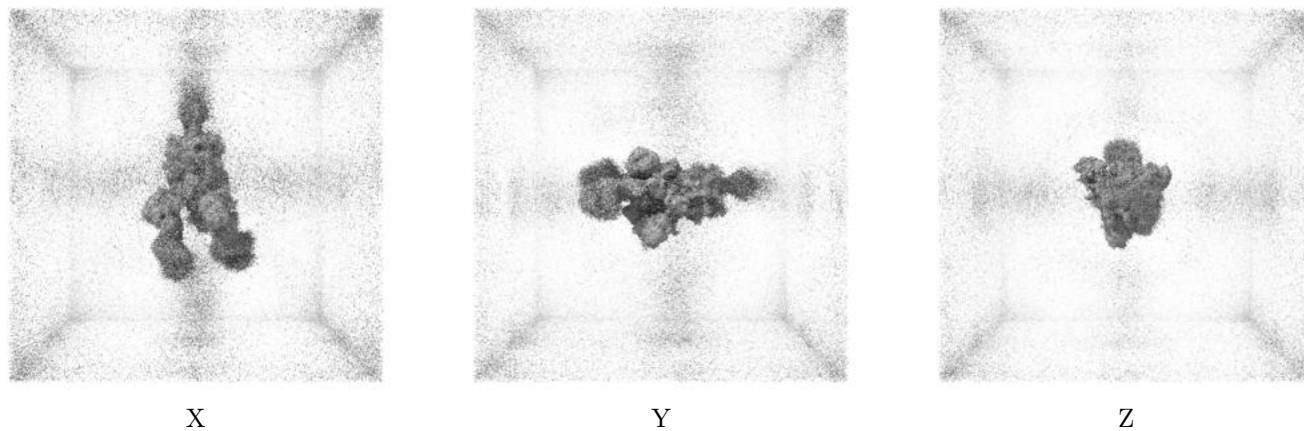
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0601. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

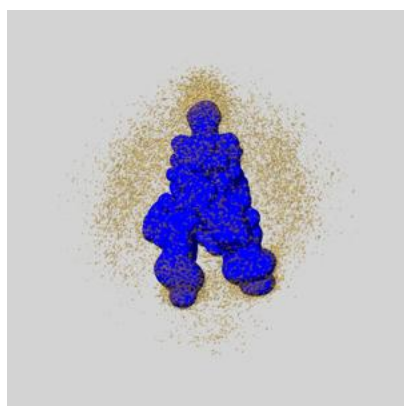
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

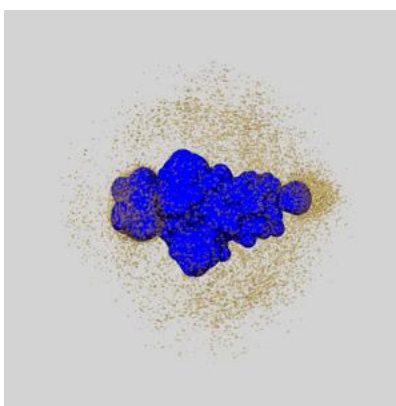
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

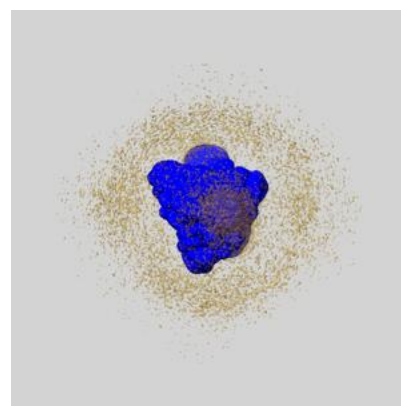
6.6.1 emd_37636_msk_1.map [i](#)



X



Y

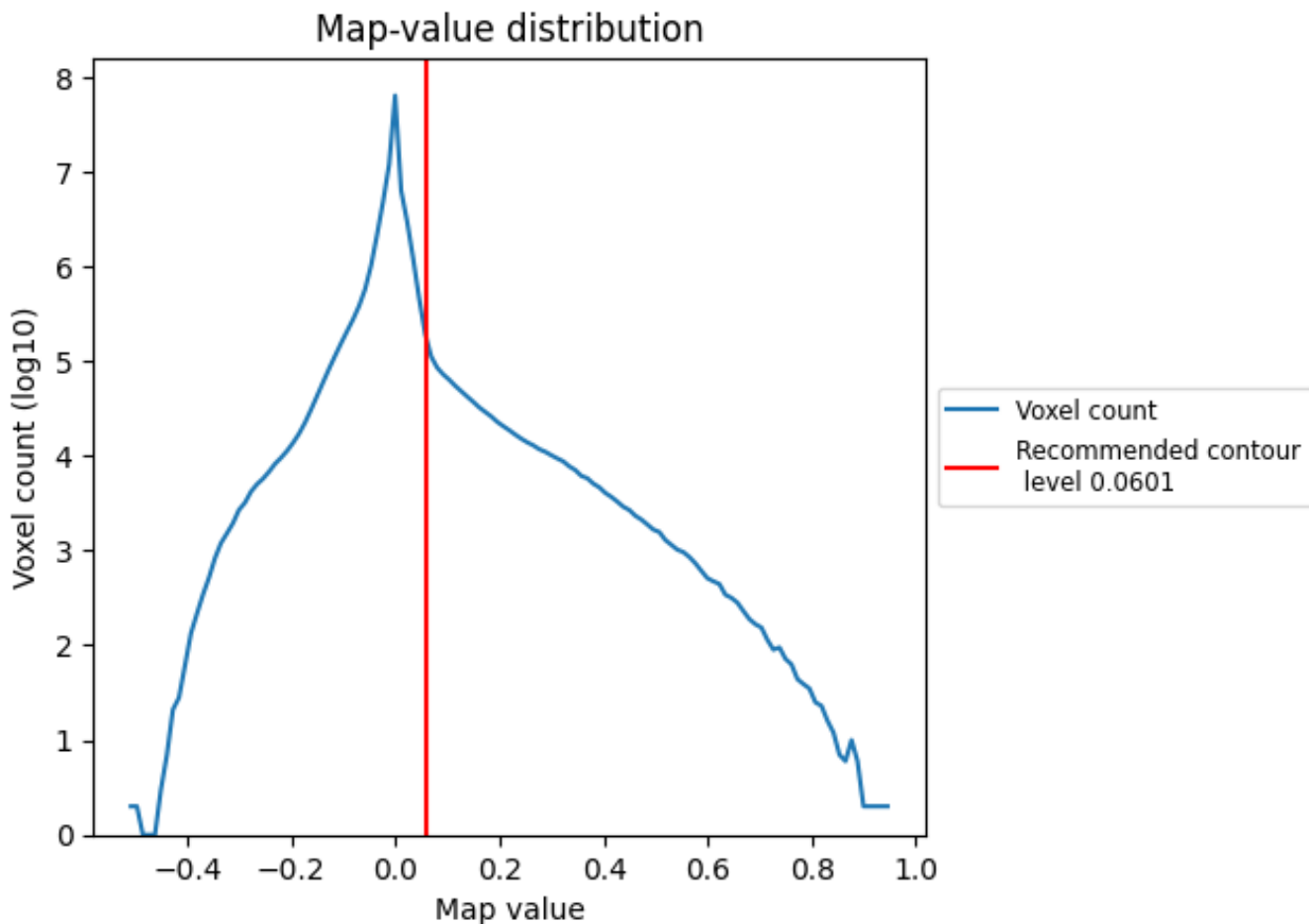


Z

7 Map analysis [i](#)

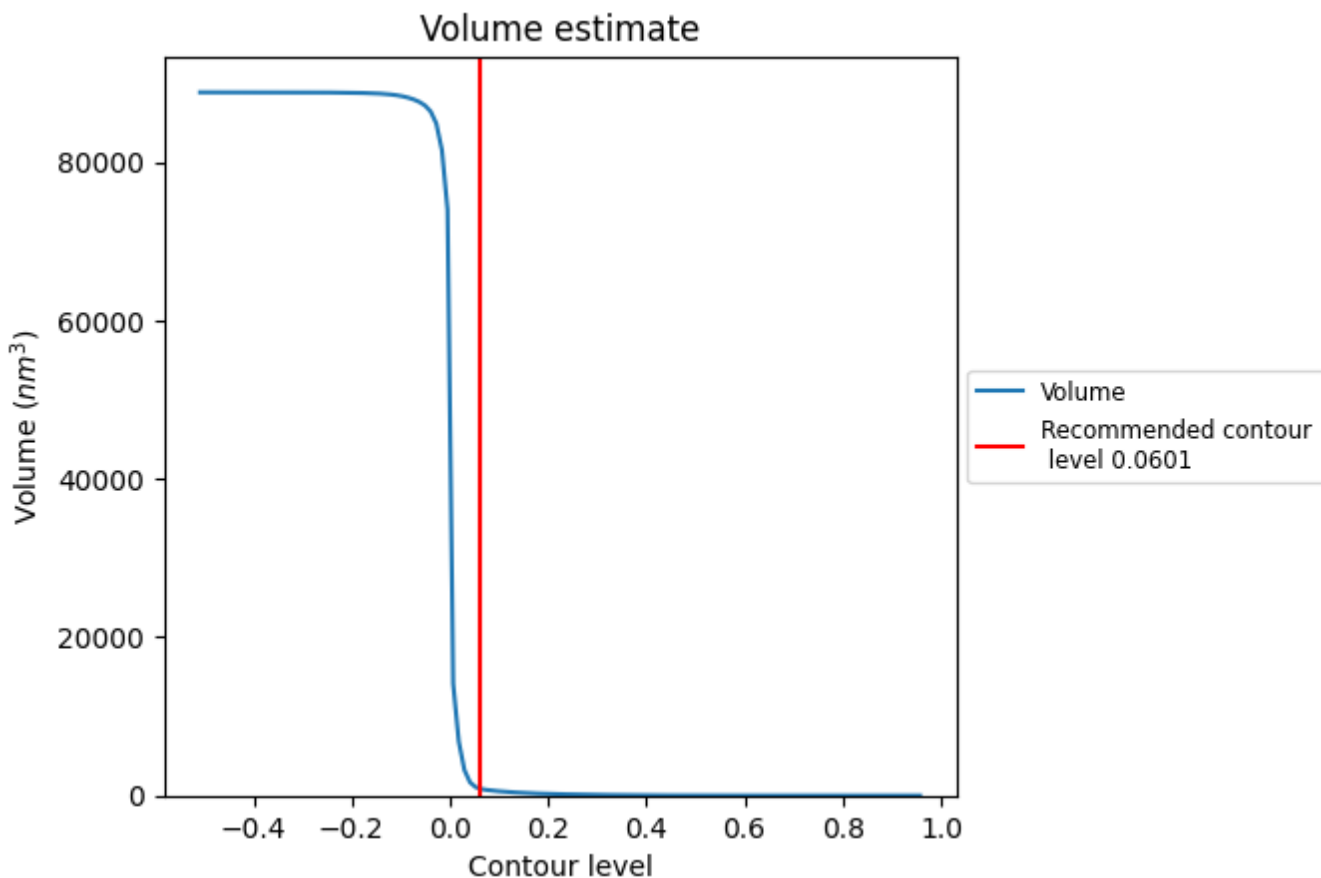
This section contains the results of statistical analysis of the map.

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.

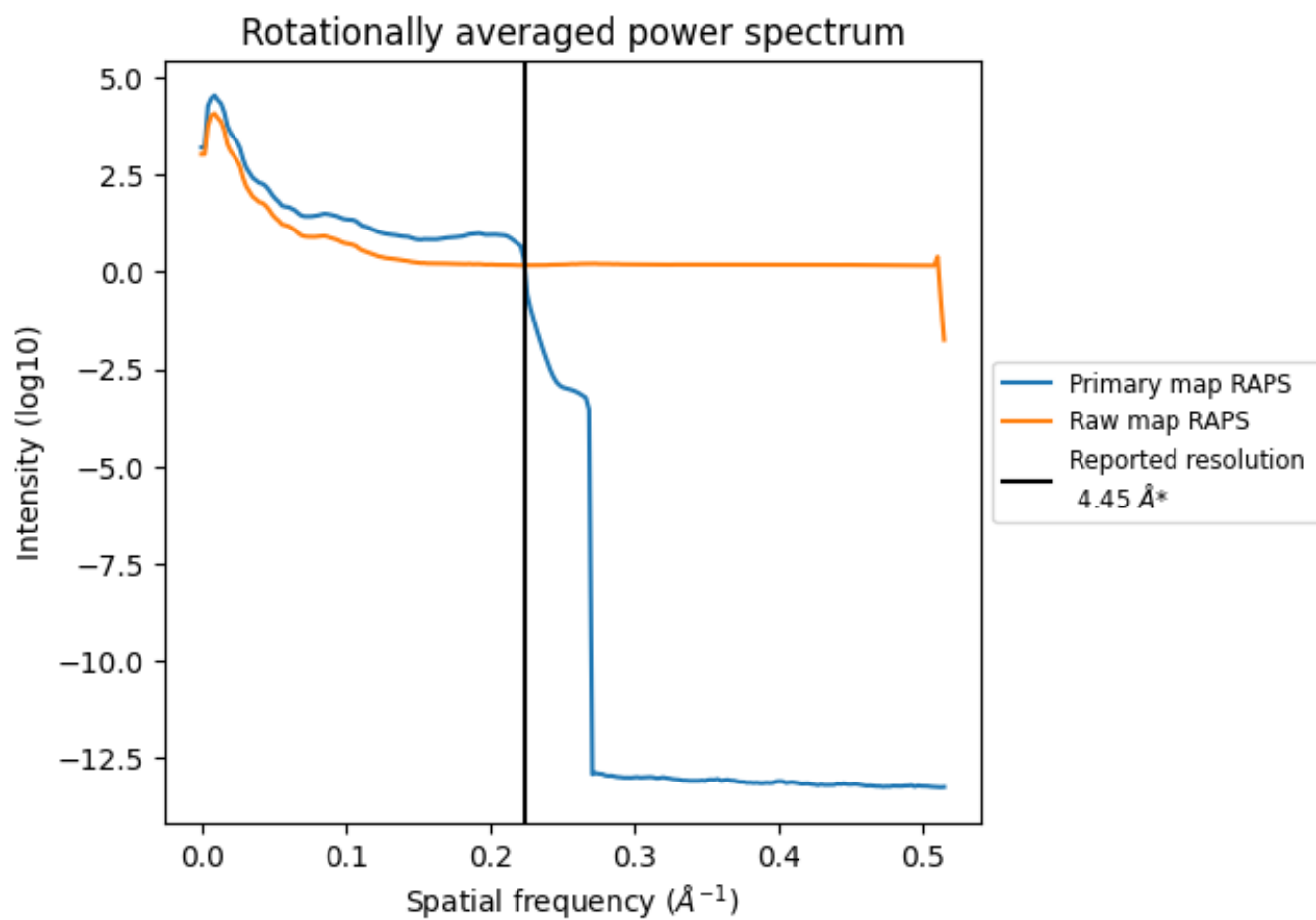
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 907 nm^3 ; this corresponds to an approximate mass of 819 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

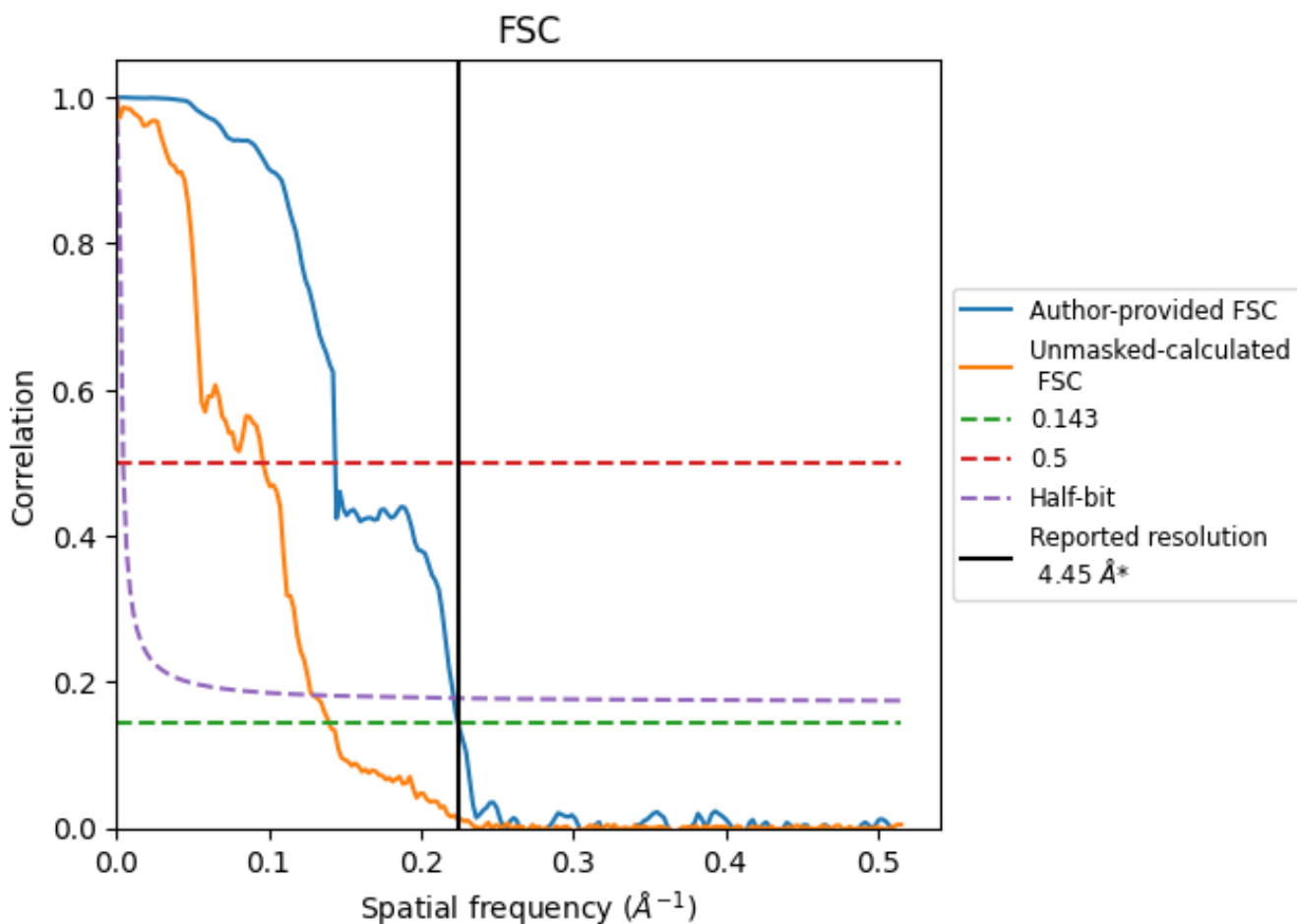


*Reported resolution corresponds to spatial frequency of 0.225 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.225 Å⁻¹

8.2 Resolution estimates [i](#)

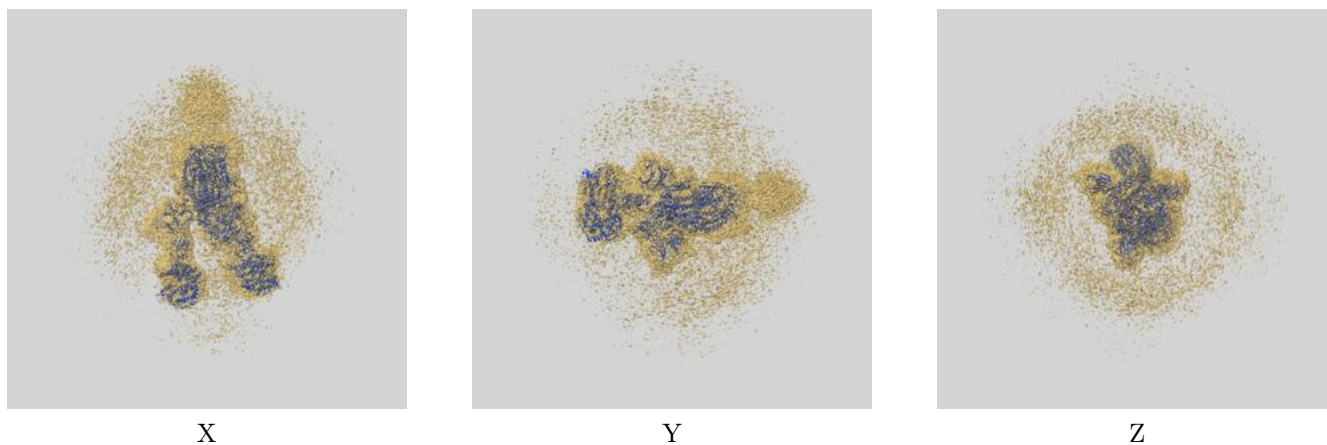
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.45	-	-
Author-provided FSC curve	4.45	6.96	4.51
Unmasked-calculated*	7.15	10.38	7.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.15 differs from the reported value 4.45 by more than 10 %

9 Map-model fit [i](#)

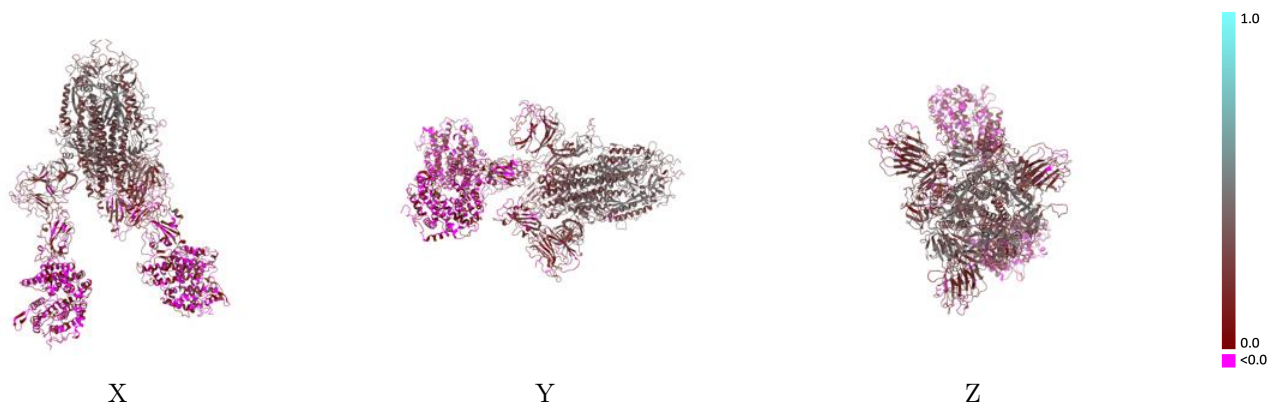
This section contains information regarding the fit between EMDB map EMD-37636 and PDB model 8WLZ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



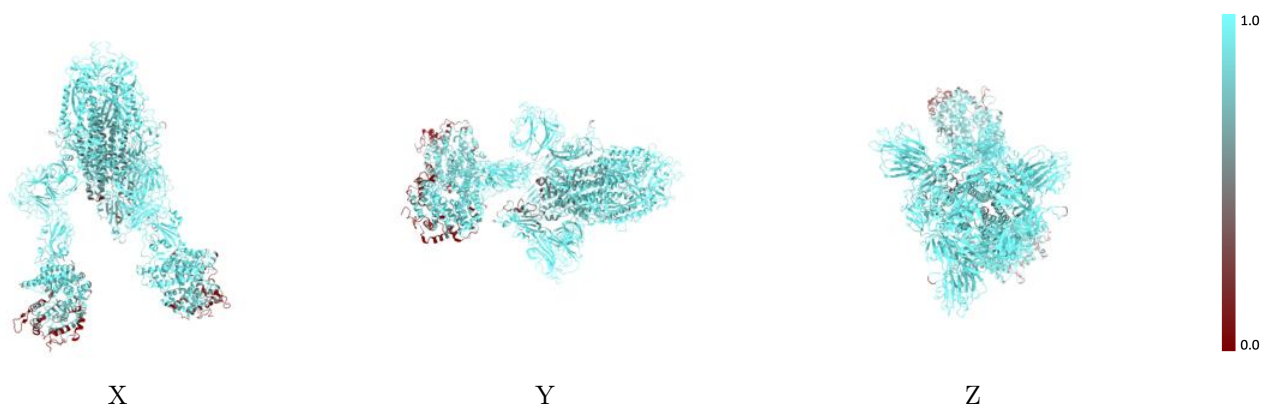
The images above show the 3D surface view of the map at the recommended contour level 0.0601 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



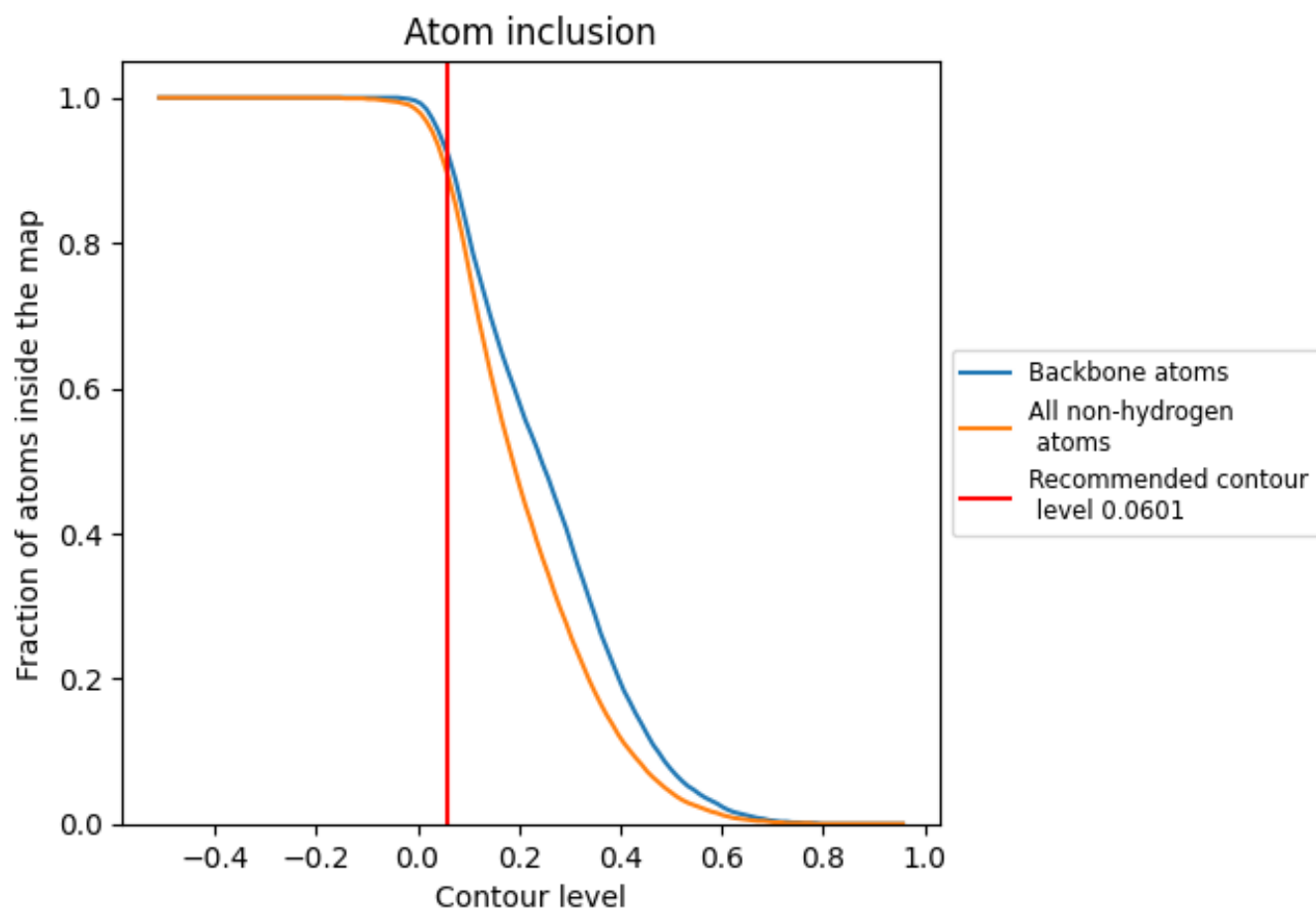
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0601).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0601) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.2130
A	 0.9530	 0.2700
B	 0.9250	 0.2790
C	 0.9630	 0.2720
D	 0.7320	 0.0420
E	 1.0000	 0.3710
F	 1.0000	 0.3540
G	 0.7690	 0.0550
H	 1.0000	 0.3030
I	 1.0000	 0.4230
J	 1.0000	 0.3640
K	 1.0000	 0.1880
L	 0.2500	 0.0710
M	 0.9740	 0.3160
N	 1.0000	 0.3800
O	 1.0000	 0.3320
P	 1.0000	 0.4000
Q	 1.0000	 0.2760
R	 1.0000	 0.3870
S	 1.0000	 0.3150
T	 0.9640	 0.3260
U	 1.0000	 0.2990

