



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:37 PM UTC

PDB ID : 5W9H / pdb_00005w9h
EMDB ID : EMD-8783
Title : MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors : Pallesen, J.; Ward, A.B.
Deposited on : 2017-06-23
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

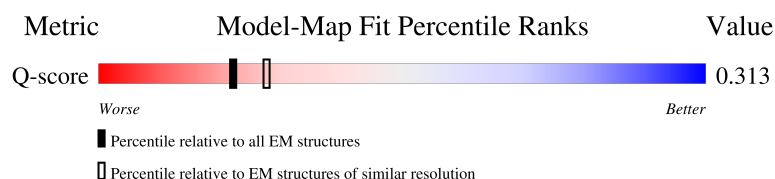
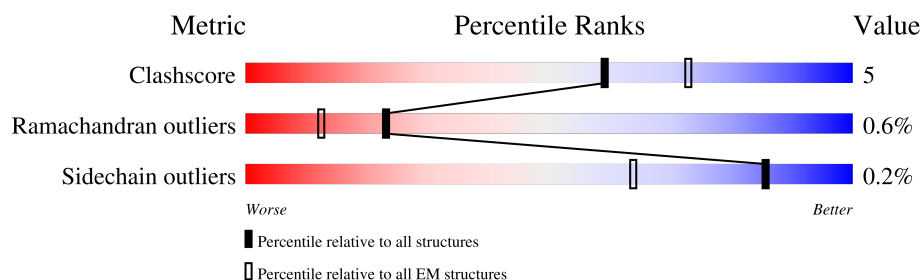
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	1329	
1	D	1329	
1	G	1329	
1	p	1329	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	q	1329	
1	r	1329	
2	B	233	
2	E	233	
2	H	233	
3	C	218	
3	F	218	
3	I	218	
4	J	2	
4	K	2	
4	L	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	
4	Y	2	
4	Z	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	a	2	50% 100%
4	b	2	100%
4	c	2	100%
4	d	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33840 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 MERS S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	D	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	G	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	p	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	q	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	r	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	PHE	LEU	conflict	UNP W5ZZF5
A	748	ALA	ARG	conflict	UNP W5ZZF5
A	751	GLY	ARG	conflict	UNP W5ZZF5
A	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
A	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
A	1292	GLY	-	expression tag	UNP W5ZZF5
A	1293	SER	-	expression tag	UNP W5ZZF5
A	1294	GLY	-	expression tag	UNP W5ZZF5
A	1295	TYR	-	expression tag	UNP W5ZZF5
A	1296	ILE	-	expression tag	UNP W5ZZF5
A	1297	PRO	-	expression tag	UNP W5ZZF5
A	1298	GLU	-	expression tag	UNP W5ZZF5
A	1299	ALA	-	expression tag	UNP W5ZZF5
A	1300	PRO	-	expression tag	UNP W5ZZF5
A	1301	ARG	-	expression tag	UNP W5ZZF5
A	1302	ASP	-	expression tag	UNP W5ZZF5
A	1303	GLY	-	expression tag	UNP W5ZZF5
A	1304	GLN	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1305	ALA	-	expression tag	UNP W5ZZF5
A	1306	TYR	-	expression tag	UNP W5ZZF5
A	1307	VAL	-	expression tag	UNP W5ZZF5
A	1308	ARG	-	expression tag	UNP W5ZZF5
A	1309	LYS	-	expression tag	UNP W5ZZF5
A	1310	ASP	-	expression tag	UNP W5ZZF5
A	1311	GLY	-	expression tag	UNP W5ZZF5
A	1312	GLU	-	expression tag	UNP W5ZZF5
A	1313	TRP	-	expression tag	UNP W5ZZF5
A	1314	VAL	-	expression tag	UNP W5ZZF5
A	1315	LEU	-	expression tag	UNP W5ZZF5
A	1316	LEU	-	expression tag	UNP W5ZZF5
A	1317	SER	-	expression tag	UNP W5ZZF5
A	1318	THR	-	expression tag	UNP W5ZZF5
A	1319	PHE	-	expression tag	UNP W5ZZF5
A	1320	LEU	-	expression tag	UNP W5ZZF5
A	1321	GLY	-	expression tag	UNP W5ZZF5
A	1322	ARG	-	expression tag	UNP W5ZZF5
A	1323	SER	-	expression tag	UNP W5ZZF5
A	1324	LEU	-	expression tag	UNP W5ZZF5
A	1325	GLU	-	expression tag	UNP W5ZZF5
A	1326	VAL	-	expression tag	UNP W5ZZF5
A	1327	LEU	-	expression tag	UNP W5ZZF5
A	1328	PHE	-	expression tag	UNP W5ZZF5
A	1329	GLN	-	expression tag	UNP W5ZZF5
D	506	PHE	LEU	conflict	UNP W5ZZF5
D	748	ALA	ARG	conflict	UNP W5ZZF5
D	751	GLY	ARG	conflict	UNP W5ZZF5
D	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
D	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
D	1292	GLY	-	expression tag	UNP W5ZZF5
D	1293	SER	-	expression tag	UNP W5ZZF5
D	1294	GLY	-	expression tag	UNP W5ZZF5
D	1295	TYR	-	expression tag	UNP W5ZZF5
D	1296	ILE	-	expression tag	UNP W5ZZF5
D	1297	PRO	-	expression tag	UNP W5ZZF5
D	1298	GLU	-	expression tag	UNP W5ZZF5
D	1299	ALA	-	expression tag	UNP W5ZZF5
D	1300	PRO	-	expression tag	UNP W5ZZF5
D	1301	ARG	-	expression tag	UNP W5ZZF5
D	1302	ASP	-	expression tag	UNP W5ZZF5
D	1303	GLY	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1304	GLN	-	expression tag	UNP W5ZZF5
D	1305	ALA	-	expression tag	UNP W5ZZF5
D	1306	TYR	-	expression tag	UNP W5ZZF5
D	1307	VAL	-	expression tag	UNP W5ZZF5
D	1308	ARG	-	expression tag	UNP W5ZZF5
D	1309	LYS	-	expression tag	UNP W5ZZF5
D	1310	ASP	-	expression tag	UNP W5ZZF5
D	1311	GLY	-	expression tag	UNP W5ZZF5
D	1312	GLU	-	expression tag	UNP W5ZZF5
D	1313	TRP	-	expression tag	UNP W5ZZF5
D	1314	VAL	-	expression tag	UNP W5ZZF5
D	1315	LEU	-	expression tag	UNP W5ZZF5
D	1316	LEU	-	expression tag	UNP W5ZZF5
D	1317	SER	-	expression tag	UNP W5ZZF5
D	1318	THR	-	expression tag	UNP W5ZZF5
D	1319	PHE	-	expression tag	UNP W5ZZF5
D	1320	LEU	-	expression tag	UNP W5ZZF5
D	1321	GLY	-	expression tag	UNP W5ZZF5
D	1322	ARG	-	expression tag	UNP W5ZZF5
D	1323	SER	-	expression tag	UNP W5ZZF5
D	1324	LEU	-	expression tag	UNP W5ZZF5
D	1325	GLU	-	expression tag	UNP W5ZZF5
D	1326	VAL	-	expression tag	UNP W5ZZF5
D	1327	LEU	-	expression tag	UNP W5ZZF5
D	1328	PHE	-	expression tag	UNP W5ZZF5
D	1329	GLN	-	expression tag	UNP W5ZZF5
G	506	PHE	LEU	conflict	UNP W5ZZF5
G	748	ALA	ARG	conflict	UNP W5ZZF5
G	751	GLY	ARG	conflict	UNP W5ZZF5
G	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
G	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
G	1292	GLY	-	expression tag	UNP W5ZZF5
G	1293	SER	-	expression tag	UNP W5ZZF5
G	1294	GLY	-	expression tag	UNP W5ZZF5
G	1295	TYR	-	expression tag	UNP W5ZZF5
G	1296	ILE	-	expression tag	UNP W5ZZF5
G	1297	PRO	-	expression tag	UNP W5ZZF5
G	1298	GLU	-	expression tag	UNP W5ZZF5
G	1299	ALA	-	expression tag	UNP W5ZZF5
G	1300	PRO	-	expression tag	UNP W5ZZF5
G	1301	ARG	-	expression tag	UNP W5ZZF5
G	1302	ASP	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	1303	GLY	-	expression tag	UNP W5ZZF5
G	1304	GLN	-	expression tag	UNP W5ZZF5
G	1305	ALA	-	expression tag	UNP W5ZZF5
G	1306	TYR	-	expression tag	UNP W5ZZF5
G	1307	VAL	-	expression tag	UNP W5ZZF5
G	1308	ARG	-	expression tag	UNP W5ZZF5
G	1309	LYS	-	expression tag	UNP W5ZZF5
G	1310	ASP	-	expression tag	UNP W5ZZF5
G	1311	GLY	-	expression tag	UNP W5ZZF5
G	1312	GLU	-	expression tag	UNP W5ZZF5
G	1313	TRP	-	expression tag	UNP W5ZZF5
G	1314	VAL	-	expression tag	UNP W5ZZF5
G	1315	LEU	-	expression tag	UNP W5ZZF5
G	1316	LEU	-	expression tag	UNP W5ZZF5
G	1317	SER	-	expression tag	UNP W5ZZF5
G	1318	THR	-	expression tag	UNP W5ZZF5
G	1319	PHE	-	expression tag	UNP W5ZZF5
G	1320	LEU	-	expression tag	UNP W5ZZF5
G	1321	GLY	-	expression tag	UNP W5ZZF5
G	1322	ARG	-	expression tag	UNP W5ZZF5
G	1323	SER	-	expression tag	UNP W5ZZF5
G	1324	LEU	-	expression tag	UNP W5ZZF5
G	1325	GLU	-	expression tag	UNP W5ZZF5
G	1326	VAL	-	expression tag	UNP W5ZZF5
G	1327	LEU	-	expression tag	UNP W5ZZF5
G	1328	PHE	-	expression tag	UNP W5ZZF5
G	1329	GLN	-	expression tag	UNP W5ZZF5
p	506	PHE	LEU	conflict	UNP W5ZZF5
p	748	ALA	ARG	conflict	UNP W5ZZF5
p	751	GLY	ARG	conflict	UNP W5ZZF5
p	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
p	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
p	1292	GLY	-	expression tag	UNP W5ZZF5
p	1293	SER	-	expression tag	UNP W5ZZF5
p	1294	GLY	-	expression tag	UNP W5ZZF5
p	1295	TYR	-	expression tag	UNP W5ZZF5
p	1296	ILE	-	expression tag	UNP W5ZZF5
p	1297	PRO	-	expression tag	UNP W5ZZF5
p	1298	GLU	-	expression tag	UNP W5ZZF5
p	1299	ALA	-	expression tag	UNP W5ZZF5
p	1300	PRO	-	expression tag	UNP W5ZZF5
p	1301	ARG	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
p	1302	ASP	-	expression tag	UNP W5ZZF5
p	1303	GLY	-	expression tag	UNP W5ZZF5
p	1304	GLN	-	expression tag	UNP W5ZZF5
p	1305	ALA	-	expression tag	UNP W5ZZF5
p	1306	TYR	-	expression tag	UNP W5ZZF5
p	1307	VAL	-	expression tag	UNP W5ZZF5
p	1308	ARG	-	expression tag	UNP W5ZZF5
p	1309	LYS	-	expression tag	UNP W5ZZF5
p	1310	ASP	-	expression tag	UNP W5ZZF5
p	1311	GLY	-	expression tag	UNP W5ZZF5
p	1312	GLU	-	expression tag	UNP W5ZZF5
p	1313	TRP	-	expression tag	UNP W5ZZF5
p	1314	VAL	-	expression tag	UNP W5ZZF5
p	1315	LEU	-	expression tag	UNP W5ZZF5
p	1316	LEU	-	expression tag	UNP W5ZZF5
p	1317	SER	-	expression tag	UNP W5ZZF5
p	1318	THR	-	expression tag	UNP W5ZZF5
p	1319	PHE	-	expression tag	UNP W5ZZF5
p	1320	LEU	-	expression tag	UNP W5ZZF5
p	1321	GLY	-	expression tag	UNP W5ZZF5
p	1322	ARG	-	expression tag	UNP W5ZZF5
p	1323	SER	-	expression tag	UNP W5ZZF5
p	1324	LEU	-	expression tag	UNP W5ZZF5
p	1325	GLU	-	expression tag	UNP W5ZZF5
p	1326	VAL	-	expression tag	UNP W5ZZF5
p	1327	LEU	-	expression tag	UNP W5ZZF5
p	1328	PHE	-	expression tag	UNP W5ZZF5
p	1329	GLN	-	expression tag	UNP W5ZZF5
q	506	PHE	LEU	conflict	UNP W5ZZF5
q	748	ALA	ARG	conflict	UNP W5ZZF5
q	751	GLY	ARG	conflict	UNP W5ZZF5
q	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
q	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
q	1292	GLY	-	expression tag	UNP W5ZZF5
q	1293	SER	-	expression tag	UNP W5ZZF5
q	1294	GLY	-	expression tag	UNP W5ZZF5
q	1295	TYR	-	expression tag	UNP W5ZZF5
q	1296	ILE	-	expression tag	UNP W5ZZF5
q	1297	PRO	-	expression tag	UNP W5ZZF5
q	1298	GLU	-	expression tag	UNP W5ZZF5
q	1299	ALA	-	expression tag	UNP W5ZZF5
q	1300	PRO	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
q	1301	ARG	-	expression tag	UNP W5ZZF5
q	1302	ASP	-	expression tag	UNP W5ZZF5
q	1303	GLY	-	expression tag	UNP W5ZZF5
q	1304	GLN	-	expression tag	UNP W5ZZF5
q	1305	ALA	-	expression tag	UNP W5ZZF5
q	1306	TYR	-	expression tag	UNP W5ZZF5
q	1307	VAL	-	expression tag	UNP W5ZZF5
q	1308	ARG	-	expression tag	UNP W5ZZF5
q	1309	LYS	-	expression tag	UNP W5ZZF5
q	1310	ASP	-	expression tag	UNP W5ZZF5
q	1311	GLY	-	expression tag	UNP W5ZZF5
q	1312	GLU	-	expression tag	UNP W5ZZF5
q	1313	TRP	-	expression tag	UNP W5ZZF5
q	1314	VAL	-	expression tag	UNP W5ZZF5
q	1315	LEU	-	expression tag	UNP W5ZZF5
q	1316	LEU	-	expression tag	UNP W5ZZF5
q	1317	SER	-	expression tag	UNP W5ZZF5
q	1318	THR	-	expression tag	UNP W5ZZF5
q	1319	PHE	-	expression tag	UNP W5ZZF5
q	1320	LEU	-	expression tag	UNP W5ZZF5
q	1321	GLY	-	expression tag	UNP W5ZZF5
q	1322	ARG	-	expression tag	UNP W5ZZF5
q	1323	SER	-	expression tag	UNP W5ZZF5
q	1324	LEU	-	expression tag	UNP W5ZZF5
q	1325	GLU	-	expression tag	UNP W5ZZF5
q	1326	VAL	-	expression tag	UNP W5ZZF5
q	1327	LEU	-	expression tag	UNP W5ZZF5
q	1328	PHE	-	expression tag	UNP W5ZZF5
q	1329	GLN	-	expression tag	UNP W5ZZF5
r	506	PHE	LEU	conflict	UNP W5ZZF5
r	748	ALA	ARG	conflict	UNP W5ZZF5
r	751	GLY	ARG	conflict	UNP W5ZZF5
r	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
r	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
r	1292	GLY	-	expression tag	UNP W5ZZF5
r	1293	SER	-	expression tag	UNP W5ZZF5
r	1294	GLY	-	expression tag	UNP W5ZZF5
r	1295	TYR	-	expression tag	UNP W5ZZF5
r	1296	ILE	-	expression tag	UNP W5ZZF5
r	1297	PRO	-	expression tag	UNP W5ZZF5
r	1298	GLU	-	expression tag	UNP W5ZZF5
r	1299	ALA	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
r	1300	PRO	-	expression tag	UNP W5ZZF5
r	1301	ARG	-	expression tag	UNP W5ZZF5
r	1302	ASP	-	expression tag	UNP W5ZZF5
r	1303	GLY	-	expression tag	UNP W5ZZF5
r	1304	GLN	-	expression tag	UNP W5ZZF5
r	1305	ALA	-	expression tag	UNP W5ZZF5
r	1306	TYR	-	expression tag	UNP W5ZZF5
r	1307	VAL	-	expression tag	UNP W5ZZF5
r	1308	ARG	-	expression tag	UNP W5ZZF5
r	1309	LYS	-	expression tag	UNP W5ZZF5
r	1310	ASP	-	expression tag	UNP W5ZZF5
r	1311	GLY	-	expression tag	UNP W5ZZF5
r	1312	GLU	-	expression tag	UNP W5ZZF5
r	1313	TRP	-	expression tag	UNP W5ZZF5
r	1314	VAL	-	expression tag	UNP W5ZZF5
r	1315	LEU	-	expression tag	UNP W5ZZF5
r	1316	LEU	-	expression tag	UNP W5ZZF5
r	1317	SER	-	expression tag	UNP W5ZZF5
r	1318	THR	-	expression tag	UNP W5ZZF5
r	1319	PHE	-	expression tag	UNP W5ZZF5
r	1320	LEU	-	expression tag	UNP W5ZZF5
r	1321	GLY	-	expression tag	UNP W5ZZF5
r	1322	ARG	-	expression tag	UNP W5ZZF5
r	1323	SER	-	expression tag	UNP W5ZZF5
r	1324	LEU	-	expression tag	UNP W5ZZF5
r	1325	GLU	-	expression tag	UNP W5ZZF5
r	1326	VAL	-	expression tag	UNP W5ZZF5
r	1327	LEU	-	expression tag	UNP W5ZZF5
r	1328	PHE	-	expression tag	UNP W5ZZF5
r	1329	GLN	-	expression tag	UNP W5ZZF5

- Molecule 2 is a protein called G4 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	E	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	H	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

- Molecule 3 is a protein called G4 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	111	Total	C	N	O	S	0	0
			835	522	143	166	4		
3	F	111	Total	C	N	O	S	0	0
			835	522	143	166	4		
3	I	111	Total	C	N	O	S	0	0
			835	522	143	166	4		

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



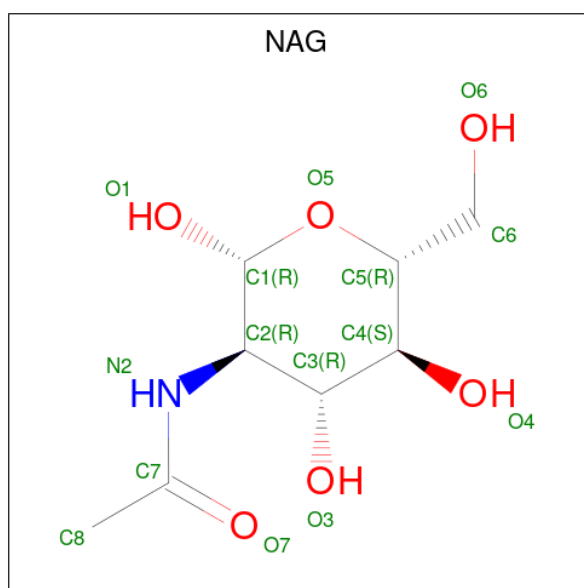
Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

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

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

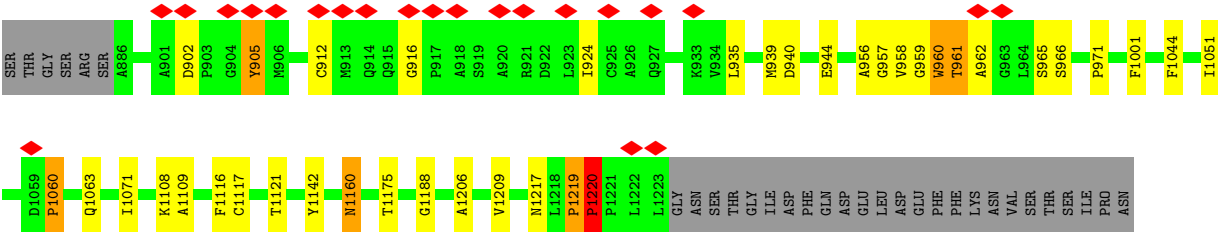


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	p	1	Total	C	N	O	0
			14	8	1	5	

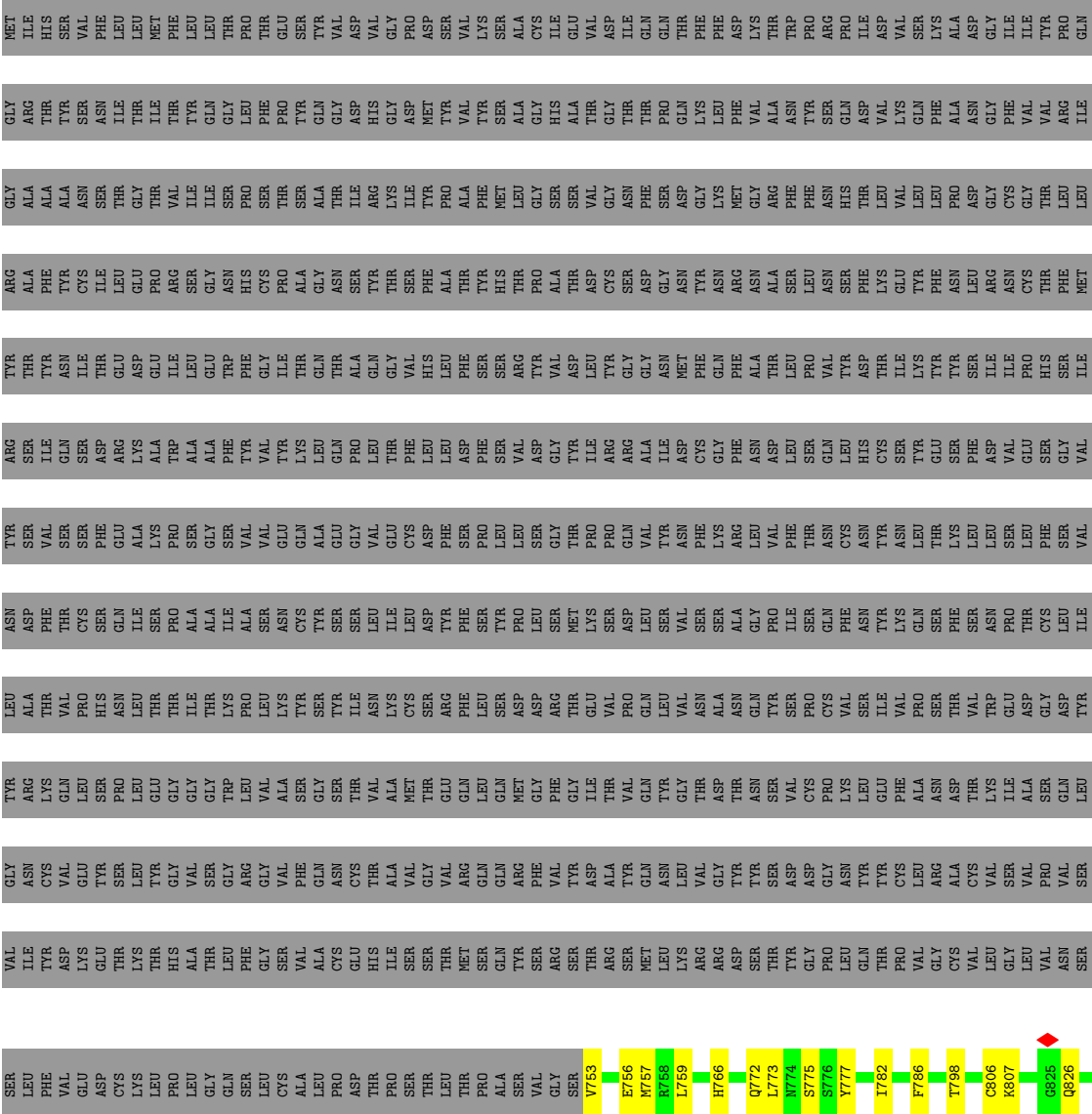
Continued on next page...

Continued from previous page...

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

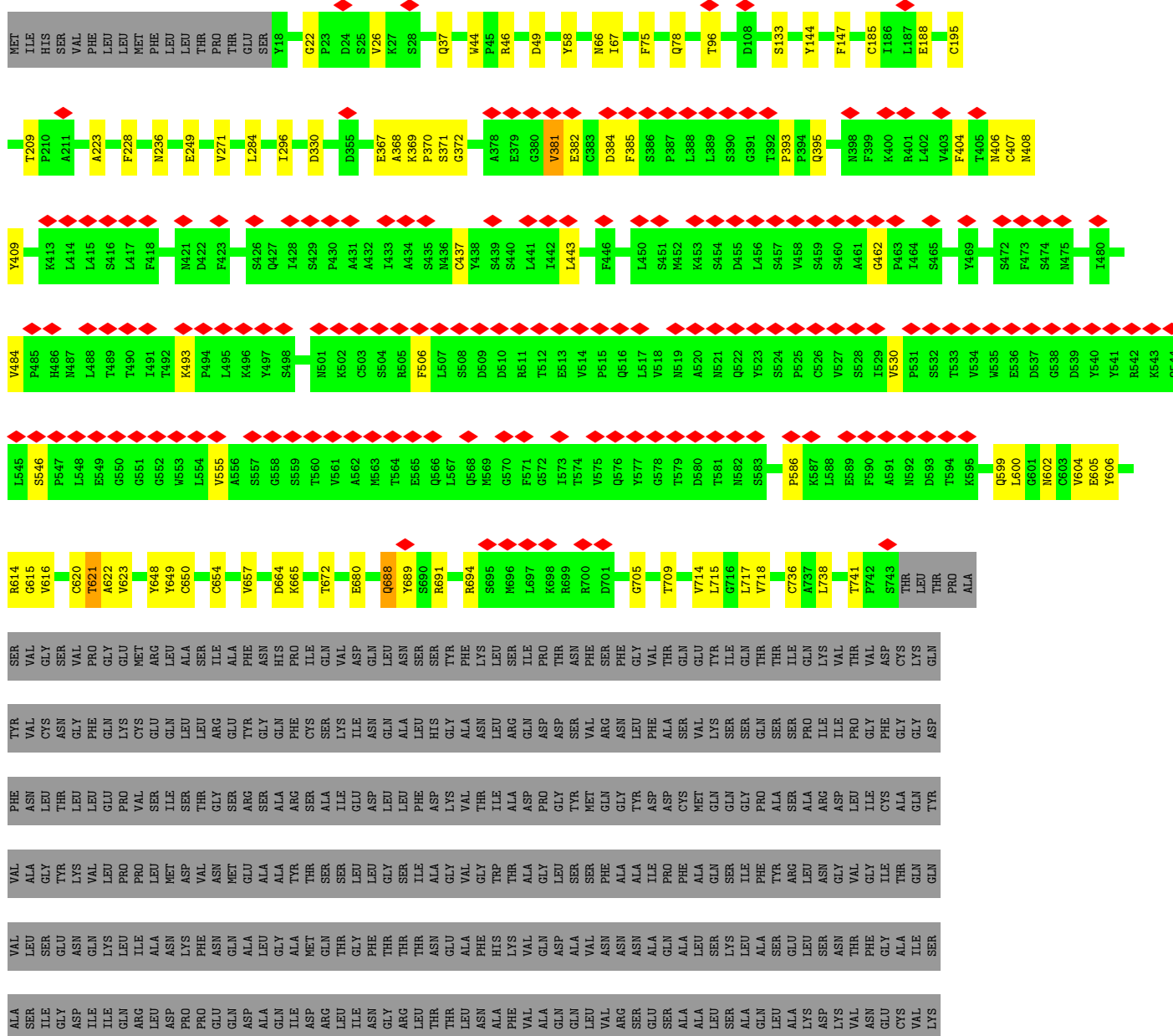


• Molecule 1: MERS S

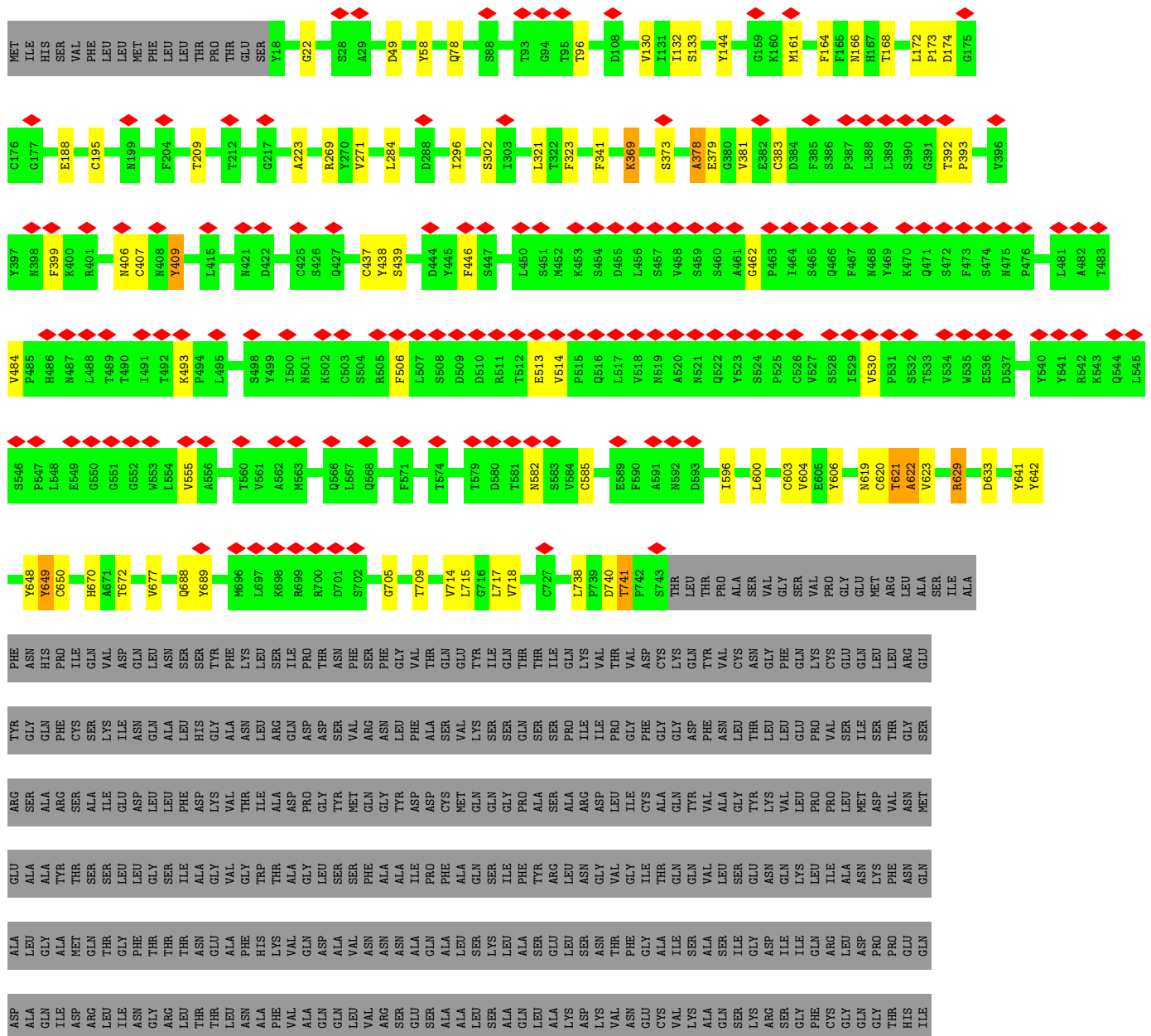




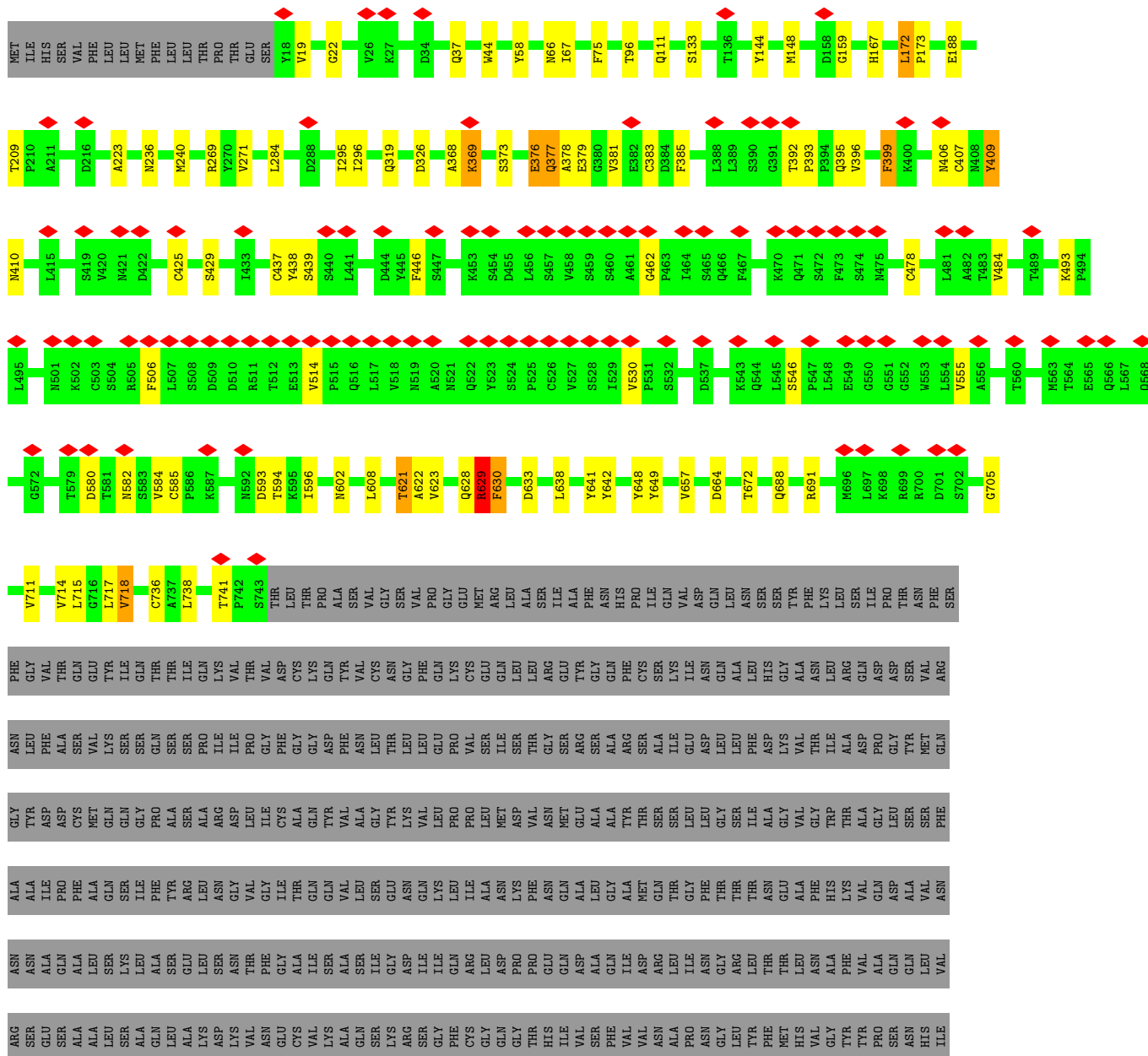
- Molecule 1: MERS S

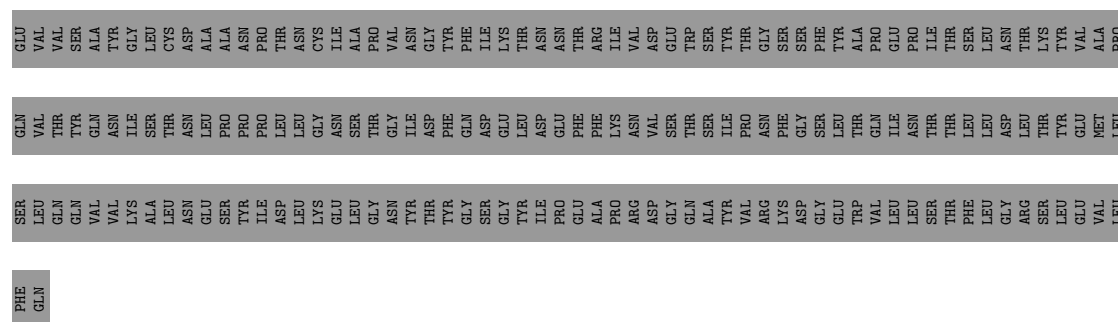


- Molecule 1: MERS S

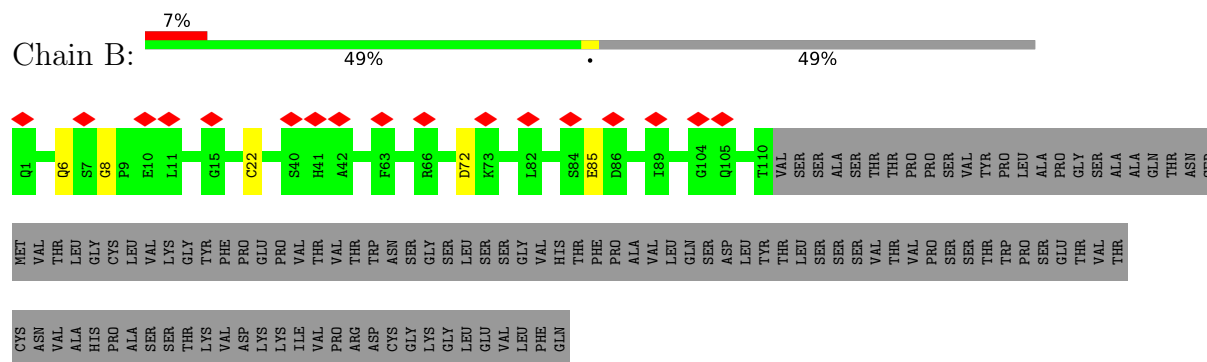


- Molecule 1: MERS S

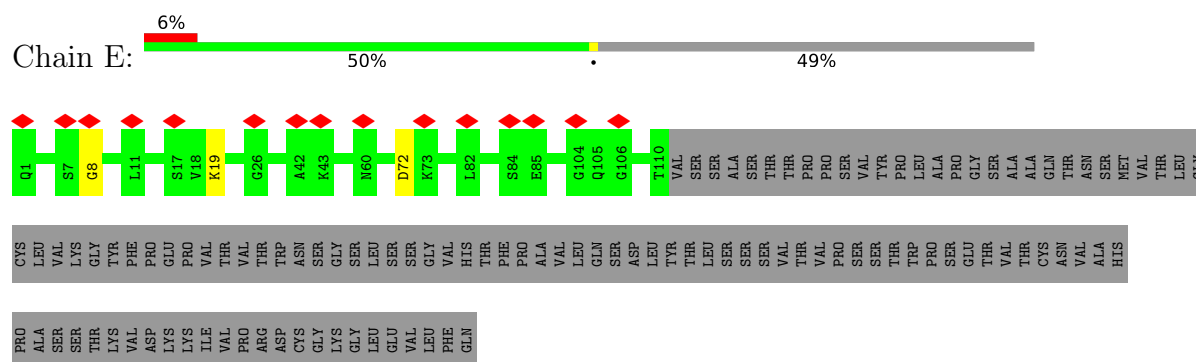




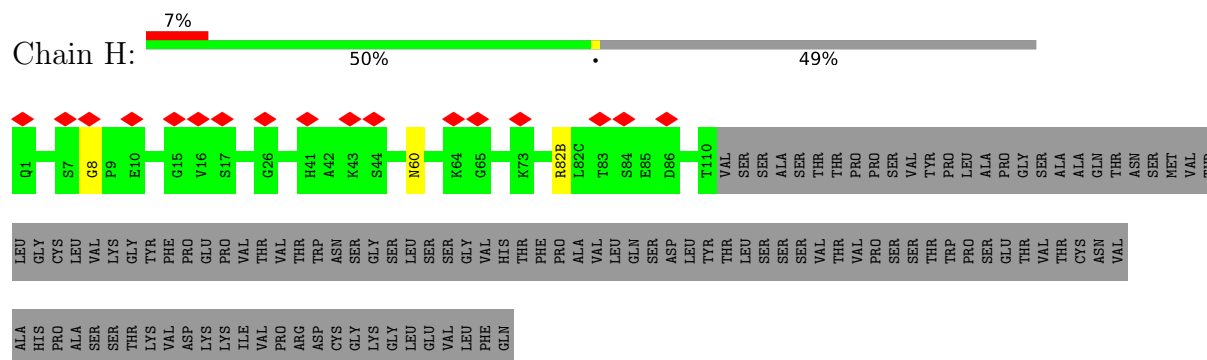
- Molecule 2: G4 VH



- Molecule 2: G4 VH



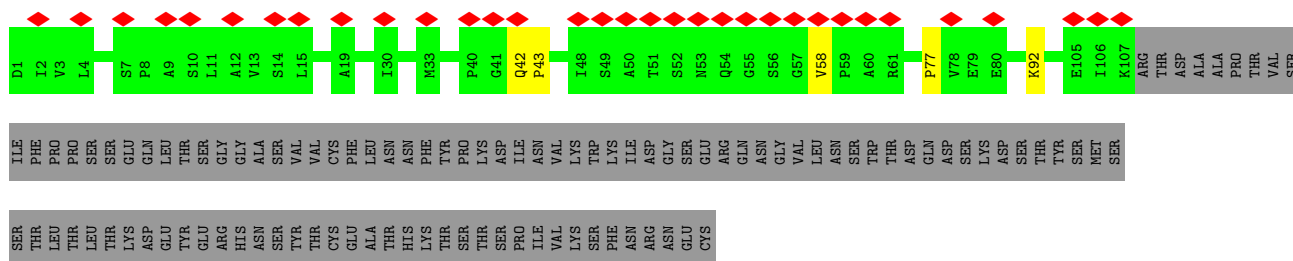
- Molecule 2: G4 VH



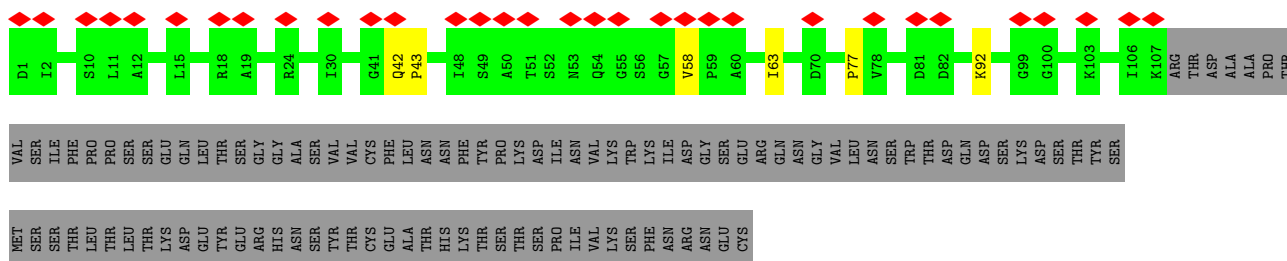
- Molecule 3: G4 VL



- Molecule 3: G4 VL



- Molecule 3: G4 VL



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



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



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



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



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



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



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



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



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

Chain R:  50% 50%



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

Chain S:  50% 50%



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

Chain T:  50% 50%



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

Chain U:  100%



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

Chain V:  50% 50%



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

Chain W:  50% 50%

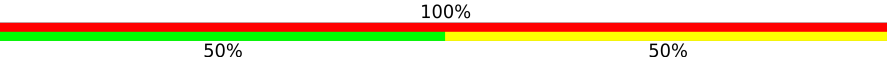


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%



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

Chain Y:  50% 100% 50%

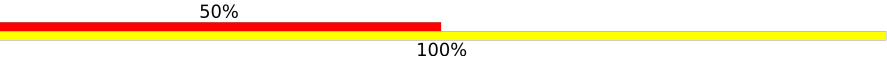


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 50%

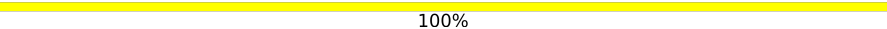


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 100%

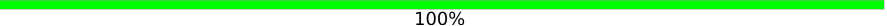


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%



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

Chain c:  100%



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

Chain d:  50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	310.08, 310.08, 310.08	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.95	0/3618	1.20	30/4921 (0.6%)
1	D	0.93	0/3618	1.18	30/4921 (0.6%)
1	G	0.95	0/3618	1.24	37/4921 (0.8%)
1	p	0.80	2/5803 (0.0%)	1.30	68/7901 (0.9%)
1	q	0.80	0/5803	1.31	74/7901 (0.9%)
1	r	0.82	3/5803 (0.1%)	1.35	87/7901 (1.1%)
2	B	0.72	0/972	1.11	2/1317 (0.2%)
2	E	0.73	0/972	1.15	4/1317 (0.3%)
2	H	0.75	0/972	1.16	4/1317 (0.3%)
3	C	0.75	0/852	1.30	8/1153 (0.7%)
3	F	0.76	0/852	1.36	8/1153 (0.7%)
3	I	0.76	0/852	1.40	9/1153 (0.8%)
All	All	0.84	5/33735 (0.0%)	1.27	361/45876 (0.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	r	584	VAL	CA-C	-7.22	1.44	1.52
1	p	437	CYS	CA-C	6.53	1.61	1.52
1	p	185	CYS	N-CA	6.00	1.53	1.45
1	r	437	CYS	C-O	5.65	1.30	1.23
1	r	585	CYS	N-CA	-5.03	1.39	1.46

All (361) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	688	GLN	N-CA-C	11.02	123.30	111.28
3	I	42	GLN	CA-C-N	10.19	127.00	119.66
3	I	42	GLN	C-N-CA	10.19	127.00	119.66
1	G	961	THR	CA-C-N	10.14	140.90	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	961	THR	C-N-CA	10.14	140.90	121.54
1	q	284	LEU	CA-C-N	9.60	129.25	119.56
1	q	284	LEU	C-N-CA	9.60	129.25	119.56
3	C	42	GLN	CA-C-N	9.57	126.55	119.66
3	C	42	GLN	C-N-CA	9.57	126.55	119.66
1	r	144	TYR	CA-C-N	9.40	129.35	119.85
1	r	144	TYR	C-N-CA	9.40	129.35	119.85
3	C	58	VAL	CA-C-N	9.27	129.84	119.92
3	C	58	VAL	C-N-CA	9.27	129.84	119.92
1	r	284	LEU	CA-C-N	9.08	128.73	119.56
1	r	284	LEU	C-N-CA	9.08	128.73	119.56
2	E	8	GLY	CA-C-N	9.07	129.01	119.85
2	E	8	GLY	C-N-CA	9.07	129.01	119.85
1	r	437	CYS	O-C-N	-8.99	112.67	123.19
1	q	144	TYR	CA-C-N	8.89	128.83	119.85
1	q	144	TYR	C-N-CA	8.89	128.83	119.85
2	H	8	GLY	CA-C-N	8.81	128.75	119.85
2	H	8	GLY	C-N-CA	8.81	128.75	119.85
3	F	42	GLN	CA-C-N	8.62	125.95	119.66
3	F	42	GLN	C-N-CA	8.62	125.95	119.66
1	q	393	PRO	CA-C-N	8.55	128.50	120.03
1	q	393	PRO	C-N-CA	8.55	128.50	120.03
3	I	58	VAL	CA-C-N	8.52	128.47	120.03
3	I	58	VAL	C-N-CA	8.52	128.47	120.03
1	p	144	TYR	CA-C-N	8.49	128.42	119.85
1	p	144	TYR	C-N-CA	8.49	128.42	119.85
3	F	58	VAL	CA-C-N	8.46	128.40	120.03
3	F	58	VAL	C-N-CA	8.46	128.40	120.03
1	G	1156	CYS	N-CA-C	8.39	121.46	108.96
1	r	393	PRO	CA-C-N	8.37	128.30	119.85
1	r	393	PRO	C-N-CA	8.37	128.30	119.85
1	r	96	THR	CA-C-N	8.35	128.38	119.78
1	r	96	THR	C-N-CA	8.35	128.38	119.78
1	p	462	GLY	CA-C-N	8.33	128.06	119.56
1	p	462	GLY	C-N-CA	8.33	128.06	119.56
1	p	393	PRO	CA-C-N	8.33	128.28	120.03
1	p	393	PRO	C-N-CA	8.33	128.28	120.03
1	p	209	THR	CA-C-N	8.24	127.97	119.56
1	p	209	THR	C-N-CA	8.24	127.97	119.56
1	r	22	GLY	CA-C-N	8.24	128.26	119.78
1	r	22	GLY	C-N-CA	8.24	128.26	119.78
1	D	965	SER	CB-CA-C	-8.17	94.17	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	q	96	THR	CA-C-N	8.16	128.19	119.78
1	q	96	THR	C-N-CA	8.16	128.19	119.78
1	q	373	SER	N-CA-C	8.12	121.39	110.35
1	A	902	ASP	CA-C-N	8.10	128.12	119.78
1	A	902	ASP	C-N-CA	8.10	128.12	119.78
1	r	530	VAL	CA-C-N	8.10	128.58	119.92
1	r	530	VAL	C-N-CA	8.10	128.58	119.92
1	A	935	LEU	CA-C-N	8.03	125.44	119.66
1	A	935	LEU	C-N-CA	8.03	125.44	119.66
1	q	209	THR	CA-C-N	7.98	127.70	119.56
1	q	209	THR	C-N-CA	7.98	127.70	119.56
1	q	741	THR	CA-C-N	7.98	128.00	119.78
1	q	741	THR	C-N-CA	7.98	128.00	119.78
1	D	935	LEU	CA-C-N	7.97	125.39	119.66
1	D	935	LEU	C-N-CA	7.97	125.39	119.66
1	p	738	LEU	CA-C-N	7.96	127.89	119.85
1	p	738	LEU	C-N-CA	7.96	127.89	119.85
1	r	741	THR	CA-C-N	7.95	127.97	119.78
1	r	741	THR	C-N-CA	7.95	127.97	119.78
1	r	392	THR	CA-C-N	7.90	125.42	119.66
1	r	392	THR	C-N-CA	7.90	125.42	119.66
1	p	284	LEU	CA-C-N	7.88	127.60	119.56
1	p	284	LEU	C-N-CA	7.88	127.60	119.56
1	r	493	LYS	CA-C-N	7.88	127.81	119.85
1	r	493	LYS	C-N-CA	7.88	127.81	119.85
1	r	484	VAL	CA-C-N	7.84	127.85	119.78
1	r	484	VAL	C-N-CA	7.84	127.85	119.78
1	r	399	PHE	N-CA-C	7.80	121.24	110.24
1	r	705	GLY	CA-C-N	7.79	127.72	119.85
1	r	705	GLY	C-N-CA	7.79	127.72	119.85
1	p	530	VAL	CA-C-N	7.69	128.15	119.92
1	p	530	VAL	C-N-CA	7.69	128.15	119.92
1	q	530	VAL	CA-C-N	7.68	127.69	119.78
1	q	530	VAL	C-N-CA	7.68	127.69	119.78
1	A	939	MET	N-CA-C	7.62	120.47	111.71
1	A	1142	TYR	CA-C-N	7.62	127.63	119.78
1	A	1142	TYR	C-N-CA	7.62	127.63	119.78
1	p	384	ASP	CA-C-N	7.52	135.27	122.26
1	p	384	ASP	C-N-CA	7.52	135.27	122.26
1	G	1219	PRO	N-CA-C	7.50	119.85	110.70
1	q	462	GLY	CA-C-N	7.49	127.20	119.56
1	q	462	GLY	C-N-CA	7.49	127.20	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	43	PRO	CA-C-N	7.43	127.36	119.85
3	F	43	PRO	C-N-CA	7.43	127.36	119.85
1	q	493	LYS	CA-C-N	7.41	127.33	119.85
1	q	493	LYS	C-N-CA	7.41	127.33	119.85
1	p	96	THR	CA-C-N	7.37	127.37	119.78
1	p	96	THR	C-N-CA	7.37	127.37	119.78
1	r	462	GLY	CA-C-N	7.37	127.08	119.56
1	r	462	GLY	C-N-CA	7.37	127.08	119.56
1	G	912	CYS	CA-C-N	7.28	134.21	120.97
1	G	912	CYS	C-N-CA	7.28	134.21	120.97
1	G	753	VAL	CA-C-N	7.27	127.27	119.78
1	G	753	VAL	C-N-CA	7.27	127.27	119.78
3	I	58	VAL	N-CA-C	7.24	117.14	108.45
1	r	688	GLN	CA-C-N	7.23	134.71	121.70
1	r	688	GLN	C-N-CA	7.23	134.71	121.70
1	q	133	SER	CA-C-N	7.22	126.93	119.56
1	q	133	SER	C-N-CA	7.22	126.93	119.56
1	p	493	LYS	CA-C-N	7.22	127.14	119.85
1	p	493	LYS	C-N-CA	7.22	127.14	119.85
1	r	209	THR	CA-C-N	7.19	128.83	119.84
1	r	209	THR	C-N-CA	7.19	128.83	119.84
1	p	133	SER	CA-C-N	7.15	126.85	119.56
1	p	133	SER	C-N-CA	7.15	126.85	119.56
1	G	902	ASP	CA-C-N	7.10	127.10	119.78
1	G	902	ASP	C-N-CA	7.10	127.10	119.78
1	D	1142	TYR	CA-C-N	7.08	127.07	119.78
1	D	1142	TYR	C-N-CA	7.08	127.07	119.78
1	r	236	ASN	CA-C-N	-7.06	111.40	121.50
1	r	236	ASN	C-N-CA	-7.06	111.40	121.50
1	r	406	ASN	CA-C-N	-7.05	110.30	121.87
1	r	406	ASN	C-N-CA	-7.05	110.30	121.87
1	r	133	SER	CA-C-N	7.04	126.74	119.56
1	r	133	SER	C-N-CA	7.04	126.74	119.56
1	p	741	THR	CA-C-N	7.03	127.02	119.78
1	p	741	THR	C-N-CA	7.03	127.02	119.78
1	q	406	ASN	CA-C-N	-6.98	110.42	121.87
1	q	406	ASN	C-N-CA	-6.98	110.42	121.87
1	r	373	SER	N-CA-C	6.97	120.32	110.50
1	r	584	VAL	CB-CA-C	-6.96	102.53	110.96
2	B	8	GLY	CA-C-N	6.91	126.89	119.78
2	B	8	GLY	C-N-CA	6.91	126.89	119.78
1	G	924	ILE	CA-C-N	-6.91	109.51	121.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	924	ILE	C-N-CA	-6.91	109.51	121.66
1	D	1219	PRO	N-CA-C	6.89	119.11	110.70
1	G	1142	TYR	CA-C-N	6.89	126.81	119.85
1	G	1142	TYR	C-N-CA	6.89	126.81	119.85
1	q	378	ALA	CA-C-N	6.80	133.95	121.70
1	q	378	ALA	C-N-CA	6.80	133.95	121.70
1	q	514	VAL	CA-C-N	6.79	126.78	119.78
1	q	514	VAL	C-N-CA	6.79	126.78	119.78
1	p	688	GLN	CA-C-N	6.78	133.90	121.70
1	p	688	GLN	C-N-CA	6.78	133.90	121.70
1	G	766	HIS	CA-C-N	6.75	126.74	119.78
1	G	766	HIS	C-N-CA	6.75	126.74	119.78
1	D	924	ILE	CA-C-N	-6.75	109.50	122.06
1	D	924	ILE	C-N-CA	-6.75	109.50	122.06
1	r	446	PHE	N-CA-C	6.75	119.12	108.79
1	r	369	LYS	CA-C-N	6.70	126.68	119.78
1	r	369	LYS	C-N-CA	6.70	126.68	119.78
1	G	1218	LEU	CA-C-N	6.70	127.28	120.38
1	G	1218	LEU	C-N-CA	6.70	127.28	120.38
1	q	22	GLY	CA-C-N	6.69	126.67	119.78
1	q	22	GLY	C-N-CA	6.69	126.67	119.78
1	q	399	PHE	N-CA-C	6.67	119.65	110.24
3	I	43	PRO	CA-C-N	6.66	126.64	119.78
3	I	43	PRO	C-N-CA	6.66	126.64	119.78
3	F	58	VAL	N-CA-C	6.65	116.43	108.45
1	p	22	GLY	CA-C-N	6.62	126.60	119.78
1	p	22	GLY	C-N-CA	6.62	126.60	119.78
1	A	1160	ASN	CA-C-N	6.61	128.10	119.84
1	A	1160	ASN	C-N-CA	6.61	128.10	119.84
1	A	912	CYS	N-CA-C	-6.61	104.86	113.12
1	A	924	ILE	CA-C-N	-6.60	110.28	120.31
1	A	924	ILE	C-N-CA	-6.60	110.28	120.31
1	D	1160	ASN	CA-C-N	6.60	128.09	119.84
1	D	1160	ASN	C-N-CA	6.60	128.09	119.84
1	G	935	LEU	CA-C-N	6.59	124.47	119.66
1	G	935	LEU	C-N-CA	6.59	124.47	119.66
1	q	604	VAL	N-CA-C	6.54	118.86	109.51
1	p	271	VAL	N-CA-C	6.50	117.15	111.56
1	A	859	SER	CA-C-N	6.49	126.46	119.78
1	A	859	SER	C-N-CA	6.49	126.46	119.78
1	q	58	TYR	CA-C-N	6.47	126.44	119.78
1	q	58	TYR	C-N-CA	6.47	126.44	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	484	VAL	CA-C-N	6.42	126.39	119.78
1	p	484	VAL	C-N-CA	6.42	126.39	119.78
1	p	623	VAL	CA-C-N	-6.42	114.25	121.83
1	p	623	VAL	C-N-CA	-6.42	114.25	121.83
1	q	629	ARG	CB-CA-C	-6.38	97.72	110.42
1	r	37	GLN	N-CA-C	6.37	119.90	111.75
1	q	409	TYR	N-CA-C	6.33	118.57	109.14
1	p	26	VAL	N-CA-C	6.32	117.06	110.62
1	q	392	THR	CA-C-N	6.29	124.19	119.66
1	q	392	THR	C-N-CA	6.29	124.19	119.66
3	C	43	PRO	CA-C-N	6.28	126.20	119.85
3	C	43	PRO	C-N-CA	6.28	126.20	119.85
1	p	185	CYS	CA-C-O	-6.28	114.74	121.45
1	G	1058	LEU	N-CA-C	6.24	119.35	109.50
1	q	585	CYS	CA-C-N	6.24	126.20	119.78
1	q	585	CYS	C-N-CA	6.24	126.20	119.78
1	D	965	SER	N-CA-C	6.23	124.07	110.80
1	q	484	VAL	CA-C-N	6.23	126.19	119.78
1	q	484	VAL	C-N-CA	6.23	126.19	119.78
1	p	75	PHE	CA-C-N	6.22	126.13	119.85
1	p	75	PHE	C-N-CA	6.22	126.13	119.85
1	p	188	GLU	CA-C-N	6.21	126.18	119.78
1	p	188	GLU	C-N-CA	6.21	126.18	119.78
1	r	484	VAL	N-CA-C	6.19	113.95	108.63
1	q	302	SER	CA-C-N	6.16	128.75	120.50
1	q	302	SER	C-N-CA	6.16	128.75	120.50
1	r	319	GLN	CA-C-N	6.14	127.52	119.84
1	r	319	GLN	C-N-CA	6.14	127.52	119.84
1	p	185	CYS	O-C-N	6.14	130.16	123.10
1	p	236	ASN	CA-C-N	-6.13	112.73	121.50
1	p	236	ASN	C-N-CA	-6.13	112.73	121.50
1	r	296	ILE	CA-C-N	6.11	126.02	119.85
1	r	296	ILE	C-N-CA	6.11	126.02	119.85
1	r	584	VAL	O-C-N	-6.08	115.52	122.94
1	q	738	LEU	CA-C-N	6.07	126.04	119.78
1	q	738	LEU	C-N-CA	6.07	126.04	119.78
1	D	766	HIS	CA-C-N	6.07	126.03	119.78
1	D	766	HIS	C-N-CA	6.07	126.03	119.78
1	D	1044	PHE	CA-CB-CG	-6.03	107.77	113.80
1	A	1060	PRO	N-CA-C	6.03	118.05	110.70
1	G	1163	ASN	CB-CG-ND2	-6.01	107.38	116.40
1	p	296	ILE	CA-C-N	6.01	125.92	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	296	ILE	C-N-CA	6.01	125.92	119.85
1	G	1060	PRO	N-CA-C	5.99	118.01	110.70
1	A	766	HIS	CA-C-N	5.99	125.94	119.78
1	A	766	HIS	C-N-CA	5.99	125.94	119.78
1	p	546	SER	CA-C-N	5.98	125.86	119.28
1	p	546	SER	C-N-CA	5.98	125.86	119.28
1	G	1206	ALA	CA-C-N	5.96	125.92	119.78
1	G	1206	ALA	C-N-CA	5.96	125.92	119.78
1	r	269	ARG	N-CA-C	5.96	117.78	111.28
1	q	369	LYS	CB-CA-C	-5.95	106.97	111.20
1	A	916	GLY	CA-C-N	5.95	125.86	119.85
1	A	916	GLY	C-N-CA	5.95	125.86	119.85
1	p	736	CYS	N-CA-C	-5.94	100.11	108.96
1	p	705	GLY	CA-C-N	5.93	125.89	119.78
1	p	705	GLY	C-N-CA	5.93	125.89	119.78
1	r	657	VAL	CA-C-N	5.92	125.88	119.78
1	r	657	VAL	C-N-CA	5.92	125.88	119.78
1	p	195	CYS	CA-C-N	5.91	125.61	119.05
1	p	195	CYS	C-N-CA	5.91	125.61	119.05
1	q	705	GLY	CA-C-N	5.84	125.80	119.78
1	q	705	GLY	C-N-CA	5.84	125.80	119.78
1	q	438	TYR	N-CA-C	5.83	117.94	109.07
1	q	296	ILE	CA-C-N	5.83	125.74	119.85
1	q	296	ILE	C-N-CA	5.83	125.74	119.85
1	q	603	CYS	CA-C-N	5.83	128.54	120.49
1	q	603	CYS	C-N-CA	5.83	128.54	120.49
1	G	916	GLY	CA-C-N	5.83	125.73	119.85
1	G	916	GLY	C-N-CA	5.83	125.73	119.85
1	A	1044	PHE	CA-CB-CG	-5.82	107.98	113.80
1	r	738	LEU	CA-C-N	5.82	125.72	119.85
1	r	738	LEU	C-N-CA	5.82	125.72	119.85
1	r	44	TRP	CA-C-N	5.81	125.71	119.85
1	r	44	TRP	C-N-CA	5.81	125.71	119.85
1	D	807	LYS	N-CA-C	-5.78	106.27	113.55
1	r	368	ALA	N-CA-C	5.76	119.61	112.58
1	p	688	GLN	N-CA-C	5.75	118.66	111.24
1	r	649	TYR	CA-C-N	-5.74	112.88	122.64
1	r	649	TYR	C-N-CA	-5.74	112.88	122.64
3	F	92	LYS	N-CA-C	5.71	117.51	111.28
1	r	173	PRO	CA-C-N	-5.71	114.72	122.77
1	r	173	PRO	C-N-CA	-5.71	114.72	122.77
1	p	58	TYR	CA-C-N	5.70	125.65	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	58	TYR	C-N-CA	5.70	125.65	119.78
1	D	1193	ALA	CA-C-N	5.69	125.64	119.78
1	D	1193	ALA	C-N-CA	5.69	125.64	119.78
1	q	341	PHE	CA-CB-CG	-5.67	108.13	113.80
1	r	641	TYR	N-CA-C	5.67	118.44	108.75
1	q	688	GLN	CA-C-N	5.64	131.85	121.70
1	q	688	GLN	C-N-CA	5.64	131.85	121.70
1	q	321	LEU	N-CA-C	5.63	118.44	110.50
1	D	912	CYS	CA-C-N	5.63	129.25	120.75
1	D	912	CYS	C-N-CA	5.63	129.25	120.75
1	G	807	LYS	N-CA-C	-5.62	106.47	113.55
1	p	44	TRP	CA-C-N	5.61	125.52	119.85
1	p	44	TRP	C-N-CA	5.61	125.52	119.85
1	r	438	TYR	N-CA-C	5.60	117.69	109.24
1	D	1060	PRO	N-CA-C	5.58	117.51	110.70
1	q	269	ARG	N-CA-C	5.58	117.36	111.28
1	r	271	VAL	N-CA-C	5.58	116.36	111.56
1	G	936	PRO	CA-C-N	5.57	125.52	119.78
1	G	936	PRO	C-N-CA	5.57	125.52	119.78
1	r	399	PHE	CA-CB-CG	-5.56	108.24	113.80
1	D	1113	ARG	N-CA-C	5.55	118.10	111.71
1	r	58	TYR	CA-C-N	5.55	125.50	119.78
1	r	58	TYR	C-N-CA	5.55	125.50	119.78
1	r	188	GLU	CA-C-N	5.52	125.46	119.78
1	r	188	GLU	C-N-CA	5.52	125.46	119.78
3	C	92	LYS	N-CA-C	5.51	117.29	111.28
1	D	782	ILE	CA-C-N	5.51	125.42	119.85
1	D	782	ILE	C-N-CA	5.51	125.42	119.85
1	p	657	VAL	N-CA-C	5.50	113.48	107.60
1	q	195	CYS	CA-C-N	5.49	125.14	119.05
1	q	195	CYS	C-N-CA	5.49	125.14	119.05
1	r	223	ALA	N-CA-C	5.47	116.92	111.07
1	p	46	ARG	CA-C-N	5.45	125.39	119.78
1	p	46	ARG	C-N-CA	5.45	125.39	119.78
1	G	1044	PHE	CA-CB-CG	-5.44	108.36	113.80
1	p	484	VAL	N-CA-C	5.42	113.30	108.63
1	r	172	LEU	CA-C-N	5.42	125.33	119.85
1	r	172	LEU	C-N-CA	5.42	125.33	119.85
1	p	649	TYR	CA-C-N	-5.42	113.38	122.92
1	p	649	TYR	C-N-CA	-5.42	113.38	122.92
1	r	546	SER	CA-C-N	5.39	125.22	119.28
1	r	546	SER	C-N-CA	5.39	125.22	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1206	ALA	CA-C-N	5.39	125.33	119.78
1	A	1206	ALA	C-N-CA	5.39	125.33	119.78
1	r	75	PHE	CA-C-N	5.38	125.28	119.85
1	r	75	PHE	C-N-CA	5.38	125.28	119.85
1	r	409	TYR	N-CA-C	5.38	117.36	109.24
1	q	188	GLU	CA-C-N	5.36	125.30	119.78
1	q	188	GLU	C-N-CA	5.36	125.30	119.78
1	p	223	ALA	N-CA-C	5.34	116.78	111.07
1	q	649	TYR	CA-C-N	-5.34	113.02	122.74
1	q	649	TYR	C-N-CA	-5.34	113.02	122.74
1	D	936	PRO	CA-C-N	5.32	125.22	119.85
1	D	936	PRO	C-N-CA	5.32	125.22	119.85
1	q	437	CYS	O-C-N	-5.32	116.99	123.10
1	r	585	CYS	CA-C-N	5.31	125.25	119.78
1	r	585	CYS	C-N-CA	5.31	125.25	119.78
1	r	167	HIS	CA-CB-CG	5.30	119.10	113.80
1	r	514	VAL	CA-C-N	5.29	125.23	119.78
1	r	514	VAL	C-N-CA	5.29	125.23	119.78
1	r	173	PRO	N-CA-C	-5.29	102.97	111.38
1	G	1193	ALA	CA-C-N	5.28	125.22	119.78
1	G	1193	ALA	C-N-CA	5.28	125.22	119.78
1	q	271	VAL	N-CA-C	5.28	116.55	112.12
1	D	1206	ALA	CA-C-N	5.25	125.19	119.78
1	D	1206	ALA	C-N-CA	5.25	125.19	119.78
1	G	970	ILE	CA-C-N	5.25	125.19	119.78
1	G	970	ILE	C-N-CA	5.25	125.19	119.78
1	A	912	CYS	CA-C-N	5.25	128.68	120.75
1	A	912	CYS	C-N-CA	5.25	128.68	120.75
1	q	172	LEU	CA-C-N	5.23	125.16	119.78
1	q	172	LEU	C-N-CA	5.23	125.16	119.78
1	D	753	VAL	CA-C-N	5.22	125.16	119.78
1	D	753	VAL	C-N-CA	5.22	125.16	119.78
1	q	223	ALA	N-CA-C	5.20	116.64	111.07
1	p	147	PHE	N-CA-C	5.19	117.08	109.24
1	G	1156	CYS	CA-C-O	5.18	126.99	121.45
1	p	406	ASN	CA-C-N	-5.17	113.39	121.87
1	p	406	ASN	C-N-CA	-5.17	113.39	121.87
1	r	736	CYS	N-CA-CB	-5.17	102.81	110.37
1	q	173	PRO	CA-C-N	-5.17	115.72	123.00
1	q	173	PRO	C-N-CA	-5.17	115.72	123.00
1	D	798	THR	N-CA-C	5.15	117.01	109.24
1	A	798	THR	N-CA-C	5.14	117.00	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	q	709	THR	CA-C-N	5.13	124.92	119.28
1	q	709	THR	C-N-CA	5.13	124.92	119.28
1	A	1219	PRO	N-CA-C	5.10	116.92	110.70
1	A	1217	ASN	N-CA-C	5.09	116.94	107.99
3	I	63	ILE	N-CA-C	5.07	115.07	107.51
2	E	19	LYS	CA-C-N	5.07	130.75	122.69
2	E	19	LYS	C-N-CA	5.07	130.75	122.69
1	q	323	PHE	N-CA-C	5.07	117.09	109.23
1	r	429	SER	CA-C-N	5.07	124.57	119.19
1	r	429	SER	C-N-CA	5.07	124.57	119.19
1	A	905	TYR	CB-CA-C	-5.07	110.34	117.23
3	I	92	LYS	N-CA-C	5.06	116.80	111.28
1	p	709	THR	CA-C-N	5.06	124.84	119.28
1	p	709	THR	C-N-CA	5.06	124.84	119.28
1	A	1188	GLY	N-CA-C	-5.05	106.08	112.54
2	H	82(B)	ARG	N-CA-C	5.02	118.06	111.28
2	H	60	ASN	N-CA-C	-5.02	102.85	110.28
1	r	19	VAL	N-CA-C	5.01	116.05	109.58
3	C	87	PHE	N-CA-C	5.01	117.22	108.76
1	A	1220	PRO	N-CA-C	5.00	116.81	110.70
1	G	1156	CYS	O-C-N	-5.00	117.35	123.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3545	0	3464	51	0
1	D	3545	0	3465	45	0
1	G	3545	0	3463	16	0
1	p	5658	0	5413	68	0
1	q	5658	0	5417	55	0
1	r	5658	0	5414	77	0
2	B	948	0	904	3	0
2	E	948	0	904	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	948	0	904	0	0
3	C	835	0	816	2	0
3	F	835	0	816	0	0
3	I	835	0	816	0	0
4	J	28	0	25	0	0
4	K	28	0	25	1	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	T	28	0	25	1	0
4	U	28	0	25	2	0
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	1	0
4	Y	28	0	25	0	0
4	Z	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
4	d	28	0	25	0	0
5	A	14	0	13	0	0
5	D	14	0	13	0	0
5	G	14	0	13	1	0
5	p	84	0	78	0	0
5	q	84	0	78	1	0
5	r	84	0	78	1	0
All	All	33840	0	32594	299	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 5.

All (299) 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:p:371:SER:CB	1:p:604:VAL:HG12	1.31	1.59
1:p:371:SER:HB3	1:p:604:VAL:CG1	1.18	1.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:580:ASP:CB	1:r:629:ARG:CG	1.89	1.50
1:r:580:ASP:HB3	1:r:629:ARG:CG	1.50	1.35
1:r:580:ASP:HB3	1:r:629:ARG:CB	1.58	1.33
1:p:381:VAL:HG11	1:p:408:ASN:N	1.42	1.31
1:q:506:PHE:CE2	1:q:555:VAL:HG21	1.71	1.25
1:p:381:VAL:CG1	1:p:408:ASN:N	2.00	1.24
1:p:381:VAL:CG1	1:p:408:ASN:H	1.53	1.22
1:D:905:TYR:CE1	1:D:936:PRO:HB3	1.53	1.18
1:r:580:ASP:CB	1:r:629:ARG:HG3	1.67	1.16
1:p:381:VAL:HG11	1:p:407:CYS:C	1.73	1.13
1:r:580:ASP:CB	1:r:629:ARG:HG2	1.61	1.13
1:q:506:PHE:CZ	1:q:555:VAL:HG21	1.86	1.10
1:p:381:VAL:HB	1:p:408:ASN:CB	1.75	1.09
1:r:580:ASP:HB2	1:r:629:ARG:CG	1.65	1.07
1:p:381:VAL:HB	1:p:408:ASN:HB2	1.09	1.05
1:r:714:VAL:HG21	1:r:717:LEU:HD22	1.31	1.05
1:r:580:ASP:HB3	1:r:629:ARG:HB2	1.36	1.02
1:r:580:ASP:CA	1:r:629:ARG:HG3	1.88	1.02
1:p:371:SER:HB3	1:p:604:VAL:HG13	1.42	1.00
1:A:1121:THR:HA	1:D:964:LEU:HD13	1.44	0.99
1:r:621:THR:O	1:r:648:TYR:HB3	1.63	0.99
1:D:905:TYR:HE1	1:D:936:PRO:HB3	1.28	0.99
1:D:905:TYR:CE1	1:D:936:PRO:CB	2.45	0.98
1:p:381:VAL:HG12	1:p:408:ASN:H	1.26	0.98
1:A:958:VAL:HG11	1:A:1108:LYS:O	1.65	0.96
1:p:371:SER:CA	1:p:604:VAL:HG12	1.97	0.95
1:p:621:THR:HG22	1:p:622:ALA:H	1.30	0.94
1:q:620:CYS:SG	1:q:648:TYR:CD2	2.61	0.94
1:r:580:ASP:HB2	1:r:629:ARG:HG2	0.94	0.93
1:A:961:THR:HG22	1:A:962:ALA:H	1.32	0.91
1:A:1121:THR:HA	1:D:964:LEU:CD1	2.01	0.90
1:p:371:SER:CB	1:p:604:VAL:CG1	2.08	0.89
1:p:381:VAL:CG1	1:p:407:CYS:HA	2.01	0.89
1:r:630:PHE:HB3	1:r:638:LEU:HD11	1.55	0.88
1:p:506:PHE:CE2	1:p:555:VAL:HG21	2.09	0.87
1:A:1121:THR:HG22	1:D:964:LEU:HB3	1.56	0.87
1:r:580:ASP:HA	1:r:629:ARG:HG3	1.55	0.87
1:p:381:VAL:CB	1:p:408:ASN:CB	2.51	0.86
1:p:506:PHE:CZ	1:p:555:VAL:HG21	2.09	0.86
1:A:958:VAL:CG1	1:A:1108:LYS:O	2.25	0.85
1:q:714:VAL:HG21	1:q:717:LEU:HD12	1.58	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:381:VAL:CG1	1:p:407:CYS:CA	2.57	0.83
1:D:964:LEU:O	1:D:965:SER:OG	1.97	0.82
1:q:506:PHE:CE2	1:q:555:VAL:CG2	2.59	0.82
1:r:622:ALA:HB1	1:r:642:TYR:OH	1.78	0.82
1:A:1121:THR:HG22	1:D:964:LEU:CD1	2.10	0.81
1:G:1160:ASN:OD1	1:G:1162:THR:OG1	1.97	0.81
1:p:372:GLY:O	1:p:604:VAL:HB	1.81	0.80
1:D:957:GLY:CA	1:D:968:ALA:HB3	2.15	0.77
1:r:506:PHE:CZ	1:r:555:VAL:HG21	2.20	0.76
1:A:961:THR:HG22	1:A:962:ALA:N	2.01	0.76
1:q:620:CYS:CB	1:q:650:CYS:SG	2.74	0.76
1:D:957:GLY:HA3	1:D:968:ALA:HB3	1.68	0.75
1:q:620:CYS:HB3	1:q:650:CYS:SG	2.26	0.75
1:p:381:VAL:HG11	1:p:407:CYS:CA	2.15	0.75
1:r:629:ARG:HB3	1:r:630:PHE:CD2	2.21	0.74
1:q:506:PHE:CD2	1:q:555:VAL:HG21	2.23	0.73
1:D:775:SER:HB3	1:D:777:TYR:CE1	2.24	0.72
1:q:369:LYS:O	1:q:369:LYS:HG2	1.89	0.72
1:D:960:TRP:O	1:D:961:THR:OG1	2.07	0.72
1:p:372:GLY:O	1:p:604:VAL:CB	2.39	0.71
1:q:620:CYS:SG	1:q:649:TYR:CA	2.79	0.70
1:A:1121:THR:HG22	1:D:964:LEU:CB	2.21	0.70
1:q:506:PHE:HE1	1:q:513:GLU:CD	2.01	0.69
1:q:620:CYS:SG	1:q:649:TYR:C	2.77	0.68
1:q:506:PHE:CE1	1:q:513:GLU:CD	2.72	0.68
1:p:381:VAL:CB	1:p:408:ASN:HB2	2.03	0.67
1:r:580:ASP:CB	1:r:629:ARG:HB2	2.15	0.67
1:A:1121:THR:CA	1:D:964:LEU:HD13	2.22	0.67
1:r:621:THR:HG22	1:r:622:ALA:H	1.59	0.67
1:r:630:PHE:HB3	1:r:638:LEU:CD1	2.24	0.66
1:A:1121:THR:HG22	1:D:964:LEU:HD13	1.77	0.66
1:r:66:ASN:OD1	1:r:66:ASN:C	2.39	0.66
1:p:371:SER:C	1:p:604:VAL:HG12	2.20	0.66
1:p:680:GLU:N	1:p:680:GLU:OE1	2.31	0.64
1:A:804:VAL:HG12	1:A:805:ASP:N	2.12	0.64
1:A:811:CYS:SG	1:A:1051:ILE:HD13	2.37	0.64
1:p:602:ASN:O	1:p:616:VAL:HB	1.99	0.63
1:q:164:PHE:HB3	1:q:168:THR:HG21	1.81	0.63
1:p:381:VAL:HG13	1:p:407:CYS:HA	1.78	0.63
1:r:691:ARG:HA	1:r:691:ARG:NE	2.13	0.63
1:D:957:GLY:HA3	1:D:968:ALA:CB	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLU:OE1	2:B:85:GLU:N	2.32	0.61
1:G:757:MET:O	1:r:717:LEU:O	2.18	0.61
1:p:370:PRO:HB3	1:p:614:ARG:CZ	2.31	0.60
1:G:905:TYR:CE1	1:G:936:PRO:HG3	2.37	0.60
1:A:961:THR:CG2	1:A:962:ALA:H	2.04	0.60
1:A:1121:THR:HB	1:D:964:LEU:HD12	1.83	0.60
1:D:775:SER:HB3	1:D:777:TYR:CD1	2.37	0.60
1:q:620:CYS:SG	1:q:648:TYR:C	2.85	0.60
1:q:166:ASN:O	1:q:168:THR:HG23	2.01	0.60
1:r:622:ALA:C	1:r:642:TYR:OH	2.45	0.59
1:D:759:LEU:HD13	1:q:717:LEU:HD13	1.84	0.59
1:p:66:ASN:OD1	1:p:66:ASN:C	2.46	0.59
1:r:376:GLU:HB2	1:r:608:LEU:CD2	2.33	0.59
1:D:757:MET:O	1:q:717:LEU:O	2.20	0.59
1:p:616:VAL:HG13	1:p:616:VAL:O	2.02	0.59
1:A:1121:THR:CB	1:D:964:LEU:HD12	2.33	0.59
1:r:628:GLN:O	1:r:629:ARG:HB2	2.01	0.59
1:A:811:CYS:SG	1:A:1051:ILE:CD1	2.92	0.58
1:D:905:TYR:HE1	1:D:936:PRO:CB	2.02	0.57
1:r:506:PHE:CE2	1:r:555:VAL:HG21	2.39	0.57
1:p:371:SER:HB3	1:p:604:VAL:HG12	0.60	0.57
1:A:1121:THR:CG2	1:D:964:LEU:CD1	2.83	0.57
1:p:621:THR:O	1:p:648:TYR:HB3	2.05	0.56
1:r:621:THR:O	1:r:648:TYR:CB	2.47	0.56
1:p:620:CYS:CB	1:p:650:CYS:SG	2.93	0.56
1:r:630:PHE:CD2	1:r:630:PHE:N	2.73	0.56
1:q:621:THR:O	1:q:622:ALA:HB2	2.05	0.56
1:A:1121:THR:CB	1:D:964:LEU:CD1	2.84	0.56
1:p:385:PHE:CE1	1:p:404:PHE:CE2	2.94	0.56
1:r:159:GLY:HA3	5:r:1404:NAG:H83	1.87	0.56
1:r:240:MET:C	1:r:240:MET:SD	2.89	0.55
1:p:368:ALA:O	1:p:688:GLN:O	2.24	0.55
1:A:805:ASP:OD1	1:A:807:LYS:HB3	2.07	0.55
1:q:506:PHE:HD1	1:q:513:GLU:HG3	1.72	0.55
1:q:620:CYS:SG	1:q:649:TYR:HA	2.46	0.54
1:D:826:GLN:OE1	1:D:826:GLN:N	2.25	0.54
1:p:714:VAL:HB	1:p:717:LEU:HD23	1.88	0.54
1:r:622:ALA:CB	1:r:642:TYR:OH	2.53	0.54
1:p:621:THR:HG22	1:p:622:ALA:N	2.07	0.54
1:r:378:ALA:HB1	1:r:379:GLU:HG2	1.90	0.54
1:D:964:LEU:O	1:D:965:SER:CB	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:689:TYR:C	1:p:689:TYR:CD2	2.86	0.54
1:A:805:ASP:C	1:A:807:LYS:H	2.14	0.54
1:D:905:TYR:O	1:D:908:GLY:HA3	2.08	0.53
1:r:377:GLN:O	1:r:378:ALA:HB3	2.07	0.53
1:A:1209:VAL:HG12	4:K:2:NAG:H2	1.90	0.53
1:r:399:PHE:CD1	1:r:399:PHE:N	2.74	0.53
1:p:381:VAL:CG1	1:p:407:CYS:C	2.53	0.53
1:r:664:ASP:OD1	1:r:664:ASP:C	2.51	0.53
1:r:376:GLU:HB2	1:r:608:LEU:HD22	1.90	0.53
1:p:78:GLN:C	1:p:78:GLN:CD	2.77	0.53
1:r:172:LEU:O	1:r:172:LEU:HG	2.09	0.53
1:r:240:MET:SD	1:r:240:MET:O	2.67	0.53
1:G:906:MET:O	1:G:906:MET:HG2	2.08	0.52
1:p:367:GLU:O	1:p:368:ALA:HB3	2.08	0.52
1:q:606:TYR:C	1:q:606:TYR:CD1	2.87	0.52
3:C:1:ASP:C	3:C:1:ASP:OD1	2.50	0.52
1:r:714:VAL:CG2	1:r:717:LEU:HD22	2.22	0.52
1:G:1145:ASN:ND2	4:R:1:NAG:O7	2.42	0.52
1:q:672:THR:HG22	1:q:715:LEU:HB2	1.92	0.51
1:A:958:VAL:HG11	1:A:1109:ALA:HA	1.92	0.51
1:r:369:LYS:O	1:r:369:LYS:HG2	2.10	0.51
1:p:605:GLU:HA	1:p:614:ARG:HA	1.92	0.51
1:r:622:ALA:HB1	1:r:642:TYR:CZ	2.45	0.51
1:A:958:VAL:HG12	1:A:1108:LYS:O	2.09	0.51
1:r:622:ALA:HB1	1:r:642:TYR:CE1	2.46	0.51
1:q:439:SER:HA	1:q:582:ASN:HA	1.93	0.51
1:r:395:GLN:OE1	1:r:395:GLN:HA	2.11	0.51
1:p:620:CYS:SG	1:p:648:TYR:CD2	3.03	0.51
1:p:665:LYS:HD3	1:p:665:LYS:C	2.36	0.50
1:p:691:ARG:HA	1:p:691:ARG:NE	2.26	0.50
1:r:409:TYR:CD1	1:r:409:TYR:C	2.90	0.50
1:A:804:VAL:HG12	1:A:805:ASP:H	1.76	0.50
1:r:381:VAL:O	1:r:407:CYS:HB2	2.11	0.50
1:r:602:ASN:OD1	1:r:602:ASN:N	2.43	0.50
1:q:369:LYS:O	1:q:369:LYS:CG	2.56	0.50
1:r:378:ALA:HB1	1:r:379:GLU:HA	1.93	0.50
1:D:1175:THR:O	1:D:1175:THR:HG23	2.12	0.49
1:p:228:PHE:CD1	1:p:228:PHE:C	2.90	0.49
1:p:664:ASP:OD1	1:p:664:ASP:C	2.56	0.49
1:q:622:ALA:HB1	1:q:642:TYR:OH	2.12	0.49
1:r:714:VAL:HB	1:r:717:LEU:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:872:THR:HA	4:T:1:NAG:H82	1.94	0.49
1:r:439:SER:HA	1:r:582:ASN:HA	1.93	0.49
1:r:593:ASP:N	1:r:594:THR:HA	2.27	0.49
1:r:383:CYS:HB2	1:r:385:PHE:CZ	2.48	0.49
1:A:1175:THR:O	1:A:1175:THR:HG23	2.13	0.49
1:r:111:GLN:OE1	1:r:111:GLN:N	2.43	0.49
1:A:905:TYR:CE1	1:r:711:VAL:HG13	2.47	0.49
1:D:772:GLN:HG2	1:D:773:LEU:H	1.78	0.49
1:p:372:GLY:O	1:p:604:VAL:CG2	2.60	0.49
1:q:506:PHE:CD2	1:q:555:VAL:CG2	2.90	0.49
1:D:756:GLU:OE1	1:D:756:GLU:N	2.35	0.48
1:p:37:GLN:OE1	1:p:37:GLN:N	2.46	0.48
1:D:1120:GLY:O	1:D:1121:THR:OG1	2.26	0.48
1:A:1001:PHE:CD1	1:A:1001:PHE:C	2.92	0.48
1:q:383:CYS:SG	1:q:409:TYR:HB3	2.54	0.48
1:q:506:PHE:HE1	1:q:513:GLU:OE2	1.96	0.48
1:r:172:LEU:N	1:r:172:LEU:HD23	2.29	0.48
1:p:381:VAL:CB	1:p:408:ASN:N	2.72	0.48
1:A:804:VAL:CG1	1:A:805:ASP:N	2.76	0.47
1:A:826:GLN:OE1	1:A:826:GLN:N	2.28	0.47
1:p:395:GLN:OE1	1:p:395:GLN:HA	2.14	0.47
1:A:1121:THR:CG2	1:D:964:LEU:HD12	2.44	0.47
1:D:957:GLY:N	1:D:968:ALA:HB3	2.29	0.47
1:r:621:THR:HG22	1:r:622:ALA:N	2.29	0.47
1:G:759:LEU:HD13	1:r:717:LEU:HD23	1.97	0.47
1:A:810:VAL:HG12	1:A:811:CYS:SG	2.55	0.47
1:A:817:CYS:SG	1:A:1071:ILE:HD11	2.54	0.47
1:D:1173:ILE:HG13	1:D:1185:SER:OG	2.14	0.47
1:q:78:GLN:CD	1:q:78:GLN:C	2.83	0.47
1:r:172:LEU:HD23	1:r:172:LEU:H	1.78	0.47
1:A:805:ASP:C	1:A:807:LYS:N	2.73	0.47
1:p:615:GLY:HA2	1:p:654:CYS:SG	2.54	0.47
1:q:620:CYS:SG	1:q:649:TYR:N	2.88	0.47
1:p:443:LEU:HD23	1:p:443:LEU:C	2.40	0.47
1:p:67:ILE:O	1:p:67:ILE:HG13	2.14	0.47
1:q:596:ILE:C	1:q:596:ILE:HD12	2.40	0.46
1:q:620:CYS:CB	1:q:650:CYS:HG	2.28	0.46
1:r:506:PHE:CE1	1:r:555:VAL:HG21	2.49	0.46
1:A:1219:PRO:HB2	1:A:1220:PRO:HD3	1.96	0.46
1:D:806:CYS:O	1:D:806:CYS:SG	2.73	0.46
3:C:92:LYS:HD3	3:C:92:LYS:C	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1001:PHE:CD1	1:G:1001:PHE:C	2.94	0.46
1:p:599:GLN:C	1:p:600:LEU:HG	2.39	0.46
1:D:775:SER:CB	1:D:777:TYR:CE1	2.96	0.46
1:G:1161:PRO:HG3	4:U:1:NAG:H81	1.97	0.46
1:q:506:PHE:CE1	1:q:555:VAL:HG21	2.45	0.46
1:q:621:THR:O	1:q:648:TYR:HB3	2.16	0.46
1:p:330:ASP:C	1:p:330:ASP:OD1	2.58	0.46
1:q:378:ALA:HB1	1:q:379:GLU:HA	1.98	0.46
1:r:691:ARG:HA	1:r:691:ARG:HE	1.79	0.46
1:q:78:GLN:O	1:q:78:GLN:NE2	2.49	0.45
1:A:956:ALA:N	1:A:957:GLY:HA2	2.31	0.45
1:p:694:ARG:HA	1:p:694:ARG:NE	2.31	0.45
1:r:67:ILE:HG13	1:r:67:ILE:O	2.16	0.45
1:A:1060:PRO:HA	1:A:1063:GLN:HB3	1.97	0.45
1:D:959:GLY:HA3	1:D:978:TYR:CE1	2.51	0.45
1:q:633:ASP:C	1:q:633:ASP:OD1	2.59	0.45
1:G:1160:ASN:OD1	1:G:1160:ASN:C	2.58	0.45
1:A:805:ASP:HB3	1:A:808:GLN:HB2	1.98	0.45
1:A:1121:THR:CG2	1:D:964:LEU:HD13	2.44	0.45
1:r:672:THR:HG22	1:r:715:LEU:HB2	1.98	0.45
1:G:826:GLN:OE1	1:G:826:GLN:N	2.37	0.45
1:p:714:VAL:HG21	1:p:717:LEU:HG	1.98	0.45
1:r:633:ASP:OD1	1:r:633:ASP:C	2.59	0.45
1:p:381:VAL:HG12	1:p:407:CYS:HB2	1.98	0.45
1:p:665:LYS:HD3	1:p:665:LYS:O	2.17	0.45
1:G:1120:GLY:O	1:G:1121:THR:OG1	2.24	0.44
1:r:378:ALA:HB1	1:r:379:GLU:CG	2.47	0.44
1:p:49:ASP:OD1	1:p:49:ASP:C	2.59	0.44
1:G:1209:VAL:HG12	4:U:2:NAG:H2	1.98	0.44
1:r:622:ALA:CA	1:r:642:TYR:OH	2.65	0.44
1:r:326:ASP:OD1	1:r:326:ASP:C	2.61	0.44
1:r:378:ALA:CB	1:r:379:GLU:HA	2.47	0.44
1:q:629:ARG:HB3	1:q:641:TYR:CE1	2.51	0.44
1:r:580:ASP:HB3	1:r:629:ARG:HG3	1.41	0.44
1:A:1121:THR:CA	1:D:964:LEU:CD1	2.82	0.44
1:D:1060:PRO:HA	1:D:1063:GLN:HB3	2.00	0.44
1:q:622:ALA:C	1:q:642:TYR:OH	2.60	0.44
1:p:371:SER:C	1:p:604:VAL:CG1	2.91	0.44
1:p:381:VAL:HG12	1:p:408:ASN:N	1.99	0.44
1:A:872:THR:O	1:A:872:THR:HG22	2.18	0.43
1:G:806:CYS:O	1:G:806:CYS:SG	2.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:49:ASP:C	1:q:49:ASP:OD1	2.60	0.43
1:p:249:GLU:HB2	4:X:1:NAG:H62	2.00	0.43
1:q:446:PHE:CD1	1:q:446:PHE:N	2.85	0.43
1:D:777:TYR:CD1	1:D:777:TYR:N	2.86	0.43
1:p:409:TYR:O	1:p:586:PRO:HA	2.18	0.43
1:r:396:VAL:HA	1:r:399:PHE:CE1	2.53	0.43
2:B:6:GLN:HG2	2:B:22:CYS:SG	2.57	0.43
1:q:670:HIS:CD2	1:q:670:HIS:N	2.86	0.43
1:r:376:GLU:HB2	1:r:608:LEU:HD23	1.99	0.43
1:q:717:LEU:HD23	1:q:717:LEU:HA	1.81	0.43
1:r:629:ARG:HA	1:r:629:ARG:HD3	1.72	0.43
1:D:1008:MET:HA	1:D:1008:MET:HE2	2.01	0.43
1:p:606:TYR:CD1	1:p:606:TYR:C	2.97	0.43
1:r:717:LEU:O	1:r:718:VAL:HB	2.19	0.43
1:A:1160:ASN:OD1	1:A:1160:ASN:C	2.62	0.43
1:q:409:TYR:CD1	1:q:409:TYR:C	2.96	0.43
1:r:378:ALA:HB1	1:r:379:GLU:CA	2.48	0.43
1:A:875:GLU:OE1	1:A:875:GLU:N	2.35	0.42
1:A:959:GLY:O	1:A:960:TRP:HB2	2.19	0.42
1:r:425:CYS:HA	1:r:478:CYS:HA	2.00	0.42
1:q:381:VAL:O	1:q:407:CYS:HB2	2.18	0.42
1:A:826:GLN:H	1:A:826:GLN:CD	2.18	0.42
1:A:965:SER:OG	1:A:966:SER:N	2.51	0.42
1:A:1116:PHE:O	1:A:1117:CYS:HB2	2.19	0.42
1:r:383:CYS:O	1:r:385:PHE:CD2	2.72	0.42
1:p:372:GLY:O	1:p:604:VAL:HG21	2.20	0.42
1:D:773:LEU:HD23	1:D:773:LEU:HA	1.79	0.42
1:q:174:ASP:C	1:q:174:ASP:OD1	2.63	0.42
1:q:600:LEU:N	1:q:600:LEU:HD12	2.35	0.42
1:p:672:THR:HG22	1:p:715:LEU:HB2	2.01	0.42
1:q:161:MET:HA	5:q:1406:NAG:H81	2.02	0.42
1:q:620:CYS:SG	1:q:648:TYR:O	2.78	0.41
1:A:960:TRP:O	1:A:961:THR:HB	2.20	0.41
1:D:786:PHE:CD2	1:D:786:PHE:C	2.99	0.41
1:G:875:GLU:H	1:G:875:GLU:CD	2.28	0.41
1:A:971:PRO:HB3	5:G:1401:NAG:H81	2.03	0.41
1:p:381:VAL:CB	1:p:408:ASN:H	2.24	0.41
1:q:740:ASP:O	1:q:741:THR:C	2.64	0.41
1:r:295:ILE:O	1:r:295:ILE:HG23	2.19	0.41
1:A:804:VAL:CG1	1:A:805:ASP:H	2.33	0.41
1:D:826:GLN:H	1:D:826:GLN:CD	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:72:ASP:C	2:E:72:ASP:OD1	2.63	0.41
2:B:72:ASP:OD1	2:B:72:ASP:C	2.62	0.41
1:G:841:ARG:HA	1:G:841:ARG:NE	2.35	0.41
1:q:130:VAL:O	1:q:130:VAL:HG12	2.20	0.41
1:A:944:GLU:OE1	1:A:944:GLU:HA	2.21	0.40
1:r:148:MET:HE3	1:r:148:MET:HB2	1.97	0.40
1:q:132:ILE:HD12	1:q:132:ILE:HA	1.81	0.40
1:q:677:VAL:O	1:q:677:VAL:HG22	2.21	0.40
1:q:689:TYR:CD1	1:q:689:TYR:C	2.99	0.40
1:r:410:ASN:C	1:r:410:ASN:OD1	2.64	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	459/1329 (34%)	440 (96%)	15 (3%)	4 (1%)	14	48
1	D	459/1329 (34%)	440 (96%)	16 (4%)	3 (1%)	18	54
1	G	459/1329 (34%)	440 (96%)	17 (4%)	2 (0%)	30	65
1	p	724/1329 (54%)	688 (95%)	32 (4%)	4 (1%)	21	57
1	q	724/1329 (54%)	691 (95%)	29 (4%)	4 (1%)	21	57
1	r	724/1329 (54%)	693 (96%)	25 (4%)	6 (1%)	16	52
2	B	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	E	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	H	117/233 (50%)	113 (97%)	4 (3%)	0	100	100
3	C	109/218 (50%)	104 (95%)	4 (4%)	1 (1%)	14	48
3	F	109/218 (50%)	104 (95%)	4 (4%)	1 (1%)	14	48
3	I	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	14	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4227/9327 (45%)	4048 (96%)	153 (4%)	26 (1%)	23 57

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	q	622	ALA
1	r	621	THR
1	A	940	ASP
1	A	961	THR
1	p	718	VAL
1	q	621	THR
1	q	718	VAL
1	r	377	GLN
1	A	1220	PRO
1	D	1220	PRO
1	G	887	ARG
1	G	1220	PRO
1	p	382	GLU
1	q	623	VAL
1	r	629	ARG
1	D	956	ALA
1	p	621	THR
1	r	718	VAL
1	D	905	TYR
1	A	960	TRP
1	r	596	ILE
3	C	77	PRO
3	I	77	PRO
1	r	623	VAL
3	F	77	PRO
1	p	381	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/1148 (34%)	388 (100%)	0	100	100
1	D	388/1148 (34%)	388 (100%)	0	100	100
1	G	388/1148 (34%)	387 (100%)	1 (0%)	86	85
1	p	635/1148 (55%)	634 (100%)	1 (0%)	87	87
1	q	635/1148 (55%)	634 (100%)	1 (0%)	87	87
1	r	635/1148 (55%)	632 (100%)	3 (0%)	81	82
2	B	102/202 (50%)	102 (100%)	0	100	100
2	E	102/202 (50%)	102 (100%)	0	100	100
2	H	102/202 (50%)	102 (100%)	0	100	100
3	C	93/192 (48%)	93 (100%)	0	100	100
3	F	93/192 (48%)	93 (100%)	0	100	100
3	I	93/192 (48%)	93 (100%)	0	100	100
All	All	3654/8070 (45%)	3648 (100%)	6 (0%)	85	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	774	ASN
1	p	369	LYS
1	q	619	ASN
1	r	376	GLU
1	r	629	ARG
1	r	630	PHE

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

Mol	Chain	Res	Type
1	A	766	HIS
1	A	836	HIS
1	A	1208	GLN
1	A	1212	GLN
1	D	766	HIS
1	D	836	HIS
1	D	1020	HIS
1	D	1212	GLN
1	G	766	HIS
1	G	769	GLN
1	G	836	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	914	GLN
1	G	1163	ASN
1	G	1208	GLN
1	p	91	HIS
1	p	167	HIS
1	p	319	GLN
1	q	72	GLN
1	q	78	GLN
1	q	167	HIS
1	q	628	GLN
1	q	647	ASN
1	r	78	GLN
1	r	348	HIS
1	r	471	GLN
1	r	636	GLN
1	r	688	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

42 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	J	1	4,1	14,14,15	1.22	1 (7%)	17,19,21	1.23	3 (17%)
4	NAG	J	2	4	14,14,15	0.47	0	17,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	K	1	4,1	14,14,15	0.88	1 (7%)	17,19,21	0.97	1 (5%)
4	NAG	K	2	4	14,14,15	0.32	0	17,19,21	0.94	1 (5%)
4	NAG	L	1	4,1	14,14,15	0.27	0	17,19,21	0.59	0
4	NAG	L	2	4	14,14,15	0.84	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	M	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	M	2	4	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	N	1	4,1	14,14,15	0.55	0	17,19,21	0.65	0
4	NAG	N	2	4	14,14,15	0.41	0	17,19,21	0.62	0
4	NAG	O	1	4,1	14,14,15	1.14	2 (14%)	17,19,21	2.65	4 (23%)
4	NAG	O	2	4	14,14,15	0.49	0	17,19,21	0.43	0
4	NAG	P	1	4,1	14,14,15	0.50	0	17,19,21	0.62	0
4	NAG	P	2	4	14,14,15	0.46	0	17,19,21	0.34	0
4	NAG	Q	1	4,1	14,14,15	0.22	0	17,19,21	0.57	0
4	NAG	Q	2	4	14,14,15	0.95	1 (7%)	17,19,21	2.31	3 (17%)
4	NAG	R	1	4,1	14,14,15	0.37	0	17,19,21	0.73	1 (5%)
4	NAG	R	2	4	14,14,15	0.39	0	17,19,21	0.40	0
4	NAG	S	1	4,1	14,14,15	1.23	1 (7%)	17,19,21	1.29	3 (17%)
4	NAG	S	2	4	14,14,15	0.52	0	17,19,21	0.47	0
4	NAG	T	1	4,1	14,14,15	0.71	1 (7%)	17,19,21	0.64	0
4	NAG	T	2	4	14,14,15	0.35	0	17,19,21	0.49	0
4	NAG	U	1	4,1	14,14,15	0.81	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	U	2	4	14,14,15	0.40	0	17,19,21	0.74	1 (5%)
4	NAG	V	1	4,1	14,14,15	0.57	0	17,19,21	1.01	1 (5%)
4	NAG	V	2	4	14,14,15	0.44	0	17,19,21	0.54	0
4	NAG	W	1	4,1	14,14,15	1.11	1 (7%)	17,19,21	1.27	2 (11%)
4	NAG	W	2	4	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	X	1	4,1	14,14,15	1.23	1 (7%)	17,19,21	1.55	1 (5%)
4	NAG	X	2	4	14,14,15	0.92	1 (7%)	17,19,21	2.38	4 (23%)
4	NAG	Y	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	0.86	0
4	NAG	Y	2	4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	Z	1	4,1	14,14,15	0.25	0	17,19,21	1.08	1 (5%)
4	NAG	Z	2	4	14,14,15	0.33	0	17,19,21	0.54	0
4	NAG	a	1	4,1	14,14,15	1.09	1 (7%)	17,19,21	0.83	0
4	NAG	a	2	4	14,14,15	0.72	1 (7%)	17,19,21	0.62	0
4	NAG	b	1	4,1	14,14,15	0.93	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	b	2	4	14,14,15	1.42	1 (7%)	17,19,21	2.39	4 (23%)
4	NAG	c	1	4,1	14,14,15	0.63	0	17,19,21	0.66	0
4	NAG	c	2	4	14,14,15	0.42	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	d	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	2.41	3 (17%)
4	NAG	d	2	4	14,14,15	0.44	0	17,19,21	0.57	0

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

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

Continued on next page...

Continued from previous page...

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	2	NAG	C1-C2	4.67	1.58	1.52
4	X	1	NAG	O5-C1	4.34	1.51	1.43
4	J	1	NAG	O5-C1	-4.11	1.36	1.43
4	S	1	NAG	O5-C1	-4.07	1.36	1.43
4	W	1	NAG	O5-C1	-3.87	1.37	1.43
4	a	1	NAG	C1-C2	3.67	1.57	1.52
4	K	1	NAG	C1-C2	3.16	1.56	1.52
4	O	1	NAG	C1-C2	3.08	1.56	1.52
4	Q	2	NAG	C1-C2	2.97	1.56	1.52
4	L	2	NAG	C1-C2	2.97	1.56	1.52
4	b	1	NAG	O5-C1	-2.95	1.38	1.43
4	Y	1	NAG	O5-C1	-2.85	1.38	1.43
4	X	2	NAG	C1-C2	2.82	1.56	1.52
4	U	1	NAG	C1-C2	2.76	1.56	1.52
4	d	1	NAG	C1-C2	2.49	1.55	1.52
4	O	1	NAG	O5-C1	2.46	1.47	1.43
4	M	1	NAG	O5-C1	-2.45	1.39	1.43
4	T	1	NAG	O5-C1	-2.41	1.39	1.43
4	a	2	NAG	O5-C1	2.17	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	1	NAG	C2-N2-C7	8.30	134.02	122.90
4	X	2	NAG	C2-N2-C7	8.27	133.98	122.90
4	Q	2	NAG	C2-N2-C7	8.24	133.95	122.90
4	O	1	NAG	C2-N2-C7	8.23	133.93	122.90
4	b	2	NAG	C2-N2-C7	7.99	133.60	122.90
4	X	1	NAG	C1-O5-C5	6.05	120.29	112.19
4	O	1	NAG	C1-O5-C5	4.30	117.95	112.19
4	O	1	NAG	C1-C2-N2	4.18	117.02	110.43
4	d	1	NAG	C1-C2-N2	4.03	116.78	110.43
4	X	2	NAG	C1-C2-N2	3.77	116.37	110.43
4	b	2	NAG	C1-C2-N2	3.57	116.06	110.43
4	Q	2	NAG	C1-C2-N2	3.53	116.00	110.43
4	M	1	NAG	C2-N2-C7	3.42	127.48	122.90
4	K	2	NAG	C1-O5-C5	3.36	116.69	112.19
4	W	1	NAG	C2-N2-C7	3.34	127.38	122.90
4	Z	1	NAG	C2-N2-C7	3.28	127.30	122.90
4	L	2	NAG	C1-O5-C5	3.14	116.40	112.19
4	V	1	NAG	C2-N2-C7	3.08	127.03	122.90
4	b	2	NAG	C1-O5-C5	2.88	116.04	112.19
4	S	1	NAG	C4-C3-C2	2.58	114.80	111.02
4	U	2	NAG	C1-O5-C5	2.56	115.62	112.19
4	S	1	NAG	O3-C3-C2	-2.52	104.17	109.40
4	b	1	NAG	C1-O5-C5	2.30	115.27	112.19
4	R	1	NAG	C1-O5-C5	2.30	115.27	112.19
4	J	1	NAG	C2-N2-C7	2.25	125.92	122.90
4	S	1	NAG	C1-O5-C5	-2.24	109.18	112.19
4	X	2	NAG	C1-O5-C5	2.24	115.19	112.19
4	Q	2	NAG	C8-C7-N2	2.23	119.82	116.12
4	b	2	NAG	C8-C7-N2	2.23	119.82	116.12
4	K	1	NAG	O4-C4-C5	2.22	114.79	109.32
4	W	1	NAG	C1-O5-C5	-2.19	109.26	112.19
4	d	1	NAG	C8-C7-N2	2.17	119.72	116.12
4	J	1	NAG	O3-C3-C2	-2.17	104.90	109.40
4	U	1	NAG	O4-C4-C5	2.17	114.66	109.32
4	J	1	NAG	C4-C3-C2	2.16	114.18	111.02
4	X	2	NAG	C8-C7-N2	2.14	119.67	116.12
4	O	1	NAG	C8-C7-N2	2.13	119.66	116.12

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	W	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L	1	NAG	O5-C5-C6-O6
4	d	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	O	1	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	T	2	NAG	C8-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
4	X	2	NAG	C8-C7-N2-C2
4	X	2	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
4	a	1	NAG	C8-C7-N2-C2
4	a	1	NAG	O7-C7-N2-C2
4	a	2	NAG	C8-C7-N2-C2
4	a	2	NAG	O7-C7-N2-C2
4	b	2	NAG	C8-C7-N2-C2
4	b	2	NAG	O7-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2
4	d	1	NAG	O7-C7-N2-C2
4	d	2	NAG	C8-C7-N2-C2
4	d	2	NAG	O7-C7-N2-C2
4	P	1	NAG	O5-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

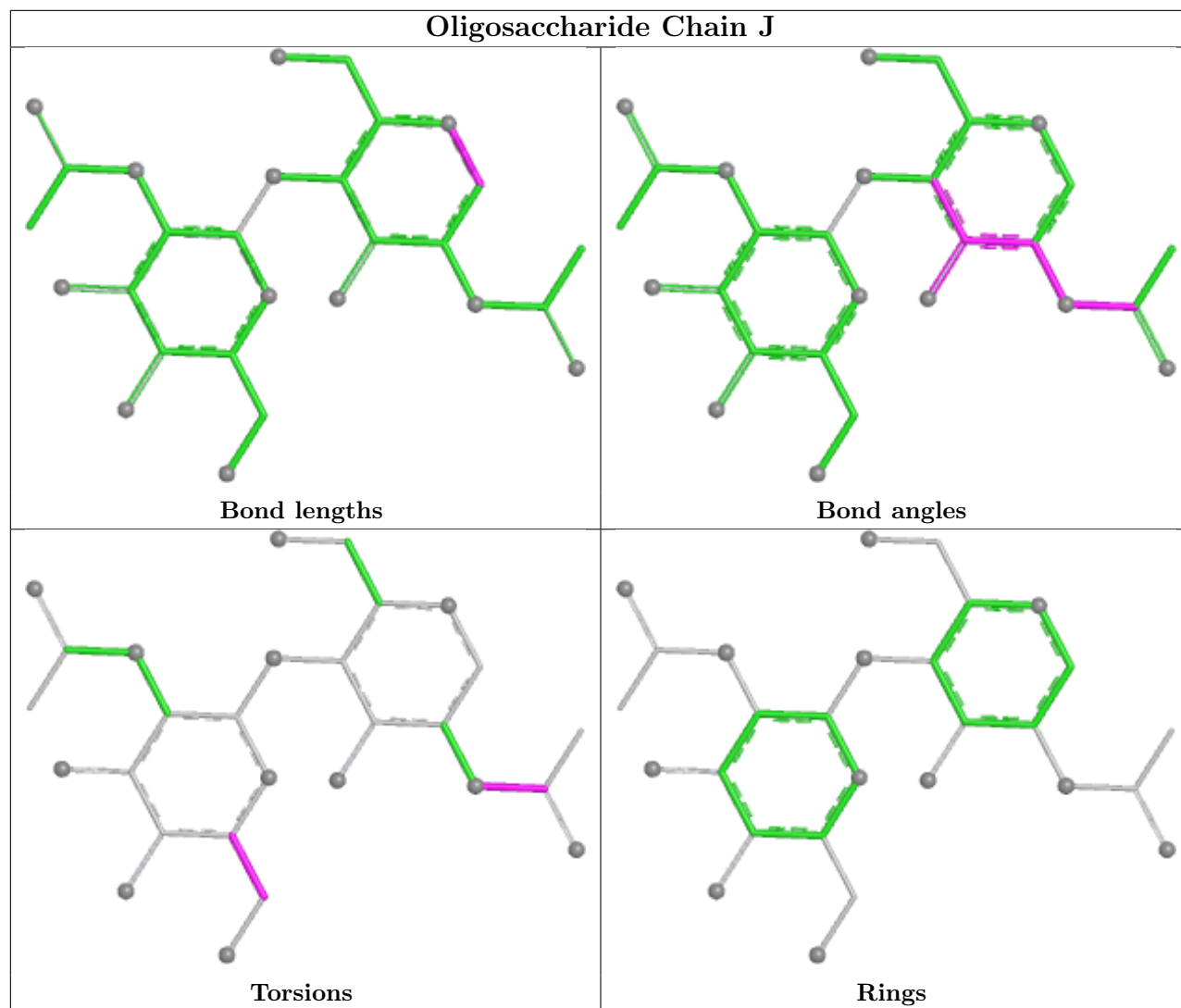
Mol	Chain	Res	Type	Atoms
4	X	1	NAG	O5-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C1-C2-N2-C7
4	Z	1	NAG	C1-C2-N2-C7
4	b	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	C3-C2-N2-C7
4	W	1	NAG	C3-C2-N2-C7
4	X	2	NAG	C3-C2-N2-C7
4	b	2	NAG	C3-C2-N2-C7
4	d	1	NAG	C3-C2-N2-C7
4	V	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C1-C2-N2-C7
4	P	1	NAG	C1-C2-N2-C7
4	Q	2	NAG	C1-C2-N2-C7
4	V	1	NAG	C1-C2-N2-C7
4	W	1	NAG	C1-C2-N2-C7
4	X	2	NAG	C1-C2-N2-C7
4	b	2	NAG	C1-C2-N2-C7
4	d	1	NAG	C1-C2-N2-C7
4	U	1	NAG	O5-C5-C6-O6
4	M	1	NAG	C3-C2-N2-C7
4	O	1	NAG	C3-C2-N2-C7
4	S	1	NAG	C3-C2-N2-C7
4	V	1	NAG	C3-C2-N2-C7
4	Z	1	NAG	C3-C2-N2-C7

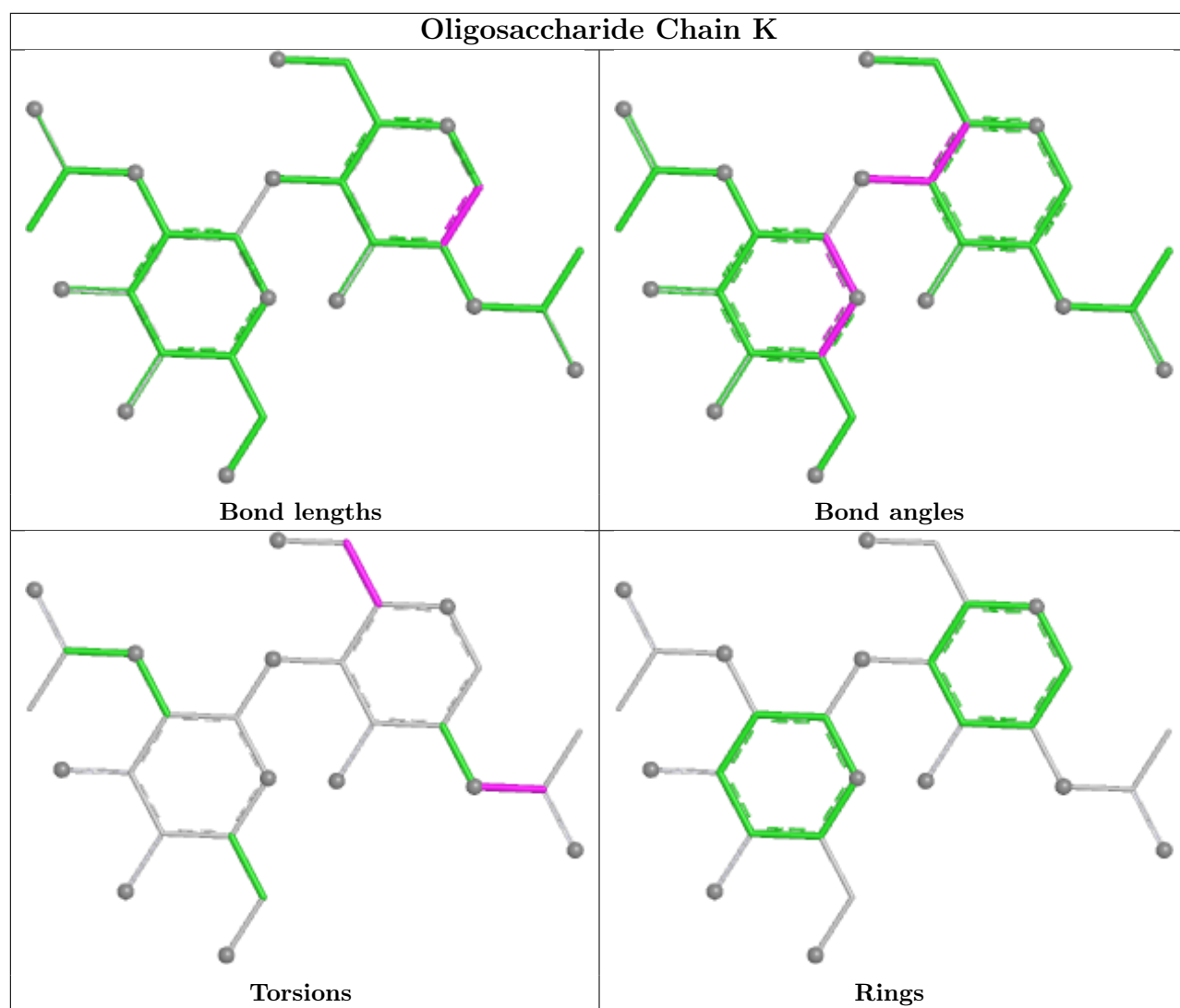
There are no ring outliers.

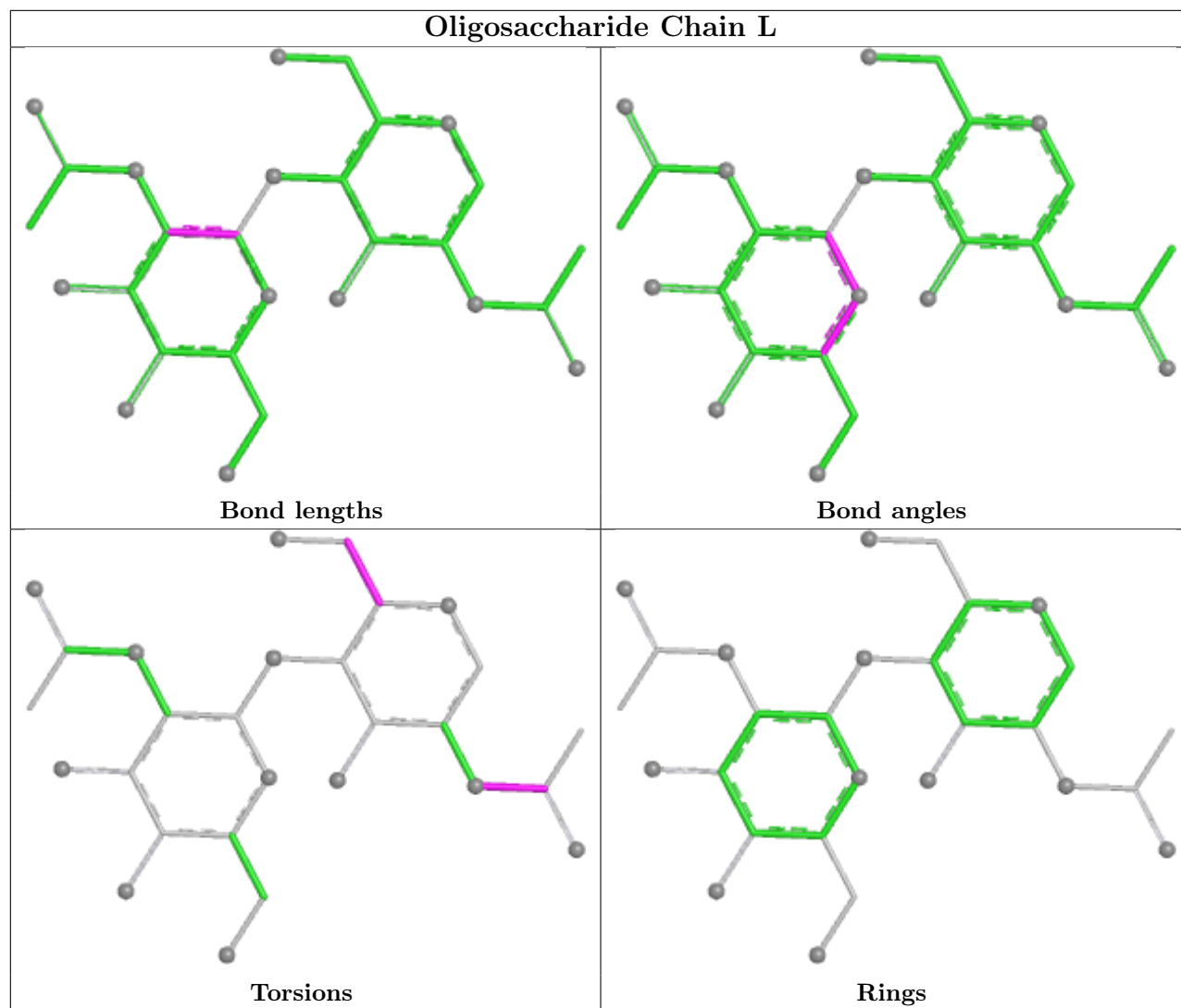
6 monomers are involved in 6 short contacts:

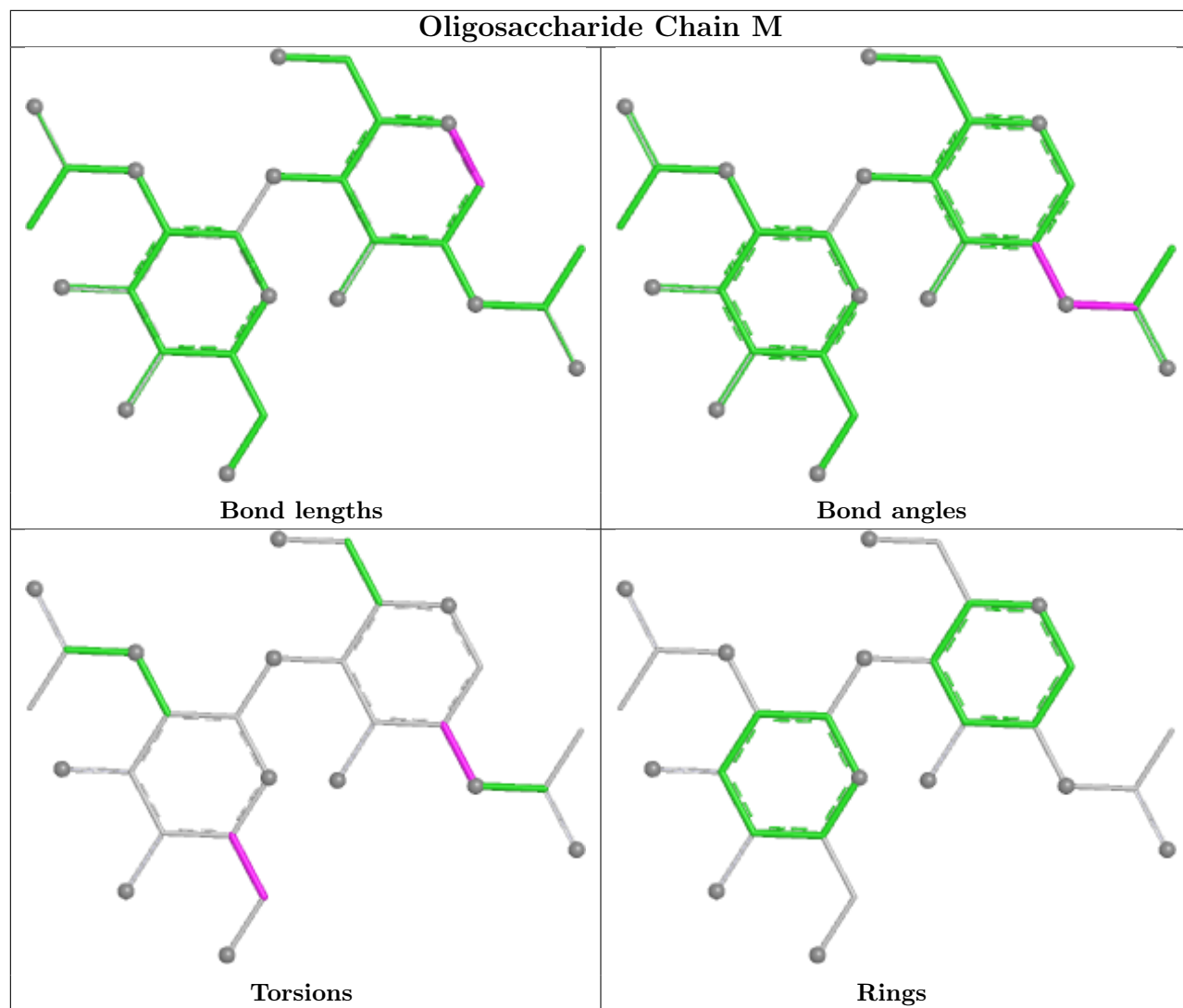
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	T	1	NAG	1	0
4	R	1	NAG	1	0
4	U	1	NAG	1	0
4	U	2	NAG	1	0
4	X	1	NAG	1	0
4	K	2	NAG	1	0

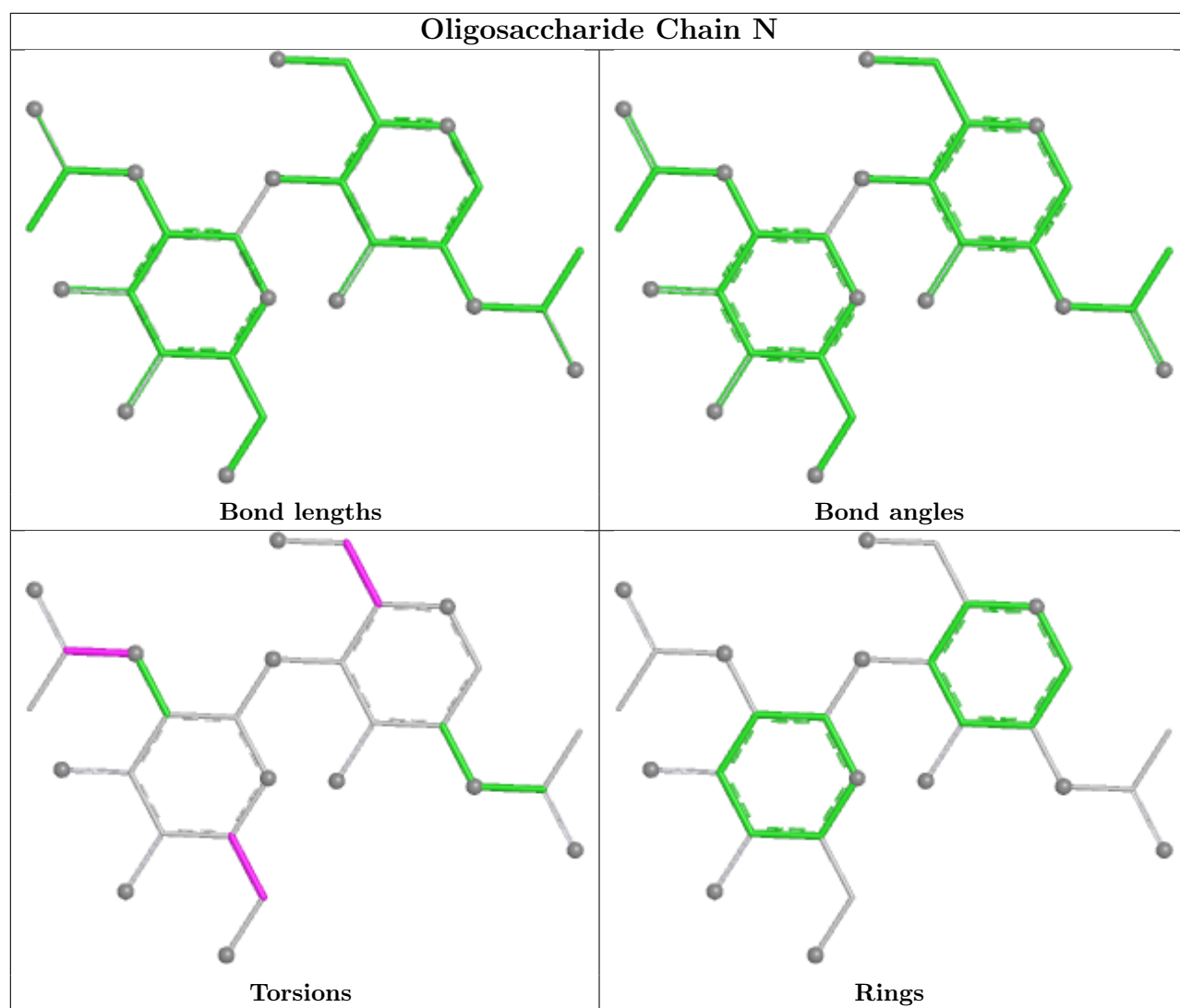
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

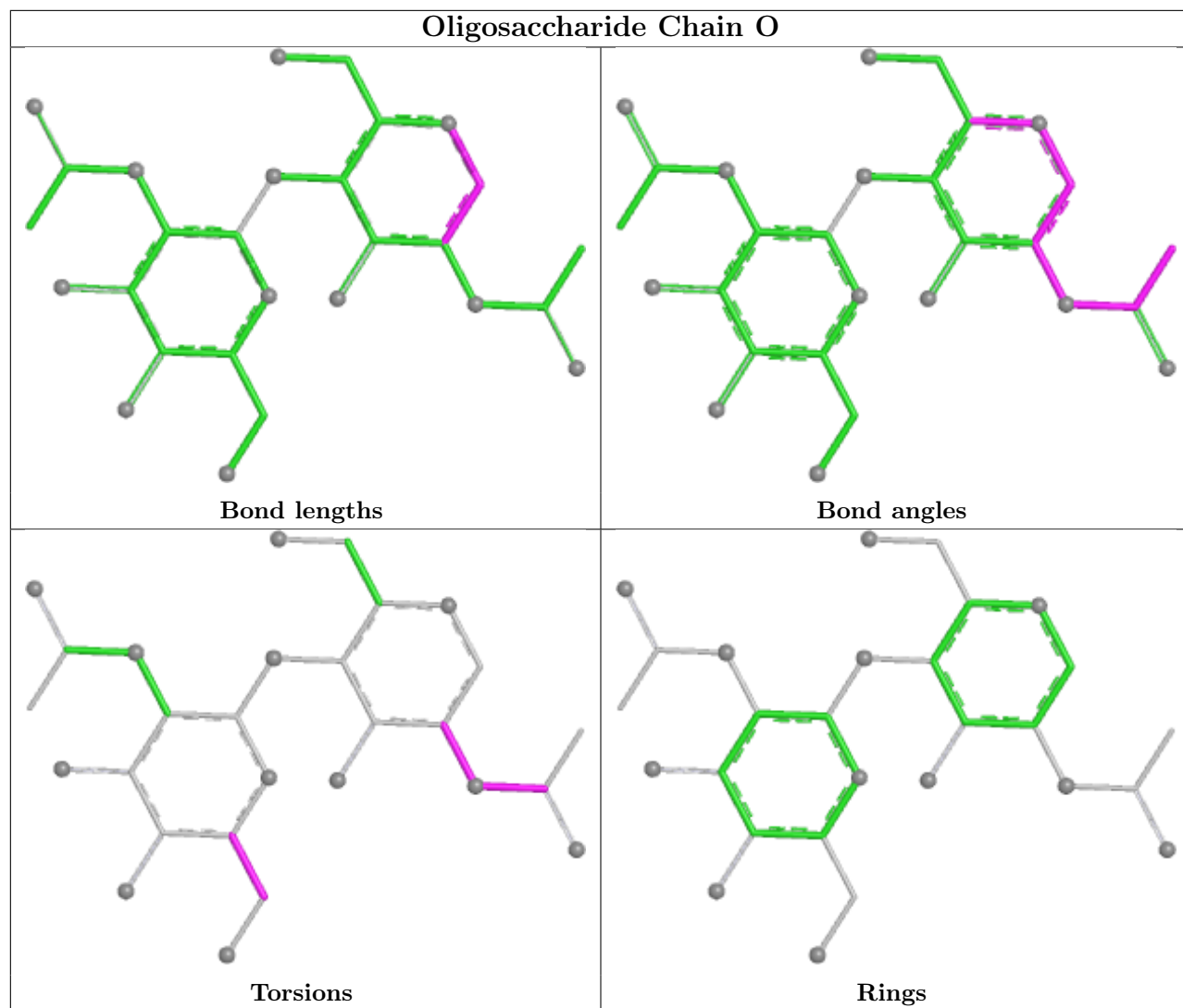


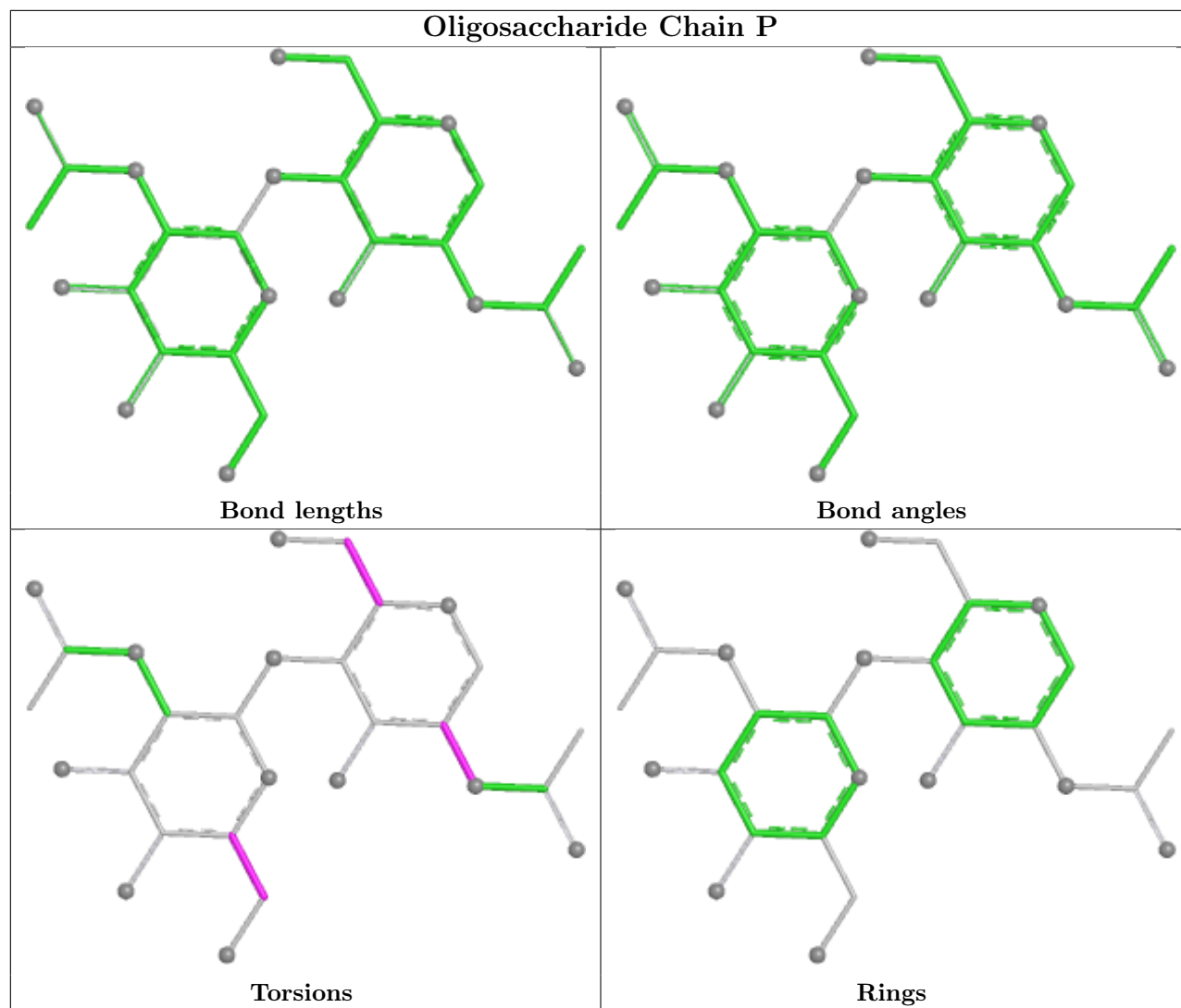


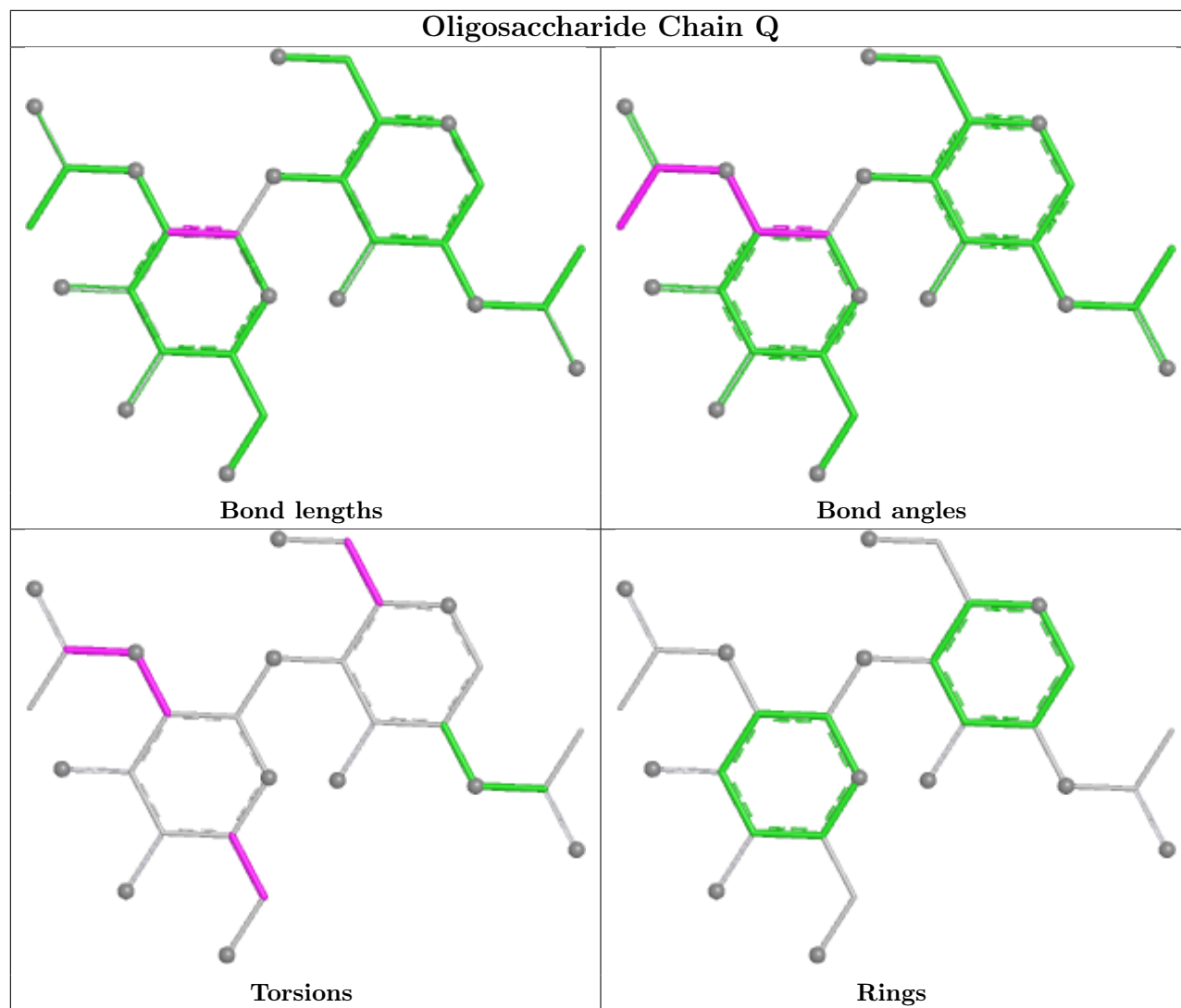


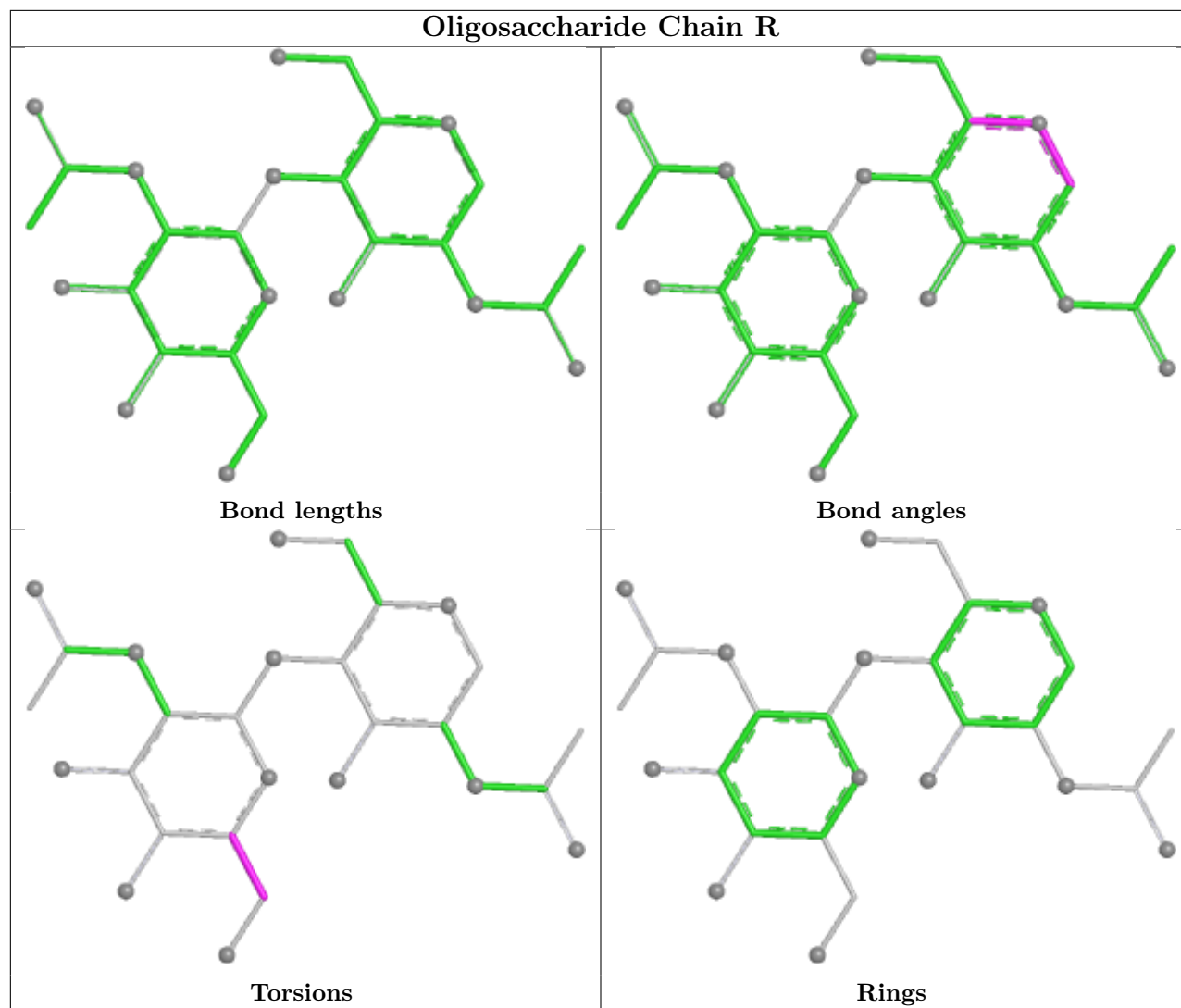


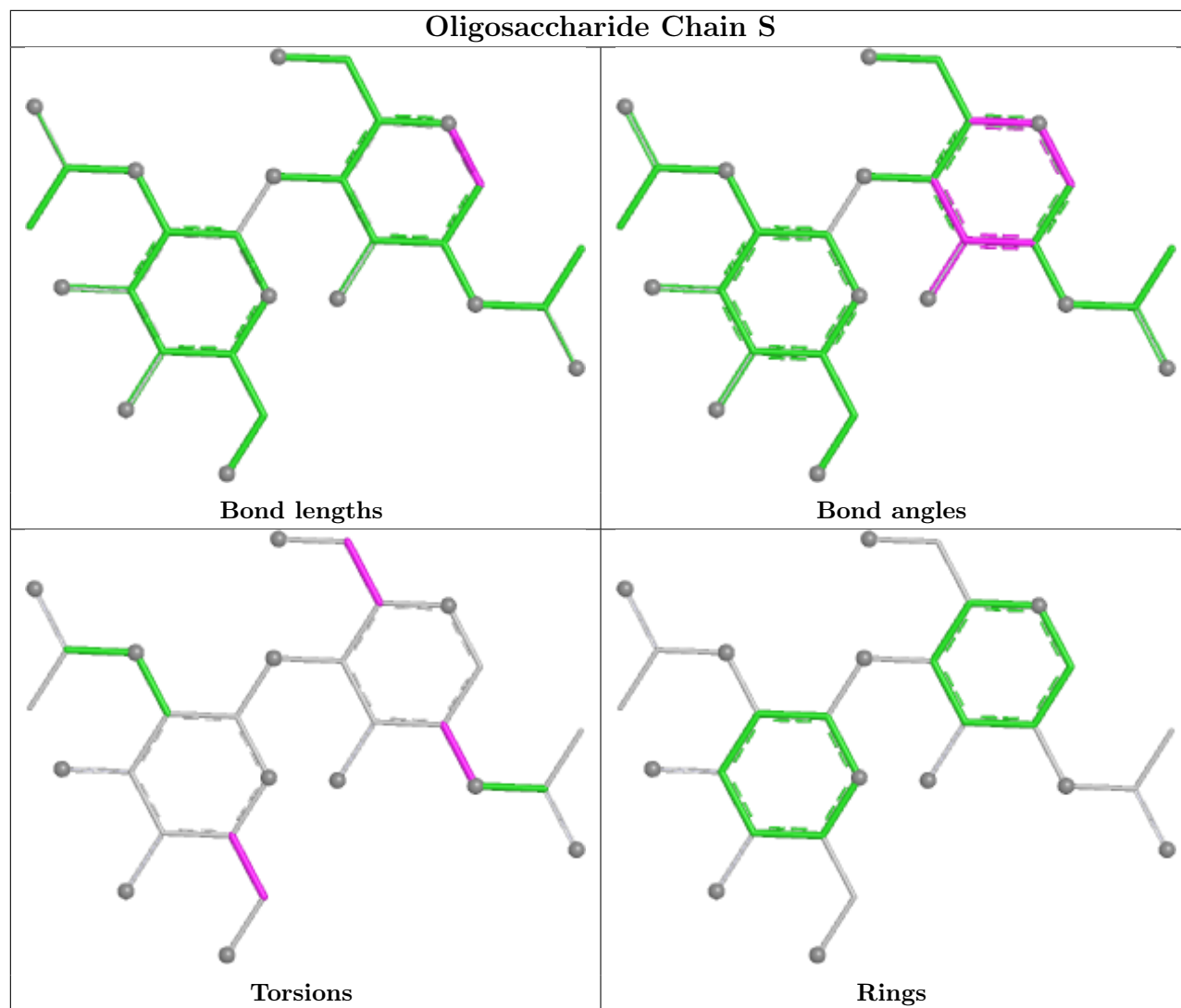


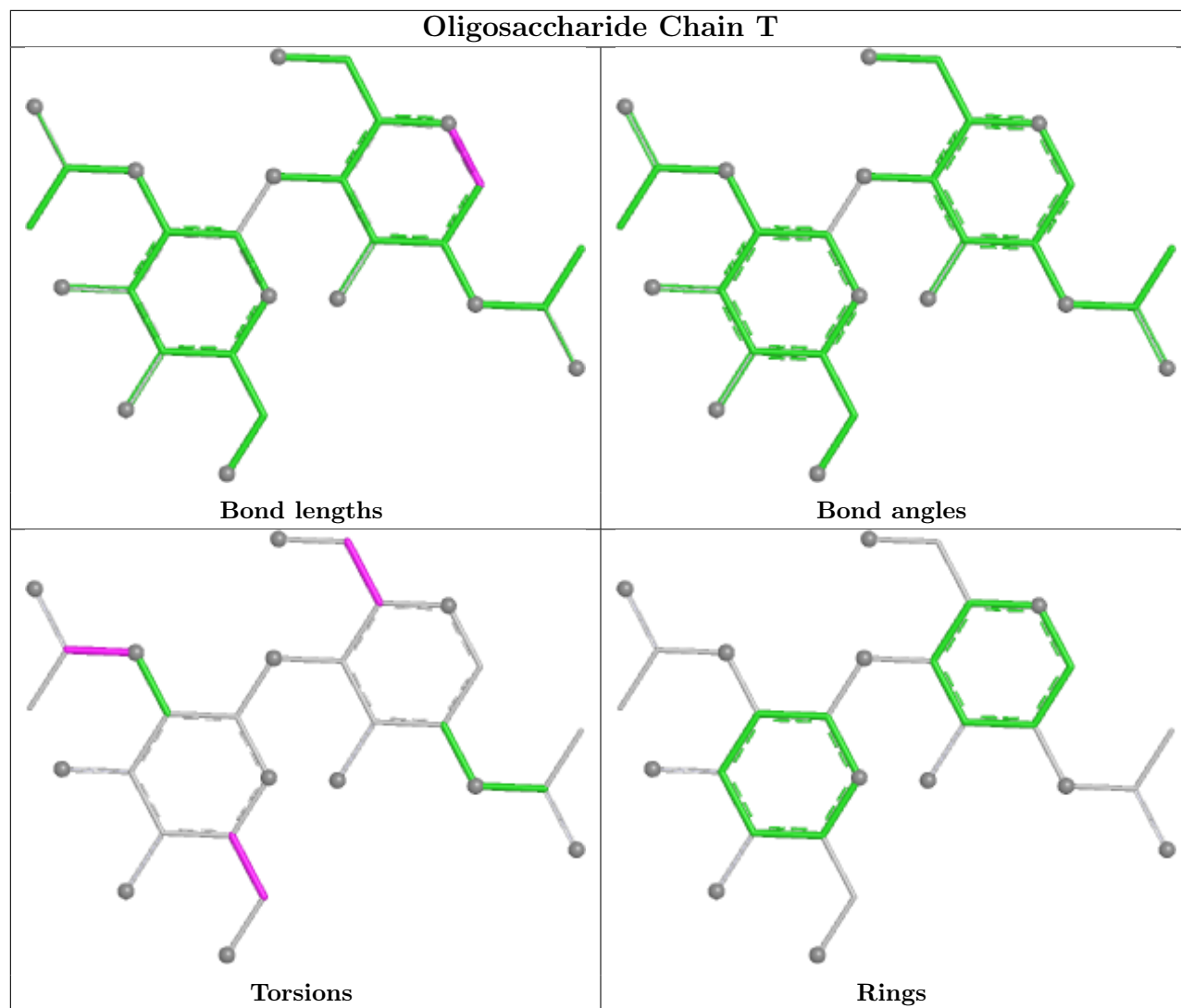


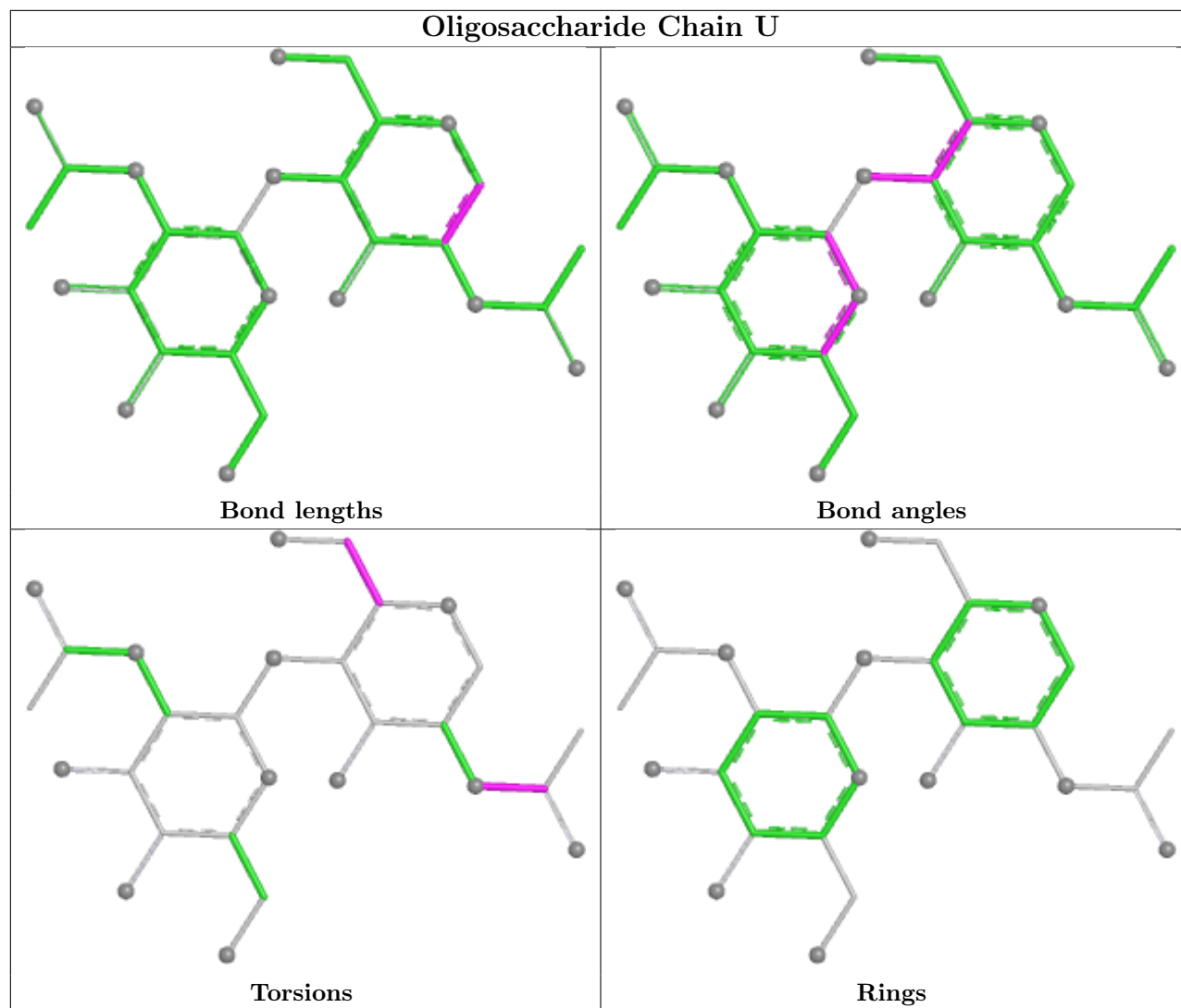


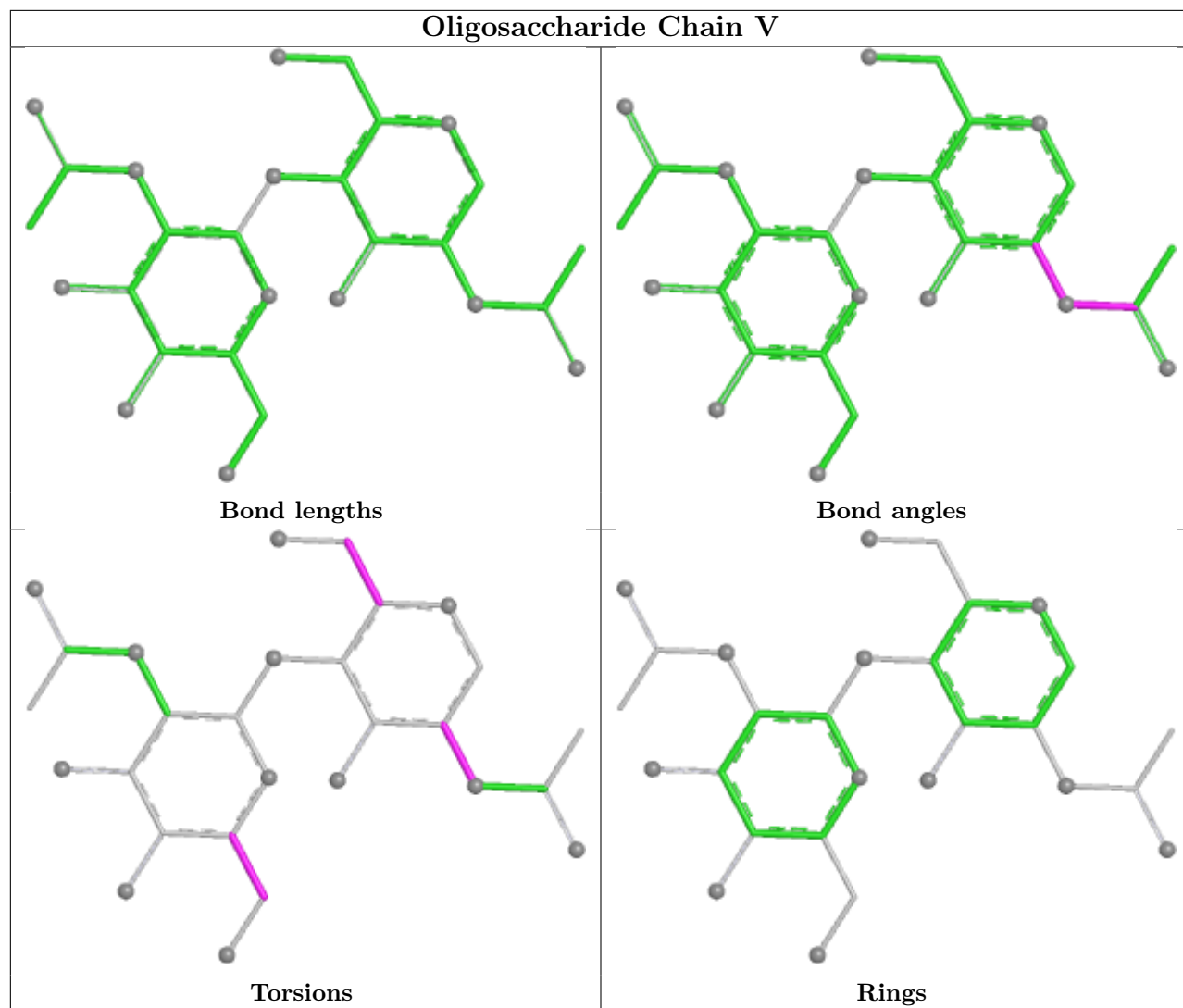


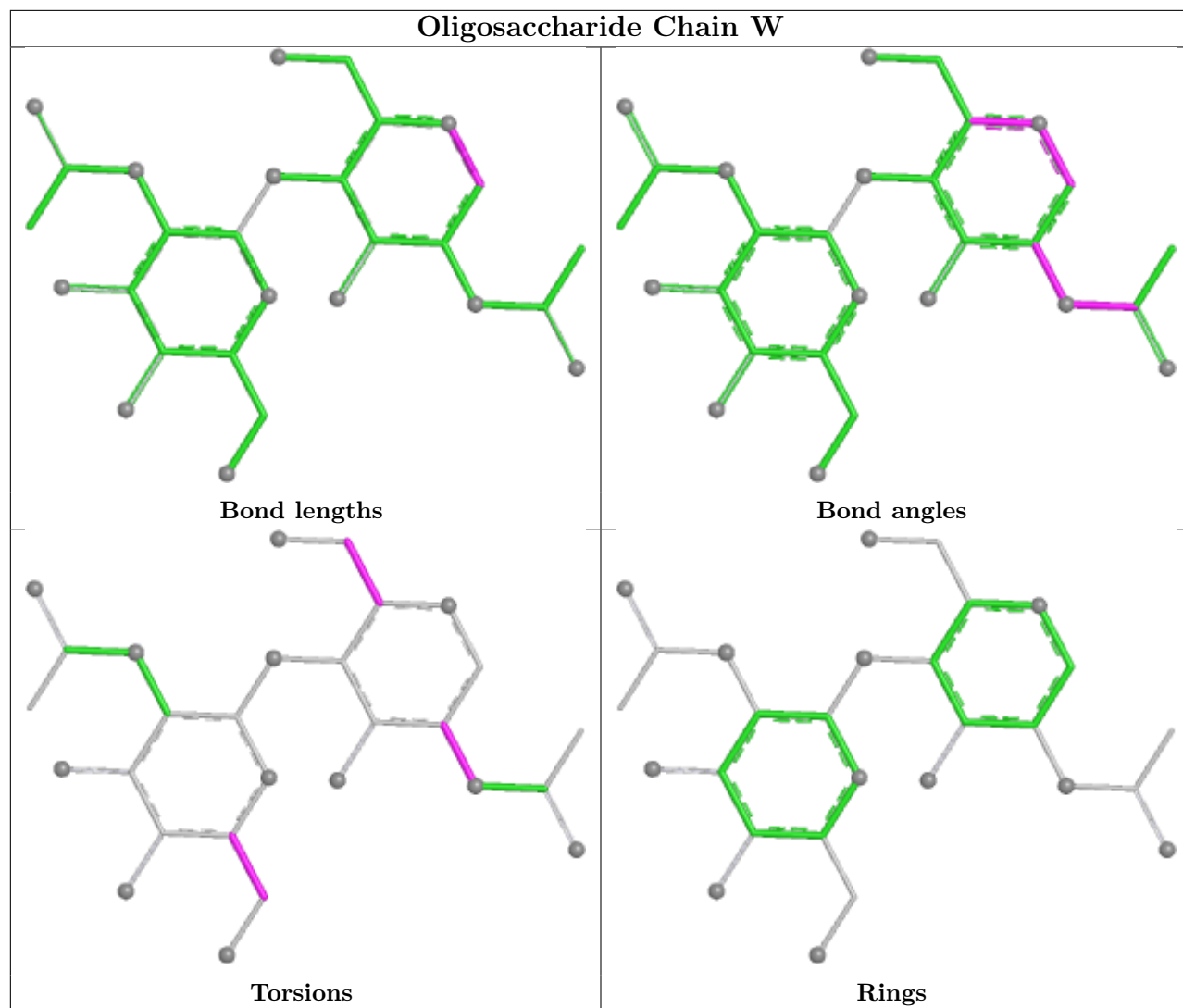


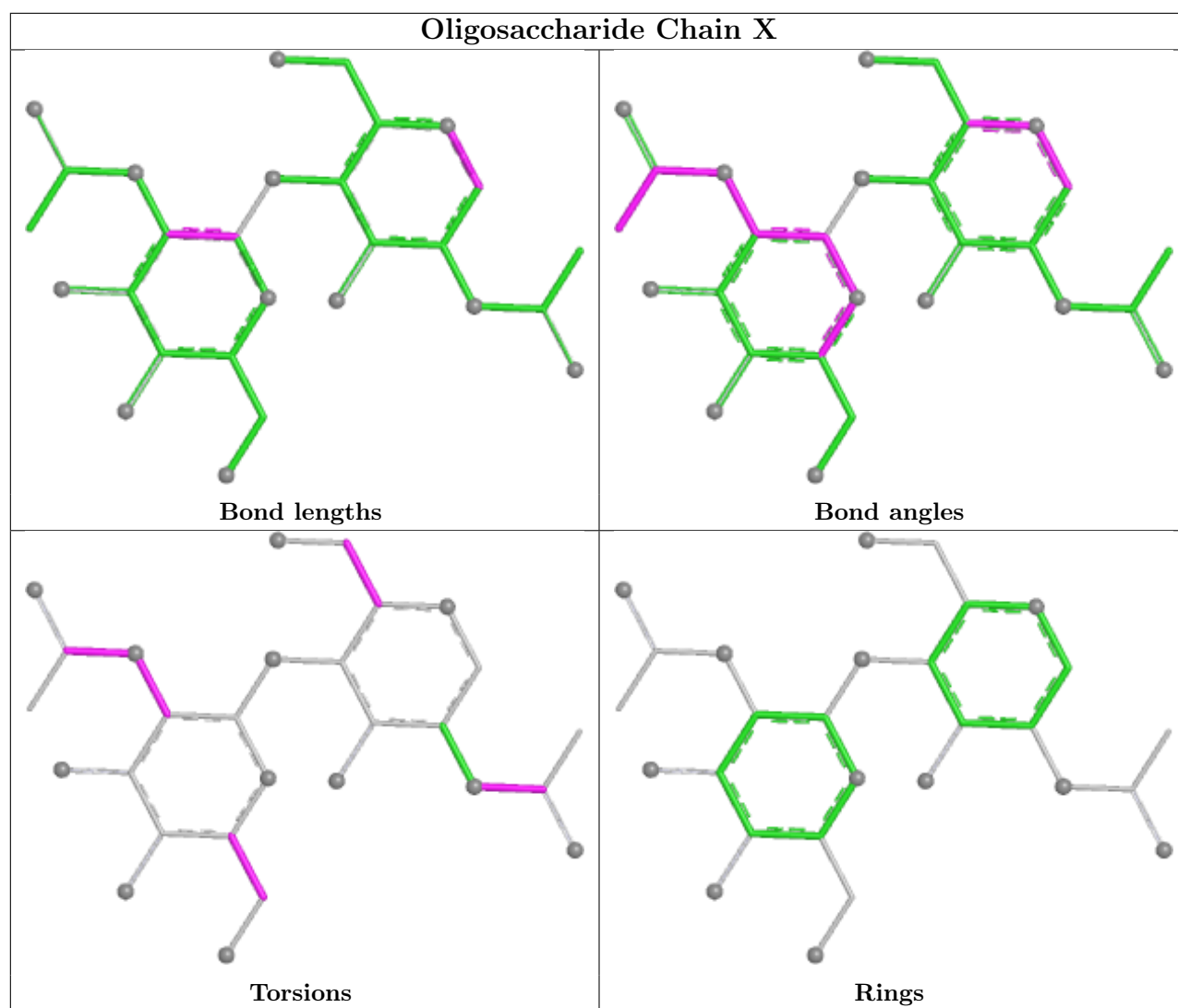


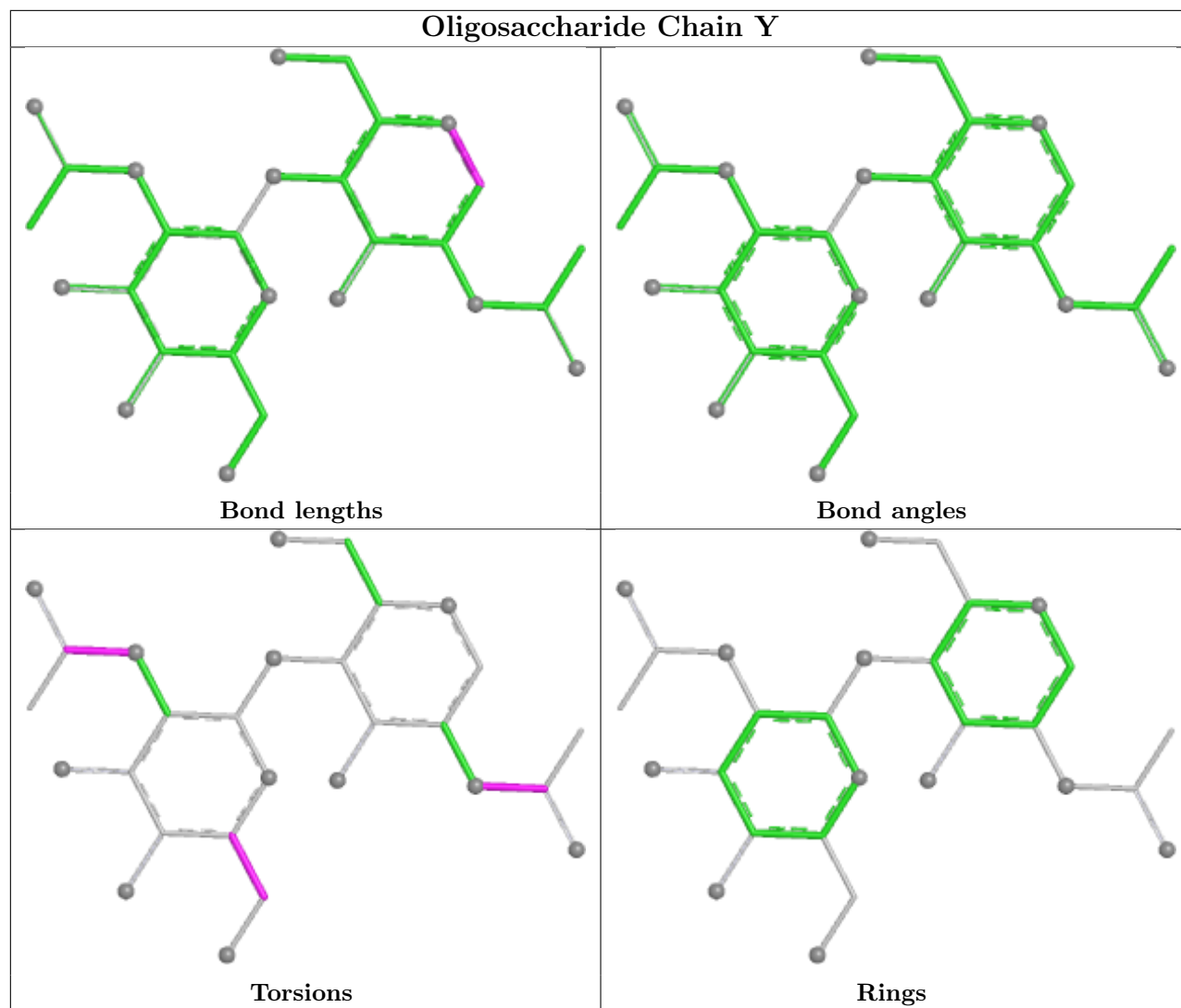


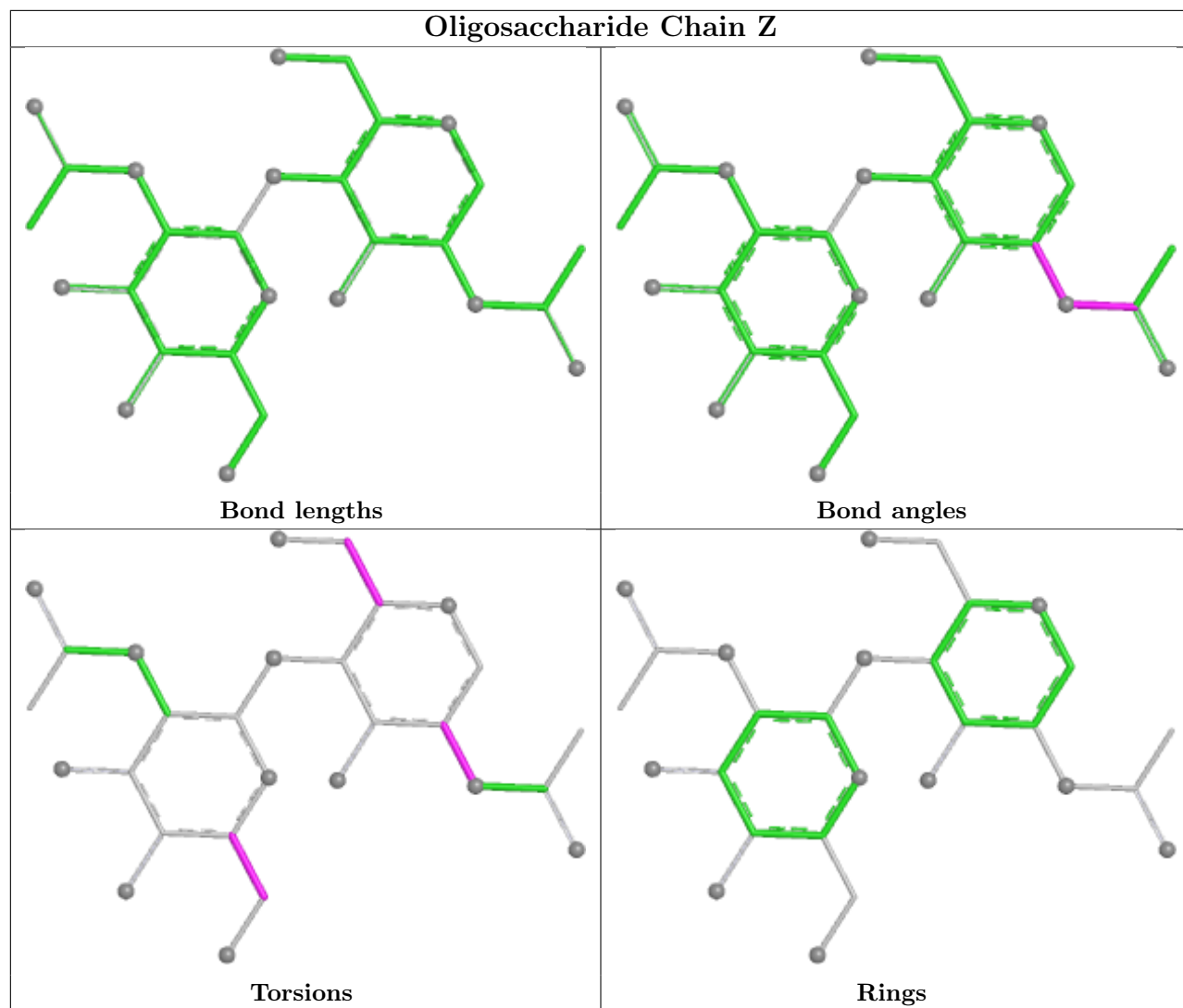


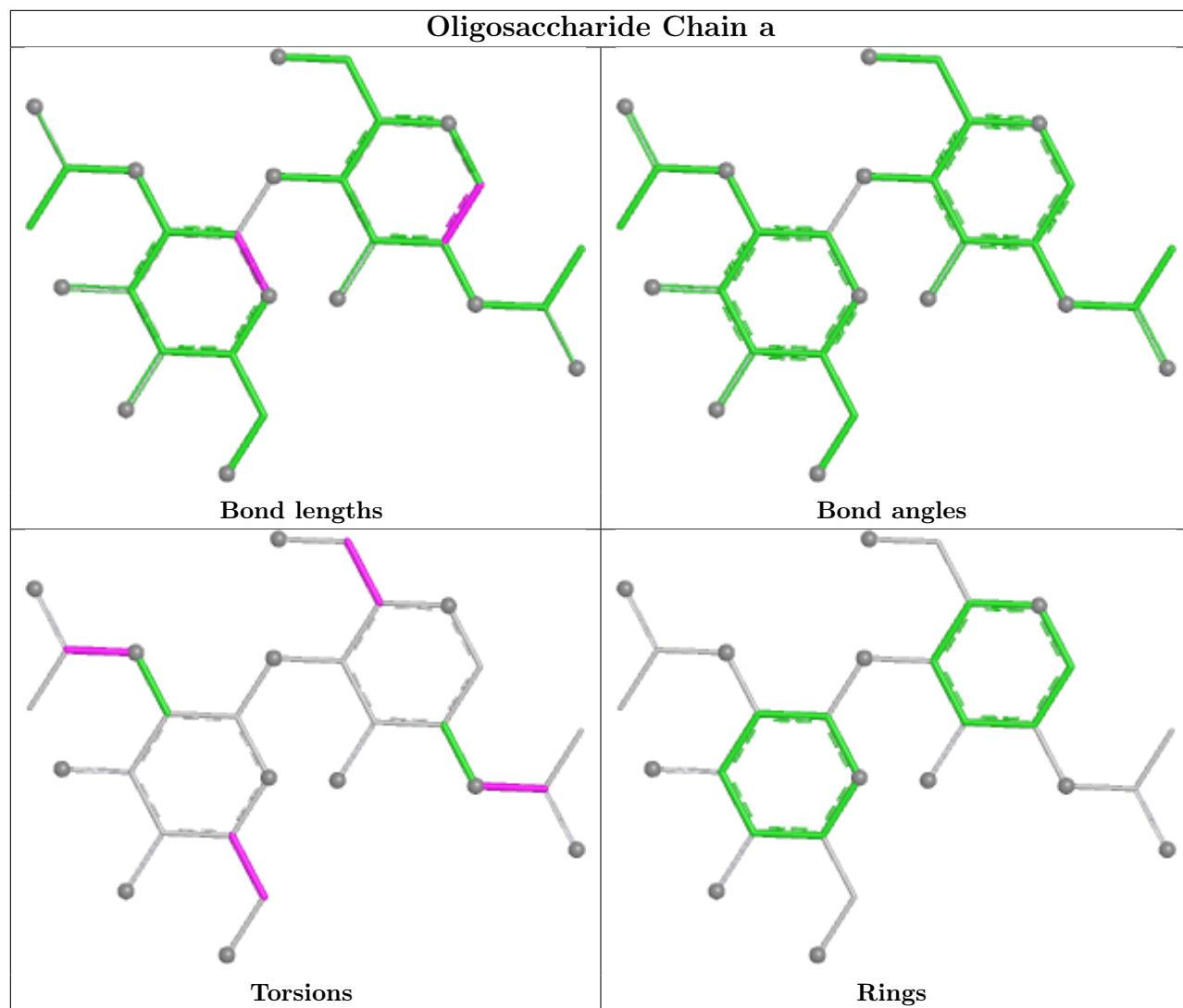


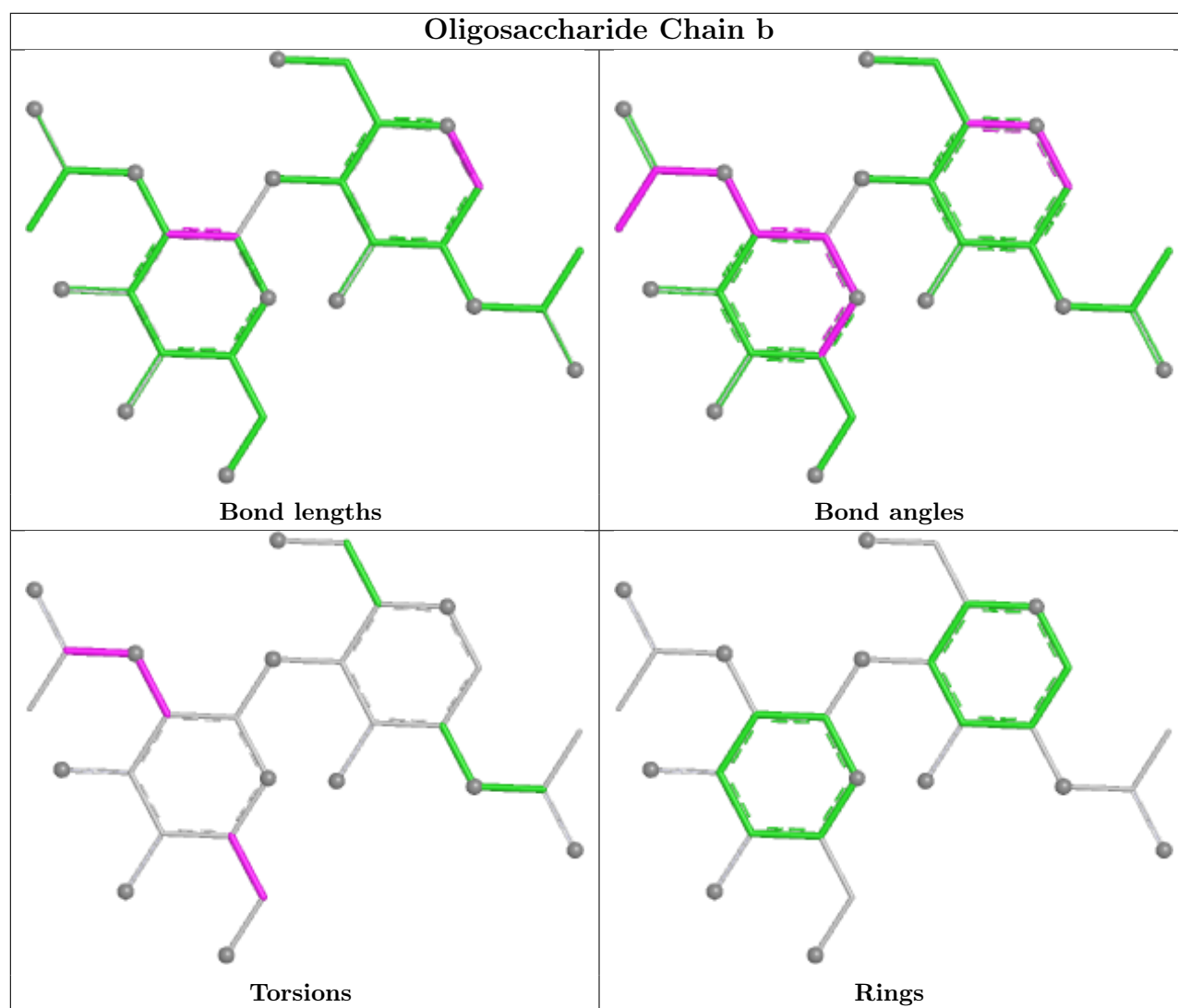


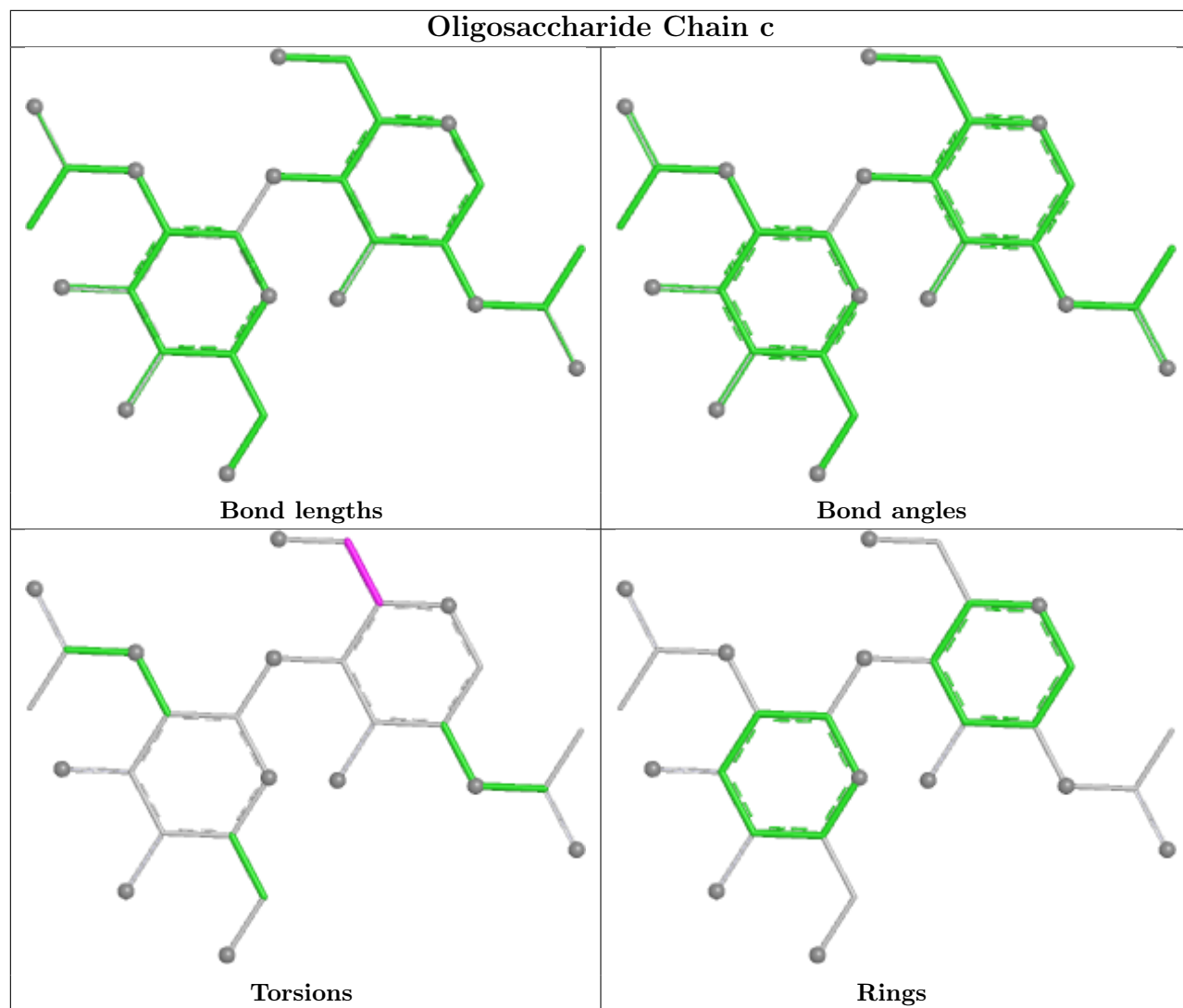


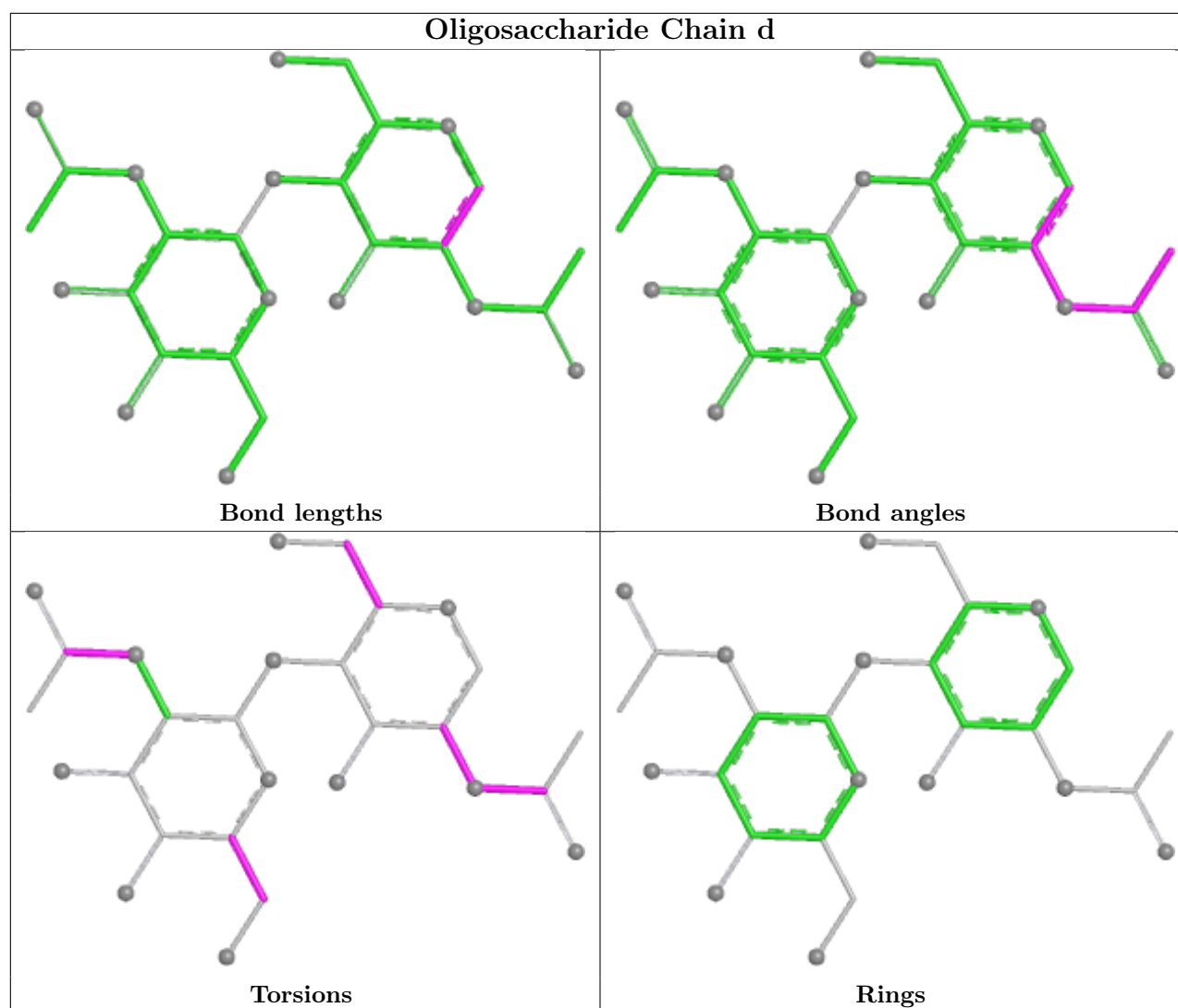












5.6 Ligand geometry [i](#)

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	q	1403	1	14,14,15	0.63	1 (7%)	17,19,21	0.53	0
5	NAG	q	1404	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	q	1406	1	14,14,15	0.45	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	p	1402	1	14,14,15	0.56	0	17,19,21	1.09	1 (5%)
5	NAG	r	1405	1	14,14,15	0.25	0	17,19,21	0.39	0
5	NAG	p	1403	1	14,14,15	0.46	0	17,19,21	0.55	0
5	NAG	r	1403	1	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
5	NAG	p	1401	1	14,14,15	0.92	1 (7%)	17,19,21	2.39	4 (23%)
5	NAG	q	1401	1	14,14,15	0.71	1 (7%)	17,19,21	0.82	1 (5%)
5	NAG	p	1404	1	14,14,15	0.37	0	17,19,21	2.04	3 (17%)
5	NAG	r	1404	1	14,14,15	0.88	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	p	1405	1	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
5	NAG	r	1406	1	14,14,15	0.25	0	17,19,21	0.55	0
5	NAG	p	1406	1	14,14,15	0.78	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	r	1402	1	14,14,15	1.35	1 (7%)	17,19,21	2.42	4 (23%)
5	NAG	q	1405	1	14,14,15	0.67	1 (7%)	17,19,21	1.25	2 (11%)
5	NAG	r	1401	1	14,14,15	0.51	0	17,19,21	1.01	1 (5%)
5	NAG	D	1401	1	14,14,15	1.51	2 (14%)	17,19,21	1.55	2 (11%)
5	NAG	q	1402	1	14,14,15	1.27	2 (14%)	17,19,21	2.73	4 (23%)
5	NAG	A	1401	1	14,14,15	0.57	0	17,19,21	0.95	1 (5%)
5	NAG	G	1401	1	14,14,15	0.73	1 (7%)	17,19,21	0.82	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	q	1403	1	-	1/6/23/26	0/1/1/1
5	NAG	q	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	q	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	p	1402	1	-	4/6/23/26	0/1/1/1
5	NAG	r	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	p	1403	1	-	4/6/23/26	0/1/1/1
5	NAG	r	1403	1	-	4/6/23/26	0/1/1/1
5	NAG	p	1401	1	-	6/6/23/26	0/1/1/1
5	NAG	q	1401	1	-	4/6/23/26	0/1/1/1
5	NAG	p	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	r	1404	1	-	4/6/23/26	0/1/1/1
5	NAG	p	1405	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	r	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	p	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	r	1402	1	-	6/6/23/26	0/1/1/1
5	NAG	q	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	r	1401	1	-	4/6/23/26	0/1/1/1
5	NAG	D	1401	1	-	3/6/23/26	0/1/1/1
5	NAG	q	1402	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	3/6/23/26	0/1/1/1
5	NAG	G	1401	1	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1401	NAG	O5-C1	4.92	1.52	1.43
5	r	1402	NAG	C1-C2	4.51	1.58	1.52
5	q	1402	NAG	O5-C1	3.48	1.49	1.43
5	r	1404	NAG	C1-C2	3.08	1.56	1.52
5	p	1401	NAG	C1-C2	2.71	1.56	1.52
5	D	1401	NAG	C1-C2	2.68	1.56	1.52
5	q	1402	NAG	C1-C2	2.65	1.55	1.52
5	G	1401	NAG	O5-C1	2.60	1.48	1.43
5	p	1406	NAG	O5-C1	2.27	1.47	1.43
5	q	1405	NAG	C1-C2	2.17	1.55	1.52
5	q	1403	NAG	C1-C2	2.05	1.55	1.52
5	q	1401	NAG	C1-C2	2.01	1.55	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	q	1402	NAG	C2-N2-C7	8.33	134.07	122.90
5	p	1401	NAG	C2-N2-C7	8.29	134.01	122.90
5	r	1402	NAG	C2-N2-C7	8.15	133.83	122.90
5	p	1404	NAG	C1-O5-C5	6.61	121.04	112.19
5	q	1402	NAG	C1-O5-C5	5.78	119.93	112.19
5	D	1401	NAG	C1-O5-C5	5.03	118.93	112.19
5	r	1402	NAG	C1-C2-N2	4.12	116.93	110.43
5	p	1404	NAG	C3-C4-C5	3.92	117.33	110.23
5	p	1401	NAG	C1-C2-N2	3.90	116.58	110.43
5	q	1402	NAG	C1-C2-N2	3.74	116.33	110.43
5	p	1402	NAG	C1-C2-N2	3.60	116.11	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1401	NAG	C2-N2-C7	3.32	127.35	122.90
5	q	1405	NAG	C2-N2-C7	3.25	127.25	122.90
5	r	1401	NAG	C2-N2-C7	3.20	127.19	122.90
5	p	1406	NAG	C1-O5-C5	3.19	116.46	112.19
5	q	1405	NAG	C1-O5-C5	3.12	116.37	112.19
5	D	1401	NAG	C2-N2-C7	3.09	127.04	122.90
5	r	1404	NAG	C2-N2-C7	2.93	126.83	122.90
5	p	1405	NAG	C1-O5-C5	2.86	116.02	112.19
5	r	1402	NAG	C1-O5-C5	2.57	115.63	112.19
5	q	1401	NAG	C1-O5-C5	2.54	115.59	112.19
5	G	1401	NAG	C1-O5-C5	2.42	115.43	112.19
5	r	1403	NAG	C1-O5-C5	2.38	115.38	112.19
5	p	1404	NAG	O5-C5-C4	2.26	116.33	110.83
5	p	1401	NAG	C1-O5-C5	2.25	115.20	112.19
5	q	1402	NAG	C8-C7-N2	2.24	119.83	116.12
5	r	1402	NAG	C8-C7-N2	2.21	119.78	116.12
5	p	1401	NAG	C8-C7-N2	2.11	119.62	116.12

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	r	1404	NAG	C4-C5-C6-O6
5	p	1401	NAG	O5-C5-C6-O6
5	r	1401	NAG	O5-C5-C6-O6
5	p	1402	NAG	O5-C5-C6-O6
5	r	1404	NAG	O5-C5-C6-O6
5	r	1401	NAG	C4-C5-C6-O6
5	p	1403	NAG	O5-C5-C6-O6
5	p	1402	NAG	C4-C5-C6-O6
5	G	1401	NAG	C8-C7-N2-C2
5	G	1401	NAG	O7-C7-N2-C2
5	p	1401	NAG	C8-C7-N2-C2
5	p	1401	NAG	O7-C7-N2-C2
5	p	1402	NAG	C8-C7-N2-C2
5	p	1402	NAG	O7-C7-N2-C2
5	p	1403	NAG	C8-C7-N2-C2
5	p	1403	NAG	O7-C7-N2-C2
5	p	1406	NAG	C8-C7-N2-C2
5	p	1406	NAG	O7-C7-N2-C2
5	q	1401	NAG	C8-C7-N2-C2
5	q	1401	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	q	1402	NAG	C8-C7-N2-C2
5	q	1402	NAG	O7-C7-N2-C2
5	q	1406	NAG	C8-C7-N2-C2
5	q	1406	NAG	O7-C7-N2-C2
5	r	1402	NAG	C8-C7-N2-C2
5	r	1402	NAG	O7-C7-N2-C2
5	r	1403	NAG	C8-C7-N2-C2
5	r	1403	NAG	O7-C7-N2-C2
5	r	1406	NAG	C8-C7-N2-C2
5	r	1406	NAG	O7-C7-N2-C2
5	r	1403	NAG	O5-C5-C6-O6
5	p	1401	NAG	C4-C5-C6-O6
5	D	1401	NAG	O5-C5-C6-O6
5	q	1401	NAG	O5-C5-C6-O6
5	r	1406	NAG	O5-C5-C6-O6
5	q	1401	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	r	1402	NAG	C4-C5-C6-O6
5	p	1405	NAG	O5-C5-C6-O6
5	r	1403	NAG	C4-C5-C6-O6
5	q	1402	NAG	O5-C5-C6-O6
5	q	1403	NAG	O5-C5-C6-O6
5	r	1402	NAG	O5-C5-C6-O6
5	A	1401	NAG	C1-C2-N2-C7
5	r	1402	NAG	C3-C2-N2-C7
5	p	1403	NAG	C4-C5-C6-O6
5	p	1404	NAG	O5-C5-C6-O6
5	D	1401	NAG	C1-C2-N2-C7
5	p	1401	NAG	C1-C2-N2-C7
5	q	1402	NAG	C1-C2-N2-C7
5	q	1405	NAG	C1-C2-N2-C7
5	r	1401	NAG	C1-C2-N2-C7
5	r	1402	NAG	C1-C2-N2-C7
5	r	1404	NAG	C1-C2-N2-C7
5	A	1401	NAG	C3-C2-N2-C7
5	D	1401	NAG	C3-C2-N2-C7
5	p	1401	NAG	C3-C2-N2-C7
5	q	1402	NAG	C3-C2-N2-C7
5	q	1405	NAG	C3-C2-N2-C7
5	r	1401	NAG	C3-C2-N2-C7
5	r	1404	NAG	C3-C2-N2-C7
5	q	1404	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	q	1406	NAG	1	0
5	r	1404	NAG	1	0
5	G	1401	NAG	1	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.

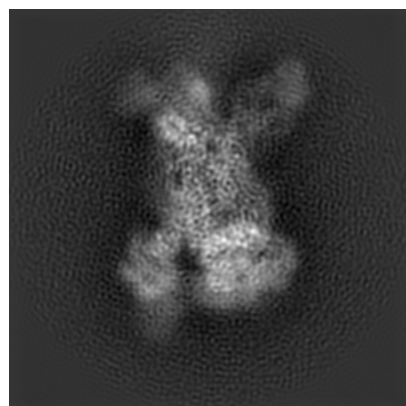
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8783. These allow visual inspection of the internal detail of the map and identification of artifacts.

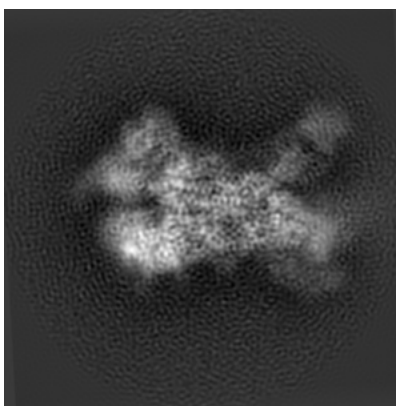
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

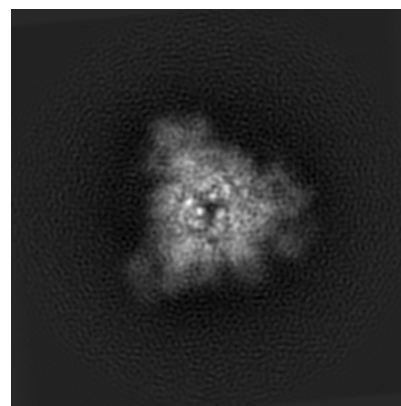
6.1.1 Primary map



X

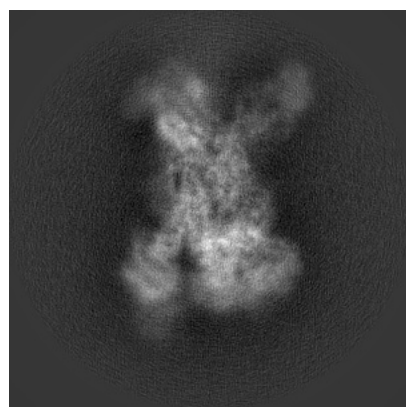


Y

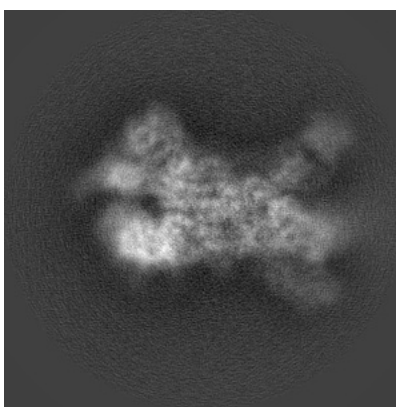


Z

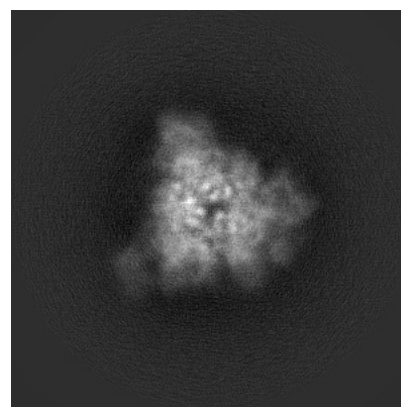
6.1.2 Raw map



X



Y

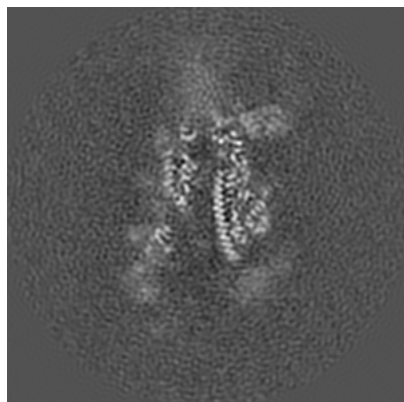


Z

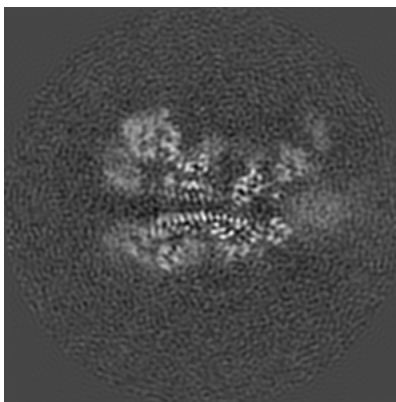
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

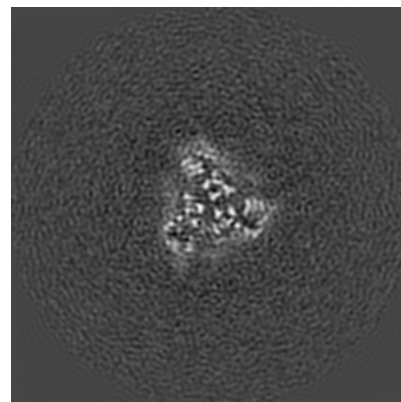
6.2.1 Primary map



X Index: 152

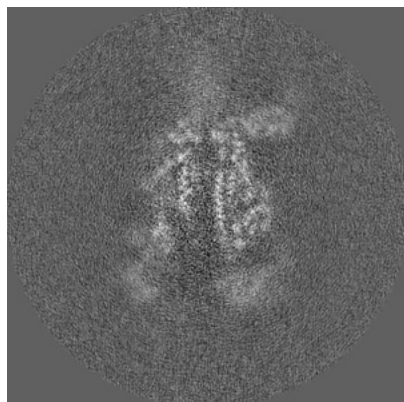


Y Index: 152

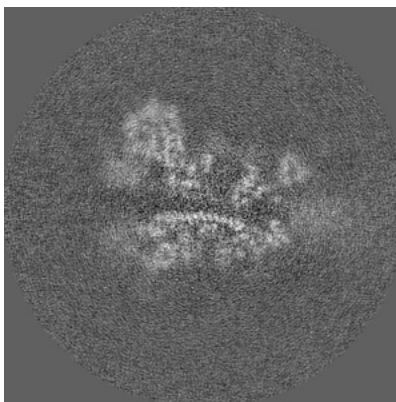


Z Index: 152

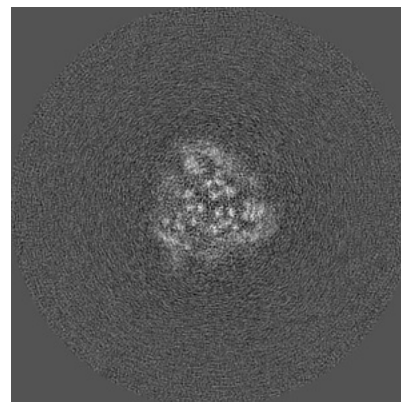
6.2.2 Raw map



X Index: 152



Y Index: 152

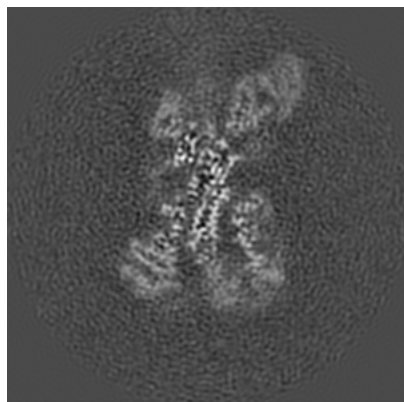


Z Index: 152

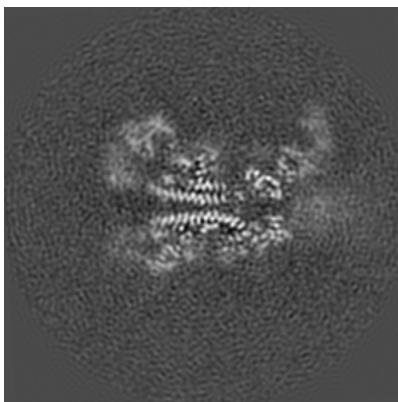
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

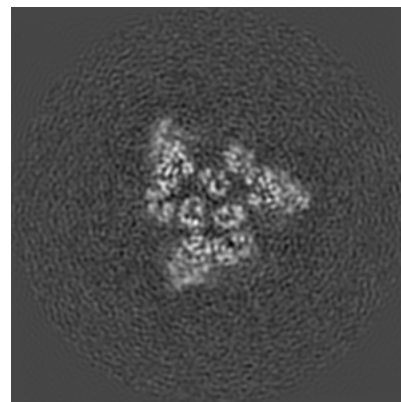
6.3.1 Primary map



X Index: 135

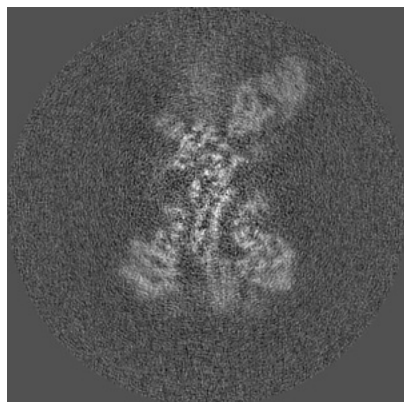


Y Index: 149

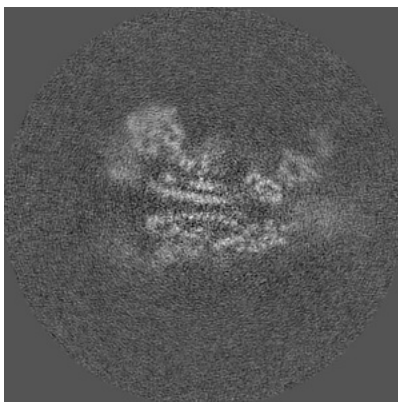


Z Index: 123

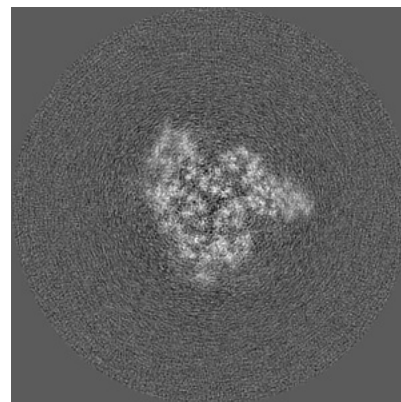
6.3.2 Raw map



X Index: 135



Y Index: 148

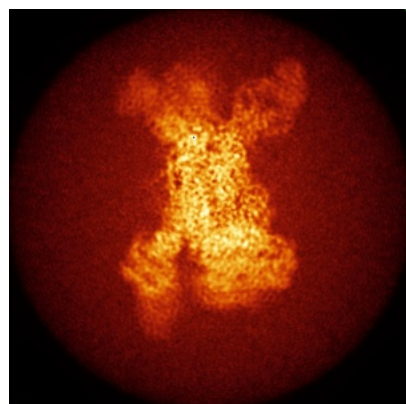


Z Index: 128

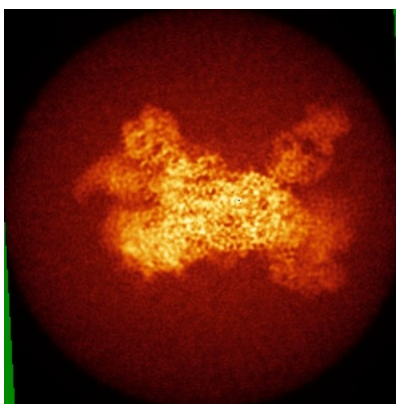
The images above show the largest variance slices of the map in three orthogonal directions.

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

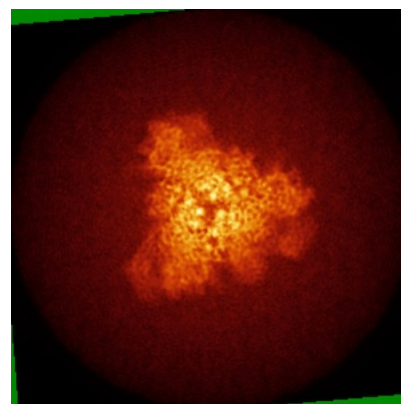
6.4.1 Primary map



X

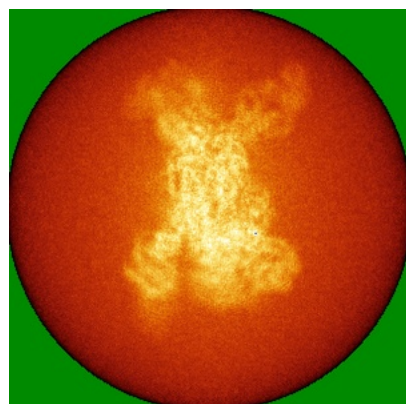


Y

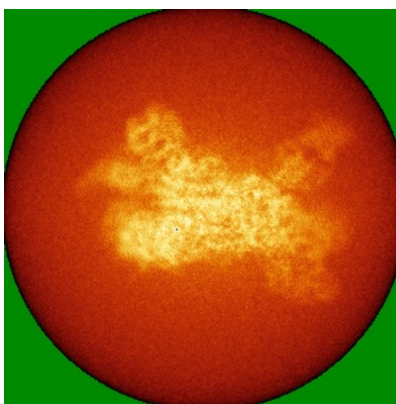


Z

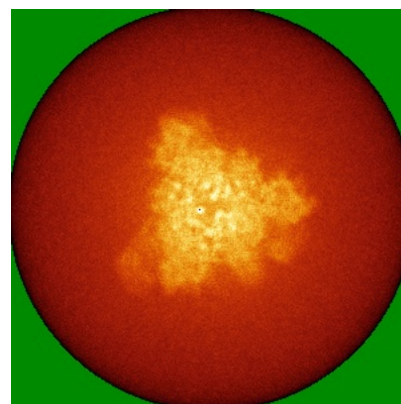
6.4.2 Raw map



X



Y

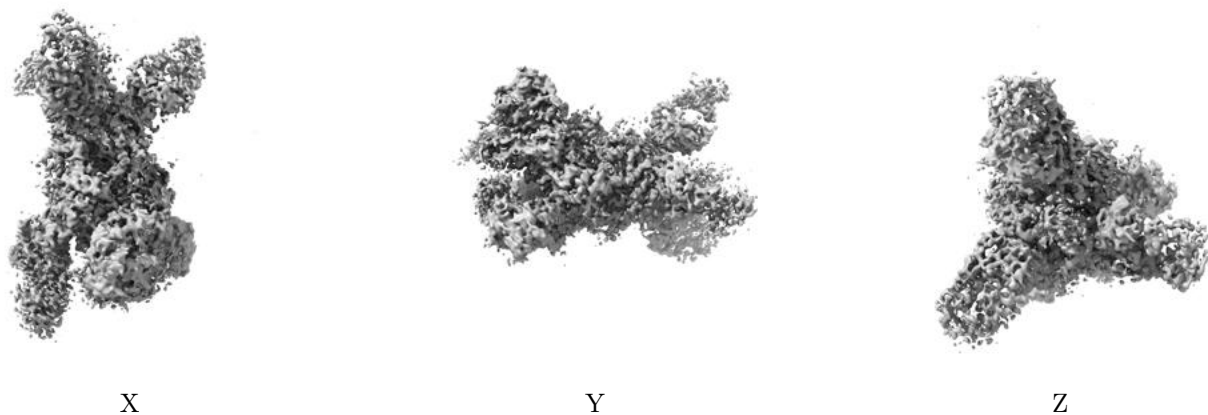


Z

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

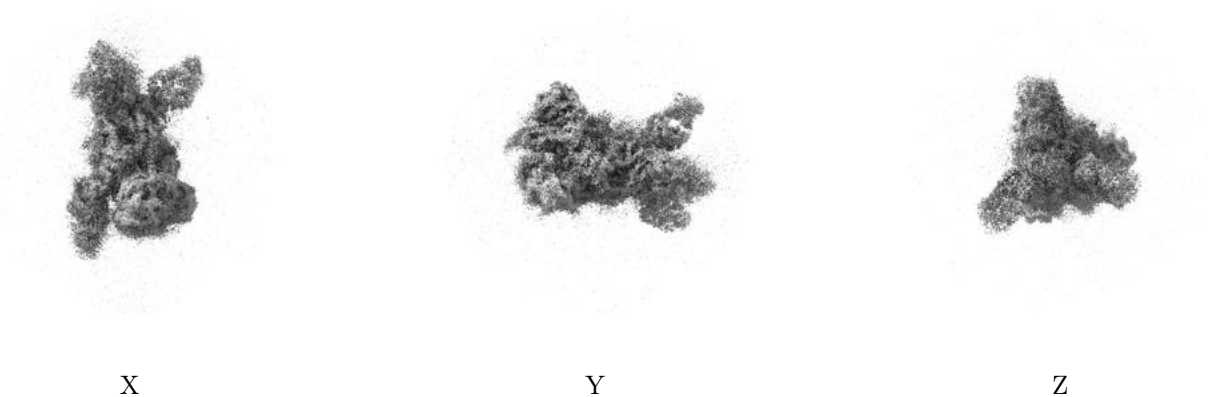
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

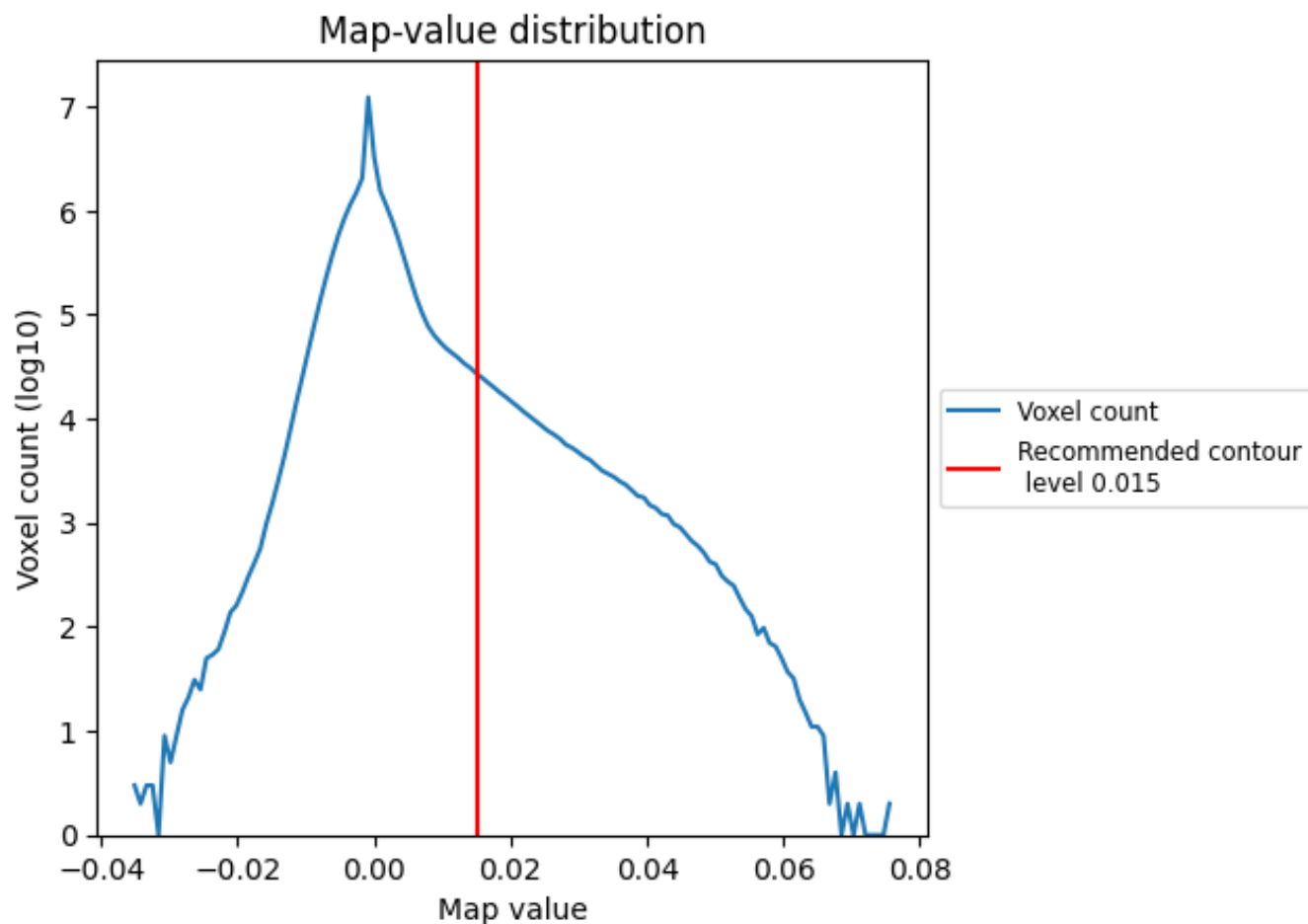
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

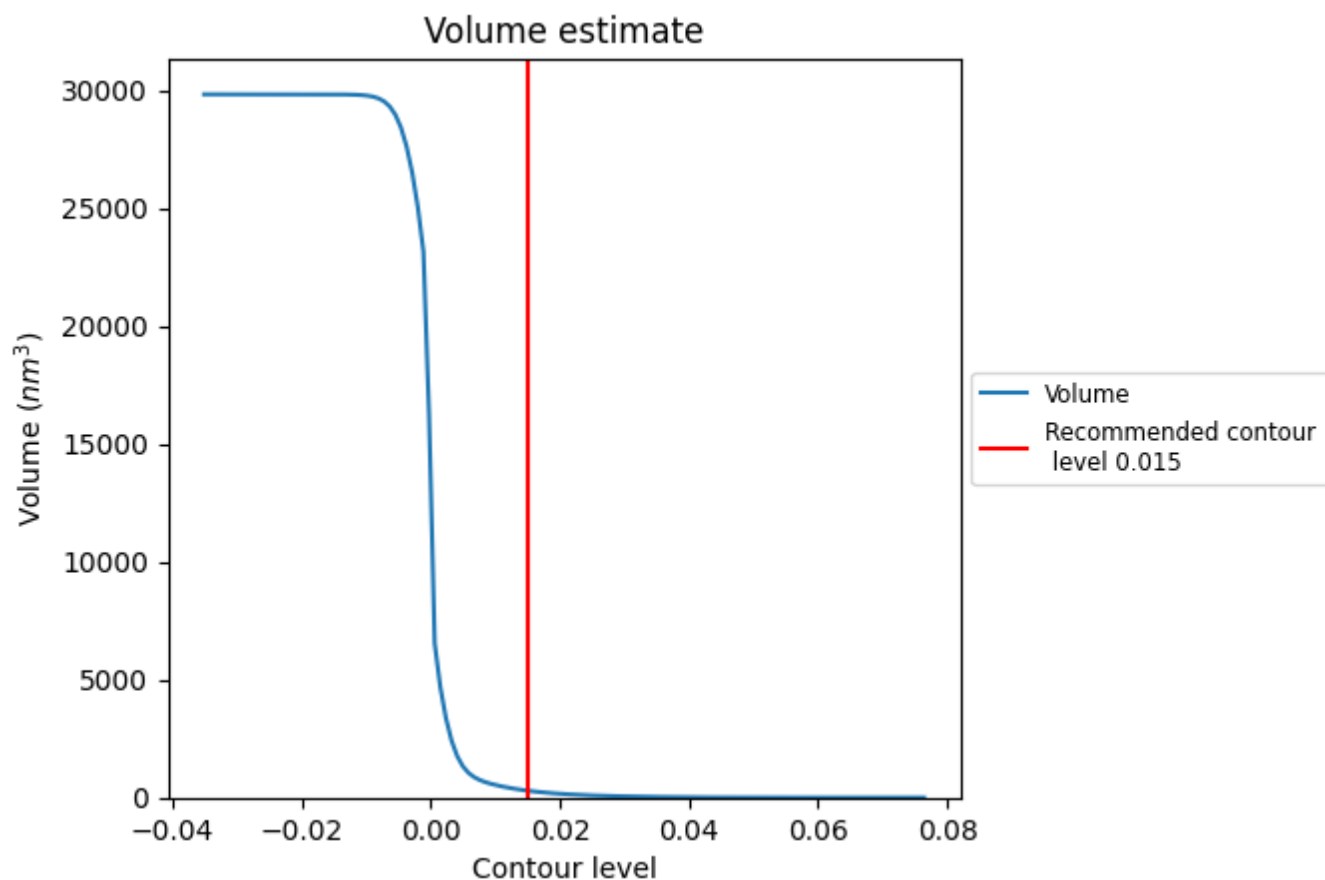
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

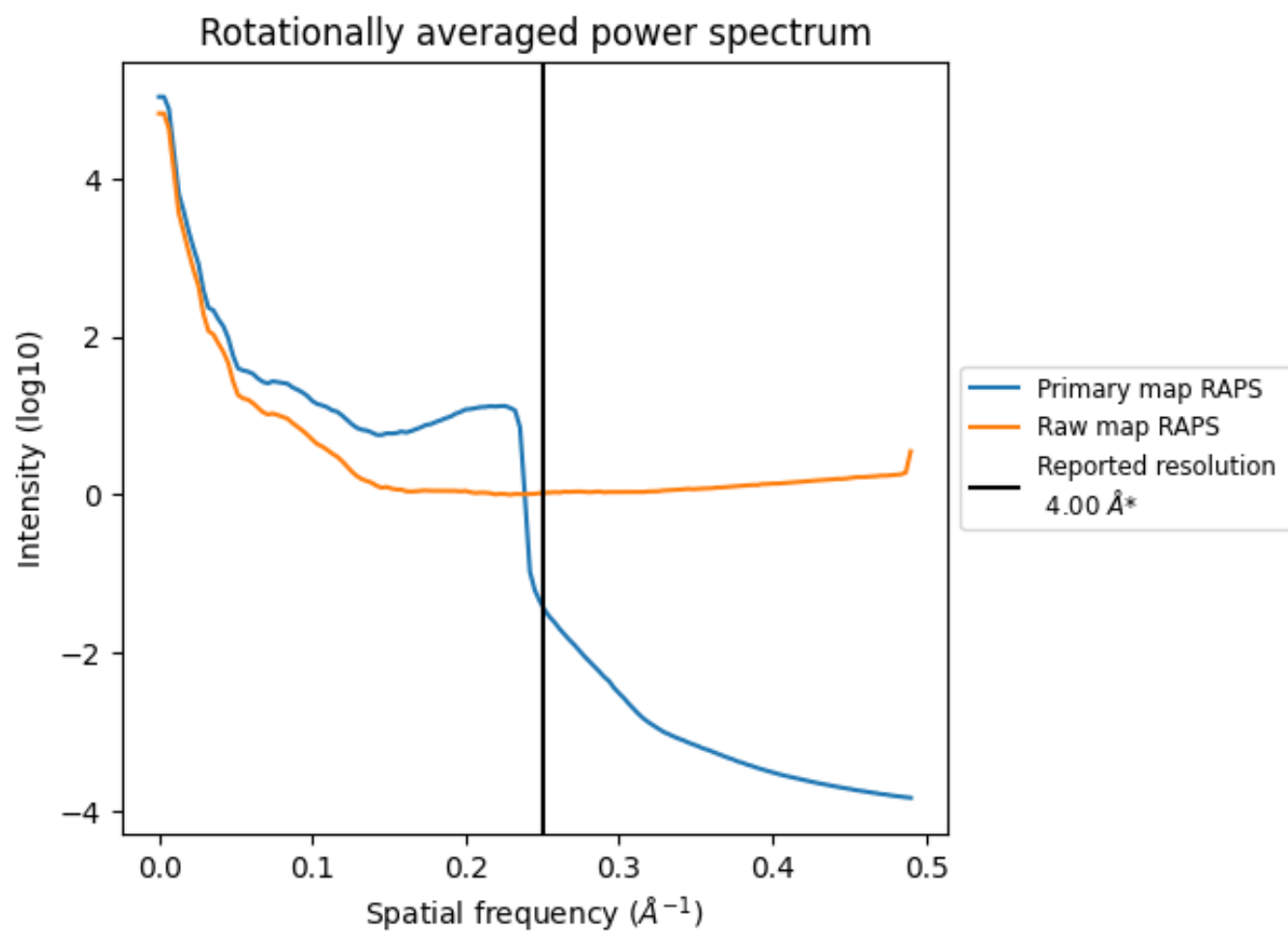
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 292 nm³; this corresponds to an approximate mass of 264 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

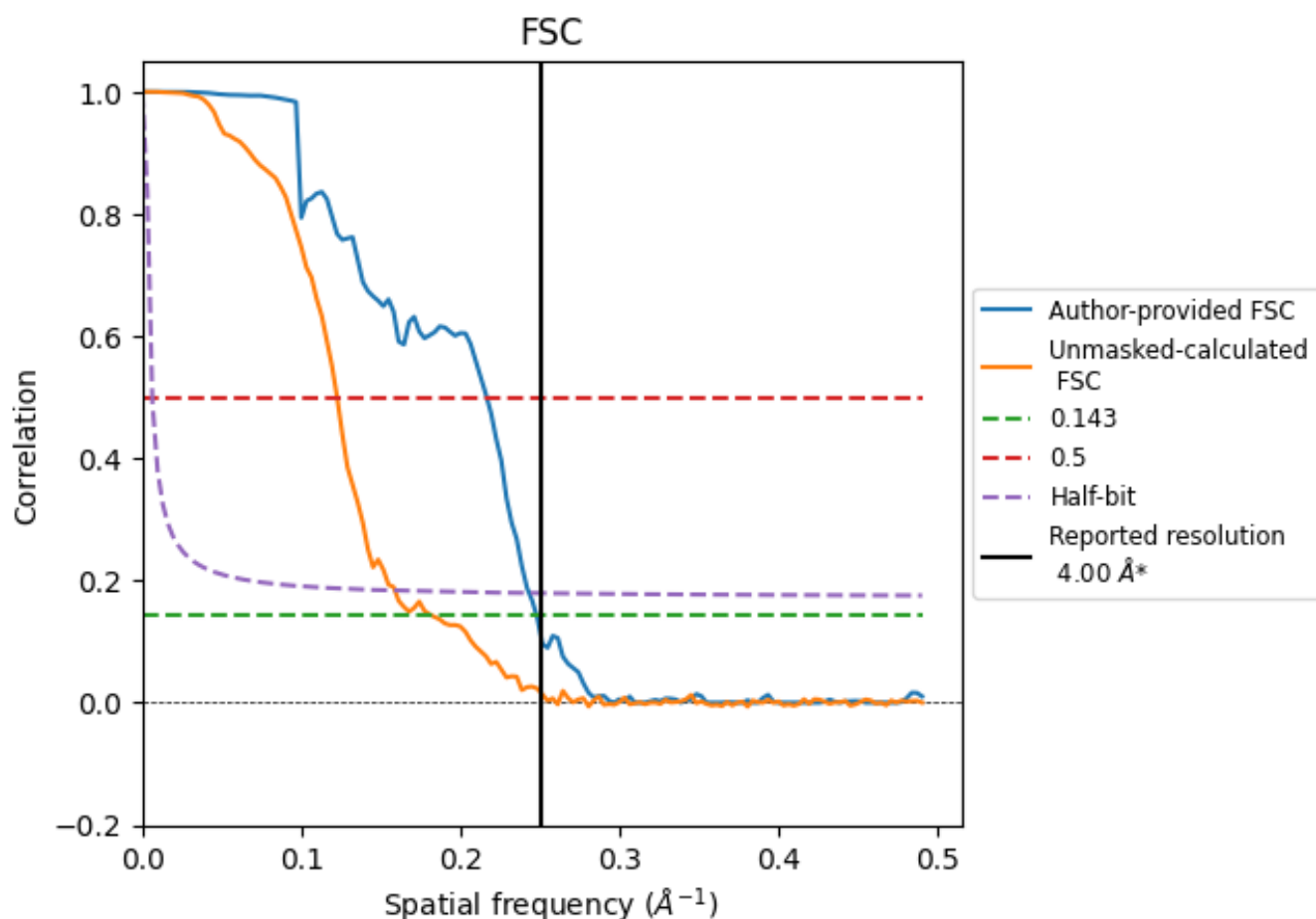


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

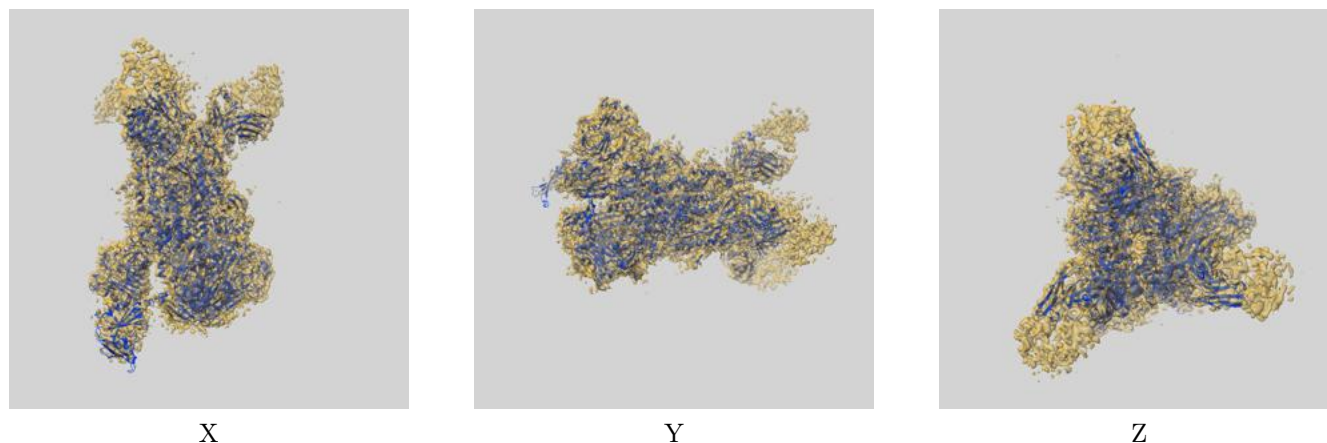
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.03	4.62	4.11
Unmasked-calculated*	5.50	8.16	6.29

*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 5.50 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

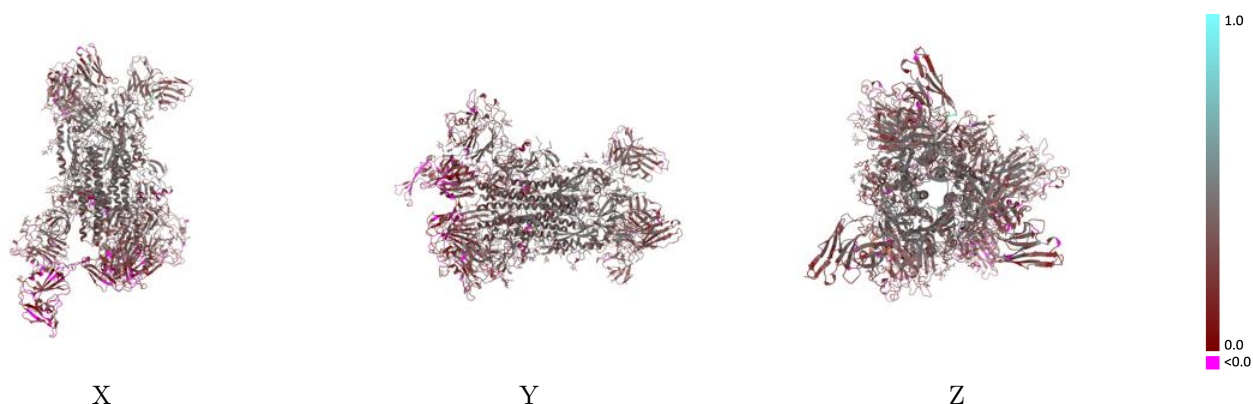
This section contains information regarding the fit between EMDB map EMD-8783 and PDB model 5W9H. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



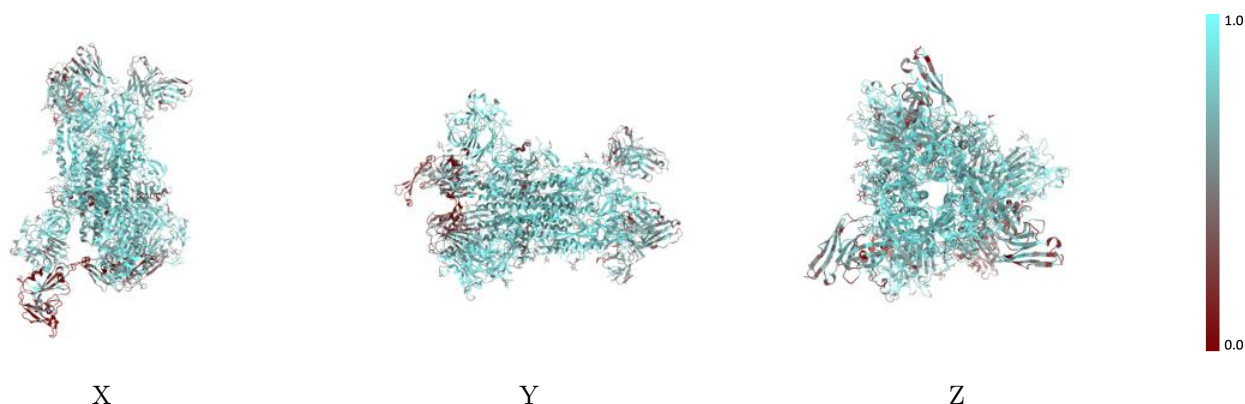
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



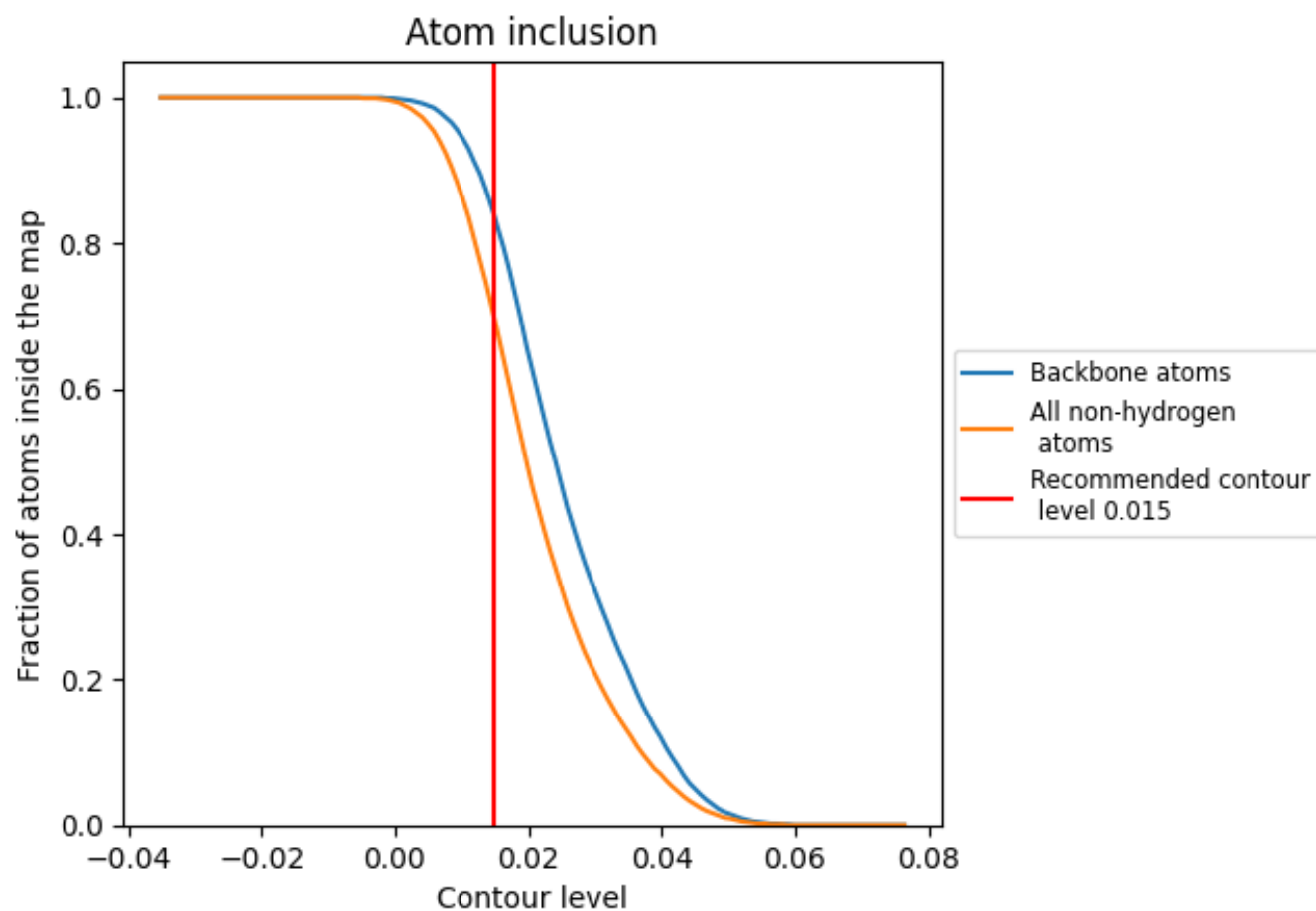
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 69% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6940	 0.3130
A	 0.7990	 0.3870
B	 0.6300	 0.3200
C	 0.5300	 0.2820
D	 0.8080	 0.3870
E	 0.6370	 0.3310
F	 0.5470	 0.2850
G	 0.7980	 0.3790
H	 0.6200	 0.3170
I	 0.5520	 0.2710
J	 0.4640	 0.3110
K	 0.7140	 0.3730
L	 0.5710	 0.3010
M	 0.6070	 0.2990
N	 0.3570	 0.2460
O	 0.5710	 0.2420
P	 0.7500	 0.3490
Q	 0.5360	 0.3550
R	 0.6070	 0.3820
S	 0.5710	 0.2480
T	 0.4290	 0.1470
U	 0.6070	 0.3000
V	 0.5000	 0.2430
W	 0.4640	 0.2440
X	 0.7500	 0.3550
Y	 0.2860	 0.2390
Z	 0.7500	 0.2740
a	 0.3210	 0.1890
b	 0.6070	 0.2630
c	 0.7140	 0.4330
d	 0.5360	 0.3250
p	 0.6420	 0.2620
q	 0.6510	 0.2670
r	 0.7030	 0.2870

