



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 02:16 pm BST

PDB ID : 6ZOZ  
EMDB ID : EMD-11331  
Title : Structure of Disulphide-stabilized SARS-CoV-2 Spike Protein Trimer (x1 disulphide-bond mutant, S383C, D985C, K986P, V987P, single Arg S1/S2 cleavage site) in Locked State  
Authors : Xiong, X.; Qu, K.; Scheres, S.H.W.; Briggs, J.A.G.  
Deposited on : 2020-07-08  
Resolution : 3.50 Å (reported)  
Based on initial model : 6VXX

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

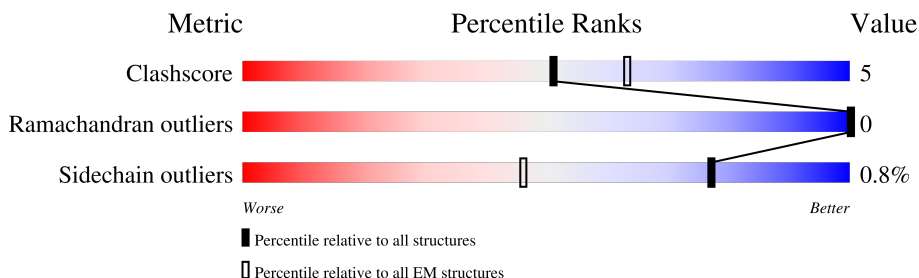
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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




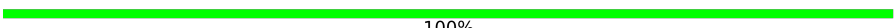
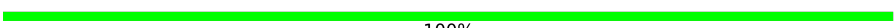



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1247	
1	B	1247	
1	C	1247	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

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Mol	Chain	Length	Quality of chain
2	I	2	 50%50%
2	J	2	 50%50%
2	K	2	 100%
2	L	2	 100%
2	M	2	 50%50%
2	N	2	 50%50%
2	O	2	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1069	Total	C	N	O	S	0	0
			8332	5317	1388	1586	41		
1	B	1069	Total	C	N	O	S	0	0
			8332	5317	1388	1586	41		
1	C	1070	Total	C	N	O	S	0	0
			8336	5319	1389	1587	41		

There are 183 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	383	CYS	SER	engineered mutation	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	981	CYS	ASP	engineered mutation	UNP P0DTC2
A	982	PRO	LYS	engineered mutation	UNP P0DTC2
A	983	PRO	VAL	engineered mutation	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2
A	1212	GLU	-	expression tag	UNP P0DTC2
A	1213	ASN	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	PHE	-	expression tag	UNP P0DTC2
A	1217	GLN	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	ILE	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	ARG	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLN	-	expression tag	UNP P0DTC2
A	1234	ALA	-	expression tag	UNP P0DTC2
A	1235	TYR	-	expression tag	UNP P0DTC2
A	1236	VAL	-	expression tag	UNP P0DTC2
A	1237	ARG	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	ASP	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	TRP	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	LEU	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	THR	-	expression tag	UNP P0DTC2
A	1248	PHE	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	383	CYS	SER	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	981	CYS	ASP	engineered mutation	UNP P0DTC2
B	982	PRO	LYS	engineered mutation	UNP P0DTC2
B	983	PRO	VAL	engineered mutation	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	SER	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2
B	1211	ARG	-	expression tag	UNP P0DTC2
B	1212	GLU	-	expression tag	UNP P0DTC2
B	1213	ASN	-	expression tag	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	PHE	-	expression tag	UNP P0DTC2
B	1217	GLN	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	GLY	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	TYR	-	expression tag	UNP P0DTC2
B	1225	ILE	-	expression tag	UNP P0DTC2
B	1226	PRO	-	expression tag	UNP P0DTC2
B	1227	GLU	-	expression tag	UNP P0DTC2
B	1228	ALA	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	ARG	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLN	-	expression tag	UNP P0DTC2
B	1234	ALA	-	expression tag	UNP P0DTC2
B	1235	TYR	-	expression tag	UNP P0DTC2
B	1236	VAL	-	expression tag	UNP P0DTC2
B	1237	ARG	-	expression tag	UNP P0DTC2
B	1238	LYS	-	expression tag	UNP P0DTC2
B	1239	ASP	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	LEU	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	THR	-	expression tag	UNP P0DTC2
B	1248	PHE	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
C	10	GLU	-	expression tag	UNP P0DTC2
C	11	THR	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	383	CYS	SER	engineered mutation	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	981	CYS	ASP	engineered mutation	UNP P0DTC2
C	982	PRO	LYS	engineered mutation	UNP P0DTC2
C	983	PRO	VAL	engineered mutation	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	SER	-	expression tag	UNP P0DTC2
C	1210	GLY	-	expression tag	UNP P0DTC2
C	1211	ARG	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	ASN	-	expression tag	UNP P0DTC2
C	1214	LEU	-	expression tag	UNP P0DTC2
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	PHE	-	expression tag	UNP P0DTC2
C	1217	GLN	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	GLY	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1224	TYR	-	expression tag	UNP P0DTC2
C	1225	ILE	-	expression tag	UNP P0DTC2
C	1226	PRO	-	expression tag	UNP P0DTC2
C	1227	GLU	-	expression tag	UNP P0DTC2
C	1228	ALA	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	ARG	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLN	-	expression tag	UNP P0DTC2
C	1234	ALA	-	expression tag	UNP P0DTC2
C	1235	TYR	-	expression tag	UNP P0DTC2
C	1236	VAL	-	expression tag	UNP P0DTC2
C	1237	ARG	-	expression tag	UNP P0DTC2
C	1238	LYS	-	expression tag	UNP P0DTC2
C	1239	ASP	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	TRP	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	LEU	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	THR	-	expression tag	UNP P0DTC2
C	1248	PHE	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2

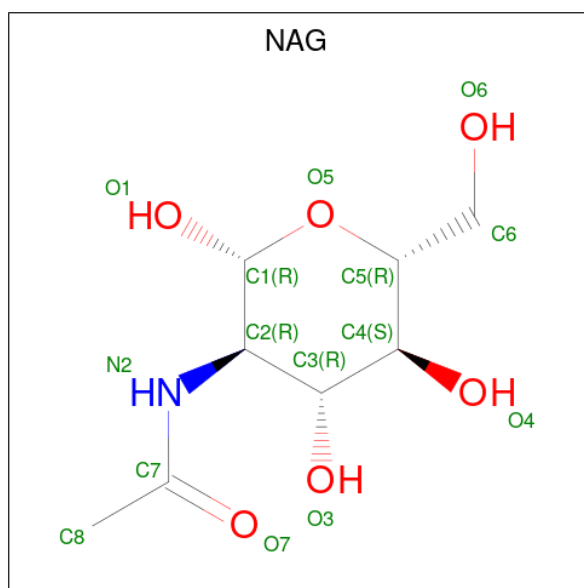
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



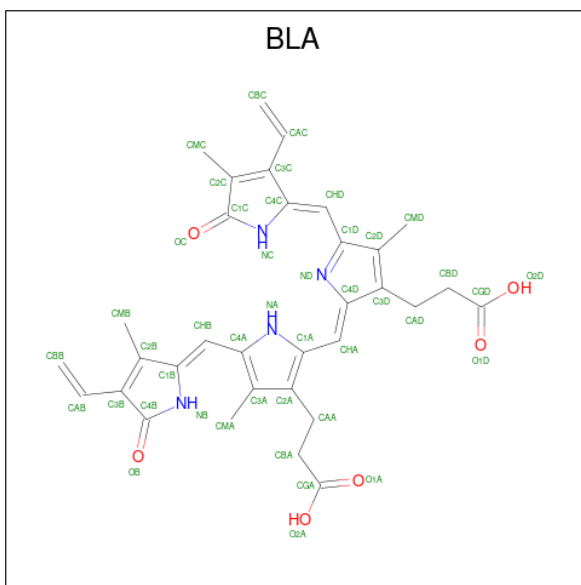
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3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

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

- Molecule 4 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula:  $C_{33}H_{34}N_4O_6$ ).

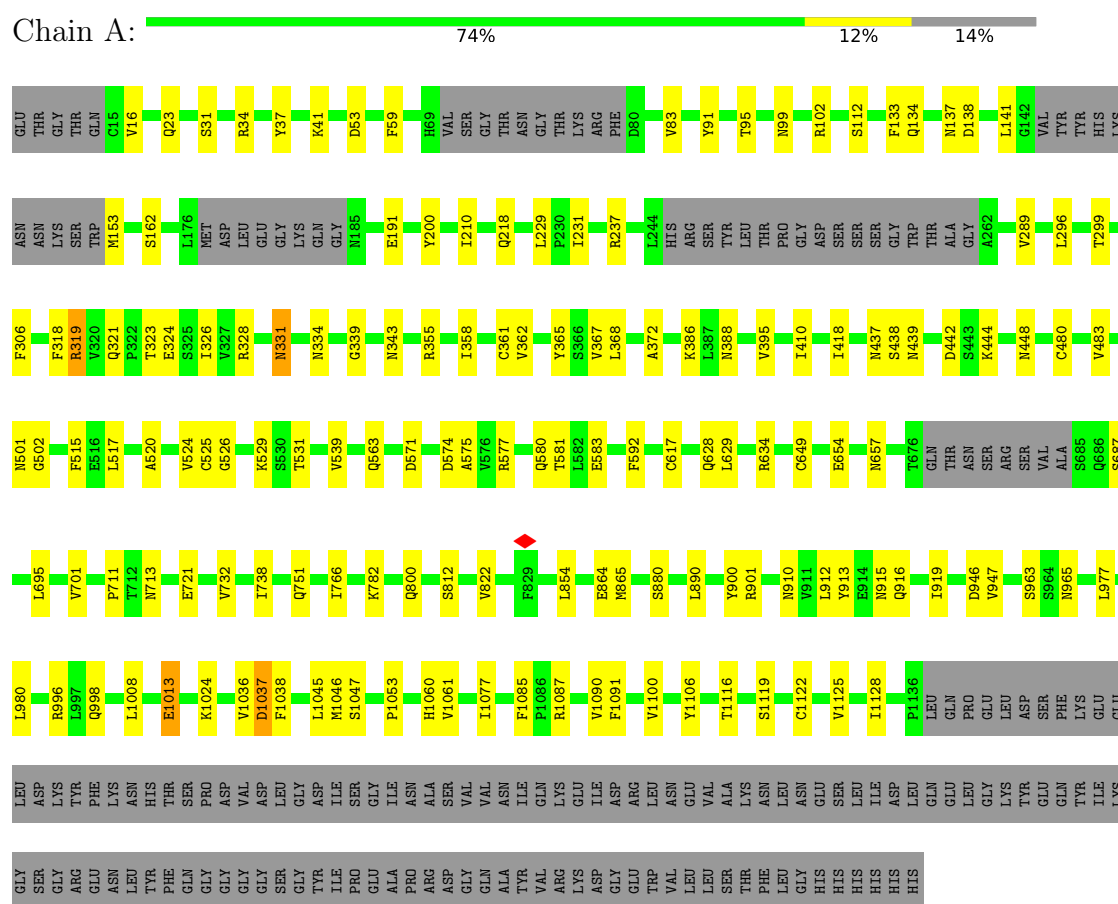


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 43	C 33	N 4	O 6	0
4	B	1	Total 43	C 33	N 4	O 6	0
4	C	1	Total 43	C 33	N 4	O 6	0

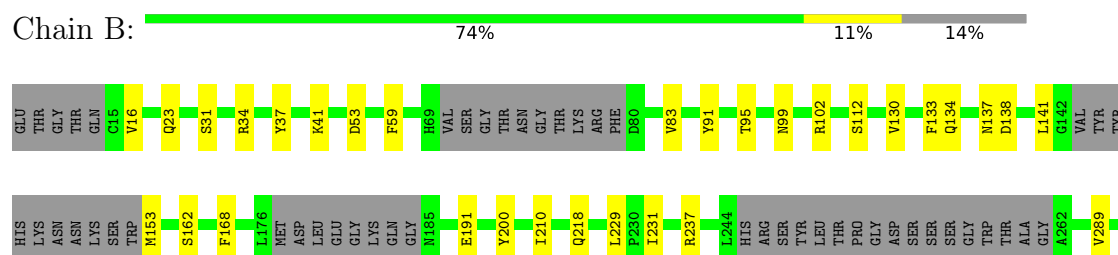
### 3 Residue-property plots

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

#### • Molecule 1: Spike glycoprotein



#### • Molecule 1: Spike glycoprotein





GLU	GLU	GLN	I919	VAL	C480	L296	GLU	TYR	GLU
LEU	LEU	PRO	D946	ALA	S885	L296	THR	THR	THR
GLY	GLY	GLU	V947	Q686	V483	T299	GLY	HIS	GLY
LYS	LYS	LEU	S963	Q686	S887	F306	LYS	ASN	THR
THR	THR	ASP	S963	S887	S887	F306	GLN	ASN	GLN
GLU	GLU	SER	S964	L695	S501	F318	ASN	ASN	C15
GLN	GLN	PHE	S964	L695	S502	F318	LYS	LYS	V16
THR	THR	LYS	N965	V701	F515	R319	SER	SER	Q23
ILE	ILE	GLU	N965	V701	E516	V320	TRP	TRP	M153
LYS	LYS	GLU	L977	P711	L517	Q321	LYS	LYS	S31
GLY	GLY	LEU	L980	T712	L517	P322	GLY	GLY	S162
SER	SER	ASP	L980	N713	A520	T323	ASP	ASP	R34
GLY	GLY	LYS	R996	N713	A520	E324	LEU	LEU	D53
ARG	ARG	TYR	R996	E721	V524	S325	GLY	GLY	F59
GLU	GLU	PHE	L997	E721	C525	S325	THR	THR	H69
ASN	ASN	LYS	Q998	V732	C525	V327	GLY	GLY	SER
LEU	LEU	ASN	V732	V732	O526	R328	LYS	LYS	GLY
THR	THR	HIS	L1008	I738	X529	N381	GLN	GLN	THR
PHE	PHE	THR	I738	I738	X530	N381	ASP	ASP	ARG
GLN	GLN	SER	E1013	Q751	S530	N381	LEU	LEU	PHE
GLY	GLY	PRO	K1024	Q751	T531	N334	GLY	GLY	D90
GLY	GLY	ASP	K1024	I766	T531	N334	THR	THR	SER
GLY	GLY	VAL	V1036	I766	V539	G339	LYS	LYS	GLY
GLY	GLY	ASP	V1036	I766	V539	G339	GLN	GLN	THR
SER	SER	LEU	D1037	K782	Q653	G339	VAL	VAL	THR
GLY	GLY	GLY	F1038	K782	Q653	N343	GLY	GLY	GLY
ILE	ILE	ASP	L1045	Q800	D571	N343	ASN	ASN	THR
PRO	PRO	SER	L1045	S812	D574	R355	LYS	LYS	GLY
GLU	GLU	ILE	S1047	S812	A575	R355	THR	THR	THR
ALA	ALA	GLY	V822	V822	V576	I358	LYS	LYS	LYS
PRO	PRO	ASN	P1053	V822	S577	C361	THR	THR	ARG
ARG	ARG	ALA	P1053	F829	S577	V362	ARG	ARG	PHE
ASP	ASP	SER	H1060	F829	Q880	L229	PHE	PHE	D90
GLY	GLY	VAL	V1077	R843	T581	P230	THR	THR	SER
GLN	GLN	VAL	I1077	R843	L582	I231	GLY	GLY	GLY
ALA	ALA	ASN	ASN	E583	V367	V83	THR	THR	THR
TYR	TYR	ILE	F1085	A848	E583	R237	LYS	LYS	LYS
VAL	VAL	GLN	P1086	A848	F592	L368	THR	THR	ARG
ARG	ARG	LYS	R1087	N852	F592	A372	ARG	ARG	THR
LYS	LYS	GLU	G853	G853	C617	L244	HIS	HIS	LYS
ASP	ASP	ILE	L854	L854	C617	L244	ARG	ARG	ARG
GLY	GLY	ASP	F1090	Q628	Q628	K386	SER	SER	N99
GLU	GLU	ARG	E864	L629	L629	L387	THR	THR	R102
TRP	TRP	LEU	M865	M865	L629	N388	LYS	LYS	LYS
VAL	VAL	ASN	S880	S880	R634	V395	LEU	LEU	LYS
LEU	LEU	GLU	Y1106	Y1106	R634	V395	THR	THR	S112
LEU	LEU	VAL	T1116	L890	C649	T410	PRO	PRO	N121
SER	SER	ALA	T1116	L890	C649	T410	ASP	ASP	LYS
THR	THR	LYS	Y900	Y900	E654	T418	SER	SER	VAL
PHE	PHE	ASN	S1119	R901	E654	T418	SER	SER	V130
LEU	LEU	LEU	G1122	N910	N657	N437	THR	THR	F133
GLY	GLY	ASN	G1122	N910	N657	N437	GLY	GLY	Q134
HIS	HIS	GLU	V1125	V911	T676	S438	TRP	TRP	N137
HIS	HIS	SER	V1125	V911	T676	S438	ALA	ALA	D1

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

Chain D:  100%



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

Chain E:  50% 50%



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

Chain F:  50% 50%



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

Chain G:  100%



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

Chain H:  100%



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

Chain I:  50% 50%



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

Chain J:  50% 50%



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

Chain K:  100%



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

Chain L:  100%



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

Chain M:  50% 50%



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

Chain N:  50% 50%



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

Chain O:  100%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	58887	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0118	Depositor
Map size (Å)	271.616, 271.616, 271.616	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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, BLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/8522	0.52	0/11603
1	B	0.31	0/8522	0.52	0/11603
1	C	0.31	0/8526	0.52	0/11608
All	All	0.31	0/25570	0.52	0/34814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8332	0	8119	101	0
1	B	8332	0	8119	97	0
1	C	8336	0	8122	103	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	1	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
3	A	182	0	169	5	0
3	B	182	0	169	5	0
3	C	182	0	169	4	0
4	A	43	0	32	0	0
4	B	43	0	32	0	0
4	C	43	0	32	0	0
All	All	26011	0	25263	270	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 (270) 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:C:657:ASN:HD21	3:C:1306:NAG:C1	1.16	1.57
1:B:657:ASN:HD21	3:B:1306:NAG:C1	1.16	1.55
1:A:657:ASN:HD21	3:A:1306:NAG:C1	1.16	1.52
1:C:657:ASN:ND2	3:C:1306:NAG:C1	1.96	1.28
1:A:657:ASN:ND2	3:A:1306:NAG:C1	1.96	1.27
1:B:657:ASN:ND2	3:B:1306:NAG:C1	1.96	1.27
1:C:321:GLN:O	1:C:628:GLN:NE2	2.15	0.80
1:B:321:GLN:O	1:B:628:GLN:NE2	2.15	0.80
1:A:321:GLN:O	1:A:628:GLN:NE2	2.15	0.79
1:A:323:THR:OG1	1:A:324:GLU:OE1	2.02	0.77
1:C:331:ASN:N	1:C:331:ASN:OD1	2.18	0.77
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.02	0.77
1:B:331:ASN:OD1	1:B:331:ASN:N	2.18	0.76
1:A:331:ASN:N	1:A:331:ASN:OD1	2.18	0.76
1:A:328:ARG:NH2	1:A:531:THR:O	2.19	0.75
1:C:328:ARG:NH2	1:C:531:THR:O	2.19	0.75
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.02	0.75
1:B:328:ARG:NH2	1:B:531:THR:O	2.19	0.74
1:A:880:SER:OG	1:A:890:LEU:O	2.04	0.74
1:B:318:PHE:O	1:B:321:GLN:NE2	2.22	0.72
1:A:318:PHE:O	1:A:321:GLN:NE2	2.22	0.72
1:B:571:ASP:OD1	1:C:963:SER:OG	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:PHE:O	1:C:321:GLN:NE2	2.22	0.72
1:A:37:TYR:OH	1:A:53:ASP:OD2	2.11	0.69
1:A:998:GLN:OE1	1:C:998:GLN:NE2	2.25	0.69
1:B:998:GLN:NE2	1:C:998:GLN:OE1	2.26	0.69
1:C:37:TYR:OH	1:C:53:ASP:OD2	2.11	0.69
1:B:37:TYR:OH	1:B:53:ASP:OD2	2.10	0.68
1:A:998:GLN:NE2	1:B:998:GLN:OE1	2.26	0.67
1:A:134:GLN:N	1:A:162:SER:OG	2.27	0.67
1:C:134:GLN:N	1:C:162:SER:OG	2.27	0.67
1:B:134:GLN:N	1:B:162:SER:OG	2.27	0.67
1:B:328:ARG:NH1	1:B:580:GLN:OE1	2.29	0.66
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.29	0.66
1:A:654:GLU:OE2	1:A:687:SER:OG	2.09	0.66
1:B:654:GLU:OE2	1:B:687:SER:OG	2.09	0.66
1:A:571:ASP:OD1	1:B:963:SER:OG	2.04	0.66
1:A:442:ASP:O	1:A:448:ASN:ND2	2.29	0.65
1:B:99:ASN:O	1:B:102:ARG:NH1	2.30	0.65
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.29	0.65
1:C:99:ASN:O	1:C:102:ARG:NH1	2.30	0.65
1:A:99:ASN:O	1:A:102:ARG:NH1	2.30	0.65
1:C:442:ASP:O	1:C:448:ASN:ND2	2.29	0.65
1:B:442:ASP:O	1:B:448:ASN:ND2	2.29	0.64
3:A:1302:NAG:O3	3:A:1302:NAG:O7	2.15	0.64
1:C:654:GLU:OE2	1:C:687:SER:OG	2.09	0.64
3:C:1302:NAG:O7	3:C:1302:NAG:O3	2.15	0.64
1:A:1024:LYS:NZ	1:A:1038:PHE:O	2.32	0.63
1:B:1024:LYS:NZ	1:B:1038:PHE:O	2.32	0.63
3:B:1302:NAG:O7	3:B:1302:NAG:O3	2.15	0.63
1:C:1024:LYS:NZ	1:C:1038:PHE:O	2.32	0.63
1:B:574:ASP:OD1	1:B:575:ALA:N	2.33	0.62
1:C:1047:SER:OG	1:C:1060:HIS:ND1	2.25	0.62
1:A:574:ASP:OD1	1:A:575:ALA:N	2.32	0.62
1:C:137:ASN:ND2	3:C:1313:NAG:O7	2.33	0.62
1:A:695:LEU:HD21	1:B:865:MET:HE3	1.82	0.62
1:C:574:ASP:OD1	1:C:575:ALA:N	2.33	0.62
1:B:137:ASN:ND2	3:B:1313:NAG:O7	2.33	0.61
1:C:324:GLU:OE1	1:C:324:GLU:N	2.33	0.61
1:A:1087:ARG:NH2	1:A:1116:THR:O	2.33	0.61
1:A:137:ASN:ND2	3:A:1313:NAG:O7	2.33	0.61
1:A:324:GLU:OE1	1:A:324:GLU:N	2.33	0.61
1:C:1087:ARG:NH2	1:C:1116:THR:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLU:OE1	1:B:324:GLU:N	2.33	0.61
1:B:1087:ARG:NH2	1:B:1116:THR:O	2.34	0.60
1:B:1047:SER:OG	1:B:1060:HIS:ND1	2.25	0.60
1:C:880:SER:OG	1:C:890:LEU:O	2.04	0.60
1:A:963:SER:OG	1:C:571:ASP:OD1	2.06	0.59
1:B:880:SER:OG	1:B:890:LEU:O	2.04	0.59
1:A:563:GLN:O	1:A:577:ARG:NH2	2.36	0.59
1:C:563:GLN:O	1:C:577:ARG:NH2	2.36	0.59
1:B:563:GLN:O	1:B:577:ARG:NH2	2.36	0.59
1:A:23:GLN:N	1:A:23:GLN:OE1	2.36	0.58
1:A:31:SER:O	1:A:59:PHE:N	2.36	0.58
1:C:23:GLN:OE1	1:C:23:GLN:N	2.36	0.58
1:C:31:SER:O	1:C:59:PHE:N	2.36	0.58
1:B:31:SER:O	1:B:59:PHE:N	2.36	0.58
1:B:23:GLN:N	1:B:23:GLN:OE1	2.36	0.57
1:C:218:GLN:OE1	1:C:218:GLN:N	2.38	0.57
1:A:218:GLN:N	1:A:218:GLN:OE1	2.38	0.57
1:B:218:GLN:N	1:B:218:GLN:OE1	2.38	0.56
1:A:695:LEU:HD21	1:B:865:MET:CE	2.35	0.56
1:A:865:MET:CE	1:C:695:LEU:HD21	2.36	0.56
1:A:721:GLU:OE2	1:A:1060:HIS:NE2	2.39	0.55
1:C:296:LEU:O	1:C:299:THR:OG1	2.24	0.55
1:A:437:ASN:OD1	1:A:438:SER:N	2.39	0.55
1:C:721:GLU:OE2	1:C:1060:HIS:NE2	2.39	0.55
1:B:437:ASN:OD1	1:B:438:SER:N	2.39	0.55
1:A:520:ALA:HB2	1:B:41:LYS:HE2	1.89	0.55
1:C:437:ASN:OD1	1:C:438:SER:N	2.39	0.54
1:C:732:VAL:HG22	1:C:854:LEU:HD23	1.89	0.54
1:C:1122:CYS:HB2	1:C:1128:ILE:HD13	1.89	0.54
1:A:41:LYS:HE2	1:C:520:ALA:HB2	1.89	0.54
1:A:617:CYS:N	1:A:649:CYS:SG	2.81	0.54
1:A:965:ASN:ND2	1:B:751:GLN:OE1	2.40	0.54
1:B:732:VAL:HG22	1:B:854:LEU:HD23	1.89	0.54
1:B:766:ILE:HD11	1:B:1008:LEU:HD23	1.89	0.54
1:A:732:VAL:HG22	1:A:854:LEU:HD23	1.89	0.54
1:A:296:LEU:O	1:A:299:THR:OG1	2.24	0.54
1:A:751:GLN:OE1	1:C:965:ASN:ND2	2.41	0.54
1:B:1122:CYS:HB2	1:B:1128:ILE:HD13	1.89	0.54
1:A:367:VAL:HG23	1:A:368:LEU:HD22	1.90	0.54
1:A:1122:CYS:HB2	1:A:1128:ILE:HD13	1.89	0.54
1:A:766:ILE:HD11	1:A:1008:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:VAL:HG23	1:B:368:LEU:HD22	1.90	0.54
1:C:617:CYS:N	1:C:649:CYS:SG	2.80	0.54
1:B:617:CYS:N	1:B:649:CYS:SG	2.81	0.53
1:B:695:LEU:HD21	1:C:865:MET:CE	2.37	0.53
1:B:721:GLU:OE2	1:B:1060:HIS:NE2	2.39	0.53
1:C:326:ILE:HD12	1:C:539:VAL:HG11	1.89	0.53
1:A:326:ILE:HD12	1:A:539:VAL:HG11	1.89	0.53
1:A:865:MET:HE3	1:C:695:LEU:HD21	1.90	0.53
1:B:326:ILE:HD12	1:B:539:VAL:HG11	1.89	0.53
1:C:367:VAL:HG23	1:C:368:LEU:HD22	1.90	0.53
1:C:766:ILE:HD11	1:C:1008:LEU:HD23	1.89	0.53
1:B:112:SER:N	1:B:133:PHE:O	2.42	0.53
1:B:525:CYS:SG	1:B:526:GLY:N	2.83	0.52
1:C:112:SER:N	1:C:133:PHE:O	2.43	0.52
1:A:1047:SER:OG	1:A:1060:HIS:ND1	2.25	0.52
1:B:965:ASN:ND2	1:C:751:GLN:OE1	2.42	0.52
1:A:525:CYS:SG	1:A:526:GLY:N	2.83	0.52
1:B:695:LEU:HD21	1:C:865:MET:HE3	1.90	0.52
1:C:141:LEU:O	1:C:153:MET:N	2.43	0.52
1:A:112:SER:N	1:A:133:PHE:O	2.43	0.52
1:C:444:LYS:N	1:C:448:ASN:OD1	2.43	0.51
1:C:525:CYS:SG	1:C:526:GLY:N	2.83	0.51
1:A:141:LEU:O	1:A:153:MET:N	2.43	0.51
1:A:444:LYS:N	1:A:448:ASN:OD1	2.43	0.51
1:A:946:ASP:OD1	1:A:947:VAL:N	2.44	0.50
1:B:229:LEU:HB3	1:B:231:ILE:HD11	1.93	0.50
1:B:296:LEU:O	1:B:299:THR:OG1	2.24	0.50
1:B:141:LEU:O	1:B:153:MET:N	2.43	0.50
1:C:229:LEU:HB3	1:C:231:ILE:HD11	1.94	0.50
1:C:629:LEU:O	1:C:634:ARG:NH1	2.44	0.50
1:C:946:ASP:OD1	1:C:947:VAL:N	2.44	0.50
1:A:913:TYR:HB3	1:C:1125:VAL:HG23	1.94	0.50
1:A:800:GLN:O	1:A:812:SER:OG	2.30	0.50
1:B:800:GLN:O	1:B:812:SER:OG	2.30	0.50
1:B:946:ASP:OD1	1:B:947:VAL:N	2.44	0.49
1:A:95:THR:OG1	1:A:210:ILE:HD11	2.13	0.49
1:A:629:LEU:O	1:A:634:ARG:NH1	2.44	0.49
1:C:95:THR:OG1	1:C:210:ILE:HD11	2.13	0.49
1:C:782:LYS:HE3	1:C:782:LYS:HA	1.95	0.49
1:A:782:LYS:HE3	1:A:782:LYS:HA	1.95	0.49
1:B:444:LYS:N	1:B:448:ASN:OD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:O	1:B:634:ARG:NH1	2.44	0.49
1:B:713:ASN:HD21	2:I:1:NAG:C7	2.26	0.49
1:B:520:ALA:HB2	1:C:41:LYS:HE2	1.96	0.48
1:C:800:GLN:O	1:C:812:SER:OG	2.30	0.48
1:A:229:LEU:HB3	1:A:231:ILE:HD11	1.94	0.48
1:B:95:THR:OG1	1:B:210:ILE:HD11	2.12	0.48
1:B:782:LYS:HA	1:B:782:LYS:HE3	1.95	0.48
1:A:910:ASN:ND2	1:C:1119:SER:OG	2.46	0.48
1:A:977:LEU:O	1:C:386:LYS:NZ	2.41	0.48
1:B:1036:VAL:HG12	1:B:1037:ASP:OD2	2.14	0.48
1:A:713:ASN:HD21	2:E:1:NAG:C7	2.26	0.48
1:C:1036:VAL:HG12	1:C:1037:ASP:OD2	2.14	0.48
1:B:437:ASN:OD1	1:B:439:ASN:N	2.47	0.47
1:B:1119:SER:OG	1:C:910:ASN:ND2	2.48	0.47
1:C:713:ASN:HD21	2:M:1:NAG:C7	2.26	0.47
1:A:386:LYS:NZ	1:B:980:LEU:O	2.44	0.47
1:C:358:ILE:HB	1:C:395:VAL:HG23	1.97	0.47
1:A:1036:VAL:HG12	1:A:1037:ASP:OD2	2.14	0.47
1:C:319:ARG:NH1	1:C:592:PHE:O	2.49	0.46
1:A:319:ARG:NH1	1:A:592:PHE:O	2.49	0.46
1:A:1119:SER:OG	1:B:910:ASN:ND2	2.48	0.46
1:A:358:ILE:HB	1:A:395:VAL:HG23	1.97	0.46
1:B:319:ARG:NH1	1:B:592:PHE:O	2.49	0.46
1:B:358:ILE:HB	1:B:395:VAL:HG23	1.97	0.46
1:A:83:VAL:HG11	1:A:237:ARG:NH2	2.31	0.46
1:A:437:ASN:OD1	1:A:439:ASN:N	2.47	0.46
1:C:901:ARG:NH1	1:C:1045:LEU:O	2.49	0.46
1:B:83:VAL:HG11	1:B:237:ARG:NH2	2.31	0.45
1:A:980:LEU:O	1:C:386:LYS:NZ	2.45	0.45
1:A:386:LYS:NZ	1:B:977:LEU:O	2.41	0.45
1:A:581:THR:O	1:A:583:GLU:N	2.50	0.45
1:A:1125:VAL:HG23	1:B:913:TYR:HB3	1.97	0.45
1:B:915:ASN:O	1:B:919:ILE:HD12	2.17	0.45
1:C:83:VAL:HG11	1:C:237:ARG:NH2	2.31	0.45
1:A:901:ARG:NH1	1:A:1045:LEU:O	2.49	0.45
1:B:901:ARG:NH1	1:B:1045:LEU:O	2.49	0.45
1:A:1122:CYS:CB	1:A:1128:ILE:HD13	2.46	0.45
1:C:915:ASN:O	1:C:919:ILE:HD12	2.17	0.45
1:B:1125:VAL:HG23	1:C:913:TYR:HB3	1.97	0.45
1:A:289:VAL:HG23	1:A:306:PHE:CZ	2.52	0.45
1:A:361:CYS:HB2	1:A:524:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:CYS:HB2	1:C:524:VAL:HG23	1.98	0.45
1:C:1122:CYS:CB	1:C:1128:ILE:HD13	2.46	0.45
1:B:289:VAL:HG23	1:B:306:PHE:CZ	2.52	0.45
1:C:437:ASN:OD1	1:C:439:ASN:N	2.47	0.45
1:A:915:ASN:O	1:A:919:ILE:HD12	2.17	0.44
1:A:738:ILE:O	1:A:996:ARG:NH1	2.50	0.44
1:B:361:CYS:HB2	1:B:524:VAL:HG23	1.98	0.44
1:A:900:TYR:OH	1:C:1090:VAL:HG11	2.17	0.44
1:B:738:ILE:O	1:B:996:ARG:NH1	2.50	0.44
1:B:581:THR:O	1:B:583:GLU:N	2.50	0.44
1:C:289:VAL:HG23	1:C:306:PHE:CZ	2.52	0.44
1:B:386:LYS:NZ	1:C:980:LEU:O	2.48	0.44
1:B:1122:CYS:CB	1:B:1128:ILE:HD13	2.46	0.44
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.51	0.43
1:B:711:PRO:O	1:B:1106:TYR:N	2.51	0.43
1:C:501:ASN:OD1	1:C:502:GLY:N	2.50	0.43
1:A:711:PRO:O	1:A:1106:TYR:N	2.52	0.43
1:B:368:LEU:O	1:B:372:ALA:N	2.51	0.43
1:C:368:LEU:O	1:C:372:ALA:N	2.51	0.43
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.34	0.43
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.51	0.43
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.51	0.43
1:A:16:VAL:HG23	1:A:138:ASP:OD2	2.19	0.43
1:B:480:CYS:O	1:B:483:VAL:HG22	2.19	0.43
1:B:912:LEU:O	1:B:916:GLN:N	2.52	0.43
1:C:16:VAL:HG23	1:C:138:ASP:OD2	2.19	0.43
1:B:501:ASN:OD1	1:B:502:GLY:N	2.50	0.43
1:C:480:CYS:O	1:C:483:VAL:HG22	2.19	0.43
1:A:480:CYS:O	1:A:483:VAL:HG22	2.19	0.43
1:B:16:VAL:HG23	1:B:138:ASP:OD2	2.19	0.43
1:B:386:LYS:NZ	1:C:977:LEU:O	2.44	0.43
1:A:1085:PHE:O	1:A:1116:THR:OG1	2.19	0.43
1:C:912:LEU:O	1:C:916:GLN:N	2.52	0.43
1:B:1090:VAL:HG11	1:C:900:TYR:OH	2.19	0.43
3:A:1305:NAG:O7	3:A:1305:NAG:O3	2.34	0.42
1:B:355:ARG:NH2	1:C:200:TYR:OH	2.52	0.42
1:A:1046:MET:HE3	1:A:1061:VAL:HG11	2.01	0.42
1:A:912:LEU:O	1:A:916:GLN:N	2.52	0.42
1:C:738:ILE:O	1:C:996:ARG:NH1	2.50	0.42
1:A:822:VAL:HG11	1:A:1053:PRO:HG2	2.02	0.42
1:C:581:THR:O	1:C:583:GLU:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1085:PHE:O	1:C:1116:THR:OG1	2.19	0.42
1:A:501:ASN:OD1	1:A:502:GLY:N	2.50	0.42
1:B:1091:PHE:CD1	1:B:1100:VAL:HG12	2.55	0.42
1:A:365:TYR:OH	1:A:388:ASN:ND2	2.53	0.42
1:B:822:VAL:HG11	1:B:1053:PRO:HG2	2.02	0.42
1:C:1091:PHE:CD1	1:C:1100:VAL:HG12	2.55	0.42
1:C:365:TYR:OH	1:C:388:ASN:ND2	2.53	0.42
3:B:1305:NAG:O7	3:B:1305:NAG:O3	2.34	0.42
1:A:355:ARG:NH2	1:B:200:TYR:OH	2.53	0.41
1:A:1090:VAL:HG11	1:B:900:TYR:OH	2.19	0.41
1:C:711:PRO:O	1:C:1106:TYR:N	2.51	0.41
1:A:200:TYR:OH	1:C:355:ARG:NH2	2.54	0.41
1:A:83:VAL:HG11	1:A:237:ARG:HH21	1.85	0.41
1:B:365:TYR:OH	1:B:388:ASN:ND2	2.53	0.41
1:B:732:VAL:HG22	1:B:854:LEU:CD2	2.51	0.41
1:C:410:ILE:HD11	1:C:418:ILE:HG21	2.03	0.41
1:A:368:LEU:O	1:A:372:ALA:N	2.51	0.41
1:B:339:GLY:O	1:B:343:ASN:N	2.51	0.41
1:C:83:VAL:HG11	1:C:237:ARG:HH21	1.85	0.41
1:C:822:VAL:HG11	1:C:1053:PRO:HG2	2.02	0.41
1:A:1091:PHE:CD1	1:A:1100:VAL:HG12	2.55	0.41
1:C:102:ARG:NE	1:C:121:ASN:O	2.51	0.41
1:A:334:ASN:O	1:A:362:VAL:HG12	2.21	0.41
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.34	0.41
1:C:919:ILE:HD12	1:C:919:ILE:H	1.87	0.41
1:C:1077:ILE:C	1:C:1128:ILE:HD11	2.41	0.41
1:B:130:VAL:HG22	1:B:168:PHE:HB3	2.04	0.40
1:B:1013:GLU:OE1	1:B:1013:GLU:HA	2.22	0.40
1:C:339:GLY:O	1:C:343:ASN:N	2.51	0.40
1:A:515:PHE:CE2	1:A:517:LEU:HD11	2.57	0.40
1:C:327:VAL:O	1:C:531:THR:N	2.49	0.40
1:C:515:PHE:CE2	1:C:517:LEU:HD11	2.57	0.40
1:A:339:GLY:O	1:A:343:ASN:N	2.51	0.40
1:A:410:ILE:HD11	1:A:418:ILE:HG21	2.03	0.40
1:A:1077:ILE:C	1:A:1128:ILE:HD11	2.41	0.40
1:B:919:ILE:HD12	1:B:919:ILE:H	1.86	0.40
1:C:334:ASN:O	1:C:362:VAL:HG12	2.21	0.40
1:C:848:ALA:O	1:C:852:ASN:ND2	2.54	0.40
1:A:919:ILE:HD12	1:A:919:ILE:H	1.87	0.40
1:A:1013:GLU:HA	1:A:1013:GLU:OE1	2.22	0.40
1:B:1085:PHE:O	1:B:1116:THR:OG1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:OH	1:C:191:GLU:OE1	2.34	0.40
1:C:130:VAL:HG22	1:C:168:PHE:HB3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1057/1247 (85%)	1018 (96%)	39 (4%)	0	100	100
1	B	1057/1247 (85%)	1018 (96%)	39 (4%)	0	100	100
1	C	1058/1247 (85%)	1018 (96%)	40 (4%)	0	100	100
All	All	3172/3741 (85%)	3054 (96%)	118 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	930/1081 (86%)	923 (99%)	7 (1%)	79	88
1	B	930/1081 (86%)	923 (99%)	7 (1%)	79	88
1	C	930/1081 (86%)	923 (99%)	7 (1%)	79	88
All	All	2790/3243 (86%)	2769 (99%)	21 (1%)	77	88

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

Mol	Chain	Res	Type
1	A	319	ARG
1	A	331	ASN
1	A	529	LYS
1	A	701	VAL
1	A	864	GLU
1	A	1013	GLU
1	A	1037	ASP
1	B	319	ARG
1	B	331	ASN
1	B	529	LYS
1	B	701	VAL
1	B	864	GLU
1	B	1013	GLU
1	B	1037	ASP
1	C	319	ARG
1	C	331	ASN
1	C	529	LYS
1	C	701	VAL
1	C	864	GLU
1	C	1013	GLU
1	C	1037	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	657	ASN
1	A	998	GLN
1	B	657	ASN
1	B	998	GLN
1	C	657	ASN
1	C	998	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	D	1	2,1	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	D	2	2	14,14,15	0.17	0	17,19,21	0.43	0
2	NAG	E	1	2,1	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	E	2	2	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	F	1	2,1	14,14,15	0.43	0	17,19,21	0.87	1 (5%)
2	NAG	F	2	2	14,14,15	0.20	0	17,19,21	0.53	0
2	NAG	G	1	2,1	14,14,15	0.23	0	17,19,21	0.36	0
2	NAG	G	2	2	14,14,15	0.19	0	17,19,21	0.39	0
2	NAG	H	1	2,1	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	H	2	2	14,14,15	0.17	0	17,19,21	0.42	0
2	NAG	I	1	2,1	14,14,15	0.28	0	17,19,21	0.57	0
2	NAG	I	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	J	1	2,1	14,14,15	0.41	0	17,19,21	0.87	1 (5%)
2	NAG	J	2	2	14,14,15	0.20	0	17,19,21	0.52	0
2	NAG	K	1	2,1	14,14,15	0.22	0	17,19,21	0.37	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.39	0
2	NAG	L	1	2,1	14,14,15	0.18	0	17,19,21	0.46	0
2	NAG	L	2	2	14,14,15	0.16	0	17,19,21	0.42	0
2	NAG	M	1	2,1	14,14,15	0.28	0	17,19,21	0.58	0
2	NAG	M	2	2	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	N	1	2,1	14,14,15	0.42	0	17,19,21	0.87	1 (5%)
2	NAG	N	2	2	14,14,15	0.19	0	17,19,21	0.52	0
2	NAG	O	1	2,1	14,14,15	0.23	0	17,19,21	0.37	0
2	NAG	O	2	2	14,14,15	0.20	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	1/6/23/26	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(°)
2	F	1	NAG	C1-O5-C5	2.39	115.43	112.19
2	N	1	NAG	C1-O5-C5	2.38	115.42	112.19
2	J	1	NAG	C1-O5-C5	2.37	115.40	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6

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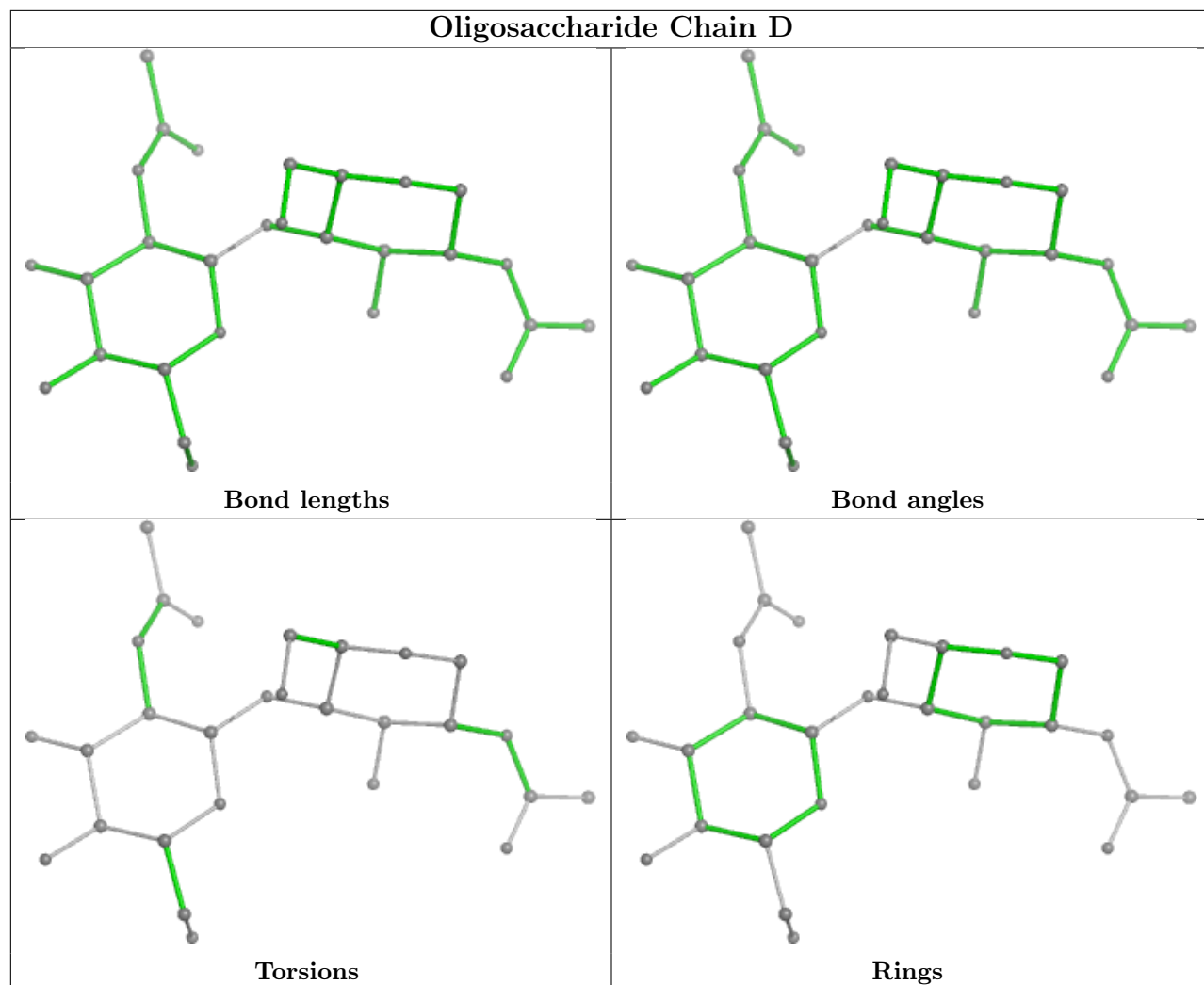
Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6

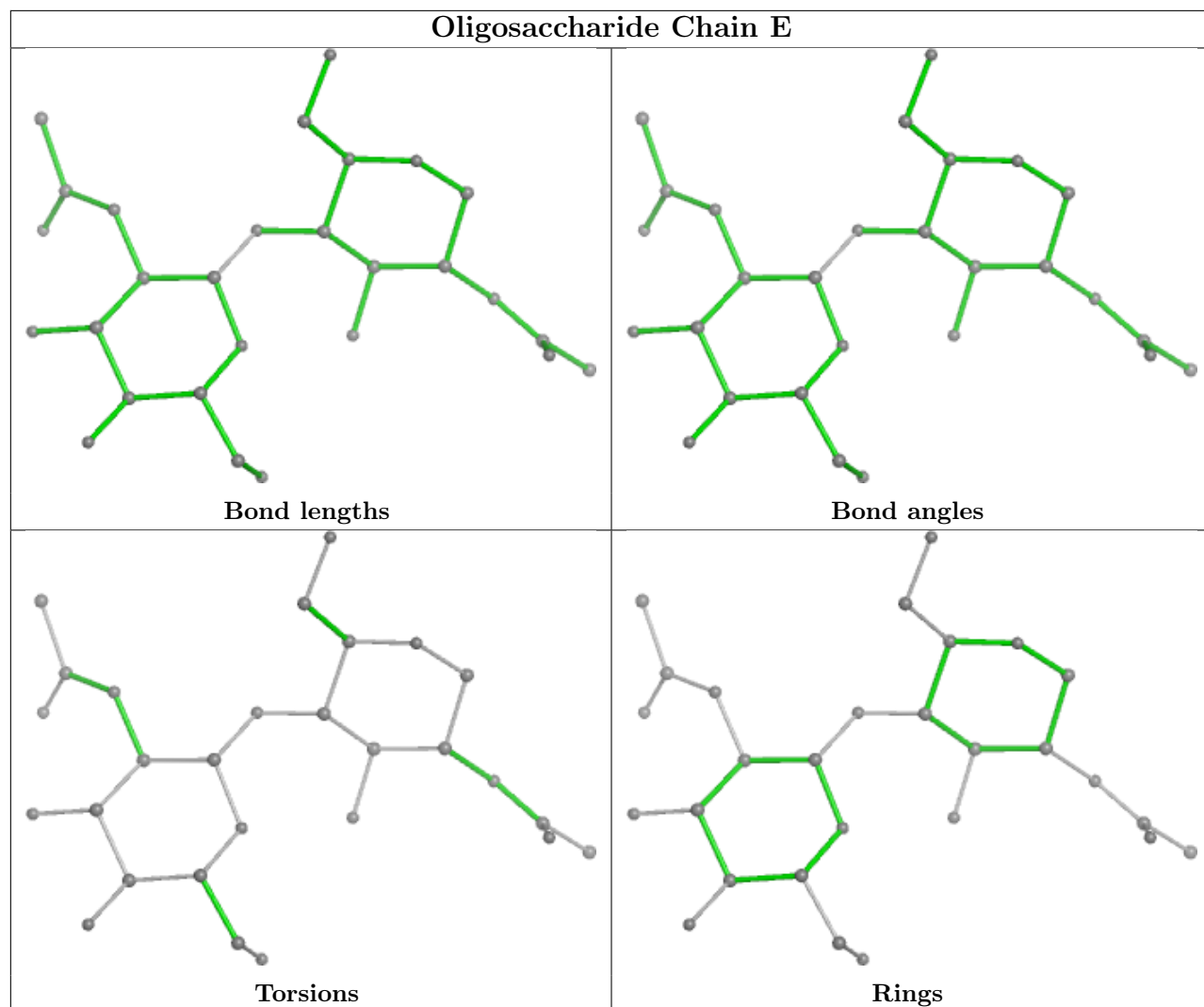
There are no ring outliers.

3 monomers are involved in 3 short contacts:

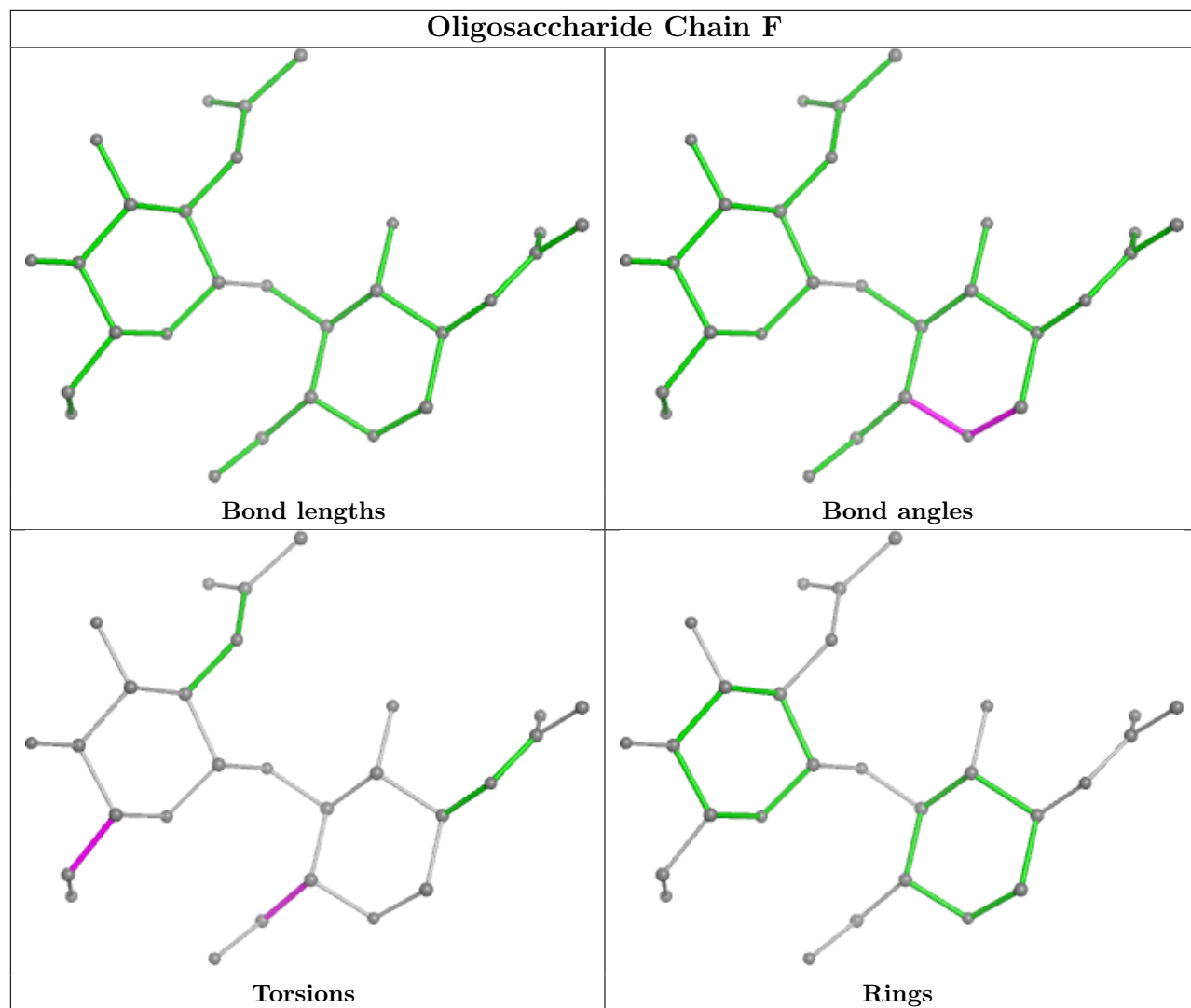
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
2	M	1	NAG	1	0
2	I	1	NAG	1	0

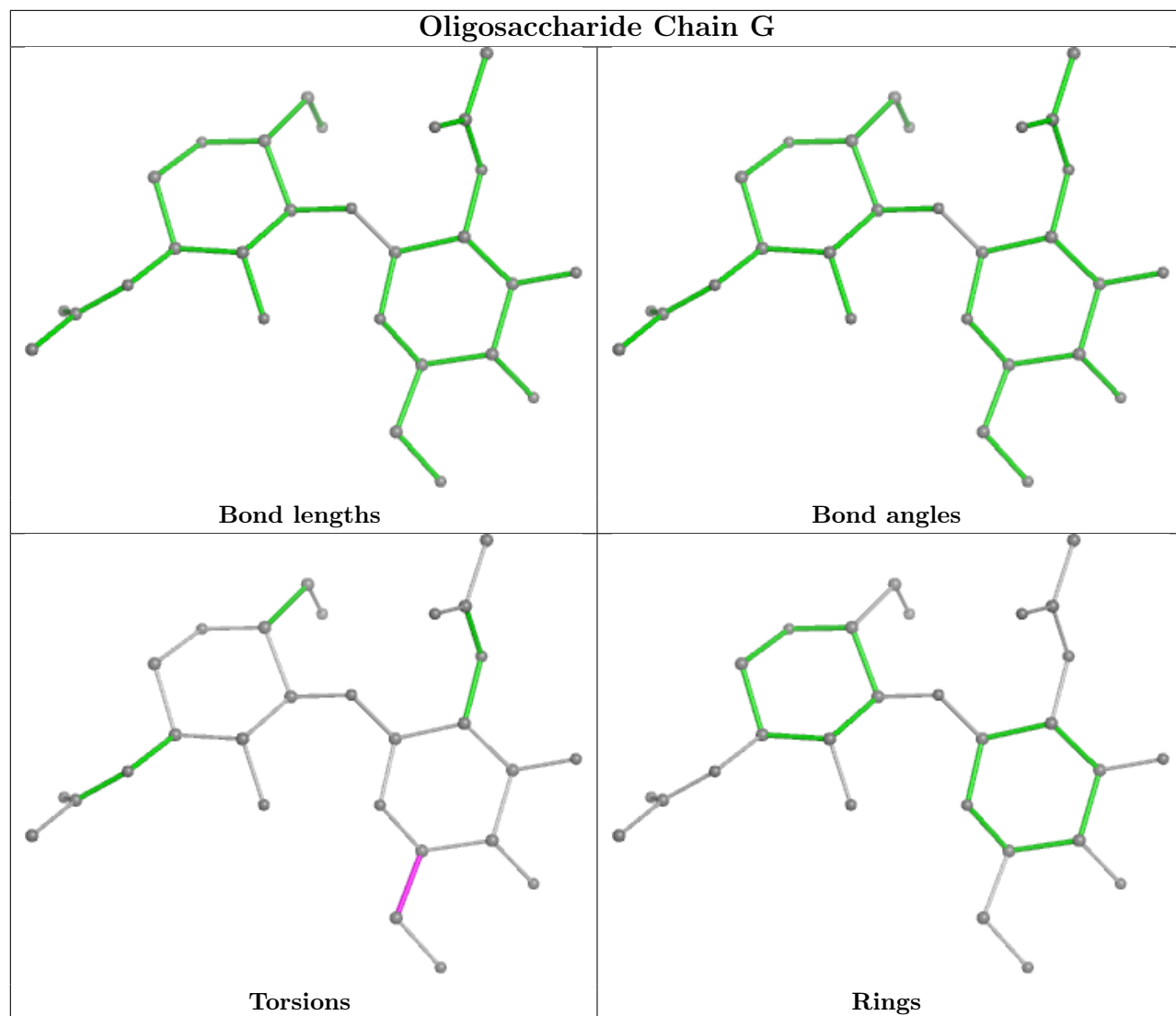
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

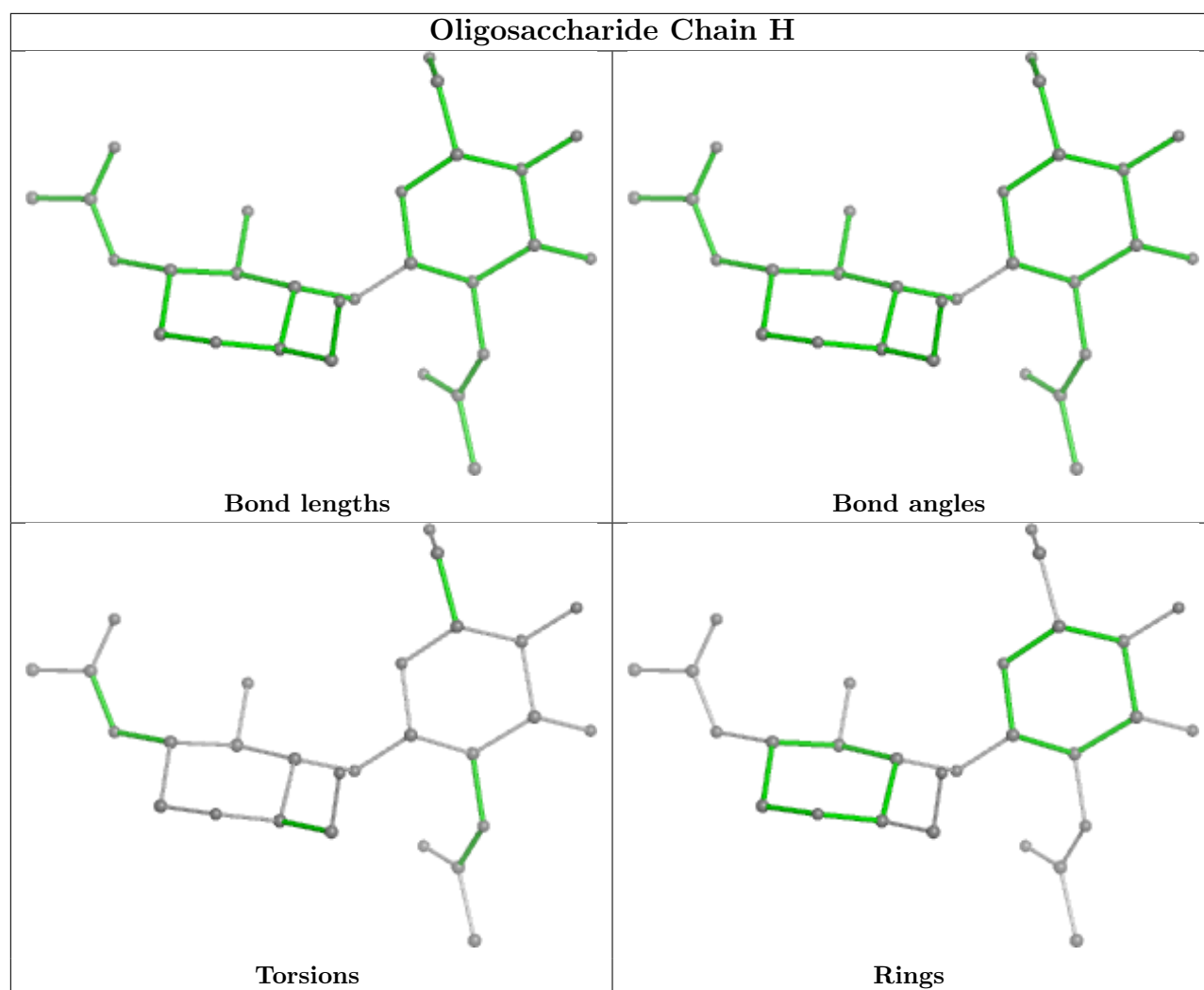


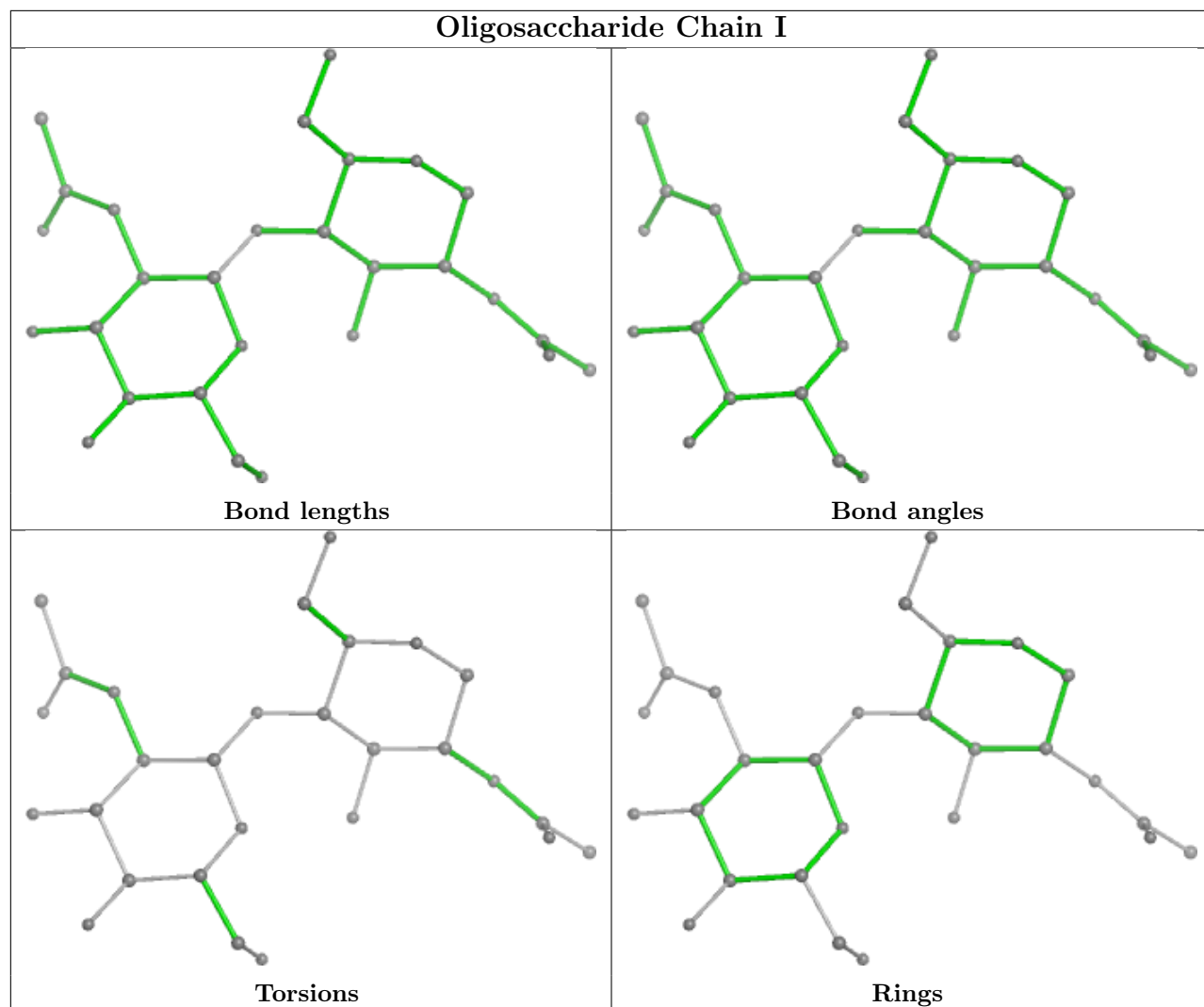


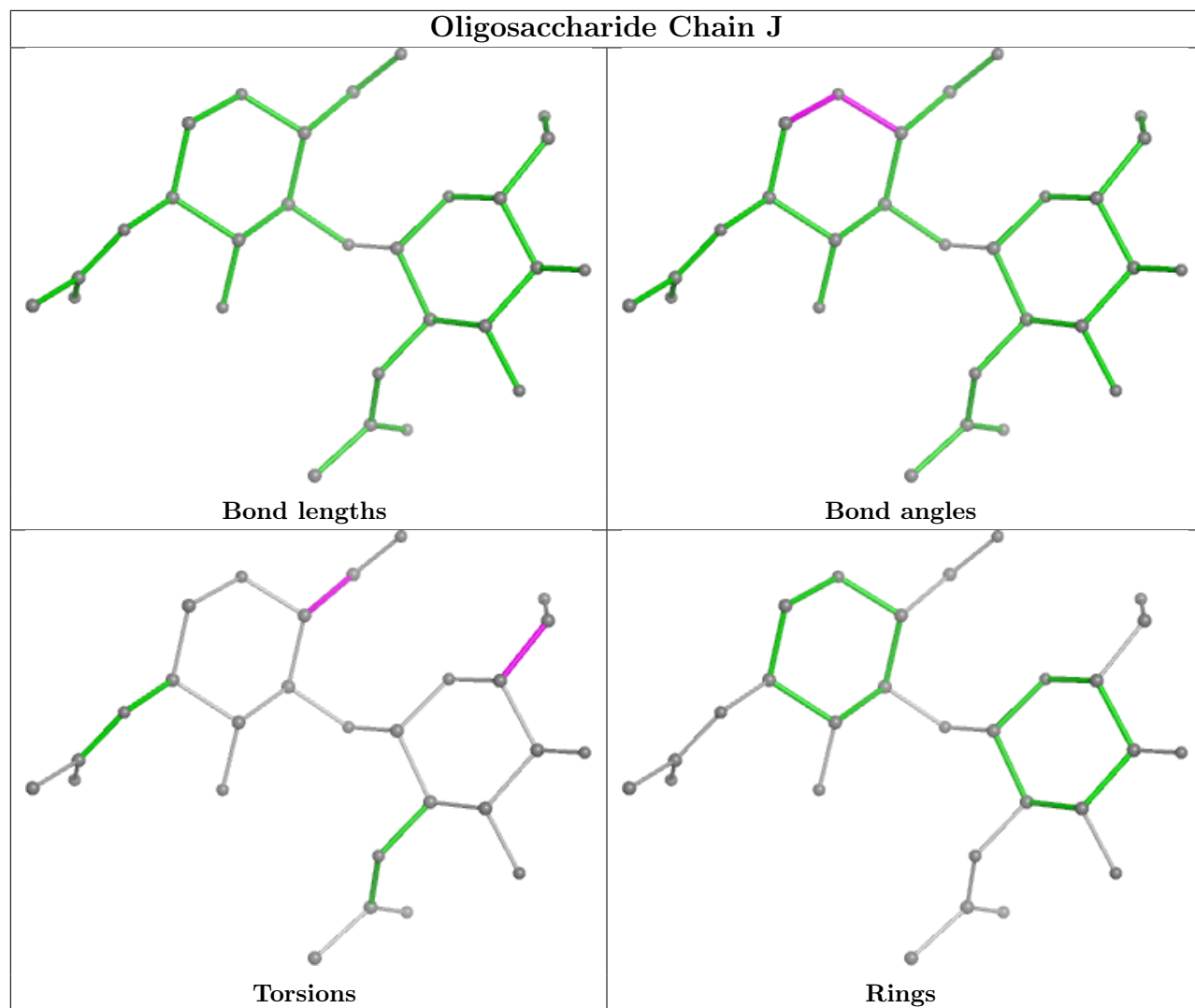


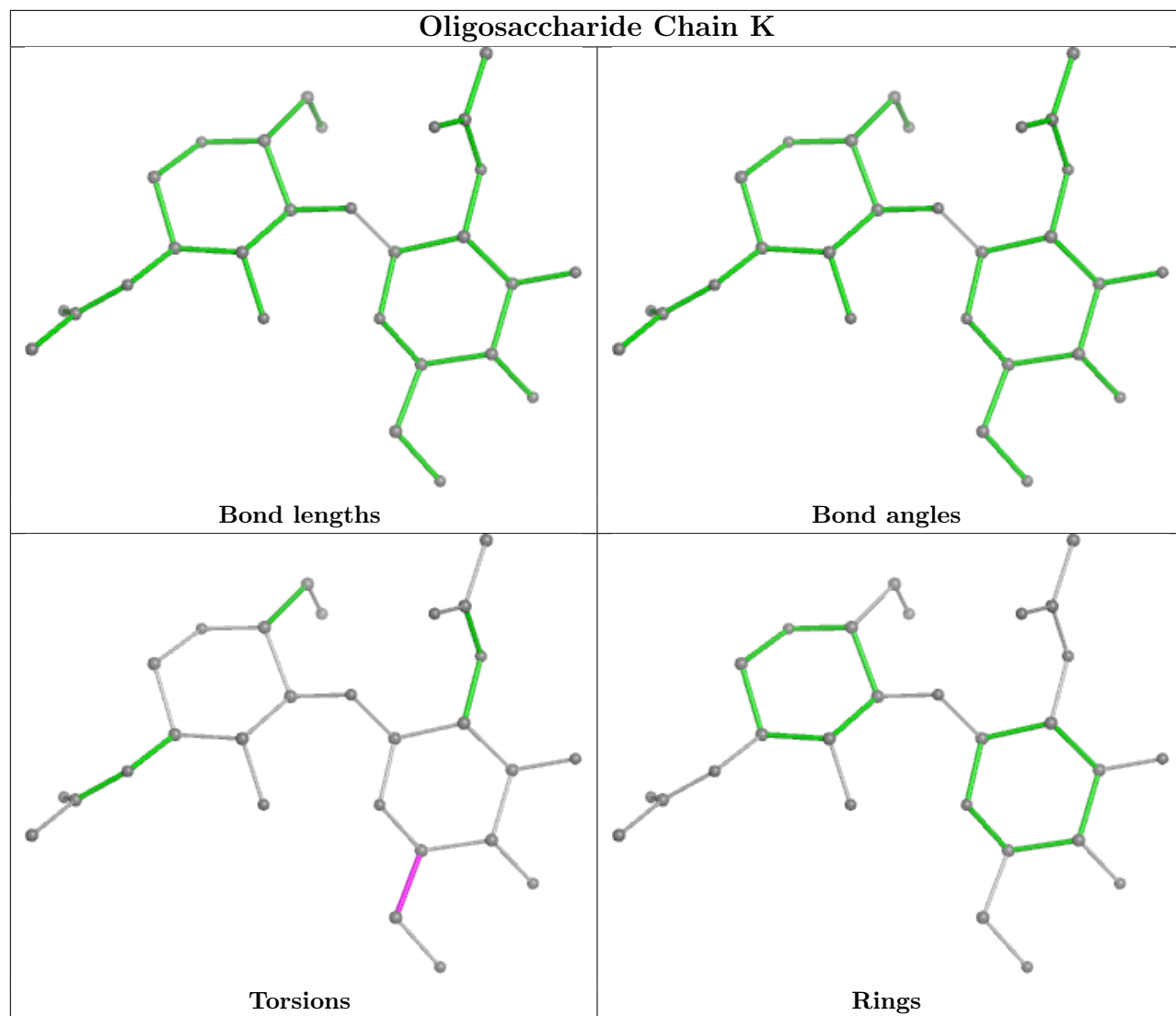


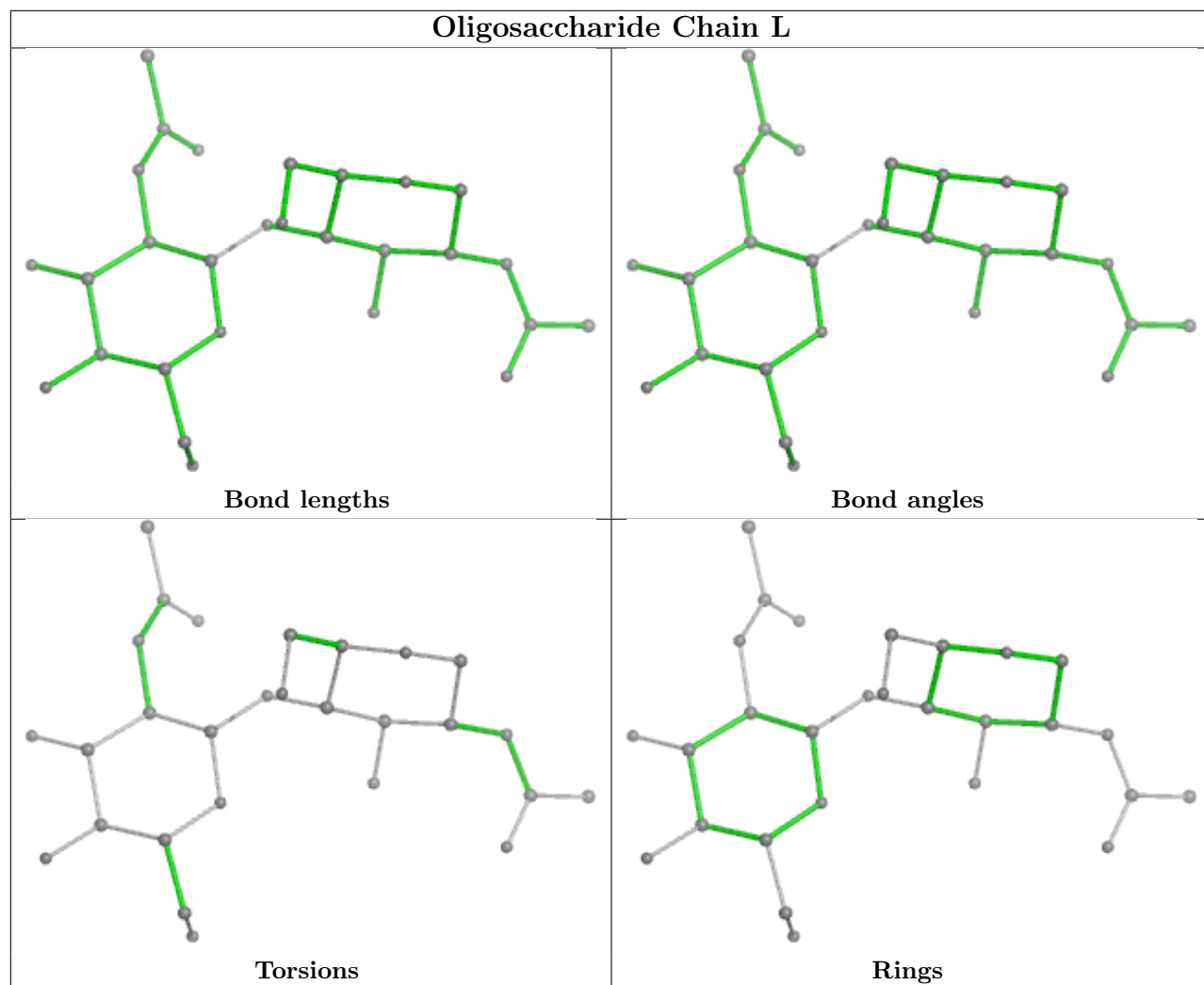


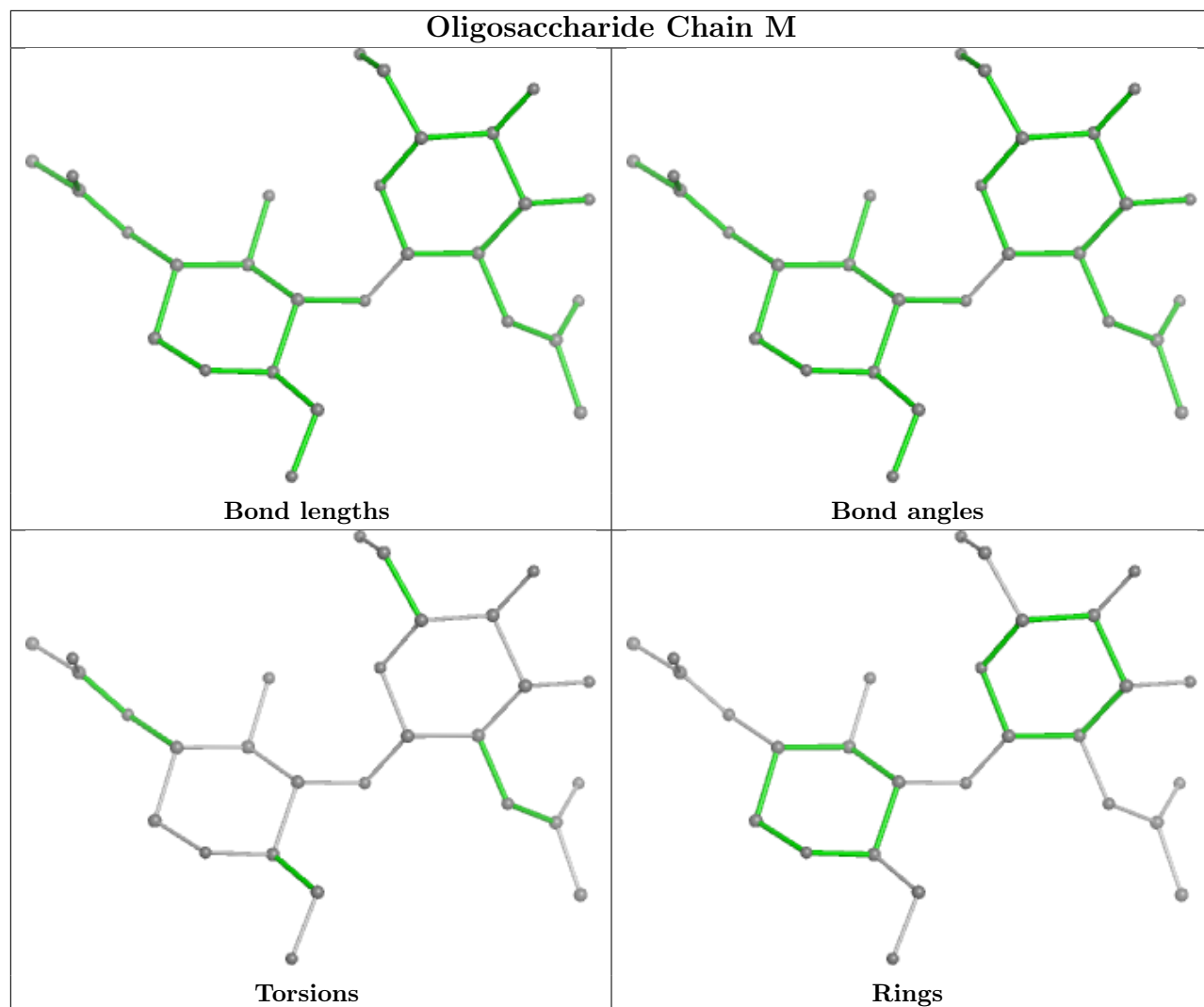




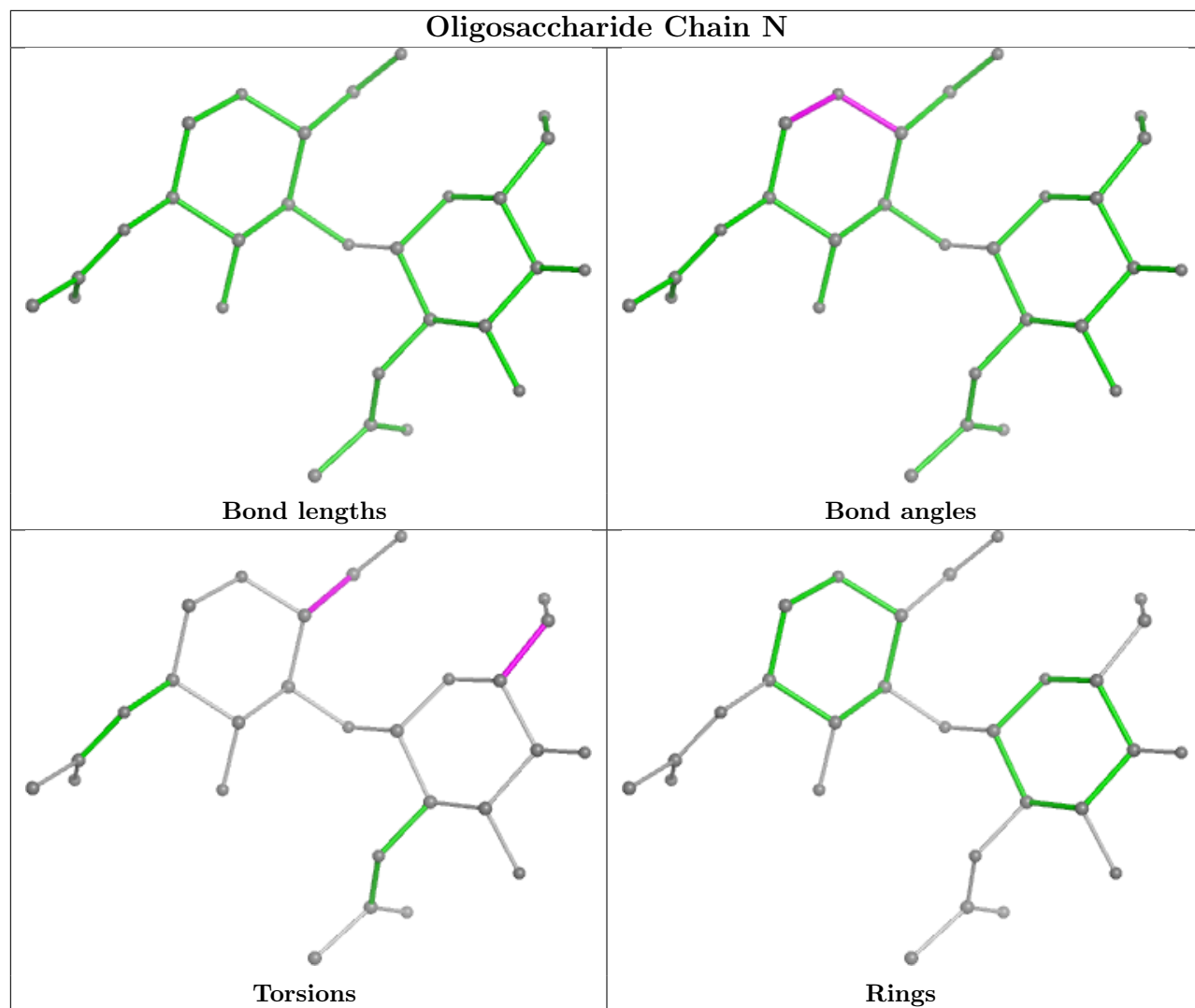


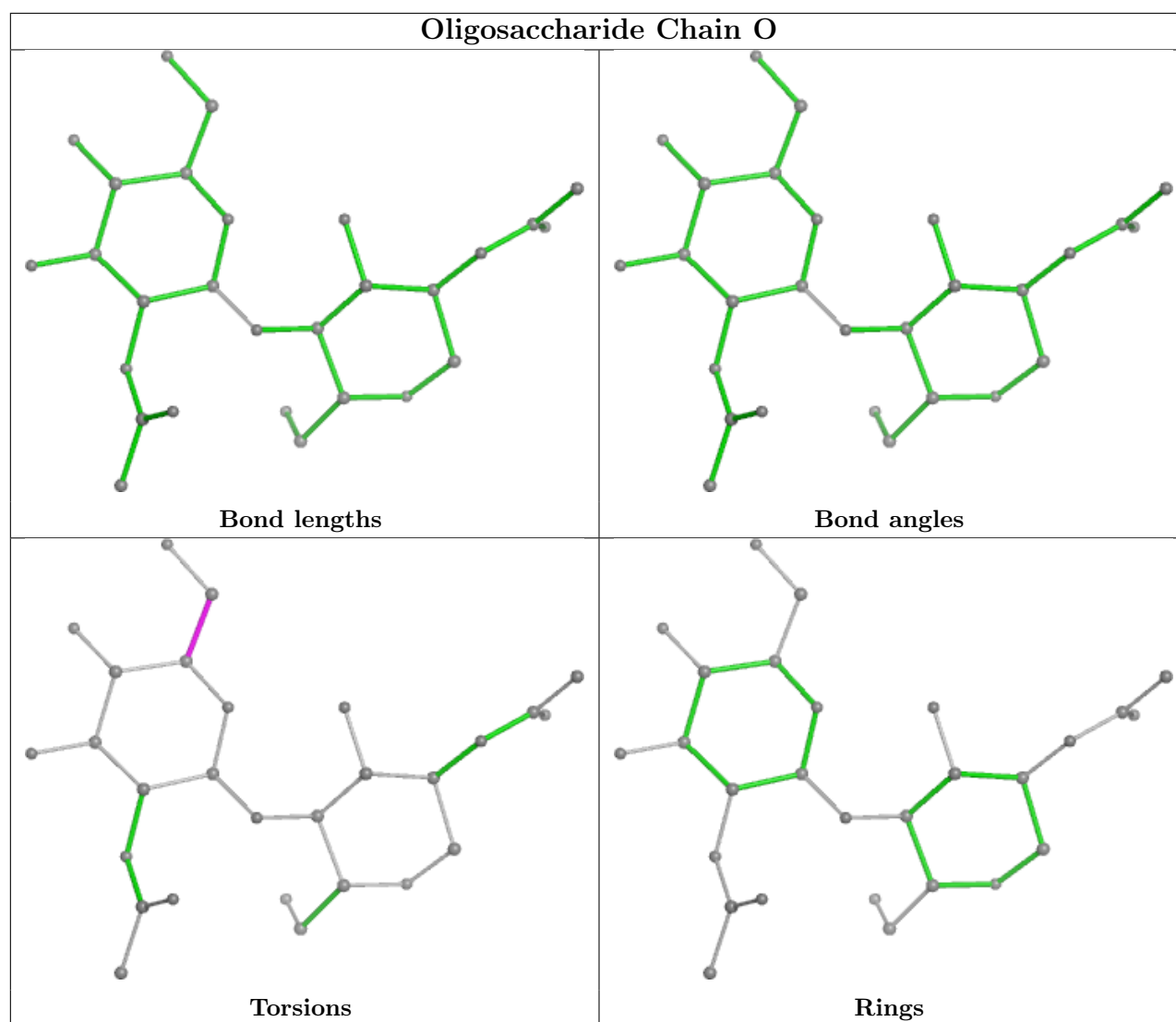












## 5.6 Ligand geometry [i](#)

42 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
4	BLA	A	1314	-	42,46,46	3.61	21 (50%)	53,67,67	1.79	10 (18%)
3	NAG	C	1309	1	14,14,15	0.17	0	17,19,21	0.39	0
3	NAG	B	1309	1	14,14,15	0.18	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1305	1	14,14,15	0.30	0	17,19,21	0.39	0
3	NAG	C	1312	1	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	B	1312	1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	A	1313	1	14,14,15	0.20	0	17,19,21	0.37	0
3	NAG	A	1303	1	14,14,15	0.53	0	17,19,21	0.86	1 (5%)
3	NAG	B	1303	1	14,14,15	0.52	0	17,19,21	0.86	1 (5%)
3	NAG	B	1313	1	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	C	1308	1	14,14,15	0.22	0	17,19,21	0.55	0
3	NAG	A	1312	1	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.56	0
3	NAG	C	1307	1	14,14,15	0.18	0	17,19,21	0.43	0
3	NAG	C	1311	1	14,14,15	0.20	0	17,19,21	0.37	0
3	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.37	0
3	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.55	0
3	NAG	B	1310	1	14,14,15	0.18	0	17,19,21	0.37	0
3	NAG	C	1306	-	14,14,15	0.45	0	17,19,21	0.44	0
3	NAG	A	1310	1	14,14,15	0.18	0	17,19,21	0.36	0
3	NAG	A	1306	-	14,14,15	0.44	0	17,19,21	0.45	0
3	NAG	C	1310	1	14,14,15	0.17	0	17,19,21	0.37	0
3	NAG	C	1301	1	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	A	1311	1	14,14,15	0.19	0	17,19,21	0.36	0
3	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	C	1302	1	14,14,15	0.39	0	17,19,21	0.40	0
3	NAG	B	1302	1	14,14,15	0.39	0	17,19,21	0.40	0
3	NAG	A	1301	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	A	1302	1	14,14,15	0.40	0	17,19,21	0.41	0
3	NAG	C	1304	1	14,14,15	0.23	0	17,19,21	0.37	0
3	NAG	B	1311	1	14,14,15	0.21	0	17,19,21	0.37	0
3	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	A	1309	1	14,14,15	0.18	0	17,19,21	0.39	0
3	NAG	B	1304	1	14,14,15	0.23	0	17,19,21	0.37	0
3	NAG	C	1303	1	14,14,15	0.53	0	17,19,21	0.87	1 (5%)
3	NAG	C	1313	1	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	B	1306	-	14,14,15	0.43	0	17,19,21	0.45	0
3	NAG	C	1305	1	14,14,15	0.31	0	17,19,21	0.39	0
3	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.40	0
3	NAG	A	1307	1	14,14,15	0.19	0	17,19,21	0.42	0
4	BLA	C	1314	-	42,46,46	3.61	21 (50%)	53,67,67	1.79	10 (18%)
4	BLA	B	1314	-	42,46,46	3.61	21 (50%)	53,67,67	1.79	10 (18%)

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	BLA	A	1314	-	-	9/26/74/74	0/4/4/4
3	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	-	-	1/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1306	-	-	1/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	-	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	BLA	C	1314	-	-	9/26/74/74	0/4/4/4
4	BLA	B	1314	-	-	9/26/74/74	0/4/4/4

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1314	BLA	C4C-NC	10.04	1.54	1.37
4	C	1314	BLA	C4C-NC	10.03	1.54	1.37
4	A	1314	BLA	C4C-NC	9.99	1.54	1.37
4	A	1314	BLA	C1B-NB	9.76	1.54	1.37
4	C	1314	BLA	C1B-NB	9.75	1.54	1.37
4	B	1314	BLA	C1B-NB	9.73	1.54	1.37
4	B	1314	BLA	C4B-NB	7.55	1.53	1.38
4	C	1314	BLA	C4B-NB	7.55	1.53	1.38
4	A	1314	BLA	C4B-NB	7.53	1.53	1.38
4	B	1314	BLA	C1C-NC	7.29	1.53	1.38
4	A	1314	BLA	C1C-NC	7.28	1.53	1.38
4	C	1314	BLA	C1C-NC	7.27	1.53	1.38
4	B	1314	BLA	C4D-ND	5.58	1.50	1.38
4	C	1314	BLA	C4D-ND	5.58	1.50	1.38
4	A	1314	BLA	C4D-ND	5.57	1.50	1.38
4	C	1314	BLA	CHD-C1D	5.54	1.53	1.40
4	A	1314	BLA	CHD-C1D	5.51	1.53	1.40
4	B	1314	BLA	CHD-C1D	5.50	1.53	1.40
4	C	1314	BLA	C3D-C2D	5.49	1.48	1.36
4	B	1314	BLA	C3D-C2D	5.48	1.48	1.36
4	A	1314	BLA	C3D-C2D	5.48	1.48	1.36
4	C	1314	BLA	C4D-C3D	5.09	1.53	1.45
4	A	1314	BLA	C4D-C3D	5.06	1.53	1.45
4	B	1314	BLA	C4D-C3D	5.04	1.53	1.45
4	B	1314	BLA	C1D-ND	4.76	1.47	1.36
4	C	1314	BLA	C1D-ND	4.74	1.47	1.36
4	A	1314	BLA	C1D-ND	4.74	1.47	1.36
4	A	1314	BLA	C1A-CHA	3.45	1.54	1.41
4	C	1314	BLA	C1A-CHA	3.45	1.54	1.41
4	B	1314	BLA	C1A-CHA	3.45	1.54	1.41
4	C	1314	BLA	C4A-CHB	3.10	1.53	1.41
4	B	1314	BLA	C4A-CHB	3.10	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1314	BLA	C4A-CHB	3.09	1.53	1.41
4	C	1314	BLA	OC-C1C	-2.86	1.18	1.23
4	B	1314	BLA	OC-C1C	-2.85	1.18	1.23
4	A	1314	BLA	OC-C1C	-2.83	1.18	1.23
4	B	1314	BLA	C3B-C2B	2.78	1.42	1.37
4	C	1314	BLA	C3B-C2B	2.75	1.42	1.37
4	A	1314	BLA	C3B-C2B	2.74	1.42	1.37
4	B	1314	BLA	C3C-C2C	2.73	1.42	1.37
4	A	1314	BLA	C3C-C2C	2.71	1.42	1.37
4	C	1314	BLA	C3C-C2C	2.70	1.42	1.37
4	B	1314	BLA	CHA-C4D	-2.66	1.32	1.35
4	A	1314	BLA	CHA-C4D	-2.65	1.32	1.35
4	C	1314	BLA	CHA-C4D	-2.65	1.32	1.35
4	A	1314	BLA	C3C-C4C	2.58	1.49	1.45
4	C	1314	BLA	C3C-C4C	2.53	1.49	1.45
4	B	1314	BLA	C3C-C4C	2.52	1.49	1.45
4	C	1314	BLA	OB-C4B	-2.52	1.18	1.23
4	C	1314	BLA	C1B-C2B	2.49	1.49	1.45
4	A	1314	BLA	C1B-C2B	2.49	1.49	1.45
4	B	1314	BLA	C1B-C2B	2.45	1.49	1.45
4	B	1314	BLA	OB-C4B	-2.45	1.18	1.23
4	A	1314	BLA	OB-C4B	-2.44	1.18	1.23
4	A	1314	BLA	CAB-C3B	2.30	1.53	1.47
4	B	1314	BLA	CAB-C3B	2.27	1.53	1.47
4	C	1314	BLA	CAB-C3B	2.26	1.53	1.47
4	A	1314	BLA	CHD-C4C	-2.12	1.32	1.38
4	C	1314	BLA	CHD-C4C	-2.11	1.32	1.38
4	B	1314	BLA	CHD-C4C	-2.09	1.32	1.38
4	C	1314	BLA	CAC-C3C	2.06	1.53	1.47
4	A	1314	BLA	CAC-C3C	2.04	1.53	1.47
4	B	1314	BLA	CAC-C3C	2.04	1.53	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1314	BLA	C1A-CHA-C4D	-7.06	120.38	128.81
4	A	1314	BLA	C1A-CHA-C4D	-7.04	120.40	128.81
4	B	1314	BLA	C1A-CHA-C4D	-7.03	120.41	128.81
4	B	1314	BLA	C3D-C4D-ND	-4.13	104.04	110.05
4	C	1314	BLA	C3D-C4D-ND	-4.13	104.05	110.05
4	A	1314	BLA	C3D-C4D-ND	-4.12	104.06	110.05
4	B	1314	BLA	C4C-CHD-C1D	-3.43	119.69	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1314	BLA	C4C-CHD-C1D	-3.43	119.71	128.08
4	A	1314	BLA	C4C-CHD-C1D	-3.42	119.72	128.08
3	C	1303	NAG	C1-O5-C5	3.19	116.52	112.19
3	B	1303	NAG	C1-O5-C5	3.17	116.49	112.19
3	A	1303	NAG	C1-O5-C5	3.17	116.48	112.19
4	C	1314	BLA	C3B-C2B-C1B	2.57	111.14	108.03
4	B	1314	BLA	C3B-C2B-C1B	2.57	111.13	108.03
4	B	1314	BLA	C4C-NC-C1C	-2.56	107.41	110.67
4	C	1314	BLA	C4C-NC-C1C	-2.55	107.43	110.67
4	A	1314	BLA	C4C-NC-C1C	-2.53	107.44	110.67
4	A	1314	BLA	C3B-C2B-C1B	2.53	111.09	108.03
4	A	1314	BLA	C1B-NB-C4B	-2.48	107.52	110.67
4	B	1314	BLA	C1B-NB-C4B	-2.46	107.54	110.67
4	B	1314	BLA	C4D-C3D-C2D	2.46	109.51	106.78
4	A	1314	BLA	C4D-C3D-C2D	2.45	109.49	106.78
4	C	1314	BLA	C1B-NB-C4B	-2.43	107.58	110.67
4	C	1314	BLA	C4D-C3D-C2D	2.42	109.47	106.78
4	B	1314	BLA	C4D-ND-C1D	2.24	110.72	106.51
4	C	1314	BLA	C4D-ND-C1D	2.23	110.72	106.51
4	A	1314	BLA	C4D-ND-C1D	2.22	110.70	106.51
4	B	1314	BLA	CHA-C4D-ND	-2.18	125.81	128.83
4	A	1314	BLA	CHA-C4D-ND	-2.15	125.84	128.83
4	C	1314	BLA	CHA-C4D-ND	-2.14	125.86	128.83
4	B	1314	BLA	CHA-C4D-C3D	2.09	130.15	125.32
4	A	1314	BLA	CHA-C4D-C3D	2.07	130.10	125.32
4	C	1314	BLA	CHA-C4D-C3D	2.06	130.09	125.32

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1314	BLA	NA-C4A-CHB-C1B
4	A	1314	BLA	C3A-C4A-CHB-C1B
4	B	1314	BLA	NA-C4A-CHB-C1B
4	B	1314	BLA	C3A-C4A-CHB-C1B
4	C	1314	BLA	NA-C4A-CHB-C1B
4	C	1314	BLA	C3A-C4A-CHB-C1B
3	A	1312	NAG	O5-C5-C6-O6
3	B	1312	NAG	O5-C5-C6-O6
3	C	1312	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1304	NAG	O5-C5-C6-O6
3	A	1302	NAG	C1-C2-N2-C7
3	B	1302	NAG	C1-C2-N2-C7
3	C	1302	NAG	C1-C2-N2-C7
3	A	1312	NAG	C4-C5-C6-O6
3	B	1312	NAG	C4-C5-C6-O6
3	C	1312	NAG	C4-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
4	A	1314	BLA	C2A-CAA-CBA-CGA
3	A	1303	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	A	1305	NAG	C1-C2-N2-C7
3	B	1305	NAG	C1-C2-N2-C7
3	C	1305	NAG	C1-C2-N2-C7
4	B	1314	BLA	C2A-CAA-CBA-CGA
4	C	1314	BLA	C2A-CAA-CBA-CGA
3	A	1305	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	A	1302	NAG	C3-C2-N2-C7
3	B	1302	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	C	1302	NAG	C3-C2-N2-C7
4	A	1314	BLA	C2C-C3C-CAC-CBC
4	B	1314	BLA	C2C-C3C-CAC-CBC
4	C	1314	BLA	C2C-C3C-CAC-CBC
3	A	1303	NAG	C3-C2-N2-C7
3	A	1305	NAG	C3-C2-N2-C7
3	B	1303	NAG	C3-C2-N2-C7
3	B	1305	NAG	C3-C2-N2-C7
3	C	1303	NAG	C3-C2-N2-C7
3	C	1305	NAG	C3-C2-N2-C7
4	A	1314	BLA	CAA-CBA-CGA-O1A
4	B	1314	BLA	CAA-CBA-CGA-O1A
4	C	1314	BLA	CAA-CBA-CGA-O1A
3	A	1307	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
4	A	1314	BLA	C4C-C3C-CAC-CBC
4	B	1314	BLA	C4C-C3C-CAC-CBC
4	C	1314	BLA	C4C-C3C-CAC-CBC
4	A	1314	BLA	CAD-CBD-CGD-O1D
4	B	1314	BLA	CAD-CBD-CGD-O1D
4	C	1314	BLA	CAD-CBD-CGD-O1D
4	A	1314	BLA	CAD-CBD-CGD-O2D
4	B	1314	BLA	CAD-CBD-CGD-O2D
4	C	1314	BLA	CAD-CBD-CGD-O2D
4	B	1314	BLA	CAA-CBA-CGA-O2A
4	C	1314	BLA	CAA-CBA-CGA-O2A
4	A	1314	BLA	CAA-CBA-CGA-O2A
3	C	1310	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	A	1307	NAG	C1-C2-N2-C7
3	C	1307	NAG	C1-C2-N2-C7

There are no ring outliers.

11 monomers are involved in 14 short contacts:

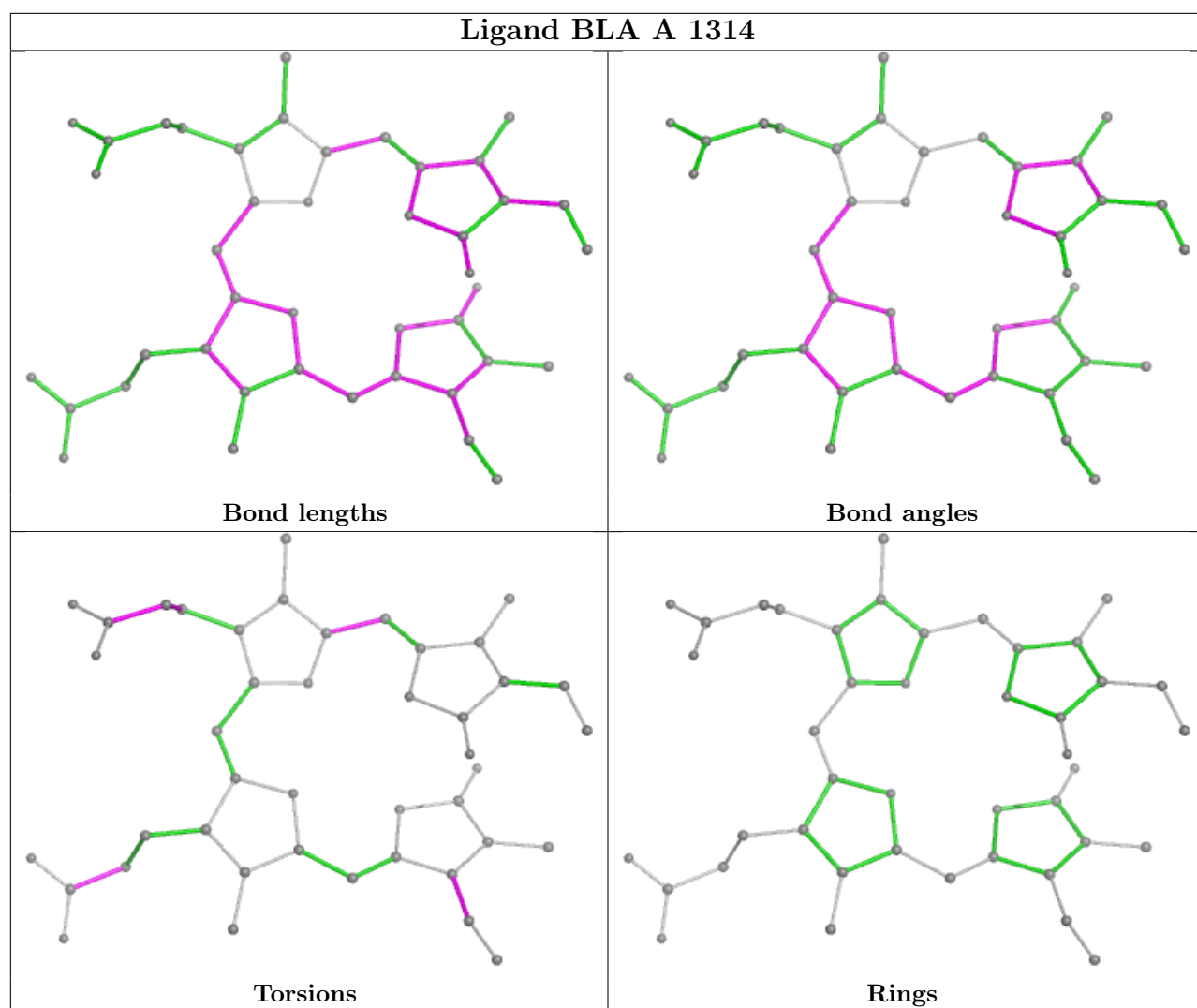
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1305	NAG	1	0
3	A	1313	NAG	1	0
3	B	1313	NAG	1	0
3	C	1306	NAG	2	0

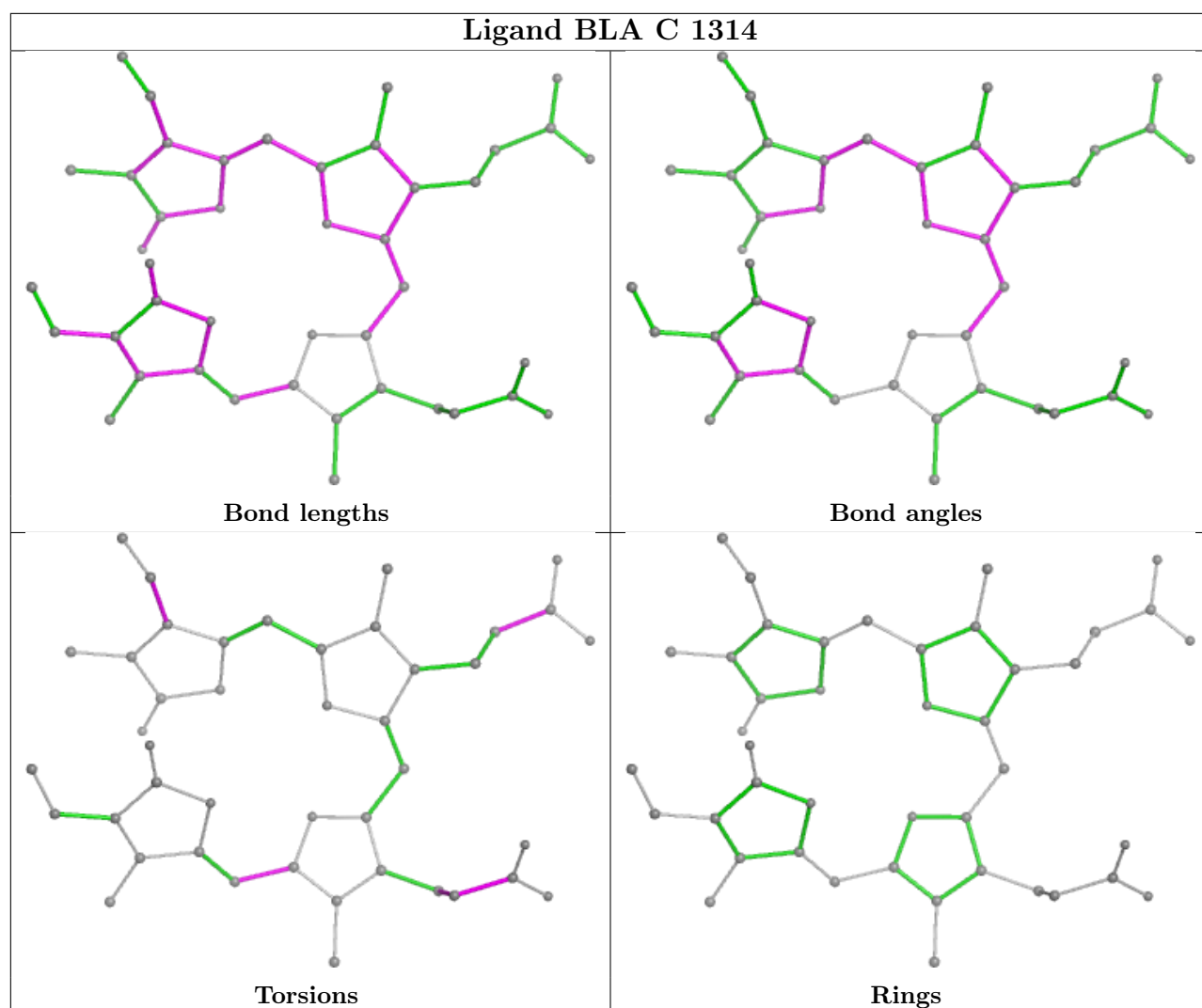
*Continued on next page...*

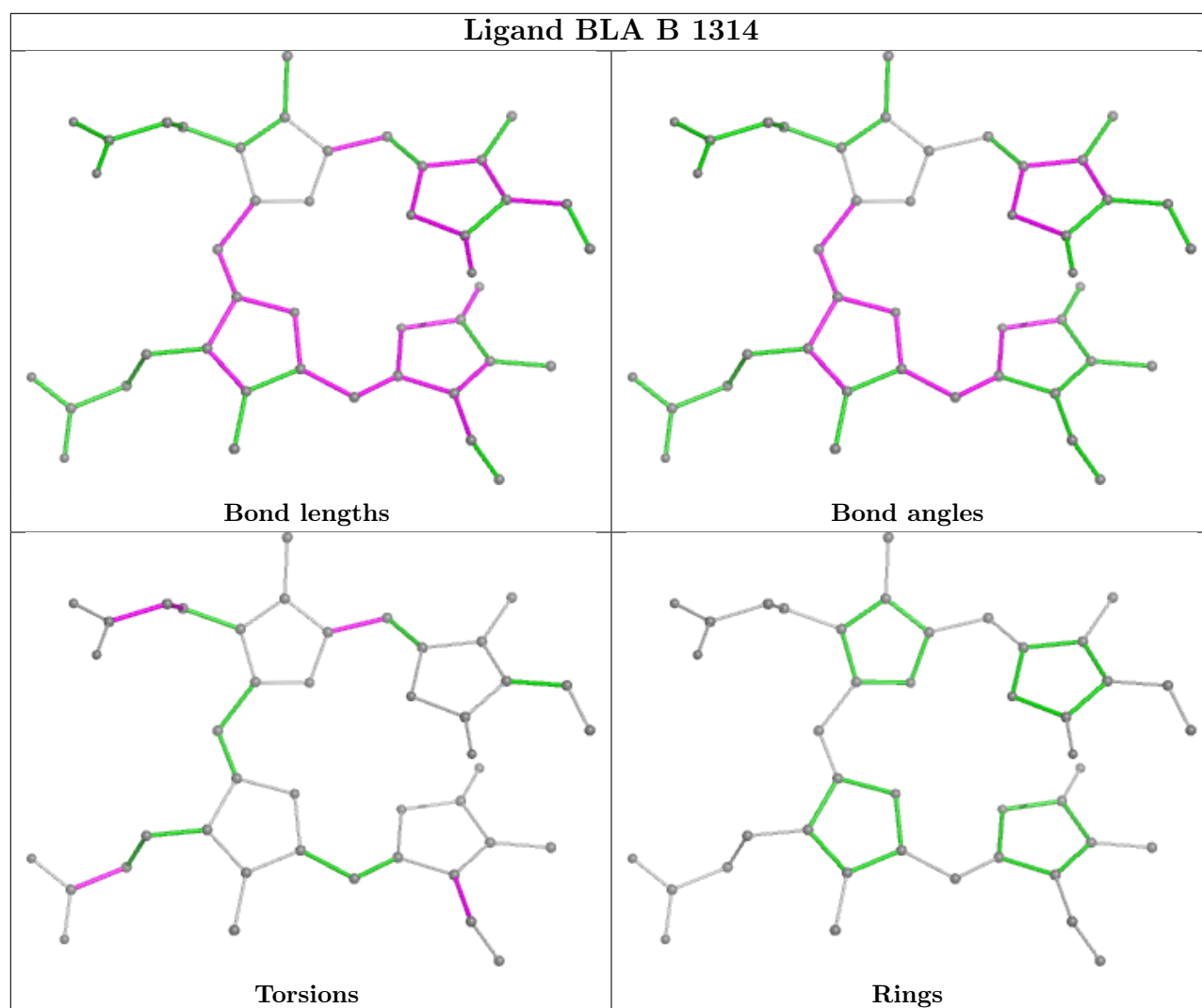
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1306	NAG	2	0
3	C	1302	NAG	1	0
3	B	1302	NAG	1	0
3	A	1302	NAG	1	0
3	C	1313	NAG	1	0
3	B	1306	NAG	2	0
3	B	1305	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

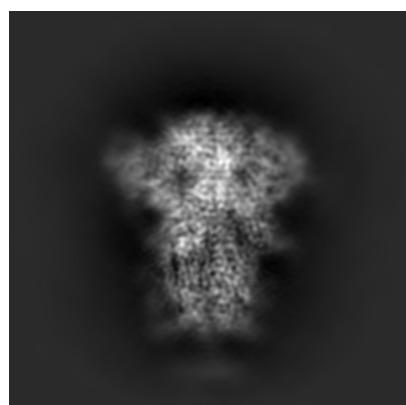
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11331. These allow visual inspection of the internal detail of the map and identification of artifacts.

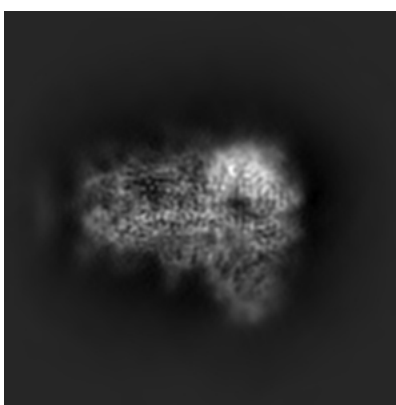
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

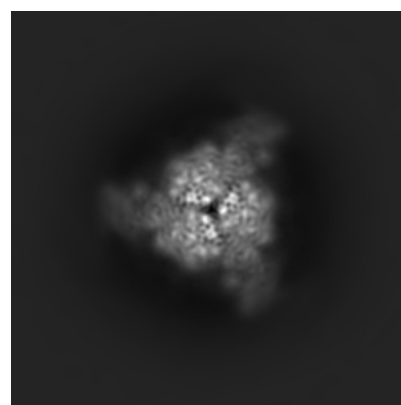
#### 6.1.1 Primary map



X



Y

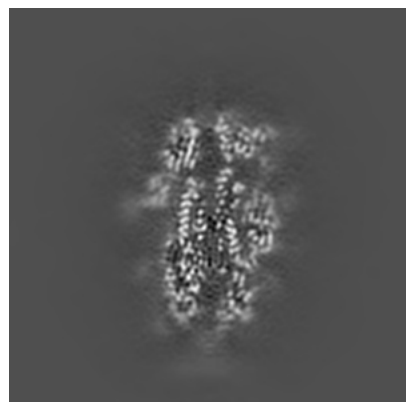


Z

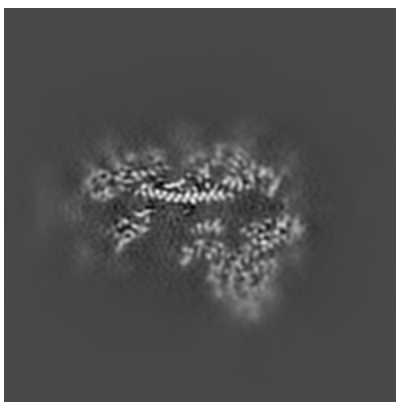
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

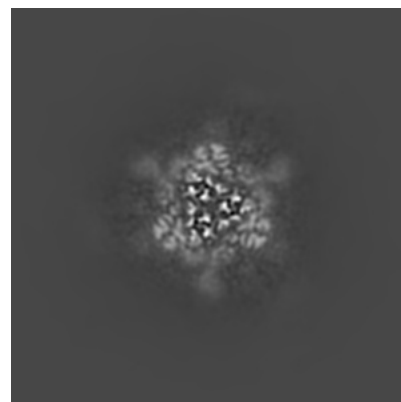
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

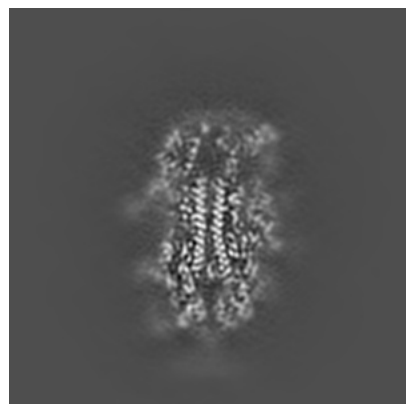


Z Index: 128

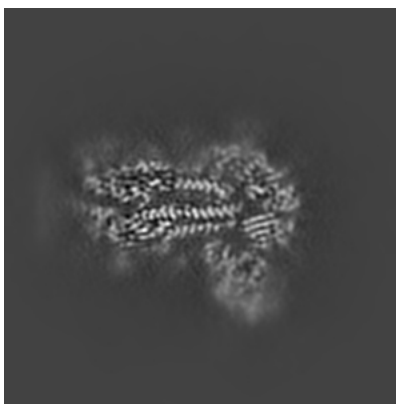
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

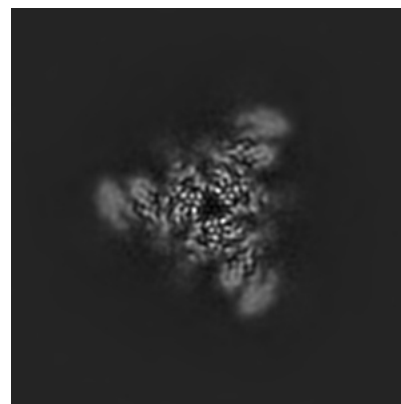
### 6.3.1 Primary map



X Index: 124



Y Index: 135

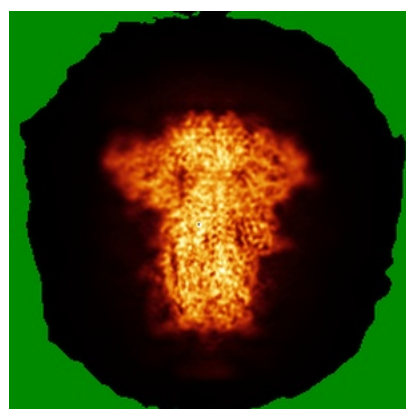


Z Index: 159

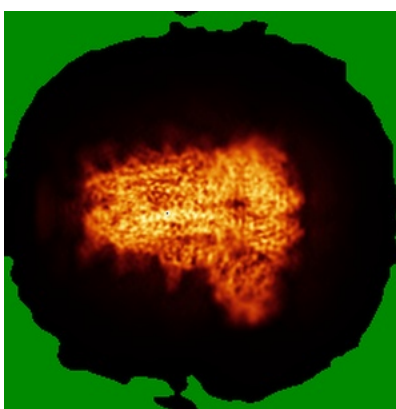
The images above show the largest variance slices of the map in three orthogonal directions.

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

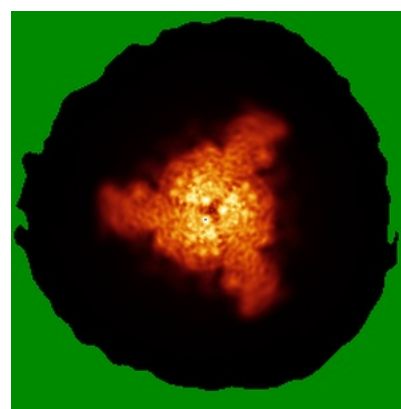
### 6.4.1 Primary map



X



Y

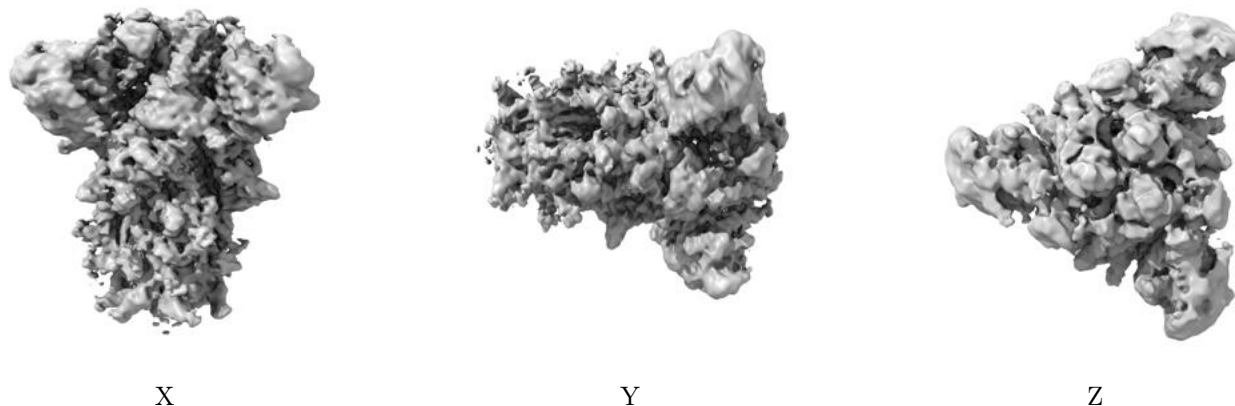


Z

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 0.0118. 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](#)

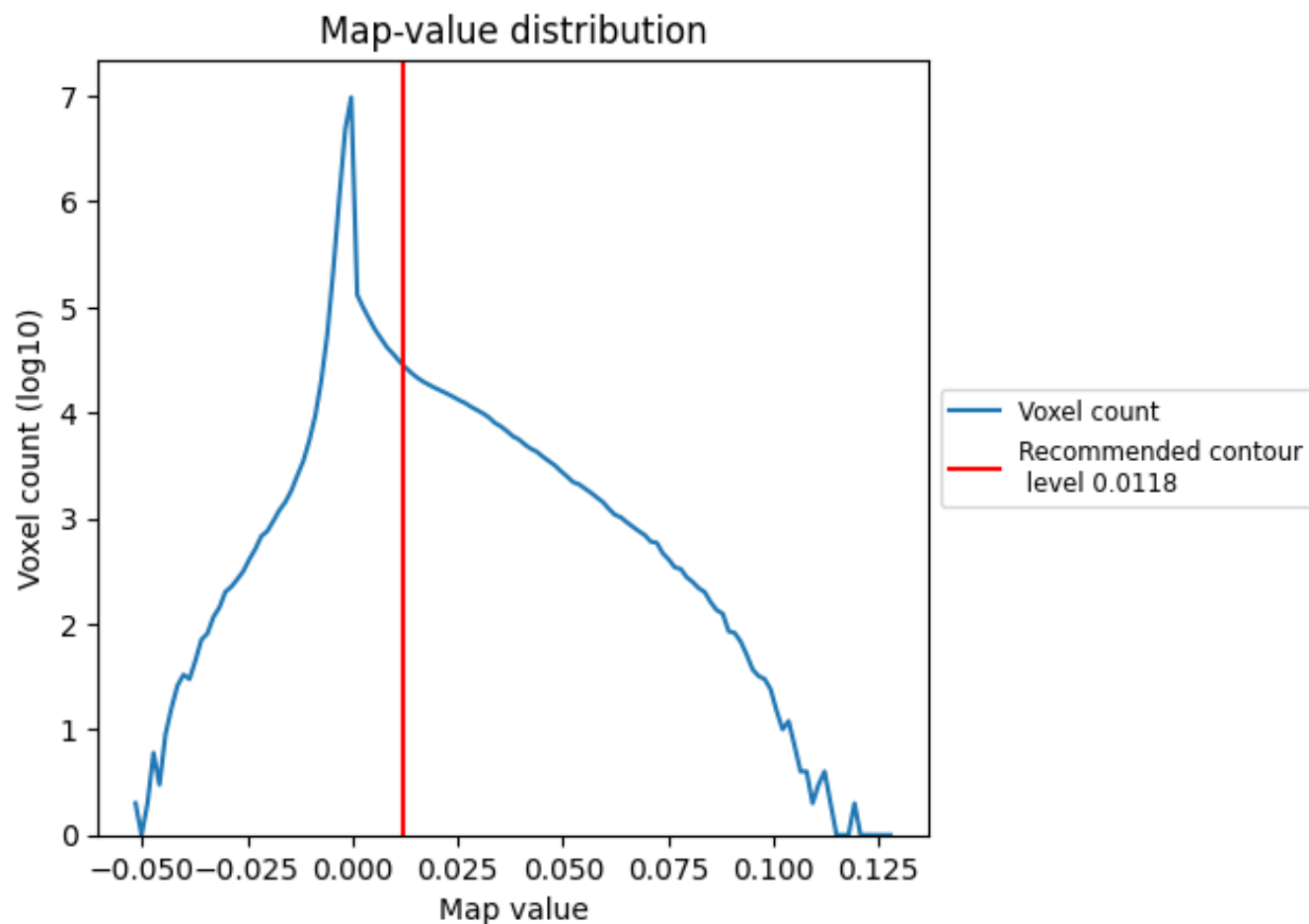
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

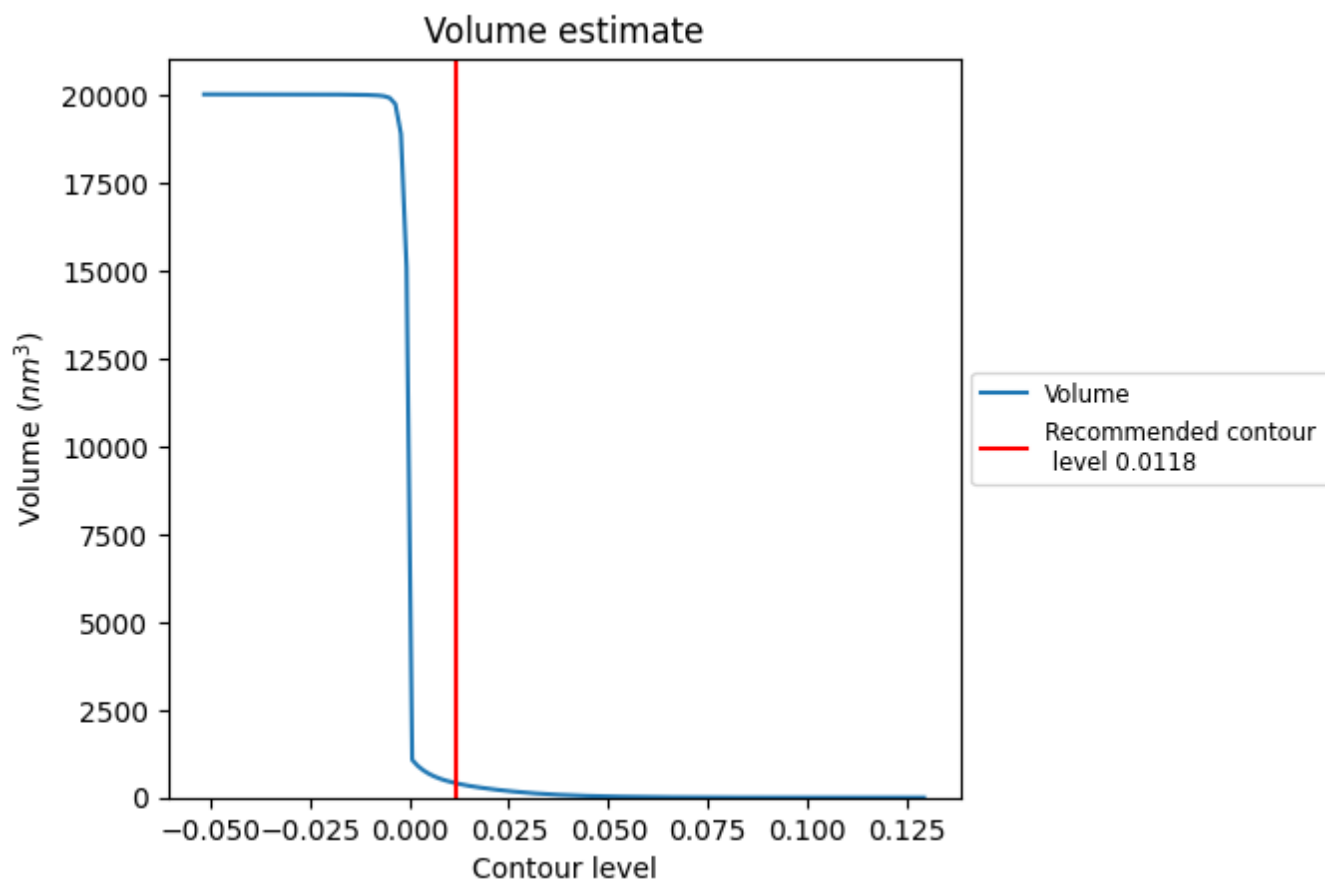
This section contains the results of statistical analysis of the map.

### 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.

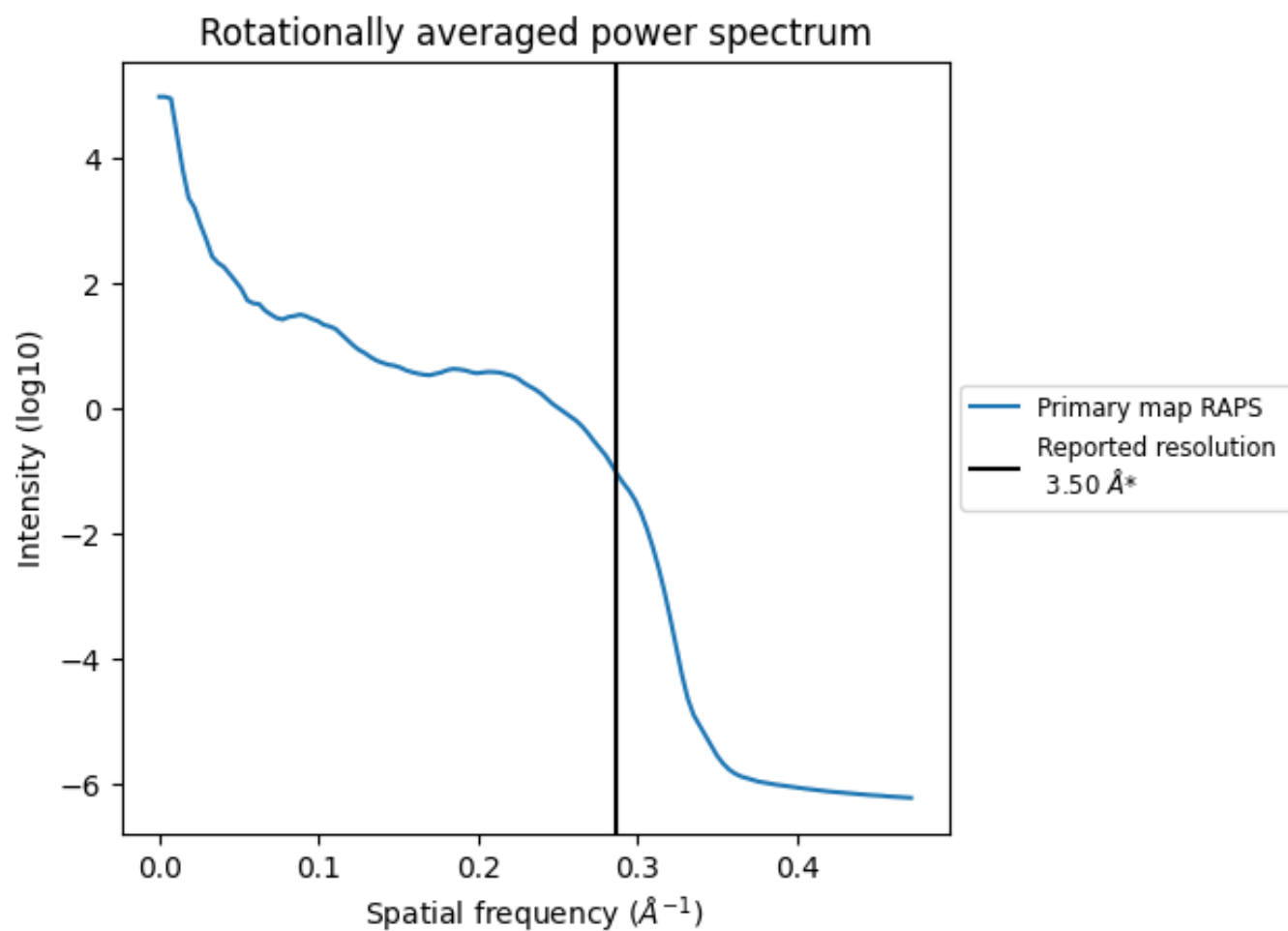
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 406  $\text{nm}^3$ ; this corresponds to an approximate mass of 367 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 0.286 Å<sup>-1</sup>

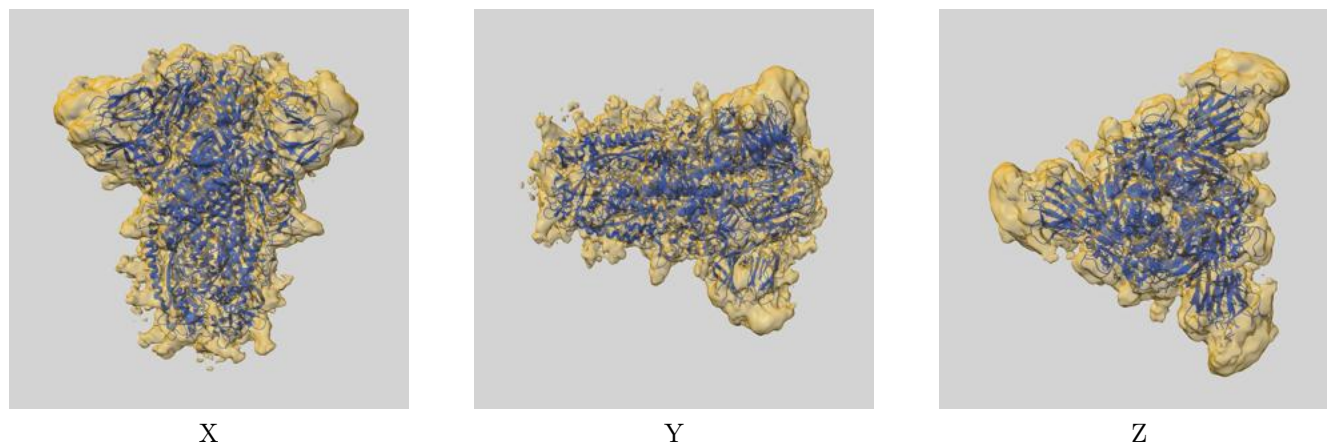
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

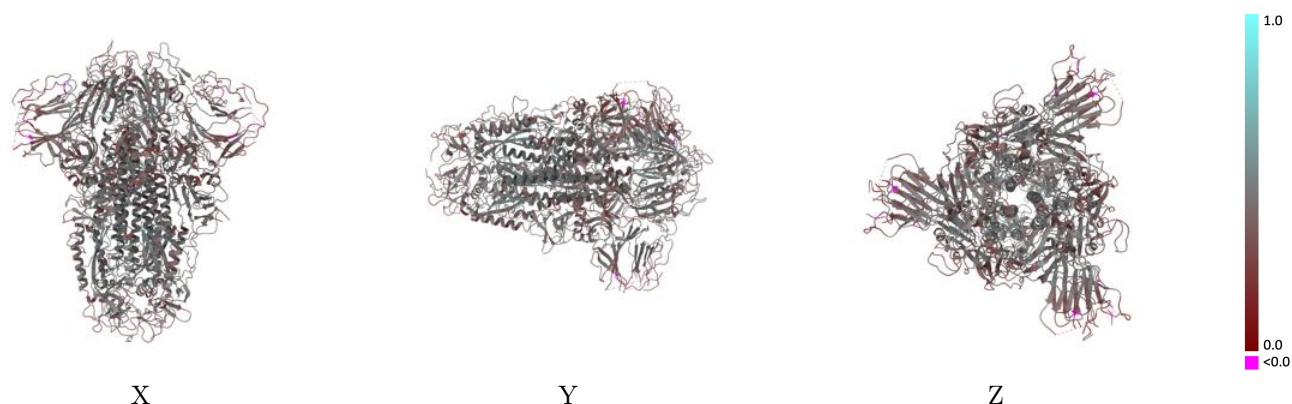
This section contains information regarding the fit between EMDB map EMD-11331 and PDB model 6Z0Z. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0118 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](#)



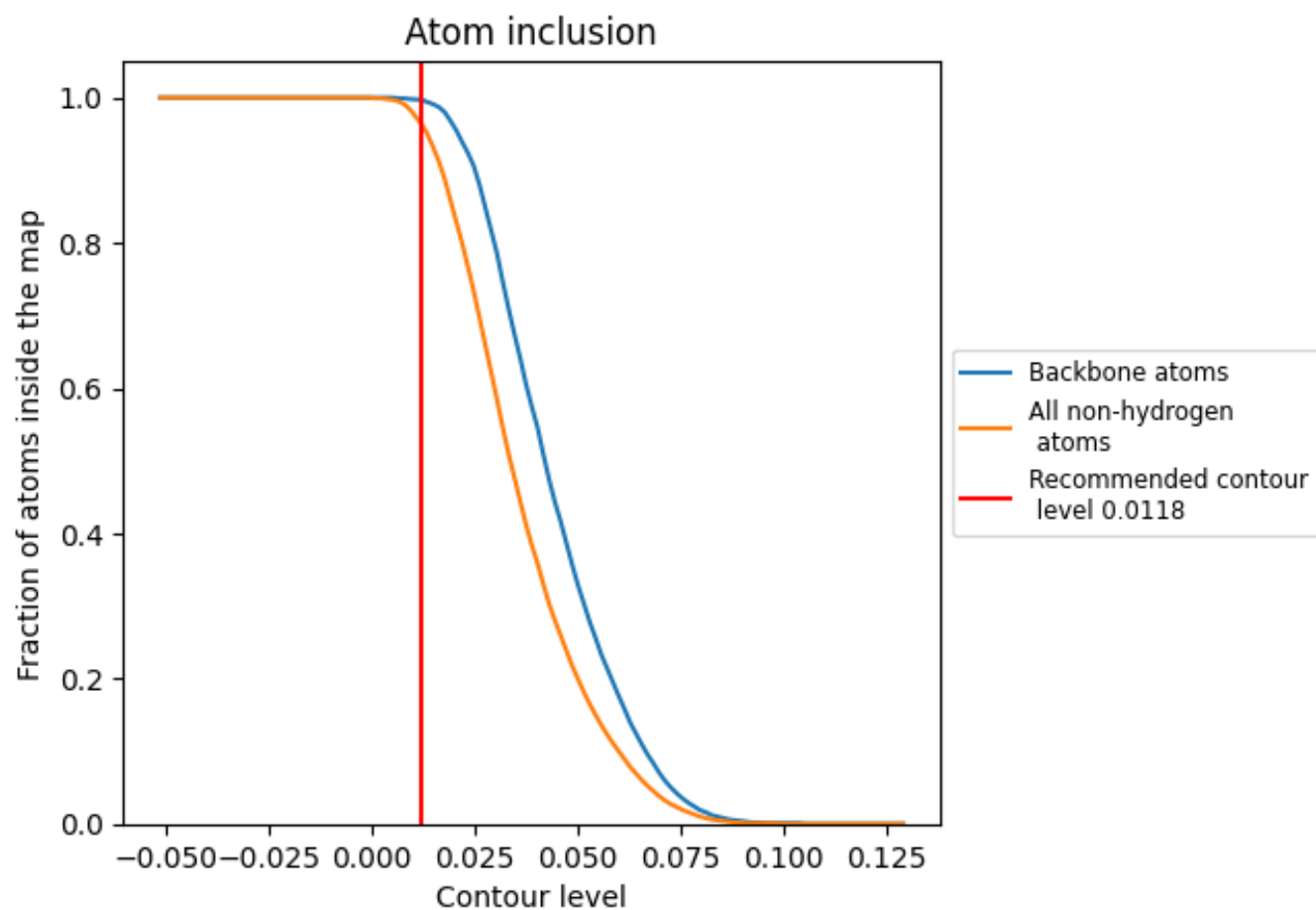
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0118).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9650	<div></div> 0.4180
A	<div></div> 0.9660	<div></div> 0.4190
B	<div></div> 0.9660	<div></div> 0.4190
C	<div></div> 0.9650	<div></div> 0.4170
D	<div></div> 1.0000	<div></div> 0.4360
E	<div></div> 0.9290	<div></div> 0.4160
F	<div></div> 0.9290	<div></div> 0.3760
G	<div></div> 0.9640	<div></div> 0.3700
H	<div></div> 1.0000	<div></div> 0.4650
I	<div></div> 0.9290	<div></div> 0.3900
J	<div></div> 0.9290	<div></div> 0.3570
K	<div></div> 0.9640	<div></div> 0.3640
L	<div></div> 1.0000	<div></div> 0.4450
M	<div></div> 0.9290	<div></div> 0.3950
N	<div></div> 0.9290	<div></div> 0.3650
O	<div></div> 0.9640	<div></div> 0.3600

