



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:26 AM UTC

PDB ID : 7WT8 / pdb_00007wt8
EMDB ID : EMD-32771
Title : SARS-CoV-2 Omicron variant spike in complex with Fab 9A8 (State 2)
Authors : Wang, X.; Wang, L.
Deposited on : 2022-02-04
Resolution : 3.60 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:

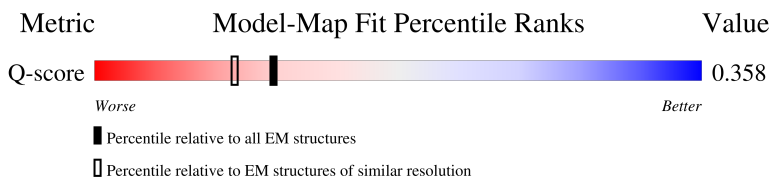
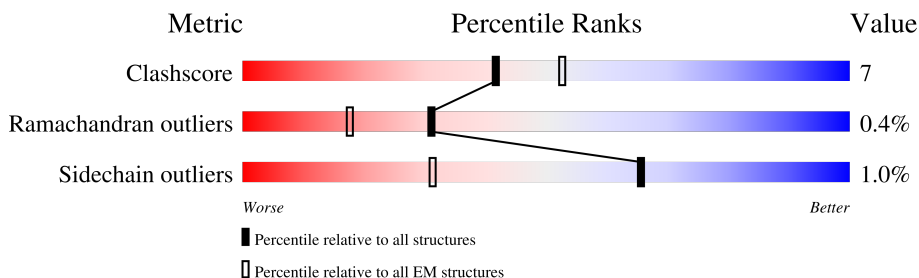
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	1270	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 74% 12% • 14%</p>
1	B	1270	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">• 70% 15% • 14%</p>
1	C	1270	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">9% 70% 16% • 14%</p>
2	D	107	<div style="display: flex; align-items: center;"> <div style="width: 75%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">75% 73% 27%</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	107	74% 77% 23%
3	H	122	66% 78% 22%
3	J	122	75% 73% 27%
4	E	2	50% 50% 50%
4	F	2	100%
4	G	2	100%
4	K	2	50% 50%
4	L	2	50% 50%
4	M	2	100%
4	N	2	50% 50% 50%
4	O	2	50% 50%
4	P	2	100%
4	Q	2	100%
4	R	2	50% 100%
4	S	2	50% 100%
4	T	2	100%
4	U	2	100%
4	V	2	100%
4	W	2	100%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 30240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1098	8632	5526	1438	1629	39	0	0
1	B	1098	8632	5526	1438	1629	39	0	0
1	C	1098	8632	5526	1438	1629	39	0	0

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	208	ILE	LEU	variant	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	212	PRO	-	insertion	UNP P0DTC2
A	213	GLU	-	insertion	UNP P0DTC2
A	336	ASP	GLY	variant	UNP P0DTC2
A	368	LEU	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	443	SER	GLY	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2
A	490	ARG	GLN	variant	UNP P0DTC2
A	493	SER	GLY	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	544	LYS	THR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	680	ALA	ARG	variant	UNP P0DTC2
A	682	ALA	ARG	variant	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	engineered mutation	UNP P0DTC2
A	853	LYS	ASN	variant	UNP P0DTC2
A	889	PRO	ALA	engineered mutation	UNP P0DTC2
A	896	PRO	ALA	engineered mutation	UNP P0DTC2
A	939	PRO	ALA	engineered mutation	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	978	PHE	LEU	variant	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	208	ILE	LEU	variant	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	212	PRO	-	insertion	UNP P0DTC2
B	213	GLU	-	insertion	UNP P0DTC2
B	336	ASP	GLY	variant	UNP P0DTC2
B	368	LEU	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	490	ARG	GLN	variant	UNP P0DTC2
B	493	SER	GLY	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	variant	UNP P0DTC2
B	544	LYS	THR	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	variant	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	680	ALA	ARG	variant	UNP P0DTC2
B	682	ALA	ARG	variant	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	814	PRO	PHE	engineered mutation	UNP P0DTC2
B	853	LYS	ASN	variant	UNP P0DTC2
B	889	PRO	ALA	engineered mutation	UNP P0DTC2
B	896	PRO	ALA	engineered mutation	UNP P0DTC2
B	939	PRO	ALA	engineered mutation	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	978	PHE	LEU	variant	UNP P0DTC2
B	983	PRO	LYS	engineered mutation	UNP P0DTC2
B	984	PRO	VAL	engineered mutation	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	208	ILE	LEU	variant	UNP P0DTC2
C	211	GLU	-	insertion	UNP P0DTC2
C	212	PRO	-	insertion	UNP P0DTC2
C	213	GLU	-	insertion	UNP P0DTC2
C	334	ASP	GLY	variant	UNP P0DTC2
C	366	LEU	SER	variant	UNP P0DTC2
C	368	PRO	SER	variant	UNP P0DTC2
C	370	PHE	SER	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	412	ASN	LYS	variant	UNP P0DTC2
C	435	LYS	ASN	variant	UNP P0DTC2
C	441	SER	GLY	variant	UNP P0DTC2
C	472	ASN	SER	variant	UNP P0DTC2
C	473	LYS	THR	variant	UNP P0DTC2
C	479	ALA	GLU	variant	UNP P0DTC2
C	488	ARG	GLN	variant	UNP P0DTC2
C	491	SER	GLY	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	TYR	ASN	variant	UNP P0DTC2
C	500	HIS	TYR	variant	UNP P0DTC2
C	542	LYS	THR	variant	UNP P0DTC2
C	609	GLY	ASP	variant	UNP P0DTC2
C	650	TYR	HIS	variant	UNP P0DTC2
C	674	LYS	ASN	variant	UNP P0DTC2
C	676	HIS	PRO	variant	UNP P0DTC2
C	678	ALA	ARG	variant	UNP P0DTC2
C	680	ALA	ARG	variant	UNP P0DTC2
C	759	LYS	ASN	variant	UNP P0DTC2
C	791	TYR	ASP	variant	UNP P0DTC2
C	812	PRO	PHE	engineered mutation	UNP P0DTC2
C	851	LYS	ASN	variant	UNP P0DTC2
C	887	PRO	ALA	engineered mutation	UNP P0DTC2
C	894	PRO	ALA	engineered mutation	UNP P0DTC2
C	937	PRO	ALA	engineered mutation	UNP P0DTC2
C	949	HIS	GLN	variant	UNP P0DTC2
C	964	LYS	ASN	variant	UNP P0DTC2
C	976	PHE	LEU	variant	UNP P0DTC2
C	981	PRO	LYS	engineered mutation	UNP P0DTC2
C	982	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called light chain of Fab 9A8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	107	Total	C	N	O	S	0	0
			831	520	137	171	3		
2	I	107	Total	C	N	O	S	0	0
			831	520	137	171	3		

- Molecule 3 is a protein called Heavy chain of Fab 9A8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	122	Total	C	N	O	S	0	0
			900	558	154	183	5		
3	J	122	Total	C	N	O	S	0	0
			900	558	154	183	5		

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



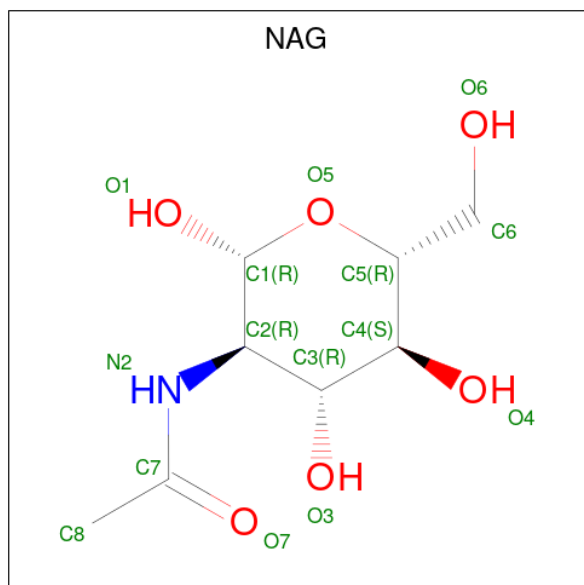
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	W	2	28	16	2	10	0	0

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



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

Continued on next page...

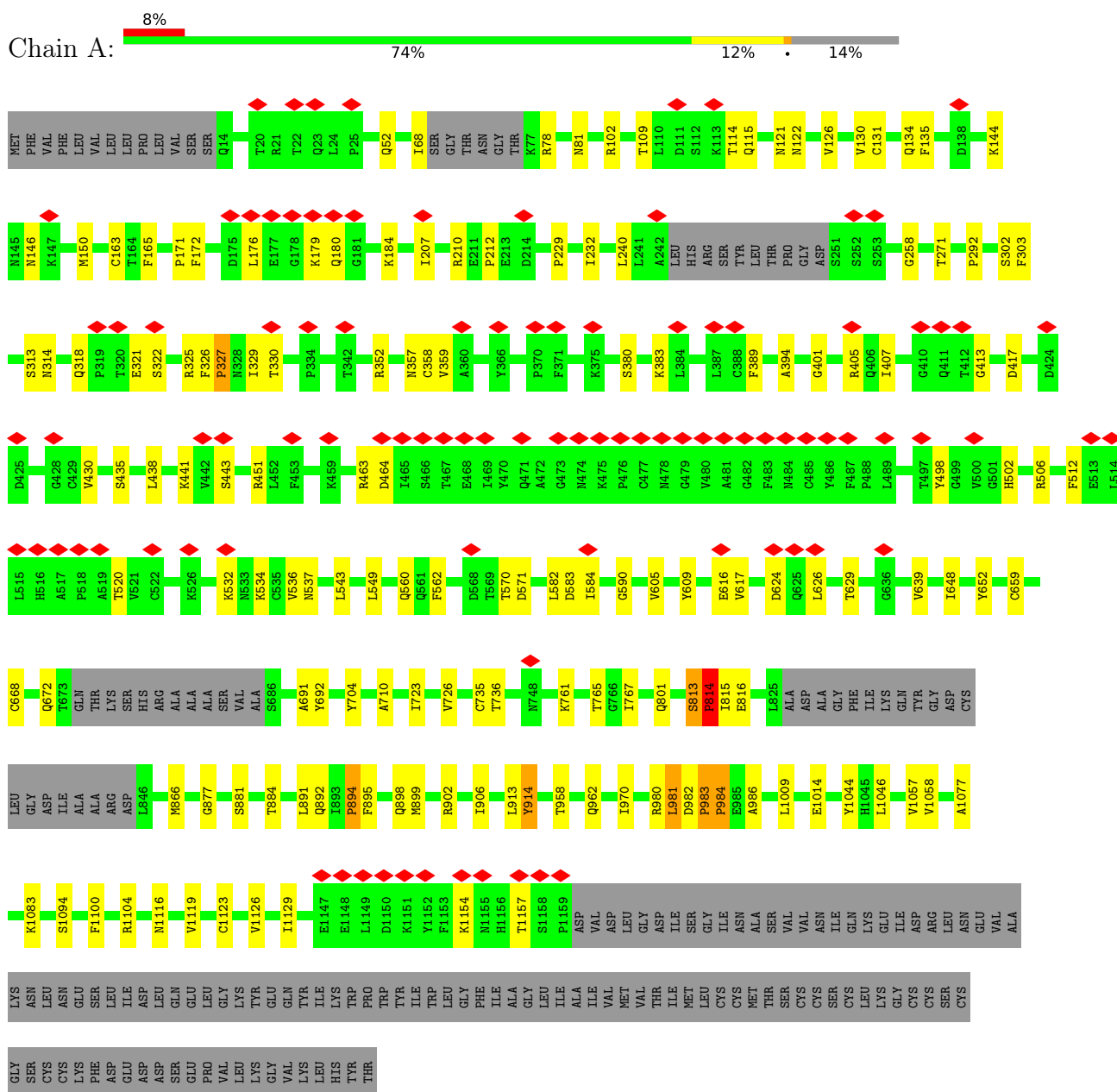
Continued from previous page...

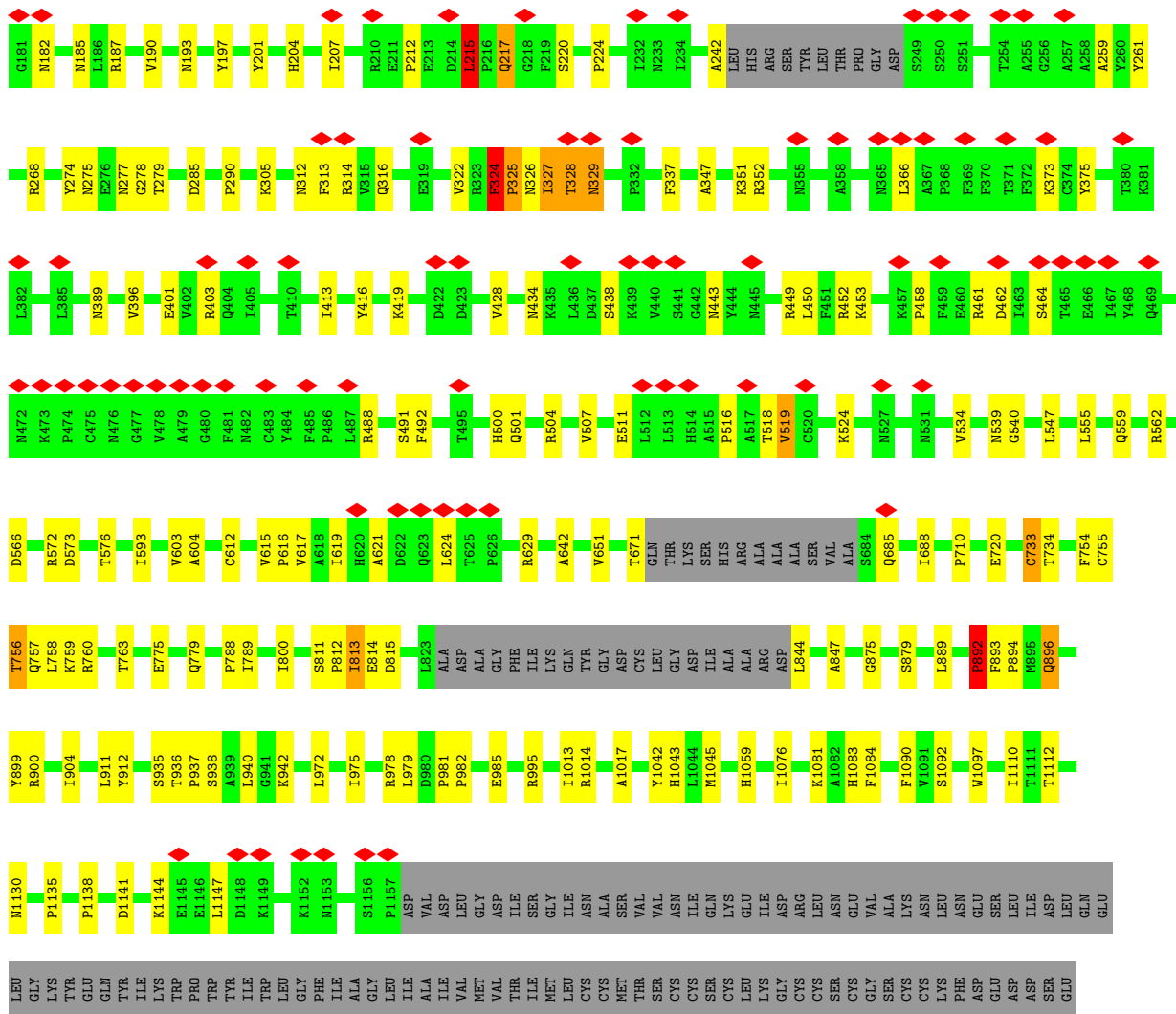
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C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

3 Residue-property plots [i](#)

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

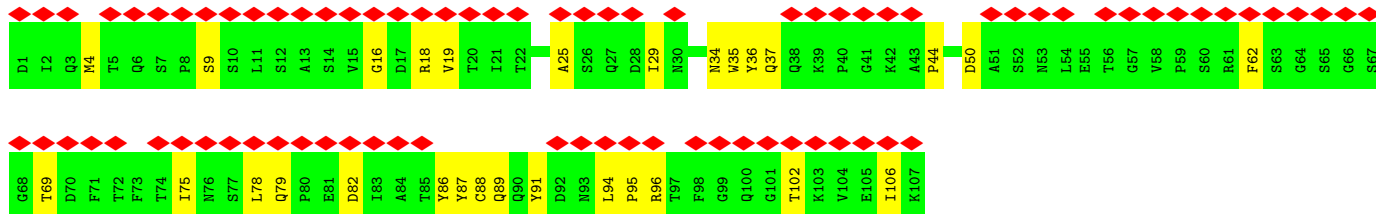
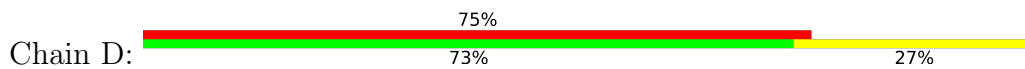
• Molecule 1: Spike glycoprotein



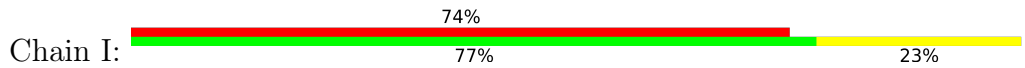


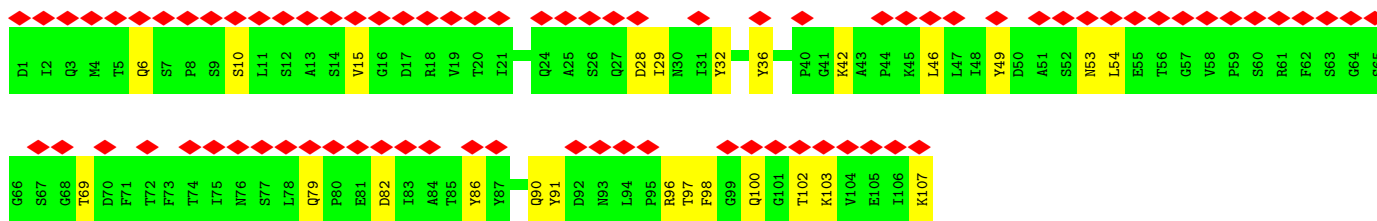
PRO VAL
 LEU LEU
 LYS LYS
 GLU VAL
 LYS LYS
 LEU LEU
 HIS HIS
 THR THR

• Molecule 2: light chain of Fab 9A8

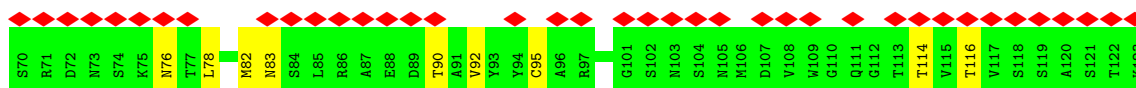
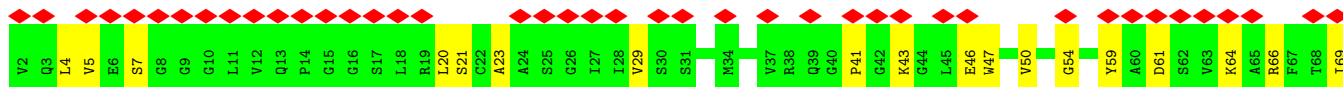
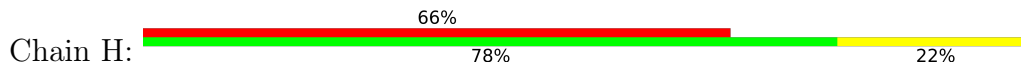


• Molecule 2: light chain of Fab 9A8

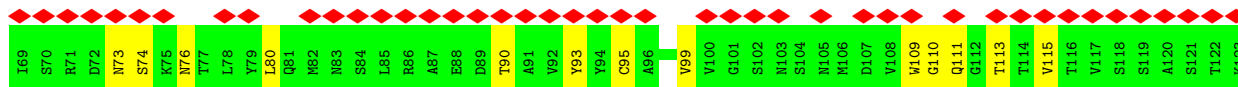
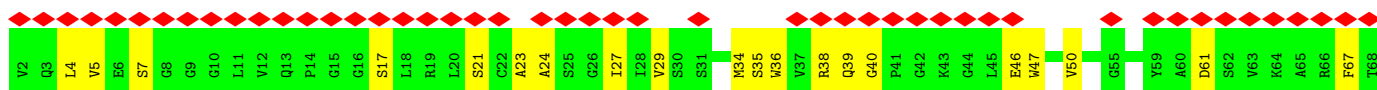
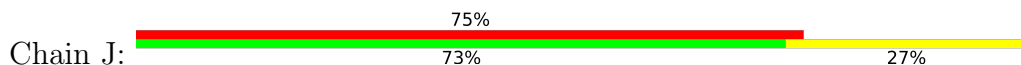




• Molecule 3: Heavy chain of Fab 9A8



• Molecule 3: Heavy chain of Fab 9A8



• 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 K:



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

Chain L:



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

Chain M:



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

Chain N:



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

Chain O:



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

Chain P:



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

Chain Q:  100%



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

Chain R:  50%
100%



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

Chain S:  50%
100%



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

Chain T:  100%



- 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:  100%



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

Chain W:  100%

3AK2
3AK3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	339195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.693	Depositor
Minimum map value	-2.049	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.42	Depositor
Map size (\AA)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	1/8842 (0.0%)	0.64	14/12033 (0.1%)
1	B	0.38	2/8842 (0.0%)	0.67	15/12033 (0.1%)
1	C	0.36	1/8842 (0.0%)	0.64	15/12033 (0.1%)
2	D	0.18	0/848	0.47	0/1151
2	I	0.20	0/848	0.52	0/1151
3	H	0.13	0/915	0.38	0/1243
3	J	0.14	0/915	0.41	0/1243
All	All	0.35	4/30052 (0.0%)	0.63	44/40887 (0.1%)

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	B	0	3
1	C	0	3
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	892	PRO	C-O	-5.76	1.16	1.23
1	B	1065	VAL	N-CA	5.08	1.49	1.45
1	A	813	SER	CA-CB	-5.07	1.47	1.54
1	B	894	PRO	C-O	-5.06	1.17	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	894	PRO	CA-C-O	-9.21	111.60	121.27
1	C	892	PRO	N-CA-CB	-9.08	95.10	103.27
1	C	763	THR	N-CA-C	-8.97	102.73	114.31
1	B	896	PRO	N-CA-C	-8.89	105.43	114.68
1	C	896	GLN	N-CA-C	-8.82	100.95	112.68
1	A	983	PRO	N-CA-C	8.07	120.54	110.70
1	C	981	PRO	N-CA-C	7.97	120.43	110.70
1	C	892	PRO	CA-C-O	-7.82	112.87	121.23
1	B	894	PRO	N-CA-CB	-7.60	95.27	103.25
1	C	814	GLU	N-CA-C	-7.40	103.20	111.71
1	A	765	THR	N-CA-C	-7.15	104.71	113.50
1	A	898	GLN	N-CA-C	-7.03	103.70	111.36
1	C	813	ILE	N-CA-C	-7.02	103.46	110.62
1	C	892	PRO	CB-CA-C	-6.90	102.95	111.64
1	B	983	PRO	N-CA-C	6.69	118.86	110.70
1	C	325	PRO	CB-CA-C	-6.58	101.28	111.22
1	A	894	PRO	CB-CA-C	-6.49	103.27	111.71
1	C	756	THR	N-CA-C	-6.46	104.24	111.28
1	B	409	PRO	CB-CA-C	-6.37	103.24	111.46
1	B	898	GLN	N-CA-C	-6.36	105.24	112.87
1	A	815	ILE	N-CA-C	-6.15	104.35	110.62
1	A	1123	CYS	CA-C-N	6.12	132.16	122.61
1	A	1123	CYS	C-N-CA	6.12	132.16	122.61
1	B	328	ASN	CB-CA-C	-6.09	102.08	111.83
1	B	809	PRO	CA-N-CD	-6.03	103.56	112.00
1	B	327	PRO	N-CA-C	5.98	120.38	111.41
1	A	986	ALA	N-CA-C	-5.91	104.84	111.28
1	B	1065	VAL	CA-C-O	-5.80	116.92	119.94
1	A	814	PRO	N-CA-CB	-5.59	97.05	103.15
1	B	816	GLU	N-CA-C	-5.58	105.29	111.71
1	A	984	PRO	CB-CA-C	-5.55	104.23	113.06
1	A	327	PRO	N-CA-C	5.49	119.92	111.57
1	C	733	CYS	CA-C-N	-5.45	112.42	120.38
1	C	733	CYS	C-N-CA	-5.45	112.42	120.38
1	B	814	PRO	N-CA-CB	-5.43	97.42	103.23
1	C	760	ARG	N-CA-C	-5.42	106.35	113.17
1	C	759	LYS	CB-CA-C	-5.36	100.37	110.01
1	B	803	LEU	CA-C-N	5.30	125.24	119.78
1	B	803	LEU	C-N-CA	5.30	125.24	119.78
1	B	328	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	914	TYR	CB-CA-C	5.13	119.41	110.68
1	C	733	CYS	CA-C-O	-5.11	115.64	120.90
1	A	895	PHE	CB-CA-C	-5.10	102.30	112.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	898	GLN	CB-CG-CD	-5.10	103.93	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	142	ASP	Peptide
1	B	521	VAL	Peptide
1	B	587	CYS	Peptide
1	C	142	ASP	Peptide
1	C	215	LEU	Peptide
1	C	324	PHE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8632	0	8443	101	0
1	B	8632	0	8442	130	0
1	C	8632	0	8442	132	0
2	D	831	0	801	20	0
2	I	831	0	801	16	0
3	H	900	0	865	16	0
3	J	900	0	865	22	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	1	0
4	M	28	0	25	0	0
4	N	28	0	25	1	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	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	0	0
5	A	126	0	117	0	0
5	B	154	0	142	0	0
5	C	154	0	143	0	0
All	All	30240	0	29461	405	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 7.

All (405) 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)
3:J:38:ARG:NH2	3:J:46:GLU:HG2	1.59	1.17
3:J:38:ARG:NH2	3:J:46:GLU:CG	2.29	0.96
1:A:441:LYS:HD3	1:A:443:SER:OG	1.68	0.94
3:J:38:ARG:HH21	3:J:46:GLU:HG2	1.31	0.91
1:C:324:PHE:CZ	1:C:540:GLY:CA	2.57	0.87
1:C:324:PHE:CZ	1:C:540:GLY:HA2	2.16	0.80
1:B:891:LEU:HD21	1:C:710:PRO:HD3	1.70	0.74
1:C:14:GLN:HG3	1:C:153:GLU:HG3	1.71	0.73
1:A:560:GLN:HE21	1:C:43:PHE:HA	1.55	0.72
1:A:130:VAL:HB	1:A:165:PHE:HB3	1.72	0.72
1:C:126:VAL:HG13	1:C:171:PRO:HA	1.73	0.71
1:A:109:THR:HG1	1:A:114:THR:HG1	1.37	0.71
1:A:914:TYR:HD2	1:B:1086:PHE:HE2	1.39	0.70
1:C:313:PHE:HB3	1:C:314:ARG:HG2	1.74	0.69
1:B:96:GLU:O	1:B:185:ASN:HB2	1.92	0.69
1:B:46:SER:HA	1:B:276:TYR:O	1.92	0.69
1:A:1126:VAL:HG21	1:C:912:TYR:HB3	1.75	0.68
2:I:49:TYR:HB2	2:I:53:ASN:HB3	1.76	0.68
1:B:799:PHE:HD2	1:B:802:ILE:HD11	1.58	0.67
1:B:737:MET:SD	1:C:312:ASN:ND2	2.68	0.67
1:C:978:ARG:HG3	1:C:979:LEU:HD12	1.77	0.67
1:C:982:PRO:O	1:C:985:GLU:HG3	1.94	0.66
3:J:5:VAL:HB	3:J:23:ALA:HB3	1.78	0.66
1:B:760:LEU:HD13	1:B:1001:LEU:HD22	1.78	0.65
1:B:970:ILE:HD12	1:B:980:ARG:HH21	1.62	0.65
1:A:532:LYS:HE2	1:A:534:LYS:HD3	1.78	0.65
1:A:326:PHE:HB3	1:A:327:PRO:HD2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:7:SER:HB2	3:H:21:SER:HB2	1.79	0.64
2:D:36:TYR:HB2	2:D:87:TYR:HB2	1.79	0.64
3:J:7:SER:HB2	3:J:21:SER:HB2	1.79	0.64
1:C:112:SER:HB3	1:C:134:GLN:HB2	1.79	0.64
1:A:52:GLN:HG3	1:A:271:THR:HG22	1.80	0.64
1:B:908:VAL:HG22	1:B:912:VAL:HG21	1.80	0.63
3:J:29:VAL:HA	3:J:34:MET:HE1	1.81	0.63
1:A:126:VAL:HG23	1:A:171:PRO:HA	1.79	0.63
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.79	0.63
1:A:292:PRO:HG3	1:A:629:THR:HG23	1.80	0.62
1:B:225:LEU:HG	1:B:226:VAL:HG23	1.81	0.62
1:C:443:ASN:HB3	1:C:492:PHE:HB2	1.82	0.62
1:C:129:LYS:NZ	1:C:163:CYS:SG	2.73	0.61
1:A:102:ARG:NH1	1:A:122:ASN:OD1	2.33	0.61
1:C:904:ILE:HD12	1:C:1042:TYR:HB3	1.82	0.60
1:B:99:ASN:O	1:B:102:ARG:NH2	2.34	0.60
1:C:337:PHE:HB3	1:C:366:LEU:HD22	1.84	0.60
1:C:97:LYS:HD3	1:C:179:LYS:HD3	1.83	0.60
1:C:324:PHE:CE2	1:C:540:GLY:HA2	2.36	0.60
1:B:914:TYR:HD2	1:C:1084:PHE:HE2	1.50	0.60
1:B:390:THR:HB	1:B:517:ALA:HB3	1.82	0.59
1:C:347:ALA:HA	1:C:461:ARG:HD3	1.83	0.59
1:B:108:THR:O	1:B:236:ARG:NH1	2.35	0.59
1:A:723:ILE:HG12	1:A:1058:VAL:HG22	1.83	0.59
1:A:914:TYR:HB3	1:B:1126:VAL:HG23	1.84	0.59
1:B:777:GLU:O	1:B:781:GLN:NE2	2.35	0.59
1:A:441:LYS:HD3	1:A:443:SER:HG	1.67	0.58
1:B:173:LEU:O	1:B:187:ARG:NH2	2.34	0.58
1:B:164:THR:O	1:C:352:ARG:NH2	2.37	0.58
2:I:10:SER:HA	2:I:103:LYS:HB2	1.86	0.58
3:H:29:VAL:HG21	3:H:76:ASN:HA	1.86	0.57
1:B:850:GLN:O	1:B:853:LYS:NZ	2.37	0.57
1:B:341:ALA:O	1:B:506:ARG:NH2	2.37	0.57
1:A:914:TYR:HD2	1:B:1086:PHE:CE2	2.20	0.57
1:C:64:TRP:HE1	1:C:259:ALA:HB1	1.70	0.57
1:C:34:ARG:NH2	1:C:220:SER:OG	2.38	0.57
1:C:775:GLU:O	1:C:779:GLN:NE2	2.37	0.57
1:C:127:VAL:HG12	1:C:168:VAL:HG22	1.85	0.57
2:D:78:LEU:HB3	2:D:106:ILE:HD12	1.86	0.57
1:C:593:ILE:HB	1:C:604:ALA:HB3	1.87	0.57
1:B:1140:PRO:HA	1:B:1143:ASP:HB2	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LYS:HG3	1:A:150:MET:H	1.70	0.56
1:C:103:GLY:HA3	1:C:120:VAL:HG12	1.88	0.56
1:C:1043:HIS:NE2	1:C:1045:MET:O	2.38	0.56
3:H:61:ASP:HA	3:H:64:LYS:HE2	1.89	0.55
2:I:6:GLN:H	2:I:100:GLN:HE22	1.52	0.55
1:C:324:PHE:CZ	1:C:540:GLY:HA3	2.42	0.55
1:C:401:GLU:HG2	1:C:413:ILE:HD13	1.88	0.55
1:A:380:SER:HB3	1:A:383:LYS:HD3	1.88	0.55
1:C:573:ASP:HB3	1:C:576:THR:O	2.07	0.55
3:H:4:LEU:HD11	3:H:95:CYS:HB2	1.89	0.55
1:A:1100:PHE:HZ	4:L:1:NAG:H62	1.72	0.55
1:B:641:GLN:NE2	1:B:642:THR:O	2.40	0.55
1:A:321:GLU:HG3	1:A:536:VAL:HG23	1.87	0.55
1:A:543:LEU:HD21	1:A:570:THR:HG21	1.88	0.55
1:B:984:PRO:O	1:B:988:VAL:HG23	2.07	0.55
1:C:187:ARG:HG3	1:C:204:HIS:HD2	1.72	0.55
1:C:534:VAL:HG21	1:C:547:LEU:HB2	1.89	0.55
2:I:86:TYR:O	2:I:102:THR:OG1	2.25	0.55
1:A:639:VAL:HG12	1:A:648:ILE:HG12	1.89	0.55
1:C:102:ARG:HG3	1:C:242:ALA:HB3	1.88	0.55
1:A:184:LYS:HD2	1:A:207:ILE:HA	1.89	0.54
1:A:314:ASN:HD21	1:A:590:GLY:H	1.55	0.54
1:B:81:ASN:O	1:B:238:GLN:NE2	2.41	0.54
1:B:658:GLU:O	1:B:692:TYR:OH	2.25	0.54
1:A:906:ILE:HD12	1:A:1044:TYR:HB3	1.87	0.54
1:A:980:ARG:NH1	1:B:514:LEU:HG	2.22	0.54
2:D:62:PHE:HZ	2:D:79:GLN:HE22	1.53	0.54
1:C:396:VAL:HG22	1:C:504:ARG:HG2	1.88	0.54
3:J:38:ARG:NH2	3:J:46:GLU:CD	2.66	0.54
1:A:982:ASP:N	1:B:380:SER:OG	2.39	0.54
1:B:499:GLY:O	1:B:503:GLN:NE2	2.38	0.54
1:B:602:SER:OG	1:B:603:ASN:N	2.40	0.54
1:C:268:ARG:NH2	1:C:285:ASP:OD2	2.41	0.54
1:C:671:THR:HG22	1:C:685:GLN:H	1.71	0.54
1:C:449:ARG:HH22	1:C:464:SER:H	1.55	0.54
1:A:435:SER:OG	1:A:506:ARG:NH1	2.41	0.54
1:A:672:GLN:OE1	1:A:692:TYR:OH	2.27	0.53
1:A:726:VAL:HG21	1:A:1057:VAL:HG23	1.90	0.53
1:C:975:ILE:HG23	1:C:979:LEU:HD13	1.90	0.53
1:B:343:ARG:NH2	1:B:447:ASN:OD1	2.42	0.53
1:B:1139:GLN:O	1:B:1143:ASP:N	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:MET:HB3	1:B:696:LEU:HD11	1.91	0.53
1:C:98:SER:HB3	1:C:179:LYS:H	1.73	0.53
1:C:110:LEU:HB3	1:C:135:PHE:HD2	1.74	0.53
1:C:1076:ILE:HD11	1:C:1130:ASN:HB3	1.90	0.53
1:B:519:ALA:O	1:B:520:THR:C	2.52	0.53
3:J:67:PHE:HB3	3:J:80:LEU:HD11	1.89	0.53
1:C:972:LEU:HD11	1:C:995:ARG:HH12	1.73	0.52
1:B:877:GLY:O	1:B:881:SER:OG	2.22	0.52
2:D:50:ASP:OD1	2:D:91:TYR:OH	2.26	0.52
1:C:733:CYS:O	1:C:734:THR:C	2.51	0.52
1:C:754:PHE:O	1:C:757:GLN:HG2	2.09	0.52
1:B:375:LYS:HZ3	1:B:408:ALA:HB2	1.74	0.52
1:C:1076:ILE:O	1:C:1083:HIS:N	2.40	0.52
1:C:1138:PRO:HA	1:C:1141:ASP:HB2	1.91	0.52
3:J:93:TYR:HE1	3:J:113:THR:HG22	1.75	0.52
1:A:549:LEU:HB3	1:A:582:LEU:HD21	1.92	0.51
1:B:358:CYS:HB2	1:B:521:VAL:HG23	1.91	0.51
1:B:620:ALA:HA	1:B:625:GLN:HG2	1.92	0.51
1:A:894:PRO:HA	1:B:704:TYR:HE1	1.75	0.51
1:B:327:PRO:HG3	1:B:576:PRO:HB3	1.90	0.51
3:H:69:ILE:HD11	3:H:78:LEU:HD21	1.93	0.51
1:B:390:THR:OG1	1:B:513:GLU:O	2.29	0.51
1:C:130:VAL:HB	1:C:165:PHE:HB3	1.93	0.51
1:C:179:LYS:NZ	1:C:182:ASN:O	2.44	0.51
3:H:66:ARG:HG3	3:H:83:ASN:H	1.75	0.51
1:B:895:PHE:N	1:B:896:PRO:HD2	2.26	0.50
1:C:322:VAL:HG11	1:C:524:LYS:HE3	1.92	0.50
1:A:616:GLU:HG2	1:A:617:VAL:HG23	1.93	0.50
1:B:719:VAL:HG22	1:B:1062:VAL:HG22	1.93	0.50
2:I:79:GLN:NE2	2:I:82:ASP:OD2	2.43	0.50
1:C:624:LEU:O	1:C:629:ARG:NH2	2.44	0.50
1:B:884:THR:HG21	1:B:891:LEU:HD22	1.94	0.50
1:C:325:PRO:O	1:C:326:ASN:C	2.55	0.50
1:A:813:SER:H	1:A:816:GLU:HB2	1.76	0.50
1:C:434:ASN:OD1	1:C:501:GLN:NE2	2.45	0.50
3:H:92:VAL:HB	3:H:114:THR:HA	1.92	0.50
1:A:68:ILE:HB	1:A:78:ARG:HB3	1.94	0.50
1:B:809:PRO:HD2	1:B:810:SER:H	1.76	0.49
2:D:18:ARG:NH1	2:D:19:VAL:O	2.44	0.49
2:D:35:TRP:HB3	2:D:37:GLN:HE22	1.77	0.49
1:A:229:PRO:HG3	1:B:354:ARG:HH21	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLN:NE2	1:A:624:ASP:OD2	2.45	0.49
1:B:1142:LEU:HA	1:B:1145:PHE:HB3	1.94	0.49
2:D:36:TYR:HB3	2:D:44:PRO:HB3	1.93	0.49
1:C:518:THR:HG23	1:C:519:VAL:HG23	1.94	0.49
1:C:539:ASN:OD1	1:C:559:GLN:NE2	2.45	0.49
1:B:144:LYS:HB2	1:B:150:MET:HB2	1.94	0.49
1:B:336:ASP:N	1:B:336:ASP:OD1	2.46	0.49
1:C:275:ASN:OD1	1:C:279:THR:N	2.38	0.49
3:H:5:VAL:HB	3:H:23:ALA:HB3	1.95	0.49
1:B:1083:LYS:HA	1:B:1122:ASN:HA	1.94	0.49
1:A:329:ILE:HG13	1:A:330:THR:H	1.77	0.48
1:A:1077:ALA:HB3	1:A:1129:ILE:HG12	1.95	0.48
1:C:720:GLU:OE2	1:C:1059:HIS:NE2	2.39	0.48
1:B:406:GLN:HE21	1:B:413:GLY:HA3	1.79	0.48
2:I:98:PHE:HE2	3:J:47:TRP:HB2	1.77	0.48
1:C:615:VAL:O	1:C:619:ILE:N	2.46	0.48
2:I:36:TYR:OH	2:I:96:ARG:NH2	2.45	0.48
2:I:42:LYS:NZ	3:J:111:GLN:OE1	2.45	0.48
1:C:562:ARG:NH1	1:C:566:ASP:OD1	2.44	0.48
1:C:875:GLY:O	1:C:879:SER:OG	2.27	0.48
1:C:316:GLN:NE2	1:C:617:VAL:O	2.46	0.48
1:B:296:THR:HG22	1:B:305:VAL:HG11	1.95	0.48
2:D:79:GLN:NE2	2:D:82:ASP:OD2	2.44	0.48
3:J:24:ALA:HB3	3:J:76:ASN:HB3	1.96	0.48
1:A:302:SER:OG	1:A:303:PHE:N	2.47	0.48
1:B:352:ARG:NH1	1:B:393:TYR:OH	2.46	0.48
1:B:376:CYS:HA	1:B:429:CYS:HB3	1.95	0.48
1:C:117:LEU:HD13	1:C:130:VAL:HG22	1.96	0.48
1:B:897:MET:C	1:B:899:MET:N	2.70	0.48
1:A:902:ARG:NH1	1:A:1046:LEU:O	2.43	0.48
2:D:29:ILE:H	2:D:69:THR:HB	1.79	0.48
1:B:454:ARG:NH2	1:B:464:ASP:OD2	2.47	0.47
1:B:471:GLN:NE2	1:B:475:LYS:O	2.47	0.47
1:C:193:ASN:HA	1:C:197:TYR:O	2.13	0.47
1:C:1144:LYS:HD3	1:C:1147:LEU:HD12	1.96	0.47
1:A:313:SER:OG	1:A:314:ASN:N	2.47	0.47
1:A:314:ASN:ND2	1:A:590:GLY:O	2.47	0.47
1:C:450:LEU:HD13	1:C:488:ARG:HD3	1.95	0.47
2:D:36:TYR:OH	2:D:96:ARG:NH2	2.48	0.47
1:A:914:TYR:CD2	1:B:1086:PHE:HE2	2.27	0.47
1:A:877:GLY:O	1:A:881:SER:OG	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:GLN:HE22	1:B:416:ALA:H	1.63	0.47
1:B:518:PRO:O	1:B:519:ALA:HB3	2.13	0.47
1:B:1142:LEU:O	1:B:1146:LYS:N	2.42	0.47
1:C:108:THR:HB	1:C:114:THR:HG21	1.97	0.47
1:C:327:ILE:O	1:C:328:THR:C	2.57	0.47
3:H:47:TRP:HZ2	3:H:50:VAL:HB	1.80	0.47
1:A:210:ARG:HB2	1:A:212:PRO:HD2	1.97	0.47
1:A:583:ASP:OD2	1:A:584:ILE:N	2.48	0.47
1:A:1104:ARG:HH21	1:C:899:TYR:HE2	1.62	0.47
1:C:324:PHE:HZ	1:C:540:GLY:CA	2.19	0.47
1:C:651:VAL:HG21	1:C:688:ILE:HD12	1.97	0.47
1:B:307:LYS:HG3	1:B:597:PRO:HA	1.95	0.47
1:B:1145:PHE:O	1:B:1149:LEU:N	2.44	0.47
1:C:438:SER:OG	1:C:492:PHE:O	2.31	0.47
1:C:844:LEU:HD12	1:C:847:ALA:HB3	1.97	0.47
1:A:704:TYR:HE1	1:C:892:PRO:HA	1.79	0.46
1:A:438:LEU:HB2	1:A:506:ARG:HH12	1.79	0.46
1:C:612:CYS:HA	1:C:615:VAL:HG13	1.97	0.46
1:A:866:MET:HE1	1:B:666:GLY:HA3	1.96	0.46
1:B:894:PRO:HB3	1:B:896:PRO:HD2	1.96	0.46
1:C:44:ARG:HB2	1:C:274:TYR:HD2	1.80	0.46
1:B:42:VAL:HG11	1:C:562:ARG:HD2	1.98	0.46
1:C:324:PHE:CZ	1:C:540:GLY:N	2.82	0.46
1:C:896:GLN:HE21	1:C:900:ARG:HE	1.63	0.46
1:A:144:LYS:HD2	1:A:144:LYS:HA	1.70	0.46
1:A:1014:GLU:OE2	1:C:1014:ARG:NH2	2.48	0.46
2:I:29:ILE:HG22	2:I:69:THR:HA	1.97	0.46
1:A:210:ARG:HH21	1:A:212:PRO:HG2	1.81	0.46
1:B:96:GLU:OE2	1:B:98:SER:OG	2.33	0.46
1:C:1076:ILE:HG23	1:C:1083:HIS:HB2	1.98	0.46
1:A:131:CYS:HA	1:A:163:CYS:HB2	1.97	0.46
1:B:125:ASN:HA	1:B:171:PRO:HD3	1.98	0.46
1:B:292:PRO:HB2	1:B:605:VAL:HG21	1.97	0.46
1:A:407:ILE:HG12	1:A:430:VAL:HG11	1.97	0.45
1:B:68:ILE:HD13	1:B:259:ALA:HB2	1.98	0.45
1:B:130:VAL:HB	1:B:165:PHE:HB3	1.99	0.45
1:B:744:THR:O	1:B:747:SER:OG	2.33	0.45
1:B:855:LEU:HD21	1:B:959:LEU:HD23	1.97	0.45
1:A:983:PRO:N	1:A:984:PRO:HD2	2.31	0.45
1:B:415:ILE:HA	1:B:419:ASN:HD22	1.81	0.45
1:C:190:VAL:HG12	1:C:201:TYR:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1144:LYS:HA	1:C:1147:LEU:HB2	1.96	0.45
3:H:20:LEU:HD23	3:H:82:MET:HE1	1.98	0.45
1:A:451:ARG:NH2	1:A:464:ASP:O	2.38	0.45
1:A:352:ARG:HH22	1:A:394:ALA:H	1.65	0.45
1:A:401:GLY:O	1:A:405:ARG:NH1	2.47	0.45
1:A:571:ASP:HB2	1:A:584:ILE:HG13	1.98	0.45
1:C:351:LYS:HD2	1:C:351:LYS:HA	1.69	0.45
1:C:419:LYS:HG2	1:C:458:PRO:HG3	1.98	0.45
1:C:1090:PHE:HE1	1:C:1110:ILE:HD12	1.81	0.45
2:D:34:ASN:HB2	2:D:89:GLN:HE21	1.82	0.45
1:A:413:GLY:H	1:A:417:ASP:HB2	1.80	0.45
1:A:652:TYR:HA	1:A:691:ALA:HB3	1.99	0.45
3:J:27:ILE:O	3:J:76:ASN:ND2	2.47	0.45
1:B:663:ILE:HB	1:B:667:ILE:HB	1.97	0.45
1:B:1079:CYS:HB2	1:B:1123:CYS:HB3	1.78	0.45
1:C:141:LEU:HB3	1:C:242:ALA:HB2	1.99	0.45
1:C:491:SER:O	1:C:500:HIS:NE2	2.50	0.45
1:B:145:ASN:O	1:B:146:ASN:C	2.59	0.45
1:B:375:LYS:NZ	1:B:408:ALA:HB2	2.31	0.45
1:C:290:PRO:HB2	1:C:603:VAL:HG21	1.98	0.45
3:J:61:ASP:N	3:J:61:ASP:OD1	2.50	0.45
3:J:39:GLN:NE2	3:J:40:GLY:O	2.49	0.45
1:B:327:PRO:HA	1:B:577:GLN:HG2	1.98	0.45
1:C:539:ASN:ND2	1:C:572:ARG:O	2.45	0.45
3:J:4:LEU:HD13	3:J:110:GLY:HA3	1.99	0.45
1:A:144:LYS:HE2	1:A:150:MET:HB2	1.99	0.44
1:C:1081:LYS:HE3	1:C:1081:LYS:HB2	1.78	0.44
1:A:176:LEU:O	1:A:179:LYS:NZ	2.50	0.44
1:B:799:PHE:CD2	1:B:802:ILE:HD11	2.46	0.44
1:C:936:THR:HA	1:C:937:PRO:HD3	1.85	0.44
1:A:358:CYS:SG	1:A:359:VAL:N	2.88	0.44
1:B:552:SER:HB2	1:B:583:ASP:HB2	1.99	0.44
1:B:595:ILE:HB	1:B:606:ALA:HB3	1.99	0.44
1:C:328:THR:O	1:C:329:ASN:HB2	2.16	0.44
1:C:1013:ILE:O	1:C:1017:ALA:N	2.48	0.44
1:A:441:LYS:CD	1:A:443:SER:OG	2.54	0.44
1:A:389:PHE:CG	1:A:512:PHE:HB3	2.53	0.44
1:A:710:ALA:HB3	1:C:889:LEU:HB3	2.00	0.44
1:A:913:LEU:O	1:A:914:TYR:C	2.59	0.44
1:C:416:TYR:OH	3:H:54:GLY:N	2.50	0.44
2:I:15:VAL:HG22	2:I:107:LYS:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:913:LEU:O	1:B:914:TYR:C	2.61	0.44
1:A:1154:LYS:O	1:A:1157:THR:OG1	2.32	0.43
1:B:439:ASP:OD1	1:B:506:ARG:NH1	2.51	0.43
1:B:642:THR:HG21	1:B:667:ILE:HG13	1.99	0.43
1:B:802:ILE:HG22	1:B:1051:GLN:HE21	1.83	0.43
1:C:217:GLN:HE21	1:C:217:GLN:HB2	1.60	0.43
1:C:275:ASN:HD21	1:C:277:ASN:HB2	1.82	0.43
1:C:978:ARG:HG3	1:C:979:LEU:N	2.32	0.43
1:A:801:GLN:O	1:A:814:PRO:HD2	2.19	0.43
1:B:67:VAL:O	1:B:259:ALA:HA	2.18	0.43
1:C:942:LYS:HE2	1:C:942:LYS:HB3	1.81	0.43
2:D:4:MET:SD	2:D:4:MET:N	2.92	0.43
1:B:789:PRO:HA	1:B:790:PRO:HD3	1.89	0.43
1:C:275:ASN:OD1	1:C:278:GLY:N	2.48	0.43
1:A:121:ASN:HD21	1:A:172:PHE:HB2	1.83	0.43
2:D:16:GLY:H	2:D:78:LEU:HG	1.84	0.43
1:B:816:GLU:OE2	1:B:1052:SER:HB3	2.18	0.43
1:C:911:LEU:HD12	1:C:911:LEU:HA	1.84	0.43
1:A:352:ARG:HB2	1:A:463:ARG:HH22	1.83	0.43
1:A:380:SER:HB2	1:B:452:LEU:HD12	2.01	0.43
1:A:498:TYR:HB3	1:A:502:HIS:HB2	2.00	0.43
1:B:1094:SER:HB3	1:B:1099:TRP:CD2	2.53	0.43
1:A:357:ASN:H	1:A:520:THR:HG22	1.84	0.43
1:A:543:LEU:HD12	1:A:543:LEU:HA	1.86	0.43
1:A:970:ILE:HD12	1:A:981:LEU:HD11	2.00	0.43
1:B:134:GLN:HB3	1:B:158:SER:H	1.83	0.43
1:B:543:LEU:HD11	1:B:570:THR:HG21	2.00	0.43
1:B:895:PHE:N	1:B:896:PRO:CD	2.82	0.43
1:B:99:ASN:ND2	1:B:175:ASP:H	2.16	0.43
1:C:44:ARG:HH11	1:C:274:TYR:HE2	1.67	0.43
2:D:94:LEU:HA	2:D:95:PRO:HA	1.82	0.43
1:B:441:LYS:HB3	1:B:445:ASN:HB2	2.01	0.43
1:B:673:THR:HG22	1:B:687:GLN:HG3	2.00	0.43
1:B:613:ASN:OD1	1:B:614:CYS:N	2.50	0.42
1:B:859:PRO:HG3	1:C:642:ALA:HA	2.00	0.42
1:B:1143:ASP:O	1:B:1147:GLU:N	2.50	0.42
1:C:35:GLY:HA3	1:C:56:LEU:HB3	2.01	0.42
2:I:32:TYR:HB3	2:I:91:TYR:CE2	2.54	0.42
1:A:81:ASN:OD1	1:A:81:ASN:N	2.51	0.42
1:A:609:TYR:HE2	1:A:648:ILE:HD12	1.83	0.42
1:B:519:ALA:O	1:B:521:VAL:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:LYS:NZ	1:B:788:THR:O	2.47	0.42
1:C:305:LYS:HE3	1:C:305:LYS:HB2	1.91	0.42
1:C:616:PRO:HA	1:C:619:ILE:HB	2.00	0.42
1:A:891:LEU:HD13	1:B:712:PRO:HD3	2.01	0.42
1:B:411:GLN:HE21	1:B:411:GLN:HB2	1.58	0.42
1:B:898:GLN:OE1	1:B:902:ARG:NH1	2.53	0.42
1:B:947:ASP:HA	1:B:950:ASN:HB2	2.00	0.42
1:C:452:ARG:NE	1:C:462:ASP:OD2	2.39	0.42
1:C:1112:THR:H	1:C:1135:PRO:HD3	1.84	0.42
1:B:131:CYS:HB3	1:B:133:PHE:CE1	2.54	0.42
1:B:193:ASN:HB2	1:B:234:ILE:HD12	2.01	0.42
1:C:621:ALA:HB1	1:C:629:ARG:HE	1.85	0.42
3:J:73:ASN:OD1	3:J:74:SER:N	2.53	0.42
1:A:134:GLN:NE2	1:A:135:PHE:O	2.52	0.42
1:A:767:ILE:HD11	1:A:1009:LEU:HD23	2.01	0.42
1:B:787:LYS:HZ1	1:B:790:PRO:HG3	1.84	0.42
1:C:169:SER:OG	1:C:170:GLN:N	2.52	0.42
3:J:36:TRP:NE1	3:J:95:CYS:SG	2.91	0.42
1:A:180:GLN:HG3	1:A:258:GLY:HA2	2.01	0.42
1:C:389:ASN:HB3	1:C:511:GLU:HB3	2.01	0.42
1:C:428:VAL:HG12	1:C:507:VAL:HA	2.01	0.42
1:B:811:LYS:HD3	1:B:811:LYS:HA	1.80	0.42
1:C:453:LYS:HE2	1:C:453:LYS:HB2	1.84	0.42
1:C:755:CYS:O	1:C:756:THR:C	2.60	0.42
2:I:28:ASP:HA	2:I:69:THR:HB	2.02	0.42
2:I:90:GLN:NE2	2:I:97:THR:OG1	2.38	0.42
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.89	0.42
1:B:385:ASN:OD1	1:B:385:ASN:N	2.51	0.42
1:C:201:TYR:CG	1:C:224:PRO:HA	2.54	0.42
2:D:19:VAL:HG21	2:D:75:ILE:HG13	2.02	0.42
1:A:1094:SER:O	1:A:1094:SER:OG	2.38	0.42
1:B:722:GLU:OE1	1:B:1061:HIS:NE2	2.49	0.42
1:C:44:ARG:HB2	1:C:274:TYR:CD2	2.55	0.42
1:C:555:LEU:HD23	1:C:555:LEU:HA	1.90	0.42
2:D:35:TRP:NE1	2:D:88:CYS:SG	2.93	0.42
3:J:90:THR:HA	3:J:115:VAL:O	2.20	0.42
1:B:122:ASN:HB2	1:B:127:VAL:HG23	2.02	0.41
1:B:1146:LYS:HD2	1:B:1149:LEU:HD23	2.02	0.41
1:C:893:PHE:N	1:C:894:PRO:HD2	2.34	0.41
2:D:86:TYR:O	2:D:102:THR:OG1	2.36	0.41
3:H:61:ASP:OD1	3:H:61:ASP:N	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:THR:O	1:A:962:GLN:HG2	2.20	0.41
1:B:914:TYR:O	1:B:915:GLU:C	2.61	0.41
1:A:115:GLN:HG2	1:A:232:ILE:HG21	2.02	0.41
1:A:624:ASP:HB3	1:A:626:LEU:HD23	2.01	0.41
1:A:1116:ASN:OD1	1:A:1116:ASN:N	2.54	0.41
1:B:341:ALA:HB3	1:B:344:PHE:HE1	1.85	0.41
1:C:93:ALA:HB3	1:C:261:TYR:HB2	2.02	0.41
2:I:46:LEU:HD11	3:J:99:VAL:HG12	2.02	0.41
1:A:1083:LYS:HD3	1:A:1119:VAL:HG21	2.01	0.41
2:D:9:SER:HA	2:D:102:THR:HG22	2.01	0.41
2:I:46:LEU:HG	3:J:109:TRP:HE1	1.85	0.41
1:B:617:VAL:HG23	1:B:618:PRO:HD3	2.01	0.41
1:B:1136:ASP:OD2	1:B:1139:GLN:HG2	2.20	0.41
3:H:59:TYR:HE2	3:H:64:LYS:HA	1.85	0.41
1:A:102:ARG:HH11	1:A:122:ASN:HA	1.86	0.41
1:A:560:GLN:NE2	1:C:43:PHE:HA	2.31	0.41
1:B:982:ASP:HB2	1:B:983:PRO:HD2	2.01	0.41
1:C:40:ASP:OD2	1:C:44:ARG:NH2	2.45	0.41
1:C:373:LYS:HE3	1:C:375:TYR:HE2	1.86	0.41
1:C:403:ARG:HH22	2:D:94:LEU:HB2	1.85	0.41
1:C:812:PRO:O	1:C:815:ASP:N	2.54	0.41
1:C:1092:SER:HB3	1:C:1097:TRP:CD2	2.56	0.41
1:C:1141:ASP:HA	1:C:1144:LYS:HB2	2.03	0.41
1:A:543:LEU:HD22	1:A:562:PHE:CE1	2.56	0.41
1:B:46:SER:CA	1:B:276:TYR:O	2.66	0.41
1:B:534:LYS:HE3	1:B:534:LYS:HB2	1.91	0.41
1:C:96:GLU:O	1:C:185:ASN:HB2	2.20	0.41
3:H:46:GLU:OE2	3:H:47:TRP:N	2.54	0.41
2:I:53:ASN:OD1	2:I:54:LEU:N	2.54	0.41
1:A:659:CYS:HB2	1:A:668:CYS:HB3	1.56	0.40
1:B:84:LEU:HA	1:B:85:PRO:HD3	1.96	0.40
1:B:423:PRO:HD2	1:B:426:PHE:HB2	2.02	0.40
1:B:755:SER:O	1:B:755:SER:OG	2.34	0.40
1:B:914:TYR:HD2	1:C:1084:PHE:CE2	2.34	0.40
1:B:1113:THR:HB	1:B:1137:PRO:HG3	2.02	0.40
1:C:788:PRO:HG2	1:C:789:ILE:HD12	2.02	0.40
1:A:322:SER:HA	1:A:537:ASN:HB3	2.02	0.40
1:A:735:CYS:SG	1:A:736:THR:N	2.94	0.40
1:B:141:LEU:HD13	1:B:141:LEU:HA	1.91	0.40
2:D:4:MET:HA	2:D:25:ALA:HA	2.02	0.40
3:H:90:THR:HA	3:H:116:THR:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:THR:O	1:B:331:ASN:HB2	2.21	0.40
1:B:368:LEU:HD13	4:N:1:NAG:H3	2.02	0.40
1:C:516:PRO:HG2	1:C:518:THR:HG22	2.02	0.40
1:C:935:SER:O	1:C:936:THR:C	2.65	0.40
1:A:292:PRO:HB2	1:A:605:VAL:HG21	2.03	0.40
3:J:35:SER:HB3	3:J:50:VAL:HG23	2.02	0.40
1:A:146:ASN:OD1	1:A:146:ASN:N	2.53	0.40
1:B:170:GLN:NE2	1:B:171:PRO:O	2.51	0.40
3:H:41:PRO:O	3:H:43:LYS:NZ	2.55	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	1088/1270 (86%)	991 (91%)	97 (9%)	0	100	100
1	B	1088/1270 (86%)	1012 (93%)	69 (6%)	7 (1%)	21	54
1	C	1088/1270 (86%)	1011 (93%)	71 (6%)	6 (1%)	21	54
2	D	105/107 (98%)	93 (89%)	12 (11%)	0	100	100
2	I	105/107 (98%)	91 (87%)	14 (13%)	0	100	100
3	H	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
3	J	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
All	All	3714/4268 (87%)	3418 (92%)	283 (8%)	13 (0%)	31	61

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	ASN
1	B	520	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	894	PRO
1	C	215	LEU
1	B	143	HIS
1	B	540	PHE
1	C	212	PRO
1	C	328	THR
1	C	329	ASN
1	B	331	ASN
1	B	914	TYR
1	C	207	ILE
1	C	519	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	967/1113 (87%)	960 (99%)	7 (1%)	76	78
1	B	967/1113 (87%)	955 (99%)	12 (1%)	63	73
1	C	967/1113 (87%)	954 (99%)	13 (1%)	61	72
2	D	94/94 (100%)	94 (100%)	0	100	100
2	I	94/94 (100%)	94 (100%)	0	100	100
3	H	98/100 (98%)	98 (100%)	0	100	100
3	J	98/100 (98%)	97 (99%)	1 (1%)	68	75
All	All	3285/3727 (88%)	3252 (99%)	33 (1%)	65	75

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	ARG
1	A	761	LYS
1	A	814	PRO
1	A	884	THR
1	A	892	GLN
1	A	899	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	981	LEU
1	B	141	LEU
1	B	151	GLU
1	B	411	GLN
1	B	425	ASP
1	B	759	GLN
1	B	813	SER
1	B	884	THR
1	B	894	PRO
1	B	936	SER
1	B	942	LEU
1	B	987	GLU
1	B	1069	GLU
1	C	141	LEU
1	C	151	GLU
1	C	215	LEU
1	C	217	GLN
1	C	324	PHE
1	C	327	ILE
1	C	758	LEU
1	C	800	ILE
1	C	811	SER
1	C	813	ILE
1	C	892	PRO
1	C	938	SER
1	C	940	LEU
3	J	17	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	121	ASN
1	A	238	GLN
1	A	625	GLN
1	A	850	GLN
1	A	1002	GLN
1	B	134	GLN
1	B	367	ASN
1	B	406	GLN
1	B	411	GLN
1	B	414	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	553	ASN
1	B	560	GLN
1	B	577	GLN
1	B	801	GLN
1	B	952	ASN
1	B	1008	GLN
1	B	1033	GLN
1	B	1051	GLN
1	C	134	GLN
1	C	143	HIS
1	C	217	GLN
1	C	799	GLN
1	C	896	GLN
1	C	930	GLN
1	C	948	ASN
1	C	1120	ASN
2	D	37	GLN
2	D	53	ASN
3	H	103	ASN
3	J	32	ASN
3	J	39	GLN
3	J	81	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](#)

32 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	E	1	1,4	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
4	NAG	E	2	4	14,14,15	0.33	0	17,19,21	0.50	0
4	NAG	F	1	1,4	14,14,15	0.37	0	17,19,21	0.59	0
4	NAG	F	2	4	14,14,15	0.41	0	17,19,21	0.53	0
4	NAG	G	1	1,4	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	G	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	K	1	1,4	14,14,15	0.59	0	17,19,21	1.41	1 (5%)
4	NAG	K	2	4	14,14,15	0.43	0	17,19,21	0.44	0
4	NAG	L	1	1,4	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	L	2	4	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	M	1	1,4	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	M	2	4	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	N	1	1,4	14,14,15	0.19	0	17,19,21	0.46	0
4	NAG	N	2	4	14,14,15	0.37	0	17,19,21	0.54	0
4	NAG	O	1	1,4	14,14,15	0.30	0	17,19,21	0.84	1 (5%)
4	NAG	O	2	4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	P	1	1,4	14,14,15	0.34	0	17,19,21	0.52	0
4	NAG	P	2	4	14,14,15	0.29	0	17,19,21	0.44	0
4	NAG	Q	1	1,4	14,14,15	0.17	0	17,19,21	0.48	0
4	NAG	Q	2	4	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	R	1	1,4	14,14,15	0.25	0	17,19,21	0.50	0
4	NAG	R	2	4	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	S	1	1,4	14,14,15	0.32	0	17,19,21	0.46	0
4	NAG	S	2	4	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	T	1	1,4	14,14,15	0.27	0	17,19,21	0.57	0
4	NAG	T	2	4	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	U	1	1,4	14,14,15	0.32	0	17,19,21	0.49	0
4	NAG	U	2	4	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	V	1	1,4	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	V	2	4	14,14,15	0.23	0	17,19,21	0.47	0
4	NAG	W	1	1,4	14,14,15	0.25	0	17,19,21	0.50	0
4	NAG	W	2	4	14,14,15	0.28	0	17,19,21	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1	NAG	C1-O5-C5	5.39	119.42	112.19
4	O	1	NAG	C2-N2-C7	2.57	126.35	122.90
4	E	1	NAG	C2-N2-C7	2.51	126.27	122.90

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	W	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	S	2	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	O	1	NAG	C1-C2-N2-C7
4	E	1	NAG	C3-C2-N2-C7
4	T	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

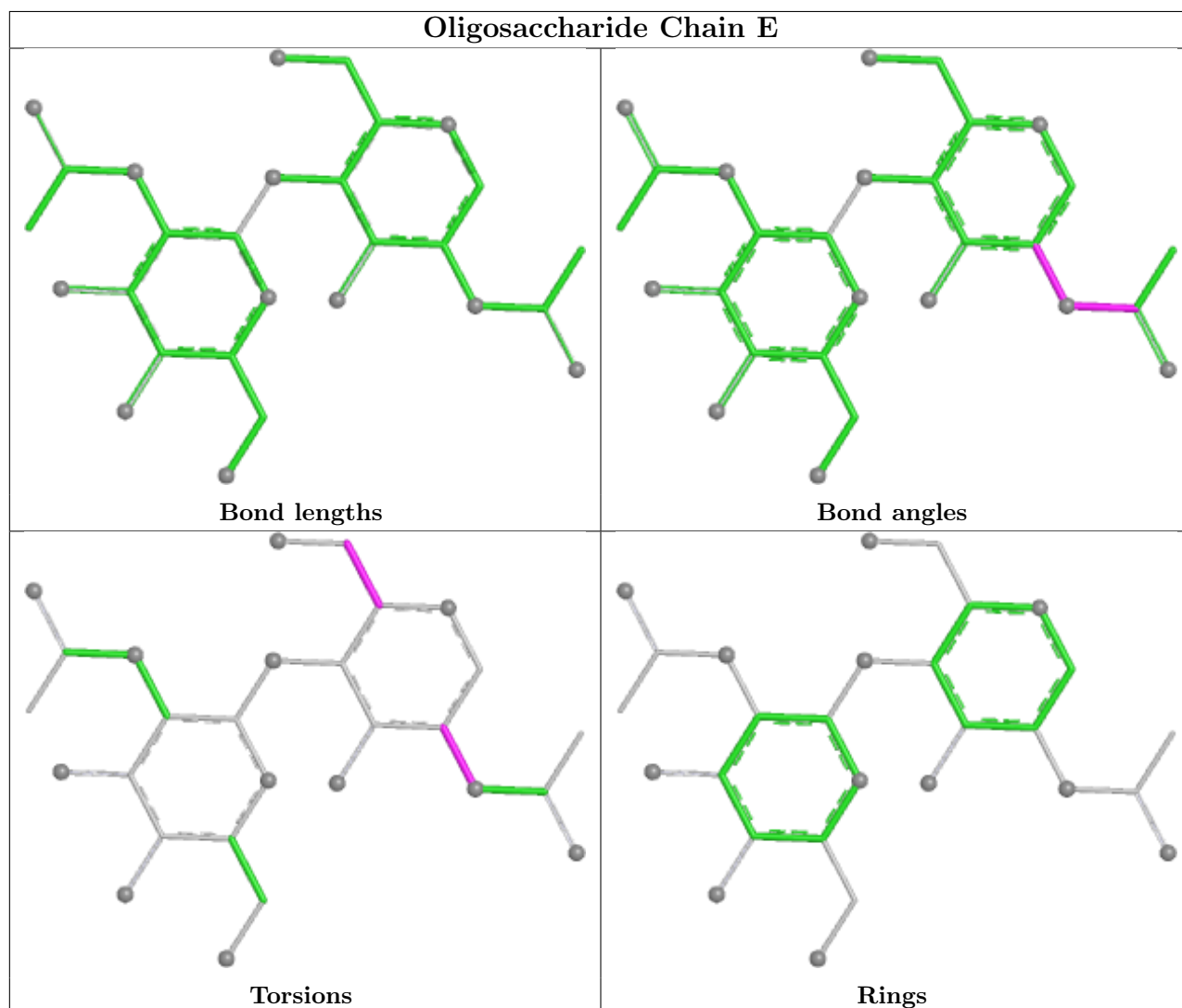
Mol	Chain	Res	Type	Atoms
4	O	1	NAG	C3-C2-N2-C7
4	V	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6

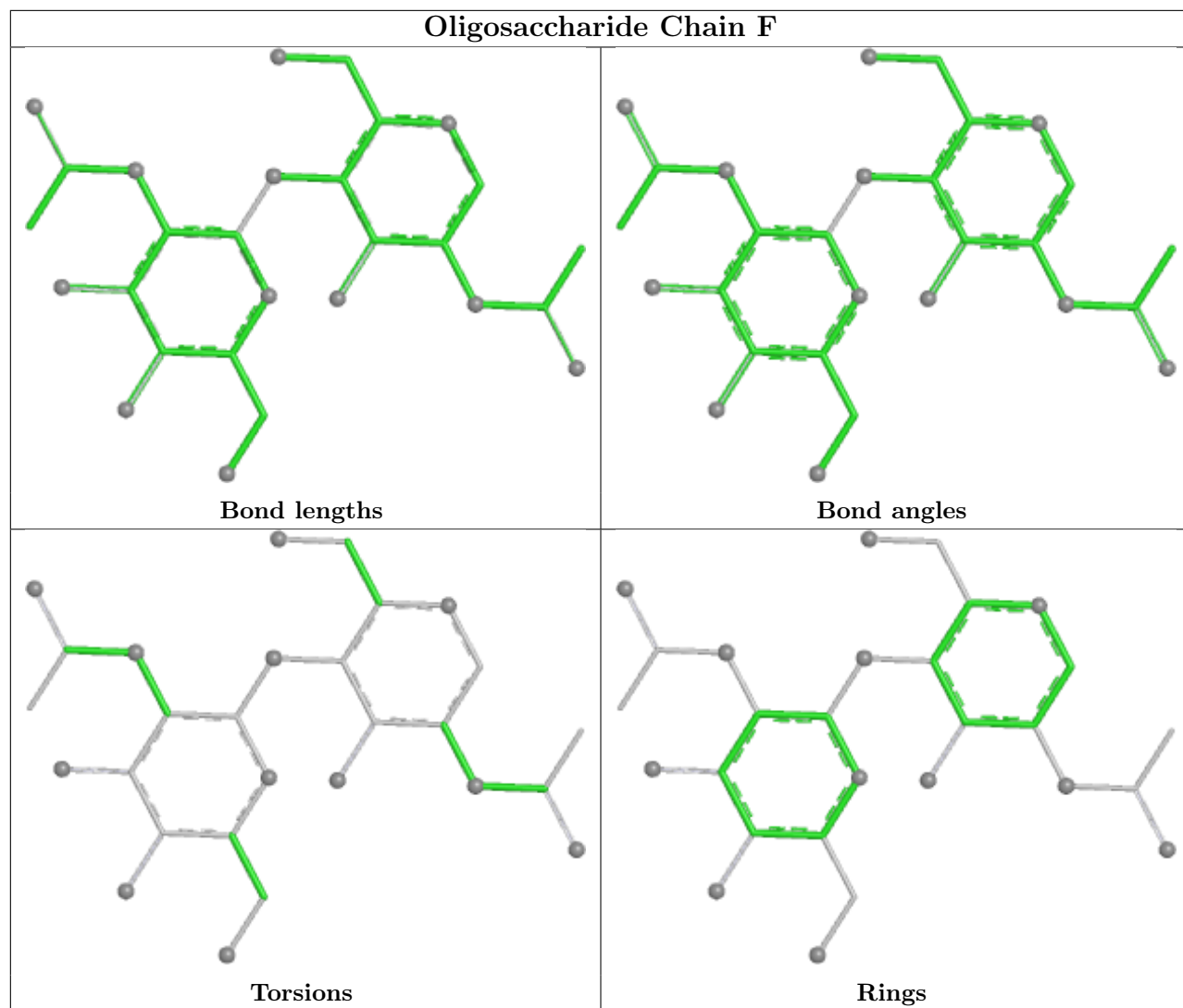
There are no ring outliers.

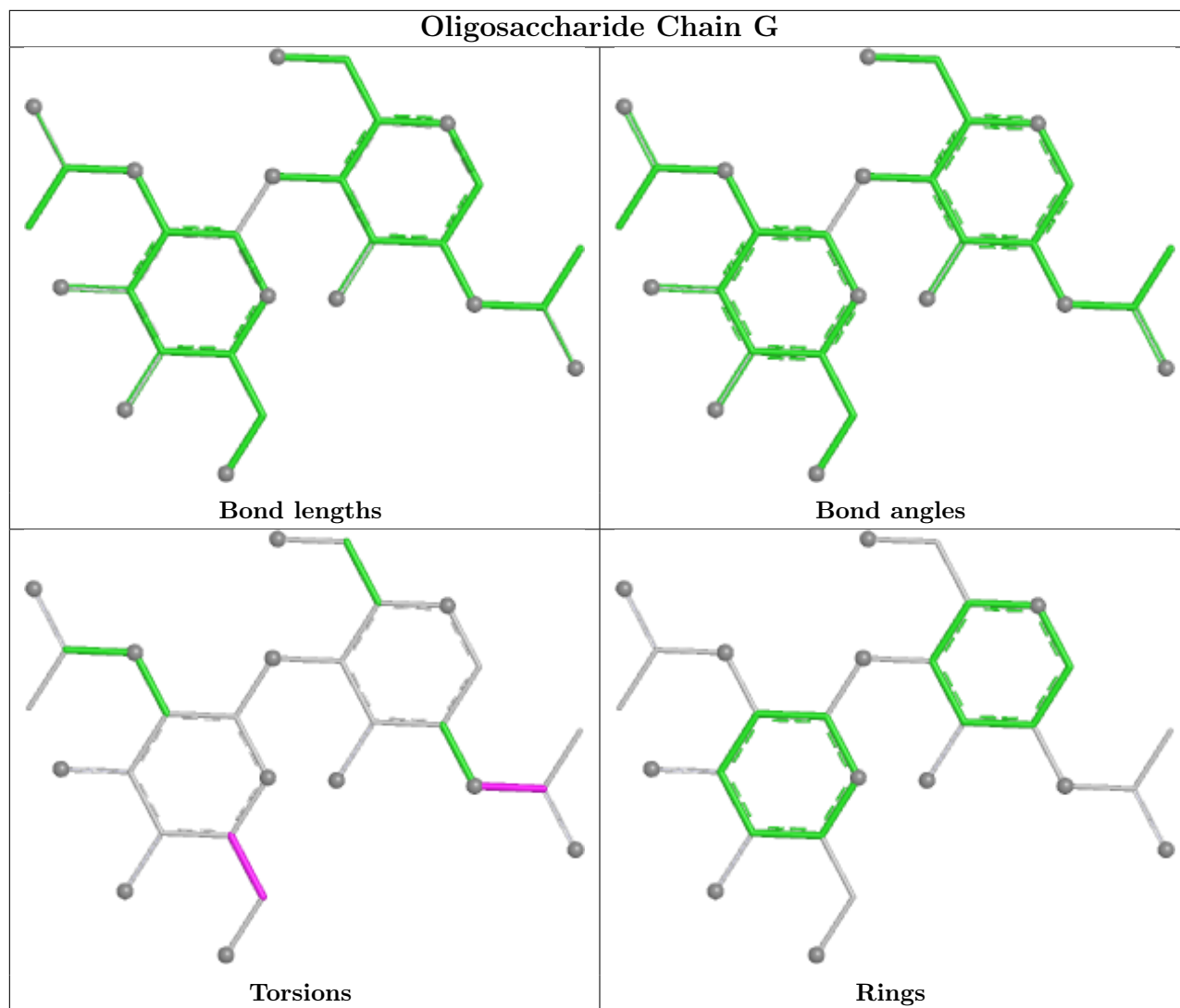
2 monomers are involved in 2 short contacts:

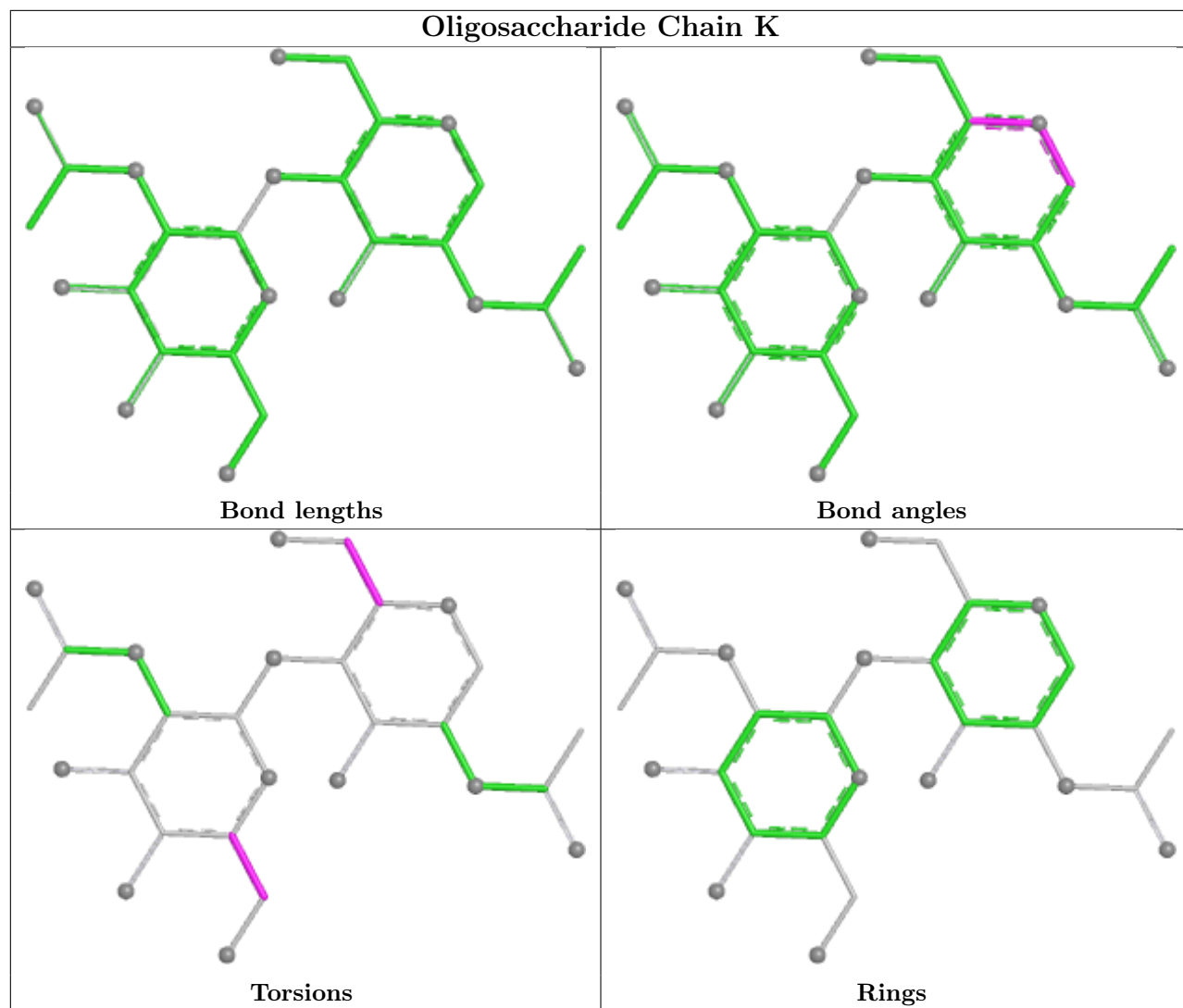
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1	NAG	1	0
4	N	1	NAG	1	0

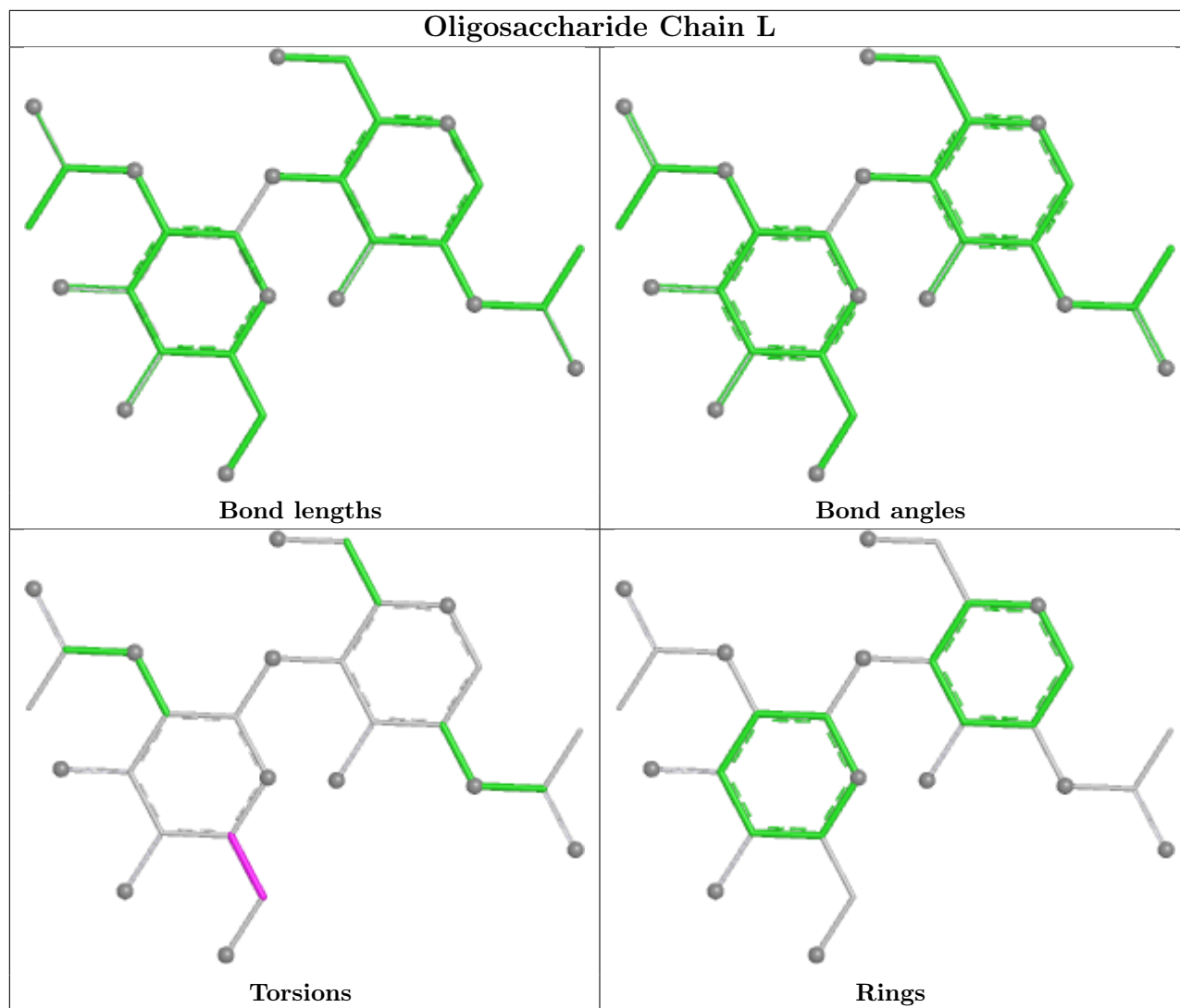
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

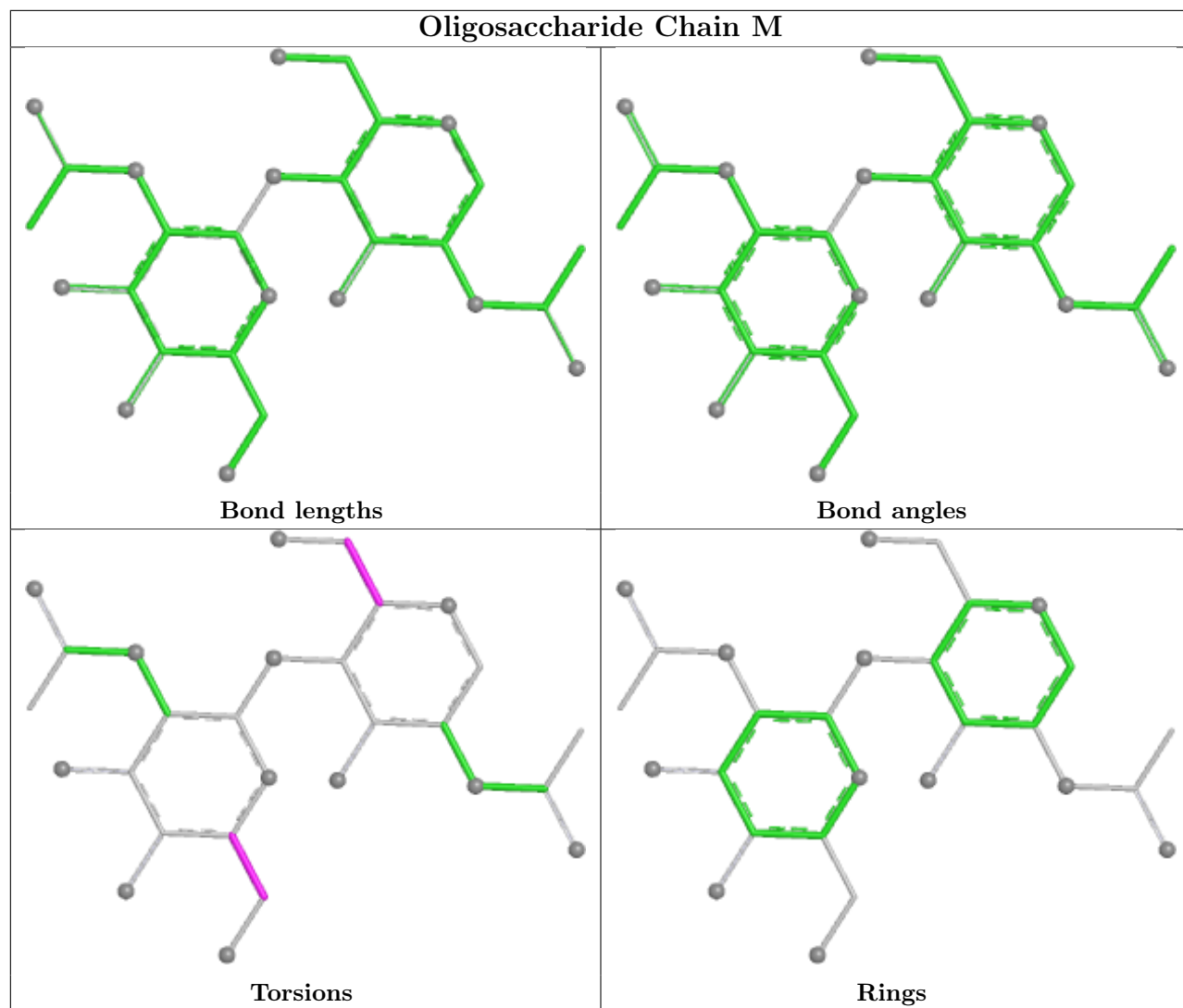


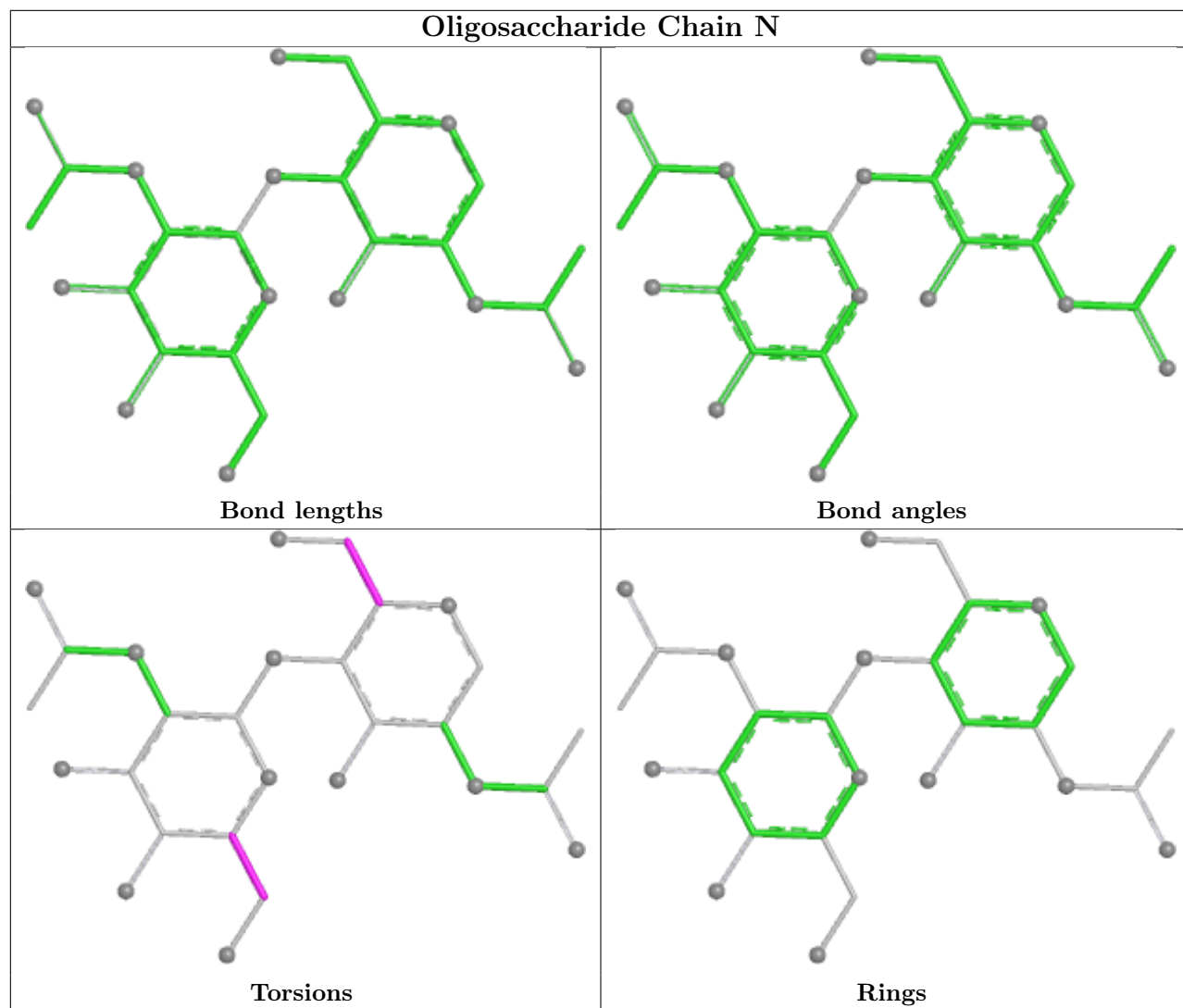


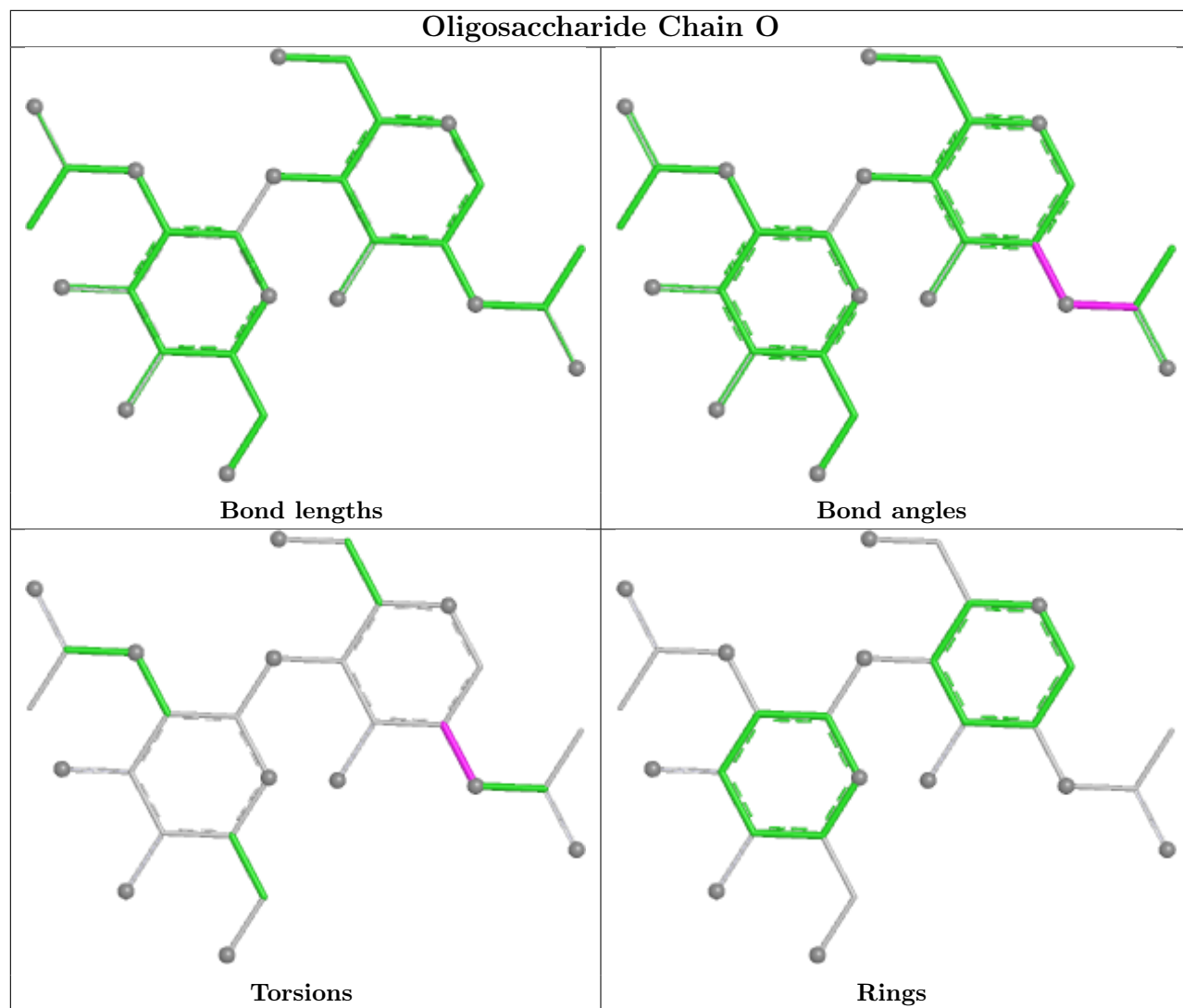


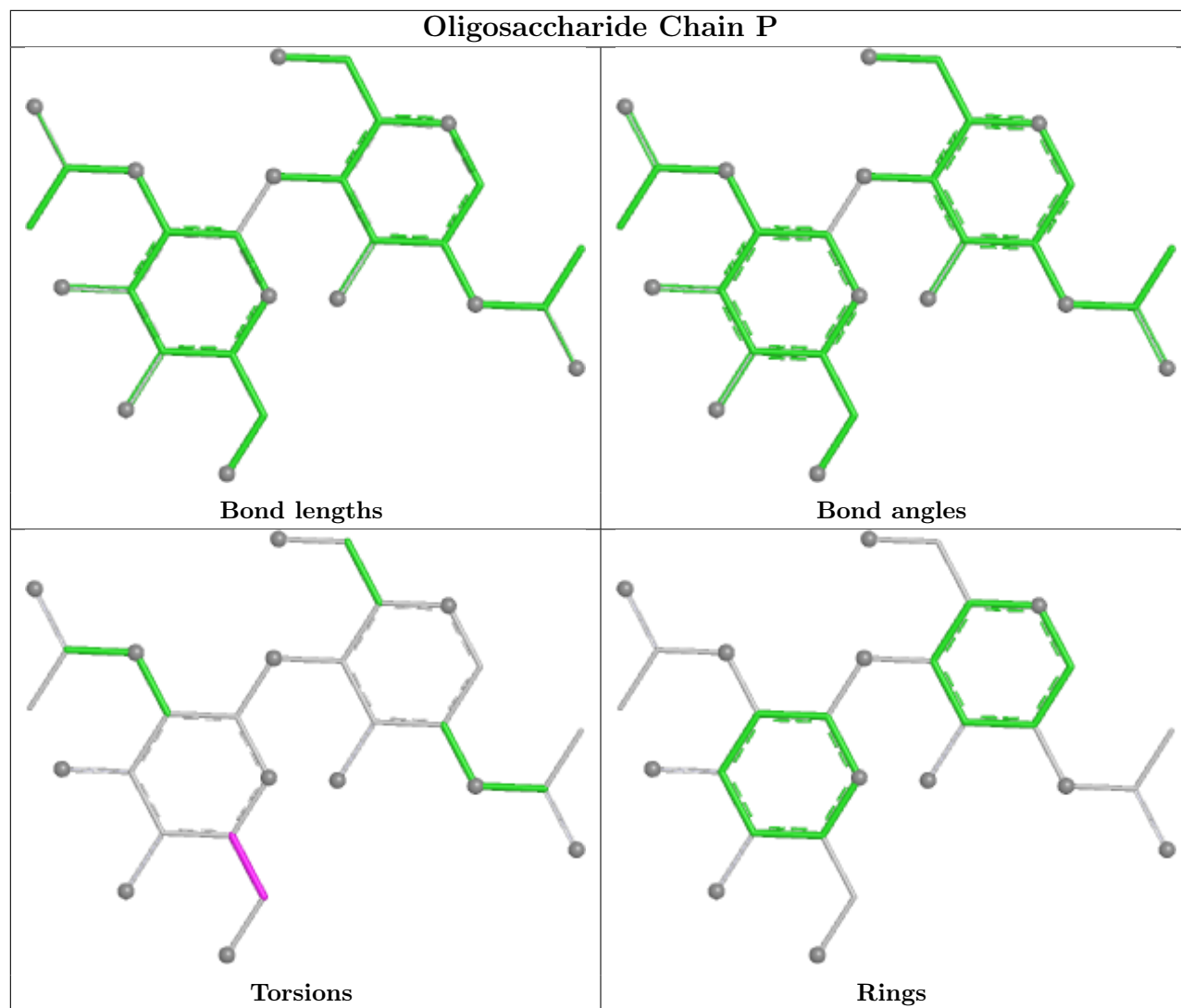


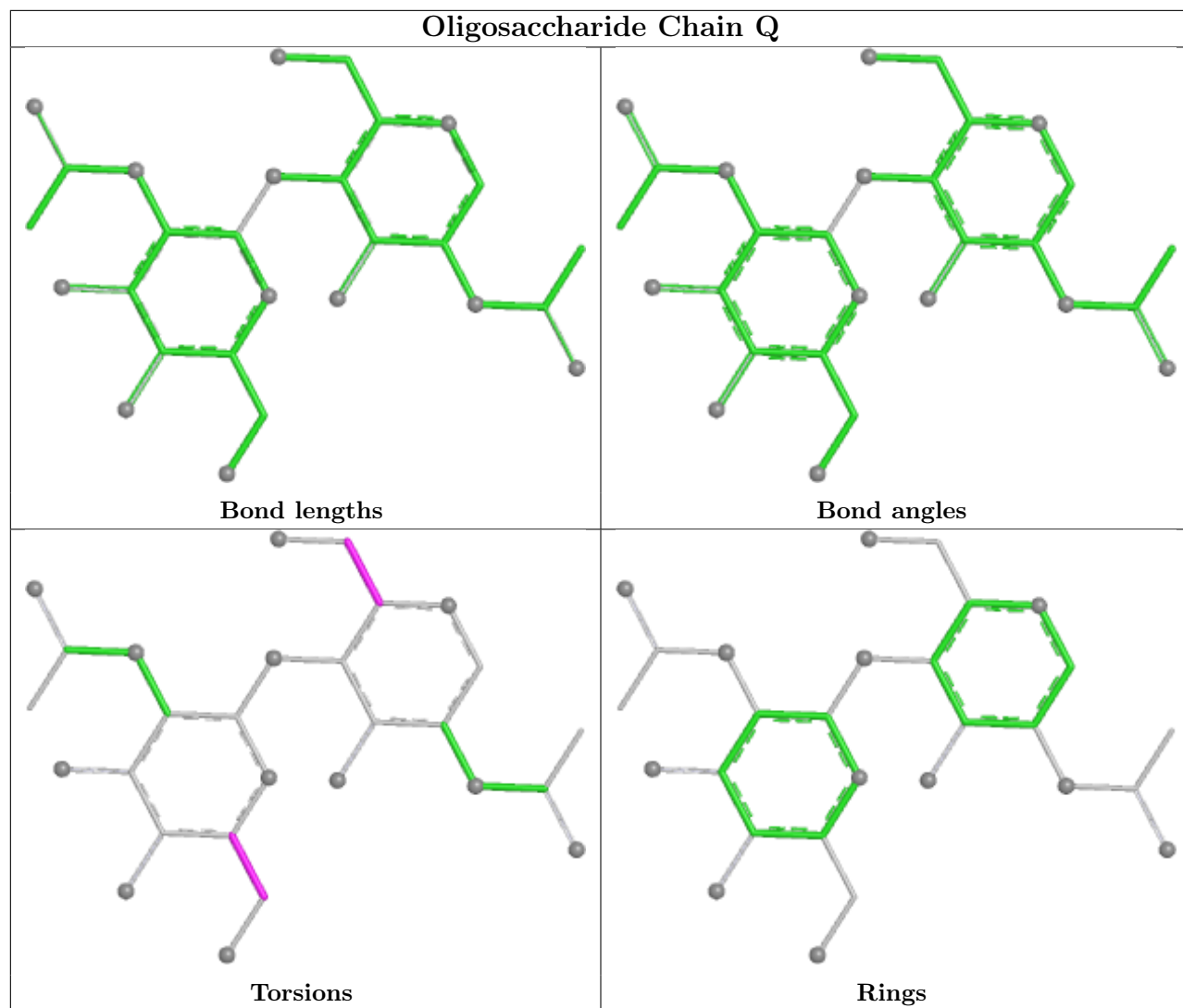


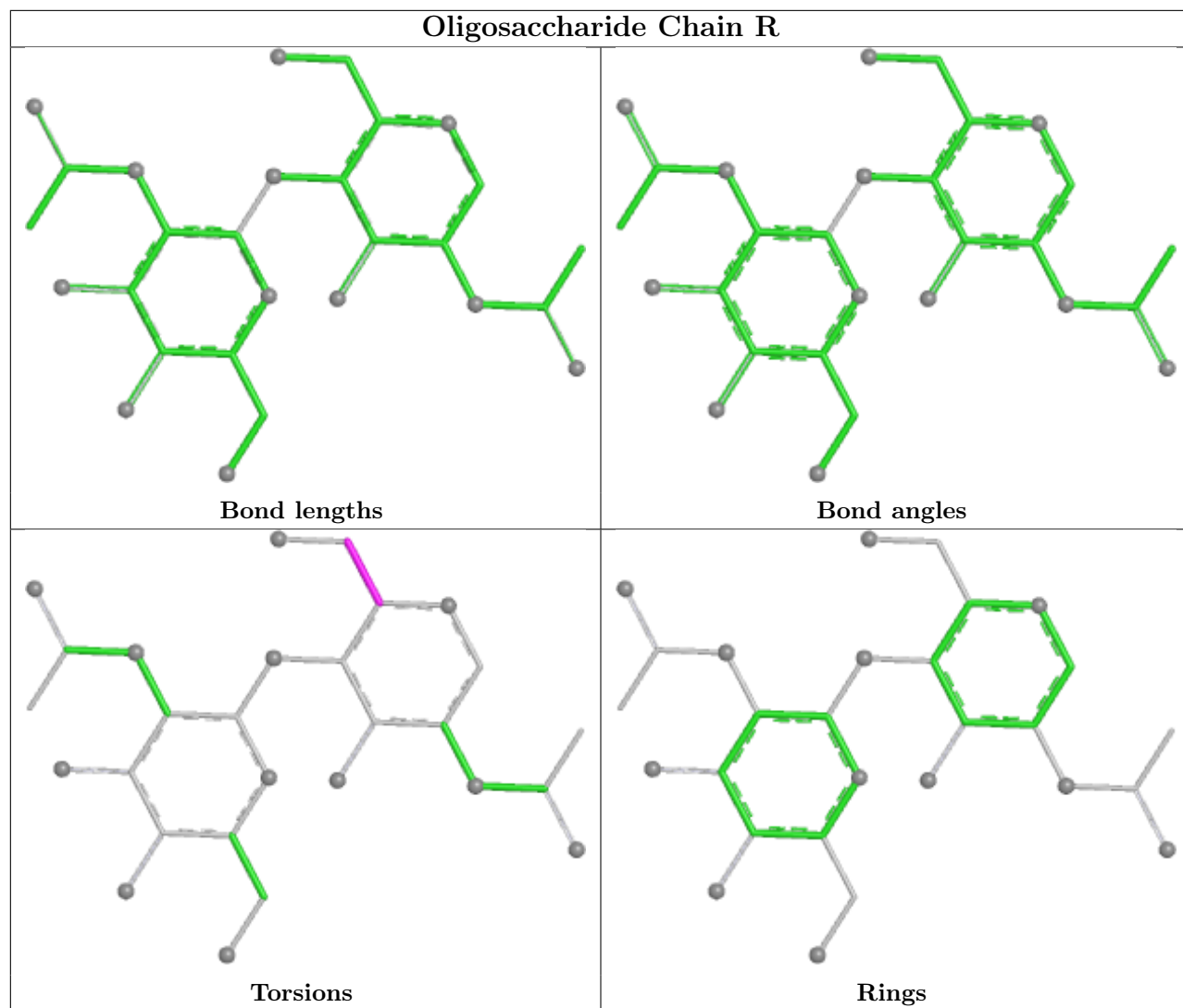


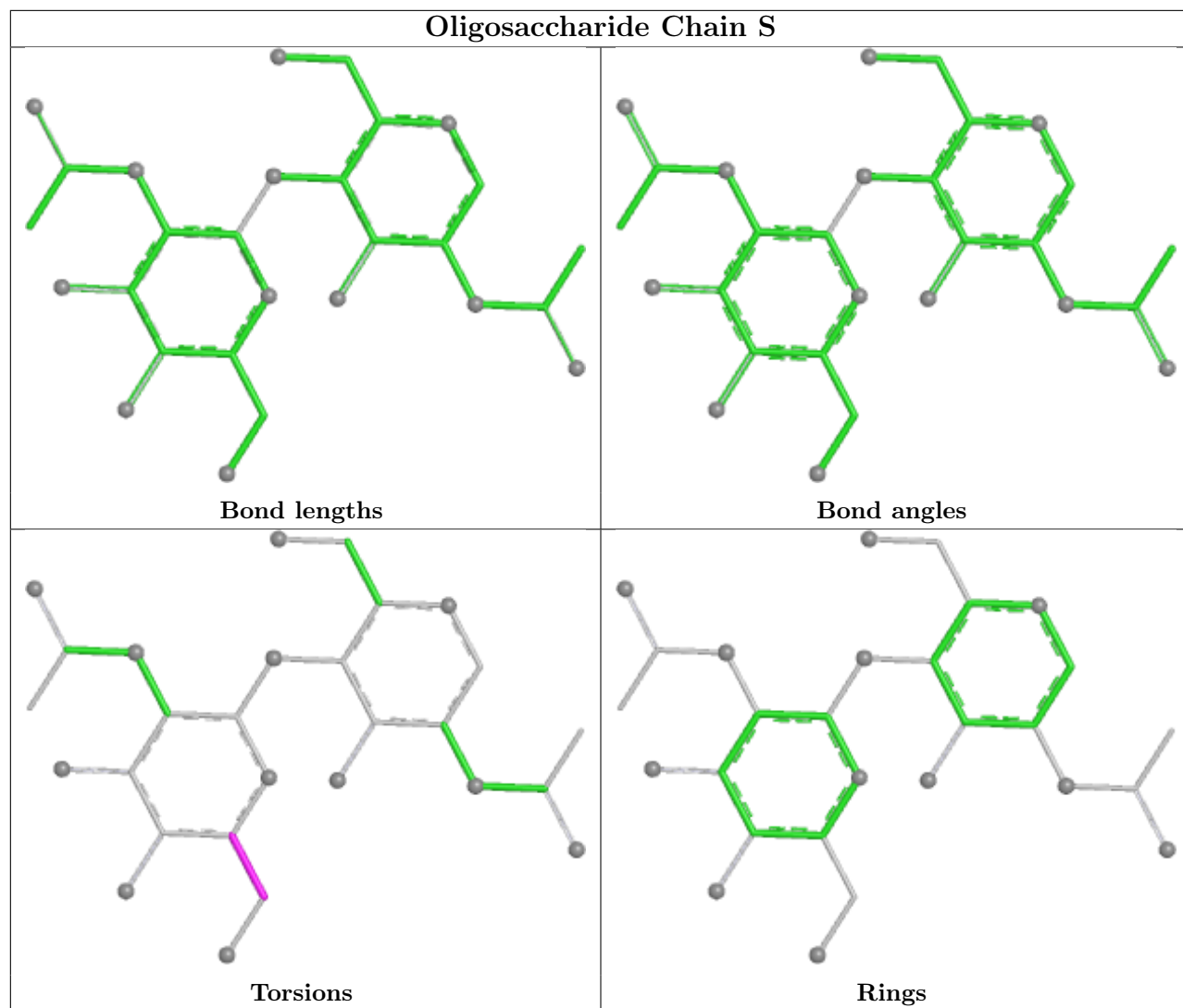


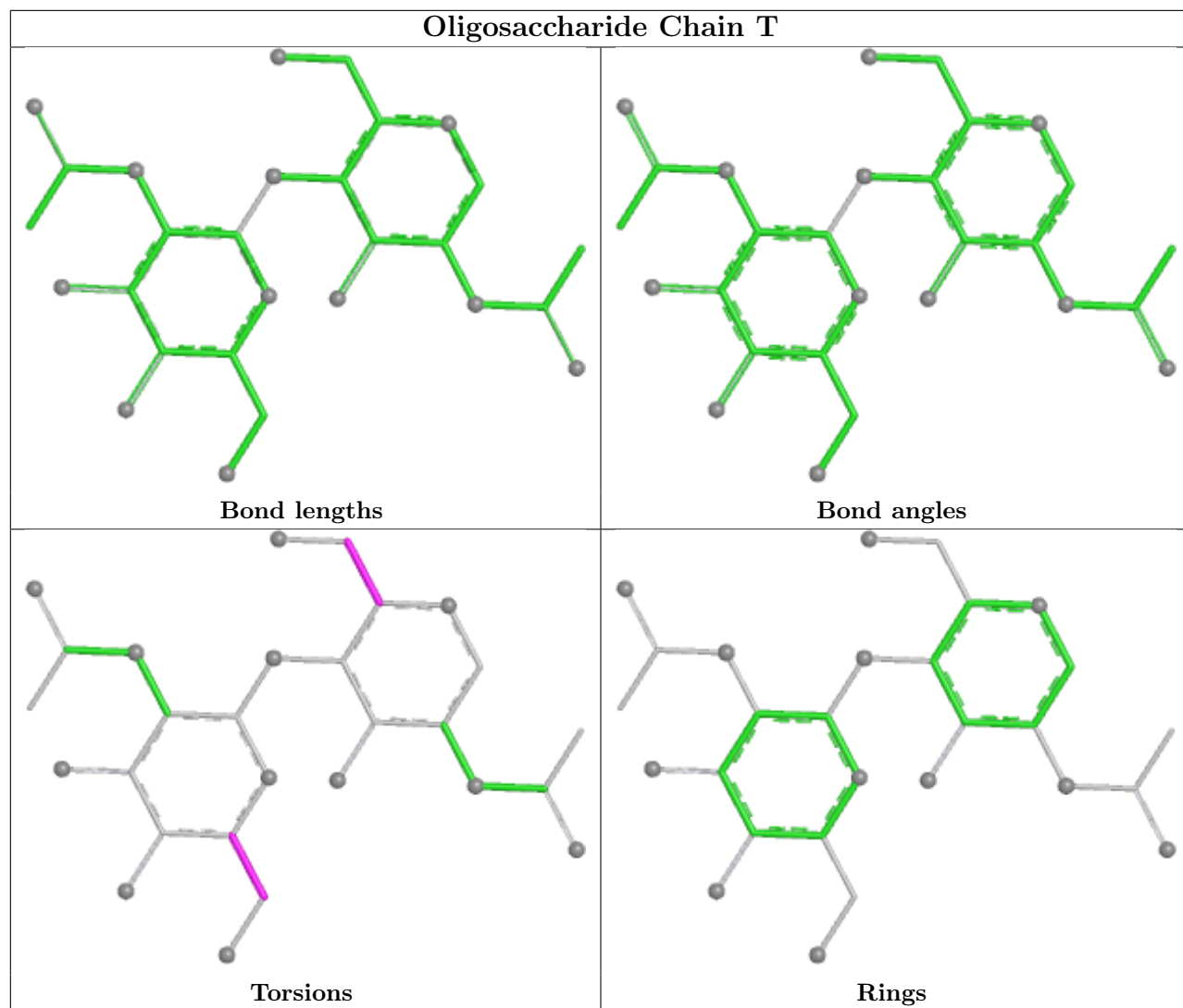


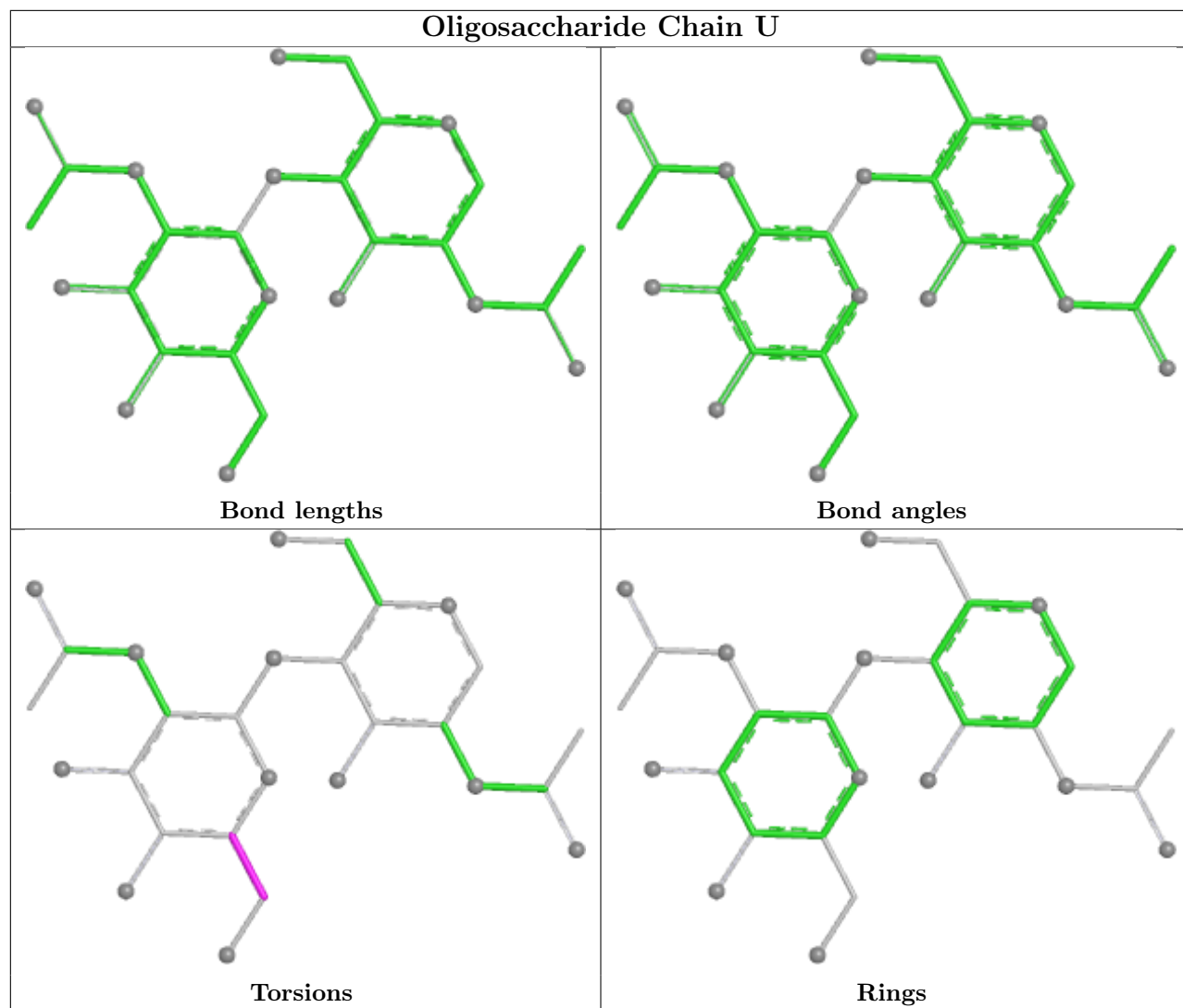


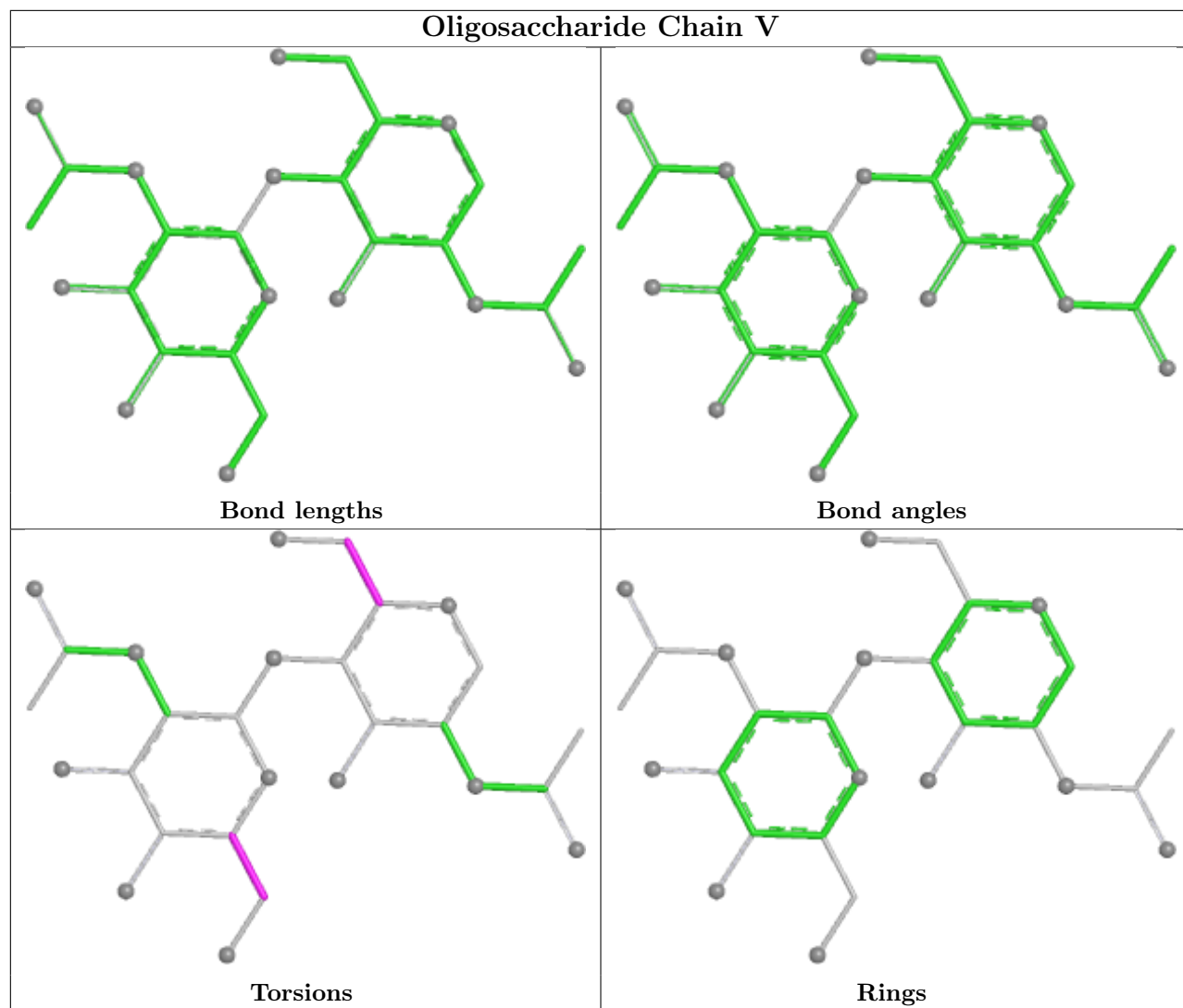


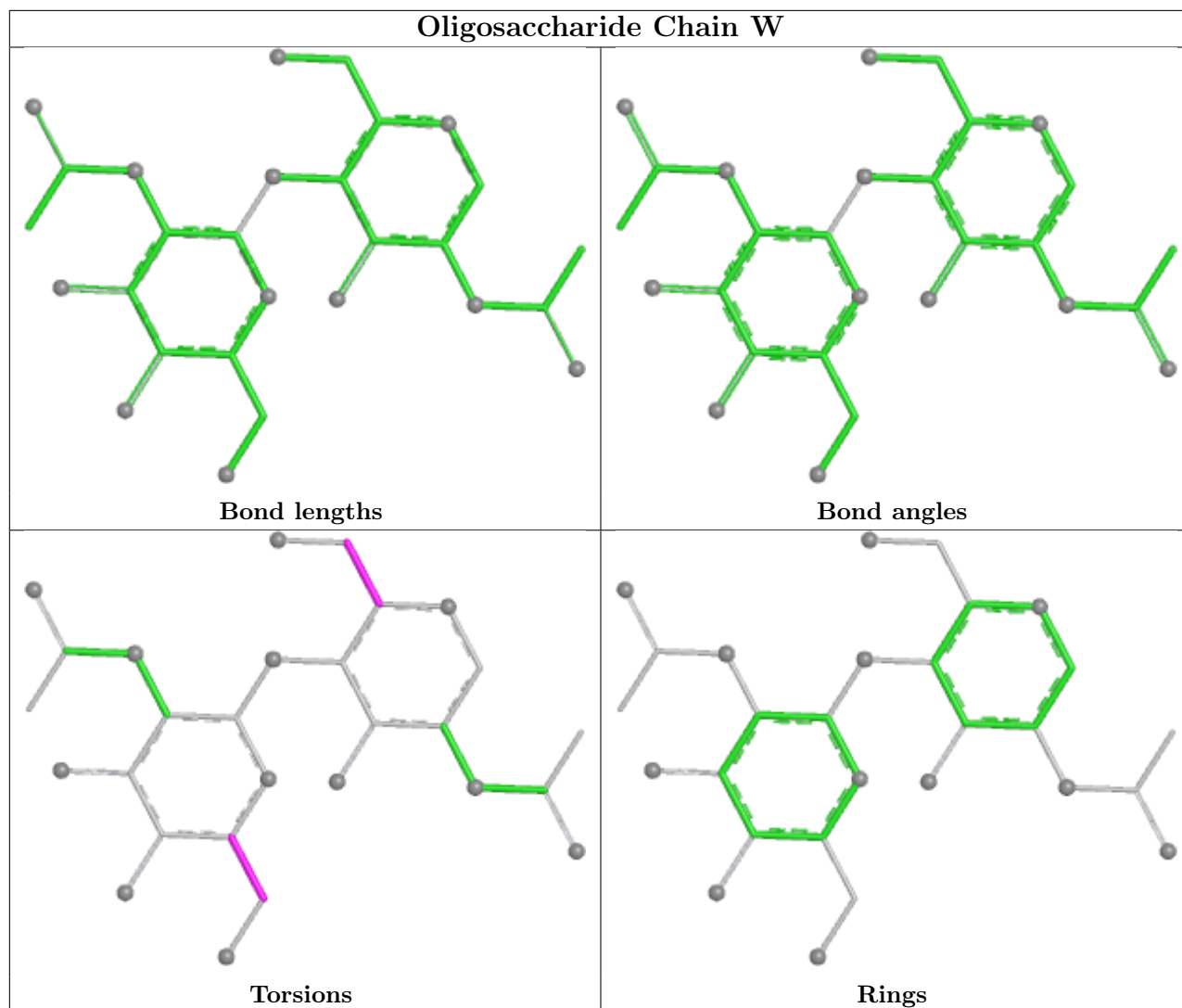












5.6 Ligand geometry [i](#)

31 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	C	1308	1	14,14,15	0.29	0	17,19,21	0.51	0
5	NAG	C	1307	1	14,14,15	0.47	0	17,19,21	0.37	0
5	NAG	C	1302	1	14,14,15	0.30	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1301	1	14,14,15	0.29	0	17,19,21	0.46	0
5	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	A	1303	1	14,14,15	0.36	0	17,19,21	0.47	0
5	NAG	C	1309	1	14,14,15	0.35	0	17,19,21	0.47	0
5	NAG	B	1308	1	14,14,15	0.30	0	17,19,21	0.49	0
5	NAG	C	1311	1	14,14,15	0.28	0	17,19,21	0.47	0
5	NAG	B	1309	1	14,14,15	0.27	0	17,19,21	0.41	0
5	NAG	A	1309	1	14,14,15	0.30	0	17,19,21	0.43	0
5	NAG	C	1304	1	14,14,15	0.35	0	17,19,21	0.51	0
5	NAG	C	1306	1	14,14,15	0.33	0	17,19,21	0.46	0
5	NAG	A	1305	1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	B	1305	-	14,14,15	0.58	0	17,19,21	0.53	0
5	NAG	A	1301	1	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	A	1308	1	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	C	1301	1	14,14,15	0.29	0	17,19,21	0.49	0
5	NAG	B	1306	1	14,14,15	0.26	0	17,19,21	0.56	0
5	NAG	B	1307	1	14,14,15	0.26	0	17,19,21	0.49	0
5	NAG	B	1310	1	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	C	1310	1	14,14,15	0.40	0	17,19,21	0.47	0
5	NAG	B	1302	1	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	B	1303	1	14,14,15	0.39	0	17,19,21	0.52	0
5	NAG	C	1305	1	14,14,15	0.26	0	17,19,21	0.51	0
5	NAG	B	1304	1	14,14,15	0.39	0	17,19,21	0.87	1 (5%)
5	NAG	A	1307	1	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	A	1304	1	14,14,15	0.27	0	17,19,21	0.42	0
5	NAG	B	1311	1	14,14,15	0.54	0	17,19,21	1.53	1 (5%)
5	NAG	A	1306	1	14,14,15	0.31	0	17,19,21	0.50	0
5	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.69	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	C	1308	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1303	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
5	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1311	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	1311	NAG	C1-O5-C5	5.78	119.94	112.19
5	B	1304	NAG	C2-N2-C7	2.58	126.36	122.90
5	C	1303	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1307	NAG	C4-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	B	1307	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	C	1310	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	C	1310	NAG	O5-C5-C6-O6
5	B	1311	NAG	O5-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	B	1311	NAG	C4-C5-C6-O6
5	C	1311	NAG	C4-C5-C6-O6
5	B	1310	NAG	C4-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	A	1301	NAG	C8-C7-N2-C2
5	A	1301	NAG	O7-C7-N2-C2
5	A	1302	NAG	C8-C7-N2-C2
5	A	1302	NAG	O7-C7-N2-C2
5	B	1310	NAG	C8-C7-N2-C2
5	B	1310	NAG	O7-C7-N2-C2
5	B	1311	NAG	C8-C7-N2-C2
5	B	1311	NAG	O7-C7-N2-C2
5	C	1303	NAG	C8-C7-N2-C2
5	C	1303	NAG	O7-C7-N2-C2
5	C	1304	NAG	C8-C7-N2-C2
5	C	1304	NAG	O7-C7-N2-C2
5	C	1308	NAG	C8-C7-N2-C2
5	C	1308	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1305	NAG	O5-C5-C6-O6
5	C	1311	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	B	1304	NAG	C1-C2-N2-C7
5	B	1307	NAG	C1-C2-N2-C7
5	B	1309	NAG	C1-C2-N2-C7
5	B	1304	NAG	C3-C2-N2-C7
5	A	1306	NAG	C4-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

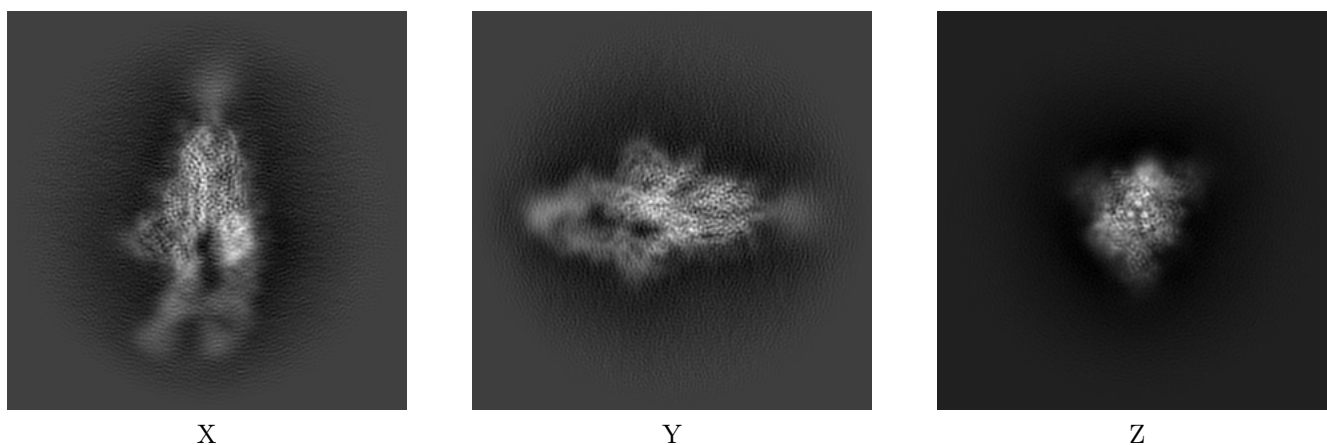
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32771. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

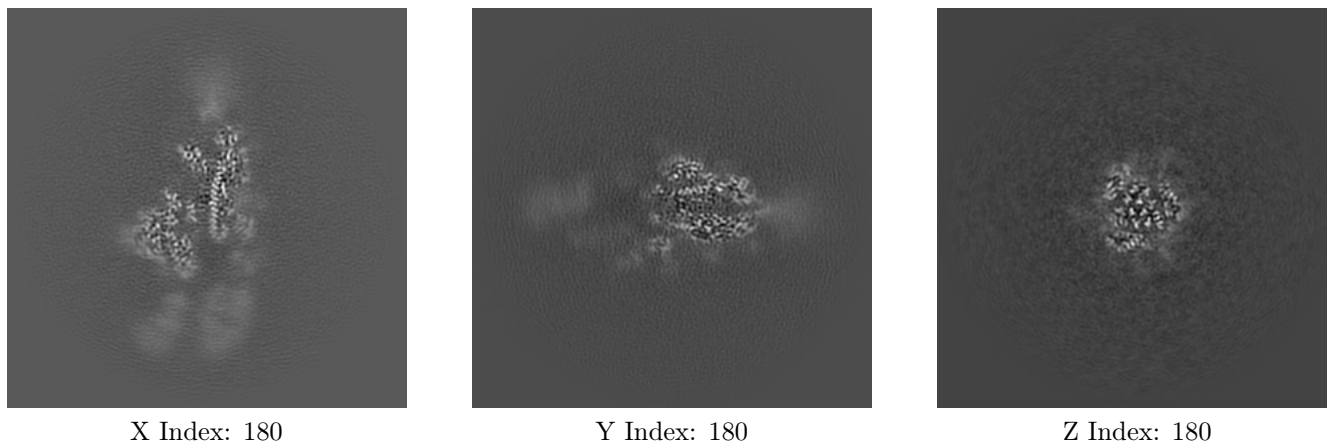
6.1.1 Primary map



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

6.2 Central slices [i](#)

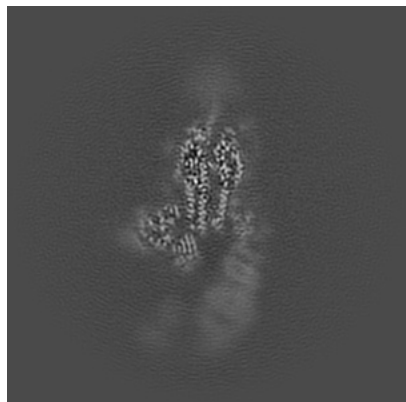
6.2.1 Primary map



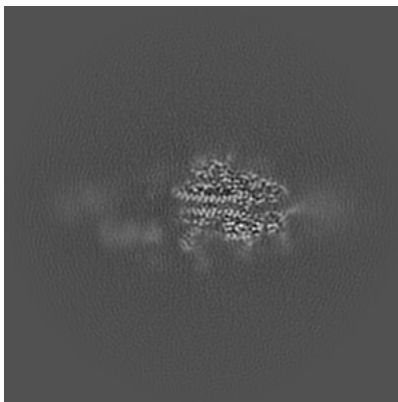
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

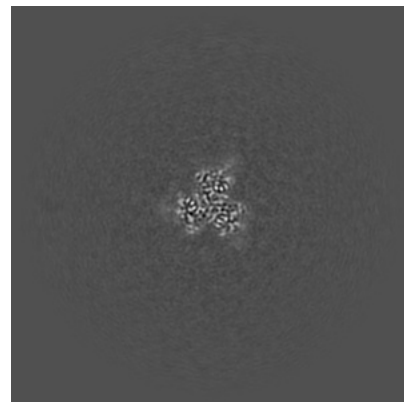
6.3.1 Primary map



X Index: 188



Y Index: 175

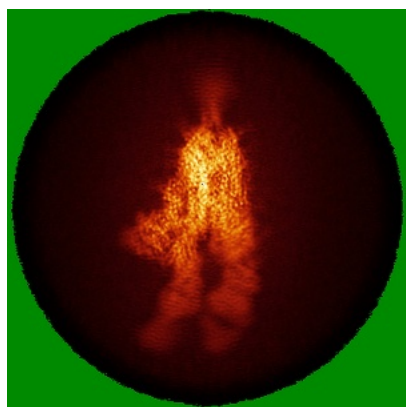


Z Index: 216

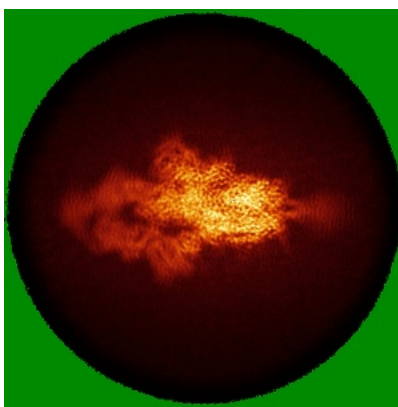
The images above show the largest variance slices of the map in three orthogonal directions.

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

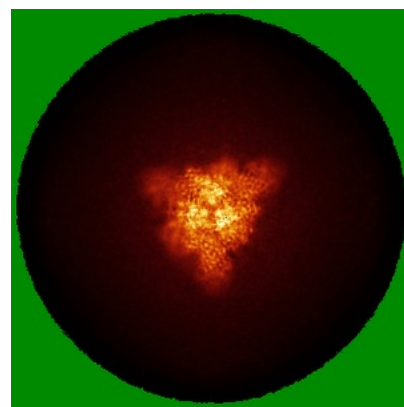
6.4.1 Primary map



X



Y

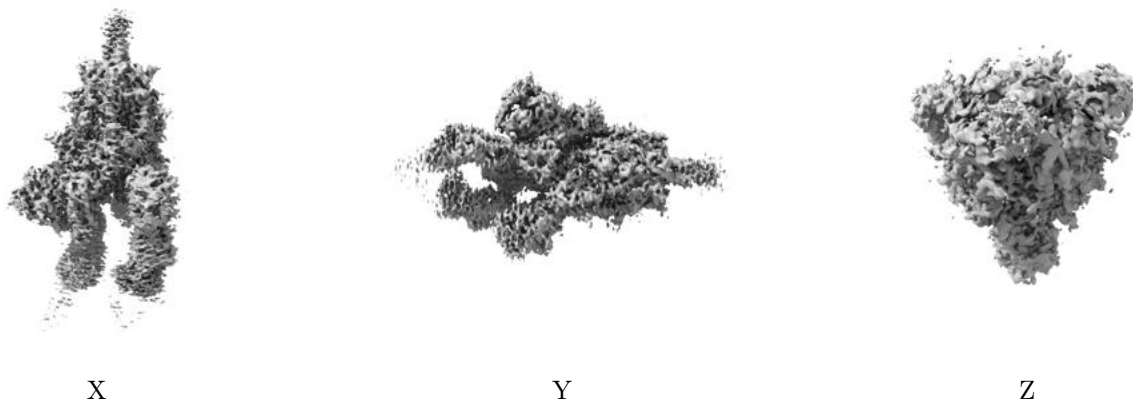


Z

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 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

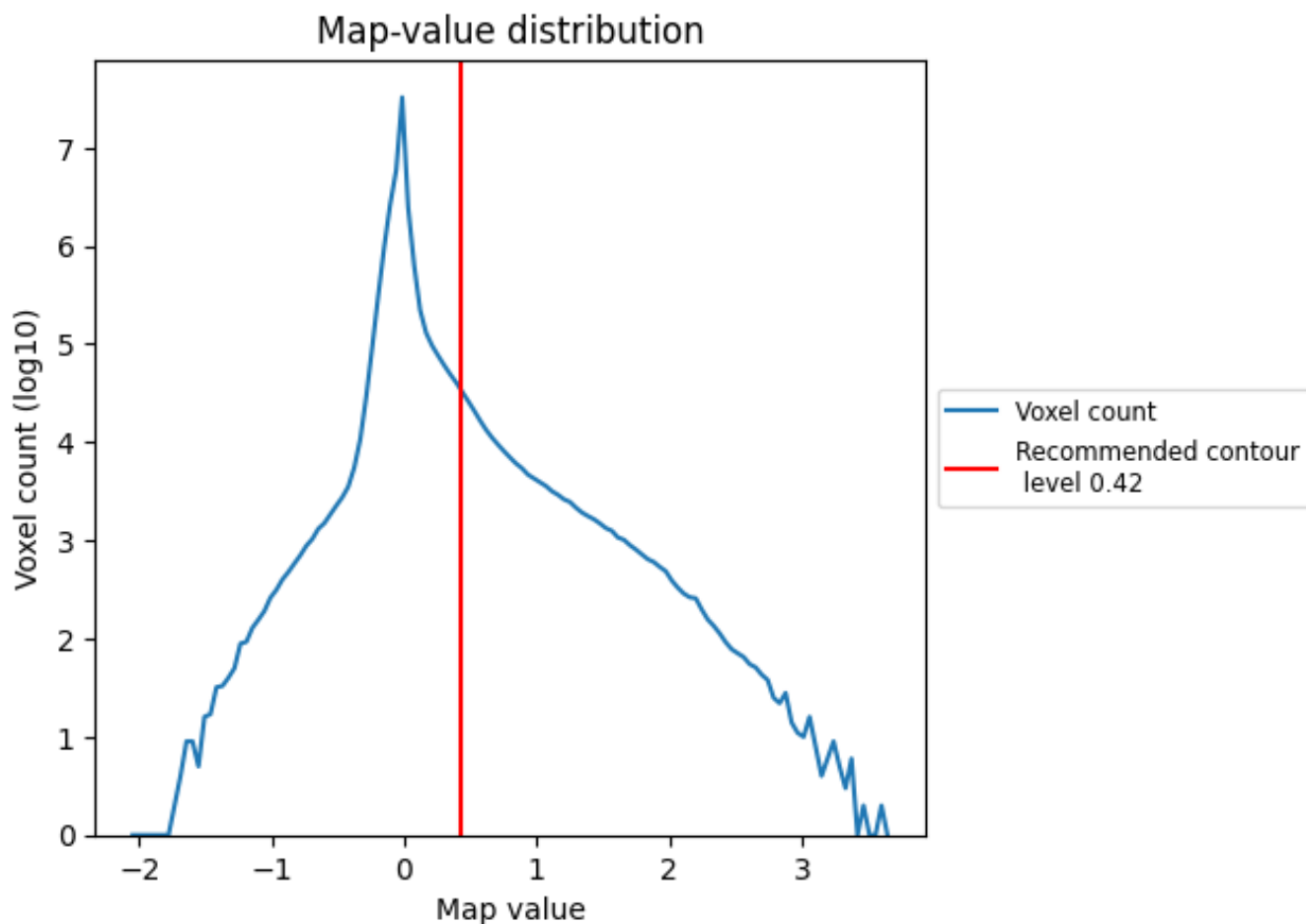
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

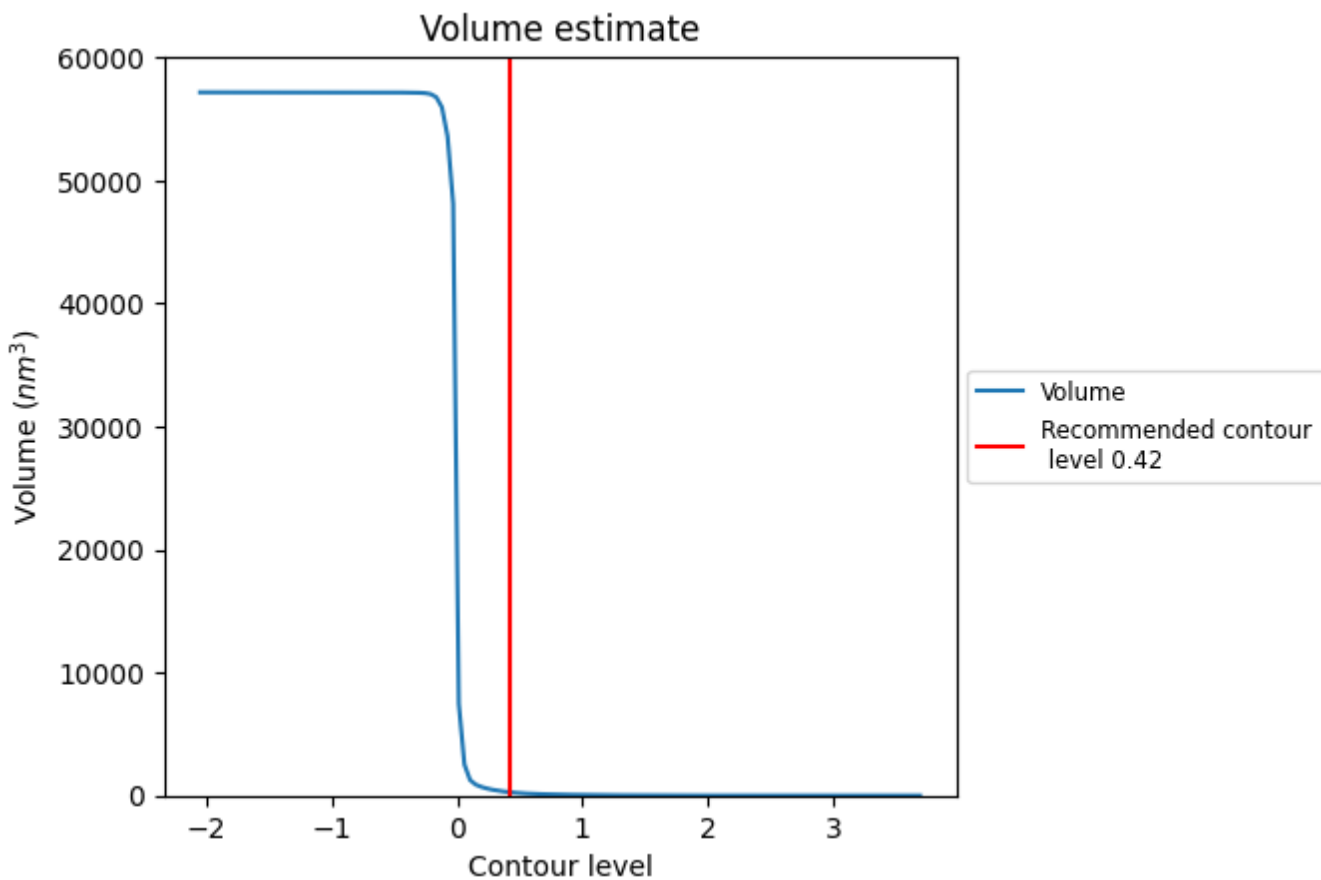
This section contains the results of statistical analysis of the map.

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.

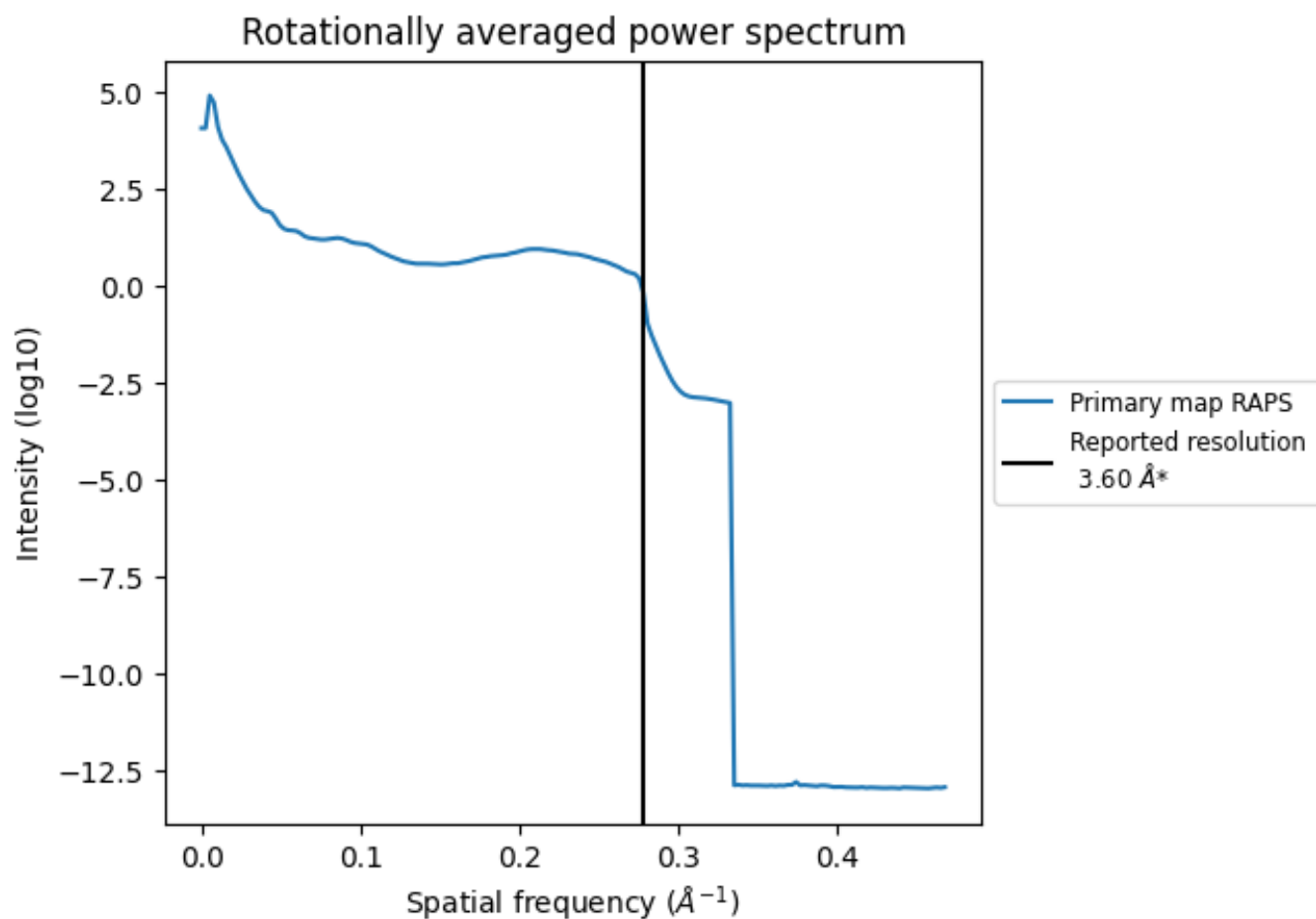
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 271 nm³; this corresponds to an approximate mass of 245 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 0.278 Å⁻¹

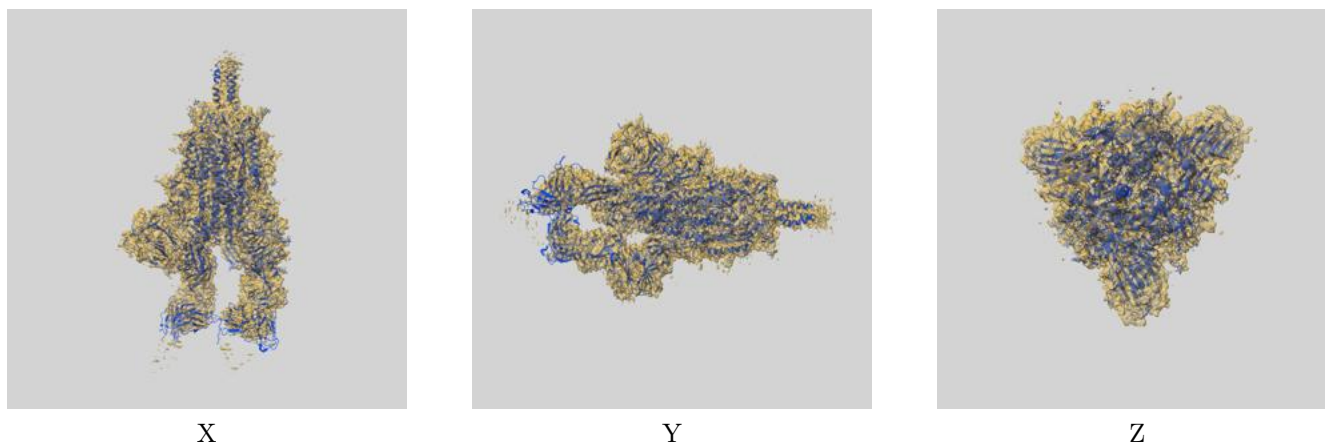
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

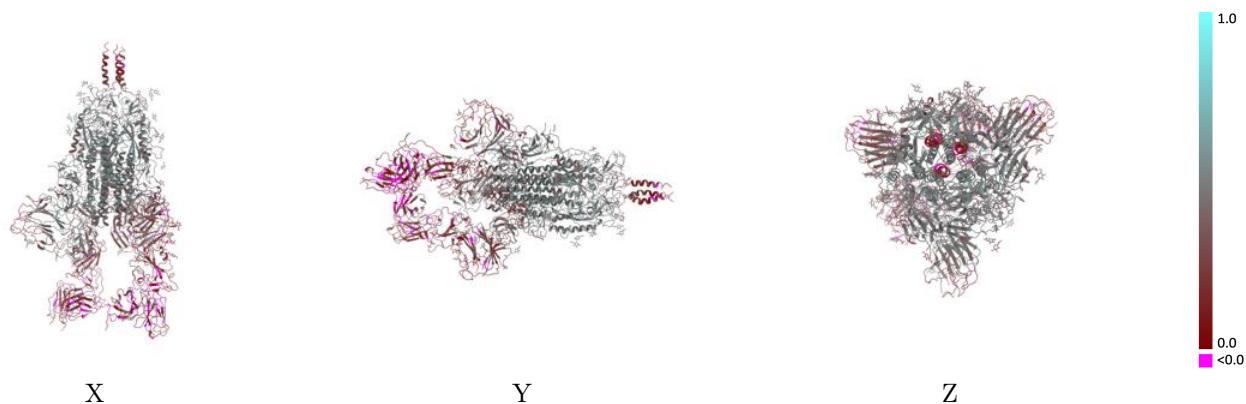
This section contains information regarding the fit between EMDB map EMD-32771 and PDB model 7WT8. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



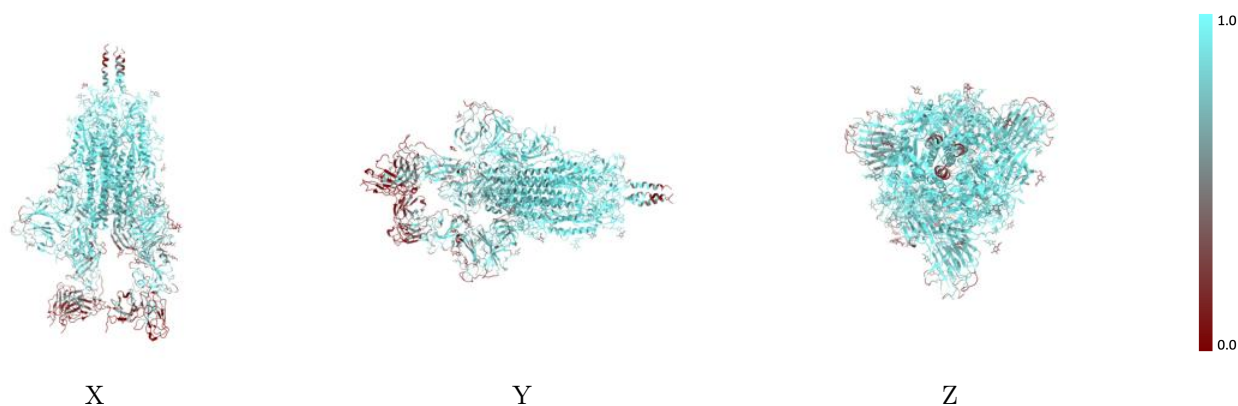
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



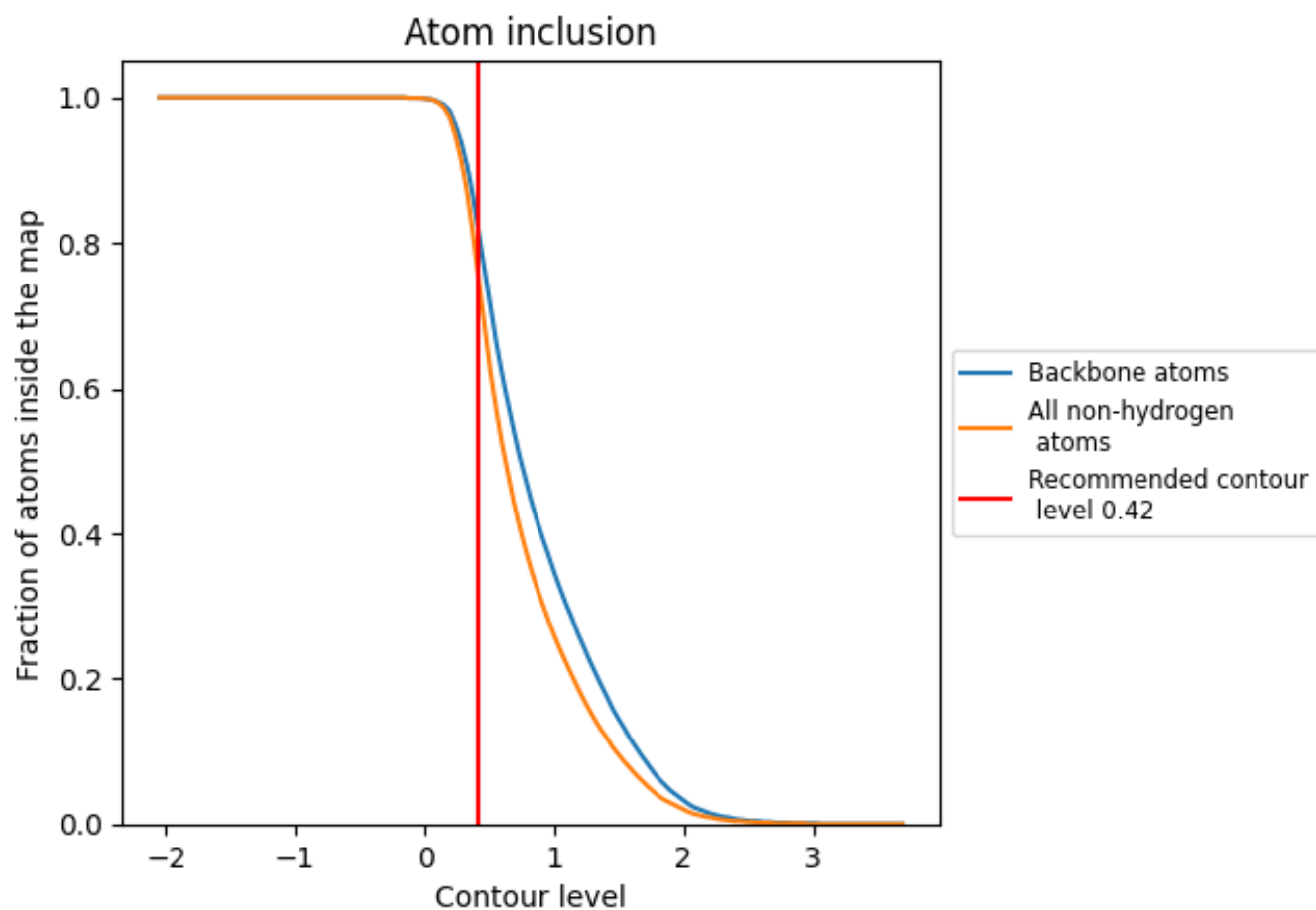
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.42).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7450	 0.3580
A	 0.8110	 0.3940
B	 0.8430	 0.4120
C	 0.7700	 0.3560
D	 0.2520	 0.0980
E	 0.5000	 0.3190
F	 0.6790	 0.3090
G	 0.9290	 0.5190
H	 0.2910	 0.1260
I	 0.2760	 0.1480
J	 0.2350	 0.1410
K	 0.8930	 0.4390
L	 0.7500	 0.4130
M	 0.6790	 0.4150
N	 0.5000	 0.3310
O	 0.7500	 0.4850
P	 0.8210	 0.4040
Q	 0.8210	 0.4870
R	 0.6070	 0.4150
S	 0.2860	 0.1640
T	 0.7500	 0.4630
U	 0.9290	 0.4480
V	 0.8210	 0.4000
W	 0.6790	 0.4240

