



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 08:48 PM JST

PDB ID : 7XNS
EMDB ID : EMD-33325
Title : SARS-CoV-2 Omicron BA.2.12.1 variant spike
Authors : Wang, X.; Wang, L.
Deposited on : 2022-04-29
Resolution : 3.48 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
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

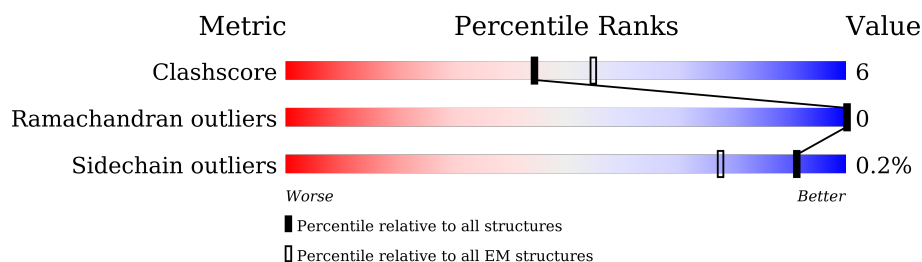
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.48 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 ≥ 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> <div>23%</div> <div>73%</div> <div>13%</div> <div>14%</div> </div>
1	B	1270	<div> <div>23%</div> <div>74%</div> <div>12%</div> <div>14%</div> </div>
1	C	1270	<div> <div>23%</div> <div>73%</div> <div>13%</div> <div>14%</div> </div>
2	D	2	<div> <div>100%</div> <div>100%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>100%</div> </div>
2	G	2	<div> <div>50%</div> <div>100%</div> </div>
2	H	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	2	<div> <div>50%</div> <div>100%</div> </div>
2	J	2	<div> <div>50%</div> <div>50%</div> </div>
2	K	2	<div> <div>50%</div> <div>50%</div> </div>
2	L	2	<div> <div>100%</div> </div>
2	M	2	<div> <div>50%</div> <div>100%</div> </div>
2	N	2	<div> <div>50%</div> <div>50%</div> </div>
2	O	2	<div> <div>50%</div> <div>100%</div> </div>
2	P	2	<div> <div>100%</div> </div>
2	Q	2	<div> <div>50%</div> <div>50%</div> </div>
2	R	2	<div> <div>100%</div> </div>
2	S	2	<div> <div>50%</div> <div>100%</div> </div>
2	T	2	<div> <div>50%</div> <div>50%</div> </div>
2	U	2	<div> <div>50%</div> <div>100%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26595 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	1095	Total	C	N	O	S	0	0
			8557	5471	1425	1623	38		
1	B	1095	Total	C	N	O	S	0	0
			8557	5471	1425	1623	38		
1	C	1095	Total	C	N	O	S	0	0
			8557	5471	1425	1623	38		

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	GLN	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	TYR	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	685	ALA	ARG	variant	UNP P0DTC2
A	704	LEU	SER	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
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B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	GLN	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	TYR	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	variant	UNP P0DTC2
B	685	ALA	ARG	variant	UNP P0DTC2
B	704	LEU	SER	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	GLN	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	679	TYR	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	variant	UNP P0DTC2
C	685	ALA	ARG	variant	UNP P0DTC2
C	704	LEU	SER	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

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



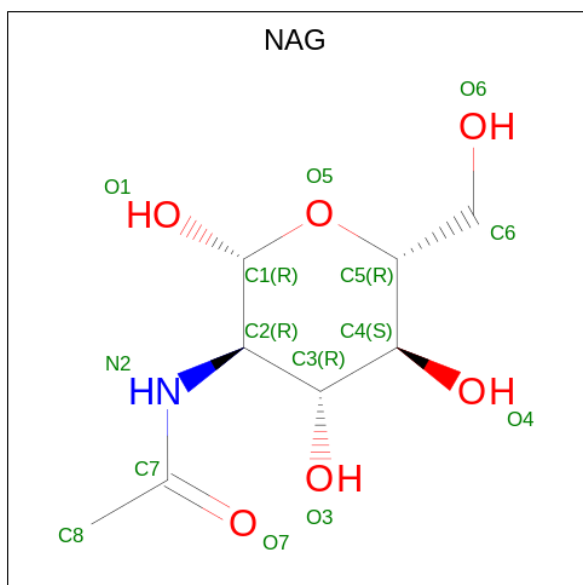
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16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

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Mol	Chain	Residues	Atoms				AltConf	Trace
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		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	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	

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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	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	
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	

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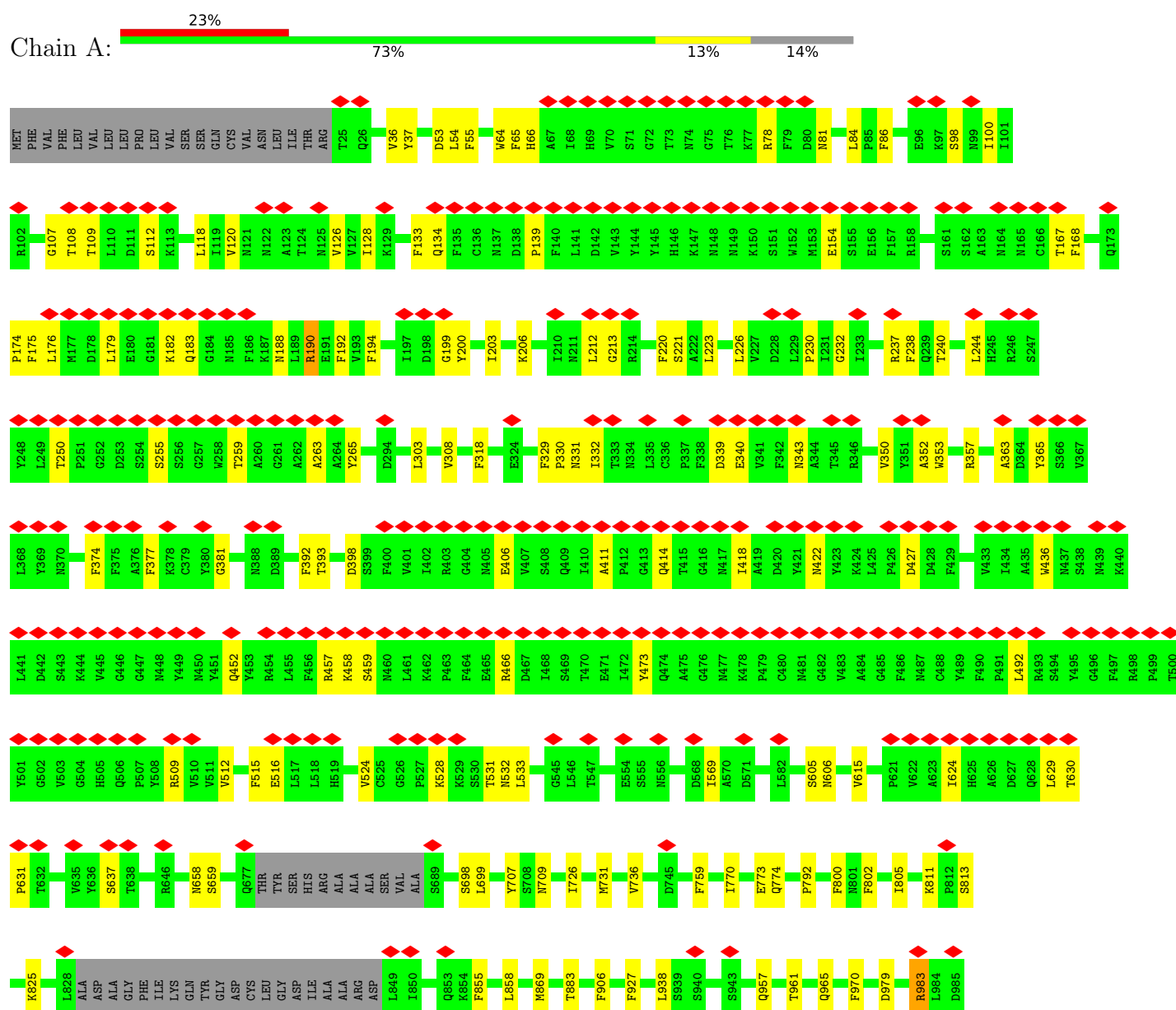
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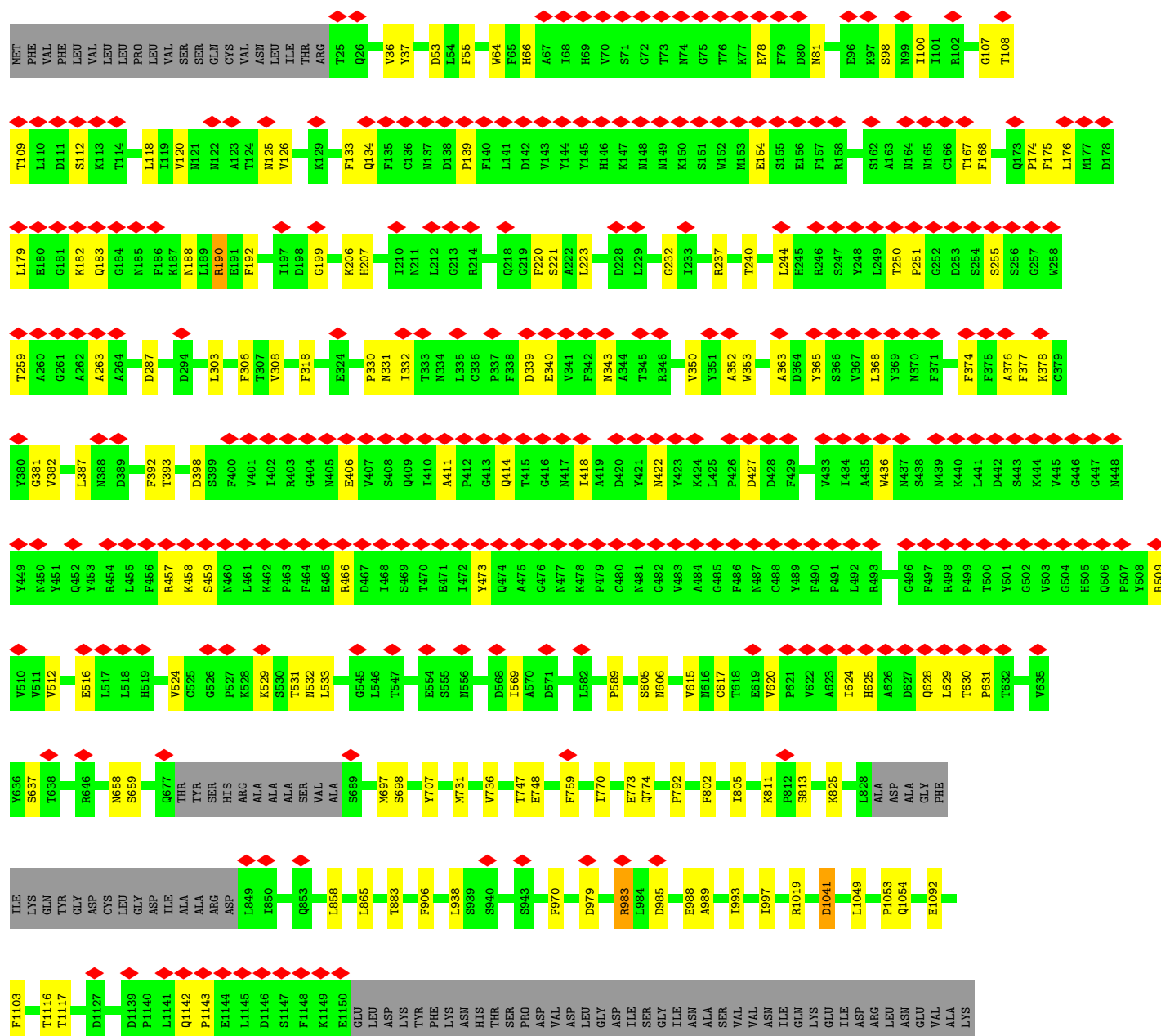
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

3 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





[illegible]

Chain C:



ILE	ASP	A989	K825	V635	V503	S443	A376	G257	F175	T108	ARG	T25
ALA	LEU	E990	L328	V636	G504	K444	F377	W258	L176	T109	THR	Q26
ILE	GLY		L328	S637	H505	V445	K378	T259	M177	D110	ASN	V36
VAL	ASP	I993	ALA	S637	H505	V445	K378	T259	M177	D110	GLN	D53
VAL	SER	I997	ASP	T638	G506	G446	C379	A260	D178	D111	CYS	F55
THR	GLY		ALA	T638	G507	G447	Y380	G261	L179	S112	LEU	
ILE	GLY	R1019	GLY	R646	H508	N448	G381	A262	E180	K113	LEU	
MET	ASN		ILE		R509	Y449	K386	A263	G181		LEU	
LEU	ALA	D1041	LYS	N658	V510	N450	L387	A264	K182	L118	PRO	
CYS	SER		GLN	S659	V511	Y451	N388	Y265	Q183	I119	LEU	
CYS	VAL	K1045	TYR		V512	Q452	D389			V120	LEU	
MET	VAL		GLY	Q677		Y453		D294	G184	N121	SER	
THR	ASN	L1049	ASP	THR	E516	R454	T383		N185	N122	SER	
SER	ILE		CYS	TYR	L517	L455	Y396	L303	F186	A123	GLN	
CYS	GLN	P1053	LEU	TYR	L518	F456	D398	V308	K187	T124	VAL	
CYS	LYS	Q1054	GLY	HIS	H519	R457	A397		N188		ASN	
SER	GLU		ASP	ARG		R457	D398	F318	L189	N125	ILE	
CYS	ILE	V1061	ILE	ALA	G526	K458	S399		R190	V126	THR	
LYS	ARG	V1065	ALA	ALA	P527	N459	F400	E324	E191	I127	THR	
GLY	LEU		ALA	ALA	K528	M460	V401		F192	K129	ARG	
CYS	ASN	E1092	ARG	VAL		L461	I402	F329	I197	F133	ARG	
CYS	GLU		ASP	VAL	K529	L461	I402	P330	D198	Q134	ARG	
SER	VAL	S1097	ALA	ALA	S530	K462	R403	N331	G199		ARG	
GLY	ALA		S689	S689	T531	P463	C404	T332		F135	ARG	
CYS	LYS	W1102	LYS	S698	N532	P464	N405	T333	K206	C136	ARG	
SER	ASN	F1103	GLY	S698	L533	E465	E406	N334	H207	N137	ARG	
CYS	LEU		Y707	Y707	K537	R466	V407	L335		D138	ARG	
CYS	ASN	T1116	LYS	Y722		D467	S408	C336	I210	P139	ARG	
LYS	GLU	T1117	GLU	V722	G545	I468	Q409	P337	N211	F140	ARG	
PHE	SER		LEU	I726	L546	S469	I410	F338	L212	L141	ARG	
GLU	ILE	D1127	ILE	I726	T547	T470	A411	D339	G213	D142	ARG	
ASP	ASP		LYS	V736	E554	E471	P412	E340	R214	A67	ARG	
LEU	LEU	D1139	LEU	D745	S555	I472	C413	V341	F220	V143	ARG	
ASP	GLN	P1140	GLU	L1471	N556	Y473	Q414	F342	S221	V70	ARG	
SER	LEU	L1141	LYS	F759		Q474	T415	N343	L226	Y145	ARG	
PRO	LEU	Q1142	LYS	Q762	D568	A475	C416	A344	V227	H146	ARG	
VAL	GLY	L1145	GLY	I569	I569	Q476	N417	T345	D228	K147	ARG	
LEU	ILE	D1146	VAL	R765	A570	N477	I418	R346	L229	N148	ARG	
LEU	ILE	S1147	LYS	I770	D571	K478	A419	V350	G232	K150	ARG	
HIS	LYS	F1148	LYS	I770	L582	P479	D420	V351	I233	S151	ARG	
TYR	THR	K1149	PRO	E773		C480	Y421	A352	R237	W152	ARG	
THR	THR	E1150	THR	Q774	V615	N481	N422	W353		M153	ARG	
	TYR	GLU	TYR	F970	W616	G482	Y423	R357	T240	S155	ARG	
	ASP	ASP	ASP	P792	O617	V483	K424	I356	L244	E156	ARG	
	THR	LYS	LYS	F800	T618	V483	L425	S359	H245	F157	ARG	
	TYR	TYR	TYR	N801	E619	A484	P426	S359	R246	R158	ARG	
	PHE	PHE	GLY	F802	V620	G485	D427		R247		ARG	
	LYS	LYS	LYS	S982	P621	P486	D428	A363	Y248	S161	ARG	
	ASN	ASN	ASN	S983	V622	N487	F429	Y365	Y248	S98	ARG	
	HIS	HIS	HIS	K811	A623	C488	T430		R249	A163	ARG	
	SER	SER	SER	P812	I624	Y489	V433	V366	T250	N164	ARG	
	PRO	PRO	PRO	S813	H625	P490	I434	L368	P251	N165	ARG	
	VAL	VAL	VAL		A626	Q491	L492	N370	G252	C166	ARG	
					Q628	R493	W436	F371	D253	T167	ARG	
					L629	S494	N437		S254	F168	ARG	
					T630	Y495	S438	F374	S255		ARG	
					P631	Q496	N439	F375	S256	V171	ARG	
					T632	F497	R440			Q173	ARG	
						R498	L441			P174	ARG	
						P499	D442				ARG	
						T500					ARG	
						Y501					ARG	
						G502					ARG	

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

Chain D: 



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

Chain E: 



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

Chain F: 



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

Chain G: 



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

Chain H: 



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

Chain I: 



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



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



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



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



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



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



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

Chain P: 



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

Chain Q: 



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

Chain R: 



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

Chain S: 



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

Chain T: 



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

Chain U: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	364517	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.075	Depositor
Minimum map value	-1.630	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/8767	0.50	1/11941 (0.0%)
1	B	0.29	0/8767	0.49	1/11941 (0.0%)
1	C	0.28	0/8767	0.49	0/11941
All	All	0.28	0/26301	0.49	2/35823 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1041	ASP	CB-CG-OD1	7.34	124.91	118.30
1	B	1041	ASP	CB-CG-OD1	5.62	123.36	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	515	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8557	0	8317	113	0
1	B	8557	0	8317	109	0
1	C	8557	0	8317	119	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	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	1	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	1	0
2	U	28	0	25	0	0
3	A	140	0	130	3	0
3	B	140	0	130	3	0
3	C	140	0	130	3	0
All	All	26595	0	25791	327	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 6.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:HG	1:B:631:PRO:HD2	1.59	0.84
1:C:629:LEU:HG	1:C:631:PRO:HD2	1.60	0.84
1:A:629:LEU:HG	1:A:631:PRO:HD2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:ASP:O	1:C:983:ARG:HB2	1.80	0.82
1:C:659:SER:HB3	1:C:698:SER:HB2	1.64	0.80
1:B:979:ASP:O	1:B:983:ARG:HB2	1.82	0.79
1:A:979:ASP:O	1:A:983:ARG:HB2	1.83	0.79
1:A:659:SER:HB3	1:A:698:SER:HB2	1.64	0.79
1:B:659:SER:HB3	1:B:698:SER:HB2	1.66	0.77
1:B:167:THR:HG22	1:B:168:PHE:H	1.53	0.74
1:C:112:SER:HB3	1:C:134:GLN:HG3	1.71	0.73
1:A:167:THR:HG22	1:A:168:PHE:H	1.54	0.73
1:C:167:THR:HG22	1:C:168:PHE:H	1.53	0.73
1:C:624:ILE:HG13	1:C:637:SER:HA	1.73	0.71
1:A:112:SER:HB3	1:A:134:GLN:HG3	1.73	0.70
1:A:624:ILE:HG13	1:A:637:SER:HA	1.74	0.69
1:B:624:ILE:HG13	1:B:637:SER:HA	1.73	0.69
1:B:112:SER:HB3	1:B:134:GLN:HG3	1.77	0.66
1:C:66:HIS:NE2	1:C:250:THR:OG1	2.29	0.65
1:B:66:HIS:NE2	1:B:250:THR:OG1	2.29	0.65
1:B:353:TRP:O	1:B:466:ARG:NH2	2.30	0.64
1:C:569:ILE:H	1:C:569:ILE:HD12	1.62	0.64
1:B:118:LEU:HD11	1:B:120:VAL:HB	1.78	0.64
1:B:569:ILE:HD12	1:B:569:ILE:H	1.62	0.64
1:A:66:HIS:NE2	1:A:250:THR:OG1	2.29	0.64
1:A:731:MET:HG2	1:A:774:GLN:HE21	1.63	0.63
1:C:102:ARG:HH12	1:C:157:PHE:HE2	1.43	0.63
1:C:436:TRP:HE3	1:C:509:ARG:HD2	1.64	0.63
1:A:353:TRP:O	1:A:466:ARG:NH2	2.30	0.63
1:C:199:GLY:HA2	1:C:232:GLY:HA2	1.81	0.63
1:A:436:TRP:HE3	1:A:509:ARG:HD2	1.64	0.62
1:C:353:TRP:O	1:C:466:ARG:NH2	2.31	0.62
1:B:436:TRP:HE3	1:B:509:ARG:HD2	1.64	0.62
1:A:255:SER:HB3	1:A:259:THR:HG21	1.83	0.60
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.35	0.60
1:C:176:LEU:HD12	1:C:190:ARG:HH22	1.66	0.60
1:B:811:LYS:HD3	1:B:813:SER:H	1.66	0.60
1:A:811:LYS:HD3	1:A:813:SER:H	1.66	0.60
1:A:869:MET:HE1	1:B:697:MET:HB3	1.84	0.60
1:A:176:LEU:HD12	1:A:190:ARG:HH22	1.67	0.59
1:B:255:SER:HB3	1:B:259:THR:HG21	1.84	0.58
1:A:53:ASP:OD1	1:A:54:LEU:N	2.33	0.58
1:B:199:GLY:HA2	1:B:232:GLY:HA2	1.85	0.58
1:A:199:GLY:HA2	1:A:232:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:SER:HB3	1:C:259:THR:HG21	1.84	0.58
1:C:811:LYS:HD3	1:C:813:SER:H	1.68	0.58
1:B:759:PHE:HE1	1:C:965:GLN:HE21	1.52	0.58
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.36	0.57
1:C:773:GLU:OE2	1:C:1019:ARG:NE	2.30	0.57
1:A:773:GLU:OE2	1:A:1019:ARG:NE	2.30	0.57
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.36	0.57
1:C:658:ASN:ND2	1:C:659:SER:H	2.04	0.56
1:C:979:ASP:O	1:C:983:ARG:CB	2.52	0.56
1:B:825:LYS:NZ	1:B:938:LEU:O	2.29	0.56
3:B:1301:NAG:H3	3:B:1301:NAG:H83	1.88	0.56
1:B:376:ALA:HB1	1:B:378:LYS:HG3	1.88	0.55
1:B:989:ALA:O	1:B:993:ILE:HG12	2.05	0.55
1:B:770:ILE:O	1:B:774:GLN:HG2	2.06	0.55
3:C:1301:NAG:H83	3:C:1301:NAG:H3	1.88	0.55
1:C:107:GLY:O	1:C:237:ARG:HB2	2.06	0.55
1:C:330:PRO:HG2	1:C:332:ILE:HD11	1.89	0.55
1:B:773:GLU:OE1	1:B:1019:ARG:NE	2.40	0.55
1:B:176:LEU:HD12	1:B:190:ARG:HH22	1.72	0.55
1:A:993:ILE:O	1:A:997:ILE:HG12	2.08	0.54
1:A:381:GLY:O	1:C:983:ARG:NH1	2.41	0.54
1:A:731:MET:HG2	1:A:774:GLN:NE2	2.22	0.54
1:A:330:PRO:HG2	1:A:332:ILE:HD11	1.89	0.54
1:B:107:GLY:O	1:B:237:ARG:HB2	2.07	0.54
1:B:382:VAL:HG21	1:B:387:LEU:HD21	1.90	0.53
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.73	0.53
1:C:352:ALA:HA	1:C:466:ARG:HD3	1.90	0.53
1:C:376:ALA:HB1	1:C:378:LYS:HG3	1.88	0.53
3:A:1301:NAG:H83	3:A:1301:NAG:H3	1.88	0.53
1:A:352:ALA:HA	1:A:466:ARG:HD3	1.88	0.53
1:B:330:PRO:HG2	1:B:332:ILE:HD11	1.90	0.53
1:C:531:THR:HG22	1:C:532:ASN:H	1.74	0.53
1:A:957:GLN:HE21	1:C:765:ARG:CZ	2.22	0.53
1:A:770:ILE:O	1:A:774:GLN:HG2	2.09	0.52
1:A:883:THR:HG23	1:B:707:TYR:HB2	1.91	0.52
1:A:979:ASP:O	1:A:983:ARG:CB	2.56	0.52
1:A:107:GLY:O	1:A:237:ARG:HB2	2.10	0.52
1:A:707:TYR:HB2	1:C:883:THR:HG23	1.92	0.52
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.74	0.52
1:B:352:ALA:HA	1:B:466:ARG:HD3	1.90	0.52
1:A:175:PHE:HD1	1:A:226:LEU:HD23	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG11	1:B:175:PHE:HD2	1.74	0.52
1:C:339:ASP:OD1	1:C:340:GLU:N	2.43	0.52
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.74	0.52
1:C:64:TRP:HB3	1:C:263:ALA:HB3	1.92	0.52
1:B:617:CYS:HA	1:B:620:VAL:HG23	1.92	0.52
1:C:118:LEU:HD11	1:C:120:VAL:HB	1.90	0.51
1:A:66:HIS:ND1	1:A:263:ALA:HA	2.25	0.51
1:A:339:ASP:OD1	1:A:340:GLU:N	2.42	0.51
1:B:993:ILE:O	1:B:997:ILE:HG12	2.11	0.51
1:A:118:LEU:HD11	1:A:120:VAL:HB	1.91	0.51
1:B:78:ARG:HH11	1:B:244:LEU:HD22	1.74	0.51
1:B:883:THR:HG23	1:C:707:TYR:HB2	1.90	0.51
1:B:66:HIS:ND1	1:B:263:ALA:HA	2.26	0.51
1:A:78:ARG:HH11	1:A:244:LEU:HD22	1.76	0.51
1:A:36:VAL:HG21	1:A:220:PHE:CZ	2.46	0.50
1:A:154:GLU:OE1	1:A:154:GLU:N	2.44	0.50
1:B:339:ASP:OD1	1:B:340:GLU:N	2.43	0.50
1:A:81:ASN:ND2	1:A:240:THR:O	2.44	0.50
1:B:179:LEU:HB2	1:B:188:ASN:HB3	1.93	0.50
1:C:179:LEU:HB2	1:C:188:ASN:HB3	1.93	0.50
1:A:179:LEU:HB2	1:A:188:ASN:HB3	1.93	0.50
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.76	0.50
1:B:64:TRP:HB3	1:B:263:ALA:HB3	1.93	0.50
1:B:531:THR:HG22	1:B:532:ASN:H	1.76	0.50
1:B:318:PHE:HZ	1:B:615:VAL:HG11	1.77	0.50
1:C:65:PHE:HE2	1:C:84:LEU:HD21	1.77	0.50
1:C:206:LYS:NZ	1:C:221:SER:OG	2.45	0.50
1:C:190:ARG:HB3	1:C:192:PHE:CE1	2.47	0.49
1:C:139:PRO:HB2	1:C:244:LEU:HD12	1.93	0.49
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.76	0.49
1:C:993:ILE:O	1:C:997:ILE:HG12	2.13	0.49
1:C:303:LEU:HD12	1:C:308:VAL:HG12	1.94	0.49
1:A:531:THR:HG22	1:A:532:ASN:H	1.77	0.49
1:C:118:LEU:HB2	1:C:133:PHE:HE2	1.77	0.49
1:B:154:GLU:N	1:B:154:GLU:OE1	2.45	0.49
1:C:66:HIS:ND1	1:C:263:ALA:HA	2.27	0.49
1:C:154:GLU:OE1	1:C:154:GLU:N	2.45	0.49
1:A:427:ASP:N	1:A:427:ASP:OD1	2.46	0.49
1:A:1041:ASP:OD1	1:A:1041:ASP:O	2.31	0.49
1:C:437:ASN:OD1	1:C:506:GLN:NE2	2.46	0.49
1:B:1142:GLN:HB3	1:B:1143:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TRP:HB3	1:A:263:ALA:HB3	1.94	0.48
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.94	0.48
1:A:374:PHE:CE2	1:A:377:PHE:HB2	2.48	0.48
1:B:988:GLU:N	1:B:988:GLU:OE1	2.46	0.48
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.48	0.48
1:C:127:VAL:HG22	1:C:171:VAL:HG22	1.94	0.48
1:C:65:PHE:O	1:C:265:TYR:HB3	2.13	0.48
1:B:36:VAL:HG21	1:B:220:PHE:CZ	2.48	0.48
1:A:303:LEU:HD12	1:A:308:VAL:HG12	1.95	0.48
1:B:190:ARG:HB3	1:B:192:PHE:CE1	2.48	0.48
1:C:406:GLU:HG2	1:C:418:ILE:HG21	1.95	0.48
1:A:190:ARG:HB3	1:A:192:PHE:HE1	1.79	0.48
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.95	0.48
1:A:983:ARG:NH1	1:B:381:GLY:O	2.46	0.48
1:B:190:ARG:HB3	1:B:192:PHE:HE1	1.79	0.48
1:C:427:ASP:OD1	1:C:427:ASP:N	2.46	0.48
1:A:658:ASN:OD1	1:A:659:SER:N	2.40	0.48
1:B:731:MET:HG2	1:B:774:GLN:NE2	2.29	0.48
1:C:175:PHE:HD1	1:C:226:LEU:HD23	1.78	0.48
1:C:374:PHE:CE2	1:C:377:PHE:HB2	2.49	0.48
1:A:825:LYS:NZ	1:A:938:LEU:O	2.29	0.48
1:B:374:PHE:CE2	1:B:377:PHE:HB2	2.49	0.48
1:C:64:TRP:HB3	1:C:263:ALA:CB	2.44	0.48
1:A:569:ILE:HD12	1:A:569:ILE:H	1.79	0.47
1:B:427:ASP:OD1	1:B:427:ASP:N	2.46	0.47
1:B:1041:ASP:OD1	1:B:1041:ASP:O	2.32	0.47
1:C:190:ARG:HB3	1:C:192:PHE:HE1	1.78	0.47
1:B:736:VAL:HG22	1:B:858:LEU:HD13	1.95	0.47
1:C:357:ARG:HH22	1:C:359:SER:HB3	1.79	0.47
1:A:118:LEU:HB2	1:A:133:PHE:HE2	1.79	0.47
1:A:1142:GLN:HB3	1:A:1143:PRO:HD3	1.96	0.47
1:C:1142:GLN:HB3	1:C:1143:PRO:HD3	1.95	0.47
1:C:825:LYS:NZ	1:C:938:LEU:O	2.30	0.47
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.97	0.47
1:C:65:PHE:CE2	1:C:84:LEU:HD21	2.50	0.47
1:A:64:TRP:HB3	1:A:263:ALA:CB	2.44	0.47
1:B:64:TRP:HB3	1:B:263:ALA:CB	2.44	0.47
1:B:658:ASN:OD1	1:B:659:SER:N	2.40	0.47
1:C:736:VAL:HG22	1:C:858:LEU:HD13	1.97	0.47
1:A:398:ASP:OD1	1:A:512:VAL:HB	2.15	0.47
1:A:736:VAL:HG22	1:A:858:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:GLN:NE2	1:A:970:PHE:HZ	2.12	0.47
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.96	0.46
1:B:125:ASN:HA	1:B:174:PRO:HD3	1.96	0.46
1:B:303:LEU:HD12	1:B:308:VAL:HG12	1.96	0.46
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.96	0.46
1:A:393:THR:OG1	1:A:516:GLU:O	2.32	0.46
1:A:350:VAL:HG11	1:A:422:ASN:HB3	1.97	0.46
1:A:406:GLU:HG2	1:A:418:ILE:HG21	1.98	0.46
1:C:78:ARG:HH11	1:C:244:LEU:HD22	1.80	0.46
1:A:126:VAL:HG22	1:A:174:PRO:HA	1.96	0.46
1:B:350:VAL:HG11	1:B:422:ASN:HB3	1.97	0.46
1:B:81:ASN:ND2	1:B:240:THR:O	2.49	0.46
1:B:118:LEU:HB2	1:B:133:PHE:HE2	1.80	0.46
1:B:393:THR:OG1	1:B:516:GLU:OE2	2.33	0.46
1:C:108:THR:HG23	1:C:109:THR:HG23	1.97	0.46
1:C:350:VAL:HG11	1:C:422:ASN:HB3	1.96	0.46
1:C:978:ASN:HA	1:C:981:LEU:HG	1.97	0.46
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.81	0.46
1:B:436:TRP:CE3	1:B:509:ARG:HD2	2.49	0.46
1:B:532:ASN:OD1	1:B:533:LEU:N	2.42	0.46
1:A:108:THR:HG23	1:A:109:THR:HG23	1.98	0.46
1:A:200:TYR:CE2	1:A:230:PRO:HG3	2.51	0.46
1:B:331:ASN:HB3	3:B:1309:NAG:C7	2.47	0.45
1:C:167:THR:HG22	1:C:168:PHE:N	2.28	0.45
1:C:393:THR:OG1	1:C:516:GLU:O	2.33	0.45
1:C:398:ASP:OD1	1:C:512:VAL:HB	2.16	0.45
1:A:128:ILE:HD11	1:A:175:PHE:CE2	2.52	0.45
1:C:81:ASN:ND2	1:C:240:THR:O	2.50	0.45
1:A:532:ASN:OD1	1:A:533:LEU:N	2.43	0.45
1:A:86:PHE:HB2	1:A:238:PHE:HD1	1.82	0.45
1:A:988:GLU:OE1	1:A:988:GLU:N	2.50	0.45
1:C:53:ASP:HB2	1:C:55:PHE:CE2	2.51	0.45
1:C:126:VAL:HG22	1:C:174:PRO:HA	1.98	0.45
1:C:331:ASN:HB3	3:C:1309:NAG:C7	2.46	0.45
1:A:343:ASN:HB3	3:A:1310:NAG:O5	2.17	0.45
1:B:98:SER:HB3	1:B:100:ILE:HG12	1.99	0.45
1:B:393:THR:OG1	1:B:516:GLU:O	2.30	0.45
1:B:406:GLU:HG2	1:B:418:ILE:HG21	1.99	0.45
1:B:747:THR:OG1	1:B:748:GLU:OE2	2.33	0.45
1:A:331:ASN:HB3	3:A:1309:NAG:C7	2.47	0.45
1:B:630:THR:HB	1:B:631:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:ARG:NH1	1:C:459:SER:O	2.35	0.45
1:B:126:VAL:HG22	1:B:174:PRO:HA	1.98	0.45
1:B:343:ASN:HB3	3:B:1310:NAG:O5	2.16	0.45
1:C:78:ARG:NH1	1:C:244:LEU:O	2.50	0.45
1:C:1041:ASP:OD2	1:C:1045:LYS:NZ	2.35	0.45
1:C:1092:GLU:OE2	1:C:1092:GLU:HA	2.16	0.45
1:C:1103:PHE:HZ	2:T:1:NAG:H61	1.82	0.45
1:B:108:THR:HG23	1:B:109:THR:HG23	1.99	0.44
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.99	0.44
1:C:157:PHE:HE1	1:C:245:HIS:HE1	1.64	0.44
1:C:988:GLU:N	1:C:988:GLU:OE2	2.50	0.44
1:A:182:LYS:HG3	1:A:183:GLN:HG2	2.00	0.44
1:B:457:ARG:NH1	1:B:459:SER:O	2.35	0.44
1:C:137:ASN:OD1	1:C:138:ASP:N	2.46	0.44
1:C:770:ILE:O	1:C:774:GLN:HG2	2.17	0.44
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	2.00	0.44
1:B:983:ARG:NH1	1:C:381:GLY:O	2.50	0.44
1:B:182:LYS:HG3	1:B:183:GLN:HG2	1.99	0.44
1:B:398:ASP:OD1	1:B:512:VAL:HB	2.18	0.44
1:A:699:LEU:HD21	1:C:869:MET:HG2	1.99	0.44
1:B:458:LYS:HD2	1:B:473:TYR:HE1	1.83	0.44
1:B:206:LYS:NZ	1:B:221:SER:OG	2.49	0.43
1:B:759:PHE:HZ	1:C:970:PHE:HE2	1.66	0.43
1:C:343:ASN:HB3	3:C:1310:NAG:O5	2.16	0.43
1:A:212:LEU:HB3	1:A:213:GLY:H	1.55	0.43
1:A:707:TYR:HB3	1:C:792:PRO:HG2	2.01	0.43
1:C:617:CYS:HA	1:C:620:VAL:HG23	2.00	0.43
1:A:458:LYS:HD2	1:A:473:TYR:HE1	1.83	0.43
1:B:748:GLU:OE2	1:B:748:GLU:N	2.49	0.43
1:B:139:PRO:HB2	1:B:244:LEU:HD12	2.01	0.43
1:B:78:ARG:NH1	1:B:244:LEU:O	2.52	0.43
1:C:458:LYS:HD2	1:C:473:TYR:HE1	1.83	0.43
1:A:126:VAL:HG11	1:A:175:PHE:H	1.84	0.43
1:A:167:THR:HG22	1:A:168:PHE:N	2.28	0.43
1:A:353:TRP:H	1:A:466:ARG:HE	1.66	0.43
1:C:531:THR:HG22	1:C:532:ASN:N	2.34	0.43
1:C:630:THR:HB	1:C:631:PRO:HD3	1.99	0.43
1:A:37:TYR:HB3	1:A:223:LEU:HB2	2.00	0.43
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.54	0.43
1:B:287:ASP:HB3	1:B:306:PHE:HE2	1.84	0.42
1:A:65:PHE:CE2	1:A:84:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:PHE:HZ	1:B:970:PHE:HE2	1.68	0.42
1:B:529:LYS:HD2	1:B:529:LYS:HA	1.86	0.42
1:C:119:ILE:HG22	1:C:119:ILE:O	2.19	0.42
1:A:78:ARG:NH1	1:A:244:LEU:O	2.53	0.42
1:A:139:PRO:HB2	1:A:244:LEU:HD12	2.01	0.42
1:A:392:PHE:N	1:A:524:VAL:O	2.42	0.42
1:A:630:THR:HB	1:A:631:PRO:HD3	2.00	0.42
1:A:1116:THR:OG1	1:A:1117:THR:N	2.52	0.42
1:B:179:LEU:HD11	1:B:207:HIS:HB3	2.01	0.42
1:C:125:ASN:HA	1:C:174:PRO:HD3	2.00	0.42
1:C:532:ASN:OD1	1:C:533:LEU:N	2.38	0.42
1:A:329:PHE:HE2	1:A:528:LYS:HG2	1.84	0.42
1:C:182:LYS:HG3	1:C:183:GLN:HG2	2.01	0.42
1:C:318:PHE:HZ	1:C:615:VAL:HG11	1.84	0.42
1:C:989:ALA:O	1:C:993:ILE:HG12	2.19	0.42
1:A:128:ILE:HD11	1:A:175:PHE:HE2	1.85	0.42
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.84	0.42
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.54	0.42
1:A:1092:GLU:OE1	1:A:1107:ARG:NH1	2.53	0.42
1:A:531:THR:HG22	1:A:532:ASN:N	2.35	0.42
1:B:605:SER:OG	1:B:606:ASN:N	2.51	0.42
1:C:985:ASP:OD1	1:C:985:ASP:N	2.47	0.42
1:A:65:PHE:O	1:A:265:TYR:HB3	2.20	0.42
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.55	0.42
1:B:363:ALA:HB1	1:B:365:TYR:HE1	1.85	0.42
1:C:1116:THR:OG1	1:C:1117:THR:N	2.53	0.42
1:B:353:TRP:H	1:B:466:ARG:HE	1.67	0.42
1:C:368:LEU:HD11	1:C:377:PHE:CE1	2.55	0.42
1:B:531:THR:HG22	1:B:532:ASN:N	2.34	0.41
1:B:1103:PHE:HZ	2:N:1:NAG:H61	1.85	0.41
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.55	0.41
1:A:792:PRO:HG2	1:B:707:TYR:HB3	2.03	0.41
1:A:1103:PHE:HZ	2:H:1:NAG:H61	1.85	0.41
1:B:1092:GLU:OE1	1:B:1092:GLU:HA	2.21	0.41
1:C:436:TRP:CE3	1:C:509:ARG:HD2	2.49	0.41
1:A:194:PHE:HD1	1:A:203:ILE:HG12	1.85	0.41
1:B:167:THR:HG22	1:B:168:PHE:N	2.28	0.41
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	2.02	0.41
1:C:374:PHE:HE2	1:C:377:PHE:HB2	1.85	0.41
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	2.01	0.41
1:A:855:PHE:HD2	1:B:589:PRO:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:PRO:HG2	1:C:707:TYR:HB3	2.03	0.41
1:C:329:PHE:HE2	1:C:528:LYS:HG2	1.85	0.41
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.86	0.41
1:B:625:HIS:HB3	1:B:628:GLN:HB3	2.03	0.41
1:A:206:LYS:NZ	1:A:221:SER:OG	2.52	0.41
1:A:709:ASN:ND2	2:E:1:NAG:H62	2.36	0.41
1:A:990:GLU:HA	1:A:993:ILE:HG12	2.03	0.41
1:B:126:VAL:HG13	1:B:174:PRO:HA	2.02	0.41
1:B:392:PHE:N	1:B:524:VAL:O	2.48	0.41
1:B:979:ASP:O	1:B:983:ARG:CB	2.61	0.41
1:C:128:ILE:HD11	1:C:175:PHE:HE2	1.86	0.41
1:C:537:LYS:HE2	1:C:537:LYS:HB3	1.98	0.41
1:C:990:GLU:HA	1:C:993:ILE:HG12	2.02	0.41
1:A:98:SER:HB3	1:A:100:ILE:HG12	2.02	0.41
1:B:985:ASP:OD1	1:B:985:ASP:N	2.48	0.41
1:C:36:VAL:HG21	1:C:220:PHE:CE2	2.56	0.41
1:C:66:HIS:NE2	1:C:251:PRO:O	2.53	0.41
1:C:98:SER:HB3	1:C:100:ILE:HG12	2.02	0.41
1:C:179:LEU:HD11	1:C:207:HIS:HB3	2.02	0.41
1:C:353:TRP:H	1:C:466:ARG:HE	1.69	0.41
1:A:452:GLN:HG2	1:A:492:LEU:HD23	2.03	0.40
1:A:1004:LEU:HA	1:A:1004:LEU:HD23	1.90	0.40
1:A:800:PHE:HD2	1:A:927:PHE:CD2	2.39	0.40
1:B:368:LEU:HD11	1:B:377:PHE:CE2	2.55	0.40
1:C:430:THR:O	1:C:430:THR:HG23	2.21	0.40
1:A:457:ARG:NH1	1:A:459:SER:O	2.35	0.40
1:A:605:SER:OG	1:A:606:ASN:N	2.54	0.40
1:C:800:PHE:HD2	1:C:927:PHE:CD2	2.39	0.40
1:A:363:ALA:HB1	1:A:365:TYR:HE1	1.87	0.40
1:A:961:THR:HG21	1:C:762:GLN:NE2	2.35	0.40
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.57	0.40
1:B:353:TRP:CH2	1:B:466:ARG:HB2	2.57	0.40
1:B:1116:THR:OG1	1:B:1117:THR:N	2.53	0.40
1:B:66:HIS:NE2	1:B:251:PRO:O	2.54	0.40
1:B:865:LEU:HD23	1:B:865:LEU:HA	1.96	0.40
1:C:357:ARG:HG3	1:C:396:TYR:CE1	2.57	0.40
1:C:363:ALA:HB1	1:C:365:TYR:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1089/1270 (86%)	1035 (95%)	54 (5%)	0	100	100
1	B	1089/1270 (86%)	1037 (95%)	52 (5%)	0	100	100
1	C	1089/1270 (86%)	1038 (95%)	51 (5%)	0	100	100
All	All	3267/3810 (86%)	3110 (95%)	157 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	952/1109 (86%)	950 (100%)	2 (0%)	92	96
1	B	952/1109 (86%)	950 (100%)	2 (0%)	92	96
1	C	952/1109 (86%)	949 (100%)	3 (0%)	91	96
All	All	2856/3327 (86%)	2849 (100%)	7 (0%)	91	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	A	983	ARG
1	B	190	ARG
1	B	983	ARG
1	C	190	ARG

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Mol	Chain	Res	Type
1	C	658	ASN
1	C	983	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	774	GLN
1	A	957	GLN
1	B	148	ASN
1	C	148	ASN

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 ⓘ

36 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	1,2	14,14,15	0.22	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	E	1	1,2	14,14,15	0.34	0	17,19,21	1.30	1 (5%)
2	NAG	E	2	2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	F	1	1,2	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	F	2	2	14,14,15	0.17	0	17,19,21	0.48	0
2	NAG	G	1	1,2	14,14,15	0.19	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	2	2	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	H	1	1,2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	H	2	2	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	I	1	1,2	14,14,15	0.48	0	17,19,21	0.63	0
2	NAG	I	2	2	14,14,15	0.19	0	17,19,21	0.51	0
2	NAG	J	1	1,2	14,14,15	0.27	0	17,19,21	0.61	1 (5%)
2	NAG	J	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	K	1	1,2	14,14,15	0.35	0	17,19,21	1.30	1 (5%)
2	NAG	K	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	L	1	1,2	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	L	2	2	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	M	1	1,2	14,14,15	0.18	0	17,19,21	0.44	0
2	NAG	M	2	2	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	N	1	1,2	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	N	2	2	14,14,15	0.23	0	17,19,21	0.40	0
2	NAG	O	1	1,2	14,14,15	0.47	0	17,19,21	0.63	0
2	NAG	O	2	2	14,14,15	0.19	0	17,19,21	0.50	0
2	NAG	P	1	1,2	14,14,15	0.20	0	17,19,21	0.49	0
2	NAG	P	2	2	14,14,15	0.21	0	17,19,21	0.41	0
2	NAG	Q	1	1,2	14,14,15	0.35	0	17,19,21	1.29	1 (5%)
2	NAG	Q	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	R	1	1,2	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	R	2	2	14,14,15	0.18	0	17,19,21	0.49	0
2	NAG	S	1	1,2	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	S	2	2	14,14,15	0.23	0	17,19,21	0.40	0
2	NAG	T	1	1,2	14,14,15	0.18	0	17,19,21	0.44	0
2	NAG	T	2	2	14,14,15	0.24	0	17,19,21	0.39	0
2	NAG	U	1	1,2	14,14,15	0.45	0	17,19,21	0.64	0
2	NAG	U	2	2	14,14,15	0.18	0	17,19,21	0.51	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	C1-O5-C5	4.80	118.70	112.19
2	E	1	NAG	C1-O5-C5	4.79	118.68	112.19
2	Q	1	NAG	C1-O5-C5	4.76	118.65	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6

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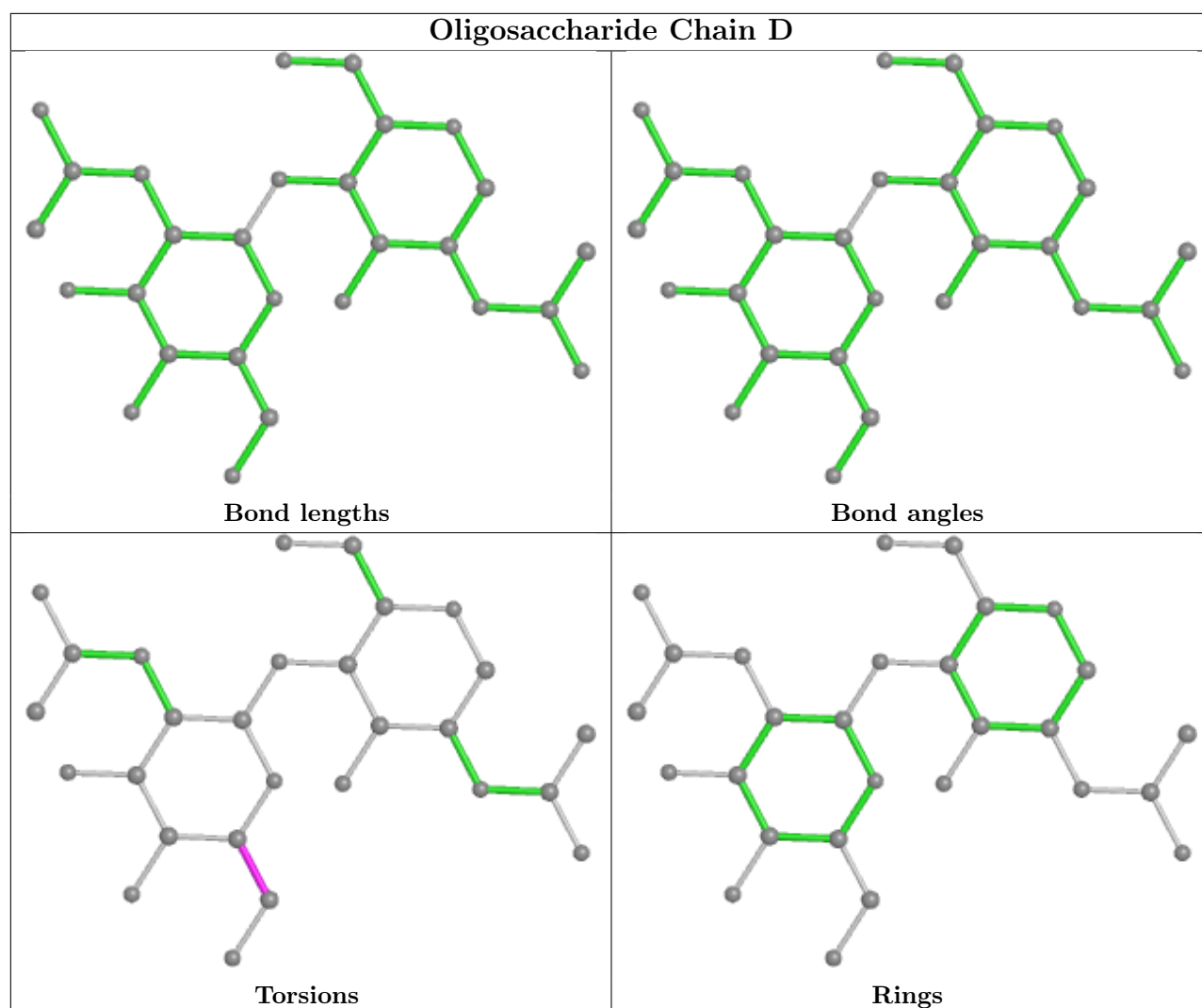
Mol	Chain	Res	Type	Atoms
2	K	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C3-C2-N2-C7
2	O	1	NAG	C3-C2-N2-C7
2	U	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C4-C5-C6-O6

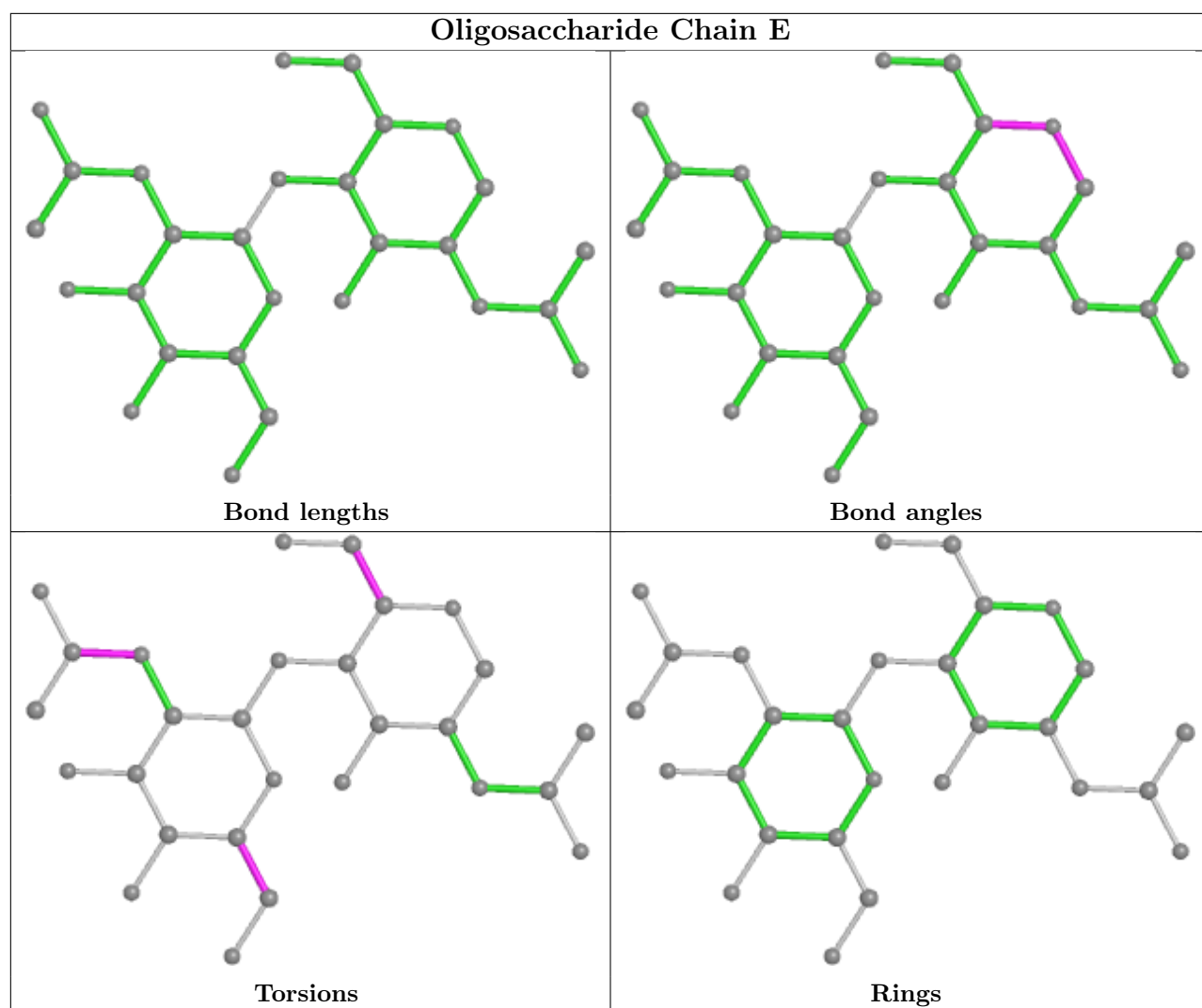
There are no ring outliers.

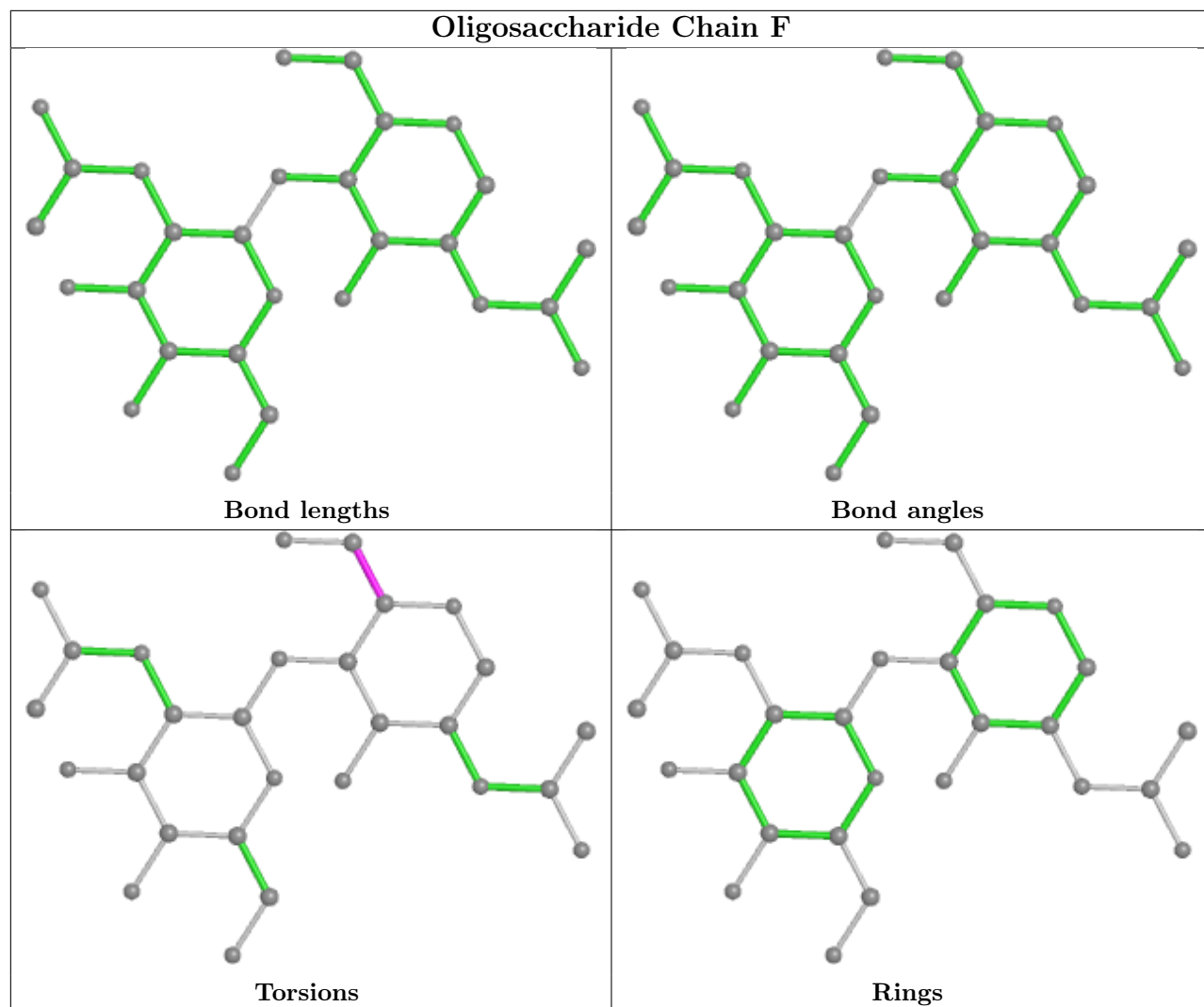
4 monomers are involved in 4 short contacts:

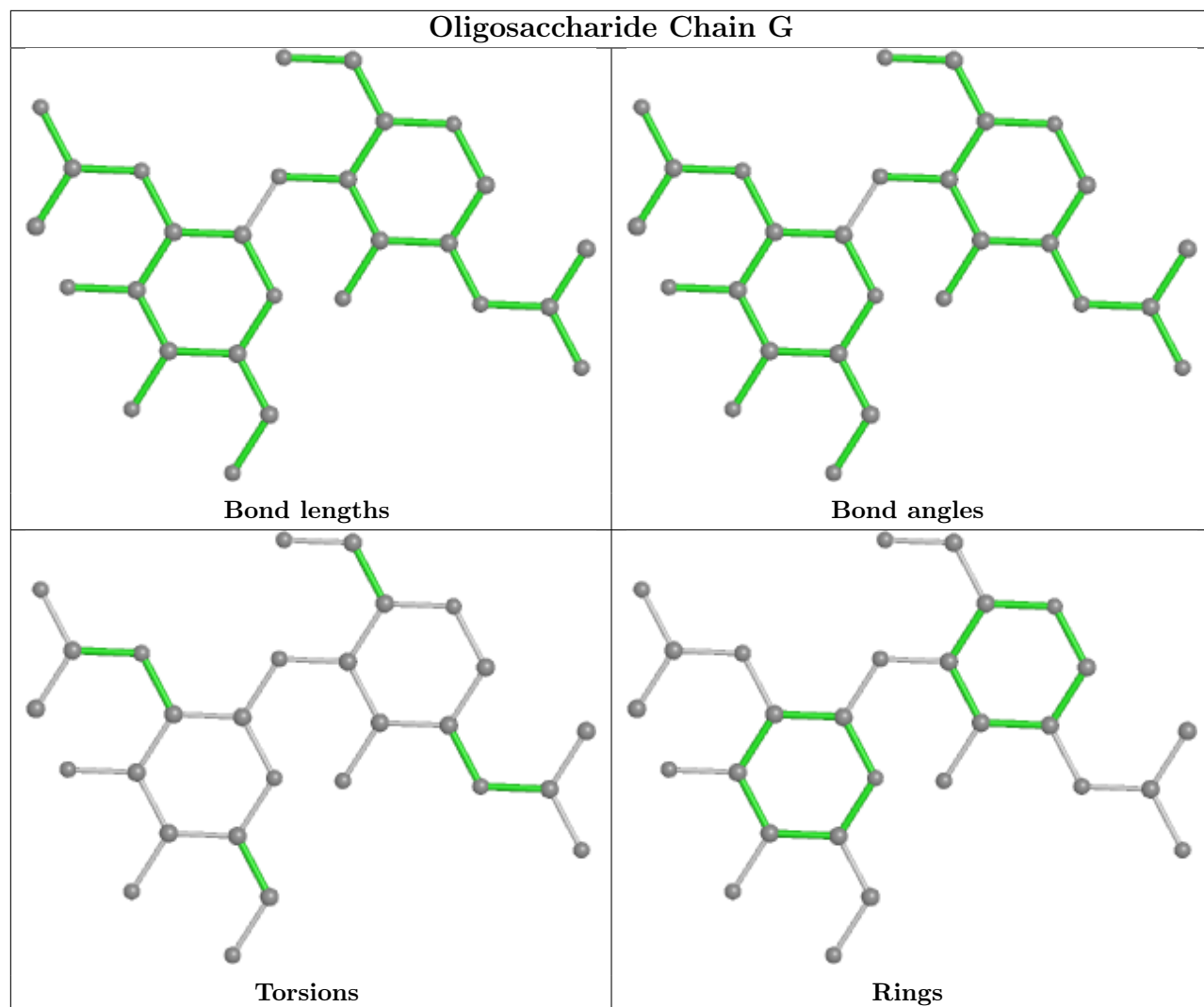
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
2	H	1	NAG	1	0
2	N	1	NAG	1	0
2	T	1	NAG	1	0

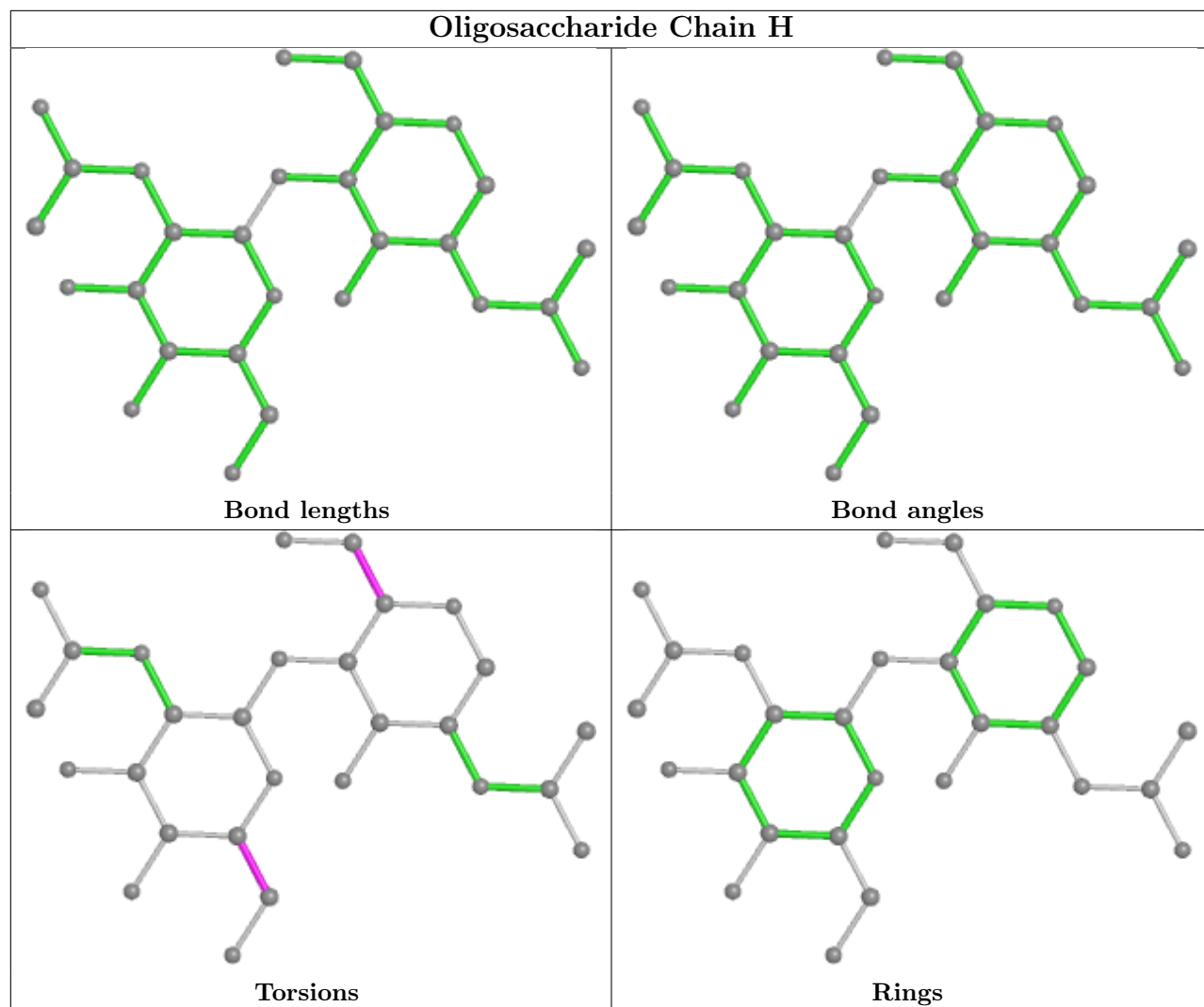
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

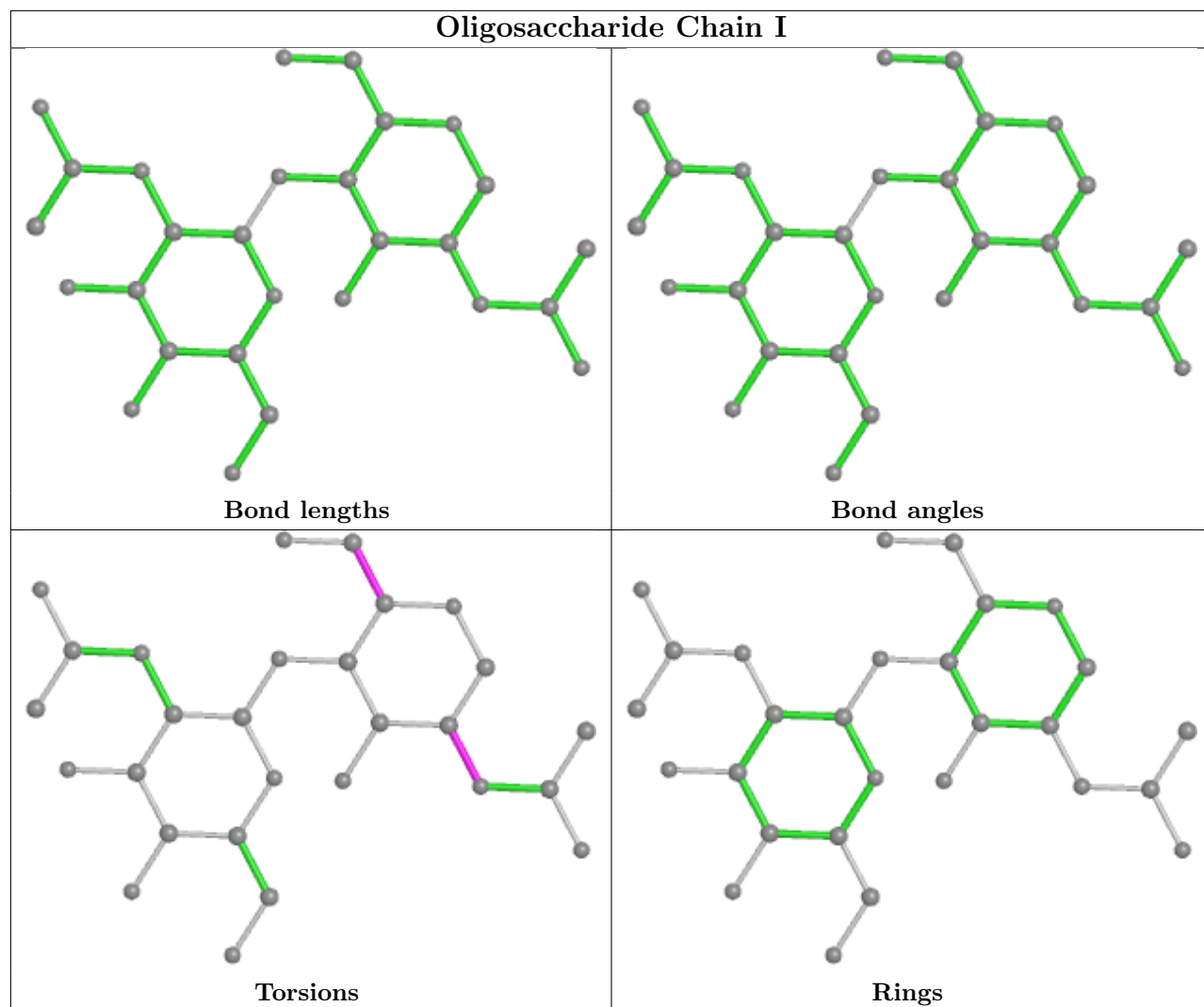


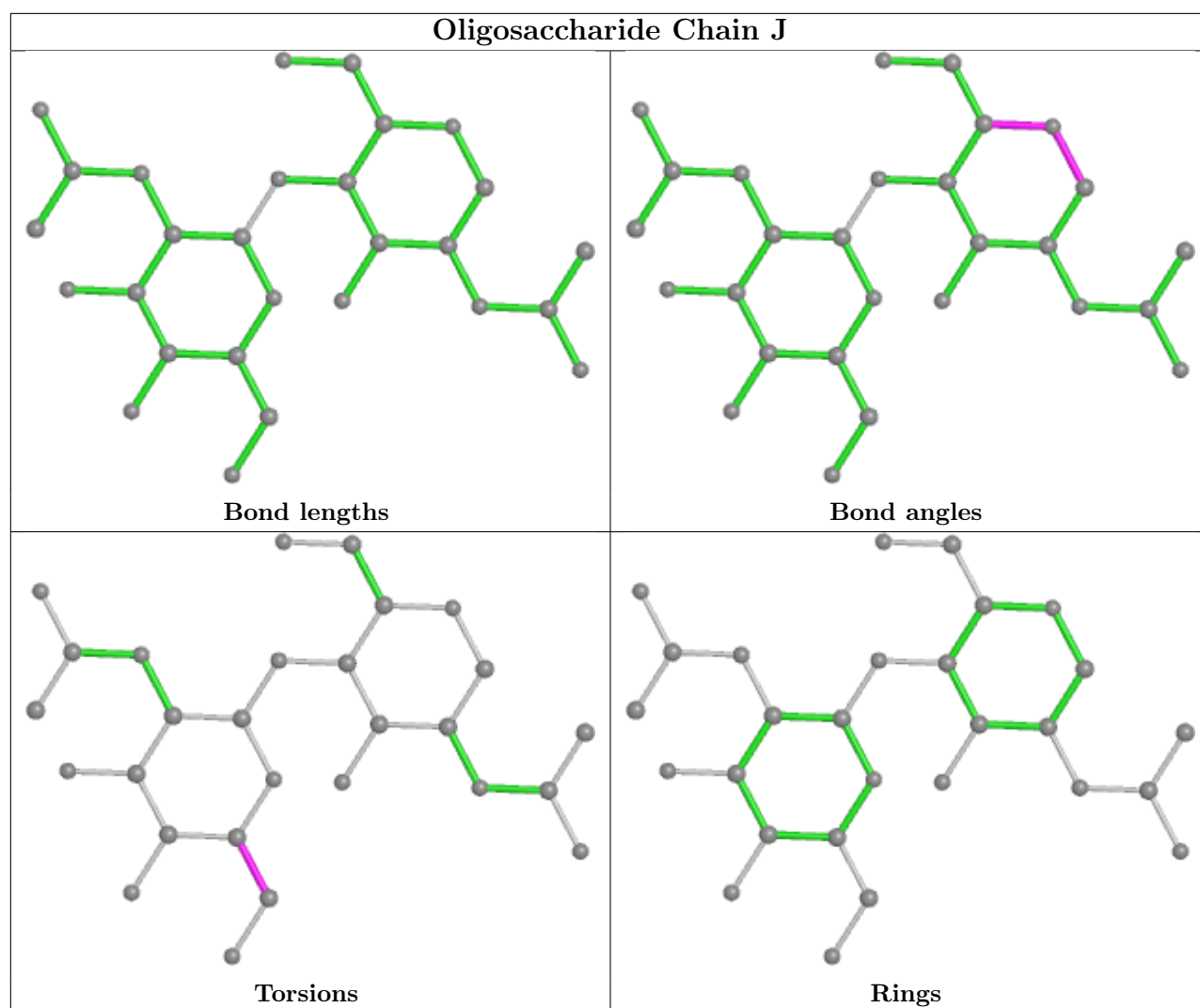


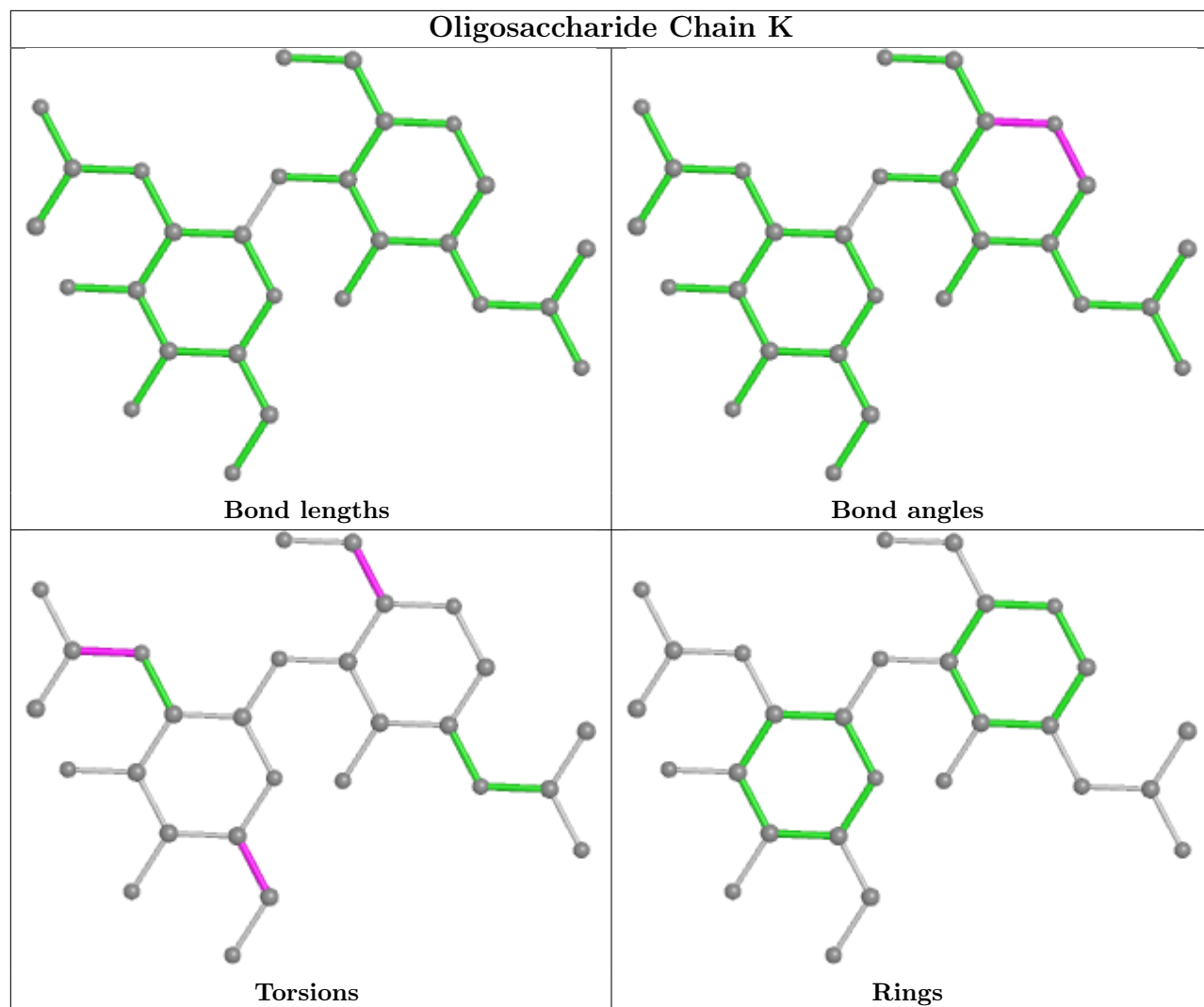


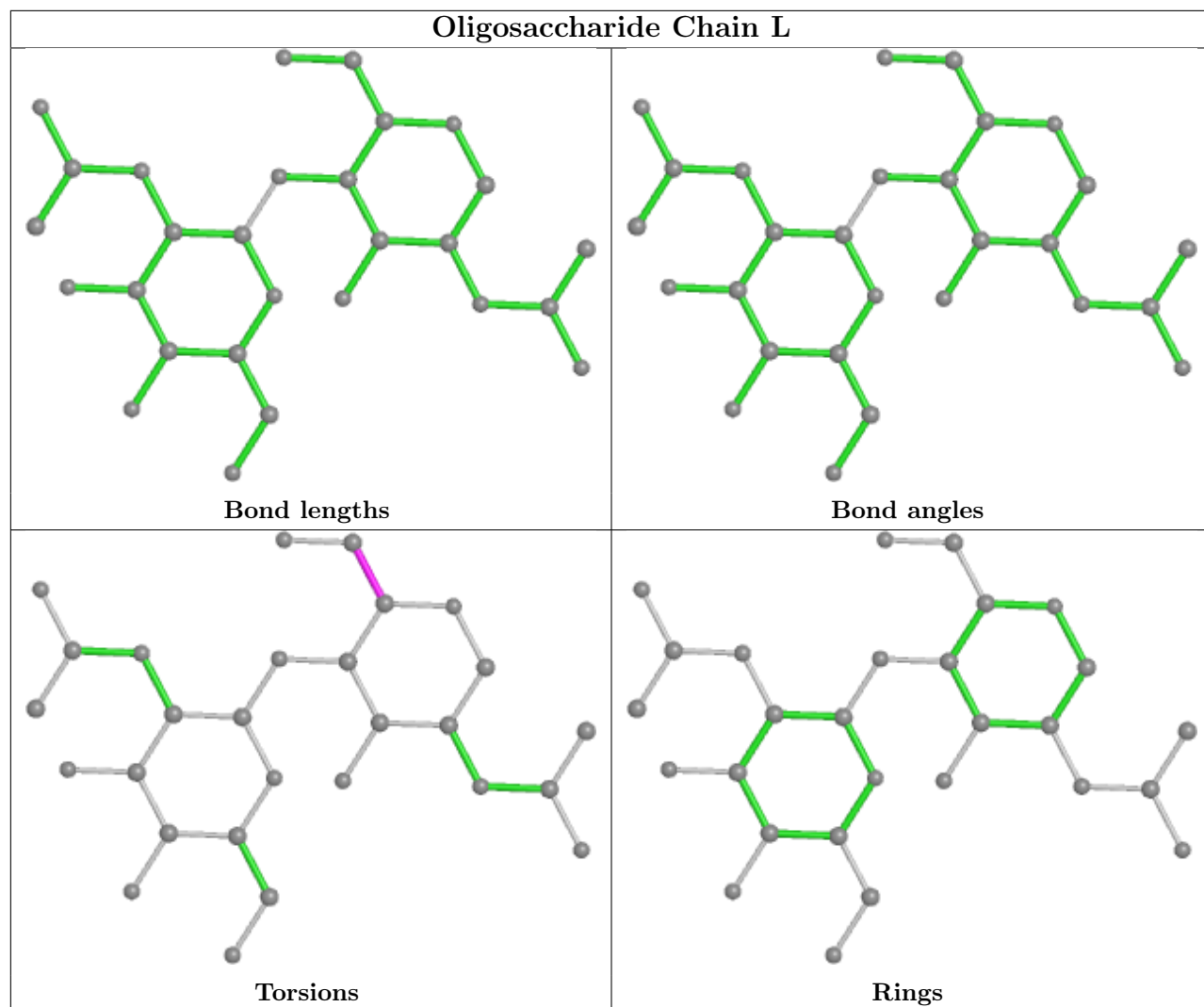


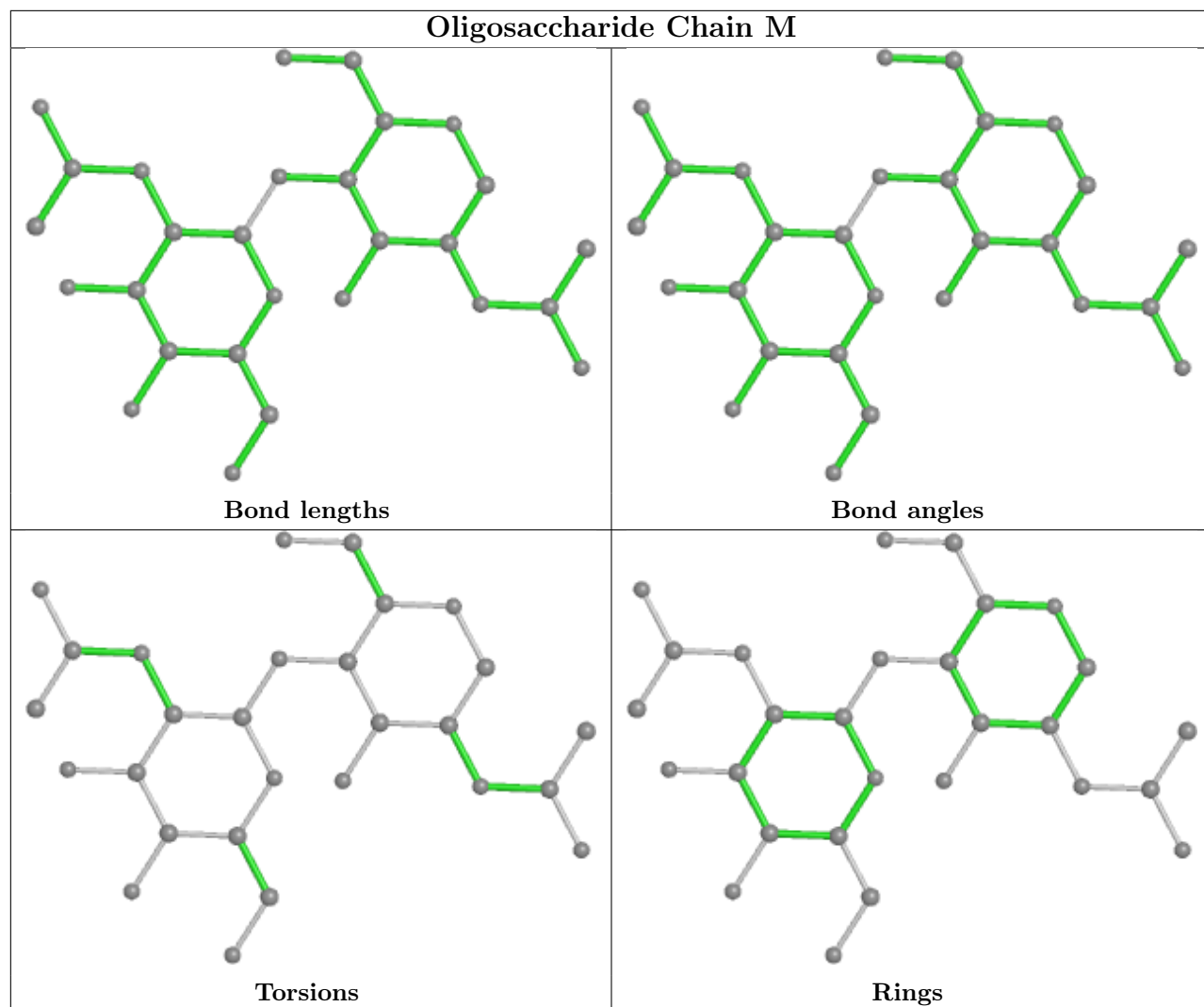


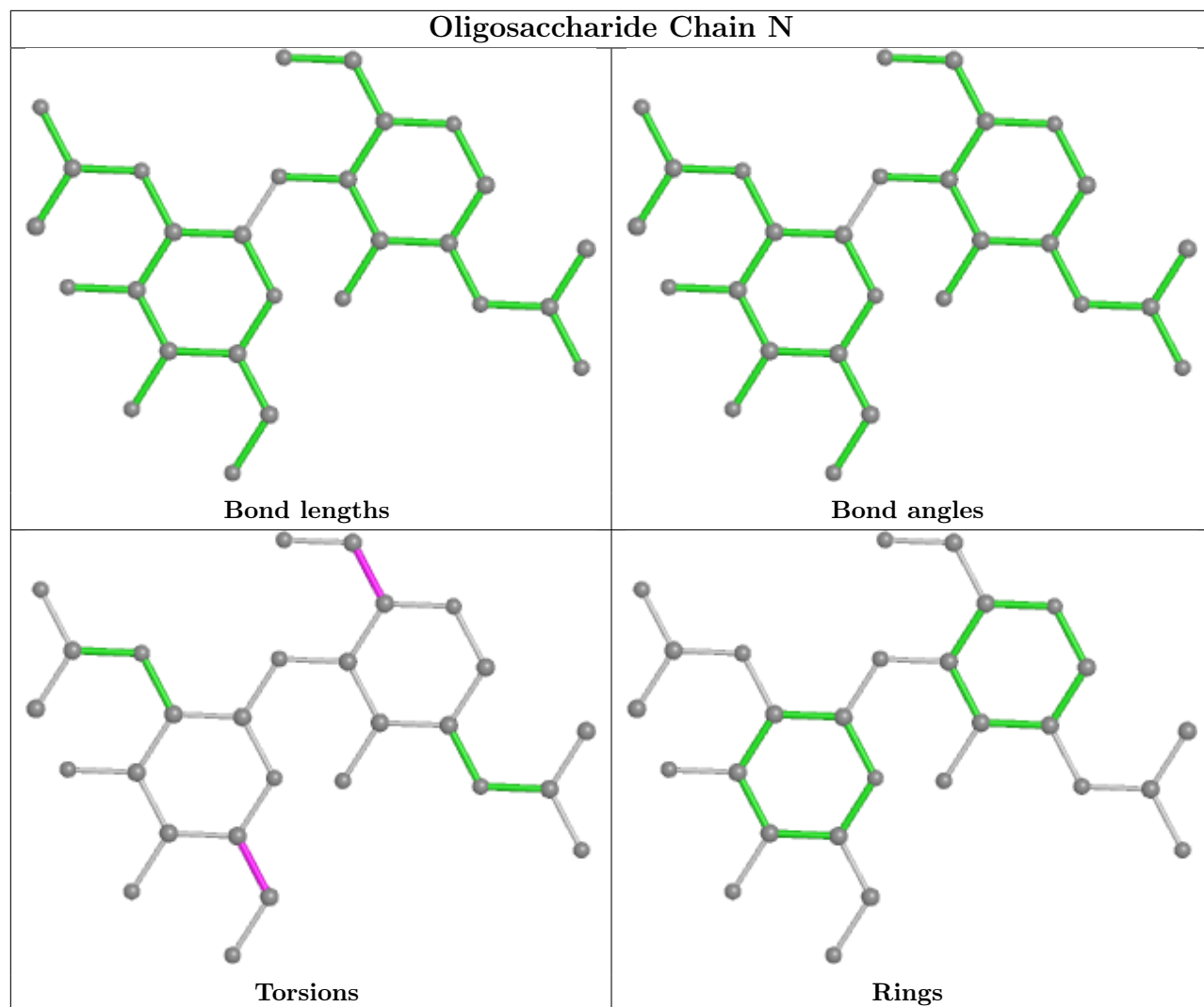


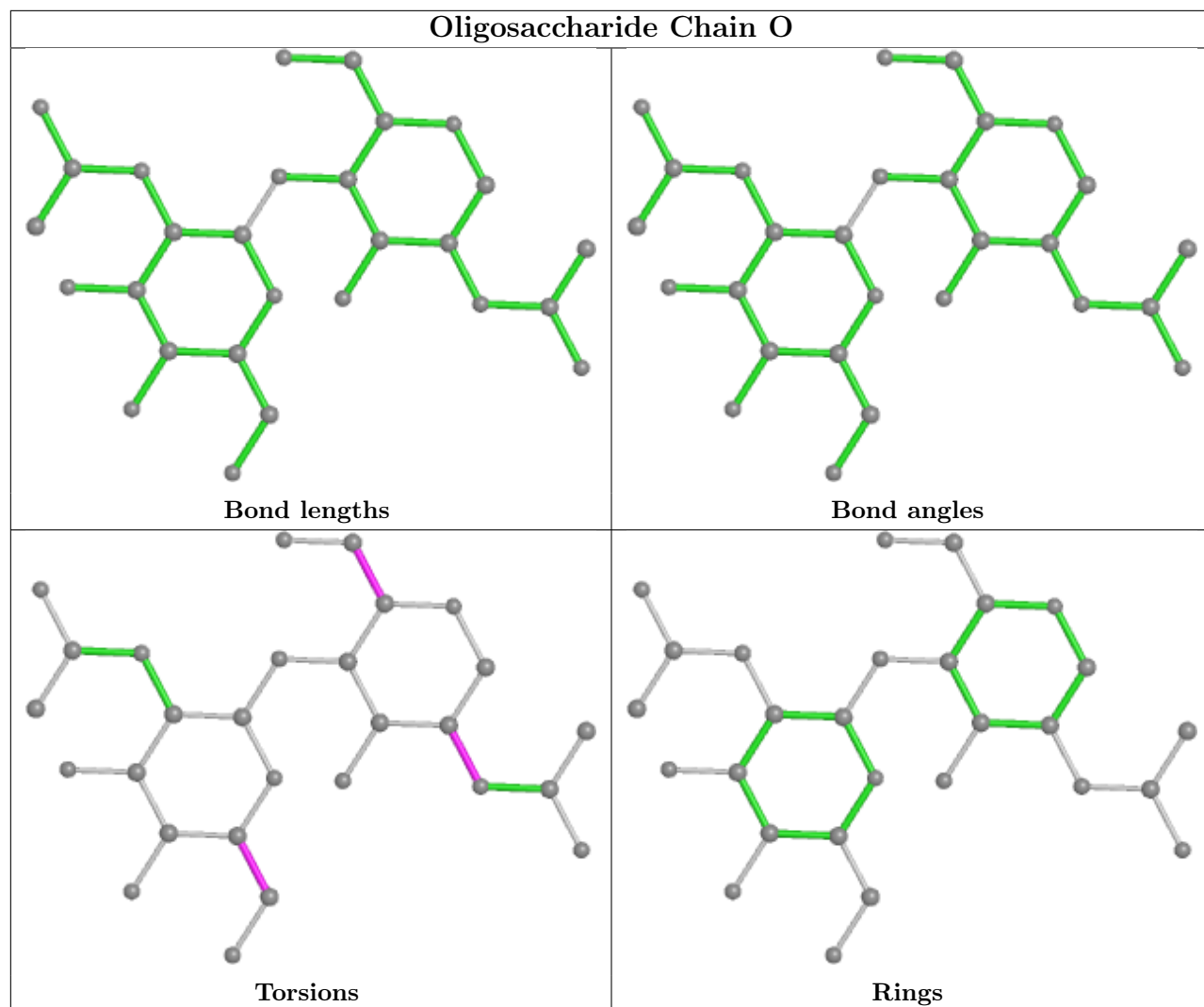


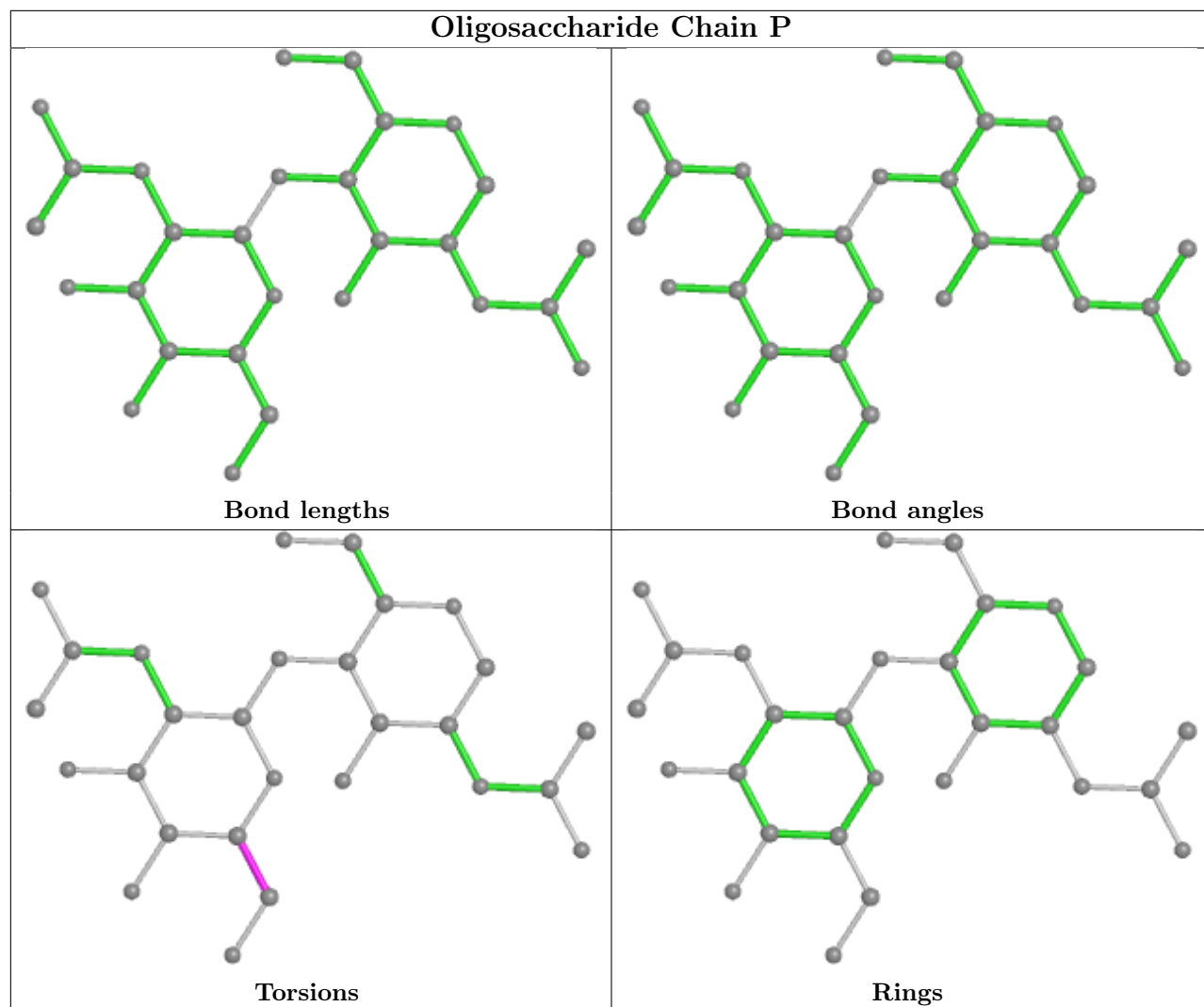


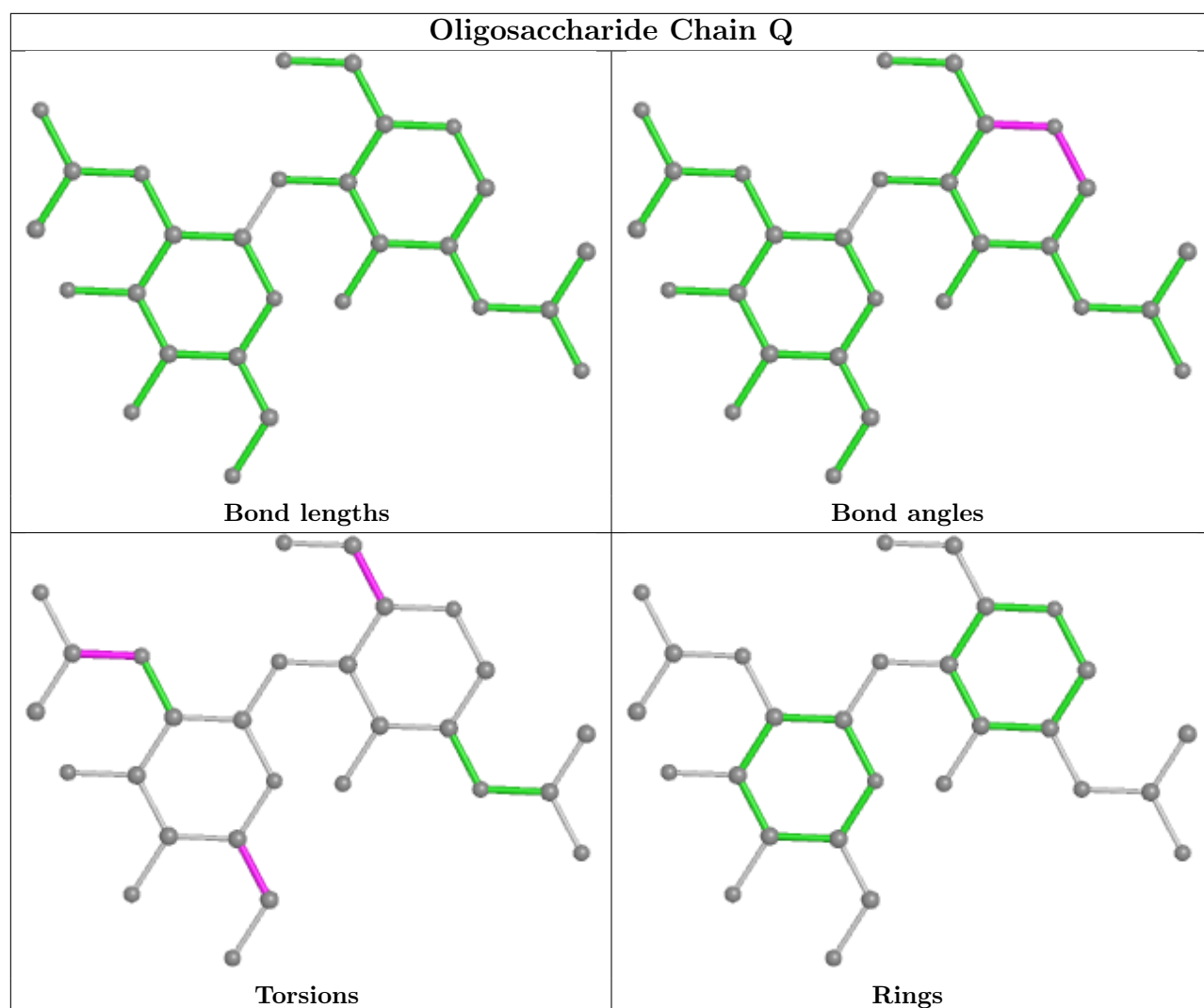


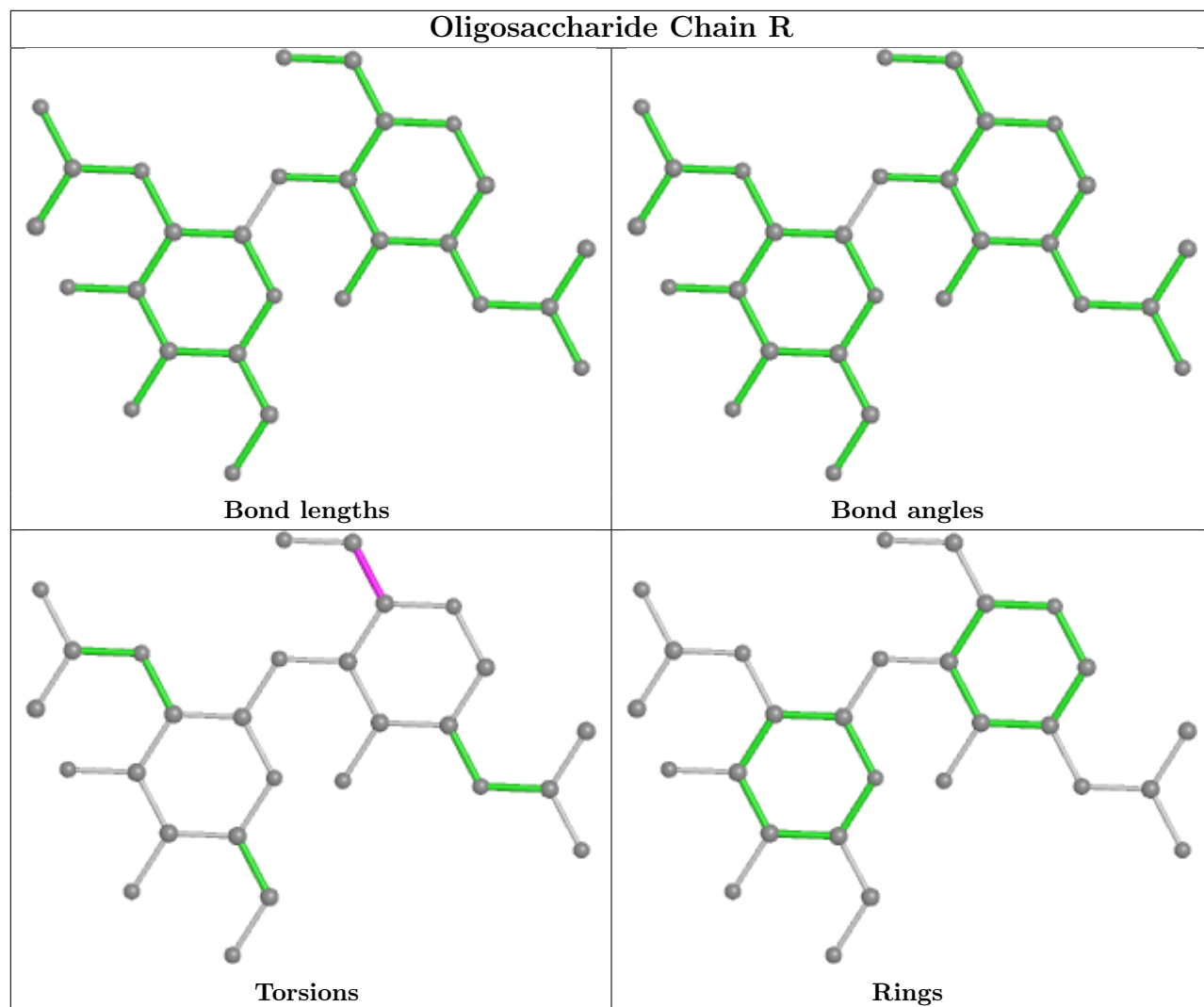


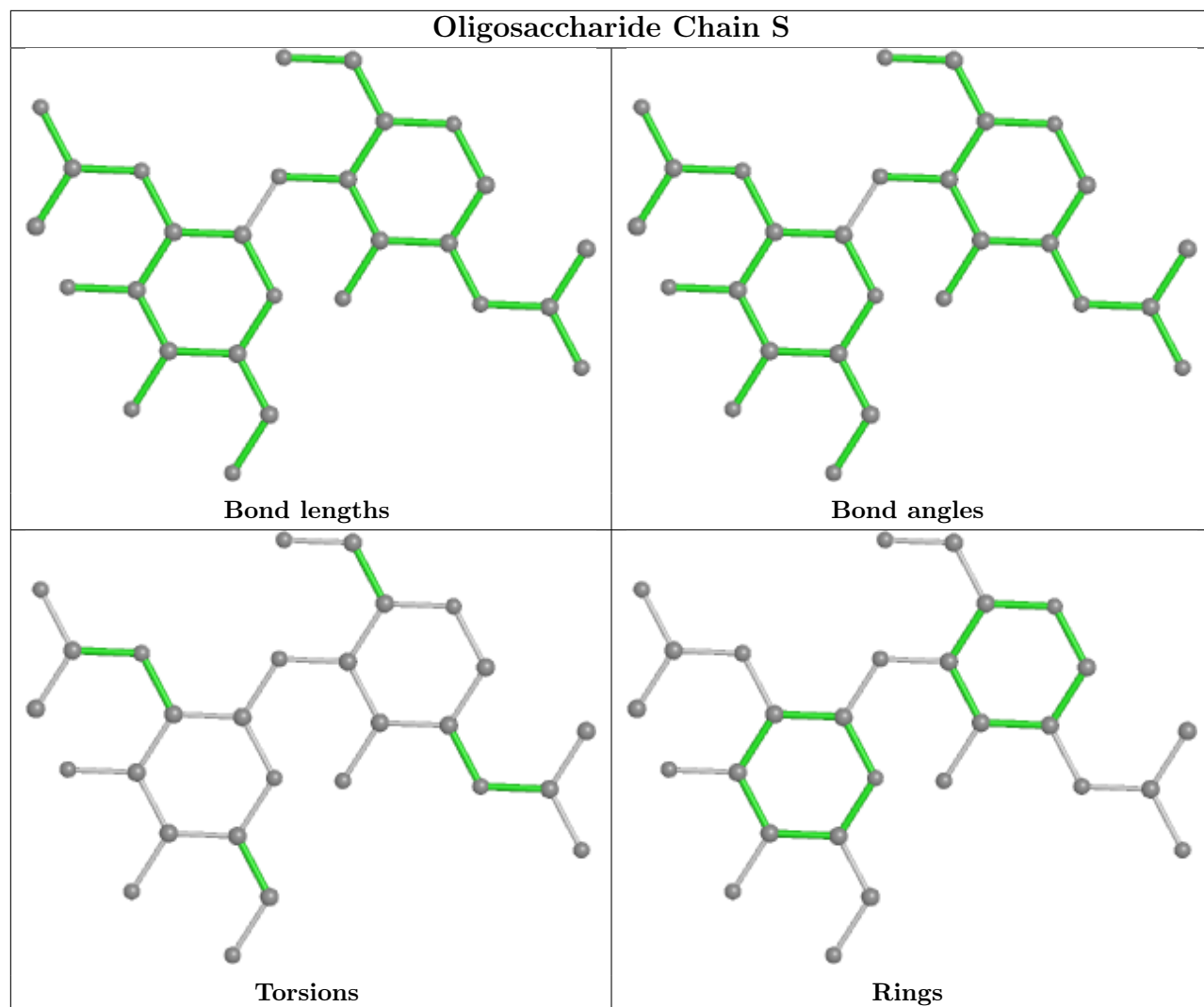


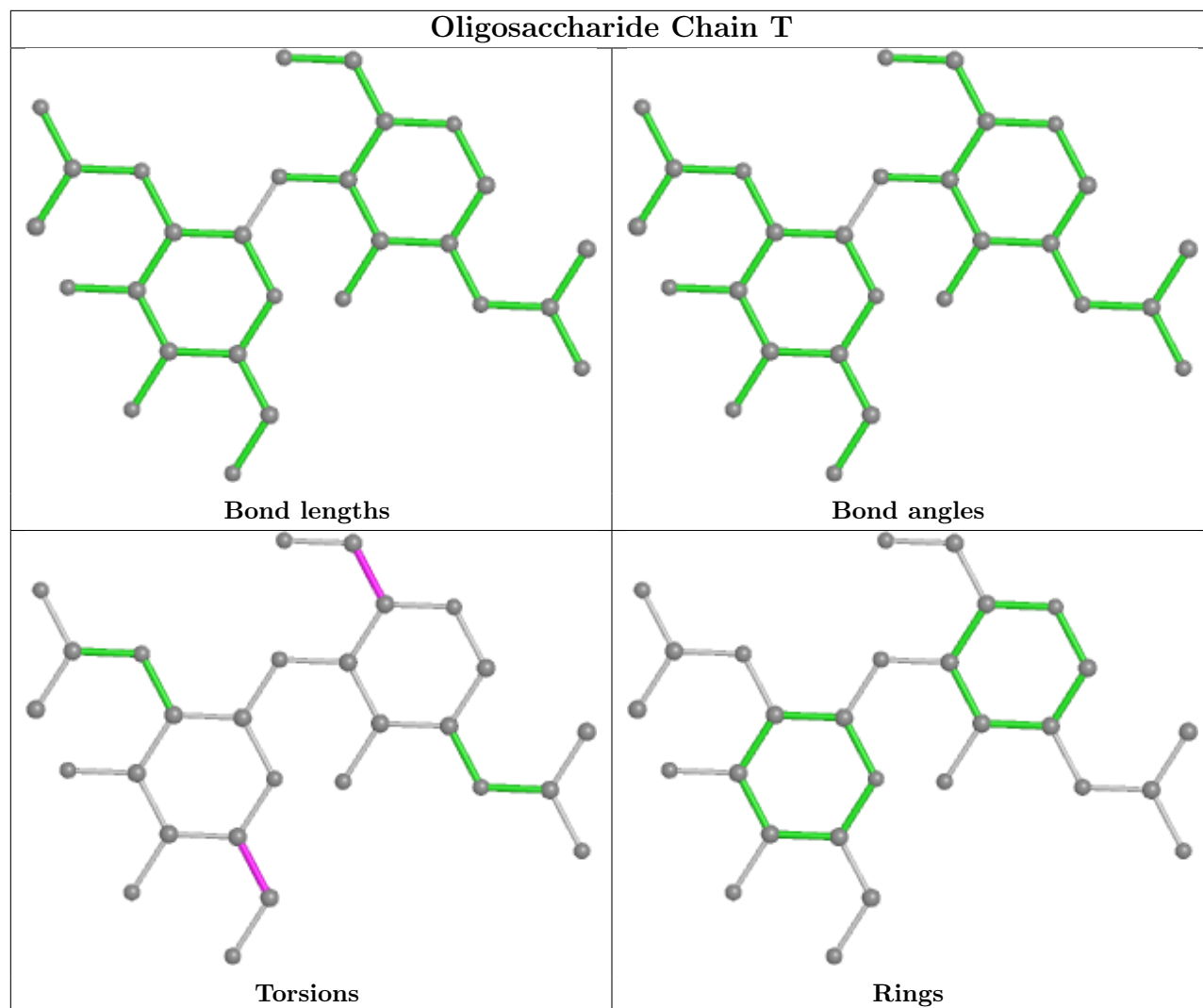


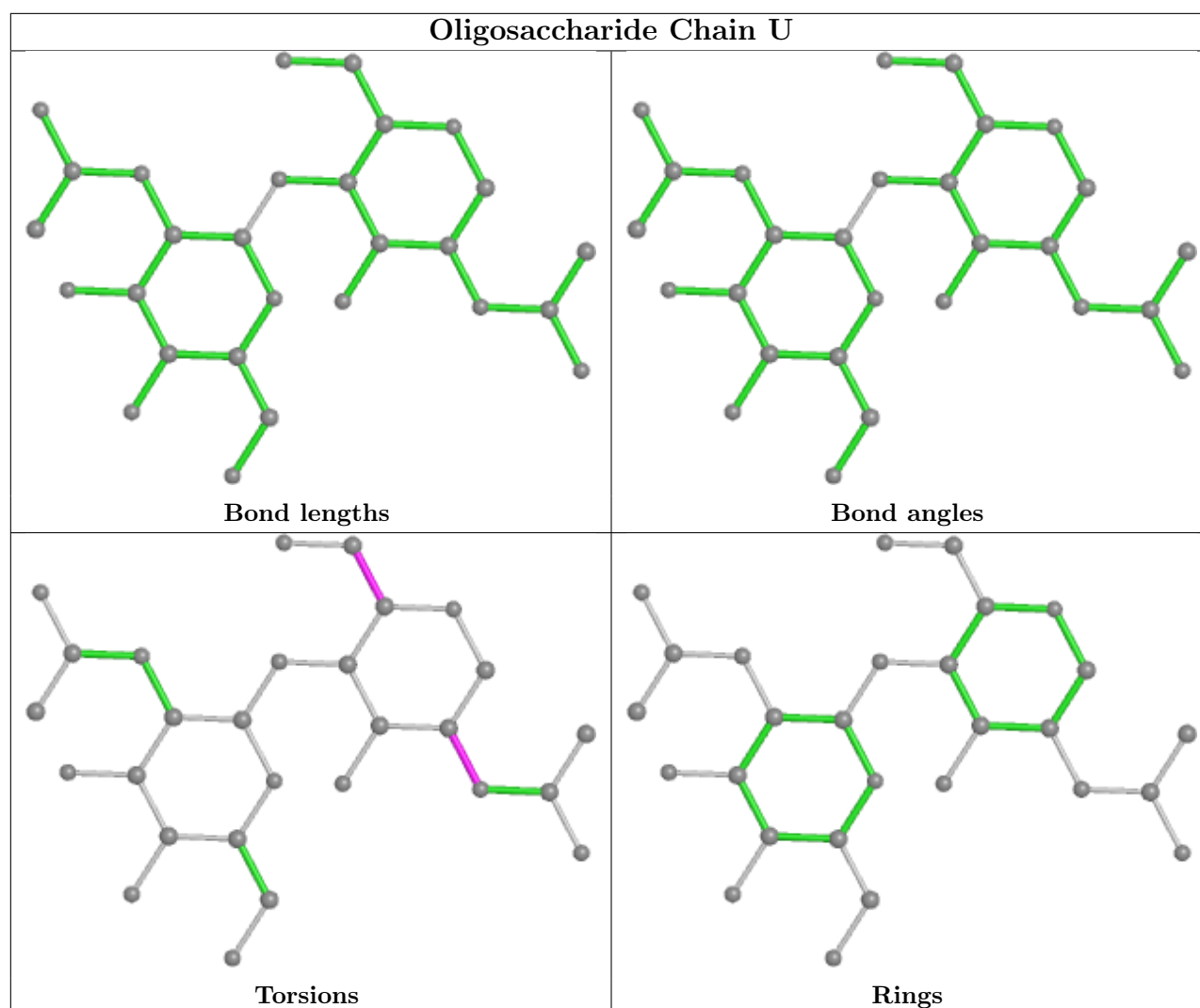












5.6 Ligand geometry [i](#)

30 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	$\# Z > 2$
3	NAG	A	1306	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	A	1308	1	14,14,15	0.18	0	17,19,21	0.41	0
3	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1307	1	14,14,15	0.16	0	17,19,21	0.55	0
3	NAG	B	1301	1	14,14,15	0.45	0	17,19,21	1.23	1 (5%)
3	NAG	A	1309	1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	C	1301	1	14,14,15	0.45	0	17,19,21	1.23	2 (11%)
3	NAG	A	1307	1	14,14,15	0.17	0	17,19,21	0.53	0
3	NAG	A	1302	1	14,14,15	0.18	0	17,19,21	0.43	0
3	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	B	1306	1	14,14,15	0.18	0	17,19,21	0.46	0
3	NAG	A	1310	1	14,14,15	0.28	0	17,19,21	0.43	0
3	NAG	B	1305	1	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	C	1306	1	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	C	1308	1	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	B	1303	1	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	B	1309	1	14,14,15	0.35	0	17,19,21	0.55	0
3	NAG	A	1305	1	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	C	1305	1	14,14,15	0.30	0	17,19,21	0.50	0
3	NAG	C	1304	1	14,14,15	0.17	0	17,19,21	0.41	0
3	NAG	C	1309	1	14,14,15	0.34	0	17,19,21	0.54	0
3	NAG	A	1301	1	14,14,15	0.43	0	17,19,21	1.23	1 (5%)
3	NAG	B	1308	1	14,14,15	0.17	0	17,19,21	0.42	0
3	NAG	B	1307	1	14,14,15	0.16	0	17,19,21	0.54	0
3	NAG	B	1302	1	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	A	1303	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	C	1302	1	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	C	1310	1	14,14,15	0.27	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1307	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	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1301	NAG	C2-N2-C7	4.30	129.02	122.90
3	A	1301	NAG	C2-N2-C7	4.28	129.00	122.90
3	C	1301	NAG	C2-N2-C7	4.27	128.98	122.90
3	C	1301	NAG	C1-C2-N2	2.02	113.94	110.49

There are no chirality outliers.

All (62) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	C4-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	A	1309	NAG	C3-C2-N2-C7
3	B	1309	NAG	C3-C2-N2-C7
3	C	1309	NAG	C3-C2-N2-C7
3	A	1305	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1301	NAG	C3-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	C	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1310	NAG	1	0
3	B	1301	NAG	1	0
3	A	1309	NAG	1	0
3	C	1301	NAG	1	0
3	A	1310	NAG	1	0
3	B	1309	NAG	1	0
3	C	1309	NAG	1	0
3	A	1301	NAG	1	0
3	C	1310	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

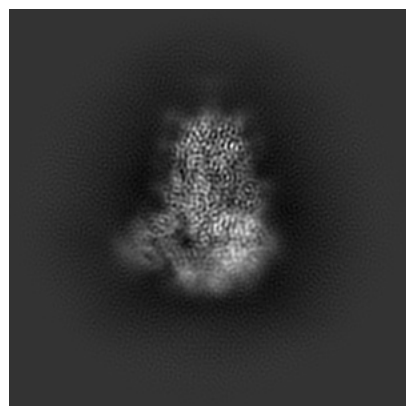
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33325. These allow visual inspection of the internal detail of the map and identification of artifacts.

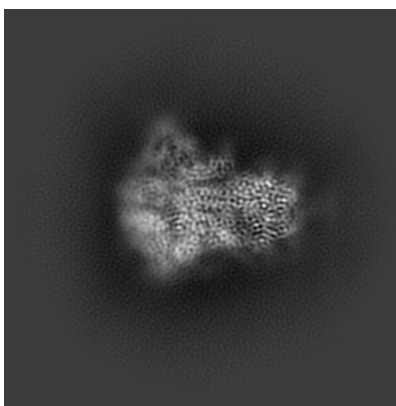
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

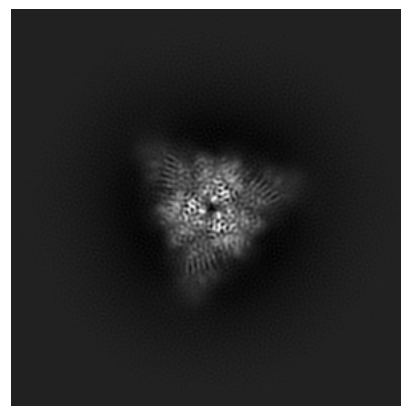
6.1.1 Primary map



X

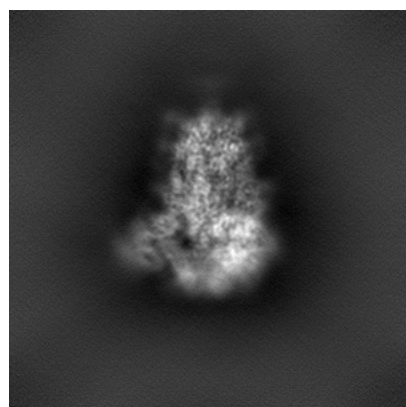


Y

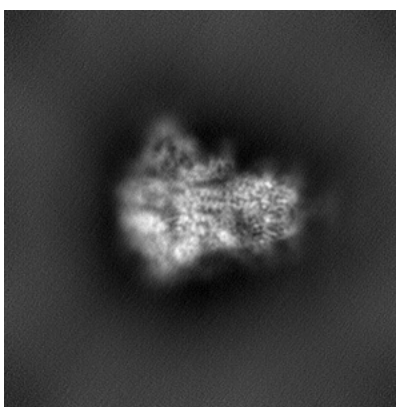


Z

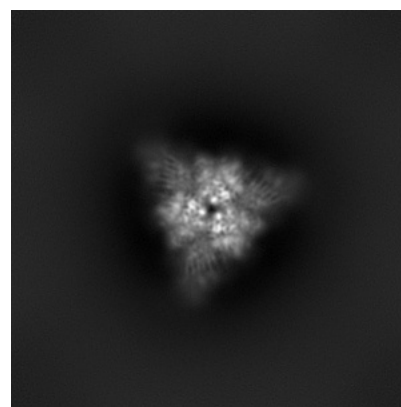
6.1.2 Raw map



X



Y

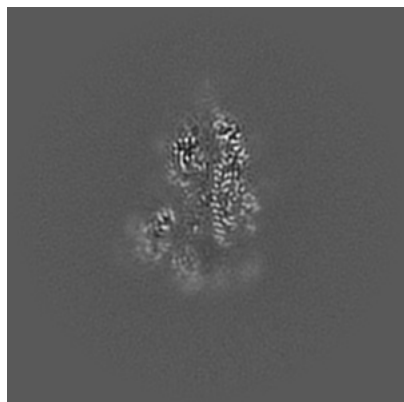


Z

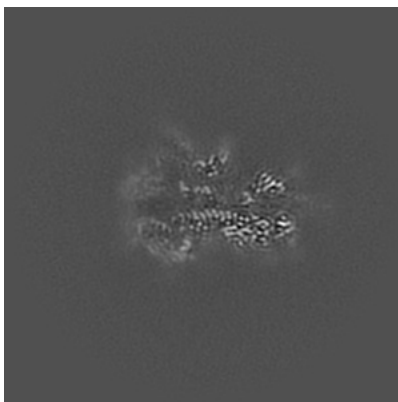
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

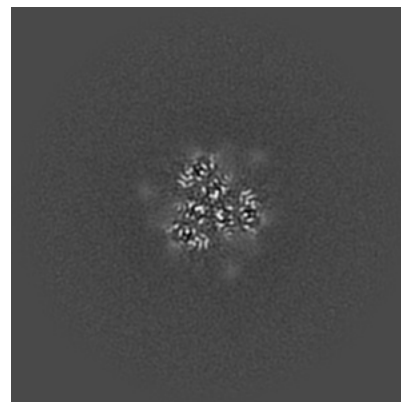
6.2.1 Primary map



X Index: 160

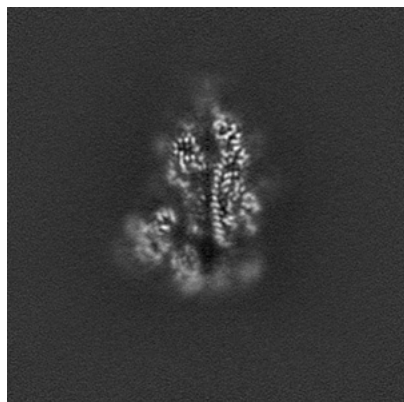


Y Index: 160

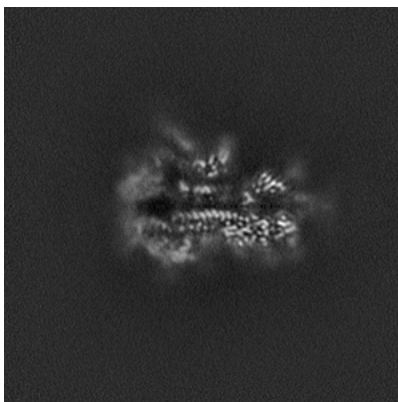


Z Index: 160

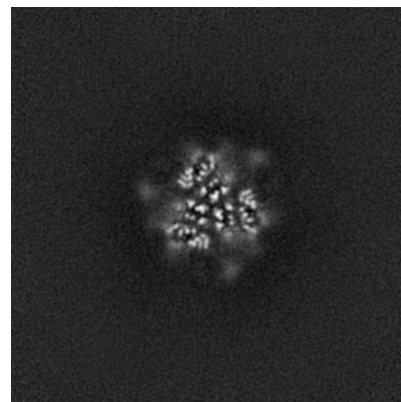
6.2.2 Raw map



X Index: 160



Y Index: 160

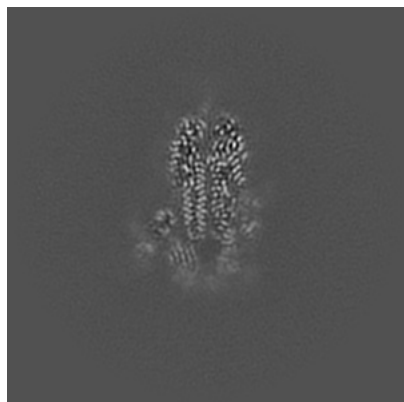


Z Index: 160

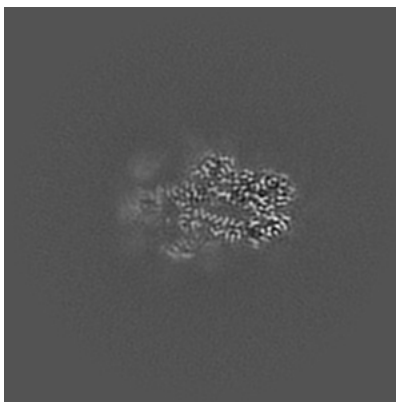
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

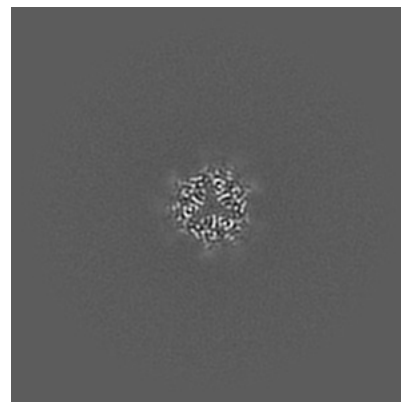
6.3.1 Primary map



X Index: 165

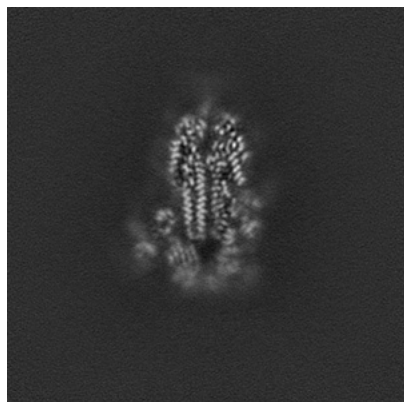


Y Index: 149

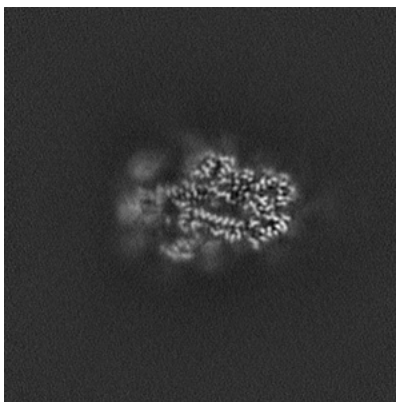


Z Index: 208

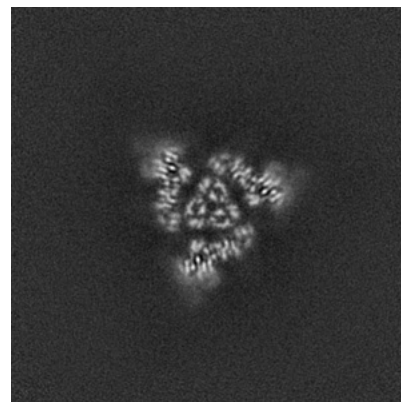
6.3.2 Raw map



X Index: 165



Y Index: 149

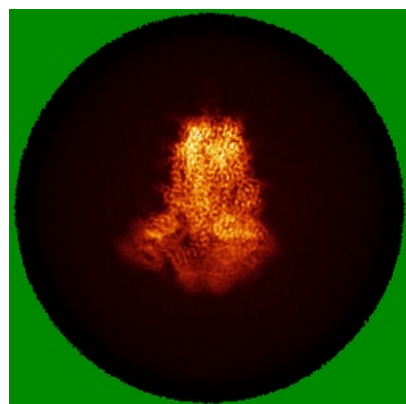


Z Index: 141

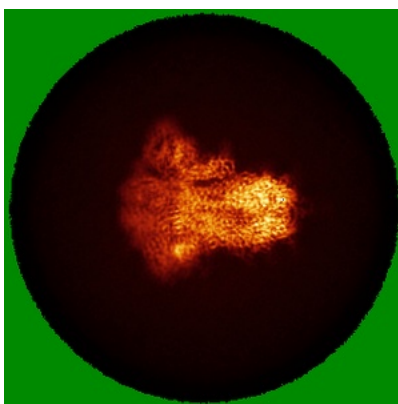
The images above show the largest variance slices of the map in three orthogonal directions.

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

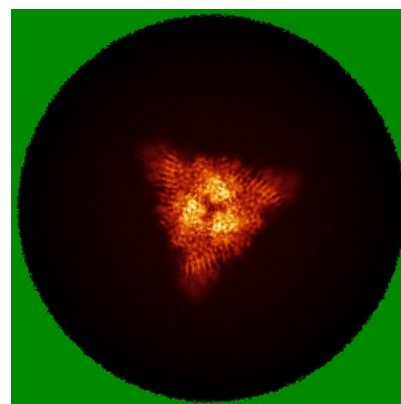
6.4.1 Primary map



X

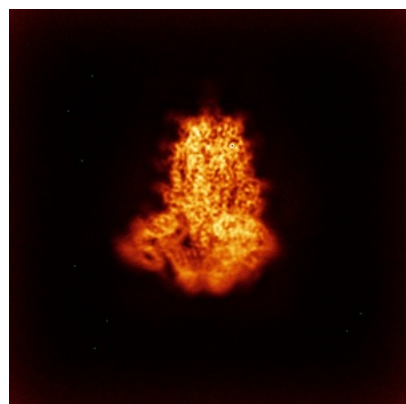


Y

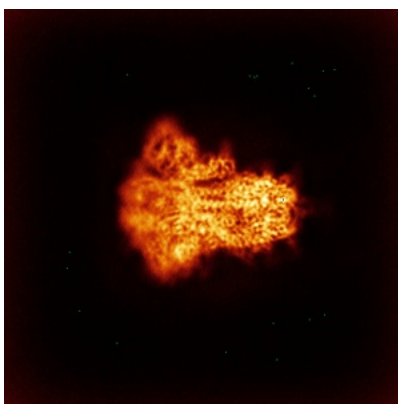


Z

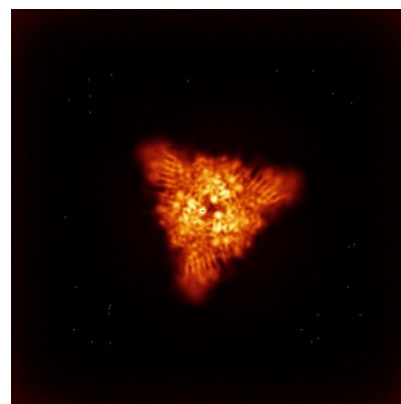
6.4.2 Raw map



X



Y

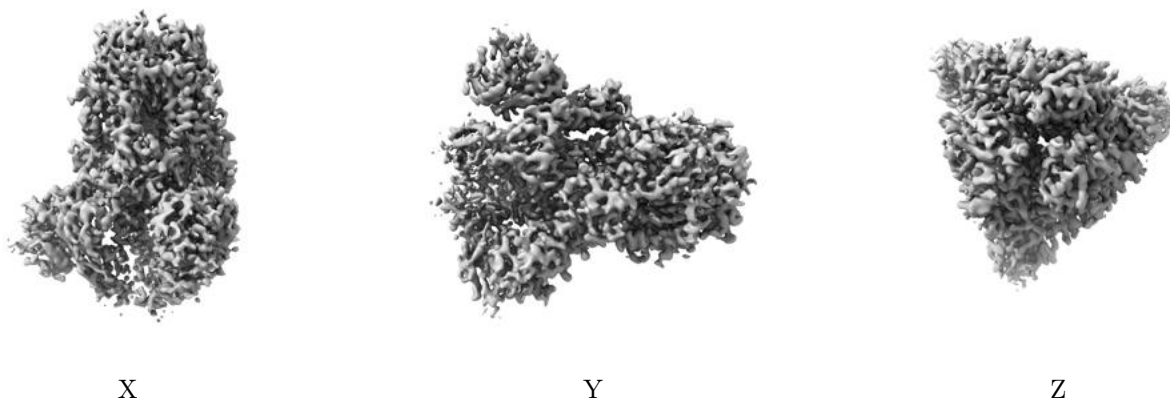


Z

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

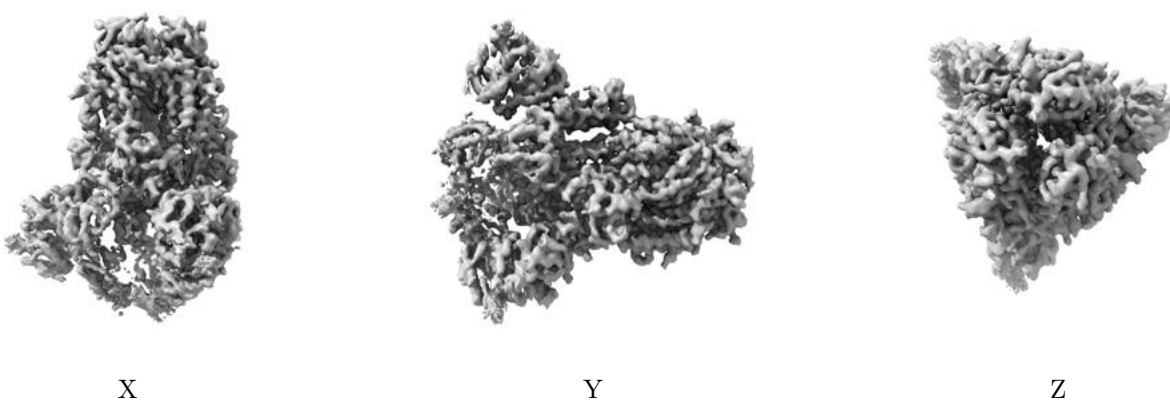
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

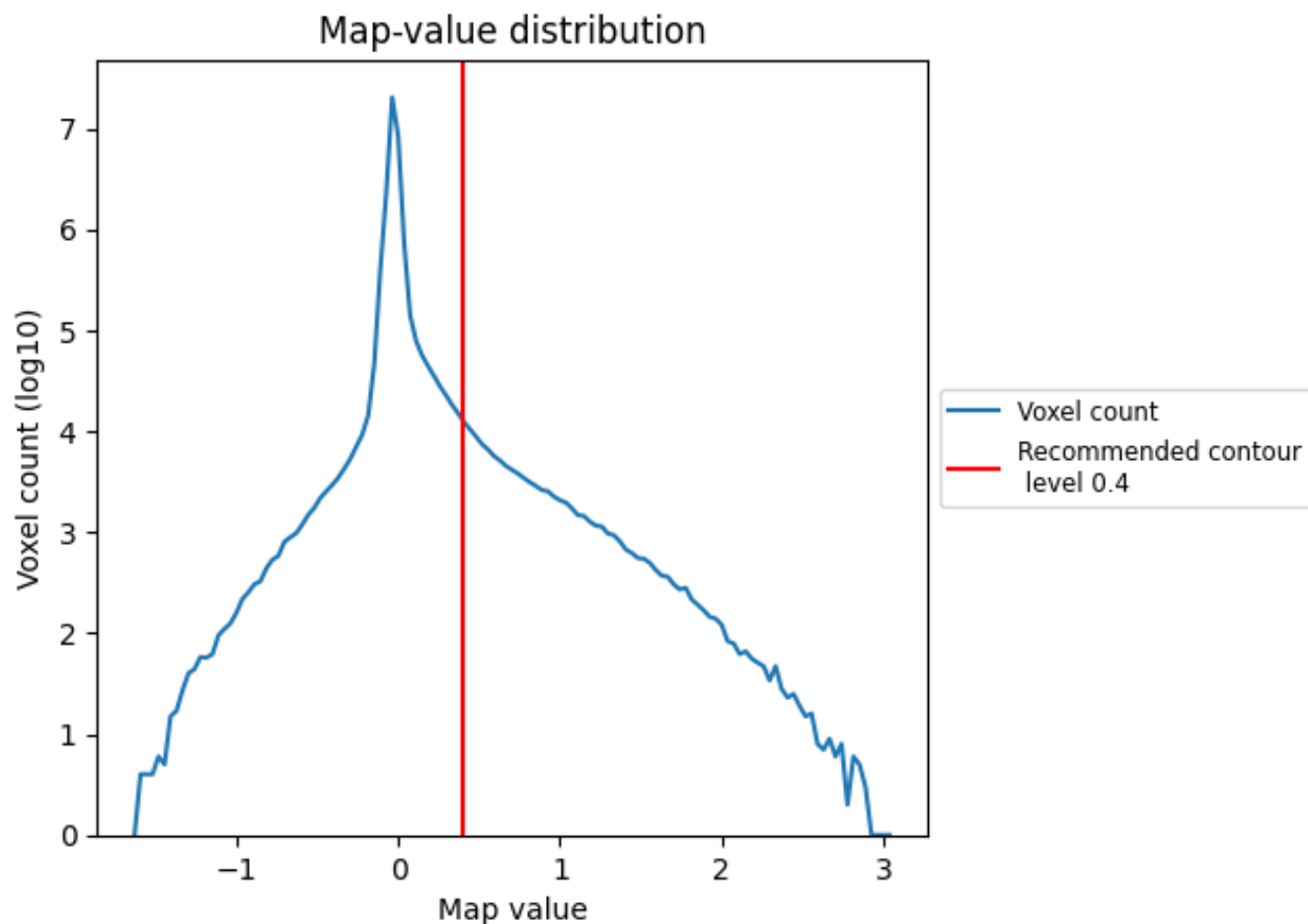
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

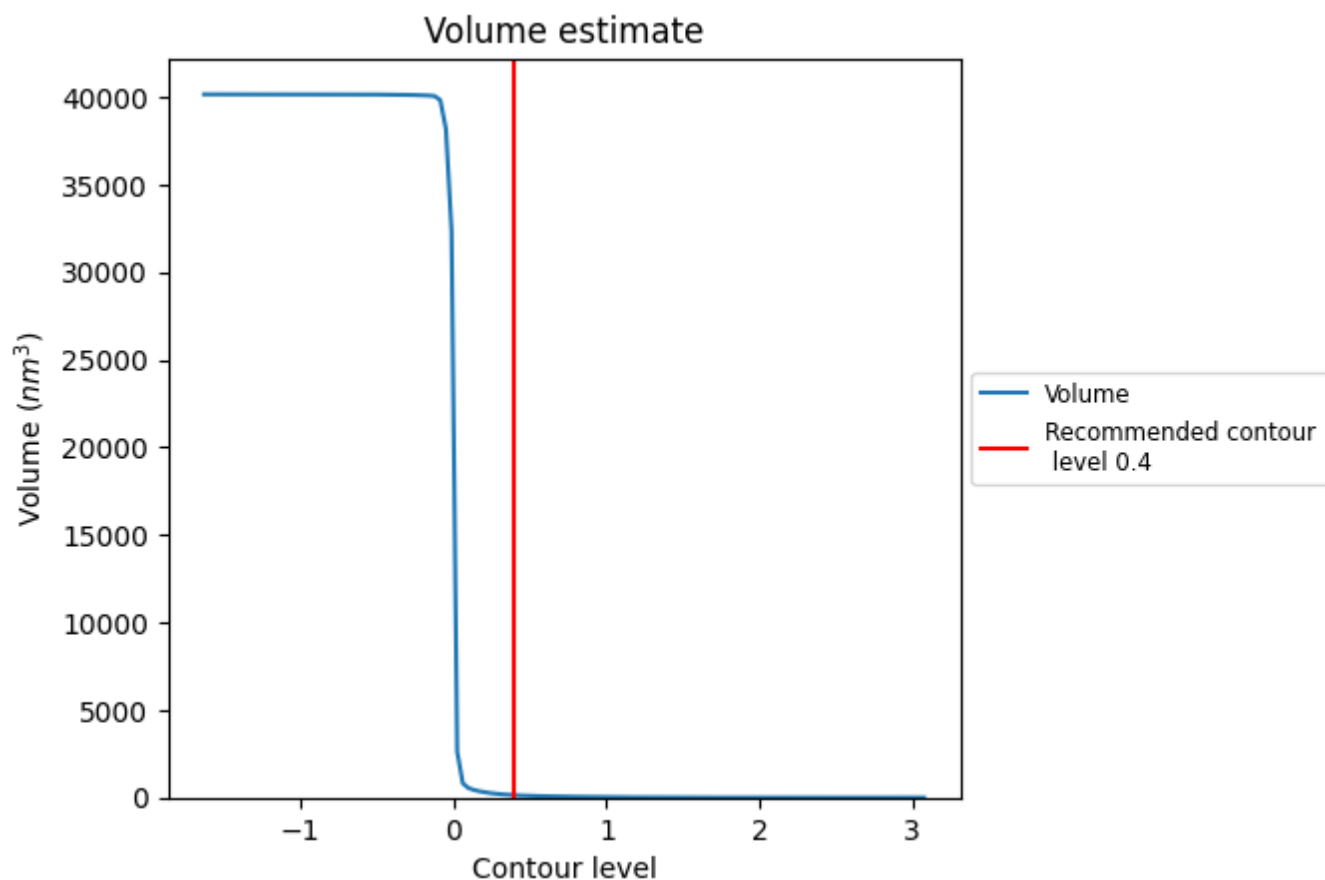
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

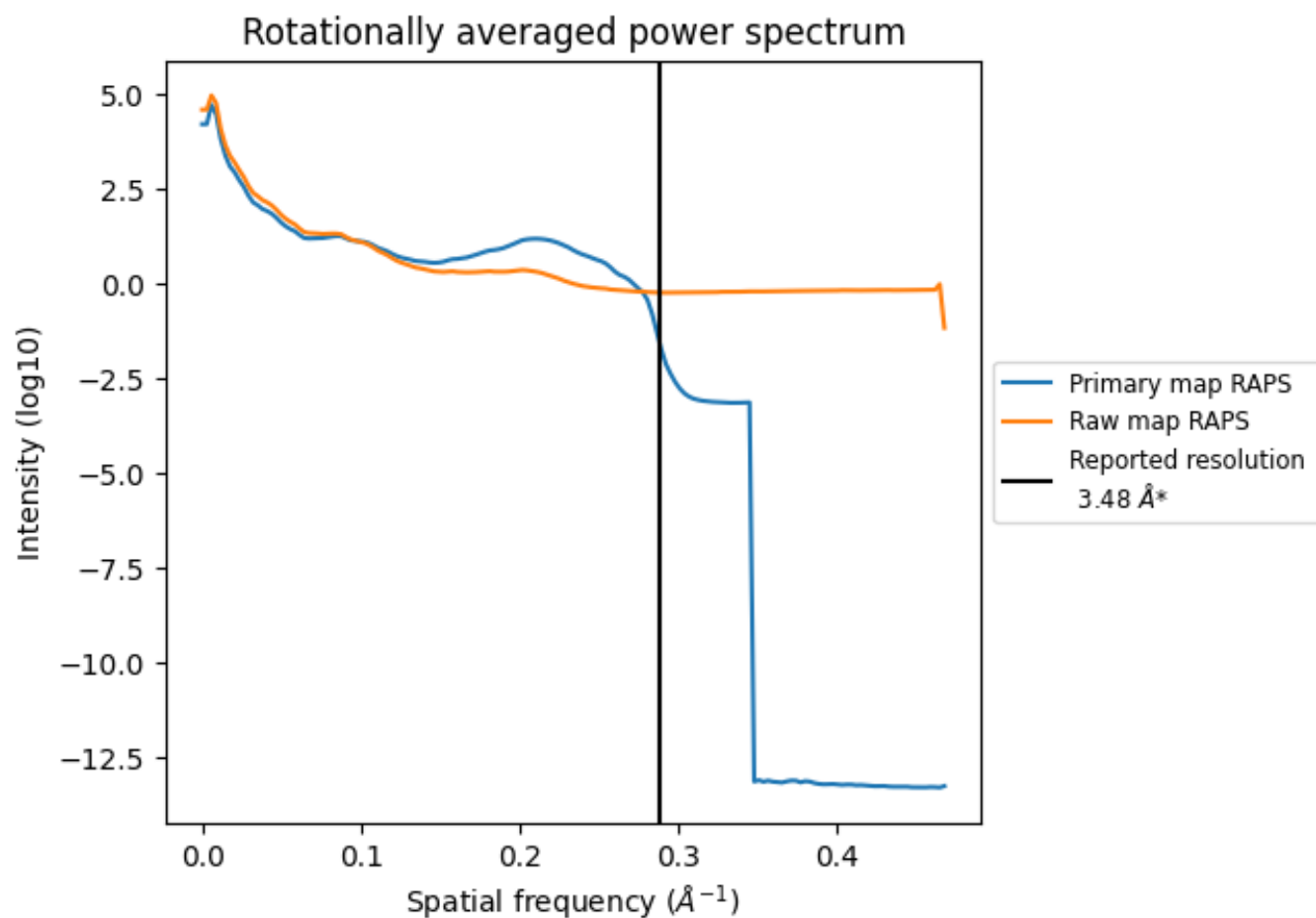
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm^3 ; this corresponds to an approximate mass of 122 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 ⓘ

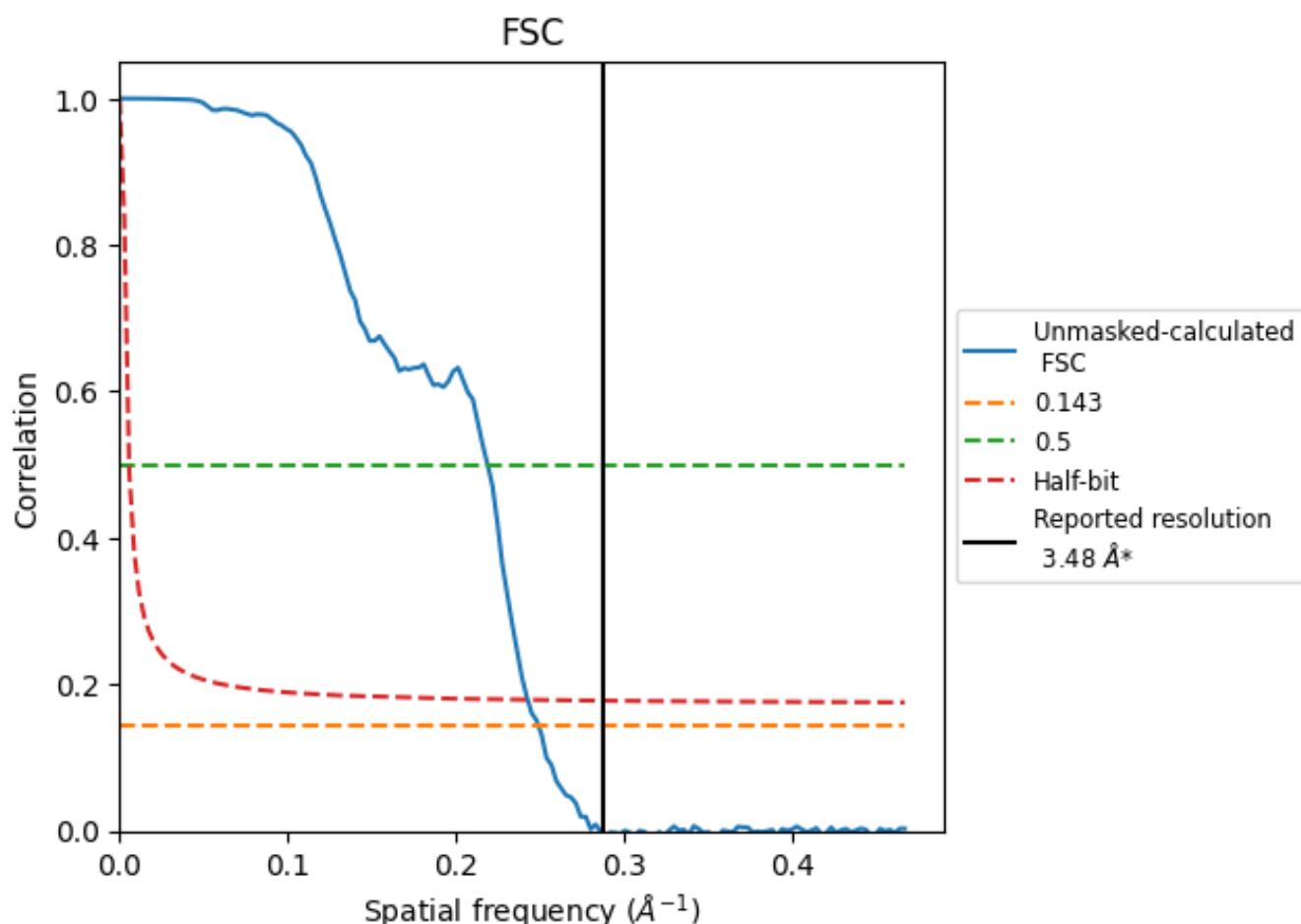


*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

8.2 Resolution estimates [i](#)

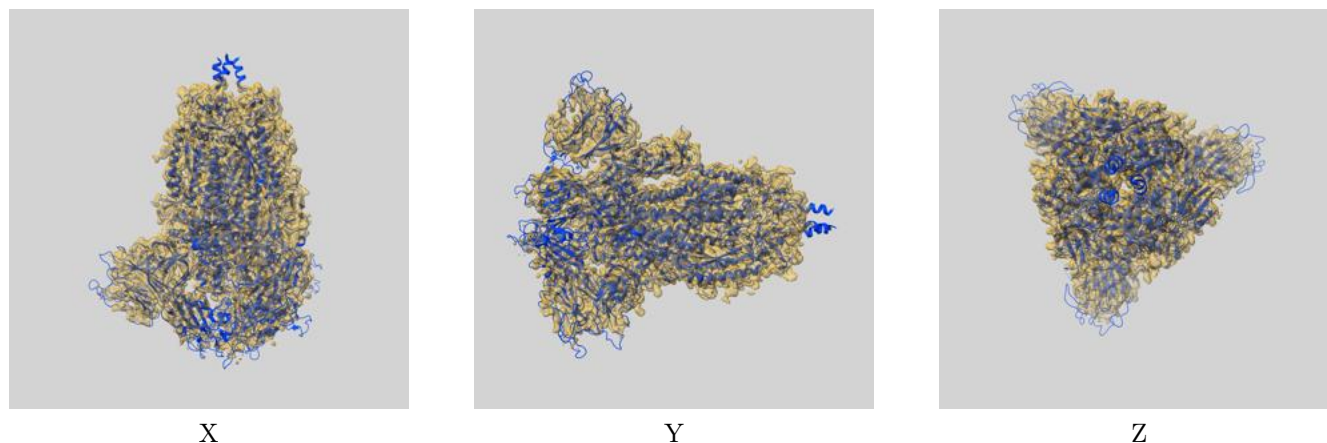
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	4.56	4.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.48 by more than 10 %

9 Map-model fit [i](#)

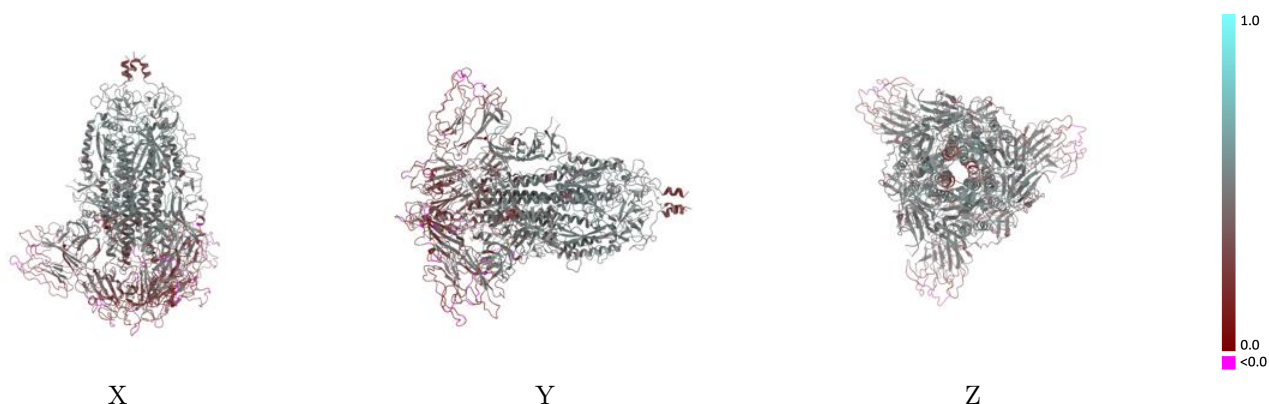
This section contains information regarding the fit between EMDB map EMD-33325 and PDB model 7XNS. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



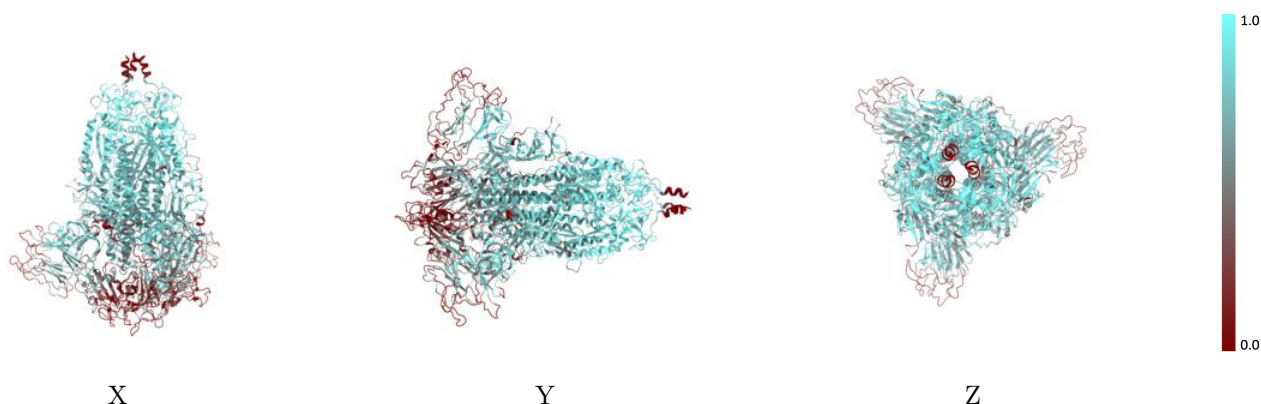
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



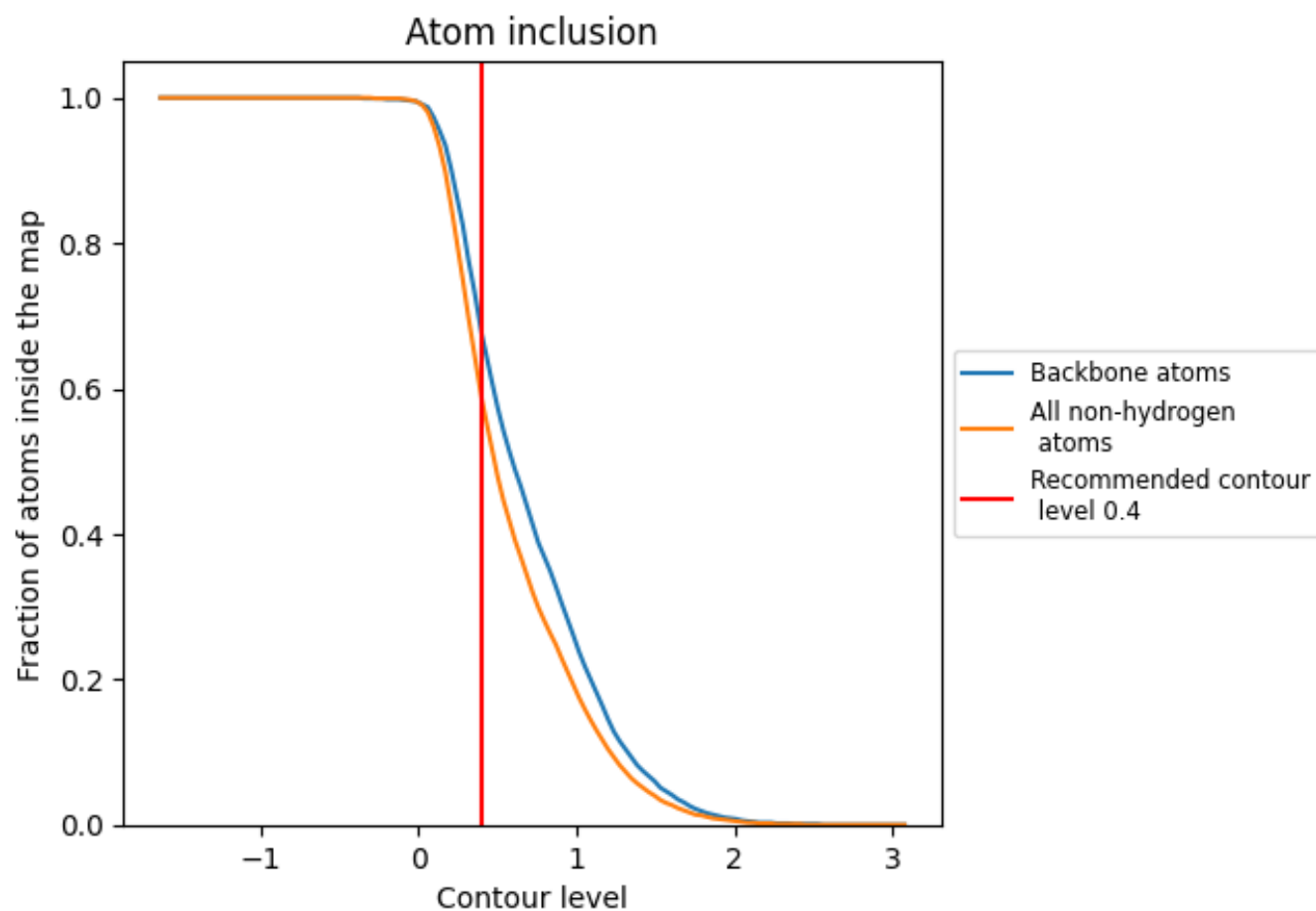
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 59% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.4020
A	 0.5910	 0.4040
B	 0.5920	 0.4040
C	 0.5910	 0.4040
D	 0.1430	 0.1490
E	 0.2500	 0.0810
F	 0.7140	 0.4630
G	 0.5360	 0.3610
H	 0.3570	 0.4030
I	 0.2860	 0.3060
J	 0.1070	 0.1780
K	 0.2500	 0.0950
L	 0.7500	 0.4730
M	 0.5000	 0.3580
N	 0.3570	 0.3960
O	 0.2860	 0.3050
P	 0.1430	 0.1700
Q	 0.2500	 0.0870
R	 0.7140	 0.4510
S	 0.5360	 0.3520
T	 0.3570	 0.3970
U	 0.2860	 0.2910

