



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 08:23 AM UTC

PDB ID : 8ELJ / pdb_00008elj
EMDB ID : EMD-28228
Title : SARS-CoV-2 spike glycoprotein in complex with the ICO-hu23 neutralizing antibody Fab fragment
Authors : Yee, A.W.; Morizumi, T.; Kim, K.; Kuo, A.; Ernst, O.P.
Deposited on : 2022-09-24
Resolution : 3.60 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

A user guide is available at

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

The types of validation reports are described at

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

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

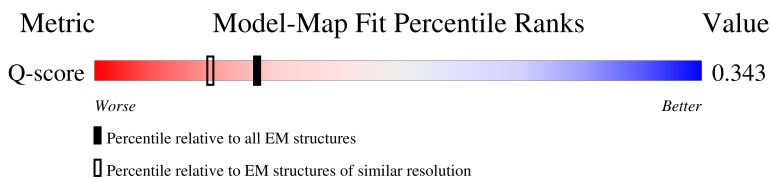
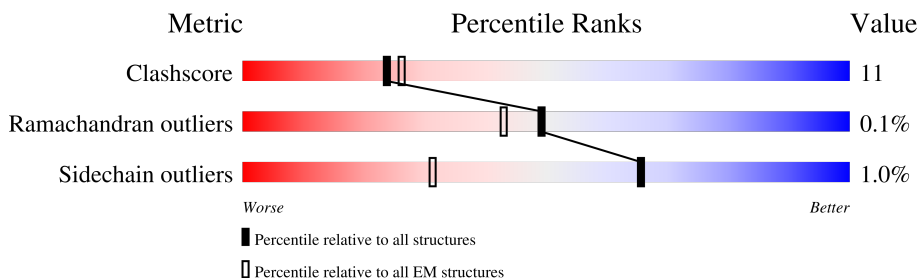
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1256	
1	B	1256	
1	C	1256	
2	S	234	

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Mol	Chain	Length	Quality of chain
2	U	234	
2	W	234	
3	T	216	
3	V	216	
3	X	216	
4	E	2	
4	F	2	
4	G	2	
4	H	2	
4	J	2	
4	K	2	
4	L	2	
4	M	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29463 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	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		
1	B	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		
1	C	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P0DTC2
A	-5	LYS	-	expression tag	UNP P0DTC2
A	-4	TRP	-	expression tag	UNP P0DTC2
A	-3	VAL	-	expression tag	UNP P0DTC2
A	-2	THR	-	expression tag	UNP P0DTC2
A	-1	PHE	-	expression tag	UNP P0DTC2
A	0	ILE	-	expression tag	UNP P0DTC2
A	1	SER	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	PHE	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	PHE	-	expression tag	UNP P0DTC2
A	7	SER	-	expression tag	UNP P0DTC2
A	8	SER	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	TYR	-	expression tag	UNP P0DTC2
A	11	SER	-	expression tag	UNP P0DTC2
A	12	ALA	-	expression tag	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	VAL	-	expression tag	UNP P0DTC2
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLY	-	expression tag	UNP P0DTC2
A	1242	SER	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
B	-6	MET	-	initiating methionine	UNP P0DTC2
B	-5	LYS	-	expression tag	UNP P0DTC2
B	-4	TRP	-	expression tag	UNP P0DTC2
B	-3	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	THR	-	expression tag	UNP P0DTC2
B	-1	PHE	-	expression tag	UNP P0DTC2
B	0	ILE	-	expression tag	UNP P0DTC2
B	1	SER	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	3	LEU	-	expression tag	UNP P0DTC2
B	4	PHE	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	PHE	-	expression tag	UNP P0DTC2
B	7	SER	-	expression tag	UNP P0DTC2
B	8	SER	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	TYR	-	expression tag	UNP P0DTC2
B	11	SER	-	expression tag	UNP P0DTC2
B	12	ALA	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	ILE	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	GLU	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	ARG	-	expression tag	UNP P0DTC2
B	1222	ASP	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLN	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	VAL	-	expression tag	UNP P0DTC2
B	1228	ARG	-	expression tag	UNP P0DTC2
B	1229	LYS	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLU	-	expression tag	UNP P0DTC2
B	1233	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1234	VAL	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	THR	-	expression tag	UNP P0DTC2
B	1239	PHE	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLY	-	expression tag	UNP P0DTC2
B	1242	SER	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
C	-6	MET	-	initiating methionine	UNP P0DTC2
C	-5	LYS	-	expression tag	UNP P0DTC2
C	-4	TRP	-	expression tag	UNP P0DTC2
C	-3	VAL	-	expression tag	UNP P0DTC2
C	-2	THR	-	expression tag	UNP P0DTC2
C	-1	PHE	-	expression tag	UNP P0DTC2
C	0	ILE	-	expression tag	UNP P0DTC2
C	1	SER	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	LEU	-	expression tag	UNP P0DTC2
C	4	PHE	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	PHE	-	expression tag	UNP P0DTC2
C	7	SER	-	expression tag	UNP P0DTC2
C	8	SER	-	expression tag	UNP P0DTC2
C	9	ALA	-	expression tag	UNP P0DTC2
C	10	TYR	-	expression tag	UNP P0DTC2
C	11	SER	-	expression tag	UNP P0DTC2
C	12	ALA	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	ILE	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	GLU	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	ARG	-	expression tag	UNP P0DTC2
C	1222	ASP	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLN	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	VAL	-	expression tag	UNP P0DTC2
C	1228	ARG	-	expression tag	UNP P0DTC2
C	1229	LYS	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLU	-	expression tag	UNP P0DTC2
C	1233	TRP	-	expression tag	UNP P0DTC2
C	1234	VAL	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	THR	-	expression tag	UNP P0DTC2
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLY	-	expression tag	UNP P0DTC2
C	1242	SER	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called ICO-hu23 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	120	Total	C	N	O	S	0	0
			956	614	161	175	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	120	Total	C	N	O	S	0	0
			956	614	161	175	6		
2	W	120	Total	C	N	O	S	0	0
			956	614	161	175	6		

- Molecule 3 is a protein called ICO-hu23 antibody Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	108	Total	C	N	O	S	0	0
			790	490	130	167	3		
3	V	108	Total	C	N	O	S	0	0
			790	490	130	167	3		
3	X	108	Total	C	N	O	S	0	0
			790	490	130	167	3		

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



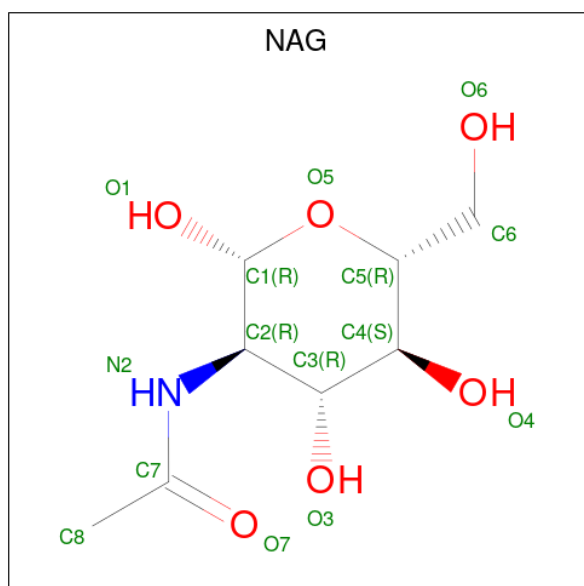
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16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

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

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



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

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

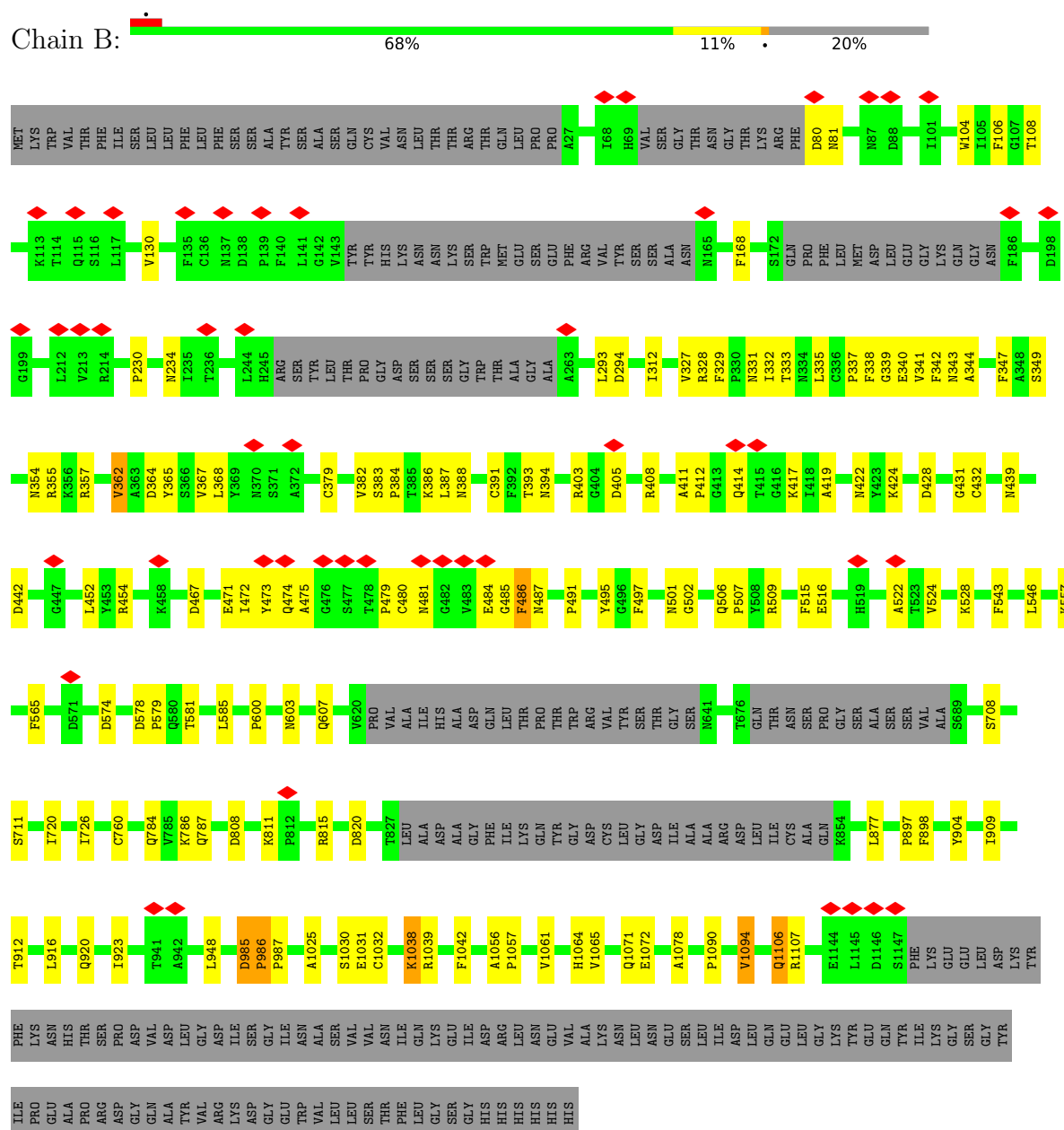
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	C	1	14	8	1	5	0

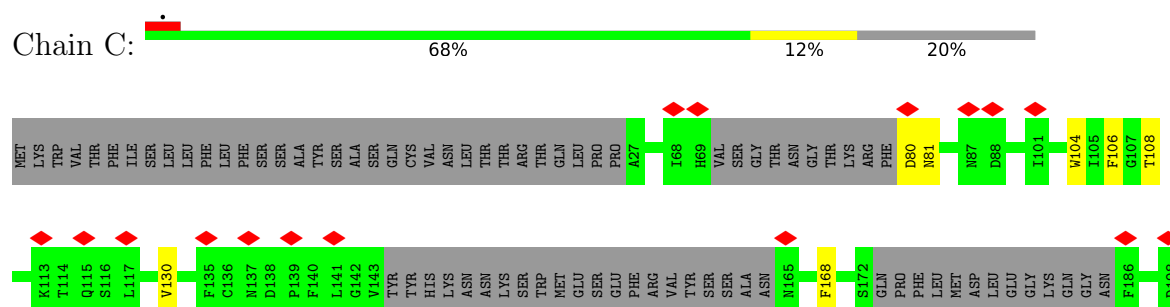
- Molecule 1: Spike glycoprotein

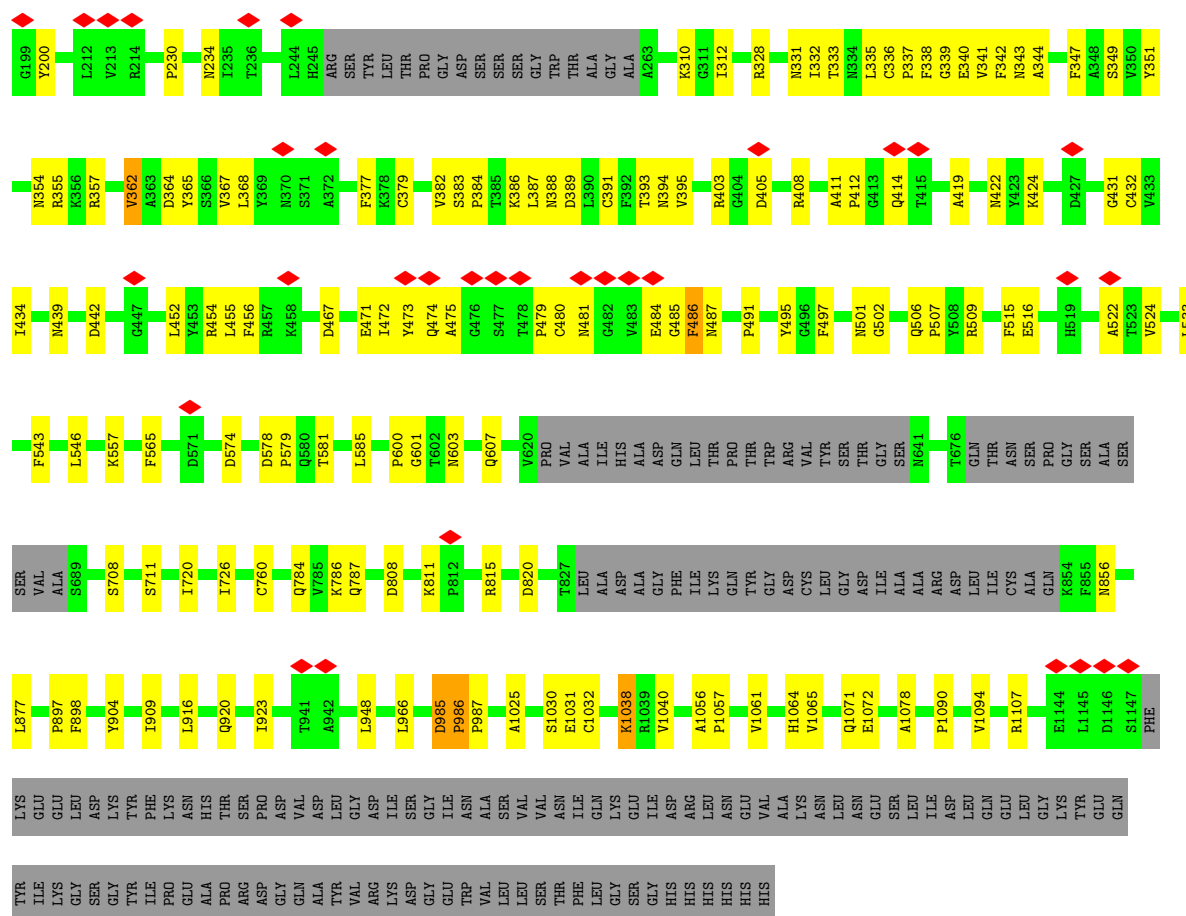
Chain B:



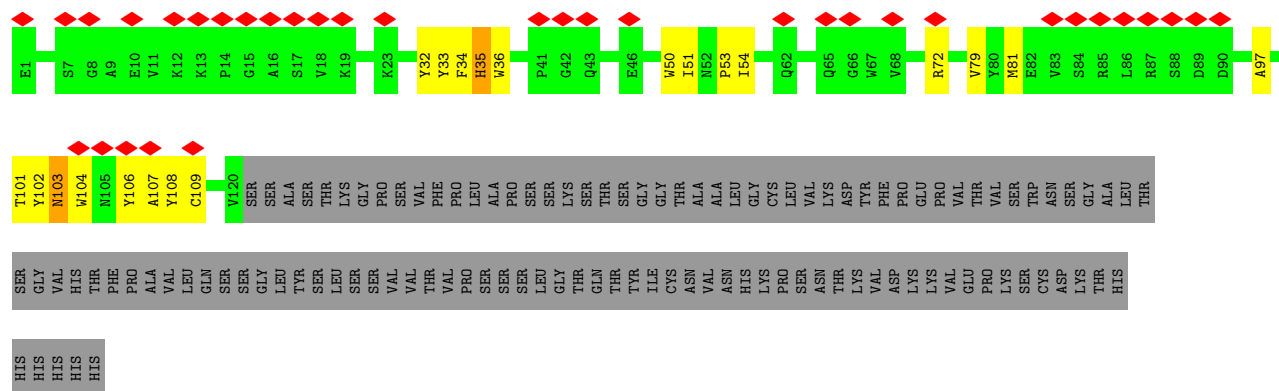
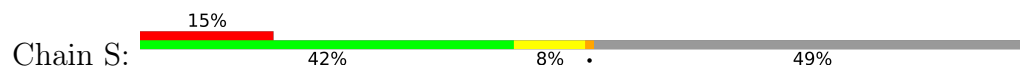
- Molecule 1: Spike glycoprotein

Chain C:

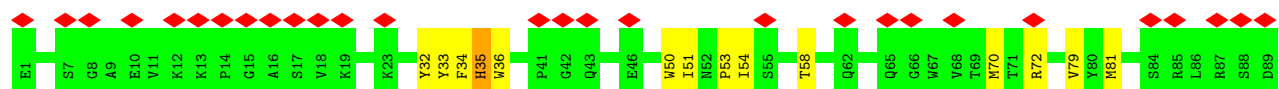
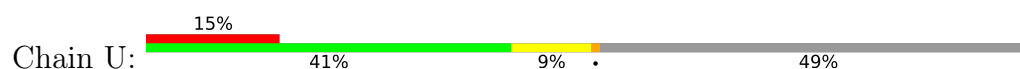


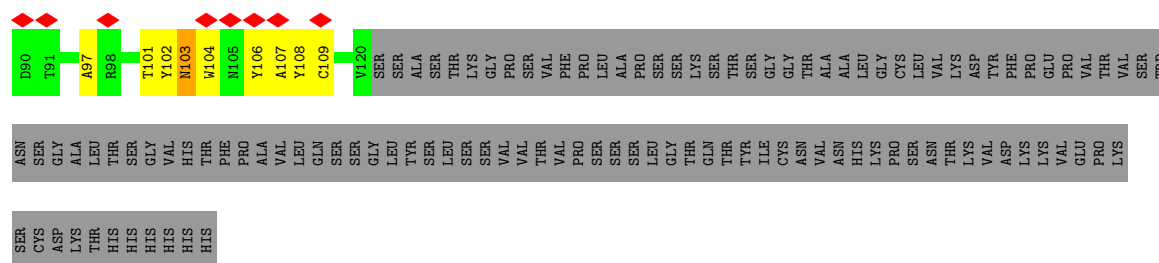


• Molecule 2: ICO-hu23 antibody Fab heavy chain

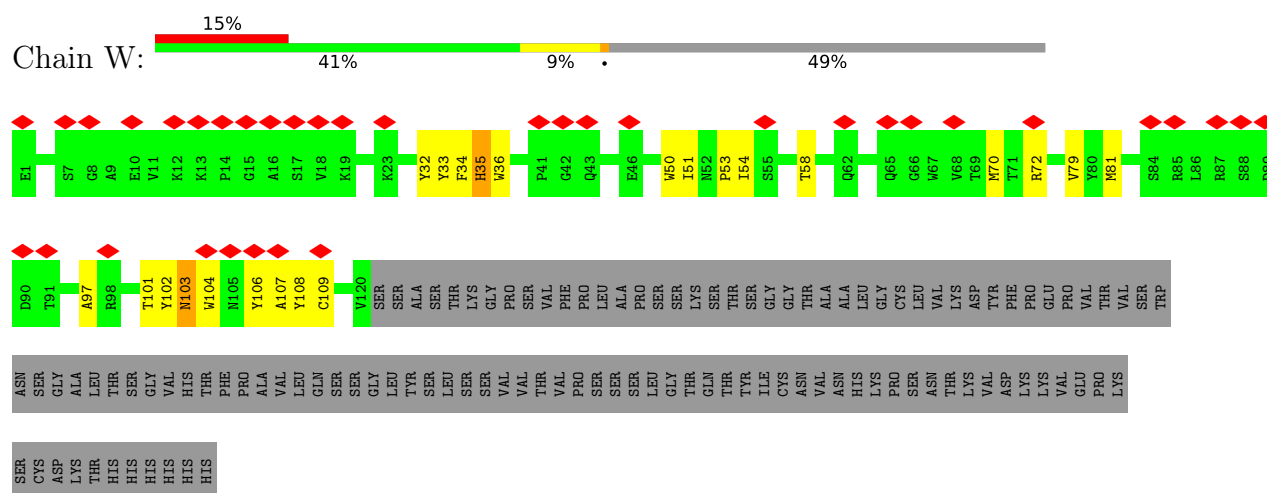


• Molecule 2: ICO-hu23 antibody Fab heavy chain

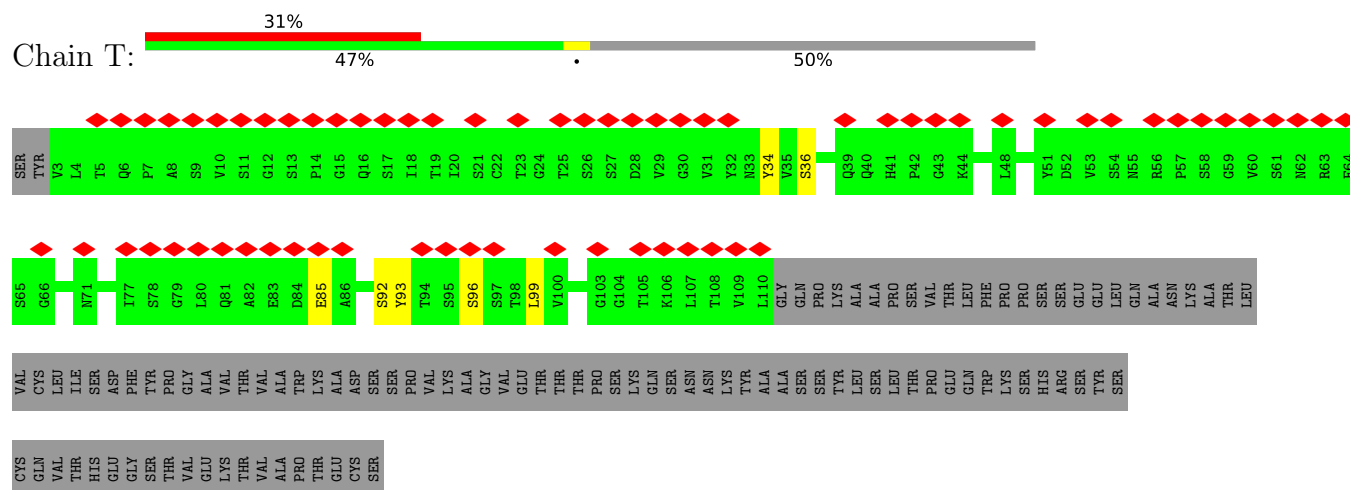




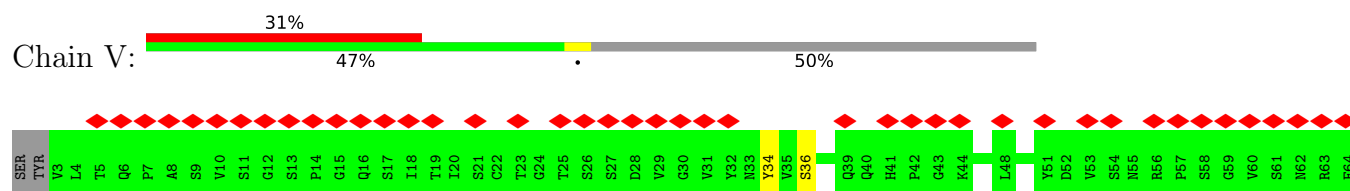
• Molecule 2: ICO-hu23 antibody Fab heavy chain

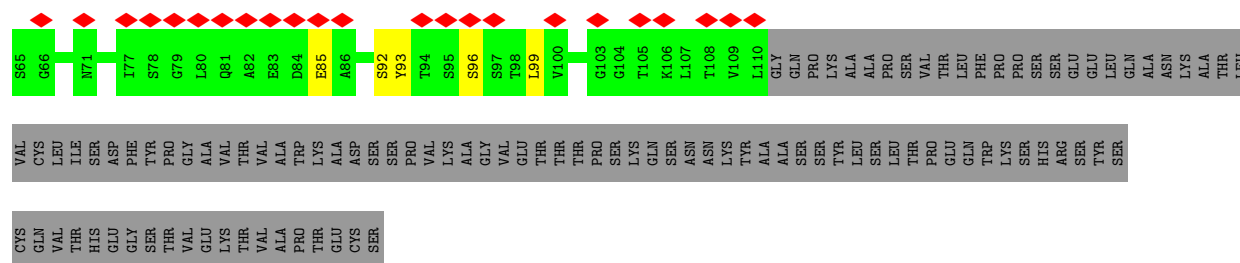


• Molecule 3: ICO-hu23 antibody Fab light chain

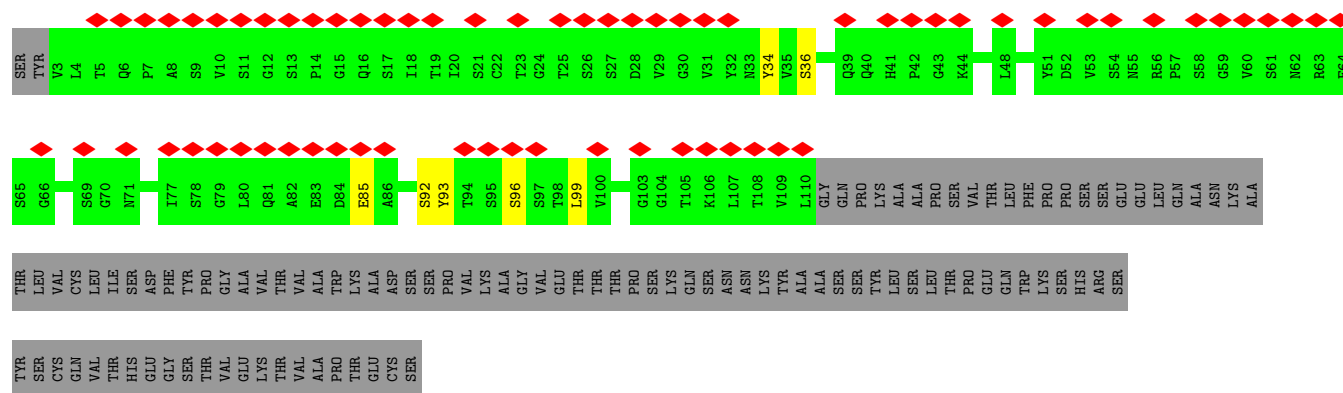


• Molecule 3: ICO-hu23 antibody Fab light chain





• Molecule 3: ICO-hu23 antibody Fab light chain



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



NAG1
NAG2

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



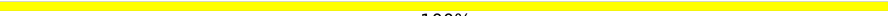
NAG1
NAG2

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



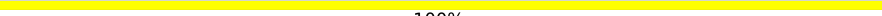
NAG1
NAG2

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

Chain H:  100%

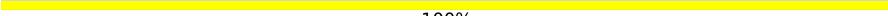
NAG1
NAG2

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

Chain J:  100%

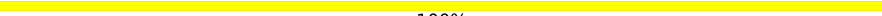
NAG1
NAG2

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

Chain K:  100%

NAG1
NAG2

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

Chain L:  100%

NAG1
NAG2

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

Chain M:  100%

NAG1
NAG2

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

Chain O:  100%

NAG1
NAG2

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

Chain P:  100%

NAG1
NAG2

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

Chain Q:  100%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	35845	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.450	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	461.7, 461.7, 461.7	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/7999	1.22	29/10885 (0.3%)
1	B	0.62	0/7999	1.22	28/10885 (0.3%)
1	C	0.63	0/7999	1.22	27/10885 (0.2%)
2	S	0.55	0/986	1.01	2/1342 (0.1%)
2	U	0.55	0/986	1.01	2/1342 (0.1%)
2	W	0.55	0/986	1.01	2/1342 (0.1%)
3	T	0.58	0/806	1.01	1/1097 (0.1%)
3	V	0.58	0/806	1.01	1/1097 (0.1%)
3	X	0.58	0/806	1.00	1/1097 (0.1%)
All	All	0.61	0/29373	1.18	93/39972 (0.2%)

There are no bond length outliers.

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	486	PHE	CA-CB-CG	8.45	122.25	113.80
1	A	486	PHE	CA-CB-CG	8.42	122.22	113.80
1	C	486	PHE	CA-CB-CG	8.42	122.22	113.80
1	B	909	ILE	N-CA-C	-7.53	105.51	112.43
1	C	909	ILE	N-CA-C	-7.51	105.52	112.43
1	A	909	ILE	N-CA-C	-7.31	105.70	112.43
1	B	331	ASN	CB-CA-C	7.18	121.59	110.67
1	A	331	ASN	CB-CA-C	7.06	121.40	110.67
2	S	35	HIS	CA-CB-CG	-7.01	106.79	113.80
1	C	331	ASN	CB-CA-C	6.96	122.40	110.77
2	W	35	HIS	CA-CB-CG	-6.96	106.83	113.80
2	U	35	HIS	CA-CB-CG	-6.96	106.84	113.80
1	C	815	ARG	CB-CG-CD	6.94	127.27	111.30
1	A	815	ARG	CB-CG-CD	6.90	127.18	111.30
1	B	815	ARG	CB-CG-CD	6.89	127.15	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	103	ASN	CA-CB-CG	6.78	119.38	112.60
1	C	985	ASP	CB-CA-C	-6.76	98.38	109.46
1	A	985	ASP	CB-CA-C	-6.75	98.40	109.46
1	B	985	ASP	CB-CA-C	-6.74	98.41	109.46
2	W	103	ASN	CA-CB-CG	6.73	119.33	112.60
2	U	103	ASN	CA-CB-CG	6.71	119.31	112.60
1	B	920	GLN	CB-CG-CD	6.54	123.72	112.60
1	C	920	GLN	CB-CG-CD	6.52	123.68	112.60
1	A	920	GLN	CB-CG-CD	6.50	123.66	112.60
1	A	1038	LYS	N-CA-CB	6.44	119.97	110.56
1	C	1090	PRO	CB-CA-C	-6.39	102.70	111.21
1	A	1107	ARG	NE-CZ-NH2	6.33	124.90	119.20
1	B	1090	PRO	CB-CA-C	-6.21	102.94	111.21
1	B	1038	LYS	N-CA-CB	6.20	119.62	110.56
1	A	1090	PRO	CB-CA-C	-6.13	103.06	111.21
1	C	1038	LYS	N-CA-CB	6.12	119.49	110.56
1	C	898	PHE	CA-CB-CG	-6.04	107.76	113.80
1	A	1071	GLN	CA-C-O	-6.01	114.08	121.11
1	C	600	PRO	N-CA-C	-5.96	102.51	111.57
1	B	898	PHE	CA-CB-CG	-5.95	107.85	113.80
1	B	1071	GLN	CA-C-O	-5.94	114.16	121.11
1	A	986	PRO	N-CA-C	5.92	117.92	110.70
1	A	600	PRO	N-CA-C	-5.92	102.57	111.57
1	B	986	PRO	N-CA-C	5.92	117.92	110.70
1	C	986	PRO	N-CA-C	5.92	117.92	110.70
1	B	600	PRO	N-CA-C	-5.91	102.59	111.57
1	A	898	PHE	CA-CB-CG	-5.89	107.91	113.80
1	B	720	ILE	CA-CB-CG1	5.84	120.33	110.40
1	A	720	ILE	CA-CB-CG1	5.82	120.29	110.40
1	B	1078	ALA	CA-C-N	5.81	125.35	119.19
1	B	1078	ALA	C-N-CA	5.81	125.35	119.19
1	C	720	ILE	CA-CB-CG1	5.76	120.20	110.40
1	A	1078	ALA	CA-C-N	5.74	125.28	119.19
1	A	1078	ALA	C-N-CA	5.74	125.28	119.19
1	C	1078	ALA	CA-C-N	5.74	125.27	119.19
1	C	1078	ALA	C-N-CA	5.74	125.27	119.19
1	C	1094	VAL	CA-C-O	-5.68	114.51	120.76
1	B	784	GLN	CB-CA-C	5.64	119.03	109.55
1	A	1065	VAL	CB-CA-C	-5.60	103.30	110.98
1	A	1064	HIS	CA-CB-CG	5.58	119.38	113.80
1	C	1064	HIS	CA-CB-CG	5.56	119.36	113.80
1	B	1065	VAL	CB-CA-C	-5.55	103.37	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1065	VAL	CB-CA-C	-5.52	103.42	110.98
1	B	1064	HIS	CA-CB-CG	5.51	119.31	113.80
1	A	1072	GLU	CB-CA-C	-5.50	98.23	109.94
3	X	85	GLU	CB-CG-CD	5.50	121.94	112.60
1	B	1072	GLU	CB-CA-C	-5.48	98.26	109.94
3	V	85	GLU	CB-CG-CD	5.48	121.91	112.60
1	A	1025	ALA	O-C-N	5.46	127.69	122.07
3	T	85	GLU	CB-CG-CD	5.46	121.87	112.60
1	C	1025	ALA	O-C-N	5.43	127.66	122.07
1	C	1072	GLU	CB-CA-C	-5.39	98.45	109.94
1	C	1071	GLN	CA-C-O	-5.35	114.85	121.11
1	A	1094	VAL	CA-C-O	-5.35	114.88	120.76
1	A	808	ASP	CA-C-N	5.29	124.95	119.56
1	A	808	ASP	C-N-CA	5.29	124.95	119.56
1	C	1107	ARG	N-CA-CB	5.26	118.44	110.28
1	C	808	ASP	CA-C-N	5.25	124.91	119.56
1	C	808	ASP	C-N-CA	5.25	124.91	119.56
1	B	808	ASP	CA-C-N	5.24	124.91	119.56
1	B	808	ASP	C-N-CA	5.24	124.91	119.56
1	B	579	PRO	CB-CA-C	-5.23	104.04	111.68
1	C	579	PRO	CB-CA-C	-5.23	104.04	111.68
1	A	80	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	1094	VAL	CA-C-O	-5.22	115.02	120.76
1	B	80	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	80	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	1025	ALA	O-C-N	5.18	127.40	122.07
1	A	579	PRO	CB-CA-C	-5.17	104.13	111.68
1	C	607	GLN	CB-CG-CD	-5.12	103.90	112.60
1	B	607	GLN	CB-CG-CD	-5.10	103.92	112.60
1	A	607	GLN	CB-CG-CD	-5.06	104.00	112.60
1	C	897	PRO	CB-CA-C	-5.06	105.14	111.56
1	A	1042	PHE	CB-CA-C	5.05	119.43	110.85
1	A	328	ARG	CB-CG-CD	-5.03	99.73	111.30
1	A	897	PRO	CB-CA-C	-5.03	105.17	111.56
1	B	897	PRO	CB-CA-C	-5.02	105.18	111.56
1	B	1042	PHE	CB-CA-C	5.02	119.38	110.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7823	0	7628	172	0
1	B	7823	0	7628	174	0
1	C	7823	0	7628	163	0
2	S	956	0	906	84	0
2	U	956	0	906	88	0
2	W	956	0	906	90	0
3	T	790	0	757	5	0
3	V	790	0	757	5	0
3	X	790	0	757	5	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
5	A	140	0	130	4	0
5	B	140	0	130	3	0
5	C	140	0	130	4	0
All	All	29463	0	28563	631	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 11.

All (631) 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:486:PHE:CB	2:S:104:TRP:CE3	1.88	1.55
1:C:486:PHE:CB	2:W:104:TRP:CE3	1.87	1.54
1:A:1094:VAL:CG2	1:A:1107:ARG:HE	1.17	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PHE:CB	2:U:104:TRP:CE3	1.89	1.51
1:A:1107:ARG:NH1	1:B:904:TYR:CE1	1.75	1.49
1:A:486:PHE:HB3	2:U:104:TRP:CE3	0.98	1.49
1:C:486:PHE:HB3	2:W:104:TRP:CE3	0.95	1.48
1:B:486:PHE:HB3	2:S:104:TRP:CE3	0.97	1.48
1:A:486:PHE:CB	2:U:104:TRP:HE3	1.25	1.43
1:C:486:PHE:CB	2:W:104:TRP:HE3	1.25	1.43
1:B:486:PHE:CB	2:S:104:TRP:HE3	1.26	1.38
2:W:51:ILE:HD11	2:W:70:MET:CB	0.91	1.37
2:U:51:ILE:HD11	2:U:70:MET:CB	0.91	1.37
1:B:328:ARG:NH1	1:B:543:PHE:HE2	1.21	1.35
2:W:53:PRO:CD	2:W:72:ARG:NH1	1.88	1.35
2:U:51:ILE:CD1	2:U:70:MET:HB3	0.87	1.34
2:S:53:PRO:CD	2:S:72:ARG:NH1	1.89	1.34
1:C:328:ARG:NH1	1:C:543:PHE:HE2	1.22	1.34
2:W:51:ILE:CD1	2:W:70:MET:HB3	0.87	1.34
1:A:328:ARG:NH1	1:A:543:PHE:HE2	1.21	1.33
2:U:53:PRO:CD	2:U:72:ARG:NH1	1.88	1.32
2:S:53:PRO:HD3	2:S:72:ARG:NH1	0.99	1.30
2:U:53:PRO:HD3	2:U:72:ARG:NH1	0.97	1.29
2:W:53:PRO:HD3	2:W:72:ARG:NH1	0.97	1.29
2:U:34:PHE:HB2	2:U:72:ARG:NH2	1.49	1.27
2:S:34:PHE:HB2	2:S:72:ARG:NH2	1.49	1.27
1:A:230:PRO:HG3	1:C:357:ARG:NH2	1.49	1.27
2:W:34:PHE:HB2	2:W:72:ARG:NH2	1.49	1.26
1:A:1094:VAL:HG22	1:A:1107:ARG:NE	1.50	1.24
1:B:357:ARG:NH2	1:C:230:PRO:HG3	1.50	1.23
1:A:357:ARG:NH2	1:B:230:PRO:HG3	1.50	1.22
1:B:328:ARG:NH1	1:B:543:PHE:CE2	2.09	1.20
1:B:335:LEU:CD2	1:B:362:VAL:HG13	1.70	1.20
1:C:328:ARG:NH1	1:C:543:PHE:CE2	2.09	1.20
1:A:328:ARG:NH1	1:A:543:PHE:CE2	2.09	1.20
1:A:335:LEU:CD2	1:A:362:VAL:HG13	1.70	1.20
1:B:486:PHE:HB3	2:S:104:TRP:CD2	1.76	1.19
1:C:486:PHE:HB3	2:W:104:TRP:CD2	1.77	1.18
1:A:1094:VAL:CG2	1:A:1107:ARG:NE	2.03	1.17
1:A:486:PHE:HB3	2:U:104:TRP:CD2	1.78	1.16
1:B:328:ARG:HH22	1:B:585:LEU:HD11	1.06	1.16
1:A:486:PHE:HA	2:U:102:TYR:CZ	1.81	1.16
1:A:335:LEU:HD23	1:A:362:VAL:HG13	1.21	1.15
1:B:329:PHE:CE1	1:B:528:LYS:HD3	1.83	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:PHE:HA	2:W:102:TYR:CZ	1.81	1.14
1:B:486:PHE:HA	2:S:102:TYR:CZ	1.82	1.13
1:C:328:ARG:HH22	1:C:585:LEU:HD11	1.06	1.13
1:A:328:ARG:HH22	1:A:585:LEU:HD11	1.06	1.13
1:C:486:PHE:HB2	2:W:104:TRP:HB2	1.12	1.12
1:B:912:THR:OG1	1:B:1106:GLN:NE2	1.81	1.11
1:A:912:THR:OG1	1:A:1106:GLN:NE2	1.83	1.11
1:C:485:GLY:HA2	2:W:103:ASN:HB3	1.11	1.10
1:B:335:LEU:HD23	1:B:362:VAL:HG13	1.21	1.09
2:U:34:PHE:N	2:U:72:ARG:HH22	1.50	1.09
1:B:486:PHE:HB2	2:S:104:TRP:HB2	1.10	1.09
2:W:34:PHE:CB	2:W:72:ARG:NH2	2.15	1.09
1:B:485:GLY:HA2	2:S:103:ASN:HB3	1.10	1.08
2:W:34:PHE:N	2:W:72:ARG:HH22	1.50	1.08
2:S:34:PHE:N	2:S:72:ARG:HH22	1.50	1.08
2:U:34:PHE:CB	2:U:72:ARG:NH2	2.15	1.08
1:A:486:PHE:HB2	2:U:104:TRP:HB2	1.10	1.08
2:S:34:PHE:CB	2:S:72:ARG:NH2	2.15	1.08
2:U:53:PRO:CD	2:U:72:ARG:HH11	1.58	1.08
2:W:34:PHE:HB2	2:W:72:ARG:HH21	0.97	1.07
1:A:485:GLY:HA2	2:U:103:ASN:HB3	1.11	1.07
2:W:53:PRO:CD	2:W:72:ARG:HH11	1.58	1.07
1:B:1107:ARG:NH2	1:C:904:TYR:CE1	2.23	1.06
2:S:34:PHE:HB2	2:S:72:ARG:HH21	0.96	1.04
1:A:328:ARG:CZ	1:A:578:ASP:OD2	2.07	1.03
1:B:328:ARG:CZ	1:B:578:ASP:OD2	2.06	1.03
2:S:34:PHE:CD2	2:S:72:ARG:CZ	2.42	1.03
2:U:34:PHE:CD2	2:U:72:ARG:CZ	2.42	1.03
1:C:328:ARG:CZ	1:C:578:ASP:OD2	2.06	1.02
1:B:1107:ARG:CZ	1:C:904:TYR:CE1	2.42	1.02
1:A:1094:VAL:HG22	1:A:1107:ARG:HE	0.87	1.02
1:A:328:ARG:CZ	1:A:543:PHE:HE2	1.73	1.01
2:W:34:PHE:CD2	2:W:72:ARG:CZ	2.42	1.01
1:C:328:ARG:CZ	1:C:543:PHE:HE2	1.73	1.01
2:U:34:PHE:HB2	2:U:72:ARG:HH21	0.97	1.01
1:A:1107:ARG:CZ	1:B:904:TYR:CE1	2.43	1.00
1:B:486:PHE:HB2	2:S:104:TRP:CB	1.91	1.00
1:B:328:ARG:CZ	1:B:543:PHE:HE2	1.74	1.00
1:A:486:PHE:HB2	2:U:104:TRP:CB	1.91	0.99
2:U:34:PHE:HD2	2:U:72:ARG:CZ	1.77	0.98
1:A:230:PRO:HG3	1:C:357:ARG:HH22	1.23	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HH22	1:A:585:LEU:CD1	1.76	0.98
1:C:486:PHE:HB2	2:W:104:TRP:CB	1.93	0.98
2:W:34:PHE:HD2	2:W:72:ARG:CZ	1.77	0.98
1:C:328:ARG:HH22	1:C:585:LEU:CD1	1.76	0.98
1:B:328:ARG:HH22	1:B:585:LEU:CD1	1.76	0.98
2:U:51:ILE:CG1	2:U:70:MET:HB3	1.94	0.97
2:S:34:PHE:HD2	2:S:72:ARG:CZ	1.76	0.97
2:W:51:ILE:CG1	2:W:70:MET:HB3	1.94	0.97
1:C:486:PHE:CA	2:W:102:TYR:CZ	2.44	0.97
1:B:328:ARG:HH11	1:B:543:PHE:HE2	1.11	0.96
1:B:486:PHE:CD2	2:S:102:TYR:HE1	1.83	0.96
1:C:486:PHE:CD2	2:W:102:TYR:HE1	1.83	0.96
2:W:51:ILE:HD11	2:W:70:MET:CG	1.96	0.96
1:C:335:LEU:HD23	1:C:362:VAL:HG13	1.46	0.96
2:S:53:PRO:CD	2:S:72:ARG:HH11	1.59	0.96
1:C:856:ASN:ND2	1:C:966:LEU:HD11	1.81	0.95
1:B:357:ARG:NH2	1:C:230:PRO:CG	2.29	0.95
1:A:230:PRO:CG	1:C:357:ARG:NH2	2.29	0.95
1:A:328:ARG:HH11	1:A:543:PHE:HE2	1.11	0.95
1:A:1107:ARG:NH1	1:B:904:TYR:HE1	1.54	0.95
1:A:486:PHE:CD2	2:U:102:TYR:HE1	1.84	0.94
2:U:51:ILE:HD11	2:U:70:MET:CG	1.96	0.94
1:B:379:CYS:HB3	1:B:432:CYS:HA	1.49	0.94
1:A:486:PHE:CA	2:U:104:TRP:CE3	2.50	0.94
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.49	0.94
2:U:51:ILE:HD13	2:U:70:MET:HB3	1.49	0.94
1:A:357:ARG:NH2	1:B:230:PRO:CG	2.30	0.93
1:B:486:PHE:CB	2:S:104:TRP:HB2	1.97	0.93
1:B:486:PHE:CA	2:S:104:TRP:CE3	2.51	0.93
1:C:328:ARG:HH11	1:C:543:PHE:HE2	1.12	0.93
1:B:486:PHE:CA	2:S:102:TYR:CZ	2.45	0.93
1:B:329:PHE:HE1	1:B:528:LYS:HD3	1.15	0.93
1:A:486:PHE:CA	2:U:102:TYR:CZ	2.45	0.92
1:A:486:PHE:CB	2:U:104:TRP:HB2	1.97	0.92
1:B:357:ARG:HH22	1:C:230:PRO:HG3	1.24	0.92
1:C:486:PHE:CA	2:W:104:TRP:CE3	2.51	0.92
2:U:51:ILE:HD11	2:U:70:MET:CA	2.00	0.92
2:U:51:ILE:CG1	2:U:70:MET:CB	2.48	0.92
1:A:357:ARG:HH22	1:B:230:PRO:HG3	1.25	0.91
1:C:379:CYS:HB3	1:C:432:CYS:HA	1.49	0.91
2:W:51:ILE:HD11	2:W:70:MET:CA	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:51:ILE:CG1	2:W:70:MET:CB	2.48	0.90
1:A:485:GLY:CA	2:U:103:ASN:HB3	2.01	0.90
1:B:485:GLY:CA	2:S:103:ASN:HB3	1.99	0.90
1:A:1094:VAL:HG22	1:A:1107:ARG:CZ	2.01	0.89
1:B:1107:ARG:NH2	1:C:904:TYR:HE1	1.68	0.89
1:C:485:GLY:CA	2:W:103:ASN:HB3	2.01	0.89
2:U:34:PHE:H	2:U:72:ARG:HH22	0.92	0.89
2:S:34:PHE:H	2:S:72:ARG:HH22	0.92	0.89
1:C:486:PHE:CB	2:W:104:TRP:HB2	2.00	0.88
1:C:486:PHE:CG	2:W:104:TRP:HE3	1.91	0.88
1:C:485:GLY:HA2	2:W:103:ASN:CB	2.02	0.87
1:B:486:PHE:CG	2:S:104:TRP:HE3	1.91	0.87
2:W:34:PHE:HD2	2:W:72:ARG:NH1	1.73	0.87
2:U:34:PHE:HD2	2:U:72:ARG:NH1	1.73	0.87
2:W:34:PHE:H	2:W:72:ARG:HH22	0.92	0.87
2:W:72:ARG:HG2	2:W:79:VAL:HG22	1.56	0.86
1:A:1107:ARG:NH1	1:B:904:TYR:CZ	2.43	0.86
2:W:34:PHE:H	2:W:72:ARG:NH2	1.74	0.86
2:W:51:ILE:HD13	2:W:70:MET:HB3	1.49	0.86
2:S:51:ILE:HG23	2:S:72:ARG:CZ	2.05	0.86
2:U:34:PHE:H	2:U:72:ARG:NH2	1.74	0.86
1:A:1094:VAL:HG23	1:A:1107:ARG:HE	1.37	0.86
2:U:53:PRO:HD3	2:U:72:ARG:HH11	1.04	0.86
1:C:486:PHE:CG	2:W:102:TYR:OH	2.29	0.86
2:S:34:PHE:H	2:S:72:ARG:NH2	1.74	0.86
2:S:72:ARG:HG2	2:S:79:VAL:HG22	1.55	0.86
1:A:486:PHE:HA	2:U:102:TYR:CE1	2.11	0.85
1:B:485:GLY:HA2	2:S:103:ASN:CB	2.01	0.85
1:C:328:ARG:NH2	1:C:585:LEU:HD11	1.91	0.85
2:S:34:PHE:HD2	2:S:72:ARG:NH1	1.72	0.85
2:U:72:ARG:HG2	2:U:79:VAL:HG22	1.56	0.85
1:B:328:ARG:NH2	1:B:585:LEU:HD11	1.92	0.85
2:W:53:PRO:HD3	2:W:72:ARG:HH11	1.04	0.85
1:A:486:PHE:CG	2:U:104:TRP:HE3	1.93	0.85
1:A:335:LEU:HD23	1:A:362:VAL:CG1	2.06	0.84
1:A:335:LEU:HD21	1:A:362:VAL:HG13	1.58	0.84
1:B:486:PHE:HA	2:S:102:TYR:CE1	2.12	0.84
2:S:51:ILE:HG23	2:S:72:ARG:NE	1.93	0.84
1:A:328:ARG:HD2	1:A:543:PHE:CE2	2.13	0.84
1:B:328:ARG:HD2	1:B:543:PHE:CE2	2.13	0.84
1:C:328:ARG:HD2	1:C:543:PHE:CE2	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:856:ASN:ND2	1:C:966:LEU:CD1	2.41	0.84
1:C:486:PHE:HA	2:W:102:TYR:CE1	2.12	0.84
2:U:53:PRO:HD3	2:U:72:ARG:HH12	1.03	0.83
1:A:485:GLY:HA2	2:U:103:ASN:CB	2.03	0.83
1:B:486:PHE:CD2	2:S:102:TYR:CE1	2.66	0.83
2:S:53:PRO:HD3	2:S:72:ARG:HH11	1.06	0.83
1:B:486:PHE:CB	2:S:104:TRP:CD2	2.49	0.83
1:C:486:PHE:CD2	2:W:102:TYR:CE1	2.66	0.83
1:B:327:VAL:CG1	1:B:528:LYS:HE2	2.09	0.83
1:B:486:PHE:CG	2:S:102:TYR:OH	2.32	0.83
1:A:328:ARG:NH2	1:A:585:LEU:HD11	1.91	0.83
1:B:486:PHE:HD2	2:S:102:TYR:HE1	1.27	0.82
1:A:486:PHE:CG	2:U:102:TYR:OH	2.32	0.82
1:B:335:LEU:HD23	1:B:362:VAL:CG1	2.06	0.81
2:S:53:PRO:HD3	2:S:72:ARG:HH12	1.02	0.81
2:W:53:PRO:HD3	2:W:72:ARG:HH12	1.03	0.81
1:A:486:PHE:CD2	2:U:102:TYR:CE1	2.68	0.81
2:W:53:PRO:CG	2:W:72:ARG:HH11	1.94	0.81
2:S:51:ILE:HG23	2:S:72:ARG:NH2	1.96	0.81
1:B:327:VAL:HG11	1:B:528:LYS:HE2	1.61	0.81
1:B:335:LEU:HD21	1:B:362:VAL:HG13	1.58	0.80
1:C:486:PHE:CB	2:W:104:TRP:CD2	2.50	0.80
1:C:486:PHE:HD2	2:W:102:TYR:HE1	1.28	0.80
2:S:53:PRO:CG	2:S:72:ARG:HH11	1.93	0.80
2:U:53:PRO:CG	2:U:72:ARG:HH11	1.94	0.80
2:W:34:PHE:N	2:W:72:ARG:NH2	2.28	0.80
1:A:1107:ARG:CZ	1:B:904:TYR:CZ	2.64	0.80
1:B:328:ARG:CZ	1:B:543:PHE:CE2	2.58	0.80
2:S:34:PHE:N	2:S:72:ARG:NH2	2.28	0.79
2:U:34:PHE:N	2:U:72:ARG:NH2	2.28	0.79
1:A:1107:ARG:HH12	1:B:904:TYR:HE1	1.16	0.79
1:C:856:ASN:HD21	1:C:966:LEU:CD1	1.95	0.78
1:B:386:LYS:NZ	1:C:985:ASP:OD1	2.15	0.78
1:A:708:SER:OG	1:A:711:SER:HB3	1.84	0.78
1:A:486:PHE:HD2	2:U:102:TYR:HE1	1.30	0.78
1:C:338:PHE:HB2	5:C:1305:NAG:H82	1.66	0.78
1:B:708:SER:OG	1:B:711:SER:HB3	1.84	0.77
1:C:328:ARG:CZ	1:C:543:PHE:CE2	2.58	0.77
1:B:328:ARG:HD2	1:B:543:PHE:CD2	2.20	0.77
2:W:34:PHE:CD2	2:W:72:ARG:NH2	2.53	0.77
1:A:328:ARG:CZ	1:A:543:PHE:CE2	2.58	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HD2	1:C:543:PHE:CD2	2.20	0.76
1:C:708:SER:OG	1:C:711:SER:HB3	1.84	0.76
1:B:486:PHE:N	2:S:104:TRP:CD2	2.54	0.76
1:A:328:ARG:HD2	1:A:543:PHE:CD2	2.20	0.76
2:U:34:PHE:CD2	2:U:72:ARG:NH2	2.53	0.76
2:S:34:PHE:CD2	2:S:72:ARG:NH2	2.53	0.75
2:W:34:PHE:CD2	2:W:72:ARG:NH1	2.53	0.75
1:A:338:PHE:HB2	5:A:1305:NAG:H82	1.67	0.75
1:B:329:PHE:HE1	1:B:528:LYS:CD	1.99	0.74
1:A:486:PHE:CB	2:U:104:TRP:CD2	2.50	0.74
2:U:34:PHE:CD2	2:U:72:ARG:NH1	2.53	0.74
1:B:367:VAL:HG13	1:B:368:LEU:HD12	1.71	0.73
1:C:368:LEU:HD11	5:C:1305:NAG:H83	1.71	0.73
1:A:386:LYS:NZ	1:B:985:ASP:OD1	2.16	0.73
2:S:72:ARG:CG	2:S:79:VAL:HG22	2.18	0.73
2:U:51:ILE:HG12	2:U:58:THR:HG22	1.69	0.73
1:A:486:PHE:N	2:U:104:TRP:CD2	2.53	0.73
2:U:72:ARG:CG	2:U:79:VAL:HG22	2.18	0.73
2:W:51:ILE:HG12	2:W:58:THR:HG22	1.69	0.73
1:A:328:ARG:NE	1:A:578:ASP:OD2	2.22	0.72
2:W:72:ARG:CD	2:W:79:VAL:HG22	2.18	0.72
2:S:72:ARG:CD	2:S:79:VAL:HG22	2.19	0.72
2:S:34:PHE:CD2	2:S:72:ARG:NH1	2.53	0.72
1:A:912:THR:HG1	1:A:1106:GLN:HE22	1.35	0.72
1:C:367:VAL:HG13	1:C:368:LEU:HD12	1.71	0.72
2:W:72:ARG:CG	2:W:79:VAL:HG22	2.18	0.72
1:A:1107:ARG:CZ	1:B:904:TYR:OH	2.38	0.72
2:U:72:ARG:CD	2:U:79:VAL:HG22	2.18	0.72
1:B:328:ARG:NE	1:B:578:ASP:OD2	2.22	0.71
1:B:391:CYS:HB3	1:B:522:ALA:HB1	1.73	0.71
1:C:328:ARG:NE	1:C:578:ASP:OD2	2.22	0.71
2:U:51:ILE:CD1	2:U:70:MET:CB	1.81	0.71
2:U:51:ILE:CD1	2:U:70:MET:HB2	2.16	0.71
1:A:367:VAL:HG13	1:A:368:LEU:HD12	1.71	0.71
1:C:486:PHE:N	2:W:104:TRP:CD2	2.55	0.71
1:B:912:THR:HG1	1:B:1106:GLN:HE22	1.38	0.71
1:C:391:CYS:HB3	1:C:522:ALA:HB1	1.72	0.71
1:B:338:PHE:HB2	5:B:1305:NAG:H82	1.73	0.70
1:C:382:VAL:HG11	1:C:387:LEU:HB3	1.74	0.70
1:A:382:VAL:HG11	1:A:387:LEU:HB3	1.74	0.70
1:A:1107:ARG:NH1	1:B:904:TYR:CD1	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ASP:OD1	1:C:386:LYS:NZ	2.16	0.69
1:A:391:CYS:HB3	1:A:522:ALA:HB1	1.73	0.69
1:B:382:VAL:HG11	1:B:387:LEU:HB3	1.74	0.69
2:W:51:ILE:CD1	2:W:70:MET:CB	1.81	0.68
1:A:484:GLU:O	2:U:103:ASN:HB2	1.94	0.68
1:A:1031:GLU:O	1:A:1031:GLU:HG3	1.93	0.68
1:C:484:GLU:O	2:W:103:ASN:HB2	1.93	0.67
1:B:383:SER:HB3	1:B:386:LYS:HD3	1.76	0.67
1:C:383:SER:HB3	1:C:386:LYS:HD3	1.76	0.67
2:U:34:PHE:CB	2:U:72:ARG:HH21	1.86	0.67
2:U:107:ALA:HB2	3:V:36:SER:HB3	1.77	0.67
2:W:51:ILE:CG1	2:W:70:MET:HB2	2.23	0.67
1:B:293:LEU:O	1:B:294:ASP:OD1	2.12	0.67
2:S:107:ALA:HB2	3:T:36:SER:HB3	1.77	0.67
1:B:357:ARG:HH22	1:C:230:PRO:CG	1.99	0.67
1:C:328:ARG:NH2	1:C:585:LEU:CD1	2.55	0.67
2:W:53:PRO:CG	2:W:72:ARG:NH1	2.56	0.67
2:U:34:PHE:CA	2:U:72:ARG:NH2	2.58	0.66
2:W:53:PRO:CD	2:W:72:ARG:HH12	1.82	0.66
1:A:383:SER:HB3	1:A:386:LYS:HD3	1.76	0.66
1:B:484:GLU:O	2:S:103:ASN:HB2	1.95	0.66
2:S:34:PHE:CA	2:S:72:ARG:NH2	2.59	0.66
1:B:328:ARG:NH2	1:B:585:LEU:CD1	2.55	0.66
2:W:107:ALA:HB2	3:X:36:SER:HB3	1.77	0.66
2:S:53:PRO:CG	2:S:72:ARG:NH1	2.55	0.65
2:U:51:ILE:CG1	2:U:70:MET:HB2	2.23	0.65
1:A:230:PRO:CG	1:C:357:ARG:HH22	1.99	0.65
1:A:368:LEU:HD11	5:A:1305:NAG:H83	1.77	0.65
2:W:34:PHE:CA	2:W:72:ARG:NH2	2.58	0.64
2:U:53:PRO:CG	2:U:72:ARG:NH1	2.56	0.64
1:A:328:ARG:NH2	1:A:585:LEU:CD1	2.55	0.64
1:C:335:LEU:HD23	1:C:362:VAL:CG1	2.25	0.63
1:C:391:CYS:HB3	1:C:522:ALA:CB	2.29	0.63
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.81	0.63
2:W:34:PHE:CG	2:W:72:ARG:NH2	2.67	0.63
1:C:412:PRO:O	1:C:414:GLN:NE2	2.32	0.63
2:S:34:PHE:CG	2:S:72:ARG:NH2	2.67	0.62
2:W:51:ILE:CD1	2:W:70:MET:HB2	2.16	0.62
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.81	0.62
1:B:412:PRO:O	1:B:414:GLN:NE2	2.32	0.62
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:51:ILE:HG23	2:S:72:ARG:HE	1.65	0.62
1:B:357:ARG:NH1	1:B:394:ASN:OD1	2.33	0.62
1:C:357:ARG:NH1	1:C:394:ASN:OD1	2.33	0.62
2:S:34:PHE:HD2	2:S:72:ARG:NH2	1.93	0.62
1:A:1094:VAL:HG22	1:A:1107:ARG:NH2	2.13	0.62
1:B:486:PHE:H	2:S:104:TRP:CG	2.17	0.62
2:U:34:PHE:CG	2:U:72:ARG:NH2	2.67	0.62
2:U:53:PRO:CD	2:U:72:ARG:HH12	1.82	0.62
1:A:391:CYS:HB3	1:A:522:ALA:CB	2.30	0.62
1:A:357:ARG:NH1	1:A:394:ASN:OD1	2.33	0.61
1:B:391:CYS:HB3	1:B:522:ALA:CB	2.30	0.61
1:C:382:VAL:CG1	1:C:387:LEU:HB3	2.30	0.61
1:A:912:THR:CB	1:A:1106:GLN:HE22	2.08	0.61
1:C:335:LEU:CD2	1:C:362:VAL:HG13	2.25	0.61
1:B:382:VAL:CG1	1:B:387:LEU:HB3	2.30	0.61
1:A:985:ASP:HB3	1:A:987:PRO:HD2	1.82	0.61
1:A:486:PHE:H	2:U:104:TRP:CG	2.17	0.61
2:S:53:PRO:CD	2:S:72:ARG:HH12	1.82	0.61
1:A:382:VAL:CG1	1:A:387:LEU:HB3	2.30	0.60
1:A:412:PRO:O	1:A:414:GLN:NE2	2.32	0.60
1:A:328:ARG:NH1	1:A:578:ASP:HB2	2.17	0.60
1:B:328:ARG:NH1	1:B:578:ASP:HB2	2.17	0.60
1:C:985:ASP:HB3	1:C:987:PRO:HD2	1.82	0.60
2:W:34:PHE:HD2	2:W:72:ARG:NH2	1.93	0.60
2:W:51:ILE:O	2:W:72:ARG:NH2	2.35	0.60
2:U:51:ILE:O	2:U:72:ARG:NH2	2.35	0.59
1:A:357:ARG:HH22	1:B:230:PRO:CG	2.01	0.59
1:B:357:ARG:HH21	1:C:230:PRO:CG	2.15	0.59
1:B:985:ASP:HB3	1:B:987:PRO:HD2	1.83	0.59
1:C:454:ARG:NH2	1:C:467:ASP:O	2.32	0.59
1:B:486:PHE:CB	2:S:104:TRP:CG	2.86	0.59
1:C:328:ARG:NH1	1:C:578:ASP:HB2	2.17	0.59
1:C:501:ASN:O	1:C:506:GLN:NE2	2.36	0.59
2:S:51:ILE:O	2:S:72:ARG:NH2	2.36	0.59
1:A:501:ASN:O	1:A:506:GLN:NE2	2.36	0.58
1:A:1094:VAL:HG23	1:A:1107:ARG:HG2	1.85	0.58
1:B:501:ASN:O	1:B:506:GLN:NE2	2.35	0.58
1:C:328:ARG:CD	1:C:543:PHE:CE2	2.86	0.58
2:S:51:ILE:HD13	2:S:72:ARG:HG3	1.85	0.58
1:A:328:ARG:NH1	1:A:578:ASP:CB	2.67	0.58
1:B:328:ARG:NH1	1:B:578:ASP:CB	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:CD	1:A:543:PHE:CE2	2.86	0.58
1:A:454:ARG:NH2	1:A:467:ASP:O	2.32	0.58
1:B:1107:ARG:CZ	1:C:904:TYR:CZ	2.86	0.58
2:U:34:PHE:HD2	2:U:72:ARG:NH2	1.93	0.58
1:C:328:ARG:NH1	1:C:578:ASP:CB	2.67	0.57
2:U:51:ILE:HG13	2:U:70:MET:SD	2.44	0.57
2:S:51:ILE:HG23	2:S:72:ARG:HH21	1.70	0.57
1:A:230:PRO:CG	1:C:357:ARG:HH21	2.14	0.57
2:W:51:ILE:HG13	2:W:70:MET:SD	2.44	0.57
1:A:486:PHE:CB	2:U:104:TRP:CG	2.86	0.57
1:B:431:GLY:HA2	1:B:515:PHE:HD2	1.70	0.57
1:C:486:PHE:H	2:W:104:TRP:CG	2.20	0.56
1:B:442:ASP:OD2	1:B:509:ARG:NE	2.39	0.56
1:C:486:PHE:CB	2:W:104:TRP:CG	2.88	0.56
1:A:414:GLN:O	1:A:424:LYS:NZ	2.38	0.56
1:C:414:GLN:O	1:C:424:LYS:NZ	2.38	0.56
1:A:1107:ARG:CZ	1:B:904:TYR:HE1	2.00	0.56
1:B:328:ARG:CD	1:B:543:PHE:CE2	2.86	0.56
1:A:442:ASP:OD2	1:A:509:ARG:NE	2.39	0.56
1:B:422:ASN:OD1	1:B:454:ARG:N	2.30	0.56
1:C:431:GLY:HA2	1:C:515:PHE:HD2	1.70	0.56
1:B:486:PHE:CD1	2:S:104:TRP:HE3	2.24	0.55
1:C:403:ARG:HB2	1:C:495:TYR:HE1	1.71	0.55
1:C:442:ASP:OD2	1:C:509:ARG:NE	2.39	0.55
1:A:357:ARG:HH21	1:B:230:PRO:CG	2.14	0.55
1:B:454:ARG:NH2	1:B:467:ASP:O	2.32	0.55
1:A:431:GLY:HA2	1:A:515:PHE:HD2	1.70	0.55
1:A:486:PHE:N	2:U:104:TRP:CE3	2.72	0.55
1:B:414:GLN:O	1:B:424:LYS:NZ	2.38	0.55
1:B:486:PHE:N	2:S:104:TRP:CE3	2.74	0.55
1:C:486:PHE:HB2	2:W:104:TRP:CG	2.42	0.55
1:A:422:ASN:OD1	1:A:454:ARG:N	2.30	0.55
1:B:403:ARG:HB2	1:B:495:TYR:HE1	1.71	0.55
1:A:403:ARG:HB2	1:A:495:TYR:HE1	1.71	0.55
1:B:486:PHE:HB2	2:S:104:TRP:CG	2.42	0.55
1:C:856:ASN:HD21	1:C:966:LEU:HD12	1.70	0.55
1:B:1031:GLU:CG	1:B:1031:GLU:O	2.53	0.54
1:B:454:ARG:HG3	1:B:491:PRO:HB2	1.89	0.54
1:C:454:ARG:HG3	1:C:491:PRO:HB2	1.89	0.54
2:U:51:ILE:HG12	2:U:70:MET:HB2	1.89	0.54
1:B:332:ILE:HG22	1:B:333:THR:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:PHE:N	2:W:104:TRP:CE3	2.74	0.54
1:B:357:ARG:NH2	1:C:230:PRO:CB	2.70	0.54
2:W:51:ILE:HG12	2:W:70:MET:HB2	1.89	0.54
1:A:357:ARG:NH2	1:B:230:PRO:CB	2.71	0.53
1:A:332:ILE:HG22	1:A:333:THR:N	2.24	0.53
1:C:1031:GLU:CG	1:C:1031:GLU:O	2.55	0.53
1:A:454:ARG:HG3	1:A:491:PRO:HB2	1.89	0.53
1:A:486:PHE:HB2	2:U:104:TRP:CG	2.42	0.53
1:C:338:PHE:CB	5:C:1305:NAG:H82	2.36	0.53
1:C:484:GLU:O	2:W:103:ASN:CB	2.57	0.53
1:C:332:ILE:HG22	1:C:333:THR:N	2.24	0.53
1:A:486:PHE:CD1	2:U:104:TRP:HE3	2.26	0.52
1:C:486:PHE:CD1	2:W:104:TRP:HE3	2.26	0.52
1:A:708:SER:HG	1:A:711:SER:HB3	1.74	0.52
1:A:230:PRO:CB	1:C:357:ARG:NH2	2.72	0.52
1:A:379:CYS:CB	1:A:432:CYS:HA	2.32	0.52
1:A:484:GLU:O	2:U:103:ASN:CB	2.57	0.52
1:B:327:VAL:HG13	1:B:528:LYS:HE2	1.89	0.52
1:B:379:CYS:CB	1:B:432:CYS:HA	2.32	0.52
1:C:422:ASN:OD1	1:C:454:ARG:N	2.30	0.52
1:A:339:GLY:O	1:A:343:ASN:HB2	2.11	0.51
1:A:497:PHE:CZ	1:A:507:PRO:HB3	2.45	0.51
1:A:912:THR:HG1	1:A:1106:GLN:NE2	2.01	0.51
2:S:36:TRP:CE2	2:S:81:MET:HB2	2.45	0.51
1:B:497:PHE:CZ	1:B:507:PRO:HB3	2.45	0.51
1:B:484:GLU:O	2:S:103:ASN:CB	2.57	0.51
2:S:51:ILE:CG2	2:S:72:ARG:HE	2.22	0.51
2:W:35:HIS:CD2	2:W:50:TRP:HB3	2.46	0.51
1:B:1031:GLU:O	1:B:1031:GLU:HG2	2.11	0.51
1:C:379:CYS:CB	1:C:432:CYS:HA	2.32	0.51
1:C:486:PHE:HA	2:W:102:TYR:CE2	2.41	0.50
2:U:36:TRP:CE2	2:U:81:MET:HB2	2.45	0.50
2:W:36:TRP:CE2	2:W:81:MET:HB2	2.45	0.50
1:C:497:PHE:CZ	1:C:507:PRO:HB3	2.45	0.50
1:B:557:LYS:NZ	1:B:574:ASP:OD2	2.43	0.50
1:B:339:GLY:O	1:B:343:ASN:HB2	2.11	0.50
1:A:1031:GLU:OE1	1:C:1040:VAL:HG23	2.12	0.50
1:A:1094:VAL:HG22	1:A:1107:ARG:HH21	1.77	0.50
2:S:35:HIS:CD2	2:S:50:TRP:HB3	2.47	0.50
1:C:339:GLY:O	1:C:343:ASN:HB2	2.11	0.50
2:S:34:PHE:CB	2:S:72:ARG:HH21	1.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ASN:OD1	2:S:104:TRP:HZ3	1.95	0.49
1:B:916:LEU:HD12	1:B:923:ILE:CD1	2.42	0.49
2:S:51:ILE:CG2	2:S:72:ARG:NE	2.72	0.49
2:U:35:HIS:CD2	2:U:50:TRP:HB3	2.46	0.49
2:W:108:TYR:CD2	3:X:99:LEU:HB2	2.48	0.49
1:B:349:SER:OG	1:B:452:LEU:O	2.30	0.49
1:B:405:ASP:O	1:B:408:ARG:NH1	2.46	0.49
2:U:108:TYR:CD2	3:V:99:LEU:HB2	2.47	0.49
1:A:365:TYR:CD2	1:A:388:ASN:HA	2.48	0.49
1:A:384:PRO:O	1:A:387:LEU:HG	2.13	0.49
1:A:916:LEU:HD12	1:A:923:ILE:CD1	2.42	0.49
1:C:916:LEU:HD12	1:C:923:ILE:CD1	2.42	0.49
1:A:557:LYS:NZ	1:A:574:ASP:OD2	2.43	0.49
1:C:349:SER:OG	1:C:452:LEU:O	2.30	0.49
1:A:349:SER:OG	1:A:452:LEU:O	2.30	0.49
1:B:365:TYR:CD2	1:B:388:ASN:HA	2.48	0.48
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.46	0.48
1:B:1094:VAL:CG2	1:B:1107:ARG:HE	2.26	0.48
1:C:384:PRO:O	1:C:387:LEU:HG	2.13	0.48
2:S:108:TYR:CD2	3:T:99:LEU:HB2	2.48	0.48
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.46	0.48
1:B:332:ILE:HG22	1:B:333:THR:H	1.77	0.48
1:B:335:LEU:CD2	1:B:362:VAL:CG1	2.65	0.48
1:C:405:ASP:O	1:C:408:ARG:NH1	2.46	0.48
1:A:405:ASP:O	1:A:408:ARG:NH1	2.46	0.48
1:B:486:PHE:HA	2:S:102:TYR:CE2	2.43	0.48
1:C:365:TYR:CD2	1:C:388:ASN:HA	2.48	0.48
1:A:338:PHE:CB	5:A:1305:NAG:H82	2.42	0.48
1:A:1094:VAL:HG23	1:A:1107:ARG:NE	2.06	0.48
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.46	0.48
1:B:384:PRO:O	1:B:387:LEU:HG	2.13	0.48
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.96	0.48
1:A:1094:VAL:HG21	1:A:1107:ARG:HE	1.51	0.48
2:W:107:ALA:HB2	3:X:36:SER:CB	2.44	0.48
1:B:332:ILE:CG2	1:B:333:THR:H	2.27	0.47
1:B:343:ASN:ND2	5:B:1305:NAG:O5	2.47	0.47
2:S:106:TYR:CG	3:T:34:TYR:HB2	2.49	0.47
1:A:986:PRO:HB2	1:A:987:PRO:HD3	1.96	0.47
2:W:106:TYR:CG	3:X:34:TYR:HB2	2.49	0.47
1:B:708:SER:HG	1:B:711:SER:HB3	1.78	0.47
2:U:106:TYR:CG	3:V:34:TYR:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:107:ALA:HB2	3:V:36:SER:CB	2.44	0.47
1:A:343:ASN:ND2	5:A:1305:NAG:O5	2.48	0.47
1:C:486:PHE:C	2:W:102:TYR:CE2	2.89	0.47
1:C:986:PRO:HB2	1:C:987:PRO:HD3	1.96	0.47
2:S:34:PHE:CG	2:S:79:VAL:HG21	2.50	0.47
2:W:34:PHE:CG	2:W:79:VAL:HG21	2.50	0.47
1:A:487:ASN:OD1	2:U:104:TRP:HZ3	1.98	0.47
1:A:486:PHE:HA	2:U:102:TYR:CE2	2.43	0.47
1:C:557:LYS:NZ	1:C:574:ASP:OD2	2.44	0.47
2:W:34:PHE:CB	2:W:72:ARG:HH21	1.86	0.47
2:U:34:PHE:CG	2:U:79:VAL:HG21	2.50	0.46
1:B:546:LEU:HD22	1:B:565:PHE:CE2	2.51	0.46
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.51	0.46
1:A:335:LEU:CD2	1:A:362:VAL:CG1	2.65	0.46
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.51	0.46
1:C:487:ASN:OD1	2:W:104:TRP:HZ3	1.99	0.46
1:C:343:ASN:ND2	5:C:1305:NAG:O5	2.48	0.46
1:A:332:ILE:HG22	1:A:333:THR:H	1.80	0.46
1:A:546:LEU:HD22	1:A:565:PHE:CE2	2.51	0.46
2:S:35:HIS:CE1	2:S:108:TYR:HB3	2.51	0.46
1:B:1094:VAL:HG22	1:B:1107:ARG:HE	1.81	0.46
2:U:35:HIS:CE1	2:U:108:TYR:HB3	2.51	0.46
1:A:340:GLU:O	1:A:344:ALA:HB2	2.16	0.45
1:A:1094:VAL:HG23	1:A:1107:ARG:CG	2.46	0.45
1:C:546:LEU:HD22	1:C:565:PHE:CE2	2.50	0.45
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.51	0.45
1:A:1094:VAL:CG2	1:A:1107:ARG:HG2	2.46	0.45
2:W:35:HIS:CE1	2:W:108:TYR:HB3	2.51	0.45
1:A:108:THR:HG23	1:A:234:ASN:O	2.16	0.45
1:B:108:THR:HG23	1:B:234:ASN:O	2.16	0.45
1:B:340:GLU:O	1:B:344:ALA:HB2	2.16	0.45
1:B:516:GLU:OE2	1:C:200:TYR:OH	2.30	0.45
1:B:578:ASP:HB3	1:B:581:THR:O	2.17	0.45
1:A:578:ASP:HB3	1:A:581:THR:O	2.17	0.45
1:A:332:ILE:CG2	1:A:333:THR:H	2.29	0.44
1:A:354:ASN:OD1	1:A:355:ARG:N	2.50	0.44
1:A:393:THR:HA	1:A:522:ALA:HA	1.98	0.44
1:B:332:ILE:CG2	1:B:333:THR:N	2.80	0.44
2:W:97:ALA:CB	2:W:109:CYS:HB3	2.47	0.44
1:C:393:THR:HA	1:C:522:ALA:HA	1.98	0.44
1:C:354:ASN:OD1	1:C:355:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:LEU:HD12	1:A:923:ILE:HD12	2.00	0.44
1:C:340:GLU:O	1:C:344:ALA:HB2	2.16	0.44
2:S:72:ARG:HG2	2:S:79:VAL:CG2	2.38	0.44
2:S:97:ALA:CB	2:S:109:CYS:HB3	2.47	0.44
1:B:393:THR:HA	1:B:522:ALA:HA	1.99	0.44
1:C:108:THR:HG23	1:C:234:ASN:O	2.16	0.44
1:C:916:LEU:HD12	1:C:923:ILE:HD12	2.00	0.44
1:C:1031:GLU:O	1:C:1031:GLU:HG2	2.18	0.44
2:S:107:ALA:HB2	3:T:36:SER:CB	2.44	0.44
1:B:354:ASN:OD1	1:B:355:ARG:N	2.50	0.44
1:B:486:PHE:C	2:S:104:TRP:CE3	2.95	0.44
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	2.00	0.44
1:A:419:ALA:O	1:A:424:LYS:HE2	2.18	0.44
1:A:486:PHE:C	2:U:104:TRP:CE3	2.96	0.44
1:C:578:ASP:HB3	1:C:581:THR:O	2.18	0.44
1:C:877:LEU:HD23	1:C:877:LEU:HA	1.89	0.44
1:B:368:LEU:HD11	5:B:1305:NAG:H83	2.00	0.44
1:B:428:ASP:OD1	1:B:428:ASP:N	2.51	0.44
1:B:486:PHE:CA	2:S:104:TRP:CD2	2.95	0.44
1:B:419:ALA:O	1:B:424:LYS:HE2	2.18	0.44
1:B:484:GLU:HG2	2:S:33:TYR:OH	2.18	0.44
1:C:332:ILE:CG2	1:C:333:THR:H	2.31	0.44
1:C:484:GLU:HG2	2:W:33:TYR:OH	2.18	0.43
2:U:97:ALA:CB	2:U:109:CYS:HB3	2.47	0.43
1:A:877:LEU:HD23	1:A:877:LEU:HA	1.88	0.43
1:A:1107:ARG:NH2	1:B:904:TYR:HE1	2.17	0.43
1:B:786:LYS:H	1:B:786:LYS:HG2	1.66	0.43
1:B:349:SER:OG	1:B:452:LEU:N	2.37	0.43
1:C:419:ALA:O	1:C:424:LYS:HE2	2.18	0.43
1:A:332:ILE:CG2	1:A:333:THR:N	2.81	0.43
1:A:471:GLU:OE1	1:A:472:ILE:N	2.52	0.43
1:A:484:GLU:HG2	2:U:33:TYR:OH	2.17	0.43
1:C:389:ASP:OD1	1:C:389:ASP:N	2.49	0.43
1:B:337:PRO:O	1:B:341:VAL:HG23	2.18	0.43
1:B:877:LEU:HD23	1:B:877:LEU:HA	1.90	0.43
1:C:1056:ALA:HB1	1:C:1057:PRO:HD2	2.01	0.43
1:A:349:SER:OG	1:A:452:LEU:N	2.37	0.43
1:C:332:ILE:HG22	1:C:333:THR:H	1.84	0.43
1:A:337:PRO:O	1:A:341:VAL:HG23	2.18	0.42
1:A:985:ASP:CB	1:A:987:PRO:HD2	2.49	0.42
1:C:471:GLU:OE1	1:C:472:ILE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:PHE:CD1	1:C:507:PRO:HD3	2.54	0.42
1:A:364:ASP:O	1:A:367:VAL:HG12	2.19	0.42
1:B:130:VAL:HG22	1:B:168:PHE:HB3	2.02	0.42
1:C:332:ILE:CG2	1:C:333:THR:N	2.81	0.42
1:C:337:PRO:O	1:C:341:VAL:HG23	2.18	0.42
2:S:51:ILE:O	2:S:72:ARG:CZ	2.68	0.42
1:A:200:TYR:OH	1:C:516:GLU:OE2	2.35	0.42
1:B:81:ASN:OD1	1:B:81:ASN:N	2.51	0.42
1:B:364:ASP:O	1:B:367:VAL:HG12	2.19	0.42
1:B:471:GLU:OE1	1:B:472:ILE:N	2.52	0.42
1:B:497:PHE:CD1	1:B:507:PRO:HD3	2.54	0.42
1:B:916:LEU:HD12	1:B:923:ILE:HD12	2.00	0.42
1:C:364:ASP:O	1:C:367:VAL:HG12	2.19	0.42
1:C:480:CYS:SG	1:C:481:ASN:N	2.92	0.42
1:C:708:SER:HG	1:C:711:SER:HB3	1.78	0.42
2:S:32:TYR:HA	2:S:101:THR:OG1	2.20	0.42
2:U:32:TYR:HA	2:U:101:THR:OG1	2.20	0.42
2:U:72:ARG:HG2	2:U:79:VAL:CG2	2.38	0.42
1:B:329:PHE:CZ	1:B:528:LYS:HD3	2.47	0.42
1:B:480:CYS:SG	1:B:481:ASN:N	2.92	0.42
1:C:130:VAL:HG22	1:C:168:PHE:HB3	2.02	0.42
1:C:985:ASP:CB	1:C:987:PRO:HD2	2.48	0.42
1:C:81:ASN:OD1	1:C:81:ASN:N	2.51	0.42
1:A:130:VAL:HG22	1:A:168:PHE:HB3	2.02	0.42
1:A:502:GLY:O	1:A:506:GLN:NE2	2.53	0.42
1:C:328:ARG:NE	1:C:543:PHE:CE2	2.88	0.42
2:S:51:ILE:CG2	2:S:72:ARG:HH21	2.31	0.42
1:C:349:SER:OG	1:C:452:LEU:N	2.37	0.42
1:C:328:ARG:NH1	1:C:578:ASP:CG	2.78	0.42
2:W:51:ILE:O	2:W:72:ARG:CZ	2.68	0.42
1:A:497:PHE:CD1	1:A:507:PRO:HD3	2.54	0.41
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.55	0.41
1:B:486:PHE:CB	2:S:104:TRP:CB	2.75	0.41
1:B:502:GLY:O	1:B:506:GLN:NE2	2.53	0.41
1:C:502:GLY:O	1:C:506:GLN:NE2	2.53	0.41
2:W:32:TYR:HA	2:W:101:THR:OG1	2.20	0.41
1:A:328:ARG:NH1	1:A:578:ASP:CG	2.78	0.41
1:A:480:CYS:SG	1:A:481:ASN:N	2.92	0.41
1:B:439:ASN:ND2	1:B:506:GLN:OE1	2.53	0.41
1:C:395:VAL:HG22	1:C:524:VAL:HG21	2.02	0.41
1:C:439:ASN:ND2	1:C:506:GLN:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:51:ILE:O	2:U:72:ARG:CZ	2.67	0.41
1:A:328:ARG:NE	1:A:543:PHE:CE2	2.88	0.41
1:A:411:ALA:O	1:A:414:GLN:HG2	2.20	0.41
1:A:439:ASN:ND2	1:A:506:GLN:OE1	2.53	0.41
1:A:1056:ALA:HB1	1:A:1057:PRO:HD2	2.01	0.41
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.49	0.41
1:B:411:ALA:O	1:B:414:GLN:HG2	2.20	0.41
1:C:328:ARG:HE	1:C:533:LEU:HD12	1.44	0.41
1:A:81:ASN:OD1	1:A:81:ASN:N	2.51	0.41
1:C:486:PHE:CA	2:W:104:TRP:CD2	2.97	0.41
1:A:338:PHE:O	1:A:342:PHE:HD1	2.03	0.41
1:A:365:TYR:HD2	1:A:388:ASN:HA	1.85	0.41
1:C:328:ARG:NH1	1:C:578:ASP:OD2	2.49	0.41
1:C:351:TYR:CE1	1:C:452:LEU:HB2	2.56	0.41
1:C:486:PHE:C	2:W:104:TRP:CE3	2.98	0.41
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.56	0.41
1:B:328:ARG:NH1	1:B:578:ASP:CG	2.78	0.41
1:C:786:LYS:HG3	1:C:787:GLN:HG3	2.03	0.41
3:V:93:TYR:CE1	3:V:96:SER:HA	2.56	0.41
2:W:33:TYR:CE2	2:W:103:ASN:HA	2.56	0.41
1:B:473:TYR:CE2	1:B:475:ALA:HB2	2.56	0.41
1:B:474:GLN:HE22	1:B:479:PRO:HA	1.86	0.41
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.56	0.41
1:C:473:TYR:CE2	1:C:475:ALA:HB2	2.55	0.41
1:B:312:ILE:O	1:B:312:ILE:HG23	2.21	0.41
1:C:411:ALA:O	1:C:414:GLN:HG2	2.21	0.41
2:U:33:TYR:CE2	2:U:103:ASN:HA	2.56	0.41
2:W:72:ARG:HG2	2:W:79:VAL:CG2	2.39	0.41
1:A:454:ARG:HA	1:A:491:PRO:O	2.21	0.41
1:A:486:PHE:CA	2:U:102:TYR:CE1	2.91	0.41
1:B:486:PHE:CD1	2:S:104:TRP:CE3	3.04	0.41
1:B:1039:ARG:HG2	1:C:1031:GLU:OE2	2.20	0.41
1:C:474:GLN:HE22	1:C:479:PRO:HA	1.86	0.41
1:A:473:TYR:CE2	1:A:475:ALA:HB2	2.56	0.41
1:B:338:PHE:O	1:B:342:PHE:HD1	2.03	0.41
1:C:312:ILE:O	1:C:312:ILE:HG23	2.21	0.41
1:A:310:LYS:HB2	1:A:601:GLY:H	1.86	0.40
1:A:455:LEU:HG	1:A:456:PHE:CE2	2.56	0.40
1:B:328:ARG:HH12	1:B:578:ASP:HB2	1.86	0.40
1:B:786:LYS:HG3	1:B:787:GLN:HG3	2.03	0.40
1:C:454:ARG:HA	1:C:491:PRO:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:93:TYR:CE1	3:T:96:SER:HA	2.56	0.40
3:X:93:TYR:CE1	3:X:96:SER:HA	2.56	0.40
1:C:455:LEU:HG	1:C:456:PHE:CE2	2.56	0.40
1:C:455:LEU:HD12	1:C:455:LEU:HA	1.89	0.40
1:B:454:ARG:HA	1:B:491:PRO:O	2.21	0.40
1:C:310:LYS:HB2	1:C:601:GLY:H	1.86	0.40
1:C:338:PHE:O	1:C:342:PHE:HD1	2.03	0.40
1:C:377:PHE:CD1	1:C:434:ILE:HG12	2.57	0.40
2:U:72:ARG:NE	2:U:79:VAL:HG22	2.36	0.40
1:A:337:PRO:O	1:A:340:GLU:HG3	2.22	0.40
1:A:1107:ARG:NE	1:B:904:TYR:OH	2.53	0.40
1:C:486:PHE:CD1	2:W:104:TRP:CE3	3.06	0.40
2:W:72:ARG:NE	2:W:79:VAL:HG22	2.36	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	986/1256 (78%)	938 (95%)	47 (5%)	1 (0%)	48	79
1	B	986/1256 (78%)	936 (95%)	49 (5%)	1 (0%)	48	79
1	C	986/1256 (78%)	937 (95%)	48 (5%)	1 (0%)	48	79
2	S	118/234 (50%)	113 (96%)	5 (4%)	0	100	100
2	U	118/234 (50%)	113 (96%)	5 (4%)	0	100	100
2	W	118/234 (50%)	113 (96%)	5 (4%)	0	100	100
3	T	106/216 (49%)	101 (95%)	5 (5%)	0	100	100
3	V	106/216 (49%)	101 (95%)	5 (5%)	0	100	100
3	X	106/216 (49%)	101 (95%)	5 (5%)	0	100	100
All	All	3630/5118 (71%)	3453 (95%)	174 (5%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1032	CYS
1	B	1032	CYS
1	C	1032	CYS

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	876/1091 (80%)	866 (99%)	10 (1%)	65	74
1	B	876/1091 (80%)	867 (99%)	9 (1%)	68	75
1	C	876/1091 (80%)	868 (99%)	8 (1%)	70	76
2	S	98/198 (50%)	97 (99%)	1 (1%)	68	75
2	U	98/198 (50%)	97 (99%)	1 (1%)	68	75
2	W	98/198 (50%)	97 (99%)	1 (1%)	68	75
3	T	91/184 (50%)	90 (99%)	1 (1%)	65	74
3	V	91/184 (50%)	90 (99%)	1 (1%)	65	74
3	X	91/184 (50%)	90 (99%)	1 (1%)	65	74
All	All	3195/4419 (72%)	3162 (99%)	33 (1%)	65	75

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

Mol	Chain	Res	Type
1	A	362	VAL
1	A	524	VAL
1	A	528	LYS
1	A	603	ASN
1	A	760	CYS
1	A	948	LEU
1	A	1030	SER
1	A	1038	LYS
1	A	1104	VAL
1	A	1106	GLN

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Mol	Chain	Res	Type
1	B	362	VAL
1	B	417	LYS
1	B	524	VAL
1	B	603	ASN
1	B	760	CYS
1	B	948	LEU
1	B	1030	SER
1	B	1038	LYS
1	B	1106	GLN
1	C	336	CYS
1	C	362	VAL
1	C	603	ASN
1	C	760	CYS
1	C	784	GLN
1	C	948	LEU
1	C	1030	SER
1	C	1038	LYS
2	S	54	ILE
3	T	92	SER
2	U	54	ILE
3	V	92	SER
2	W	54	ILE
3	X	92	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	A	388	ASN
1	A	474	GLN
1	A	690	GLN
1	A	764	ASN
1	A	907	ASN
1	A	1054	GLN
1	A	1106	GLN
1	B	317	ASN
1	B	370	ASN
1	B	388	ASN
1	B	474	GLN
1	B	675	GLN
1	B	690	GLN
1	B	764	ASN

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Mol	Chain	Res	Type
1	B	787	GLN
1	B	907	ASN
1	B	1054	GLN
1	B	1106	GLN
1	C	370	ASN
1	C	388	ASN
1	C	474	GLN
1	C	675	GLN
1	C	690	GLN
1	C	764	ASN
1	C	856	ASN
1	C	907	ASN
1	C	1054	GLN
2	S	3	GLN
2	S	35	HIS
2	S	52	ASN
2	S	65	GLN
3	T	33	ASN
3	T	41	HIS
2	U	3	GLN
2	U	35	HIS
2	U	52	ASN
2	U	65	GLN
3	V	33	ASN
3	V	41	HIS
2	W	3	GLN
2	W	35	HIS
2	W	52	ASN
2	W	65	GLN
3	X	33	ASN
3	X	41	HIS

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	$\# Z > 2$
4	NAG	E	1	4,1	14,14,15	0.80	0	17,19,21	1.53	4 (23%)
4	NAG	E	2	4	14,14,15	0.85	1 (7%)	17,19,21	1.82	4 (23%)
4	NAG	F	1	4,1	14,14,15	0.79	0	17,19,21	1.68	4 (23%)
4	NAG	F	2	4	14,14,15	0.86	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	G	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	1.32	1 (5%)
4	NAG	G	2	4	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
4	NAG	H	1	4,1	14,14,15	0.82	0	17,19,21	1.63	3 (17%)
4	NAG	H	2	4	14,14,15	0.87	1 (7%)	17,19,21	1.26	2 (11%)
4	NAG	J	1	4,1	14,14,15	0.82	0	17,19,21	1.43	4 (23%)
4	NAG	J	2	4	14,14,15	0.81	0	17,19,21	1.87	4 (23%)
4	NAG	K	1	4,1	14,14,15	0.81	0	17,19,21	1.75	4 (23%)
4	NAG	K	2	4	14,14,15	0.87	1 (7%)	17,19,21	1.02	1 (5%)
4	NAG	L	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	1.34	1 (5%)
4	NAG	L	2	4	14,14,15	0.71	0	17,19,21	1.08	1 (5%)
4	NAG	M	1	4,1	14,14,15	0.71	0	17,19,21	1.53	4 (23%)
4	NAG	M	2	4	14,14,15	0.86	1 (7%)	17,19,21	1.29	1 (5%)
4	NAG	O	1	4,1	14,14,15	0.74	0	17,19,21	1.52	4 (23%)
4	NAG	O	2	4	14,14,15	0.80	0	17,19,21	1.80	4 (23%)
4	NAG	P	1	4,1	14,14,15	0.84	0	17,19,21	1.81	4 (23%)
4	NAG	P	2	4	14,14,15	0.84	1 (7%)	17,19,21	1.03	1 (5%)
4	NAG	Q	1	4,1	14,14,15	0.78	0	17,19,21	1.32	1 (5%)
4	NAG	Q	2	4	14,14,15	0.67	0	17,19,21	1.12	1 (5%)
4	NAG	R	1	4,1	14,14,15	0.72	0	17,19,21	1.58	4 (23%)
4	NAG	R	2	4	14,14,15	0.87	1 (7%)	17,19,21	1.27	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2	NAG	C1-C2	2.22	1.55	1.52
4	E	2	NAG	C1-C2	2.13	1.55	1.52
4	G	1	NAG	C1-C2	2.12	1.55	1.52
4	M	2	NAG	C1-C2	2.10	1.55	1.52
4	L	1	NAG	C1-C2	2.10	1.55	1.52
4	F	2	NAG	C1-C2	2.08	1.55	1.52
4	H	2	NAG	C1-C2	2.08	1.55	1.52
4	R	2	NAG	C1-C2	2.05	1.55	1.52
4	P	2	NAG	C1-C2	2.04	1.55	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C1-O5-C5	5.69	119.81	112.19
4	K	1	NAG	C1-O5-C5	5.37	119.38	112.19
4	E	2	NAG	C1-O5-C5	5.32	119.32	112.19
4	O	2	NAG	C1-O5-C5	5.23	119.20	112.19
4	P	1	NAG	C1-O5-C5	5.22	119.18	112.19
4	F	1	NAG	C1-O5-C5	4.83	118.65	112.19
4	M	2	NAG	C1-O5-C5	4.10	117.68	112.19
4	G	2	NAG	C1-O5-C5	3.93	117.46	112.19
4	R	2	NAG	C1-O5-C5	3.88	117.39	112.19
4	H	2	NAG	C1-O5-C5	3.85	117.35	112.19
4	Q	2	NAG	C1-O5-C5	3.74	117.20	112.19
4	L	1	NAG	C1-O5-C5	3.72	117.17	112.19
4	R	1	NAG	C1-C2-N2	3.57	116.06	110.43
4	G	1	NAG	C1-O5-C5	3.57	116.97	112.19
4	H	1	NAG	C1-C2-N2	3.56	116.05	110.43
4	O	2	NAG	O5-C1-C2	-3.53	105.83	111.29
4	L	2	NAG	C1-O5-C5	3.48	116.86	112.19
4	P	1	NAG	O5-C1-C2	-3.46	105.94	111.29
4	E	2	NAG	O5-C1-C2	-3.46	105.94	111.29
4	O	1	NAG	C4-C3-C2	3.41	116.02	111.02
4	Q	1	NAG	C1-O5-C5	3.40	116.75	112.19
4	J	2	NAG	O5-C1-C2	-3.33	106.14	111.29
4	F	1	NAG	O5-C1-C2	-3.30	106.19	111.29
4	M	1	NAG	C1-C2-N2	3.29	115.62	110.43
4	K	1	NAG	O5-C1-C2	-3.28	106.21	111.29
4	F	2	NAG	C1-O5-C5	3.24	116.53	112.19
4	K	2	NAG	C1-O5-C5	3.23	116.51	112.19
4	P	2	NAG	C1-O5-C5	3.17	116.43	112.19
4	E	1	NAG	C4-C3-C2	3.15	115.63	111.02
4	J	1	NAG	C4-C3-C2	3.09	115.55	111.02
4	H	1	NAG	O5-C1-C2	-3.06	106.56	111.29
4	R	1	NAG	O5-C1-C2	-2.98	106.68	111.29
4	H	1	NAG	C1-O5-C5	2.96	116.15	112.19
4	M	1	NAG	C1-O5-C5	2.86	116.02	112.19
4	M	1	NAG	O5-C1-C2	-2.81	106.94	111.29
4	E	1	NAG	O5-C1-C2	2.78	115.59	111.29
4	R	1	NAG	C1-O5-C5	2.68	115.78	112.19
4	E	1	NAG	O5-C5-C6	-2.67	102.46	107.66
4	O	1	NAG	O5-C1-C2	2.63	115.36	111.29
4	P	1	NAG	C1-C2-N2	2.59	114.52	110.43
4	P	1	NAG	O3-C3-C2	2.45	114.49	109.40
4	F	1	NAG	C1-C2-N2	2.44	114.28	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	O5-C1-C2	2.44	115.06	111.29
4	O	2	NAG	C1-C2-N2	2.38	114.18	110.43
4	E	2	NAG	C1-C2-N2	2.37	114.17	110.43
4	O	1	NAG	O5-C5-C6	-2.32	103.15	107.66
4	J	1	NAG	O5-C5-C6	-2.31	103.17	107.66
4	K	1	NAG	O3-C3-C2	2.30	114.17	109.40
4	J	2	NAG	C3-C4-C5	2.28	114.37	110.23
4	J	2	NAG	C1-C2-N2	2.27	114.01	110.43
4	E	2	NAG	C3-C4-C5	2.25	114.31	110.23
4	F	1	NAG	O3-C3-C2	2.19	113.95	109.40
4	M	1	NAG	C4-C3-C2	-2.12	107.91	111.02
4	O	2	NAG	C3-C4-C5	2.11	114.06	110.23
4	R	1	NAG	C4-C3-C2	-2.10	107.95	111.02
4	K	1	NAG	C1-C2-N2	2.09	113.72	110.43
4	E	1	NAG	O5-C5-C4	2.07	115.87	110.83
4	J	1	NAG	O5-C5-C4	2.02	115.73	110.83
4	H	2	NAG	C2-N2-C7	2.01	125.60	122.90
4	O	1	NAG	O5-C5-C4	2.01	115.72	110.83

There are no chirality outliers.

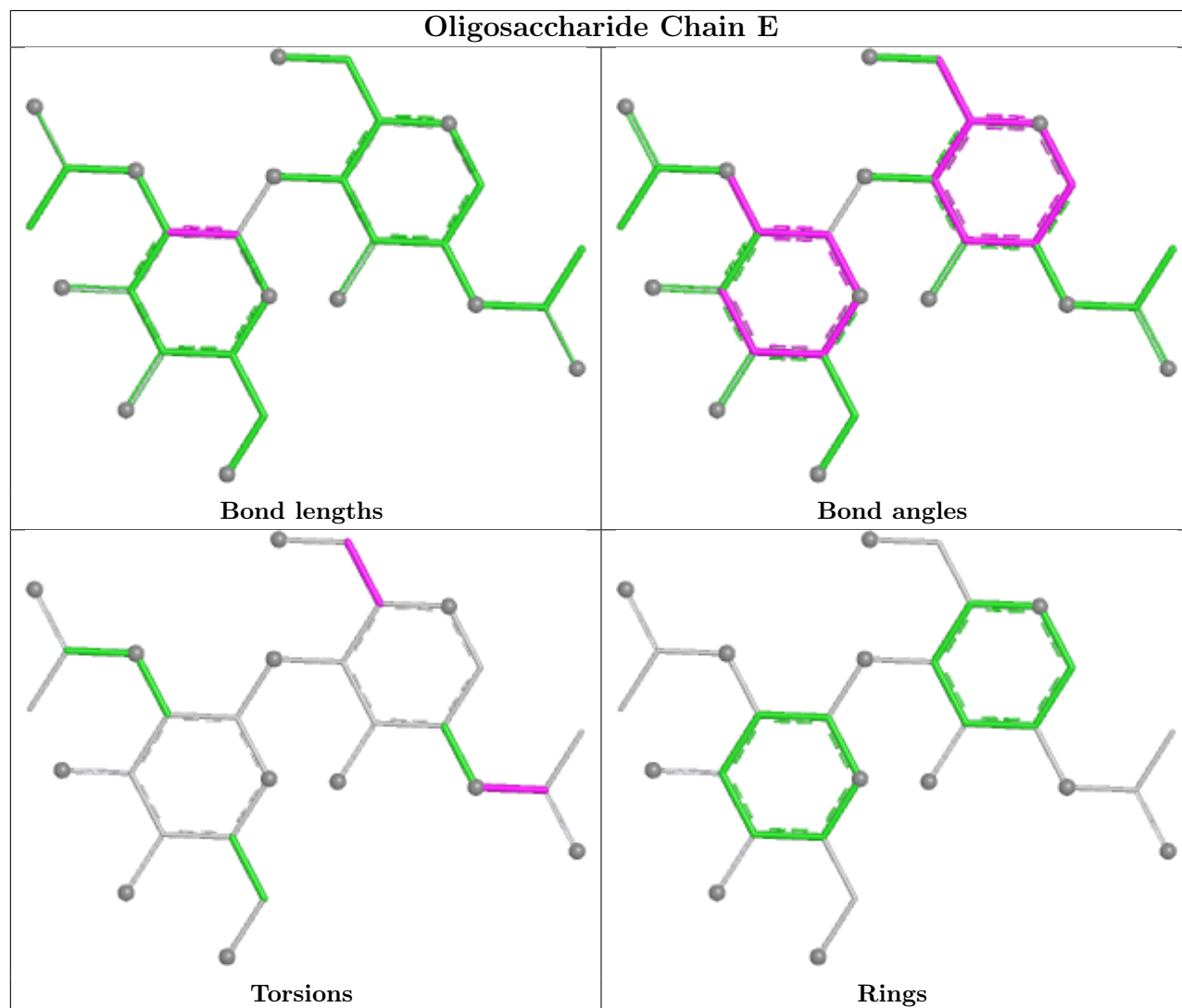
All (19) torsion outliers are listed below:

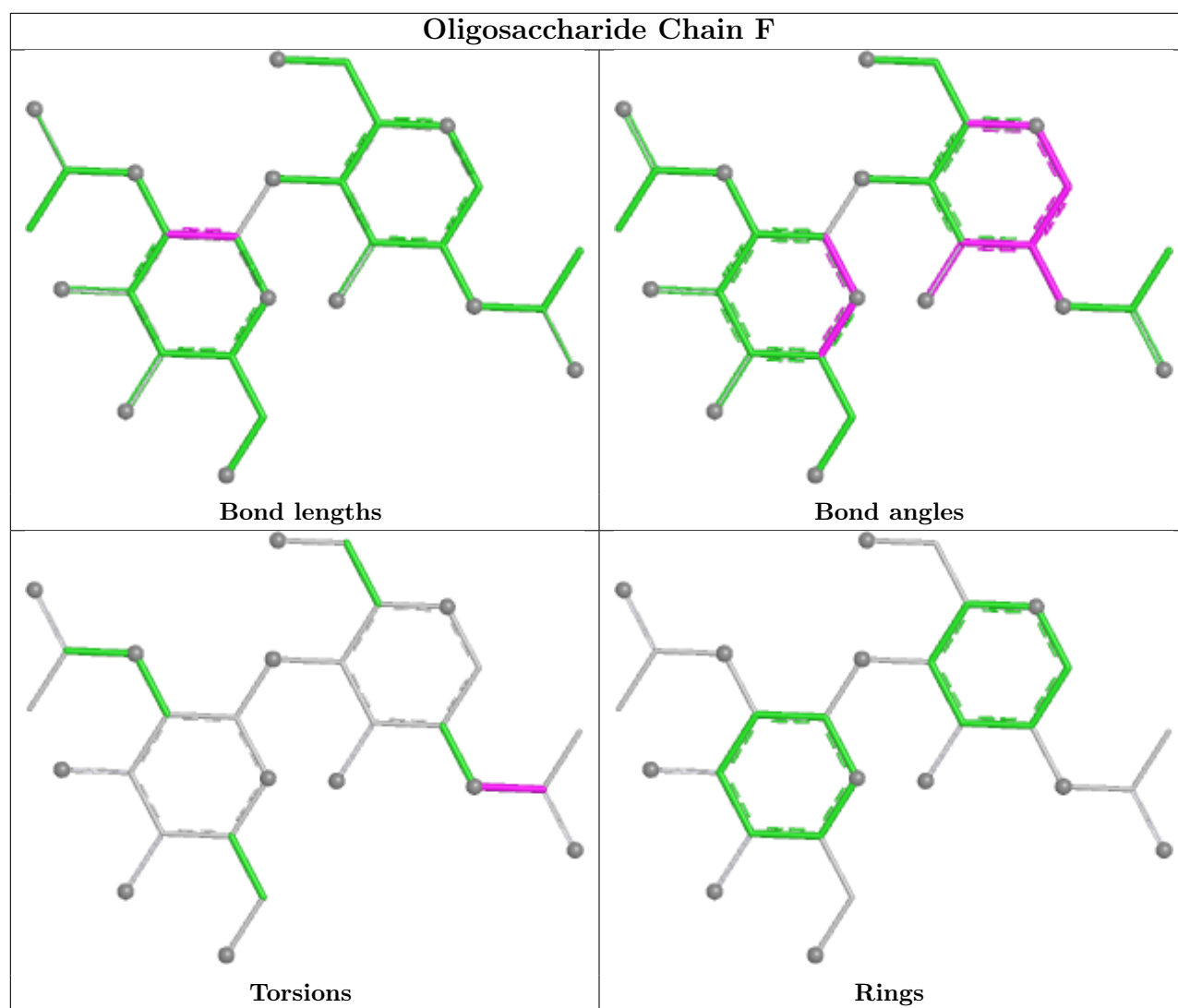
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	L	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	F	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

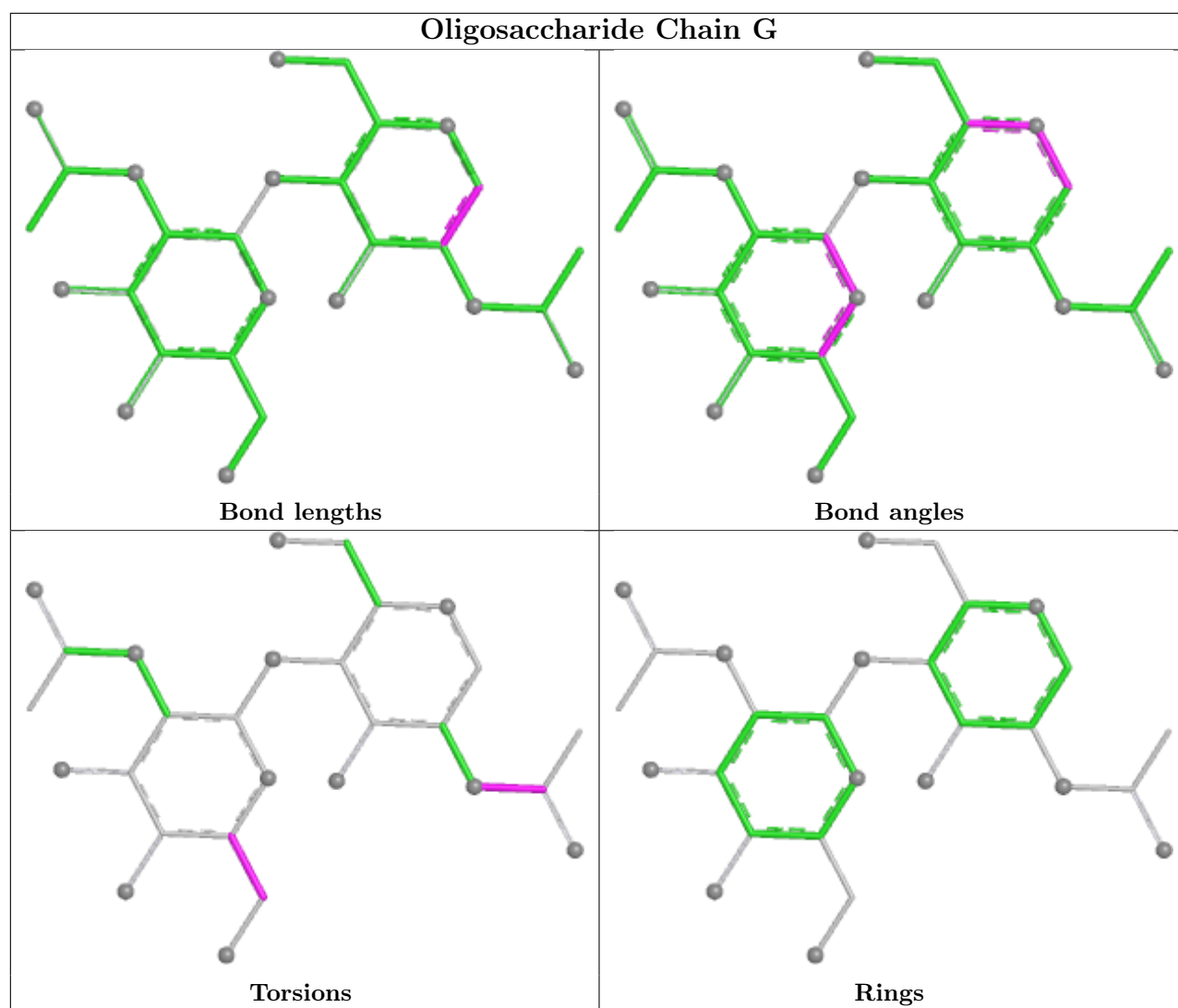
There are no ring outliers.

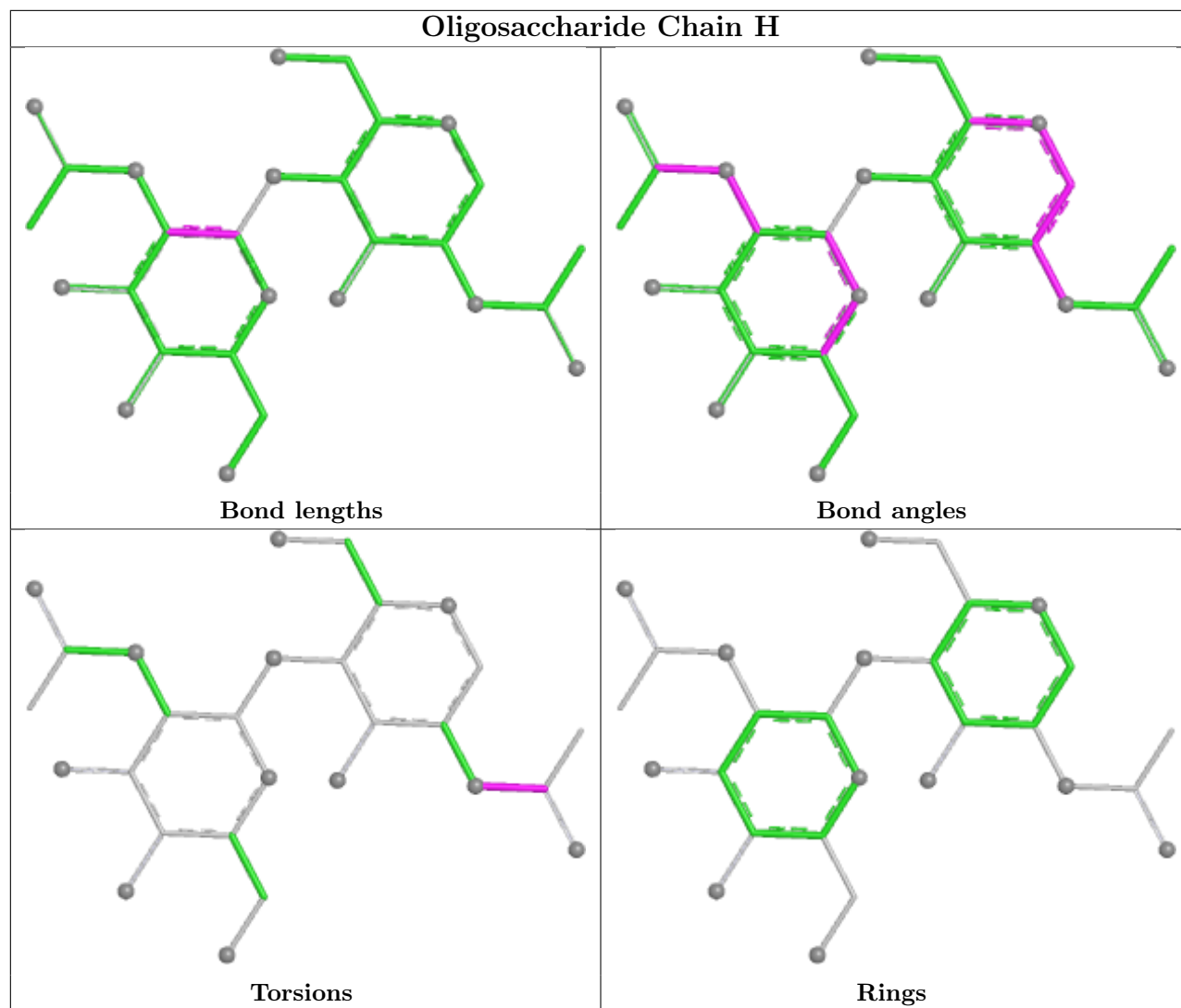
No monomer is involved in short contacts.

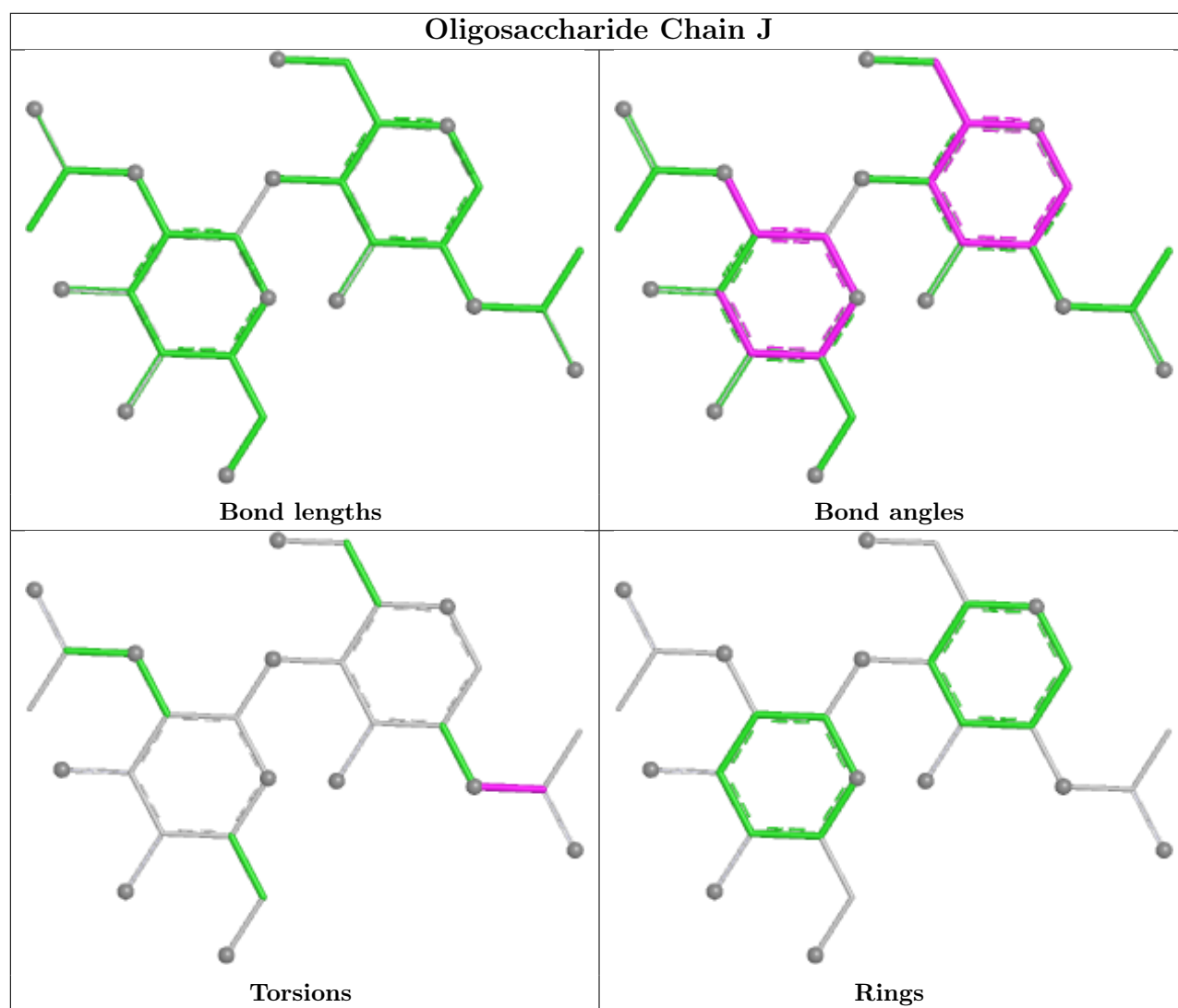
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

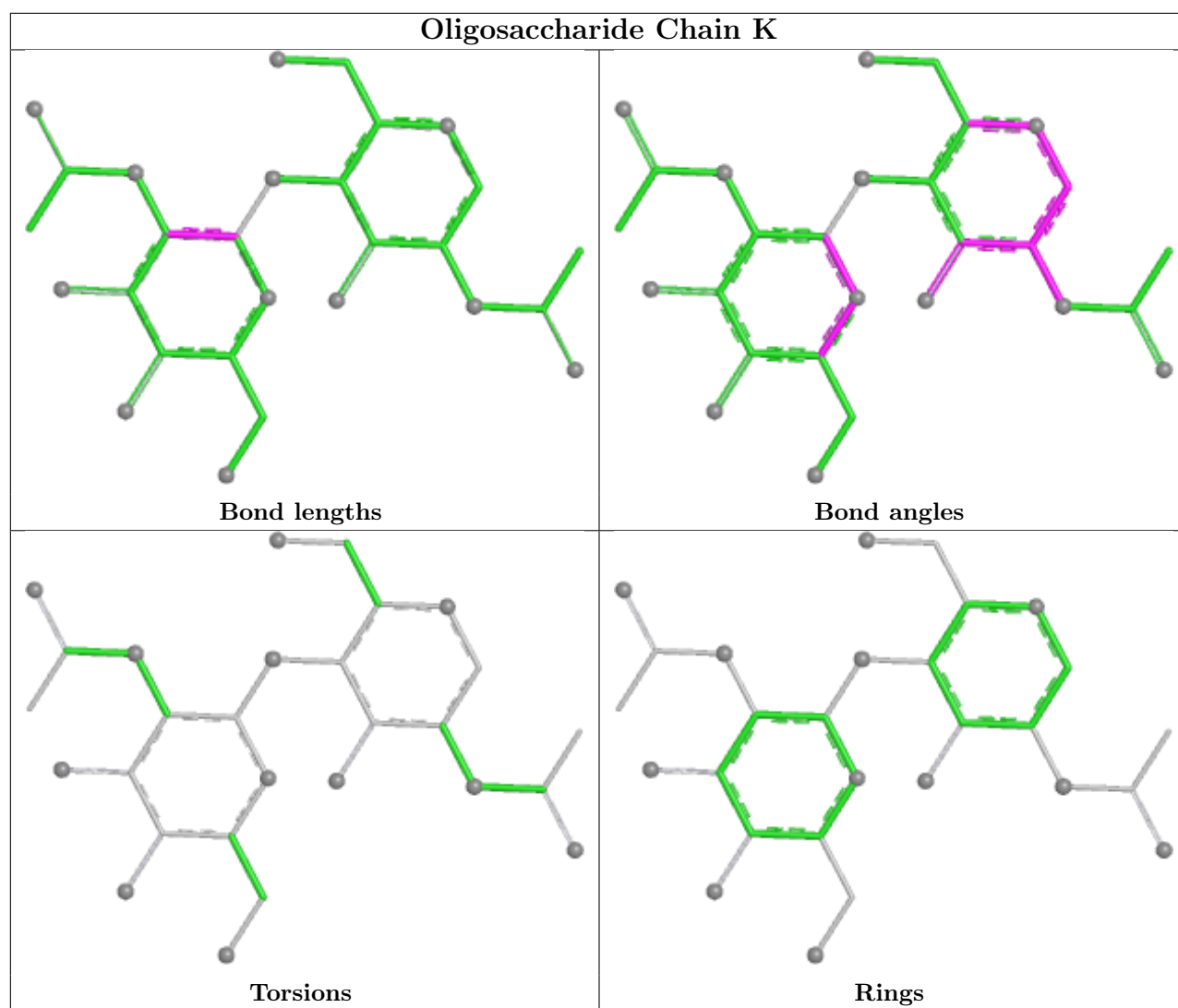


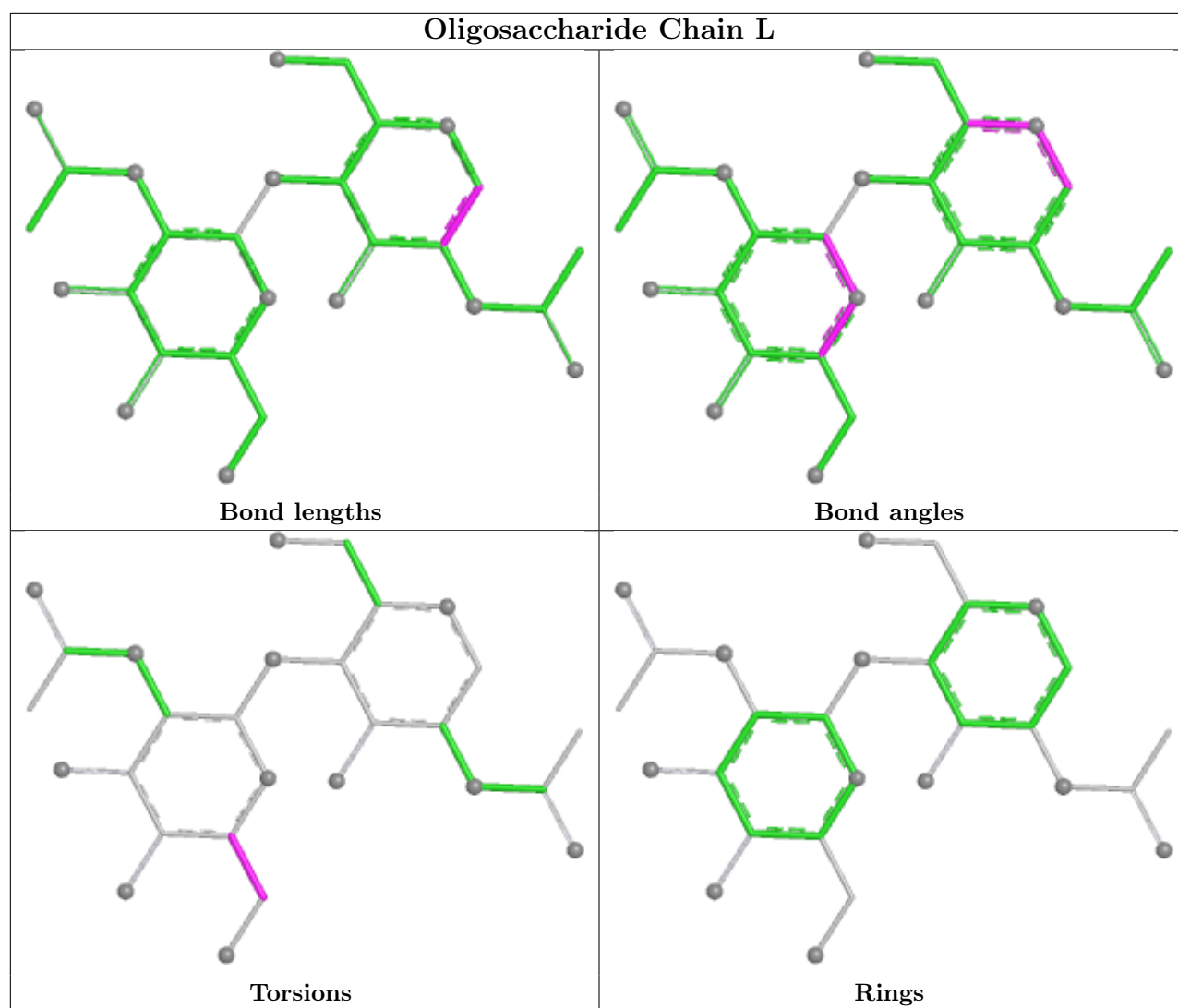


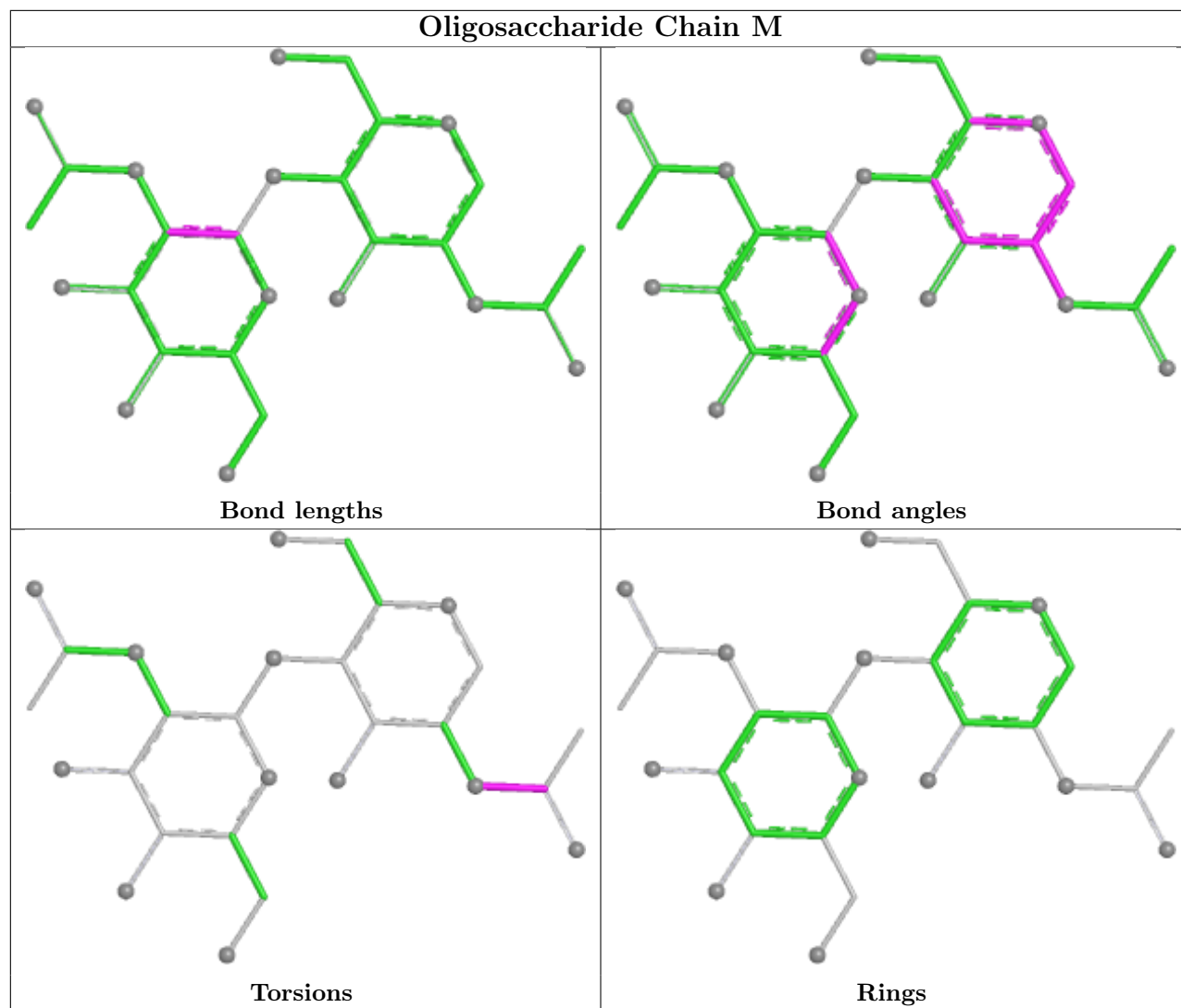


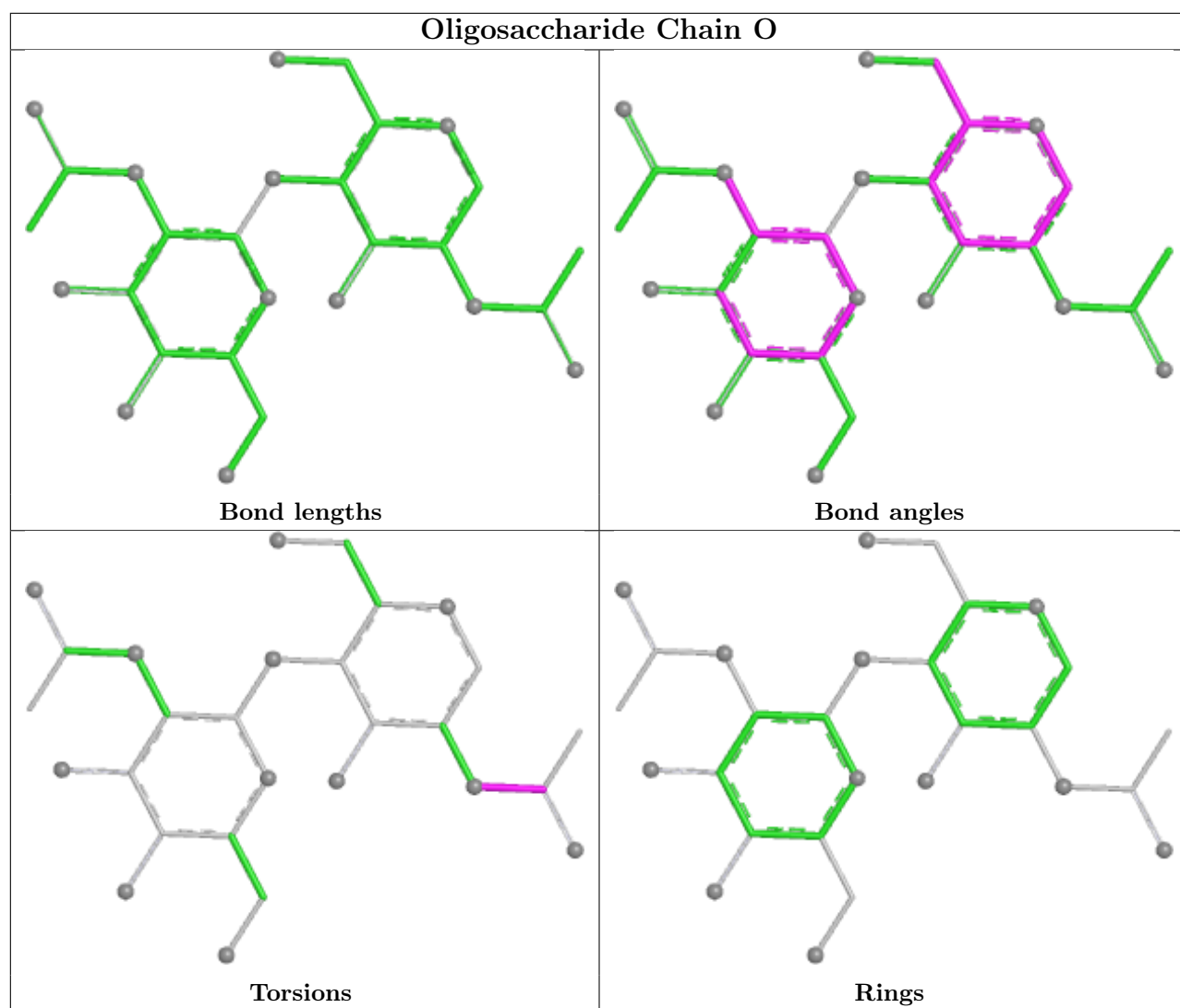


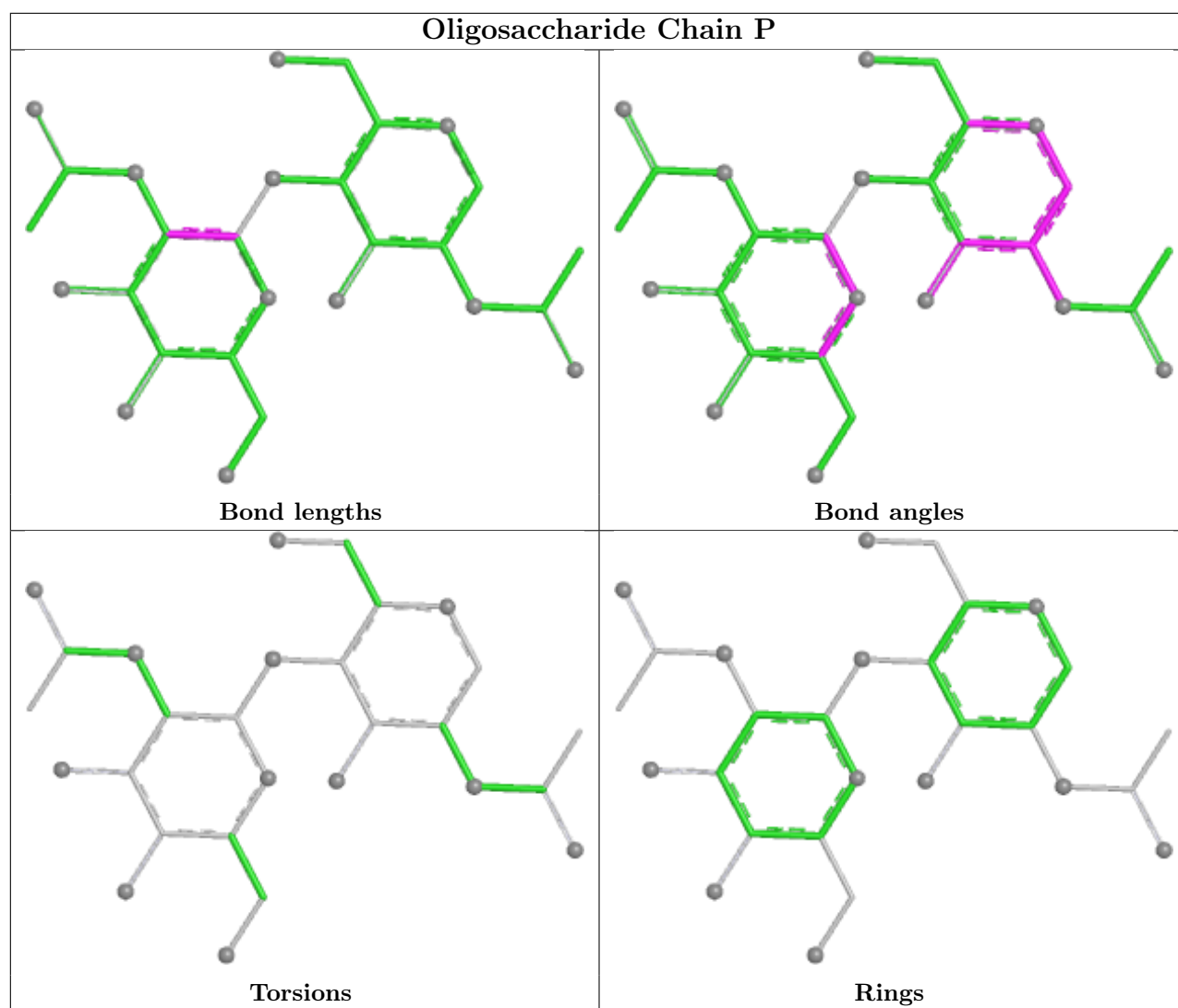


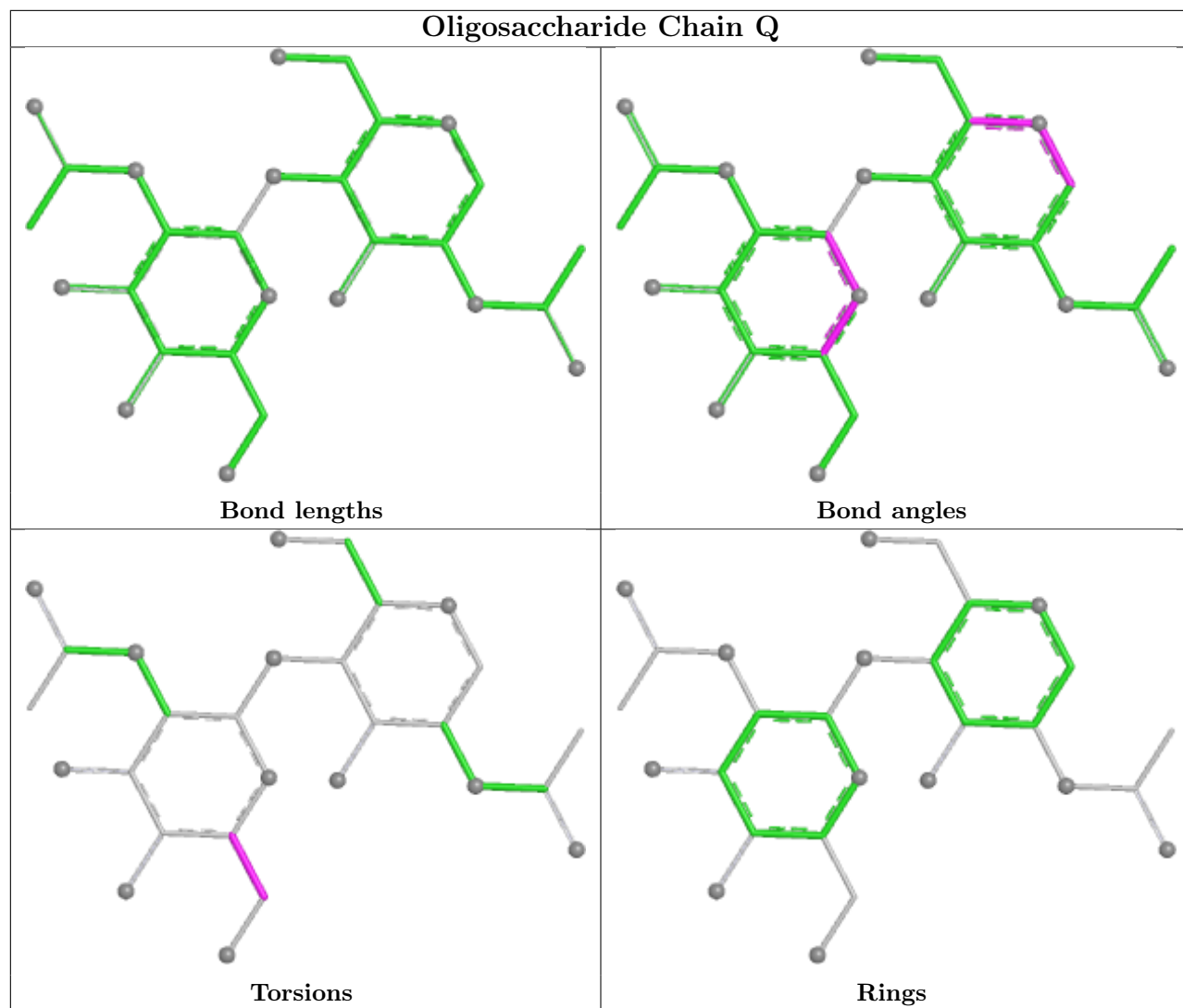


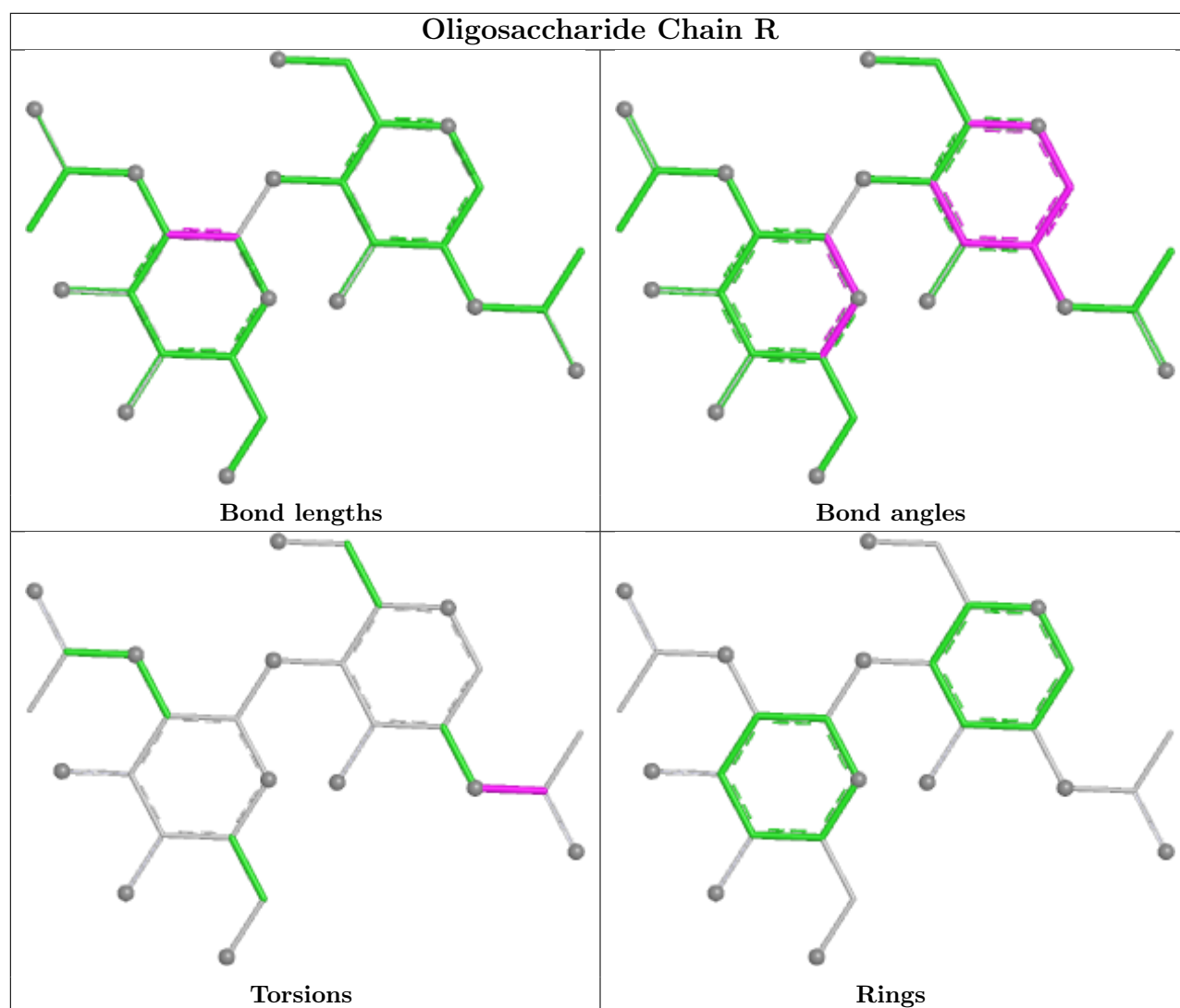












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	NAG	A	1301	1	14,14,15	0.77	0	17,19,21	0.94	1 (5%)
5	NAG	A	1303	1	14,14,15	0.85	1 (7%)	17,19,21	1.23	1 (5%)
5	NAG	A	1306	1	14,14,15	0.90	1 (7%)	17,19,21	1.12	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1305	-	14,14,15	1.46	4 (28%)	17,19,21	2.05	7 (41%)
5	NAG	B	1305	-	14,14,15	1.27	0	17,19,21	1.92	4 (23%)
5	NAG	A	1304	1	14,14,15	1.04	1 (7%)	17,19,21	2.48	3 (17%)
5	NAG	C	1301	1	14,14,15	0.78	0	17,19,21	1.03	1 (5%)
5	NAG	B	1307	1	14,14,15	0.81	1 (7%)	17,19,21	0.99	1 (5%)
5	NAG	C	1306	1	14,14,15	0.90	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	A	1308	1	14,14,15	0.76	0	17,19,21	0.90	0
5	NAG	C	1304	1	14,14,15	1.03	1 (7%)	17,19,21	2.44	4 (23%)
5	NAG	B	1309	1	14,14,15	0.72	0	17,19,21	1.32	3 (17%)
5	NAG	A	1302	1	14,14,15	1.20	1 (7%)	17,19,21	2.03	2 (11%)
5	NAG	B	1304	1	14,14,15	1.04	1 (7%)	17,19,21	2.37	4 (23%)
5	NAG	C	1303	1	14,14,15	0.86	1 (7%)	17,19,21	1.37	2 (11%)
5	NAG	C	1308	1	14,14,15	0.83	1 (7%)	17,19,21	0.89	0
5	NAG	A	1309	1	14,14,15	0.71	0	17,19,21	1.31	2 (11%)
5	NAG	A	1310	1	14,14,15	0.92	1 (7%)	17,19,21	1.73	2 (11%)
5	NAG	B	1306	1	14,14,15	0.91	1 (7%)	17,19,21	1.28	1 (5%)
5	NAG	B	1303	1	14,14,15	0.87	1 (7%)	17,19,21	1.42	2 (11%)
5	NAG	C	1302	1	14,14,15	1.19	1 (7%)	17,19,21	2.07	2 (11%)
5	NAG	C	1305	-	14,14,15	1.16	0	17,19,21	1.90	5 (29%)
5	NAG	B	1308	1	14,14,15	0.77	0	17,19,21	0.93	0
5	NAG	C	1307	1	14,14,15	0.80	1 (7%)	17,19,21	0.97	0
5	NAG	C	1309	1	14,14,15	0.72	0	17,19,21	1.31	1 (5%)
5	NAG	C	1310	1	14,14,15	0.98	1 (7%)	17,19,21	1.86	2 (11%)
5	NAG	B	1310	1	14,14,15	0.93	1 (7%)	17,19,21	1.74	2 (11%)
5	NAG	A	1307	1	14,14,15	0.84	1 (7%)	17,19,21	1.02	2 (11%)
5	NAG	B	1301	1	14,14,15	0.78	0	17,19,21	1.05	1 (5%)
5	NAG	B	1302	1	14,14,15	1.21	2 (14%)	17,19,21	2.07	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	3/6/23/26	0/1/1/1

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1302	NAG	C1-C2	2.51	1.55	1.52
5	B	1302	NAG	C1-C2	2.50	1.55	1.52
5	A	1302	NAG	C1-C2	2.47	1.55	1.52
5	C	1310	NAG	C1-C2	2.37	1.55	1.52
5	C	1304	NAG	C1-C2	2.26	1.55	1.52
5	B	1304	NAG	C1-C2	2.26	1.55	1.52
5	A	1304	NAG	C1-C2	2.26	1.55	1.52
5	A	1305	NAG	C3-C2	2.23	1.57	1.52
5	A	1310	NAG	C1-C2	2.17	1.55	1.52
5	B	1310	NAG	C1-C2	2.16	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1306	NAG	C1-C2	2.10	1.55	1.52
5	A	1306	NAG	C1-C2	2.06	1.55	1.52
5	A	1307	NAG	C1-C2	2.05	1.55	1.52
5	B	1307	NAG	C1-C2	2.04	1.55	1.52
5	A	1303	NAG	C1-C2	2.04	1.55	1.52
5	B	1303	NAG	C1-C2	2.04	1.55	1.52
5	C	1306	NAG	C1-C2	2.03	1.55	1.52
5	C	1303	NAG	C1-C2	2.03	1.55	1.52
5	A	1305	NAG	O4-C4	2.03	1.48	1.43
5	C	1308	NAG	C1-C2	2.03	1.55	1.52
5	A	1305	NAG	C1-C2	2.02	1.55	1.52
5	B	1302	NAG	C2-N2	2.01	1.49	1.46
5	A	1305	NAG	C4-C5	2.01	1.57	1.53
5	C	1307	NAG	C1-C2	2.01	1.55	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1304	NAG	C1-O5-C5	9.13	124.42	112.19
5	C	1304	NAG	C1-O5-C5	8.91	124.13	112.19
5	B	1304	NAG	C1-O5-C5	8.65	123.78	112.19
5	B	1302	NAG	C2-N2-C7	6.60	131.74	122.90
5	C	1302	NAG	C2-N2-C7	6.54	131.66	122.90
5	A	1302	NAG	C2-N2-C7	6.23	131.25	122.90
5	C	1310	NAG	C1-O5-C5	6.18	120.47	112.19
5	B	1310	NAG	C1-O5-C5	5.94	120.15	112.19
5	A	1310	NAG	C1-O5-C5	5.84	120.02	112.19
5	C	1305	NAG	C1-O5-C5	5.18	119.13	112.19
5	A	1305	NAG	C1-O5-C5	5.17	119.11	112.19
5	B	1305	NAG	C1-O5-C5	5.10	119.02	112.19
5	A	1302	NAG	C1-O5-C5	4.37	118.05	112.19
5	C	1303	NAG	C1-O5-C5	4.27	117.91	112.19
5	B	1306	NAG	C1-O5-C5	4.22	117.84	112.19
5	B	1303	NAG	C1-O5-C5	4.21	117.83	112.19
5	B	1302	NAG	C1-O5-C5	4.07	117.64	112.19
5	C	1302	NAG	C1-O5-C5	3.99	117.53	112.19
5	B	1309	NAG	C1-O5-C5	3.76	117.22	112.19
5	A	1309	NAG	C1-O5-C5	3.71	117.16	112.19
5	C	1309	NAG	C1-O5-C5	3.61	117.02	112.19
5	A	1303	NAG	C1-O5-C5	3.61	117.02	112.19
5	C	1310	NAG	C2-N2-C7	3.05	126.99	122.90
5	A	1306	NAG	C1-O5-C5	2.99	116.19	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1305	NAG	O7-C7-C8	-2.75	117.16	122.05
5	A	1310	NAG	C2-N2-C7	2.74	126.57	122.90
5	C	1305	NAG	C1-C2-N2	2.74	114.75	110.43
5	C	1301	NAG	C2-N2-C7	2.71	126.53	122.90
5	B	1310	NAG	C2-N2-C7	2.70	126.52	122.90
5	B	1301	NAG	C2-N2-C7	2.68	126.49	122.90
5	B	1305	NAG	C1-C2-N2	2.67	114.64	110.43
5	B	1305	NAG	O7-C7-C8	-2.64	117.36	122.05
5	C	1306	NAG	C1-O5-C5	2.57	115.62	112.19
5	A	1305	NAG	C1-C2-N2	2.55	114.44	110.43
5	A	1305	NAG	O7-C7-C8	-2.54	117.53	122.05
5	B	1305	NAG	C3-C4-C5	2.44	114.66	110.23
5	A	1305	NAG	C3-C4-C5	2.41	114.61	110.23
5	B	1307	NAG	C1-O5-C5	2.35	115.33	112.19
5	A	1307	NAG	C1-O5-C5	2.26	115.21	112.19
5	A	1305	NAG	C4-C3-C2	2.25	114.32	111.02
5	A	1301	NAG	C2-N2-C7	2.23	125.88	122.90
5	B	1304	NAG	C3-C4-C5	2.18	114.18	110.23
5	A	1304	NAG	O5-C5-C4	2.15	116.05	110.83
5	C	1304	NAG	O5-C5-C4	2.14	116.03	110.83
5	A	1304	NAG	C3-C4-C5	2.13	114.09	110.23
5	B	1304	NAG	O5-C5-C4	2.12	115.99	110.83
5	C	1304	NAG	C3-C4-C5	2.11	114.06	110.23
5	B	1309	NAG	O5-C1-C2	-2.10	108.03	111.29
5	C	1305	NAG	O7-C7-N2	2.10	125.70	121.98
5	A	1305	NAG	O7-C7-N2	2.06	125.63	121.98
5	A	1309	NAG	C3-C4-C5	2.06	113.96	110.23
5	B	1304	NAG	C2-N2-C7	2.05	125.65	122.90
5	B	1303	NAG	C1-C2-N2	2.04	113.64	110.43
5	A	1307	NAG	C2-N2-C7	2.03	125.62	122.90
5	C	1305	NAG	C3-C4-C5	2.03	113.91	110.23
5	B	1309	NAG	C3-C4-C5	2.03	113.90	110.23
5	C	1303	NAG	C1-C2-N2	2.02	113.61	110.43
5	A	1305	NAG	O4-C4-C5	2.02	114.29	109.32
5	C	1304	NAG	C2-N2-C7	2.01	125.60	122.90

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1302	NAG	C3-C2-N2-C7
5	B	1302	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	C	1302	NAG	C3-C2-N2-C7
5	A	1310	NAG	O5-C5-C6-O6
5	C	1310	NAG	O5-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	A	1302	NAG	C8-C7-N2-C2
5	B	1305	NAG	C4-C5-C6-O6
5	A	1302	NAG	O7-C7-N2-C2
5	C	1305	NAG	C4-C5-C6-O6
5	C	1303	NAG	C8-C7-N2-C2
5	A	1306	NAG	C1-C2-N2-C7
5	A	1308	NAG	C1-C2-N2-C7
5	B	1308	NAG	C1-C2-N2-C7
5	C	1306	NAG	C1-C2-N2-C7
5	C	1308	NAG	C1-C2-N2-C7
5	C	1303	NAG	O7-C7-N2-C2
5	B	1306	NAG	O5-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	B	1303	NAG	O7-C7-N2-C2
5	A	1303	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1305	NAG	4	0
5	B	1305	NAG	3	0
5	C	1305	NAG	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

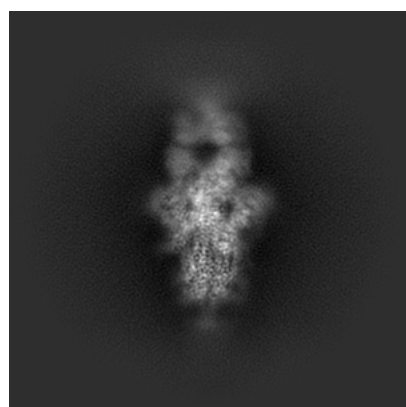
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28228. These allow visual inspection of the internal detail of the map and identification of artifacts.

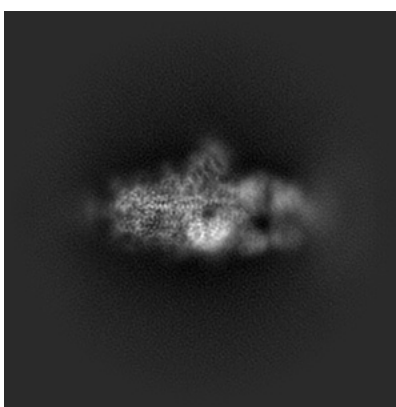
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

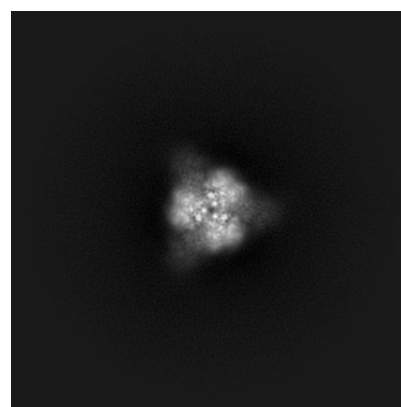
6.1.1 Primary map



X



Y

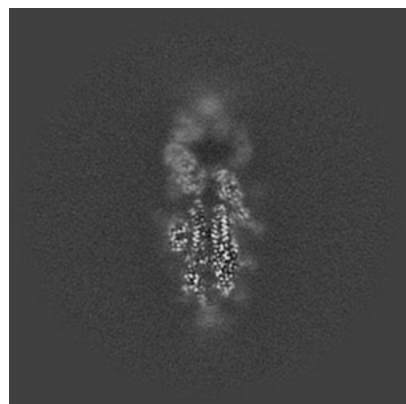


Z

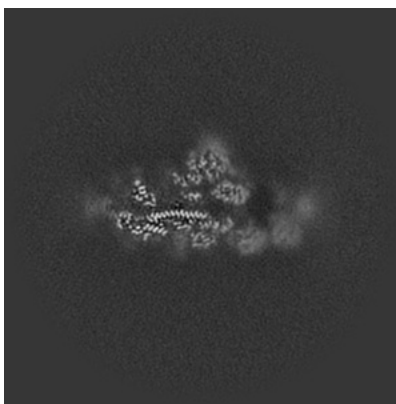
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

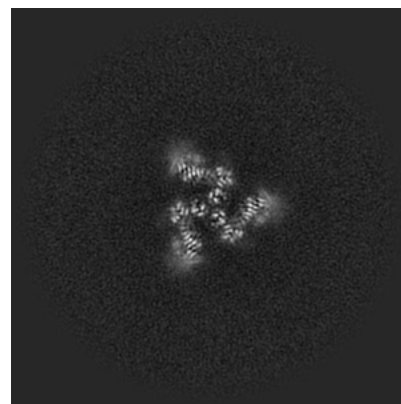
6.2.1 Primary map



X Index: 270



Y Index: 270

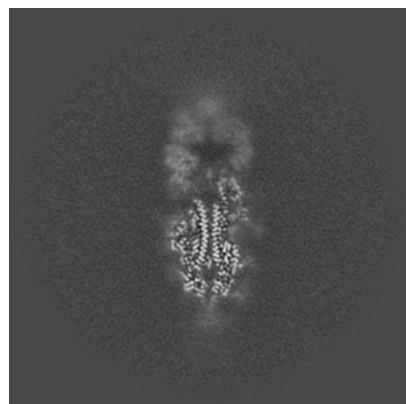


Z Index: 270

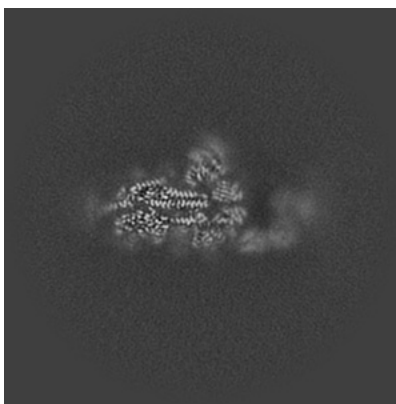
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

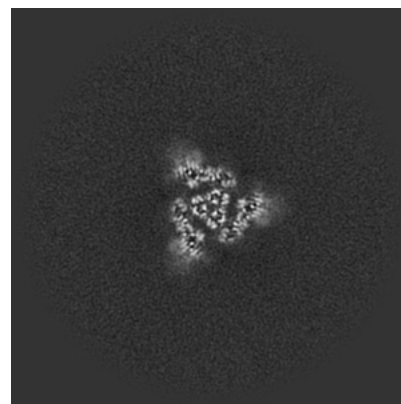
6.3.1 Primary map



X Index: 275



Y Index: 261

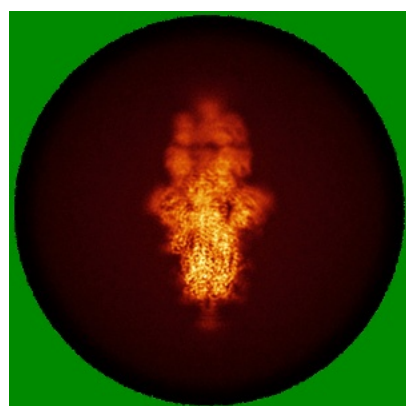


Z Index: 265

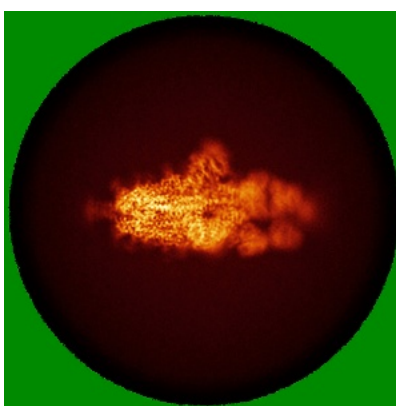
The images above show the largest variance slices of the map in three orthogonal directions.

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

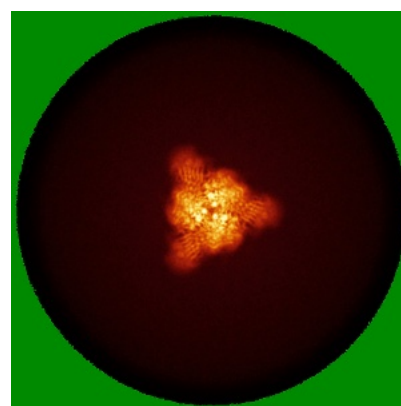
6.4.1 Primary map



X



Y

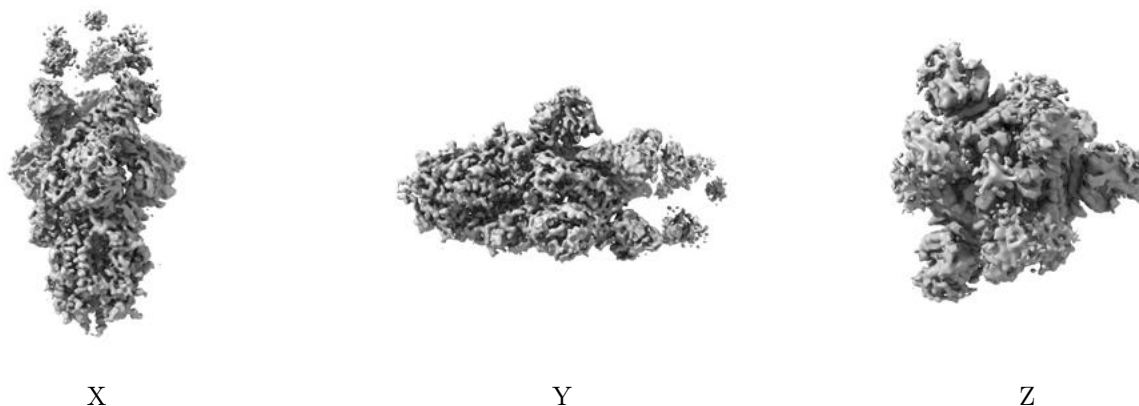


Z

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

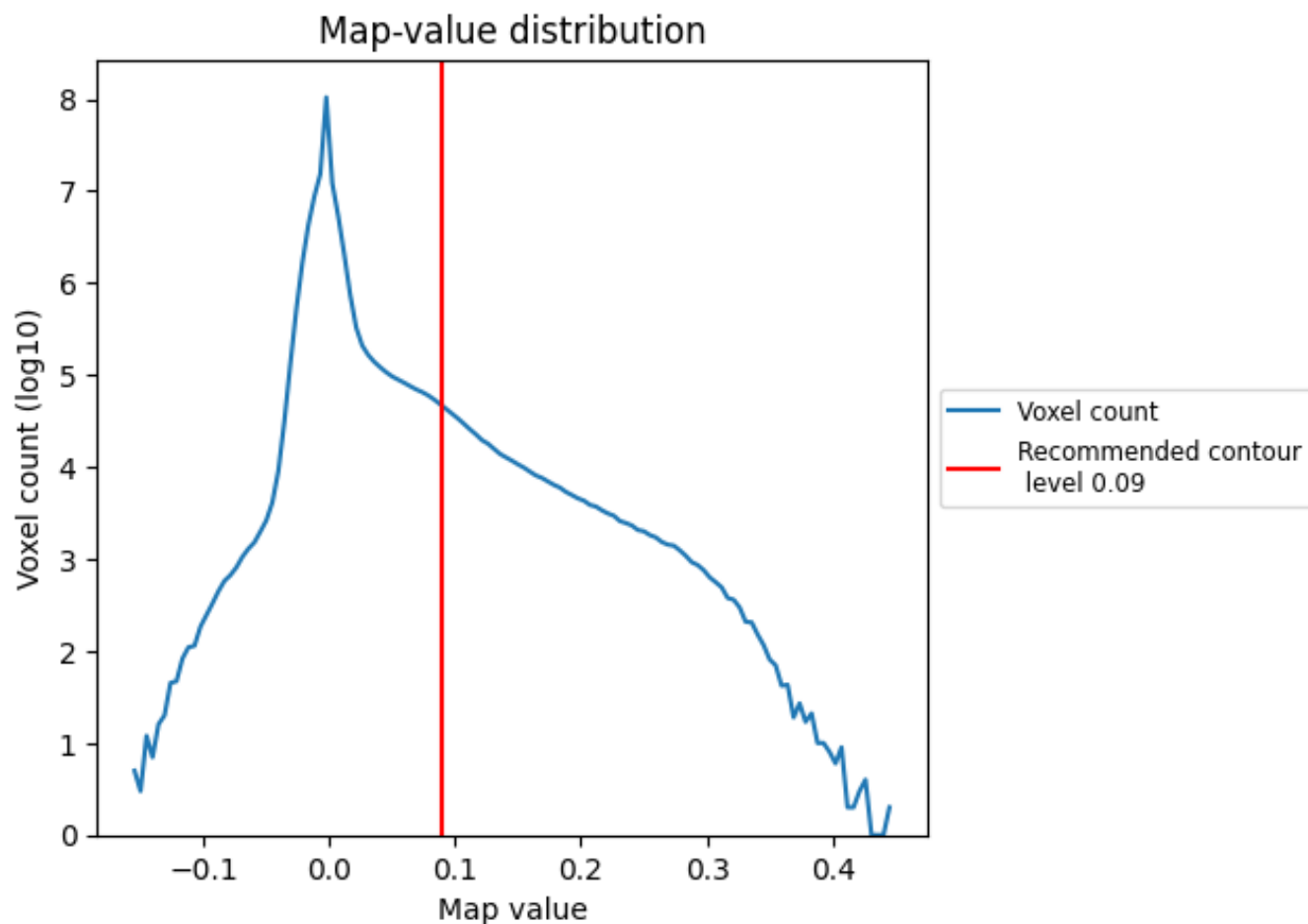
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

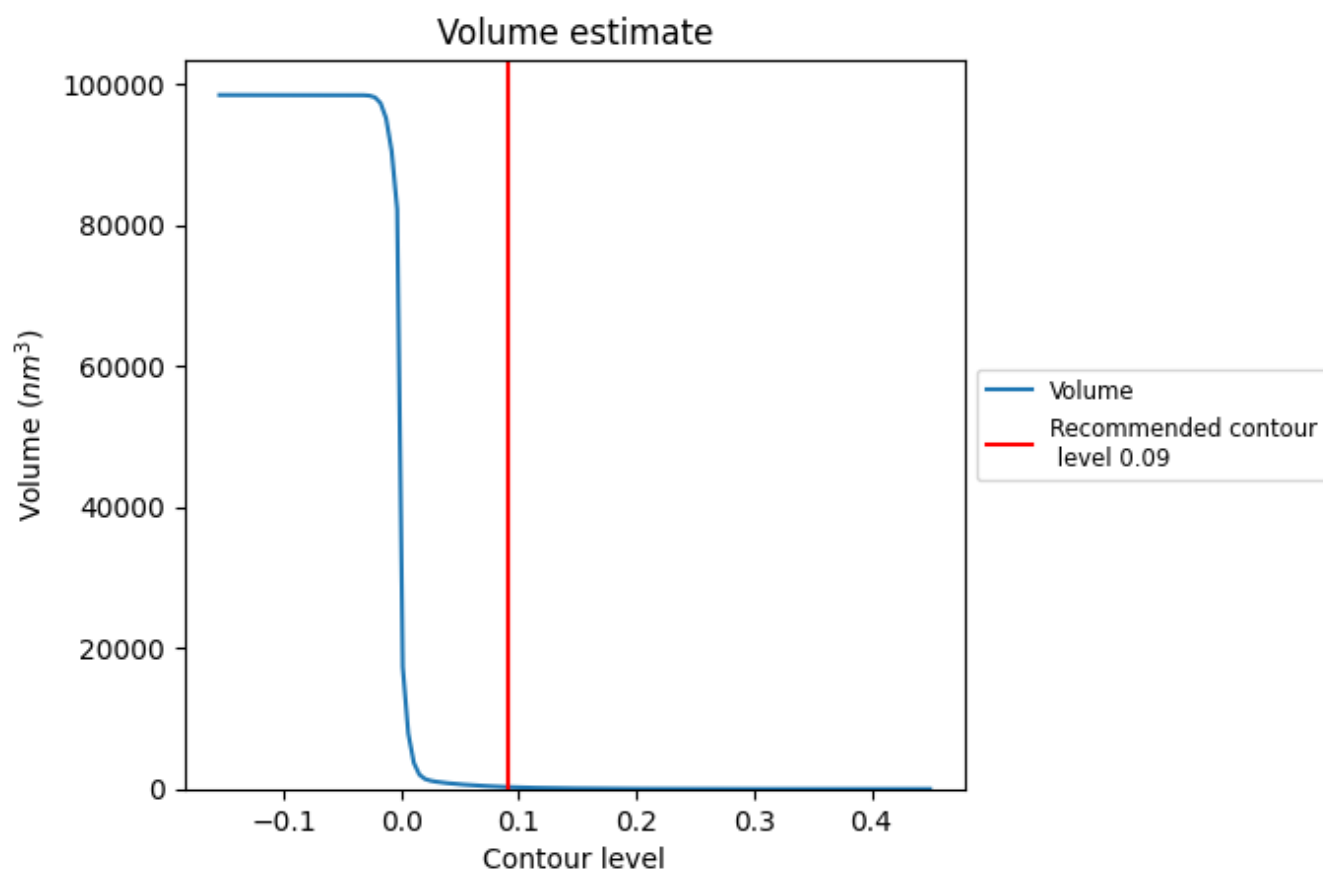
This section contains the results of statistical analysis of the map.

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.

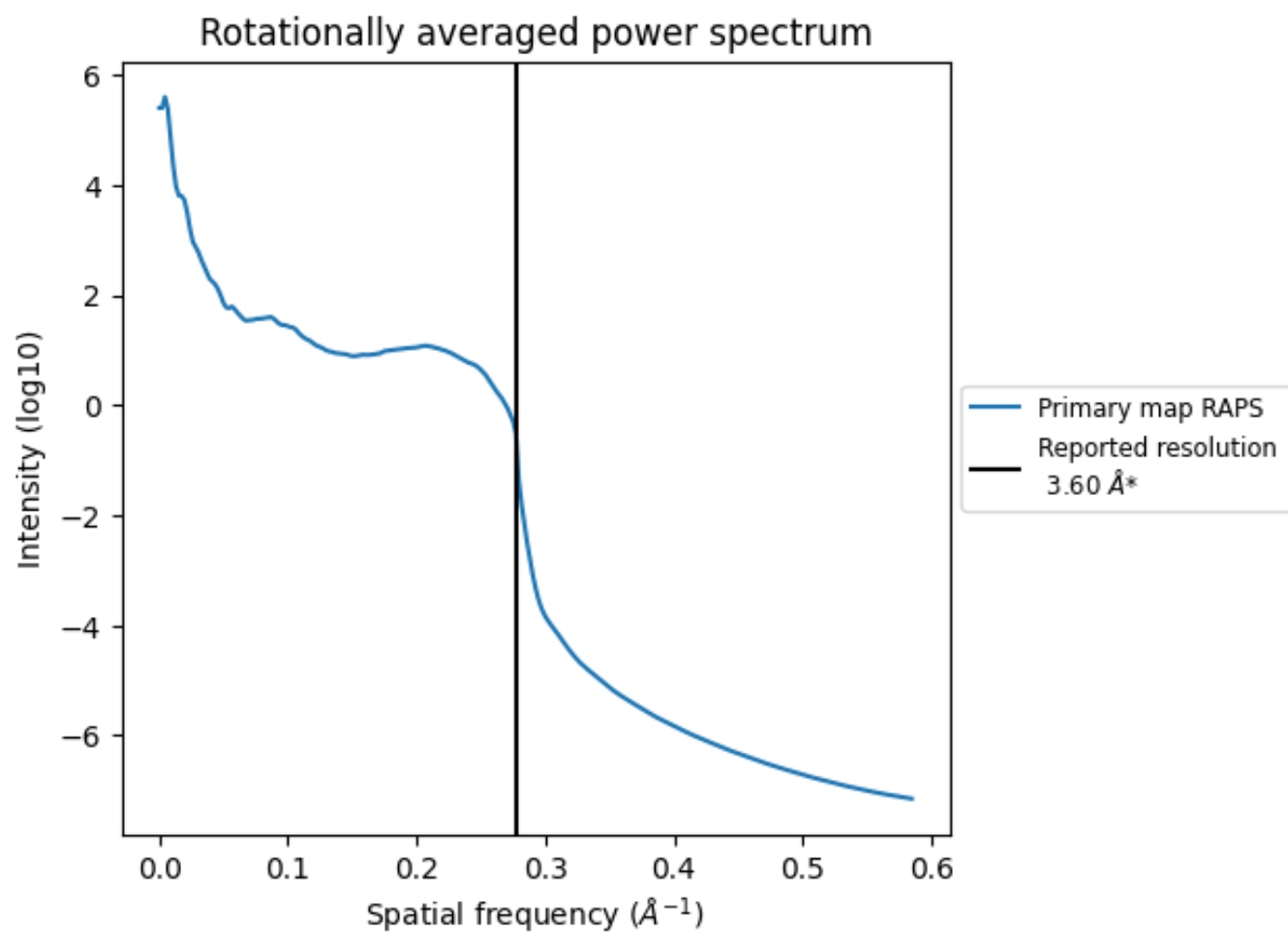
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 276 nm^3 ; this corresponds to an approximate mass of 249 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 0.278 Å⁻¹

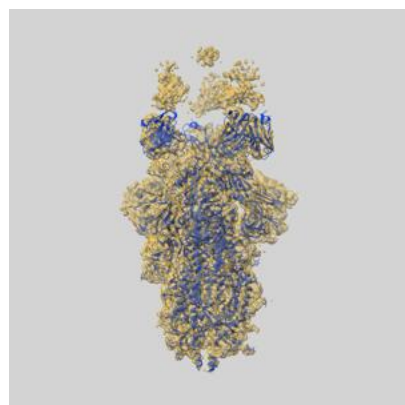
8 Fourier-Shell correlation ⓘ

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

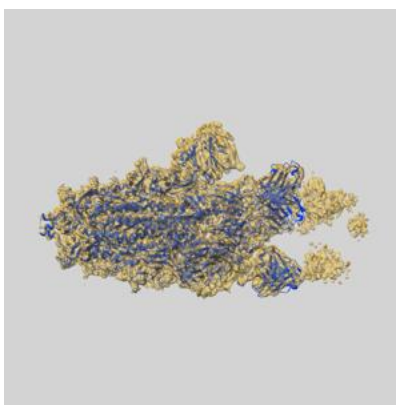
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28228 and PDB model 8ELJ. Per-residue inclusion information can be found in section 3 on page 13.

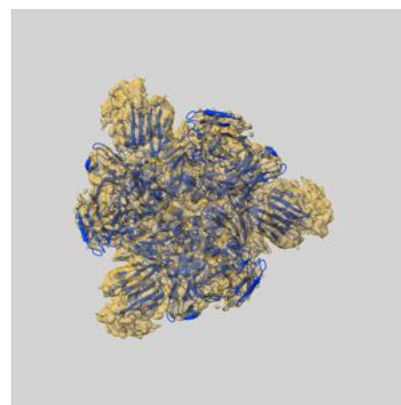
9.1 Map-model overlay [i](#)



X



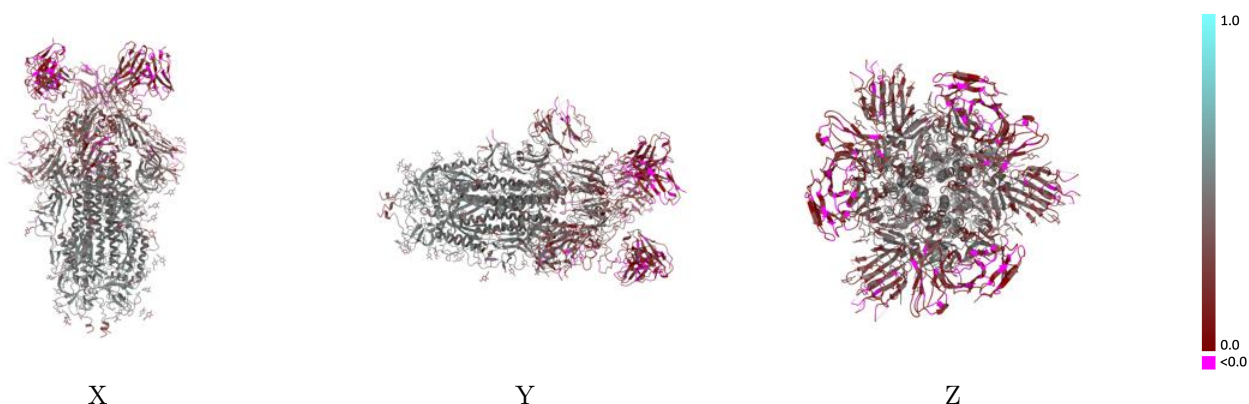
Y



Z

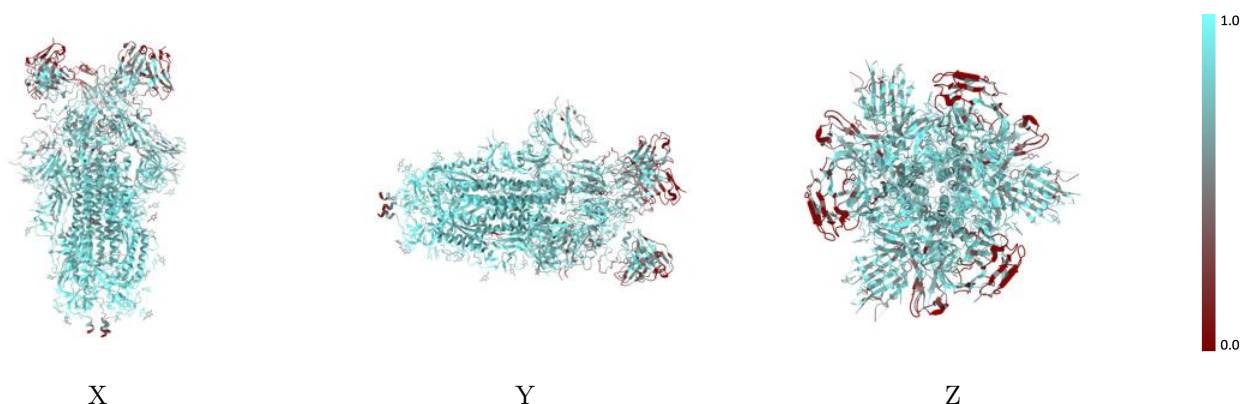
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



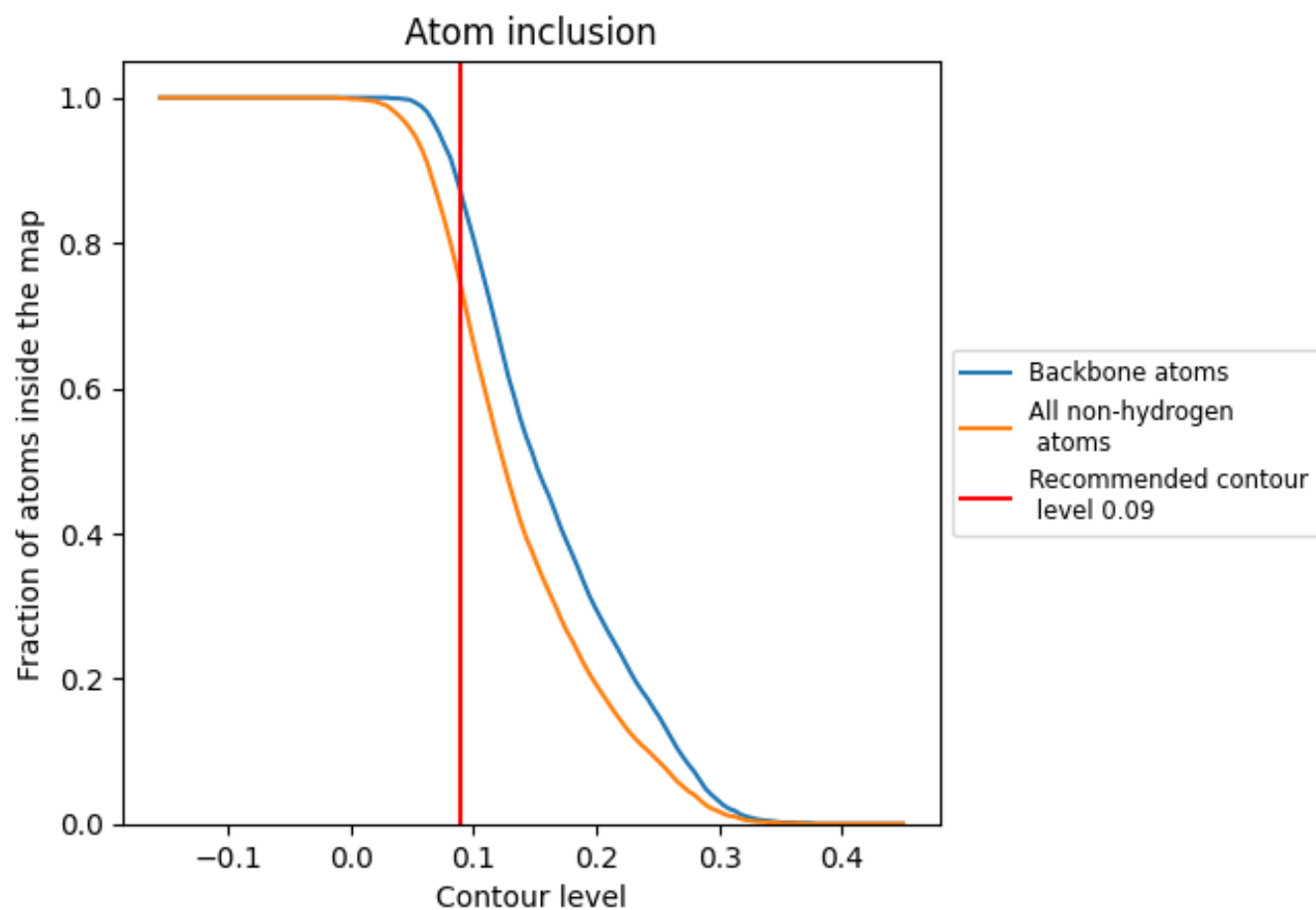
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.3430
A	 0.7990	 0.3910
B	 0.8000	 0.3920
C	 0.8000	 0.3920
E	 0.7500	 0.4640
F	 0.7500	 0.4010
G	 0.7500	 0.4130
H	 0.6790	 0.3760
J	 0.7500	 0.4660
K	 0.7500	 0.3970
L	 0.7500	 0.4220
M	 0.6790	 0.3710
O	 0.7500	 0.4660
P	 0.7500	 0.4010
Q	 0.7500	 0.4180
R	 0.6790	 0.3820
S	 0.5730	 0.1460
T	 0.3510	 0.0750
U	 0.5660	 0.1540
V	 0.3520	 0.0730
W	 0.5690	 0.1500
X	 0.3510	 0.0740

