



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:53 PM UTC

PDB ID : 7WTK / pdb\_00007wtk  
EMDB ID : EMD-32789  
Title : SARS-CoV-2 Omicron variant spike in complex with Fab XGv286  
Authors : Wang, X.; Fu, W.  
Deposited on : 2022-02-04  
Resolution : 3.60 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

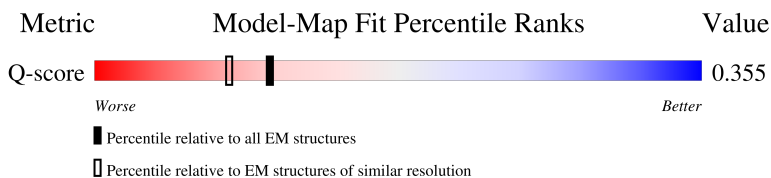
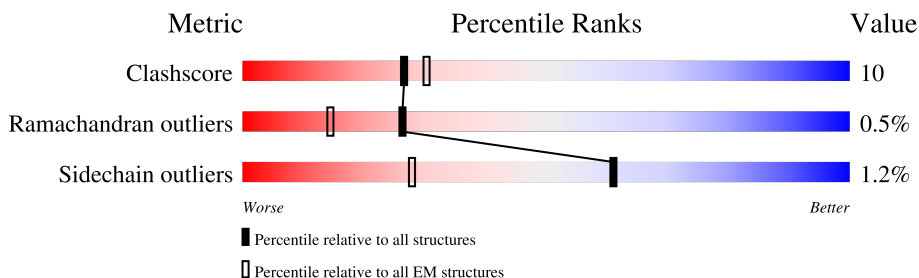
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1149	
1	B	1149	
1	C	1149	
2	G	118	

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Mol	Chain	Length	Quality of chain
2	H	118	100% 78% 22%
2	I	118	100% 84% 16%
3	J	109	43% 80% 19%
3	K	109	99% 85% 15%
3	L	109	99% 83% 17%
4	D	2	100%
4	E	2	50% 50% 50%
4	F	2	50% 50%
4	O	2	100% 100%
4	P	2	100% 100%
4	Q	2	100%
4	R	2	100% 100%
4	S	2	100%
4	V	2	100% 100%
4	W	2	100%
4	X	2	100% 50% 50%
4	Y	2	50% 50%
5	M	3	33% 67% 33%
5	N	3	67% 100%
5	T	3	67% 100%
5	U	3	67% 33% 67%
5	Z	3	33% 67% 33%
5	a	3	67% 100%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 31895 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

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

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	208	ILE	LEU	variant	UNP P0DTC2
C	211	GLU	-	insertion	UNP P0DTC2
C	212	PRO	-	insertion	UNP P0DTC2
C	213	GLU	-	insertion	UNP P0DTC2
C	341	ASP	GLY	variant	UNP P0DTC2
C	373	LEU	SER	variant	UNP P0DTC2
C	375	PRO	SER	variant	UNP P0DTC2
C	377	PHE	SER	variant	UNP P0DTC2
C	419	ASN	LYS	variant	UNP P0DTC2
C	442	LYS	ASN	variant	UNP P0DTC2
C	448	SER	GLY	variant	UNP P0DTC2
C	479	ASN	SER	variant	UNP P0DTC2
C	480	LYS	THR	variant	UNP P0DTC2
C	486	ALA	GLU	variant	UNP P0DTC2
C	495	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	498	SER	GLY	variant	UNP P0DTC2
C	500	ARG	GLN	variant	UNP P0DTC2
C	503	TYR	ASN	variant	UNP P0DTC2
C	507	HIS	TYR	variant	UNP P0DTC2
C	549	LYS	THR	variant	UNP P0DTC2
C	616	GLY	ASP	variant	UNP P0DTC2
C	657	TYR	HIS	variant	UNP P0DTC2
C	685	ALA	ARG	variant	UNP P0DTC2
C	687	ALA	ARG	variant	UNP P0DTC2
C	766	LYS	ASN	variant	UNP P0DTC2
C	798	TYR	ASP	variant	UNP P0DTC2
C	819	PRO	PHE	variant	UNP P0DTC2
C	858	LYS	ASN	variant	UNP P0DTC2
C	894	PRO	ALA	variant	UNP P0DTC2
C	901	PRO	ALA	variant	UNP P0DTC2
C	944	PRO	ALA	variant	UNP P0DTC2
C	956	HIS	GLN	variant	UNP P0DTC2
C	971	LYS	ASN	variant	UNP P0DTC2
C	983	PHE	LEU	variant	UNP P0DTC2
C	988	PRO	LYS	engineered mutation	UNP P0DTC2
C	989	PRO	VAL	engineered mutation	UNP P0DTC2
C	1165	ARG	-	expression tag	UNP P0DTC2
C	1166	ARG	-	expression tag	UNP P0DTC2
C	1167	ALA	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	208	ILE	LEU	variant	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	212	PRO	-	insertion	UNP P0DTC2
B	213	GLU	-	insertion	UNP P0DTC2
B	341	ASP	GLY	variant	UNP P0DTC2
B	373	LEU	SER	variant	UNP P0DTC2
B	375	PRO	SER	variant	UNP P0DTC2
B	377	PHE	SER	variant	UNP P0DTC2
B	419	ASN	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	442	LYS	ASN	variant	UNP P0DTC2
B	448	SER	GLY	variant	UNP P0DTC2
B	479	ASN	SER	variant	UNP P0DTC2
B	480	LYS	THR	variant	UNP P0DTC2
B	486	ALA	GLU	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	SER	GLY	variant	UNP P0DTC2
B	500	ARG	GLN	variant	UNP P0DTC2
B	503	TYR	ASN	variant	UNP P0DTC2
B	507	HIS	TYR	variant	UNP P0DTC2
B	549	LYS	THR	variant	UNP P0DTC2
B	616	GLY	ASP	variant	UNP P0DTC2
B	657	TYR	HIS	variant	UNP P0DTC2
B	685	ALA	ARG	variant	UNP P0DTC2
B	687	ALA	ARG	variant	UNP P0DTC2
B	766	LYS	ASN	variant	UNP P0DTC2
B	798	TYR	ASP	variant	UNP P0DTC2
B	819	PRO	PHE	variant	UNP P0DTC2
B	858	LYS	ASN	variant	UNP P0DTC2
B	894	PRO	ALA	variant	UNP P0DTC2
B	901	PRO	ALA	variant	UNP P0DTC2
B	944	PRO	ALA	variant	UNP P0DTC2
B	956	HIS	GLN	variant	UNP P0DTC2
B	971	LYS	ASN	variant	UNP P0DTC2
B	983	PHE	LEU	variant	UNP P0DTC2
B	988	PRO	LYS	engineered mutation	UNP P0DTC2
B	989	PRO	VAL	engineered mutation	UNP P0DTC2
B	1165	ARG	-	expression tag	UNP P0DTC2
B	1166	ARG	-	expression tag	UNP P0DTC2
B	1167	ALA	-	expression tag	UNP P0DTC2
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	208	ILE	LEU	variant	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	212	PRO	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	213	GLU	-	insertion	UNP P0DTC2
A	341	ASP	GLY	variant	UNP P0DTC2
A	373	LEU	SER	variant	UNP P0DTC2
A	375	PRO	SER	variant	UNP P0DTC2
A	377	PHE	SER	variant	UNP P0DTC2
A	419	ASN	LYS	variant	UNP P0DTC2
A	442	LYS	ASN	variant	UNP P0DTC2
A	448	SER	GLY	variant	UNP P0DTC2
A	479	ASN	SER	variant	UNP P0DTC2
A	480	LYS	THR	variant	UNP P0DTC2
A	486	ALA	GLU	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	SER	GLY	variant	UNP P0DTC2
A	500	ARG	GLN	variant	UNP P0DTC2
A	503	TYR	ASN	variant	UNP P0DTC2
A	507	HIS	TYR	variant	UNP P0DTC2
A	549	LYS	THR	variant	UNP P0DTC2
A	616	GLY	ASP	variant	UNP P0DTC2
A	657	TYR	HIS	variant	UNP P0DTC2
A	685	ALA	ARG	variant	UNP P0DTC2
A	687	ALA	ARG	variant	UNP P0DTC2
A	766	LYS	ASN	variant	UNP P0DTC2
A	798	TYR	ASP	variant	UNP P0DTC2
A	819	PRO	PHE	variant	UNP P0DTC2
A	858	LYS	ASN	variant	UNP P0DTC2
A	894	PRO	ALA	variant	UNP P0DTC2
A	901	PRO	ALA	variant	UNP P0DTC2
A	944	PRO	ALA	variant	UNP P0DTC2
A	956	HIS	GLN	variant	UNP P0DTC2
A	971	LYS	ASN	variant	UNP P0DTC2
A	983	PHE	LEU	variant	UNP P0DTC2
A	988	PRO	LYS	engineered mutation	UNP P0DTC2
A	989	PRO	VAL	engineered mutation	UNP P0DTC2
A	1165	ARG	-	expression tag	UNP P0DTC2
A	1166	ARG	-	expression tag	UNP P0DTC2
A	1167	ALA	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of XGv286.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O	S	
2	H	118	878	557	147	170	4	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	118	Total	C	N	O	S	0	0
			878	557	147	170	4		
2	I	118	Total	C	N	O	S	0	0
			878	557	147	170	4		

- Molecule 3 is a protein called Light chain of XGv286.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	109	Total	C	N	O	S	0	0
			801	495	140	164	2		
3	J	109	Total	C	N	O	S	0	0
			801	495	140	164	2		
3	K	109	Total	C	N	O	S	0	0
			801	495	140	164	2		

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



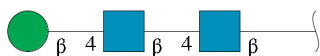
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	M	3	39	22	2	15	0	0
5	N	3	39	22	2	15	0	0
5	T	3	39	22	2	15	0	0
5	U	3	39	22	2	15	0	0
5	Z	3	39	22	2	15	0	0
5	a	3	39	22	2	15	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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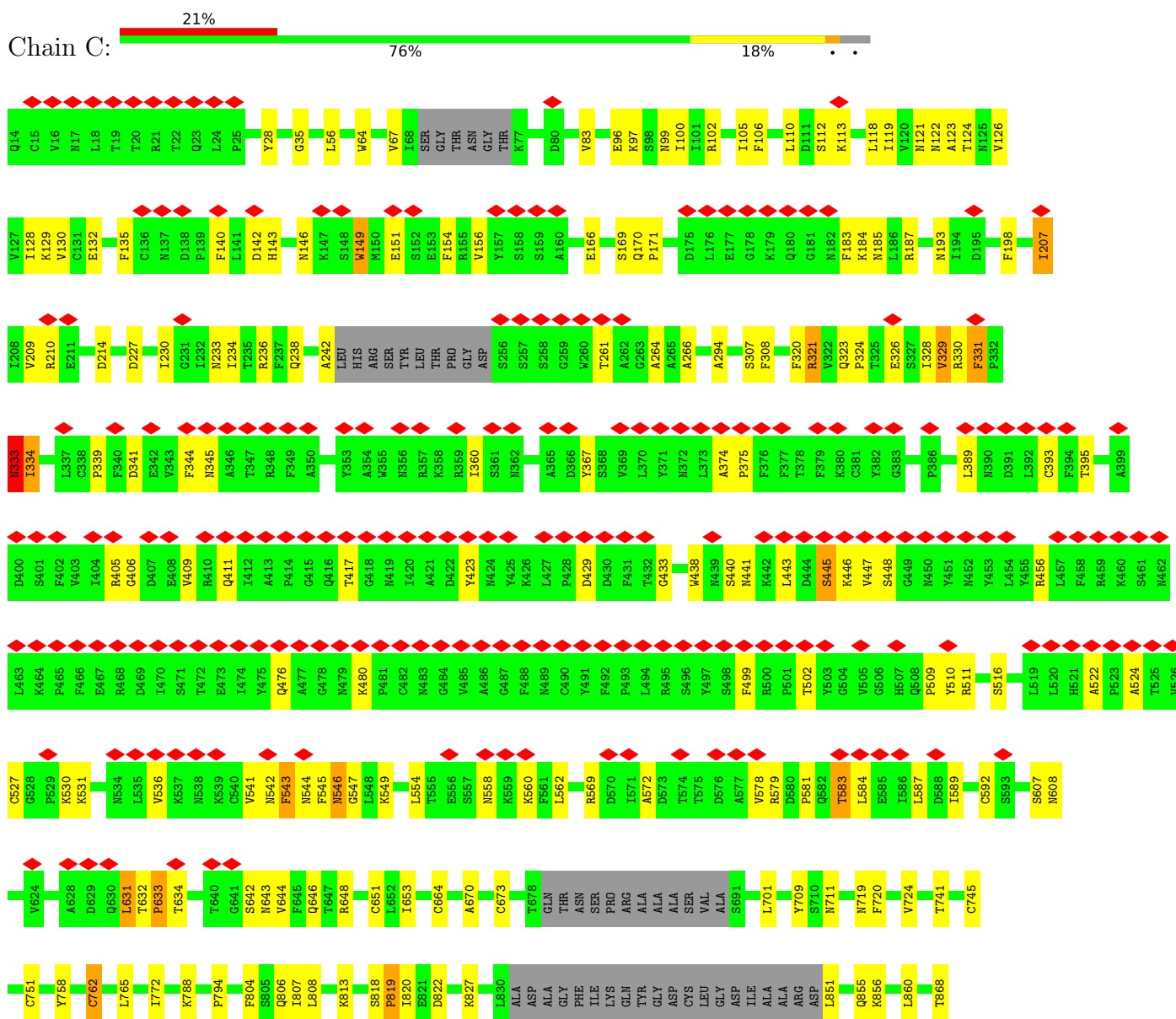
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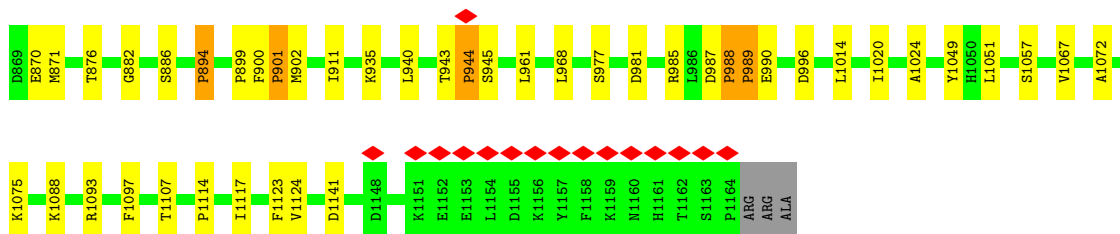
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	Total 14	8	1	5	0
6	B	1	Total 14	8	1	5	0
6	B	1	Total 14	8	1	5	0
6	B	1	Total 14	8	1	5	0
6	B	1	Total 14	8	1	5	0
6	A	1	Total 14	8	1	5	0
6	A	1	Total 14	8	1	5	0
6	A	1	Total 14	8	1	5	0
6	A	1	Total 14	8	1	5	0
6	A	1	Total 14	8	1	5	0
6	A	1	Total 14	8	1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

### 3 Residue-property plots

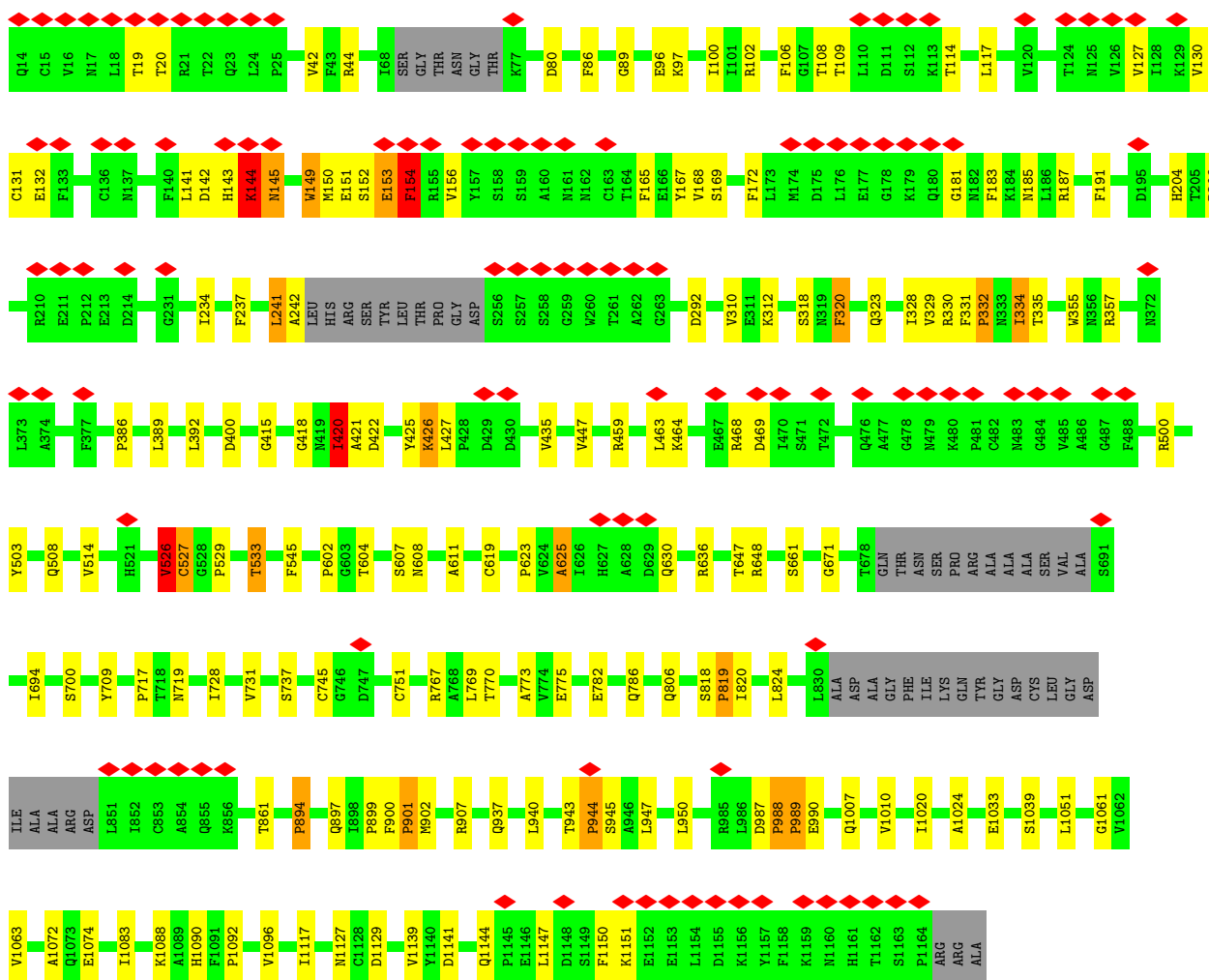
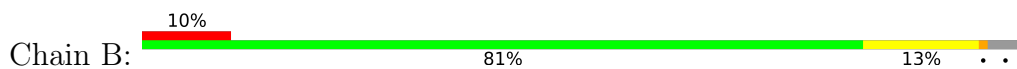
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Spike glycoprotein

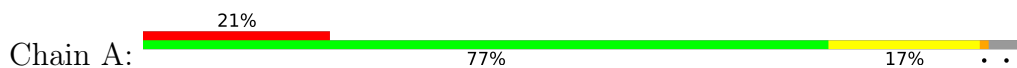


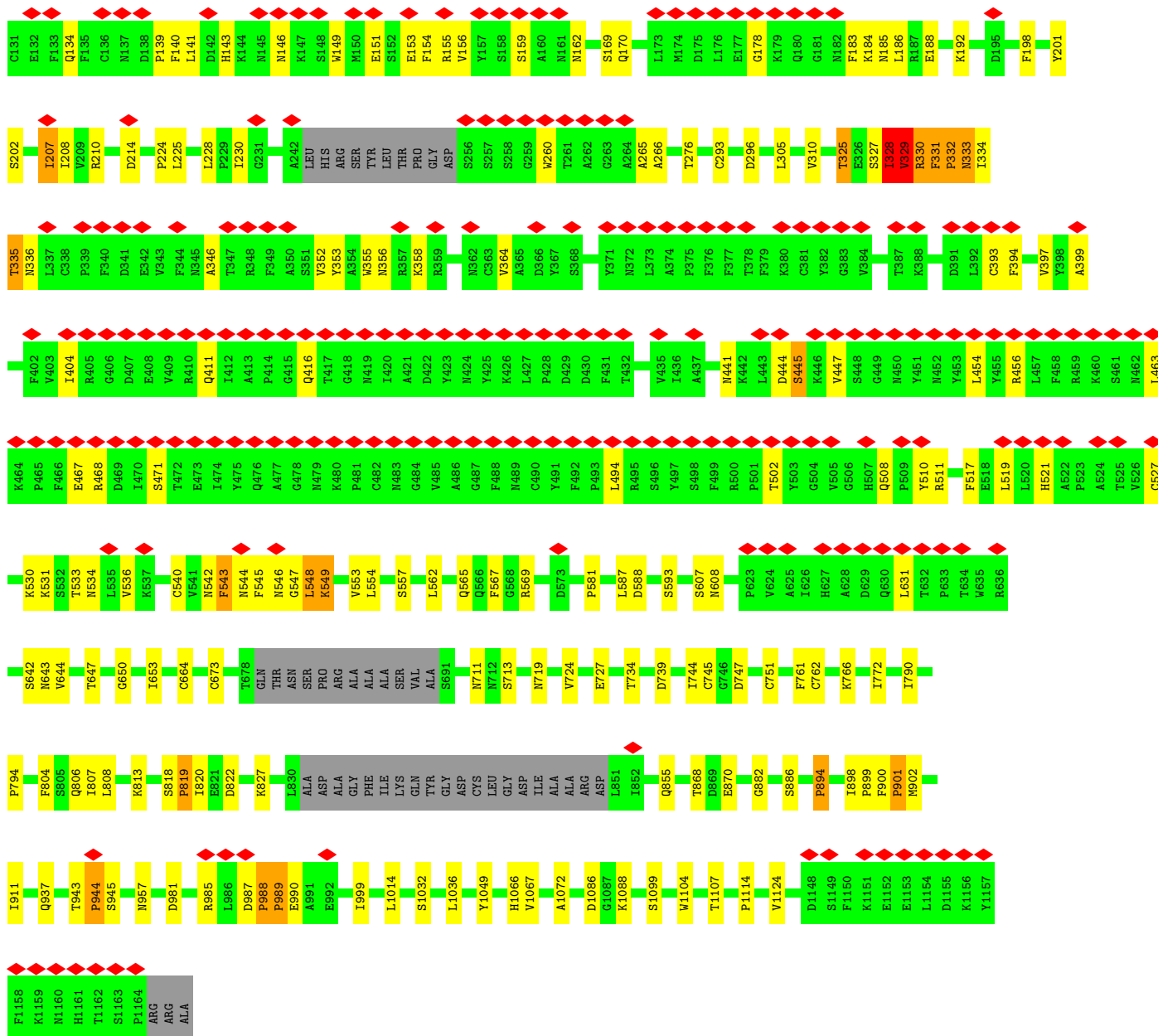


• Molecule 1: Spike glycoprotein

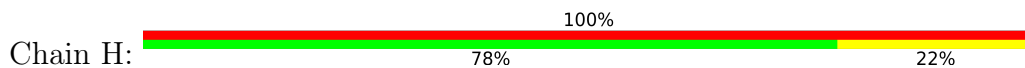


• Molecule 1: Spike glycoprotein

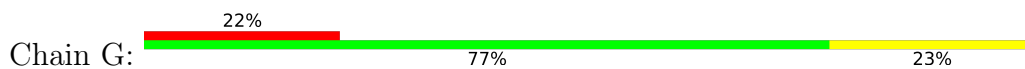


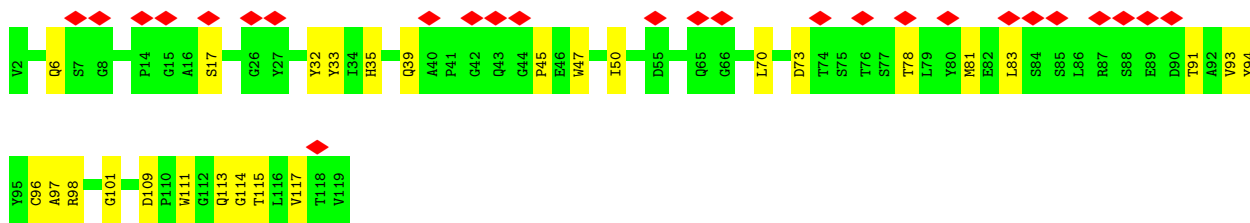


● Molecule 2: Heavy chain of XGv286

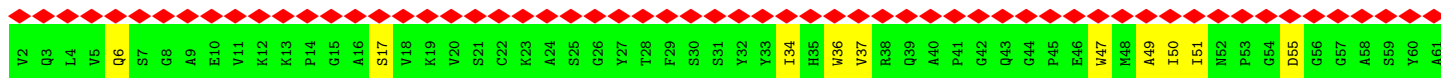
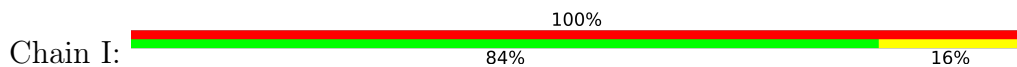


● Molecule 2: Heavy chain of XGv286

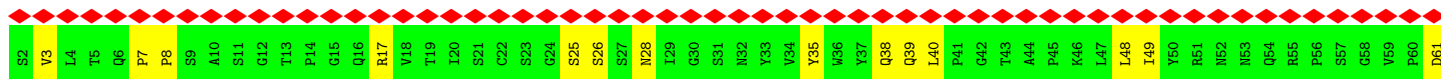
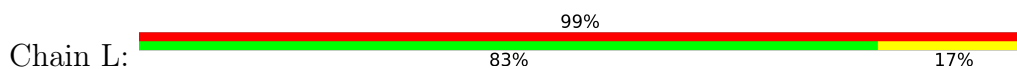




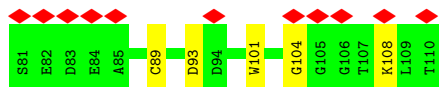
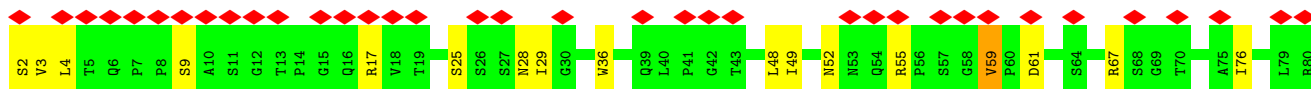
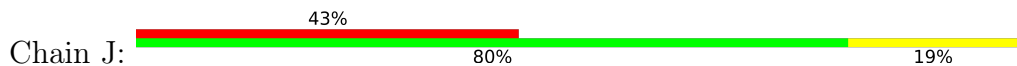
• Molecule 2: Heavy chain of XGv286



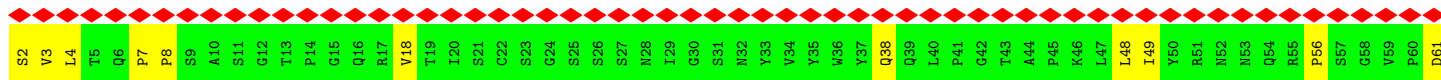
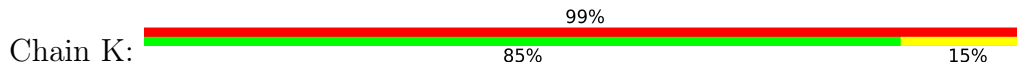
• Molecule 3: Light chain of XGv286

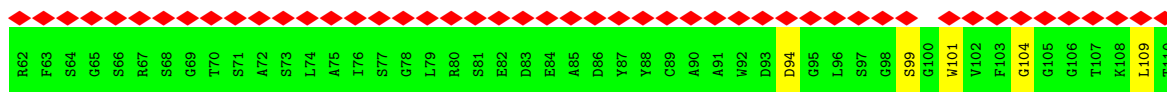


• Molecule 3: Light chain of XGv286



• Molecule 3: Light chain of XGv286





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

Chain D: 100%

MAG1  
MAG2

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

Chain E: 50%  
50% 50%

MAG1  
MAG2

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

Chain F: 50%  
50%

MAG1  
MAG2

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

Chain O: 100%  
100%

MAG1  
MAG2

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

Chain P: 100%  
100%

MAG1  
MAG2

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

Chain Q: 100%



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



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



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



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



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



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





- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	339195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	3.856	Depositor
Minimum map value	-2.203	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.07, 1.07, 1.07	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.33	1/8842 (0.0%)	0.63	15/12033 (0.1%)
1	B	0.34	0/8842	0.64	15/12033 (0.1%)
1	C	0.34	1/8842 (0.0%)	0.64	13/12033 (0.1%)
2	G	0.22	0/902	0.51	0/1232
2	H	0.18	0/902	0.39	0/1232
2	I	0.16	0/902	0.35	0/1232
3	J	0.17	0/821	0.57	1/1119 (0.1%)
3	K	0.20	0/821	0.44	0/1119
3	L	0.20	0/821	0.50	1/1119 (0.1%)
All	All	0.31	2/31695 (0.0%)	0.61	45/43152 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	761	PHE	C-O	5.20	1.30	1.24
1	C	374	ALA	C-N	5.16	1.39	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	988	PRO	CA-N-CD	-9.17	99.17	112.00
1	B	944	PRO	CA-N-CD	-9.11	99.25	112.00
1	A	988	PRO	CA-N-CD	-9.08	99.28	112.00
1	C	944	PRO	CA-N-CD	-9.05	99.33	112.00
1	A	944	PRO	CA-N-CD	-9.04	99.34	112.00
1	A	819	PRO	CA-N-CD	-9.03	99.36	112.00
1	C	901	PRO	CA-N-CD	-9.03	99.36	112.00
1	A	901	PRO	CA-N-CD	-9.02	99.37	112.00
1	C	988	PRO	CA-N-CD	-9.01	99.39	112.00
1	C	819	PRO	CA-N-CD	-8.97	99.44	112.00
1	B	901	PRO	CA-N-CD	-8.96	99.45	112.00
1	C	989	PRO	CA-N-CD	-8.96	99.46	112.00
1	B	989	PRO	CA-N-CD	-8.96	99.46	112.00
1	A	989	PRO	CA-N-CD	-8.85	99.61	112.00
1	C	894	PRO	CA-N-CD	-8.80	99.68	112.00
1	B	819	PRO	CA-N-CD	-8.80	99.67	112.00
1	A	894	PRO	CA-N-CD	-8.79	99.70	112.00
1	B	894	PRO	CA-N-CD	-8.74	99.76	112.00
1	C	633	PRO	CB-CA-C	8.51	119.14	111.40
1	B	318	SER	O-C-N	-7.47	114.01	122.75
1	C	762	CYS	CB-CA-C	7.44	123.50	110.85
1	A	329	VAL	CA-C-O	-6.94	114.51	121.45
1	B	145	ASN	CB-CA-C	6.91	124.17	110.42
1	C	581	PRO	N-CA-C	-6.62	104.71	113.65
1	C	545	PHE	CB-CA-C	-6.46	102.15	112.09
1	C	546	ASN	N-CA-C	6.42	118.42	110.91
3	J	59	VAL	N-CA-C	-6.42	103.93	109.19
1	B	418	GLY	CA-C-O	-6.16	116.17	121.04
1	A	330	ARG	N-CA-C	6.12	119.77	107.41
1	B	420	ILE	N-CA-C	-6.09	104.41	110.62
1	A	543	PHE	CA-C-N	-6.07	113.75	122.67
1	A	543	PHE	C-N-CA	-6.07	113.75	122.67
1	B	418	GLY	N-CA-C	-6.03	102.32	111.42
1	B	426	LYS	CA-C-N	5.99	136.43	121.80
1	B	426	LYS	C-N-CA	5.99	136.43	121.80
1	C	545	PHE	CA-CB-CG	5.96	119.76	113.80
1	B	422	ASP	N-CA-C	-5.81	108.00	114.62
1	A	444	ASP	CA-C-N	-5.38	115.42	123.00
1	A	444	ASP	C-N-CA	-5.38	115.42	123.00
1	A	330	ARG	CB-CA-C	-5.35	102.32	111.41
3	L	3	VAL	N-CA-C	-5.26	108.15	113.20
1	A	325	THR	CB-CA-C	5.11	120.59	110.42
1	B	320	PHE	CA-CB-CG	5.10	118.90	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	762	CYS	N-CA-CB	-5.05	102.69	110.16
1	A	761	PHE	N-CA-C	-5.03	105.50	111.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	464	LYS	Peptide
1	C	333	ASN	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8632	0	8444	219	0
1	B	8632	0	8444	157	0
1	C	8632	0	8448	199	0
2	G	878	0	817	14	0
2	H	878	0	817	17	0
2	I	878	0	817	12	0
3	J	801	0	748	14	0
3	K	801	0	748	9	0
3	L	801	0	748	12	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	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
4	S	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	1	0
5	M	39	0	34	0	0
5	N	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	39	0	34	0	0
5	U	39	0	34	1	0
5	Z	39	0	34	0	0
5	a	39	0	34	0	0
6	A	126	0	111	1	0
6	B	140	0	128	5	0
6	C	126	0	114	3	0
All	All	31895	0	30888	630	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 10.

All (630) 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:A:818:SER:OG	1:A:819:PRO:CD	1.73	1.36
1:A:943:THR:OG1	1:A:944:PRO:CD	1.74	1.33
1:B:415:GLY:HA3	1:A:988:PRO:CG	1.59	1.32
1:C:818:SER:OG	1:C:819:PRO:CD	1.81	1.28
1:A:818:SER:OG	1:A:819:PRO:HD3	1.04	1.20
1:C:818:SER:OG	1:C:819:PRO:HD3	1.06	1.19
1:A:987:ASP:OD1	1:A:988:PRO:HD3	1.04	1.18
1:C:988:PRO:HD2	1:C:989:PRO:CD	1.73	1.18
1:B:806:GLN:O	1:B:819:PRO:CD	1.93	1.16
1:C:988:PRO:CD	1:C:989:PRO:HD3	1.78	1.14
1:A:332:PRO:HD2	1:A:547:GLY:HA2	1.16	1.14
1:A:943:THR:OG1	1:A:944:PRO:HD3	0.96	1.13
1:B:989:PRO:HD2	1:B:990:GLU:H	1.14	1.12
1:B:415:GLY:HA3	1:A:988:PRO:HG2	1.26	1.12
1:A:331:PHE:H	1:A:547:GLY:HA3	1.14	1.12
1:A:987:ASP:OD1	1:A:988:PRO:CD	1.98	1.11
1:C:819:PRO:HD2	1:C:820:ILE:H	1.13	1.11
1:A:819:PRO:HD2	1:A:820:ILE:H	1.14	1.10
1:B:415:GLY:HA3	1:A:988:PRO:HG3	1.31	1.09
1:A:333:ASN:HB3	1:A:581:PRO:HB3	1.07	1.06
1:B:819:PRO:HD2	1:B:820:ILE:H	1.10	1.06
1:A:333:ASN:HB3	1:A:581:PRO:CB	1.86	1.05
1:A:989:PRO:HD2	1:A:990:GLU:H	1.22	1.04
1:A:988:PRO:CD	1:A:989:PRO:HD3	1.89	1.03
1:A:988:PRO:HD2	1:A:989:PRO:CD	1.90	1.01
1:A:331:PHE:HB2	1:A:548:LEU:HB3	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:GLN:O	1:B:819:PRO:HD2	1.65	0.96
1:B:901:PRO:HD2	1:B:902:MET:H	1.30	0.96
1:B:943:THR:OG1	1:B:944:PRO:HD3	1.64	0.96
1:C:988:PRO:HD2	1:C:989:PRO:HD3	1.34	0.95
1:A:333:ASN:CB	1:A:581:PRO:HB3	1.95	0.95
1:C:331:PHE:HB2	1:C:547:GLY:CA	1.99	0.92
1:A:806:GLN:O	1:A:819:PRO:CD	2.16	0.92
1:B:806:GLN:O	1:B:819:PRO:HD3	1.70	0.91
1:A:332:PRO:HD2	1:A:547:GLY:CA	1.99	0.91
1:C:818:SER:HG	1:C:819:PRO:HD3	1.14	0.91
1:A:328:ILE:HG13	1:A:543:PHE:HA	1.52	0.90
1:B:806:GLN:HA	1:B:819:PRO:HG2	1.54	0.89
1:A:806:GLN:O	1:A:819:PRO:CG	2.20	0.89
1:C:330:ARG:C	1:C:547:GLY:HA3	1.98	0.88
1:C:806:GLN:O	1:C:819:PRO:HG2	1.74	0.87
1:C:819:PRO:HD2	1:C:820:ILE:N	1.89	0.87
1:A:806:GLN:O	1:A:819:PRO:HG2	1.74	0.87
1:B:987:ASP:C	1:B:989:PRO:HD3	2.00	0.87
1:B:819:PRO:HD2	1:B:820:ILE:N	1.87	0.86
1:C:806:GLN:O	1:C:819:PRO:CD	2.22	0.86
1:A:819:PRO:HD2	1:A:820:ILE:N	1.89	0.86
1:B:943:THR:OG1	1:B:944:PRO:CD	2.23	0.85
1:A:943:THR:HG1	1:A:944:PRO:HD3	1.03	0.85
1:C:987:ASP:HB2	1:C:988:PRO:HD3	1.58	0.85
1:C:806:GLN:O	1:C:819:PRO:CG	2.24	0.85
1:A:987:ASP:CG	1:A:988:PRO:HD3	2.00	0.85
1:A:330:ARG:HD3	1:A:581:PRO:HD3	1.58	0.84
1:A:989:PRO:HD2	1:A:990:GLU:N	1.92	0.84
1:C:988:PRO:HD2	1:C:989:PRO:N	1.92	0.84
1:C:989:PRO:HD2	1:C:990:GLU:H	1.41	0.84
1:C:331:PHE:HB2	1:C:547:GLY:HA3	1.60	0.83
1:C:901:PRO:HD2	1:C:902:MET:H	1.41	0.82
1:A:988:PRO:HD2	1:A:989:PRO:HD3	1.52	0.81
1:A:900:PHE:N	1:A:901:PRO:HD3	1.97	0.80
1:C:331:PHE:HB2	1:C:547:GLY:HA2	1.62	0.80
1:A:899:PRO:C	1:A:901:PRO:HD3	2.06	0.80
1:B:899:PRO:HB2	1:B:901:PRO:CD	2.12	0.80
1:B:96:GLU:O	1:B:185:ASN:HB2	1.82	0.80
1:C:321:ARG:HH21	1:C:323:GLN:HA	1.44	0.79
1:C:987:ASP:HB2	1:C:989:PRO:HD3	1.65	0.79
1:C:330:ARG:HA	1:C:544:ASN:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:LYS:HD2	1:C:546:ASN:HB2	1.65	0.78
1:A:987:ASP:C	1:A:989:PRO:HD3	2.09	0.78
1:A:146:ASN:HA	1:A:260:TRP:HB2	1.65	0.78
1:C:140:PHE:HE2	1:C:142:ASP:HB2	1.46	0.78
1:A:988:PRO:CD	1:A:989:PRO:CD	2.56	0.78
1:C:988:PRO:CD	1:C:989:PRO:CD	2.46	0.78
1:A:332:PRO:CD	1:A:547:GLY:HA2	2.09	0.78
1:B:989:PRO:CD	1:B:990:GLU:H	1.96	0.77
1:A:818:SER:HG	1:A:819:PRO:HD3	0.97	0.77
1:B:819:PRO:CD	1:B:820:ILE:H	1.94	0.77
1:C:140:PHE:CE2	1:C:142:ASP:HB2	2.18	0.77
1:B:989:PRO:HD2	1:B:990:GLU:N	1.89	0.77
1:C:819:PRO:CD	1:C:820:ILE:H	1.96	0.76
1:C:440:SER:HB2	1:C:511:ARG:HD3	1.67	0.76
1:C:987:ASP:HB2	1:C:988:PRO:CD	2.15	0.76
1:A:331:PHE:N	1:A:547:GLY:HA3	1.96	0.76
1:B:415:GLY:CA	1:A:988:PRO:HG2	2.13	0.76
1:C:899:PRO:HB2	1:C:901:PRO:CD	2.16	0.76
1:A:987:ASP:CB	1:A:989:PRO:HD3	2.16	0.75
1:B:899:PRO:HB2	1:B:901:PRO:HD3	1.68	0.75
1:B:901:PRO:HD2	1:B:902:MET:N	1.97	0.75
1:C:989:PRO:HD2	1:C:990:GLU:N	2.01	0.75
1:A:819:PRO:CD	1:A:820:ILE:H	1.97	0.75
1:A:988:PRO:HD2	1:A:989:PRO:N	2.00	0.74
1:C:900:PHE:N	1:C:901:PRO:HD3	2.02	0.74
1:B:818:SER:HB3	1:B:819:PRO:HD3	1.67	0.74
2:G:94:TYR:O	2:G:114:GLY:HA2	1.87	0.74
1:A:901:PRO:HD2	1:A:902:MET:H	1.53	0.73
1:B:415:GLY:CA	1:A:988:PRO:HG3	2.13	0.73
1:A:899:PRO:C	1:A:901:PRO:CD	2.61	0.73
1:A:899:PRO:HB2	1:A:901:PRO:CD	2.18	0.72
1:A:143:HIS:HA	1:A:149:TRP:HZ3	1.54	0.72
1:B:142:ASP:CB	1:B:242:ALA:HA	2.20	0.72
1:A:329:VAL:HB	1:A:548:LEU:O	1.89	0.72
1:A:989:PRO:CD	1:A:990:GLU:H	2.00	0.71
1:B:141:LEU:HA	1:B:152:SER:HB2	1.73	0.71
1:B:900:PHE:N	1:B:901:PRO:HD3	2.06	0.71
1:C:901:PRO:HD2	1:C:902:MET:N	2.03	0.70
1:A:988:PRO:N	1:A:989:PRO:HD3	2.06	0.70
1:B:106:PHE:HB2	1:B:117:LEU:HB2	1.74	0.69
1:A:899:PRO:HB2	1:A:901:PRO:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:O	1:A:185:ASN:HB2	1.91	0.69
1:A:987:ASP:CG	1:A:989:PRO:HD3	2.18	0.69
1:A:901:PRO:HD2	1:A:902:MET:N	2.07	0.68
1:C:330:ARG:CA	1:C:544:ASN:HB3	2.22	0.68
2:G:17:SER:HA	2:G:83:LEU:O	1.93	0.68
1:A:332:PRO:HB2	1:A:545:PHE:O	1.93	0.68
1:C:328:ILE:HG23	1:C:531:LYS:HE2	1.76	0.68
1:C:333:ASN:HB2	1:C:334:ILE:HA	1.74	0.68
1:B:806:GLN:HA	1:B:819:PRO:CG	2.24	0.68
1:B:818:SER:HB3	1:B:819:PRO:CD	2.24	0.68
1:C:987:ASP:CB	1:C:989:PRO:HD3	2.25	0.67
1:B:819:PRO:CD	1:B:820:ILE:N	2.56	0.67
1:A:987:ASP:C	1:A:989:PRO:CD	2.67	0.67
1:B:329:VAL:H	1:B:533:THR:HG23	1.58	0.67
3:J:52:ASN:HD21	3:J:67:ARG:HG3	1.60	0.66
1:C:441:ASN:HB2	1:C:509:PRO:HD2	1.76	0.66
2:H:71:THR:HB	2:H:80:TYR:HB2	1.78	0.66
3:L:35:TYR:HB2	3:L:90:ALA:O	1.94	0.66
2:G:91:THR:HA	2:G:117:VAL:O	1.94	0.66
1:C:988:PRO:N	1:C:989:PRO:HD3	2.11	0.66
1:A:330:ARG:HB2	1:A:544:ASN:HB3	1.77	0.66
1:B:901:PRO:CD	1:B:902:MET:H	2.05	0.65
1:B:144:LYS:HB2	1:B:150:MET:HB3	1.77	0.65
1:B:142:ASP:HB2	1:B:242:ALA:HA	1.78	0.65
1:B:989:PRO:CD	1:B:990:GLU:N	2.58	0.65
1:A:987:ASP:HB3	1:A:989:PRO:CD	2.26	0.64
3:J:4:LEU:HD11	3:J:29:ILE:HD11	1.80	0.64
1:A:818:SER:OG	1:A:819:PRO:HD2	1.92	0.64
1:A:900:PHE:N	1:A:901:PRO:CD	2.59	0.64
1:B:142:ASP:HB2	1:B:242:ALA:O	1.97	0.64
1:A:327:SER:HA	1:A:542:ASN:HB2	1.79	0.64
1:C:446:LYS:HE2	1:C:448:SER:OG	1.98	0.64
1:B:89:GLY:HA2	1:B:191:PHE:O	1.97	0.64
3:J:17:ARG:HA	3:J:76:ILE:O	1.98	0.64
1:C:988:PRO:CD	1:C:989:PRO:N	2.60	0.64
1:C:894:PRO:HD2	1:C:894:PRO:O	1.98	0.63
1:B:894:PRO:HD2	1:B:894:PRO:O	1.98	0.63
1:C:631:LEU:HB2	1:C:633:PRO:HD2	1.81	0.63
1:C:819:PRO:CD	1:C:820:ILE:N	2.57	0.63
2:I:34:ILE:HB	2:I:51:ILE:HB	1.81	0.63
2:I:69:THR:HB	2:I:82:GLU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:PRO:C	1:B:901:PRO:HD3	2.24	0.63
1:C:530:LYS:HD2	1:C:546:ASN:CB	2.27	0.63
1:A:332:PRO:HG2	1:A:546:ASN:O	1.99	0.63
1:C:806:GLN:HA	1:C:819:PRO:HG2	1.80	0.62
1:B:901:PRO:CD	1:B:902:MET:N	2.63	0.62
1:A:989:PRO:CD	1:A:990:GLU:N	2.59	0.62
1:A:894:PRO:HD2	1:A:894:PRO:O	1.98	0.62
1:C:330:ARG:O	1:C:547:GLY:HA3	2.00	0.62
1:B:330:ARG:HD3	1:B:545:PHE:HE1	1.65	0.62
1:B:331:PHE:HB3	1:B:332:PRO:HD2	1.82	0.62
1:A:819:PRO:CD	1:A:820:ILE:N	2.58	0.62
1:C:899:PRO:HB2	1:C:901:PRO:HD3	1.81	0.62
1:C:899:PRO:C	1:C:901:PRO:HD3	2.25	0.62
1:C:943:THR:OG1	1:C:944:PRO:CD	2.48	0.62
1:A:328:ILE:HG21	1:A:546:ASN:HA	1.82	0.62
1:B:1144:GLN:HA	1:B:1147:LEU:HG	1.81	0.61
1:C:411:GLN:NE2	1:C:417:THR:O	2.33	0.61
1:C:900:PHE:N	1:C:901:PRO:CD	2.64	0.61
1:C:901:PRO:CD	1:C:902:MET:H	2.13	0.60
1:B:988:PRO:HD2	1:B:989:PRO:N	2.15	0.60
1:A:536:VAL:H	1:A:543:PHE:HZ	1.49	0.60
1:A:533:THR:HG21	1:A:543:PHE:HB2	1.83	0.60
1:A:64:TRP:HE1	1:A:266:ALA:HB1	1.67	0.60
2:G:33:TYR:HB3	2:G:50:ILE:HD11	1.84	0.60
1:B:355:TRP:O	1:B:468:ARG:NH1	2.34	0.60
1:C:806:GLN:O	1:C:819:PRO:HD2	2.02	0.60
1:A:806:GLN:O	1:A:819:PRO:HD2	2.01	0.59
1:B:987:ASP:HB2	1:B:988:PRO:HD3	1.82	0.59
1:C:326:GLU:O	1:C:542:ASN:ND2	2.35	0.59
2:I:104:TRP:HE1	3:K:101:TRP:HE1	1.48	0.59
1:B:661:SER:HB3	1:B:700:SER:HB2	1.84	0.59
2:I:71:THR:HB	2:I:80:TYR:HB2	1.85	0.59
1:C:423:TYR:HB3	1:C:456:ARG:HH12	1.68	0.59
1:C:989:PRO:CD	1:C:990:GLU:N	2.66	0.59
1:B:130:VAL:HB	1:B:165:PHE:HB3	1.85	0.58
1:C:578:VAL:HG21	1:C:589:ILE:HD12	1.85	0.58
1:B:108:THR:HG23	1:B:109:THR:HG23	1.85	0.58
1:B:944:PRO:HD2	1:B:945:SER:N	2.18	0.58
1:A:988:PRO:CD	1:A:989:PRO:N	2.66	0.58
1:C:899:PRO:C	1:C:901:PRO:CD	2.76	0.58
1:C:701:LEU:HB2	1:A:790:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:806:GLN:C	1:C:819:PRO:HG2	2.28	0.58
1:A:105:ILE:HG12	1:A:118:LEU:HG	1.85	0.58
1:C:871:MET:HE1	1:B:671:GLY:HA3	1.85	0.58
1:C:989:PRO:CD	1:C:990:GLU:H	2.13	0.58
1:A:331:PHE:H	1:A:547:GLY:CA	2.02	0.57
1:A:463:LEU:HD12	1:A:467:GLU:HB3	1.87	0.57
1:B:97:LYS:HB2	1:B:183:PHE:HA	1.85	0.57
1:B:141:LEU:HA	1:B:152:SER:CB	2.32	0.57
1:B:447:VAL:O	1:B:500:ARG:NH1	2.37	0.57
1:C:129:LYS:NZ	1:C:166:GLU:OE1	2.35	0.57
2:G:70:LEU:HD12	2:G:81:MET:HE2	1.86	0.57
1:C:724:VAL:HG22	1:C:1067:VAL:HG12	1.85	0.57
1:C:987:ASP:C	1:C:989:PRO:HD3	2.30	0.57
1:B:143:HIS:O	1:B:144:LYS:HB2	2.04	0.57
3:K:49:ILE:HA	3:K:56:PRO:HD3	1.86	0.57
1:C:35:GLY:HA3	1:C:56:LEU:HD12	1.87	0.57
1:B:987:ASP:HB2	1:B:988:PRO:CD	2.35	0.57
1:C:440:SER:H	1:C:510:TYR:HA	1.68	0.57
1:B:900:PHE:N	1:B:901:PRO:CD	2.68	0.57
1:C:562:LEU:O	1:C:579:ARG:NH2	2.37	0.57
1:A:911:ILE:HD12	1:A:1049:TYR:HB3	1.87	0.57
1:C:28:TYR:HB3	6:C:1204:NAG:H2	1.85	0.56
1:C:333:ASN:HB2	1:C:334:ILE:CA	2.35	0.56
1:C:988:PRO:HD2	1:C:989:PRO:CG	2.34	0.56
1:A:943:THR:CB	1:A:944:PRO:CD	2.81	0.56
1:C:97:LYS:HB2	1:C:183:PHE:HA	1.87	0.56
1:C:100:ILE:HD11	1:C:143:HIS:CD2	2.40	0.56
3:J:9:SER:HA	3:J:108:LYS:H	1.70	0.56
1:B:131:CYS:SG	1:B:132:GLU:N	2.78	0.56
1:B:469:ASP:N	6:B:1201:NAG:O3	2.39	0.56
3:J:28:ASN:ND2	3:J:93:ASP:O	2.39	0.56
1:A:151:GLU:HA	1:A:154:PHE:CE2	2.41	0.56
1:C:806:GLN:HA	1:C:819:PRO:CG	2.36	0.56
1:B:144:LYS:O	1:B:145:ASN:C	2.49	0.56
1:A:533:THR:HG22	1:A:534:ASN:H	1.69	0.55
1:A:68:ILE:H	1:A:78:ARG:HG2	1.71	0.55
1:A:329:VAL:C	1:A:544:ASN:HB2	2.30	0.55
1:A:540:CYS:HA	1:A:553:VAL:HG12	1.88	0.55
1:A:813:LYS:NZ	1:A:822:ASP:OD2	2.39	0.55
1:C:536:VAL:HB	1:C:541:VAL:HG21	1.87	0.55
1:A:502:THR:HA	3:K:99:SER:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:PRO:C	1:B:901:PRO:CD	2.79	0.55
1:A:987:ASP:CG	1:A:988:PRO:CD	2.70	0.55
1:C:405:ARG:HA	1:C:509:PRO:HA	1.88	0.55
1:C:806:GLN:CA	1:C:819:PRO:HG2	2.36	0.55
1:A:143:HIS:HA	1:A:149:TRP:CZ3	2.37	0.55
1:A:456:ARG:NH1	1:A:471:SER:O	2.40	0.55
1:A:329:VAL:HG23	1:A:547:GLY:O	2.06	0.55
1:A:333:ASN:HB3	1:A:581:PRO:CA	2.37	0.54
2:I:17:SER:HA	2:I:83:LEU:O	2.07	0.54
1:C:151:GLU:HA	1:C:154:PHE:CZ	2.42	0.54
1:B:806:GLN:O	1:B:819:PRO:CG	2.55	0.54
1:C:646:GLN:HA	1:C:651:CYS:HA	1.90	0.54
1:C:901:PRO:CD	1:C:902:MET:N	2.68	0.54
1:A:146:ASN:HA	1:A:260:TRP:CB	2.37	0.54
1:C:569:ARG:HB2	1:A:44:ARG:HG2	1.90	0.54
1:B:988:PRO:N	1:B:989:PRO:HD3	2.21	0.54
1:A:557:SER:HB3	1:A:588:ASP:HB2	1.89	0.54
1:A:151:GLU:HA	1:A:154:PHE:CZ	2.42	0.54
1:C:83:VAL:HG12	1:C:238:GLN:HB2	1.90	0.54
1:C:813:LYS:NZ	1:C:822:ASP:OD2	2.41	0.54
1:B:806:GLN:NE2	1:B:937:GLN:OE1	2.41	0.54
1:A:97:LYS:HB2	1:A:183:PHE:HA	1.90	0.54
1:C:806:GLN:C	1:C:819:PRO:CG	2.81	0.53
1:A:724:VAL:HG22	1:A:1067:VAL:HG12	1.90	0.53
3:J:55:ARG:HH11	3:J:59:VAL:HB	1.73	0.53
1:B:503:TYR:O	1:B:508:GLN:NE2	2.42	0.53
1:C:151:GLU:HG3	1:C:154:PHE:CE2	2.44	0.53
1:C:1088:LYS:HD3	1:C:1124:VAL:HG21	1.91	0.53
2:H:69:THR:HB	2:H:82:GLU:HB2	1.89	0.53
1:B:1117:ILE:HG22	1:B:1139:VAL:HG23	1.91	0.53
1:B:619:CYS:HB2	1:B:623:PRO:HD3	1.90	0.53
1:A:331:PHE:CB	1:A:548:LEU:H	2.22	0.53
1:C:899:PRO:HB2	1:C:901:PRO:HD2	1.88	0.53
1:C:119:ILE:HG22	1:C:128:ILE:HG12	1.90	0.53
1:C:333:ASN:CG	1:C:546:ASN:HD21	2.17	0.53
1:A:358:LYS:HB2	1:A:399:ALA:HB3	1.91	0.53
1:A:988:PRO:N	1:A:989:PRO:CD	2.69	0.53
1:C:64:TRP:HE1	1:C:266:ALA:HB1	1.73	0.52
2:H:38:ARG:NH2	2:H:90:ASP:O	2.42	0.52
1:C:130:VAL:HG21	1:C:230:ILE:HD13	1.91	0.52
1:C:395:THR:HB	1:C:522:ALA:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:ASN:HB3	1:B:1072:ALA:HB3	1.90	0.52
1:A:719:ASN:HB3	1:A:1072:ALA:HB3	1.91	0.52
1:C:804:PHE:HD1	1:C:807:ILE:HD11	1.74	0.52
1:C:868:THR:HG23	1:C:870:GLU:H	1.74	0.52
1:C:558:ASN:O	1:C:560:LYS:NZ	2.43	0.52
1:A:734:THR:OG1	1:A:957:ASN:OD1	2.26	0.52
1:A:143:HIS:CE1	1:A:149:TRP:HE3	2.26	0.52
1:A:898:ILE:HD12	1:A:899:PRO:HD2	1.92	0.52
1:B:769:LEU:HG	1:B:1010:VAL:HG23	1.92	0.52
2:G:6:GLN:NE2	2:G:96:CYS:SG	2.81	0.52
1:A:186:LEU:HD23	1:A:208:ILE:HD13	1.91	0.52
1:B:630:GLN:H	1:B:636:ARG:HH12	1.58	0.52
1:C:329:VAL:HG12	1:C:549:LYS:HA	1.92	0.51
1:C:406:GLY:HA2	1:C:409:VAL:HB	1.92	0.51
1:B:102:ARG:HD3	1:B:149:TRP:HH2	1.76	0.51
1:A:868:THR:HG23	1:A:870:GLU:H	1.74	0.51
1:C:375:PRO:HB2	1:C:438:TRP:HB2	1.93	0.51
1:A:330:ARG:HG2	1:A:330:ARG:O	2.10	0.51
1:A:901:PRO:CD	1:A:902:MET:N	2.71	0.51
1:A:562:LEU:H	1:A:565:GLN:HG3	1.76	0.51
1:C:943:THR:OG1	1:C:944:PRO:HD3	2.10	0.51
1:C:184:LYS:HD2	1:C:207:ILE:HA	1.92	0.51
1:C:644:VAL:HG12	1:C:653:ILE:HG22	1.92	0.51
1:A:141:LEU:HD11	1:A:156:VAL:HG12	1.93	0.51
2:I:37:VAL:HG12	2:I:47:TRP:HA	1.91	0.51
1:B:142:ASP:HB3	1:B:241:LEU:O	2.11	0.51
3:J:2:SER:N	3:J:93:ASP:OD1	2.44	0.51
3:J:25:SER:OG	3:J:28:ASN:OD1	2.27	0.51
1:A:331:PHE:CB	1:A:548:LEU:HB3	2.30	0.51
1:B:607:SER:OG	1:B:608:ASN:N	2.44	0.51
1:A:14:GLN:HE21	1:A:141:LEU:HG	1.74	0.51
1:A:115:GLN:NE2	1:A:162:ASN:O	2.44	0.51
2:G:32:TYR:HA	2:G:101:GLY:HA2	1.93	0.51
1:A:355:TRP:O	1:A:468:ARG:NH1	2.44	0.50
1:C:827:LYS:NZ	1:C:940:LEU:O	2.45	0.50
1:B:172:PHE:HE2	1:B:187:ARG:HE	1.59	0.50
1:A:806:GLN:HA	1:A:819:PRO:HG2	1.92	0.50
2:I:6:GLN:HG3	2:I:114:GLY:H	1.75	0.50
3:K:4:LEU:HB3	3:K:104:GLY:HA2	1.94	0.50
1:C:443:LEU:HD22	1:C:511:ARG:HE	1.76	0.50
2:H:18:VAL:HG22	2:H:86:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASP:HB2	1:B:242:ALA:CA	2.41	0.50
1:B:944:PRO:HD2	1:B:945:SER:H	1.76	0.50
1:C:67:VAL:O	1:C:264:ALA:HA	2.12	0.50
1:B:312:LYS:HG3	1:B:602:PRO:HA	1.93	0.50
1:A:34:ARG:NH1	1:A:188:GLU:OE2	2.42	0.50
1:A:441:ASN:HB2	1:A:508:GLN:HB3	1.94	0.50
1:C:804:PHE:HB3	1:C:808:LEU:HD23	1.93	0.50
1:C:818:SER:CB	1:C:819:PRO:CD	2.84	0.50
1:A:100:ILE:HD12	1:A:265:ALA:HB2	1.93	0.50
1:C:184:LYS:HE2	1:C:209:VAL:HG12	1.94	0.50
1:A:642:SER:OG	1:A:643:ASN:N	2.45	0.50
1:C:146:ASN:CB	1:C:261:THR:H	2.25	0.50
2:H:39:GLN:HG3	2:H:45:PRO:HB3	1.93	0.50
1:B:526:VAL:HG13	1:B:527:CYS:H	1.75	0.50
1:A:332:PRO:O	1:A:545:PHE:HB3	2.12	0.50
1:A:356:ASN:OD1	1:A:358:LYS:NZ	2.45	0.50
1:C:502:THR:HA	3:L:99:SER:HB2	1.94	0.49
1:A:901:PRO:CD	1:A:902:MET:H	2.21	0.49
1:C:393:CYS:HA	1:C:527:CYS:HB3	1.93	0.49
1:B:152:SER:C	1:B:154:PHE:N	2.68	0.49
1:C:719:ASN:HB3	1:C:1072:ALA:HB3	1.94	0.49
1:B:80:ASP:N	1:B:80:ASP:OD1	2.45	0.49
1:B:421:ALA:HB1	1:B:426:LYS:HB3	1.95	0.49
1:B:1147:LEU:HA	1:B:1150:PHE:HB2	1.94	0.49
1:A:607:SER:OG	1:A:608:ASN:N	2.45	0.49
1:C:876:THR:HG21	1:C:1057:SER:HB3	1.94	0.49
1:C:860:LEU:HD13	1:C:961:LEU:HD12	1.95	0.49
2:H:47:TRP:HB3	3:L:101:TRP:HB2	1.93	0.49
1:A:118:LEU:HB3	1:A:129:LYS:HB2	1.95	0.49
1:C:121:ASN:HB3	1:C:126:VAL:HG22	1.95	0.49
1:C:294:ALA:O	1:C:634:THR:OG1	2.30	0.49
1:C:988:PRO:N	1:C:989:PRO:CD	2.73	0.49
1:A:329:VAL:HG11	1:A:549:LYS:HA	1.95	0.49
2:I:6:GLN:NE2	2:I:96:CYS:SG	2.75	0.49
1:A:14:GLN:HA	1:A:140:PHE:H	1.78	0.49
1:A:154:PHE:HB2	1:A:155:ARG:HH21	1.78	0.49
3:K:2:SER:OG	3:K:3:VAL:N	2.45	0.49
1:C:193:ASN:HB3	1:C:198:PHE:HD1	1.78	0.49
1:C:851:LEU:O	1:C:855:GLN:NE2	2.46	0.49
1:B:142:ASP:HB2	1:B:242:ALA:C	2.38	0.49
1:A:184:LYS:HB3	1:A:207:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:ASP:C	1:B:989:PRO:CD	2.81	0.48
1:B:468:ARG:HB3	6:B:1201:NAG:H83	1.95	0.48
1:B:899:PRO:CB	1:B:901:PRO:HD3	2.42	0.48
1:C:476:GLN:NE2	1:C:480:LYS:O	2.46	0.48
1:B:987:ASP:N	1:B:987:ASP:OD1	2.45	0.48
1:A:330:ARG:NH1	1:A:554:LEU:HD11	2.29	0.48
1:A:818:SER:CB	1:A:819:PRO:CD	2.85	0.48
1:C:110:LEU:HB2	1:C:236:ARG:HH22	1.78	0.48
1:B:737:SER:OG	1:B:861:THR:OG1	2.32	0.48
1:A:644:VAL:HG12	1:A:653:ILE:HG12	1.95	0.48
2:I:51:ILE:HG21	2:I:79:LEU:HD22	1.96	0.48
1:C:856:LYS:HG3	1:C:860:LEU:HB2	1.96	0.48
1:B:1129:ASP:OD1	1:B:1129:ASP:N	2.47	0.48
1:A:1088:LYS:HD3	1:A:1124:VAL:HG21	1.95	0.48
1:B:782:GLU:O	1:B:786:GLN:NE2	2.46	0.48
1:B:824:LEU:HD11	1:B:947:LEU:HD11	1.96	0.48
1:A:745:CYS:HB3	1:A:751:CYS:HB3	1.56	0.48
1:C:105:ILE:HD12	1:C:118:LEU:HD12	1.96	0.48
1:C:112:SER:HA	1:C:132:GLU:HB3	1.96	0.48
1:B:154:PHE:O	1:B:156:VAL:HG13	2.14	0.48
1:B:717:PRO:HA	1:B:1074:GLU:HA	1.96	0.48
1:C:341:ASP:HA	1:C:344:PHE:HD2	1.79	0.48
1:A:198:PHE:HB3	1:A:228:LEU:HB2	1.96	0.48
1:A:210:ARG:NH2	1:A:214:ASP:OD2	2.41	0.48
1:A:14:GLN:O	1:A:139:PRO:HB3	2.14	0.47
1:C:329:VAL:C	1:C:547:GLY:H	2.22	0.47
1:C:440:SER:HB3	1:C:509:PRO:C	2.39	0.47
1:C:987:ASP:OD1	1:C:987:ASP:N	2.42	0.47
1:A:330:ARG:HH12	1:A:554:LEU:HD11	1.78	0.47
1:A:397:VAL:HG12	1:A:517:PHE:HA	1.94	0.47
1:C:96:GLU:OE1	1:C:187:ARG:NH2	2.46	0.47
1:A:276:THR:HG23	1:A:293:CYS:HB3	1.96	0.47
1:A:346:ALA:O	1:A:511:ARG:NH1	2.47	0.47
1:A:130:VAL:HG21	1:A:230:ILE:HD12	1.96	0.47
1:A:329:VAL:O	1:A:547:GLY:N	2.43	0.47
1:A:364:VAL:HG21	1:A:530:LYS:HE3	1.97	0.47
1:B:102:ARG:O	1:B:102:ARG:NH1	2.48	0.47
1:B:459:ARG:NE	6:B:1201:NAG:O6	2.42	0.47
1:B:611:ALA:HB2	1:B:694:ILE:HD11	1.96	0.47
1:A:98:SER:HA	1:A:178:GLY:HA3	1.97	0.47
1:A:454:LEU:HD12	1:A:494:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:HD2	1:C:234:ILE:HD12	1.79	0.47
1:C:122:ASN:OD1	1:C:123:ALA:N	2.45	0.47
1:B:19:THR:OG1	1:B:20:THR:N	2.48	0.47
1:B:897:GLN:OE1	1:A:713:SER:OG	2.33	0.47
1:A:124:THR:HG22	6:A:1202:NAG:HN2	1.80	0.47
1:C:320:PHE:CE1	1:C:631:LEU:HD13	2.50	0.47
1:C:794:PRO:HG3	1:B:709:TYR:HB3	1.97	0.47
1:C:944:PRO:HD2	1:C:945:SER:N	2.30	0.47
2:H:52:ASN:HB3	2:H:57:GLY:H	1.79	0.47
1:B:420:ILE:HA	1:B:420:ILE:HD12	1.68	0.47
1:A:441:ASN:O	1:A:445:SER:HB2	2.14	0.47
2:H:35:HIS:HB2	2:H:97:ALA:HB3	1.96	0.47
1:B:988:PRO:CD	1:B:989:PRO:N	2.78	0.47
2:I:36:TRP:HB2	2:I:49:ALA:HB3	1.96	0.47
1:A:727:GLU:OE2	1:A:1066:HIS:NE2	2.47	0.46
1:A:987:ASP:CB	1:A:989:PRO:CD	2.86	0.46
1:C:146:ASN:HB2	1:C:261:THR:HB	1.97	0.46
1:C:344:PHE:HB3	1:C:438:TRP:HH2	1.79	0.46
1:A:1086:ASP:O	1:A:1088:LYS:NZ	2.46	0.46
1:C:328:ILE:HD13	1:C:543:PHE:HA	1.97	0.46
1:C:395:THR:HG22	1:C:524:ALA:HB2	1.97	0.46
1:B:894:PRO:O	1:B:894:PRO:CD	2.63	0.46
1:A:804:PHE:HB3	1:A:808:LEU:HD23	1.96	0.46
1:C:429:ASP:OD1	1:C:429:ASP:N	2.47	0.46
1:B:331:PHE:O	1:B:332:PRO:C	2.59	0.46
1:C:135:PHE:HZ	1:C:156:VAL:HB	1.79	0.46
1:C:440:SER:CB	1:C:511:ARG:HD3	2.43	0.46
1:C:448:SER:HB3	2:H:57:GLY:HA3	1.98	0.46
3:L:39:GLN:NE2	3:L:40:LEU:O	2.43	0.46
1:B:625:ALA:O	1:B:636:ARG:NH2	2.34	0.46
1:A:35:GLY:HA3	1:A:56:LEU:HD12	1.97	0.46
1:A:894:PRO:O	1:A:894:PRO:CD	2.64	0.46
1:C:664:CYS:HB2	1:C:673:CYS:HB3	1.61	0.46
1:B:142:ASP:HB3	1:B:242:ALA:HA	1.96	0.46
2:G:73:ASP:OD1	2:G:78:THR:OG1	2.29	0.46
1:C:210:ARG:NH2	1:C:214:ASP:OD2	2.38	0.46
1:C:987:ASP:C	1:C:989:PRO:CD	2.88	0.46
1:B:987:ASP:CB	1:B:989:PRO:HD3	2.45	0.46
1:B:1147:LEU:O	1:B:1151:LYS:N	2.43	0.46
1:A:169:SER:OG	1:A:170:GLN:N	2.46	0.46
1:B:1020:ILE:O	1:B:1024:ALA:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASP:OD1	1:A:40:ASP:N	2.48	0.46
1:C:968:LEU:O	1:C:977:SER:OG	2.33	0.46
1:C:1093:ARG:HH21	1:C:1123:PHE:HB3	1.80	0.46
1:A:122:ASN:OD1	1:A:123:ALA:N	2.47	0.46
1:A:804:PHE:HD1	1:A:807:ILE:HD11	1.80	0.46
1:C:709:TYR:HE1	1:A:899:PRO:HA	1.80	0.46
2:H:55:ASP:OD1	2:H:55:ASP:N	2.47	0.46
1:A:806:GLN:C	1:A:819:PRO:HG2	2.37	0.46
1:A:827:LYS:NZ	1:A:943:THR:O	2.43	0.46
2:H:93:VAL:HG22	2:H:116:LEU:HD13	1.97	0.45
1:B:150:MET:HG3	1:B:151:GLU:H	1.81	0.45
1:C:169:SER:OG	1:C:170:GLN:N	2.49	0.45
1:C:745:CYS:HB3	1:C:751:CYS:HB3	1.53	0.45
2:G:97:ALA:HB2	2:G:111:TRP:CD1	2.50	0.45
1:A:202:SER:H	1:A:225:LEU:HD23	1.80	0.45
1:A:331:PHE:N	1:A:548:LEU:H	2.14	0.45
1:A:744:ILE:HG21	1:A:999:ILE:HG13	1.98	0.45
1:A:943:THR:HG23	1:A:945:SER:H	1.81	0.45
1:C:981:ASP:OD1	1:C:985:ARG:NE	2.49	0.45
1:A:394:PHE:HD1	1:A:519:LEU:HD21	1.80	0.45
1:A:531:LYS:HA	1:A:531:LYS:HD2	1.74	0.45
2:G:93:VAL:HA	2:G:115:THR:O	2.16	0.45
1:C:894:PRO:O	1:C:894:PRO:CD	2.64	0.45
1:C:307:SER:OG	1:C:308:PHE:N	2.48	0.45
1:B:141:LEU:CA	1:B:152:SER:HB2	2.45	0.45
1:A:806:GLN:OE1	1:A:937:GLN:NE2	2.49	0.45
3:L:61:ASP:OD1	3:L:61:ASP:N	2.50	0.45
1:B:1141:ASP:H	1:B:1144:GLN:NE2	2.14	0.45
1:A:772:ILE:HD11	1:A:1014:LEU:HD22	1.99	0.45
2:H:30:SER:HA	2:H:53:PRO:HB2	1.99	0.45
1:B:204:HIS:CE1	1:B:206:PRO:HG3	2.52	0.45
1:A:333:ASN:CB	1:A:581:PRO:CB	2.75	0.45
2:H:52:ASN:O	2:H:56:GLY:HA2	2.17	0.45
1:A:447:VAL:HG11	2:I:50:ILE:HG12	1.98	0.45
1:A:664:CYS:HB2	1:A:673:CYS:HB3	1.68	0.45
1:C:642:SER:OG	1:C:643:ASN:N	2.49	0.44
1:C:868:THR:HG22	1:C:871:MET:HE3	1.98	0.44
1:B:357:ARG:NH2	1:B:400:ASP:OD2	2.50	0.44
1:A:329:VAL:O	1:A:544:ASN:HB2	2.18	0.44
1:B:469:ASP:OD1	6:B:1201:NAG:O3	2.33	0.44
1:A:533:THR:CG2	1:A:543:PHE:HB2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:PHE:HB2	1:C:633:PRO:HG3	1.99	0.44
1:C:772:ILE:HD11	1:C:1014:LEU:HD22	2.00	0.44
6:C:1205:NAG:O4	6:B:1201:NAG:O7	2.36	0.44
3:L:62:ARG:NH1	3:L:77:SER:O	2.41	0.44
1:B:899:PRO:HB3	1:A:711:ASN:HA	2.00	0.44
3:J:61:ASP:OD1	3:J:61:ASP:N	2.45	0.44
1:C:100:ILE:O	1:C:242:ALA:N	2.46	0.44
1:C:977:SER:OG	1:C:977:SER:O	2.35	0.44
1:A:330:ARG:HH22	1:A:554:LEU:HG	1.82	0.44
1:A:331:PHE:HB3	1:A:548:LEU:N	2.33	0.44
1:A:647:THR:OG1	1:A:650:GLY:O	2.33	0.44
1:A:806:GLN:HA	1:A:819:PRO:CG	2.48	0.44
1:A:806:GLN:C	1:A:819:PRO:CG	2.90	0.44
1:A:988:PRO:HD2	1:A:989:PRO:CG	2.46	0.44
3:J:2:SER:OG	3:J:3:VAL:N	2.50	0.44
1:C:1141:ASP:OD1	1:C:1141:ASP:N	2.51	0.44
1:B:44:ARG:HB3	1:A:569:ARG:HB2	1.99	0.44
1:B:944:PRO:CD	1:B:945:SER:N	2.80	0.44
2:G:39:GLN:HB2	2:G:45:PRO:HB3	1.98	0.44
3:J:36:TRP:CZ3	3:J:89:CYS:HB3	2.53	0.44
1:C:882:GLY:O	1:C:886:SER:OG	2.29	0.44
3:L:48:LEU:HD23	3:L:49:ILE:HB	1.99	0.44
1:A:554:LEU:HD12	1:A:587:LEU:HD13	1.99	0.44
3:J:48:LEU:HD12	3:J:49:ILE:HB	1.99	0.44
3:K:7:PRO:HA	3:K:8:PRO:HD3	1.93	0.44
4:Y:1:NAG:H62	4:Y:2:NAG:HN2	1.83	0.44
1:C:758:TYR:OH	1:C:996:ASP:OD1	2.34	0.44
1:C:583:THR:OG1	1:C:584:LEU:N	2.51	0.44
2:H:73:ASP:N	2:H:73:ASP:OD1	2.48	0.44
1:A:201:TYR:HD1	1:A:224:PRO:HA	1.83	0.44
1:A:944:PRO:HD2	1:A:945:SER:N	2.31	0.44
1:A:899:PRO:CB	1:A:901:PRO:HD3	2.44	0.44
1:A:1099:SER:HB3	1:A:1104:TRP:CD2	2.52	0.44
3:K:61:ASP:OD1	3:K:61:ASP:N	2.48	0.44
1:A:14:GLN:NE2	1:A:153:GLU:O	2.51	0.43
1:B:1141:ASP:H	1:B:1144:GLN:HE22	1.66	0.43
1:A:411:GLN:HA	1:A:416:GLN:HG3	1.99	0.43
1:C:788:LYS:HB2	1:C:788:LYS:HE2	1.78	0.43
1:B:86:PHE:HB2	1:B:237:PHE:HD1	1.83	0.43
2:I:55:ASP:N	2:I:55:ASP:OD1	2.47	0.43
3:L:38:GLN:HB2	3:L:48:LEU:HD12	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:VAL:HG12	2:H:104:TRP:HB3	2.01	0.43
1:A:143:HIS:CE1	1:A:149:TRP:CE3	3.07	0.43
1:A:353:TYR:HE1	1:A:454:LEU:HG	1.84	0.43
1:C:113:LYS:HA	1:C:113:LYS:HD3	1.88	0.43
1:C:445:SER:OG	1:C:499:PHE:O	2.33	0.43
3:L:25:SER:OG	3:L:26:SER:N	2.51	0.43
1:B:100:ILE:CG2	1:B:241:LEU:HG	2.49	0.43
1:B:106:PHE:HB3	1:B:234:ILE:HG12	2.00	0.43
1:B:292:ASP:OD1	1:B:292:ASP:N	2.52	0.43
1:B:899:PRO:HB2	1:B:901:PRO:HD2	1.94	0.43
3:K:38:GLN:HB2	3:K:48:LEU:HD22	2.00	0.43
1:C:711:ASN:HA	1:A:899:PRO:HB3	1.99	0.43
1:B:152:SER:C	1:B:154:PHE:H	2.27	0.43
1:B:773:ALA:C	1:B:775:GLU:N	2.76	0.43
1:C:985:ARG:HG2	1:B:392:LEU:HD21	2.01	0.43
1:B:731:VAL:HG23	1:B:1061:GLY:HA2	2.01	0.43
1:B:1092:PRO:HG3	1:B:1096:VAL:HA	2.01	0.43
1:C:99:ASN:O	1:C:102:ARG:NH1	2.34	0.43
1:B:421:ALA:HA	1:B:425:TYR:O	2.18	0.43
1:B:824:LEU:HD13	1:B:940:LEU:HD23	2.00	0.43
1:B:1083:ILE:O	1:B:1090:HIS:N	2.50	0.43
1:A:328:ILE:N	1:A:542:ASN:O	2.51	0.43
1:C:911:ILE:HD12	1:C:1049:TYR:HB3	2.00	0.42
1:B:426:LYS:HG3	1:B:427:LEU:H	1.84	0.42
1:A:806:GLN:CA	1:A:819:PRO:HG2	2.48	0.42
3:K:18:VAL:HG11	3:K:109:LEU:HD11	2.01	0.42
1:B:907:ARG:NH1	1:B:1051:LEU:O	2.52	0.42
1:A:981:ASP:OD2	1:A:985:ARG:NE	2.45	0.42
1:B:181:GLY:H	1:B:183:PHE:HE1	1.67	0.42
1:B:647:THR:OG1	1:B:648:ARG:N	2.53	0.42
1:B:987:ASP:CG	1:B:989:PRO:HD3	2.44	0.42
1:C:648:ARG:NH2	1:C:670:ALA:O	2.52	0.42
1:C:1051:LEU:HB2	1:C:1067:VAL:HG23	2.00	0.42
1:A:154:PHE:HB2	1:A:155:ARG:NH2	2.34	0.42
1:B:310:VAL:H	1:B:604:THR:HG1	1.67	0.42
1:B:334:ILE:O	1:B:335:THR:HG23	2.20	0.42
1:B:1033:GLU:HB3	1:B:1039:SER:HB3	2.01	0.42
1:A:305:LEU:HD12	1:A:310:VAL:HG12	2.01	0.42
1:B:127:VAL:HA	1:B:168:VAL:HG22	2.01	0.42
1:B:950:LEU:HD21	1:B:1061:GLY:HA3	2.02	0.42
1:A:336:ASN:O	1:A:530:LYS:NZ	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:GLY:HA3	1:C:516:SER:HA	2.01	0.42
3:L:17:ARG:HE	3:L:77:SER:HB2	1.85	0.42
1:A:328:ILE:O	1:A:542:ASN:HB3	2.20	0.42
1:A:882:GLY:O	1:A:886:SER:OG	2.28	0.42
1:C:227:ASP:OD1	1:C:227:ASP:N	2.50	0.42
1:C:339:PRO:HG2	1:C:360:ILE:HD12	2.02	0.42
1:C:607:SER:OG	1:C:608:ASN:N	2.53	0.42
1:C:341:ASP:O	1:C:345:ASN:N	2.53	0.42
1:B:728:ILE:HG13	1:B:1063:VAL:HG22	2.01	0.42
1:B:100:ILE:HG21	1:B:241:LEU:HG	2.02	0.41
1:B:1007:GLN:HA	1:B:1010:VAL:HG12	2.02	0.41
1:A:355:TRP:CD1	1:A:355:TRP:H	2.37	0.41
1:B:42:VAL:HG22	1:A:567:PHE:HD2	1.85	0.41
1:B:386:PRO:HA	1:B:389:LEU:HD12	2.01	0.41
1:C:423:TYR:HB3	1:C:456:ARG:NH1	2.35	0.41
1:C:1075:LYS:HA	1:C:1075:LYS:HD2	1.91	0.41
1:A:40:ASP:OD2	1:A:44:ARG:NH2	2.53	0.41
1:A:456:ARG:HB2	1:A:494:LEU:HD23	2.02	0.41
1:A:911:ILE:HD13	1:A:911:ILE:HA	1.87	0.41
1:C:96:GLU:O	1:C:185:ASN:HB2	2.20	0.41
1:C:572:ALA:HB2	1:A:855:GLN:HB2	2.01	0.41
3:L:7:PRO:HA	3:L:8:PRO:HD3	1.90	0.41
1:B:109:THR:OG1	1:B:114:THR:OG1	2.28	0.41
1:B:745:CYS:HB3	1:B:751:CYS:HB3	1.43	0.41
1:A:327:SER:CA	1:A:542:ASN:HB2	2.48	0.41
1:B:1088:LYS:HA	1:B:1127:ASN:HA	2.01	0.41
1:A:739:ASP:N	1:A:739:ASP:OD1	2.48	0.41
1:B:988:PRO:N	1:B:989:PRO:CD	2.84	0.41
1:A:393:CYS:HA	1:A:527:CYS:HB3	2.02	0.41
1:C:100:ILE:HD11	1:C:143:HIS:HD2	1.86	0.41
1:C:367:TYR:HD1	1:C:389:LEU:HG	1.86	0.41
2:H:6:GLN:HG3	2:H:114:GLY:N	2.35	0.41
1:C:149:TRP:HA	1:C:149:TRP:CE3	2.56	0.41
1:C:326:GLU:HB2	1:C:542:ASN:H	1.85	0.41
1:C:333:ASN:N	1:C:334:ILE:HG13	2.36	0.41
1:C:1020:ILE:O	1:C:1024:ALA:N	2.46	0.41
1:B:167:TYR:CE2	1:B:169:SER:HB2	2.56	0.41
1:A:37:TYR:OH	1:A:192:LYS:NZ	2.42	0.41
1:A:134:GLN:OE1	1:A:159:SER:OG	2.31	0.41
1:A:331:PHE:HB3	1:A:548:LEU:H	1.85	0.41
1:A:508:GLN:HB2	1:A:510:TYR:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:SER:HA	1:A:1036:LEU:HD12	2.03	0.41
2:G:47:TRP:CG	3:J:101:TRP:HB2	2.56	0.41
1:C:719:ASN:OD1	1:C:720:PHE:N	2.53	0.41
2:H:12:LYS:HA	2:H:12:LYS:HD3	1.83	0.41
1:B:328:ILE:O	1:B:328:ILE:HD12	2.21	0.41
1:A:328:ILE:H	1:A:542:ASN:HB2	1.86	0.41
3:J:4:LEU:HB3	3:J:104:GLY:HA2	2.02	0.41
1:C:709:TYR:HB3	1:A:794:PRO:HG3	2.03	0.40
1:C:1107:THR:HG22	1:C:1114:PRO:HA	2.03	0.40
1:A:296:ASP:OD1	1:A:296:ASP:N	2.53	0.40
1:A:352:VAL:HG22	1:A:404:ILE:HG22	2.03	0.40
1:A:1107:THR:HG22	1:A:1114:PRO:HA	2.02	0.40
5:U:2:NAG:H61	5:U:3:BMA:H2	2.03	0.40
1:C:233:ASN:HB2	6:C:1205:NAG:H82	2.03	0.40
1:C:324:PRO:HB2	1:C:542:ASN:HD21	1.86	0.40
1:C:935:LYS:HE3	1:C:935:LYS:HB2	1.90	0.40
1:C:1097:PHE:HE1	1:C:1117:ILE:HD12	1.86	0.40
1:A:141:LEU:N	1:A:141:LEU:HD12	2.36	0.40
1:A:328:ILE:HB	1:A:544:ASN:H	1.86	0.40
2:G:35:HIS:HB2	2:G:97:ALA:HB3	2.02	0.40
2:G:98:ARG:HB3	2:G:109:ASP:HB2	2.02	0.40
1:B:463:LEU:HD12	1:B:463:LEU:HA	1.87	0.40
1:B:902:MET:HE3	1:B:902:MET:HB2	1.82	0.40
1:C:554:LEU:HD12	1:C:587:LEU:HD13	2.04	0.40
1:C:855:GLN:H	1:C:855:GLN:HG2	1.70	0.40
1:B:187:ARG:HG2	1:B:204:HIS:CD2	2.57	0.40
1:C:124:THR:HA	1:C:171:PRO:HG3	2.03	0.40
1:C:151:GLU:HG3	1:C:154:PHE:HE2	1.86	0.40
3:L:28:ASN:C	3:L:28:ASN:HD22	2.29	0.40
1:B:435:VAL:HG23	1:B:514:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1088/1149 (95%)	996 (92%)	87 (8%)	5 (0%)	24	57
1	B	1088/1149 (95%)	991 (91%)	90 (8%)	7 (1%)	21	54
1	C	1088/1149 (95%)	993 (91%)	89 (8%)	6 (1%)	21	54
2	G	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	H	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
2	I	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
3	J	107/109 (98%)	97 (91%)	10 (9%)	0	100	100
3	K	107/109 (98%)	93 (87%)	14 (13%)	0	100	100
3	L	107/109 (98%)	97 (91%)	10 (9%)	0	100	100
All	All	3933/4128 (95%)	3600 (92%)	315 (8%)	18 (0%)	26	57

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	543	PHE
1	C	445	SER
1	B	144	LYS
1	B	526	VAL
1	B	529	PRO
1	A	328	ILE
1	C	583	THR
1	B	153	GLU
1	A	331	PHE
1	C	334	ILE
1	A	335	THR
1	B	154	PHE
1	B	625	ALA
1	C	331	PHE
1	B	332	PRO
1	A	521	HIS
1	A	207	ILE
1	C	207	ILE

### 5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	967/1003 (96%)	952 (98%)	15 (2%)	55	69
1	B	967/1003 (96%)	953 (99%)	14 (1%)	59	71
1	C	967/1003 (96%)	957 (99%)	10 (1%)	68	75
2	G	89/95 (94%)	88 (99%)	1 (1%)	65	74
2	H	89/95 (94%)	89 (100%)	0	100	100
2	I	81/95 (85%)	81 (100%)	0	100	100
3	J	86/87 (99%)	86 (100%)	0	100	100
3	K	86/87 (99%)	85 (99%)	1 (1%)	63	73
3	L	86/87 (99%)	86 (100%)	0	100	100
All	All	3418/3555 (96%)	3377 (99%)	41 (1%)	61	73

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	149	TRP
1	C	321	ARG
1	C	329	VAL
1	C	333	ASN
1	C	592	CYS
1	C	631	LEU
1	C	632	THR
1	C	741	THR
1	C	762	CYS
1	C	765	LEU
1	B	144	LYS
1	B	149	TRP
1	B	153	GLU
1	B	154	PHE
1	B	241	LEU
1	B	320	PHE
1	B	323	GLN
1	B	334	ILE
1	B	420	ILE
1	B	526	VAL
1	B	527	CYS
1	B	533	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	767	ARG
1	B	770	THR
1	A	325	THR
1	A	328	ILE
1	A	329	VAL
1	A	332	PRO
1	A	333	ASN
1	A	334	ILE
1	A	335	THR
1	A	445	SER
1	A	548	LEU
1	A	549	LYS
1	A	593	SER
1	A	631	LEU
1	A	747	ASP
1	A	762	CYS
1	A	766	LYS
2	G	113	GLN
3	K	94	ASP

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	23	GLN
1	C	115	GLN
1	C	180	GLN
1	C	450	ASN
1	C	476	GLN
1	C	542	ASN
1	C	546	ASN
1	C	582	GLN
1	C	764	GLN
1	C	874	GLN
1	C	1103	HIS
3	L	28	ASN
3	L	32	ASN
1	B	99	ASN
1	B	204	HIS
1	B	489	ASN
1	B	542	ASN
1	B	630	GLN
1	B	786	GLN

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Mol	Chain	Res	Type
1	B	957	ASN
1	B	962	ASN
1	B	994	GLN
1	A	14	GLN
1	A	99	ASN
1	A	333	ASN
1	A	439	ASN
1	A	452	ASN
1	A	462	ASN
1	A	507	HIS
1	A	781	GLN
1	A	994	GLN
3	K	6	GLN
3	K	32	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

42 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	1	1,4	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	E	1	4	14,14,15	0.73	1 (7%)	17,19,21	2.11	2 (11%)
4	NAG	E	2	4	14,14,15	0.32	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	F	1	1,4	14,14,15	0.51	0	17,19,21	0.73	1 (5%)
4	NAG	F	2	4	14,14,15	0.36	0	17,19,21	0.45	0
5	NAG	M	1	1,5	14,14,15	0.20	0	17,19,21	0.48	0
5	NAG	M	2	5	14,14,15	0.26	0	17,19,21	0.46	0
5	BMA	M	3	5	11,11,12	1.33	2 (18%)	15,15,17	1.52	2 (13%)
5	NAG	N	1	1,5	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	N	2	5	14,14,15	0.32	0	17,19,21	0.40	0
5	BMA	N	3	5	11,11,12	0.68	0	15,15,17	0.79	0
4	NAG	O	1	4	14,14,15	0.43	0	17,19,21	0.38	0
4	NAG	O	2	4	14,14,15	0.31	0	17,19,21	0.46	0
4	NAG	P	1	4	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	P	2	4	14,14,15	0.31	0	17,19,21	0.47	0
4	NAG	Q	1	1,4	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	Q	2	4	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	R	1	4	14,14,15	0.21	0	17,19,21	0.54	0
4	NAG	R	2	4	14,14,15	0.36	0	17,19,21	0.40	0
4	NAG	S	1	1,4	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	S	2	4	14,14,15	0.33	0	17,19,21	0.50	0
5	NAG	T	1	1,5	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	T	2	5	14,14,15	0.23	0	17,19,21	0.49	0
5	BMA	T	3	5	11,11,12	0.64	0	15,15,17	0.83	0
5	NAG	U	1	1,5	14,14,15	0.22	0	17,19,21	0.52	0
5	NAG	U	2	5	14,14,15	0.27	0	17,19,21	0.54	0
5	BMA	U	3	5	11,11,12	0.72	0	15,15,17	0.75	0
4	NAG	V	1	1,4	14,14,15	0.44	0	17,19,21	0.43	0
4	NAG	V	2	4	14,14,15	0.33	0	17,19,21	0.45	0
4	NAG	W	1	1,4	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	W	2	4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	X	1	4	14,14,15	0.72	1 (7%)	17,19,21	2.12	2 (11%)
4	NAG	X	2	4	14,14,15	0.33	0	17,19,21	0.49	0
4	NAG	Y	1	1,4	14,14,15	0.62	0	17,19,21	1.14	1 (5%)
4	NAG	Y	2	4	14,14,15	0.44	0	17,19,21	0.50	0
5	NAG	Z	1	1,5	14,14,15	0.22	0	17,19,21	0.49	0
5	NAG	Z	2	5	14,14,15	0.25	0	17,19,21	0.45	0
5	BMA	Z	3	5	11,11,12	1.29	2 (18%)	15,15,17	1.49	1 (6%)
5	NAG	a	1	1,5	14,14,15	0.31	0	17,19,21	0.51	0
5	NAG	a	2	5	14,14,15	0.27	0	17,19,21	0.43	0
5	BMA	a	3	5	11,11,12	0.65	0	15,15,17	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4	-	5/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
4	NAG	O	1	4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	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	-	4/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	1/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	U	2	5	-	4/6/23/26	0/1/1/1
5	BMA	U	3	5	-	0/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4	-	6/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Z	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	0/2/19/22	0/1/1/1
5	NAG	a	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	3	BMA	C1-C2	2.54	1.58	1.52
5	M	3	BMA	C2-C3	2.45	1.56	1.52
5	Z	3	BMA	C1-C2	2.39	1.57	1.52
5	Z	3	BMA	C2-C3	2.33	1.56	1.52
4	E	1	NAG	C1-C2	2.24	1.55	1.52
4	X	1	NAG	C1-C2	2.20	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	1	NAG	C2-N2-C7	7.35	132.75	122.90
4	E	1	NAG	C2-N2-C7	7.34	132.74	122.90
5	M	3	BMA	C1-O5-C5	4.40	118.08	112.19
5	Z	3	BMA	C1-O5-C5	4.30	117.95	112.19
4	Y	1	NAG	C1-O5-C5	4.11	117.69	112.19
4	X	1	NAG	C1-C2-N2	3.60	116.11	110.43
4	E	1	NAG	C1-C2-N2	3.56	116.05	110.43
4	F	1	NAG	C1-O5-C5	2.38	115.37	112.19
5	M	3	BMA	C1-C2-C3	2.04	112.61	109.64

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	V	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
5	U	2	NAG	C8-C7-N2-C2
5	U	2	NAG	O7-C7-N2-C2
5	N	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6

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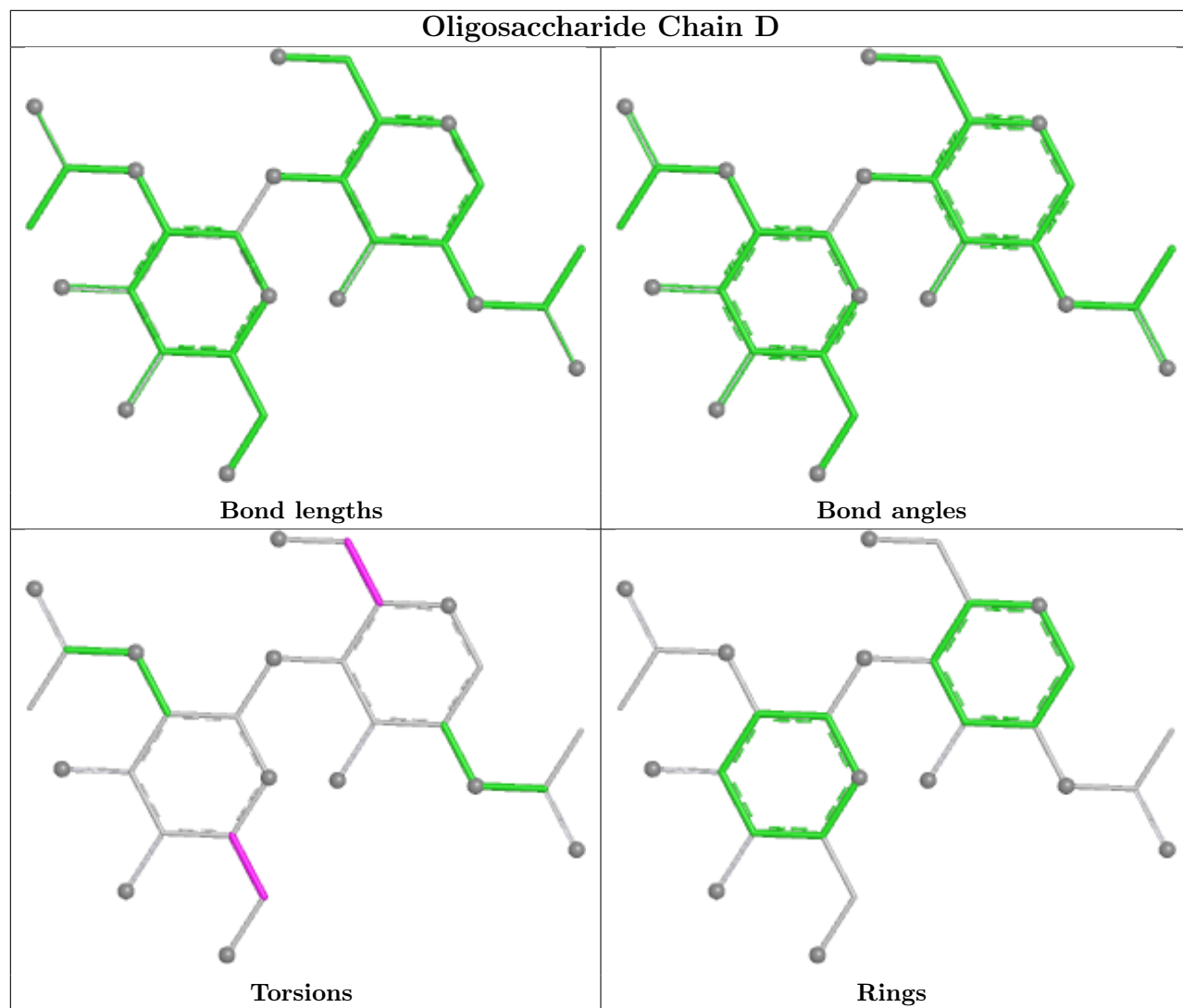
Mol	Chain	Res	Type	Atoms
4	W	1	NAG	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7
4	X	1	NAG	C1-C2-N2-C7
4	E	1	NAG	C3-C2-N2-C7
4	X	1	NAG	C3-C2-N2-C7
4	E	1	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

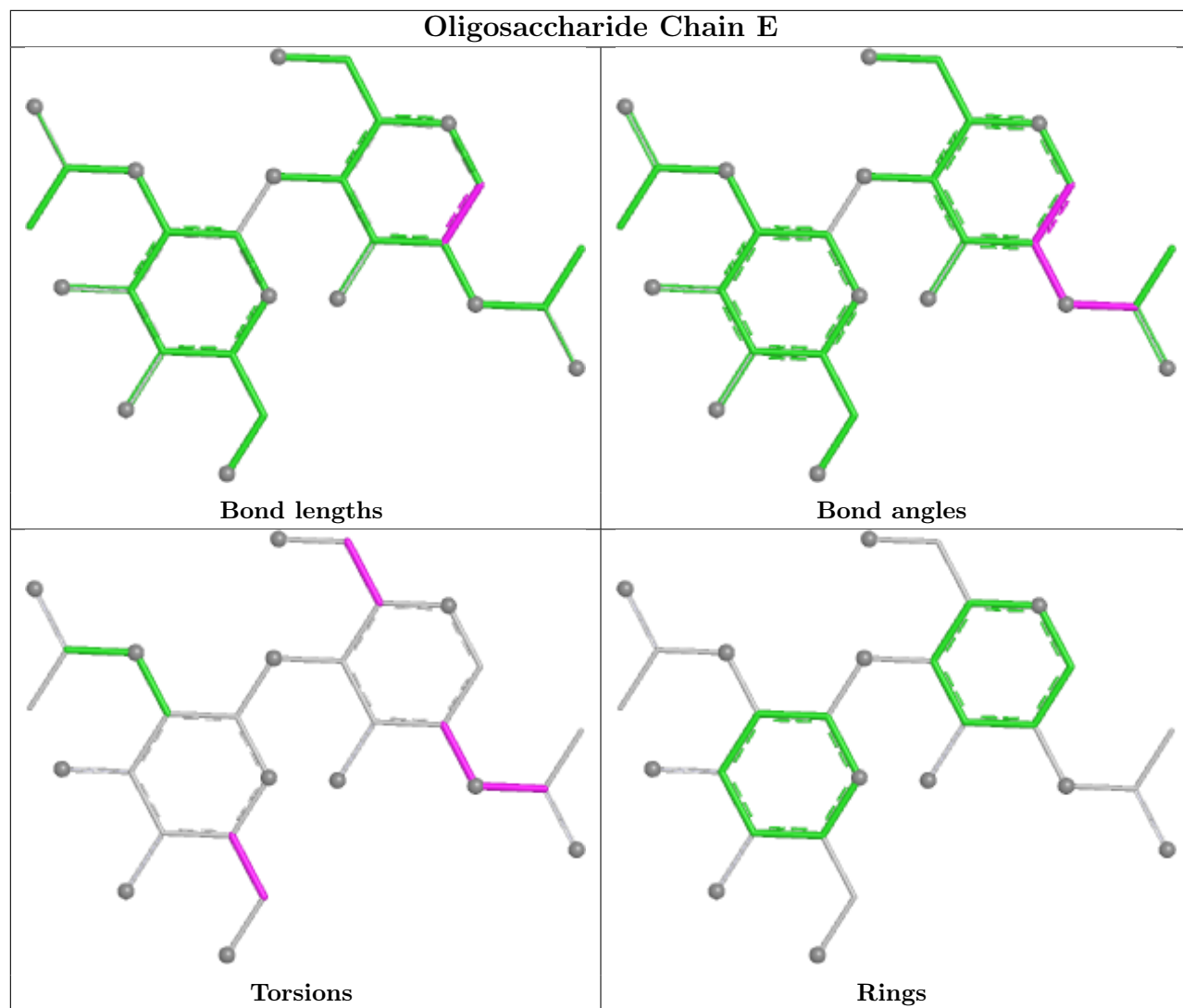
There are no ring outliers.

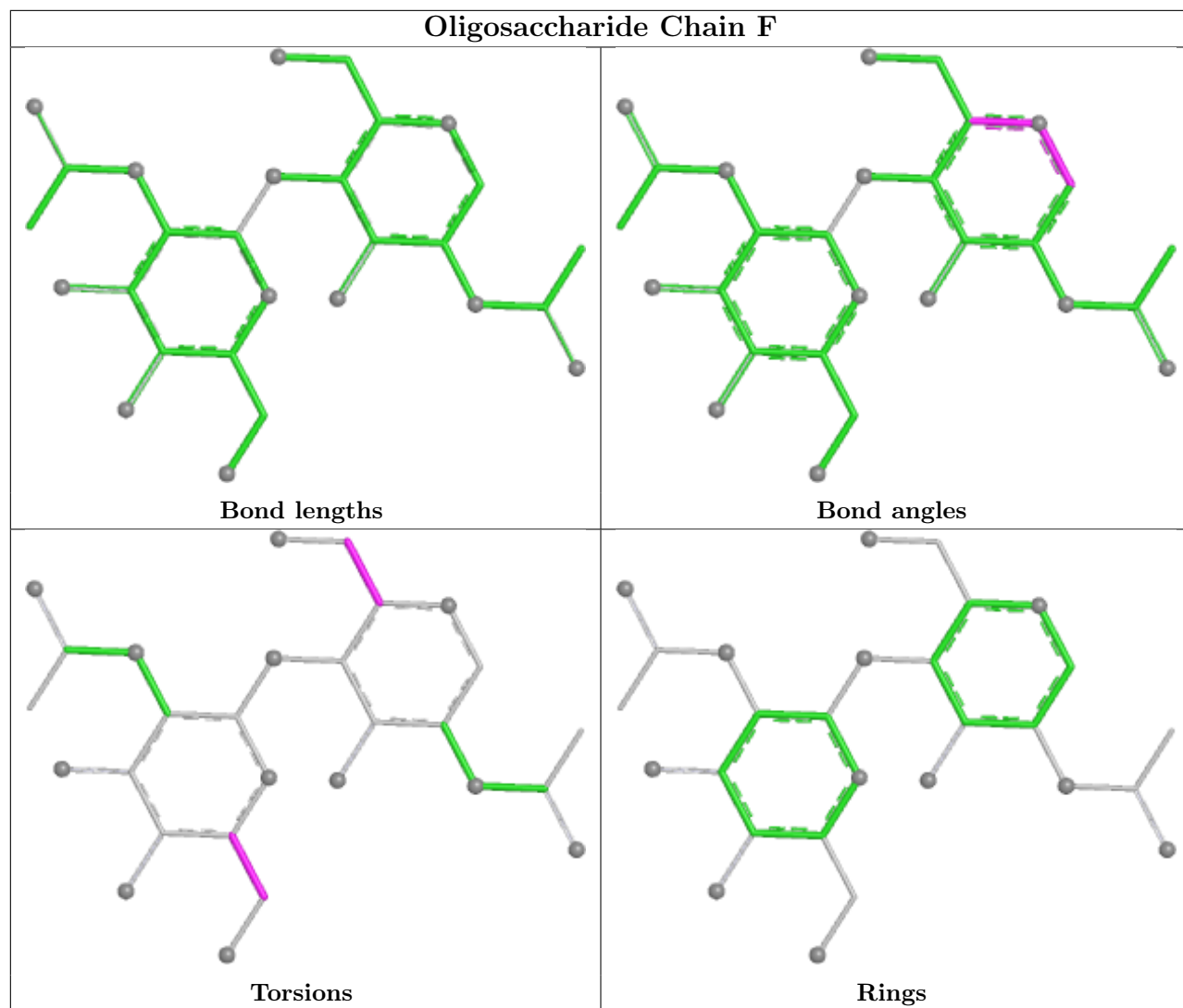
4 monomers are involved in 2 short contacts:

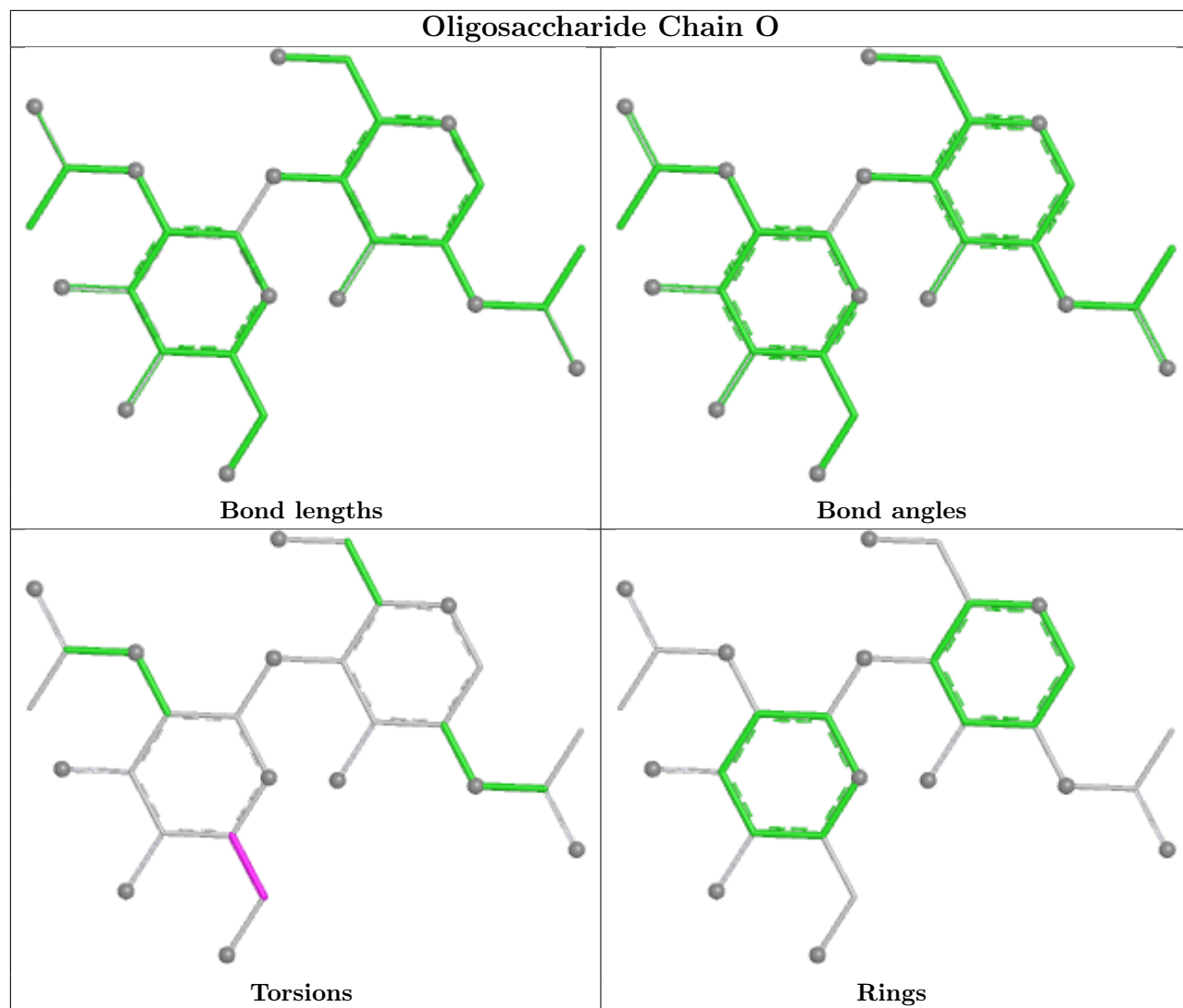
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	1	NAG	1	0
4	Y	2	NAG	1	0
5	U	2	NAG	1	0
5	U	3	BMA	1	0

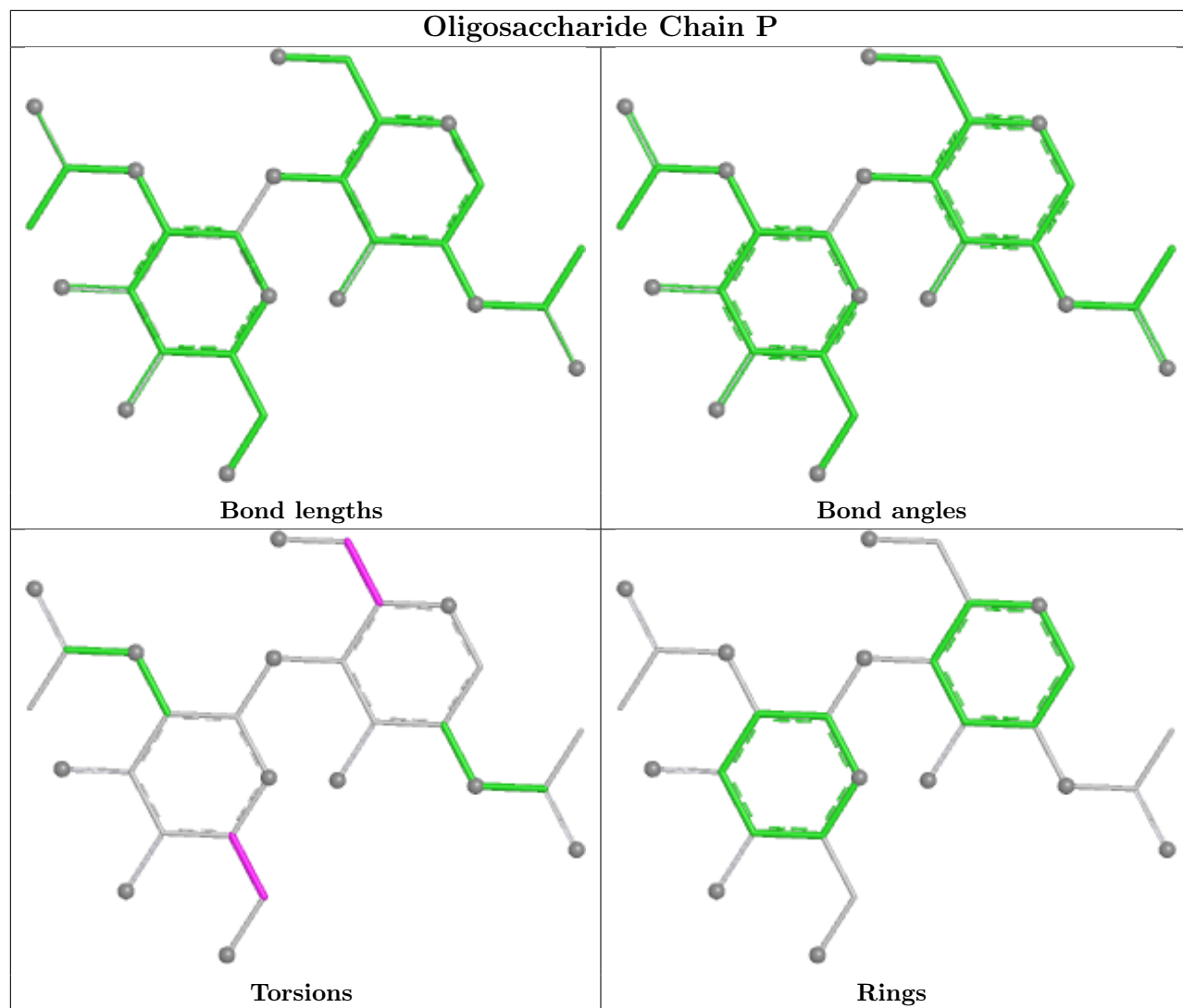
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

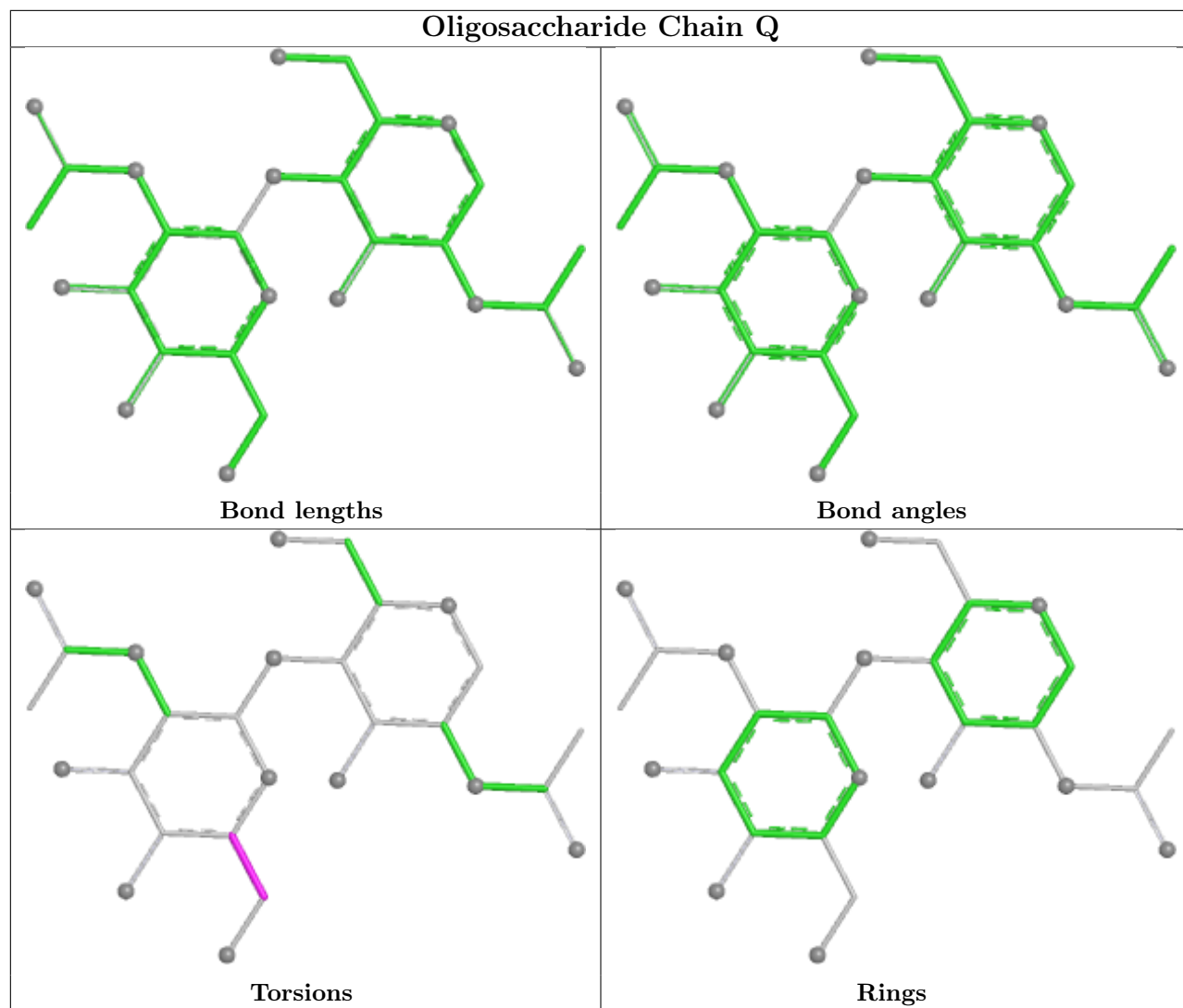


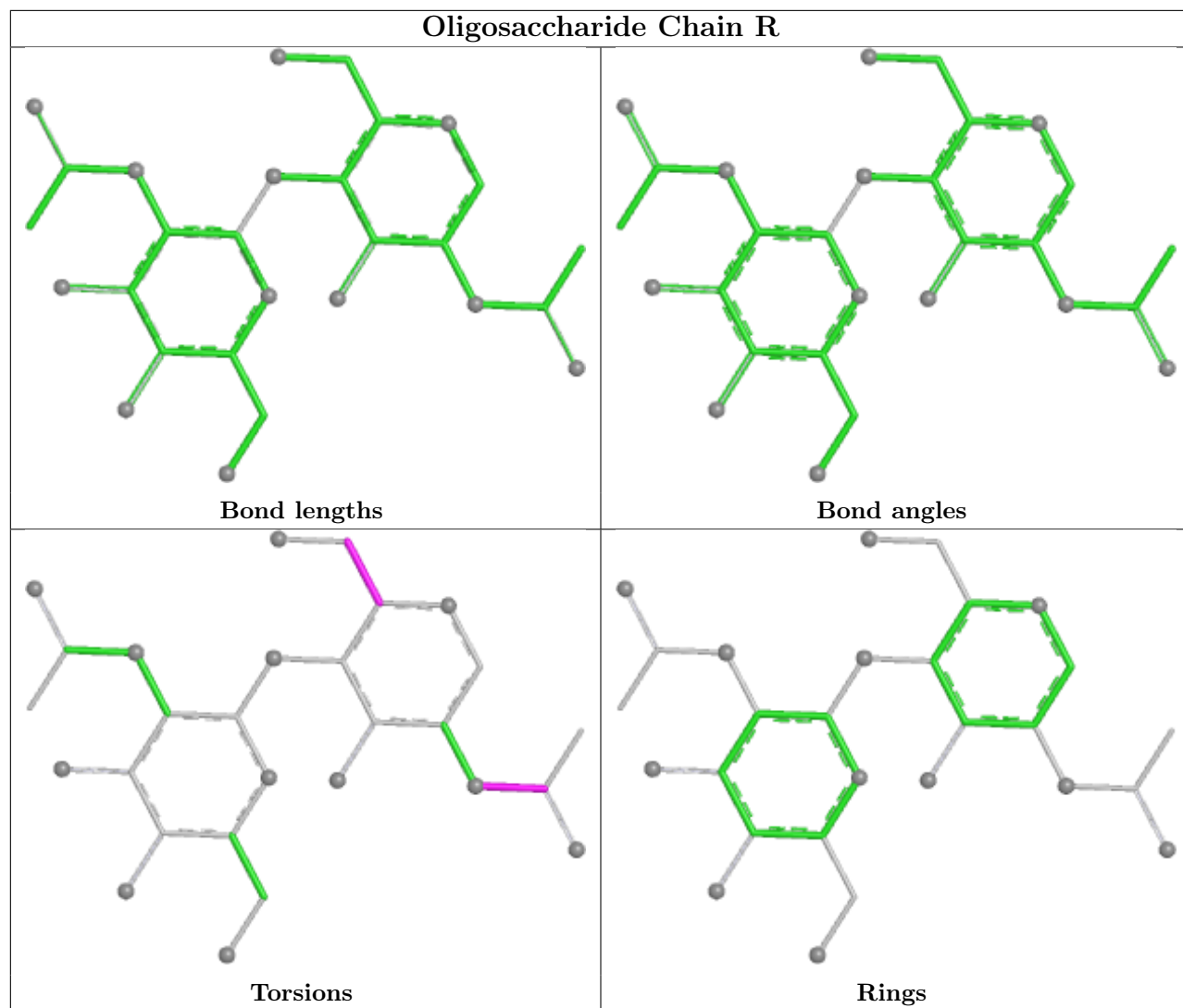


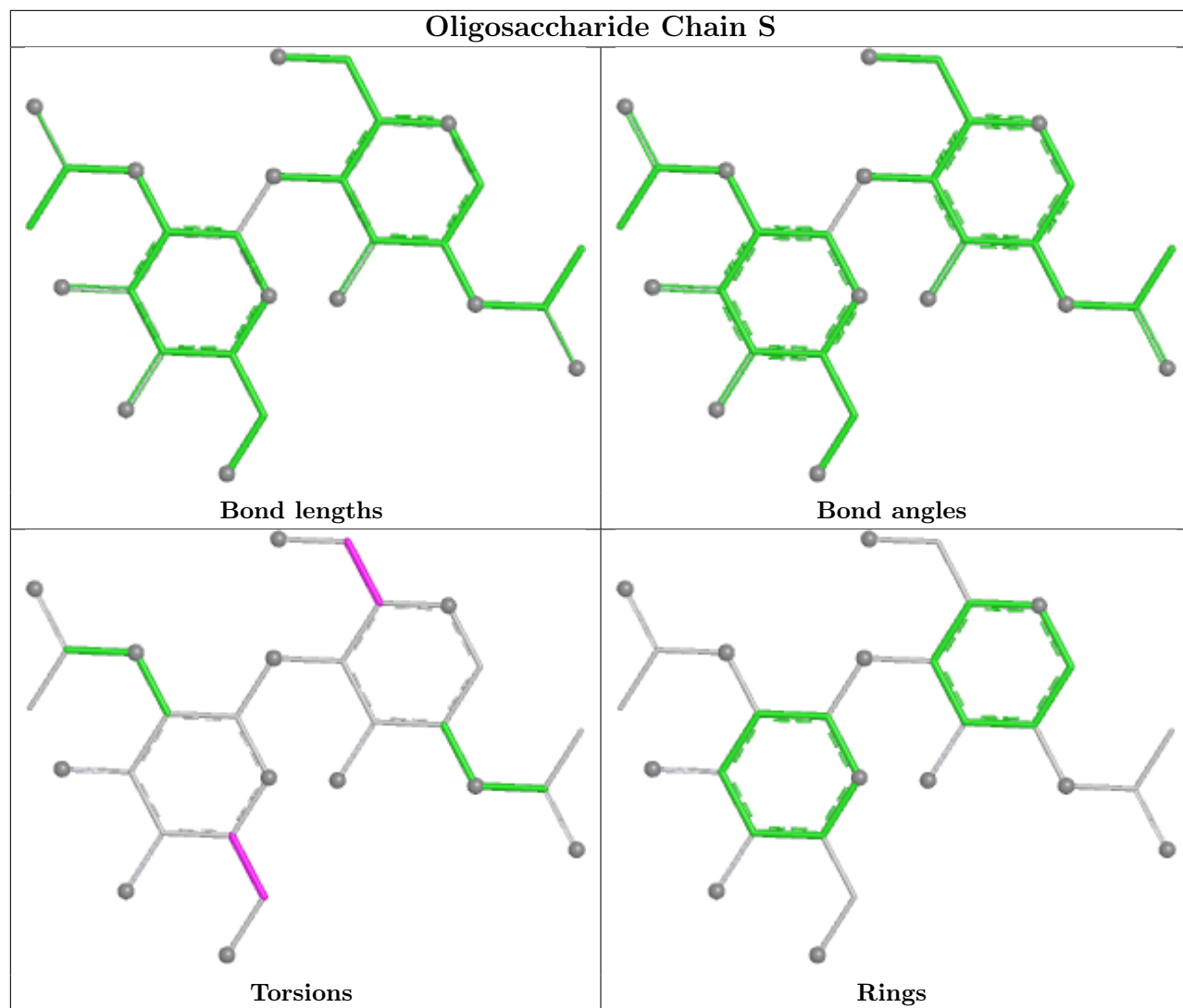


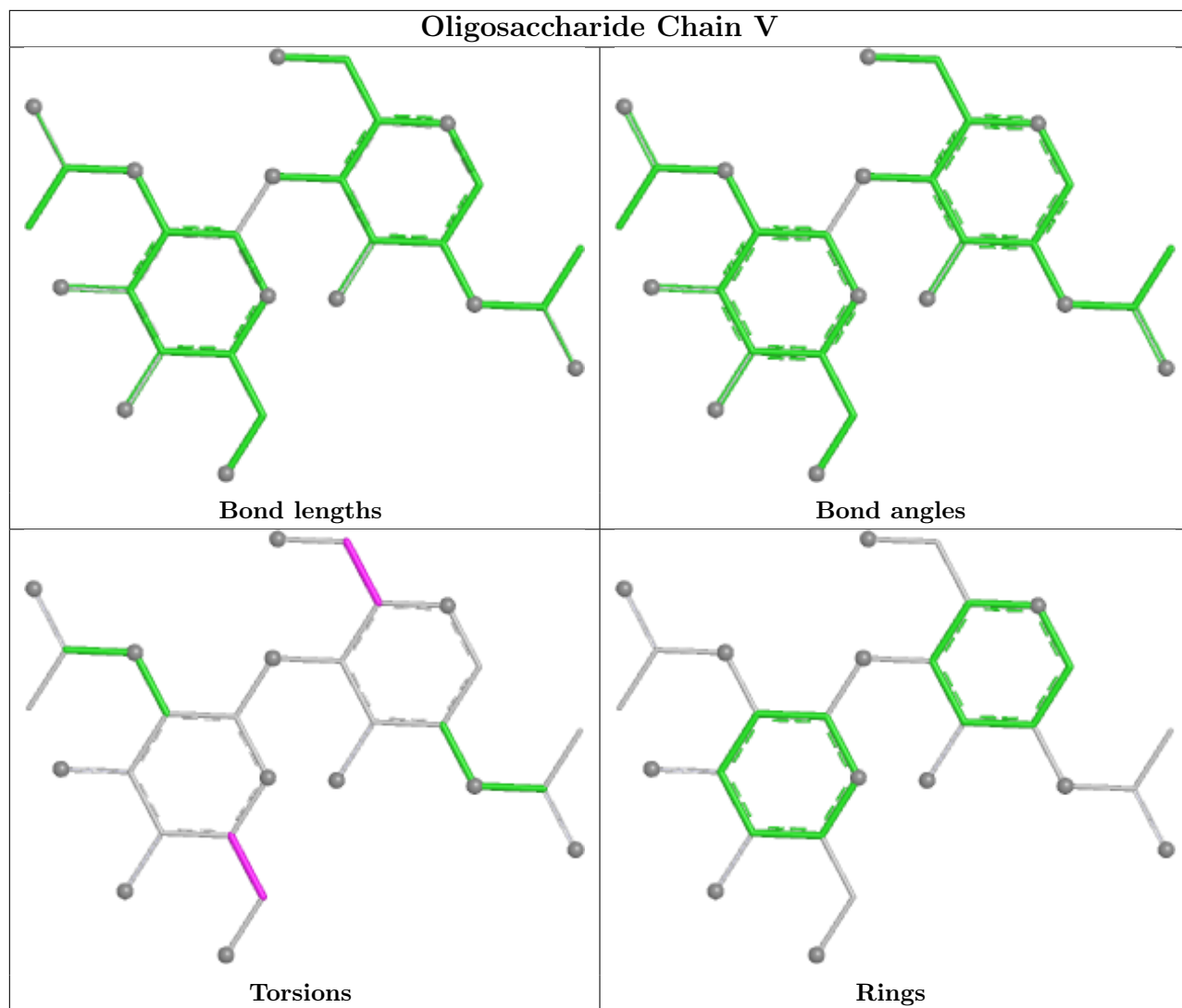


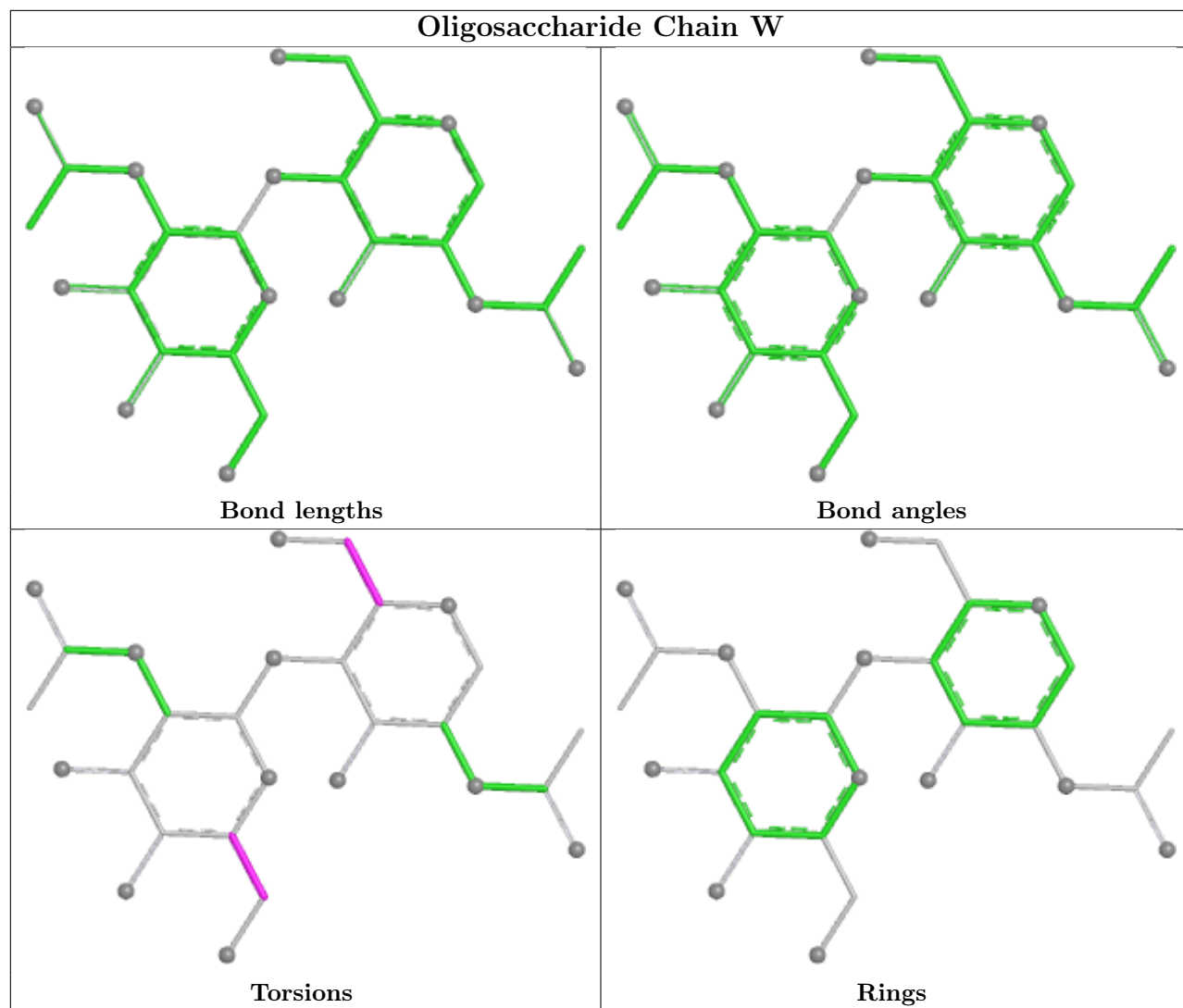


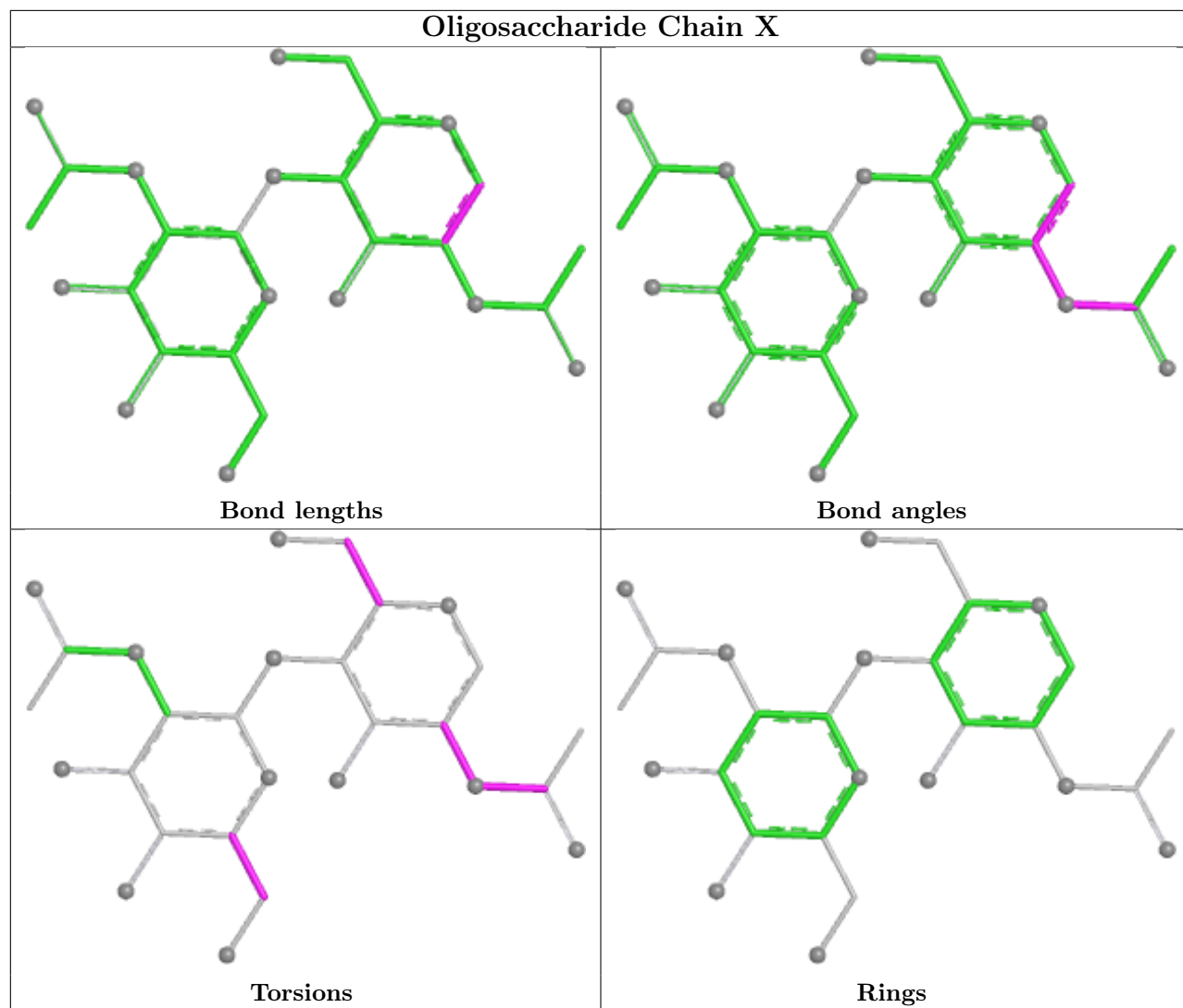


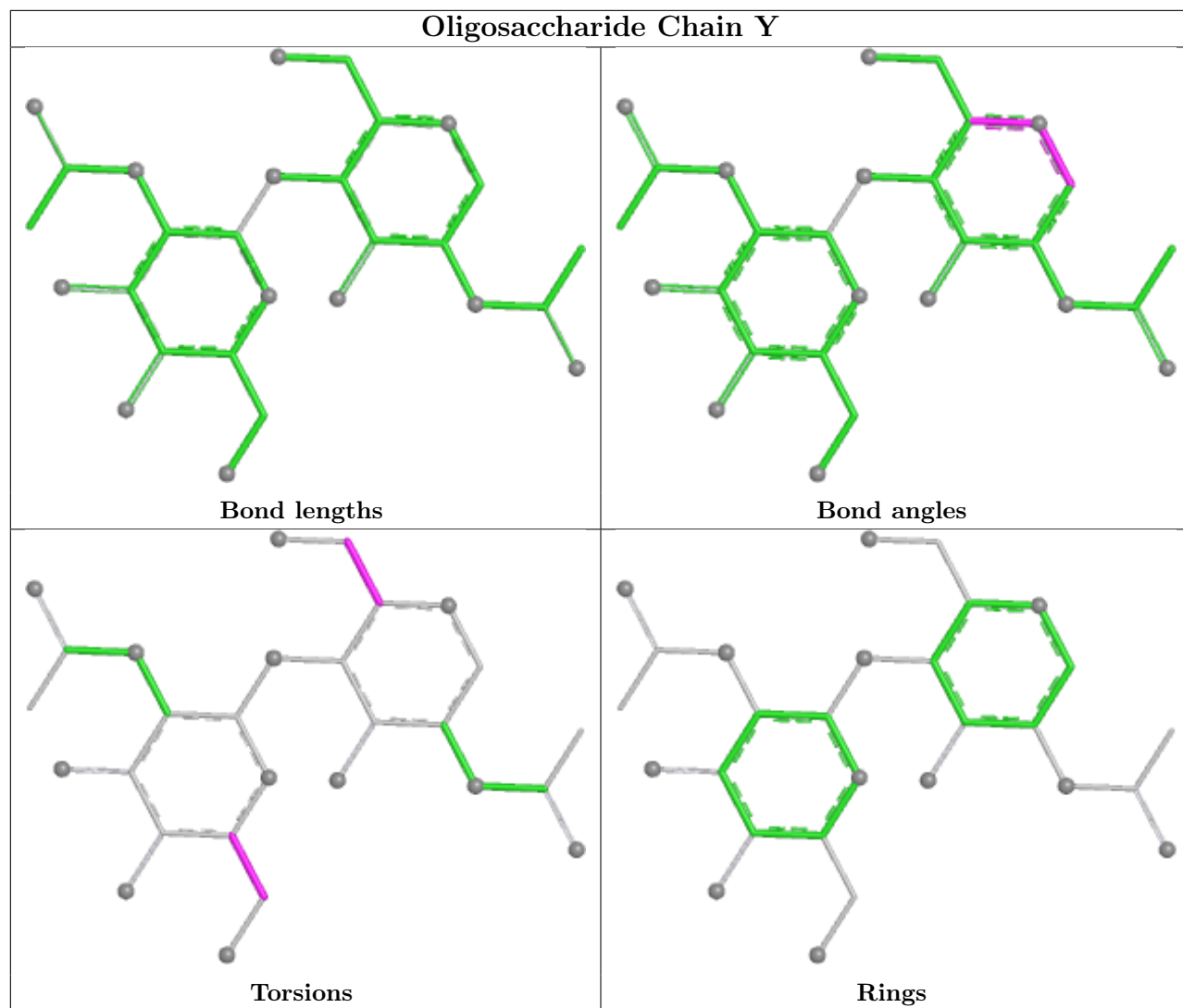


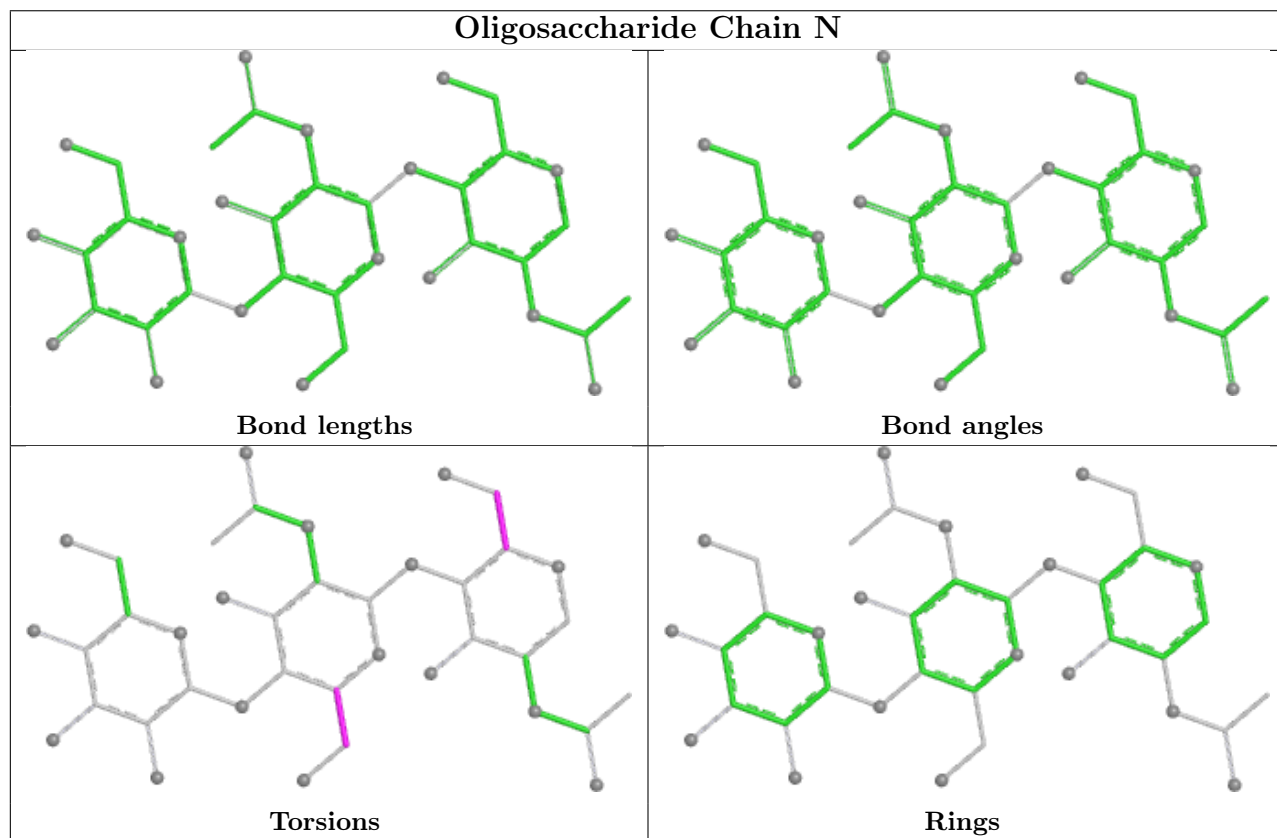
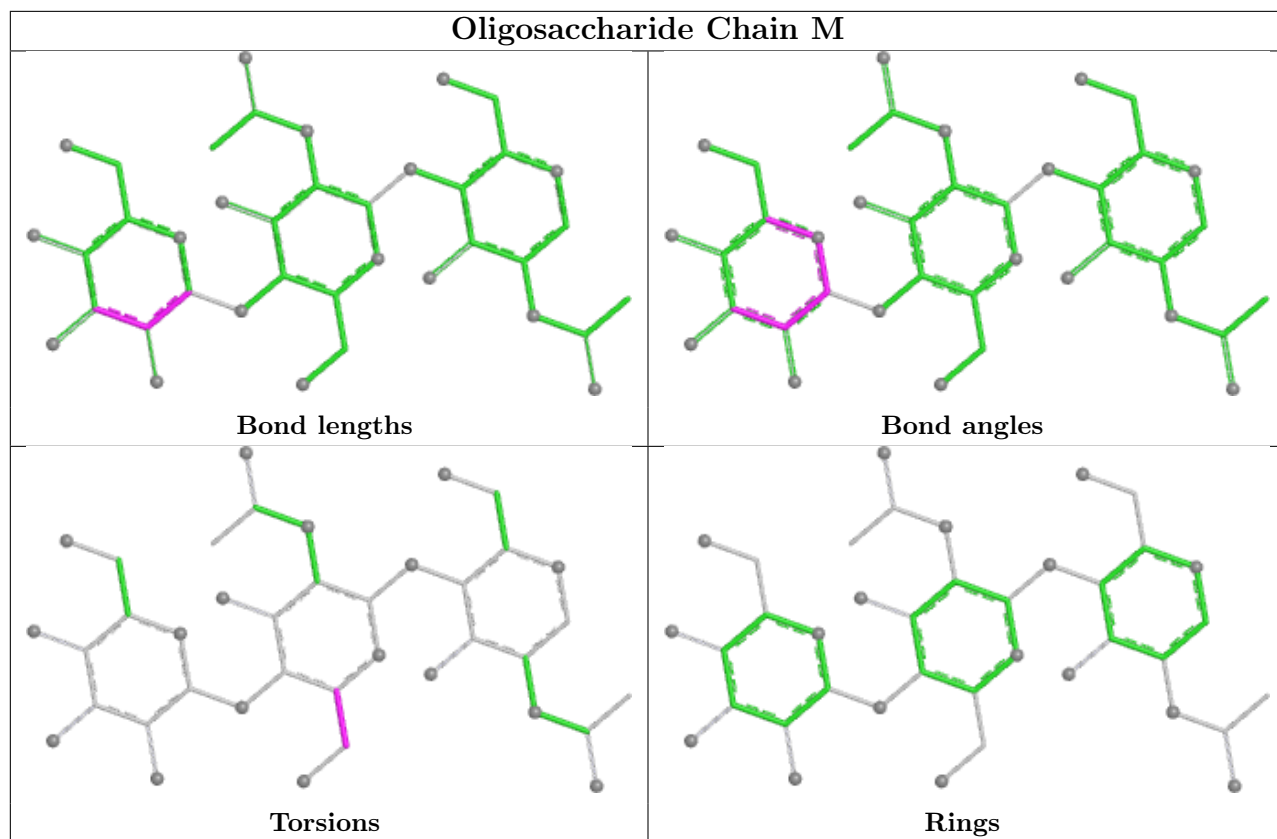


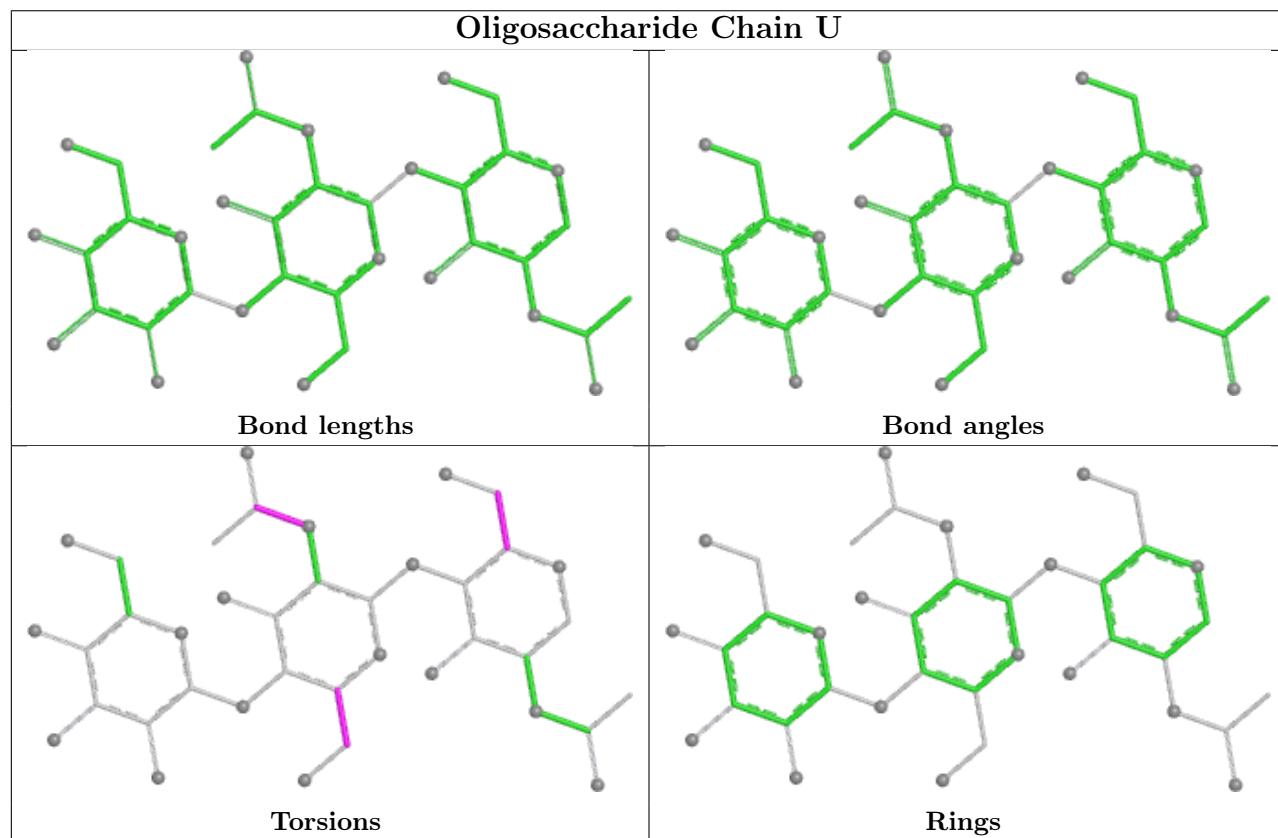
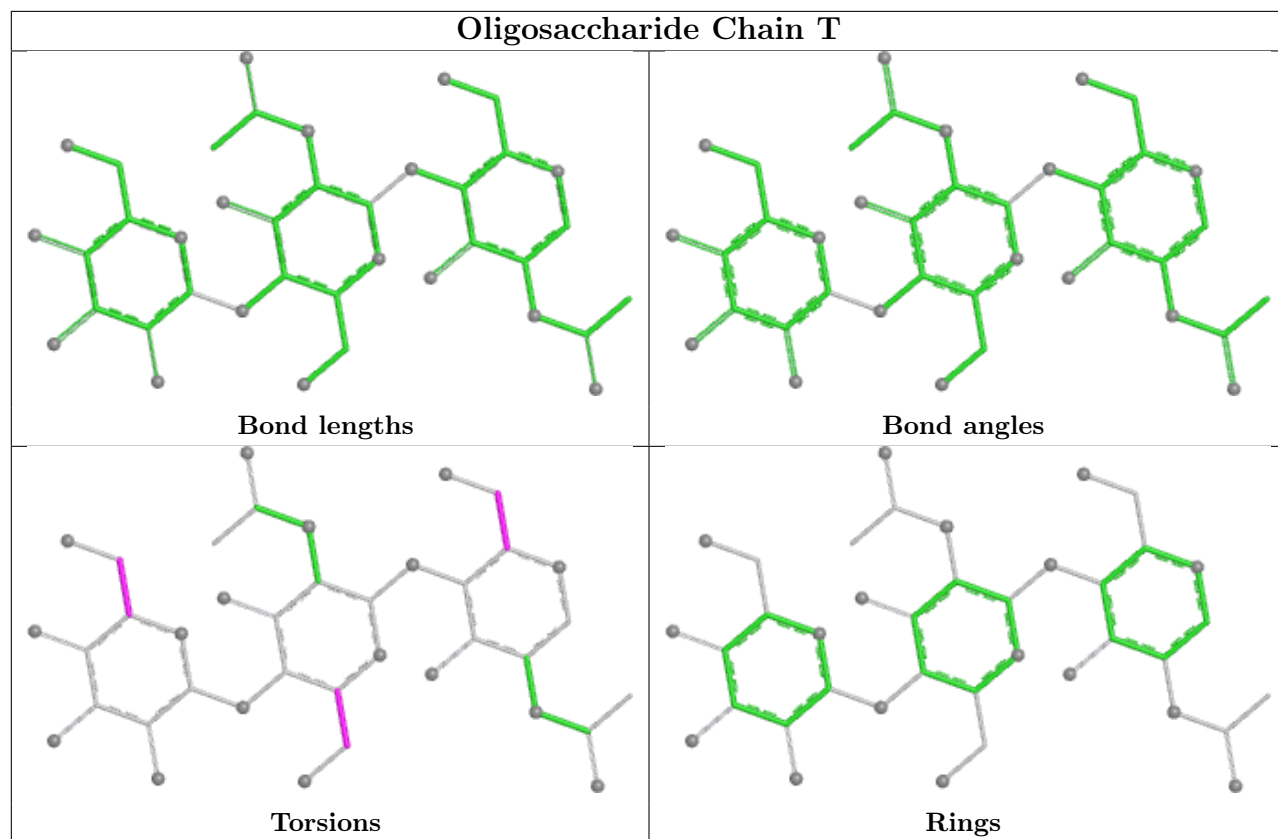


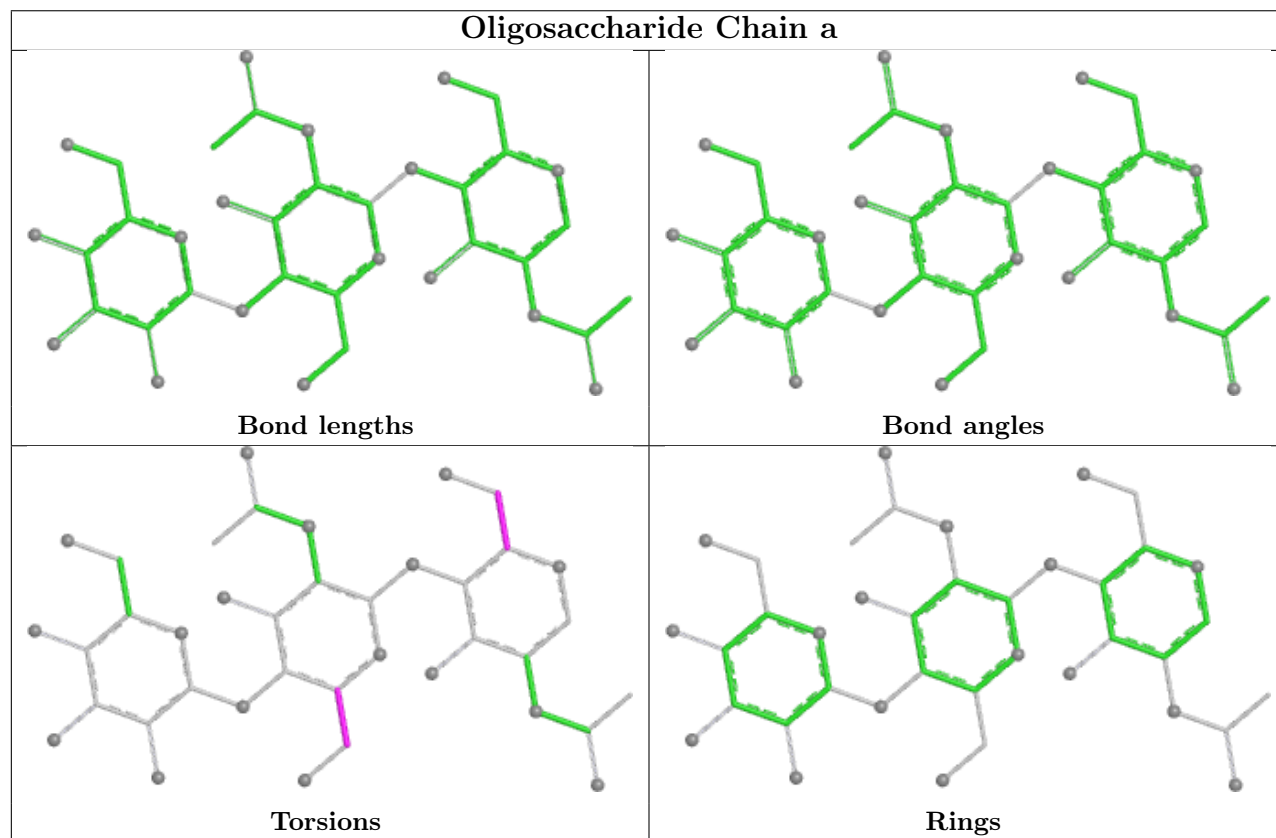
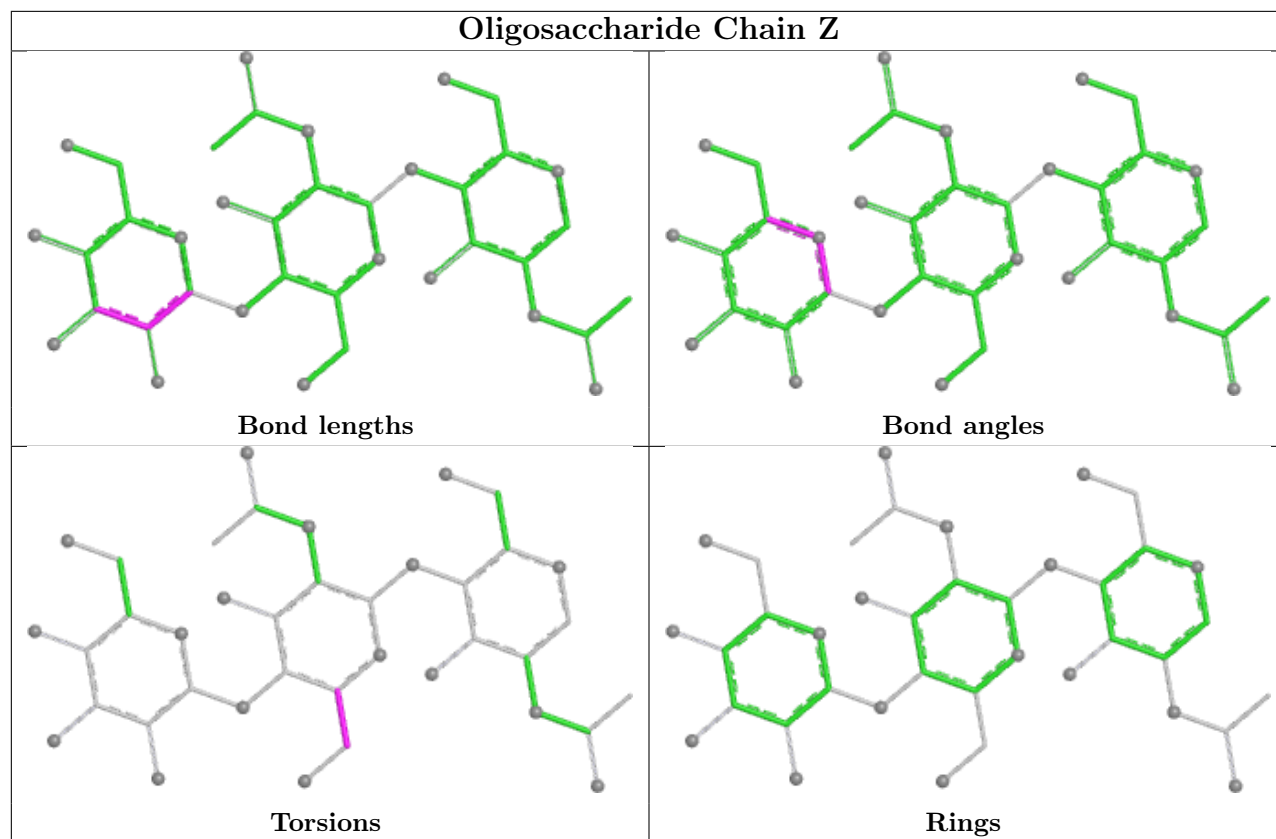












## 5.6 Ligand geometry

28 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
6	NAG	C	1204	1	14,14,15	0.56	0	17,19,21	0.75	0
6	NAG	B	1208	1	14,14,15	0.25	0	17,19,21	0.48	0
6	NAG	A	1207	1	14,14,15	0.28	0	17,19,21	0.50	0
6	NAG	B	1204	1	14,14,15	0.40	0	17,19,21	0.48	0
6	NAG	B	1202	1	14,14,15	0.34	0	17,19,21	0.46	0
6	NAG	B	1205	1	14,14,15	0.30	0	17,19,21	0.48	0
6	NAG	C	1206	1	14,14,15	0.36	0	17,19,21	0.48	0
6	NAG	C	1203	-	14,14,15	0.27	0	17,19,21	0.46	0
6	NAG	C	1201	1	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	B	1210	1	14,14,15	0.26	0	17,19,21	0.52	0
6	NAG	A	1209	1	14,14,15	0.23	0	17,19,21	0.49	0
6	NAG	A	1205	1	14,14,15	1.30	2 (14%)	17,19,21	1.20	1 (5%)
6	NAG	B	1201	-	14,14,15	0.71	0	17,19,21	1.19	2 (11%)
6	NAG	B	1203	1	14,14,15	0.23	0	17,19,21	0.48	0
6	NAG	A	1206	1	14,14,15	0.40	0	17,19,21	0.45	0
6	NAG	B	1206	1	14,14,15	0.40	0	17,19,21	0.38	0
6	NAG	A	1201	1	14,14,15	0.29	0	17,19,21	0.45	0
6	NAG	C	1207	1	14,14,15	0.28	0	17,19,21	0.50	0
6	NAG	A	1203	1	14,14,15	0.28	0	17,19,21	0.45	0
6	NAG	C	1208	1	14,14,15	0.33	0	17,19,21	0.54	0
6	NAG	C	1205	-	14,14,15	0.45	0	17,19,21	0.74	0
6	NAG	B	1209	1	14,14,15	0.28	0	17,19,21	0.48	0
6	NAG	A	1208	1	14,14,15	0.30	0	17,19,21	0.43	0
6	NAG	B	1207	1	14,14,15	1.29	2 (14%)	17,19,21	1.22	1 (5%)
6	NAG	C	1209	1	14,14,15	0.26	0	17,19,21	0.47	0
6	NAG	A	1204	1	14,14,15	0.32	0	17,19,21	0.48	0
6	NAG	A	1202	1	14,14,15	0.45	0	17,19,21	0.46	0
6	NAG	C	1202	-	14,14,15	0.24	0	17,19,21	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1204	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1208	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1207	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1204	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1202	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1205	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1206	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1203	-	-	1/6/23/26	0/1/1/1
6	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1210	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1209	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1201	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1203	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1206	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1206	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1201	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1207	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1208	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1205	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1209	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1208	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1207	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1209	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1202	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1202	-	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1205	NAG	O5-C1	3.87	1.50	1.43
6	B	1207	NAG	O5-C1	3.83	1.50	1.43
6	A	1205	NAG	C1-C2	2.70	1.56	1.52
6	B	1207	NAG	C1-C2	2.70	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1207	NAG	C1-O5-C5	4.69	118.47	112.19
6	A	1205	NAG	C1-O5-C5	4.63	118.39	112.19
6	B	1201	NAG	C2-N2-C7	-3.06	118.80	122.90
6	B	1201	NAG	C1-O5-C5	2.69	115.79	112.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1205	NAG	C4-C5-C6-O6
6	B	1209	NAG	O5-C5-C6-O6
6	B	1205	NAG	C4-C5-C6-O6
6	C	1205	NAG	O5-C5-C6-O6
6	C	1208	NAG	O5-C5-C6-O6
6	A	1203	NAG	O5-C5-C6-O6
6	C	1206	NAG	C4-C5-C6-O6
6	C	1207	NAG	O5-C5-C6-O6
6	B	1210	NAG	O5-C5-C6-O6
6	A	1205	NAG	O5-C5-C6-O6
6	C	1204	NAG	O5-C5-C6-O6
6	B	1203	NAG	O5-C5-C6-O6
6	B	1209	NAG	C4-C5-C6-O6
6	A	1203	NAG	C4-C5-C6-O6
6	A	1205	NAG	C4-C5-C6-O6
6	B	1207	NAG	O5-C5-C6-O6
6	C	1204	NAG	C4-C5-C6-O6
6	B	1205	NAG	O5-C5-C6-O6
6	C	1201	NAG	O5-C5-C6-O6
6	C	1207	NAG	C4-C5-C6-O6
6	B	1207	NAG	C4-C5-C6-O6
6	C	1206	NAG	O5-C5-C6-O6
6	B	1204	NAG	O5-C5-C6-O6
6	C	1201	NAG	C4-C5-C6-O6
6	C	1208	NAG	C4-C5-C6-O6
6	B	1210	NAG	C4-C5-C6-O6
6	C	1206	NAG	C8-C7-N2-C2
6	C	1206	NAG	O7-C7-N2-C2
6	B	1203	NAG	C8-C7-N2-C2
6	B	1203	NAG	O7-C7-N2-C2
6	B	1207	NAG	C8-C7-N2-C2
6	B	1207	NAG	O7-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	A	1206	NAG	C8-C7-N2-C2
6	A	1206	NAG	O7-C7-N2-C2
6	B	1201	NAG	O5-C5-C6-O6
6	B	1202	NAG	O5-C5-C6-O6
6	A	1204	NAG	O5-C5-C6-O6
6	B	1203	NAG	C4-C5-C6-O6
6	A	1208	NAG	C4-C5-C6-O6
6	A	1201	NAG	O5-C5-C6-O6
6	A	1206	NAG	O5-C5-C6-O6
6	A	1208	NAG	O5-C5-C6-O6
6	A	1207	NAG	C4-C5-C6-O6
6	A	1207	NAG	O5-C5-C6-O6
6	B	1206	NAG	C4-C5-C6-O6
6	C	1203	NAG	O5-C5-C6-O6
6	B	1204	NAG	C4-C5-C6-O6
6	C	1202	NAG	O5-C5-C6-O6
6	B	1202	NAG	C4-C5-C6-O6
6	A	1204	NAG	C4-C5-C6-O6
6	B	1206	NAG	O5-C5-C6-O6
6	B	1205	NAG	C1-C2-N2-C7
6	B	1210	NAG	C1-C2-N2-C7
6	B	1201	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1204	NAG	1	0
6	B	1201	NAG	5	0
6	C	1205	NAG	2	0
6	A	1202	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.

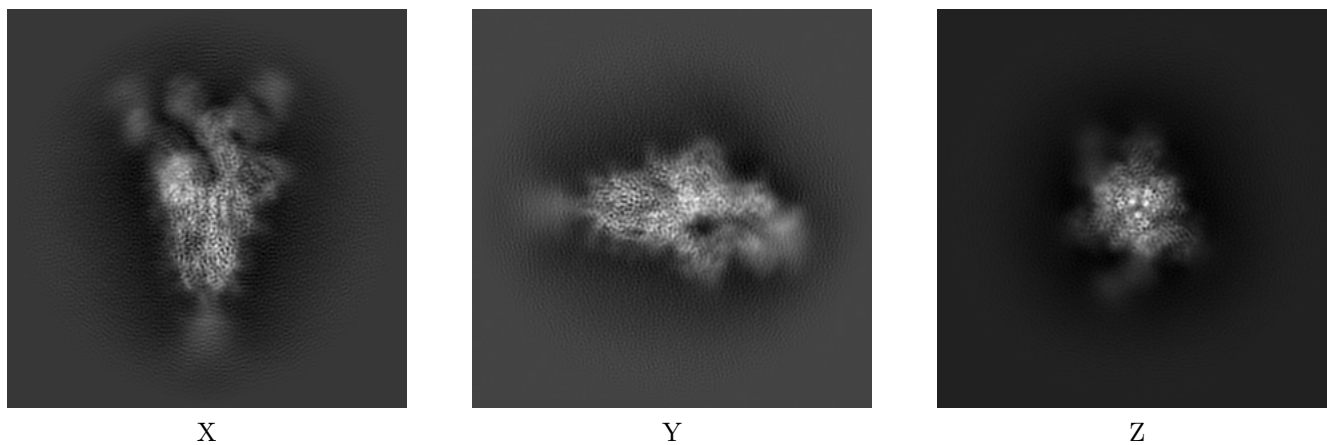
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32789. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

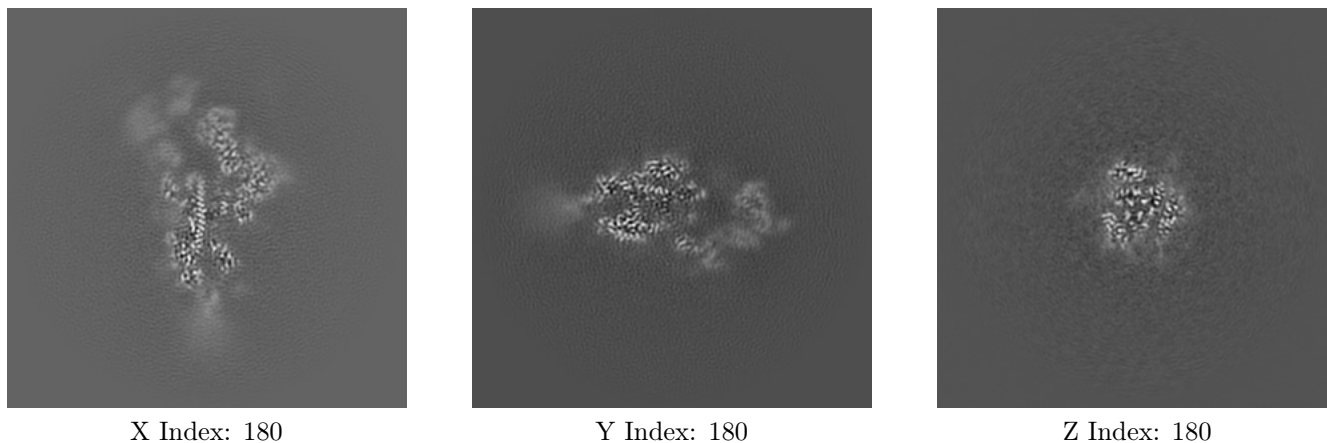
#### 6.1.1 Primary map



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

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

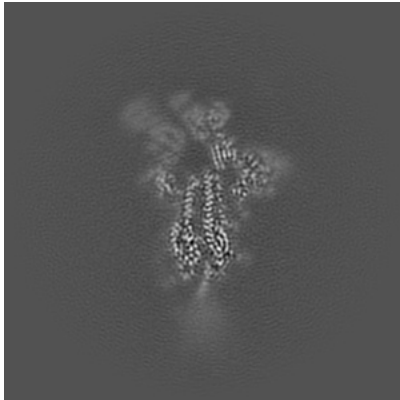
#### 6.2.1 Primary map



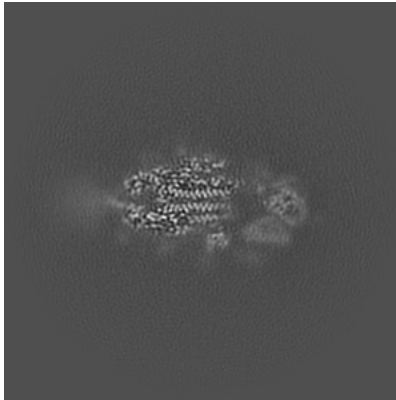
The images above show central slices of the map in three orthogonal directions.

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

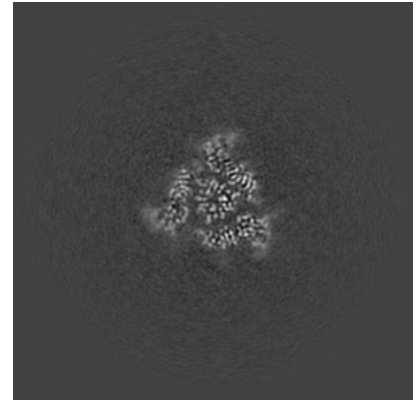
### 6.3.1 Primary map



X Index: 188



Y Index: 185

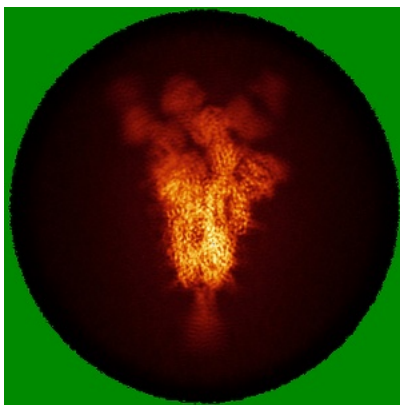


Z Index: 193

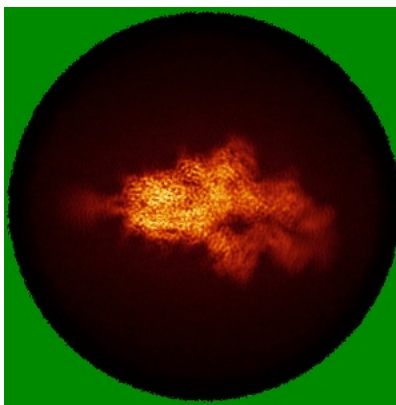
The images above show the largest variance slices of the map in three orthogonal directions.

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

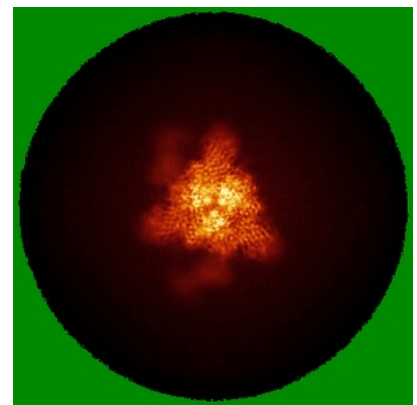
### 6.4.1 Primary map



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

This section was not generated.

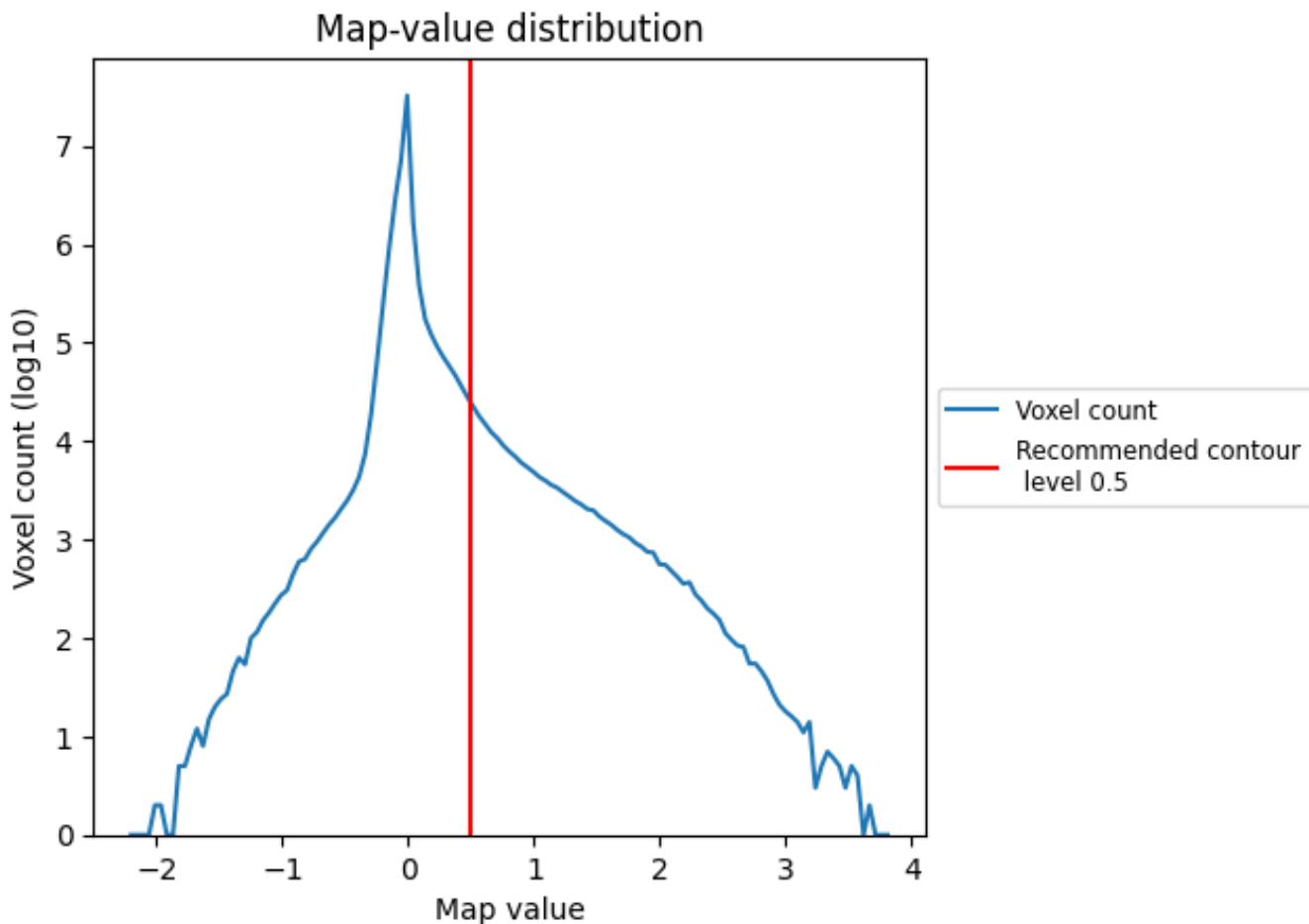
## 6.6 Mask visualisation

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

## 7 Map analysis [i](#)

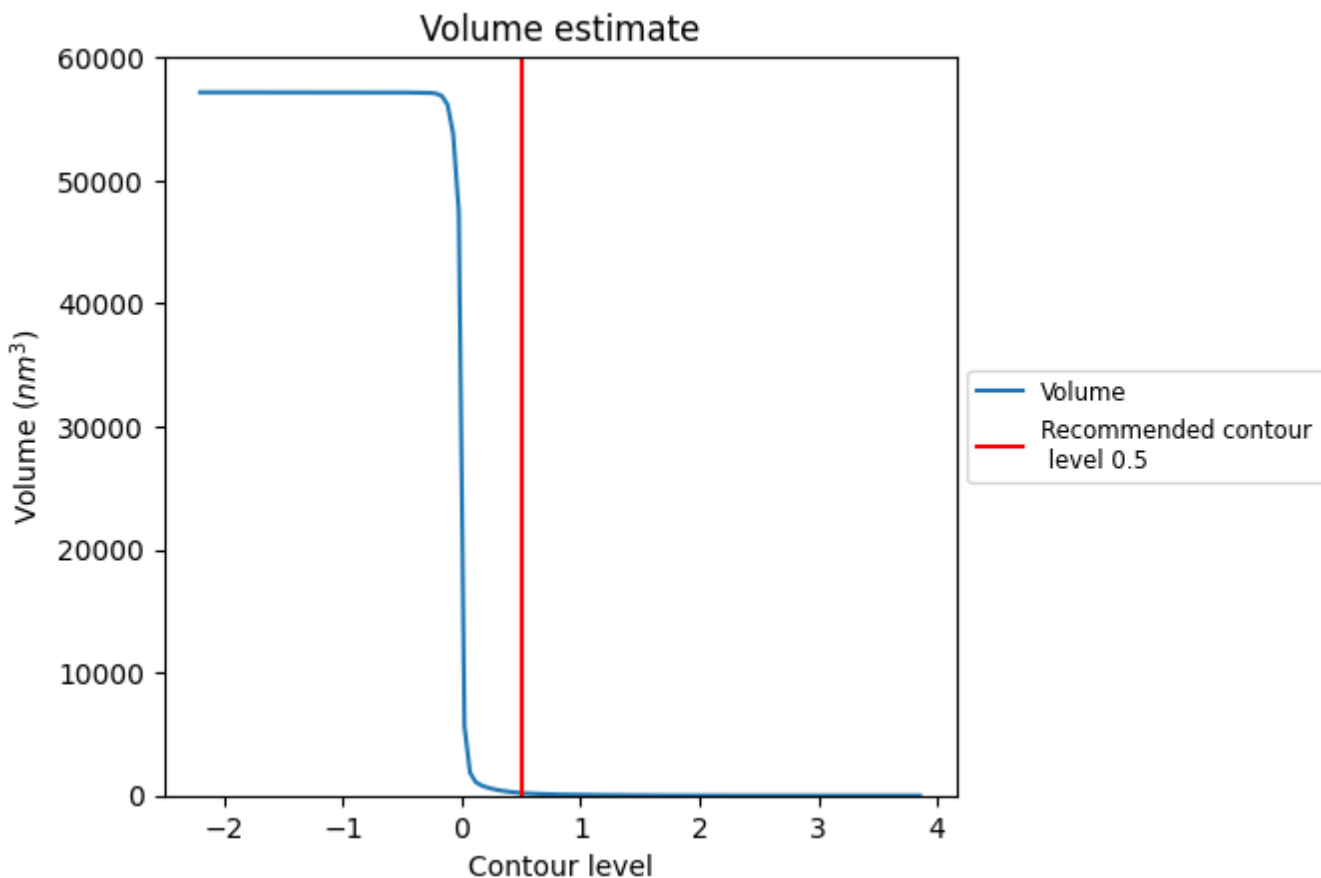
This section contains the results of statistical analysis of the map.

### 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.

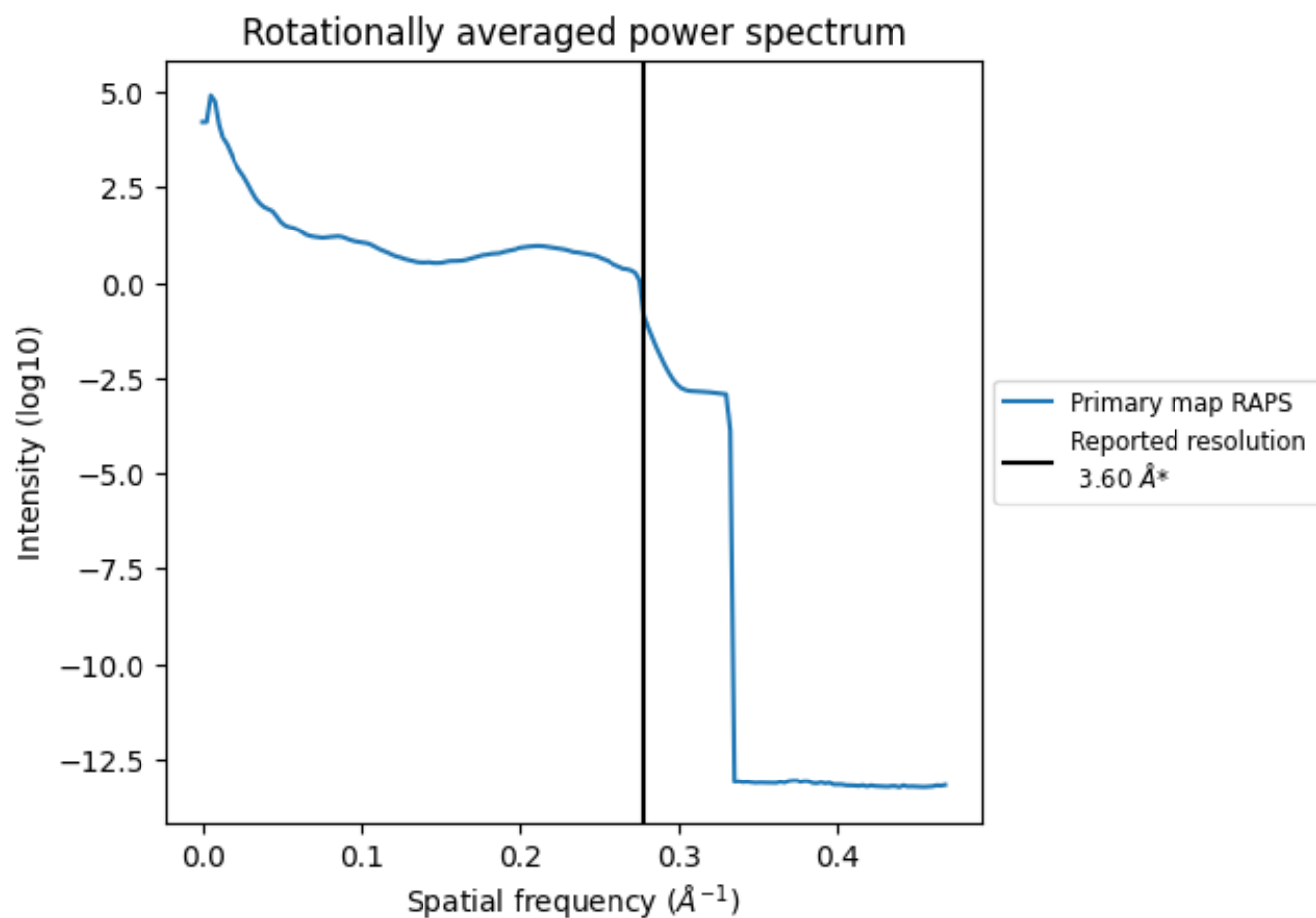
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm<sup>3</sup>; this corresponds to an approximate mass of 192 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.278 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation

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

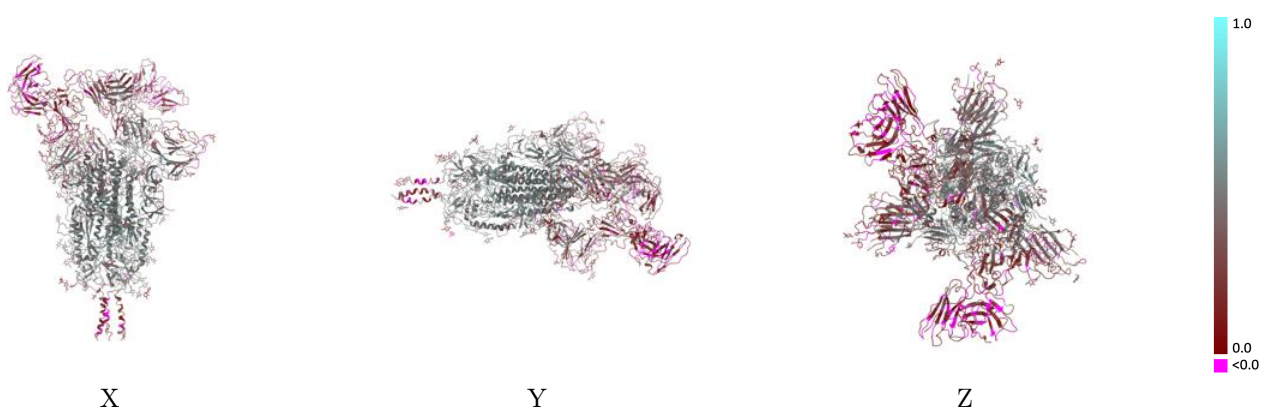
## 9 Map-model fit [\(i\)](#)

This section contains information regarding the fit between EMDB map EMD-32789 and PDB model 7WTK. Per-residue inclusion information can be found in section 3 on page 12.

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

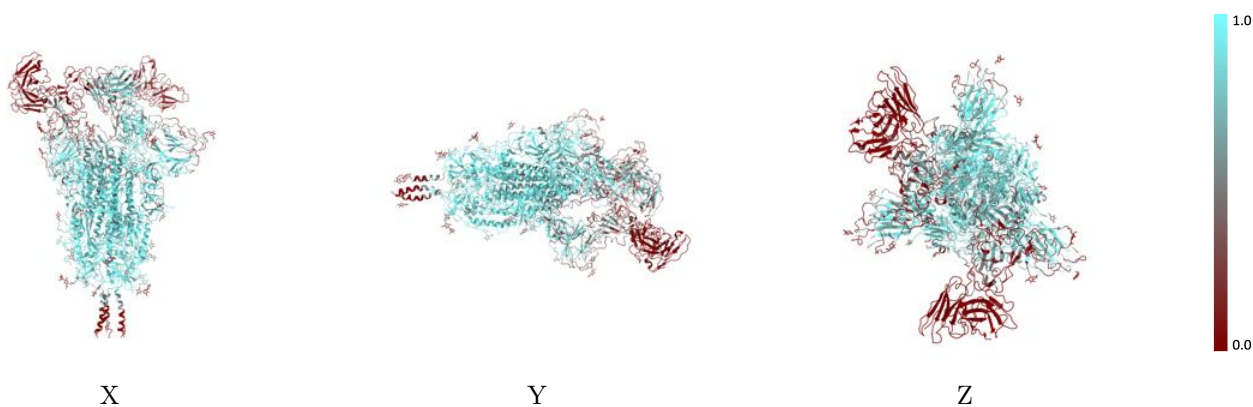
This section was not generated.

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



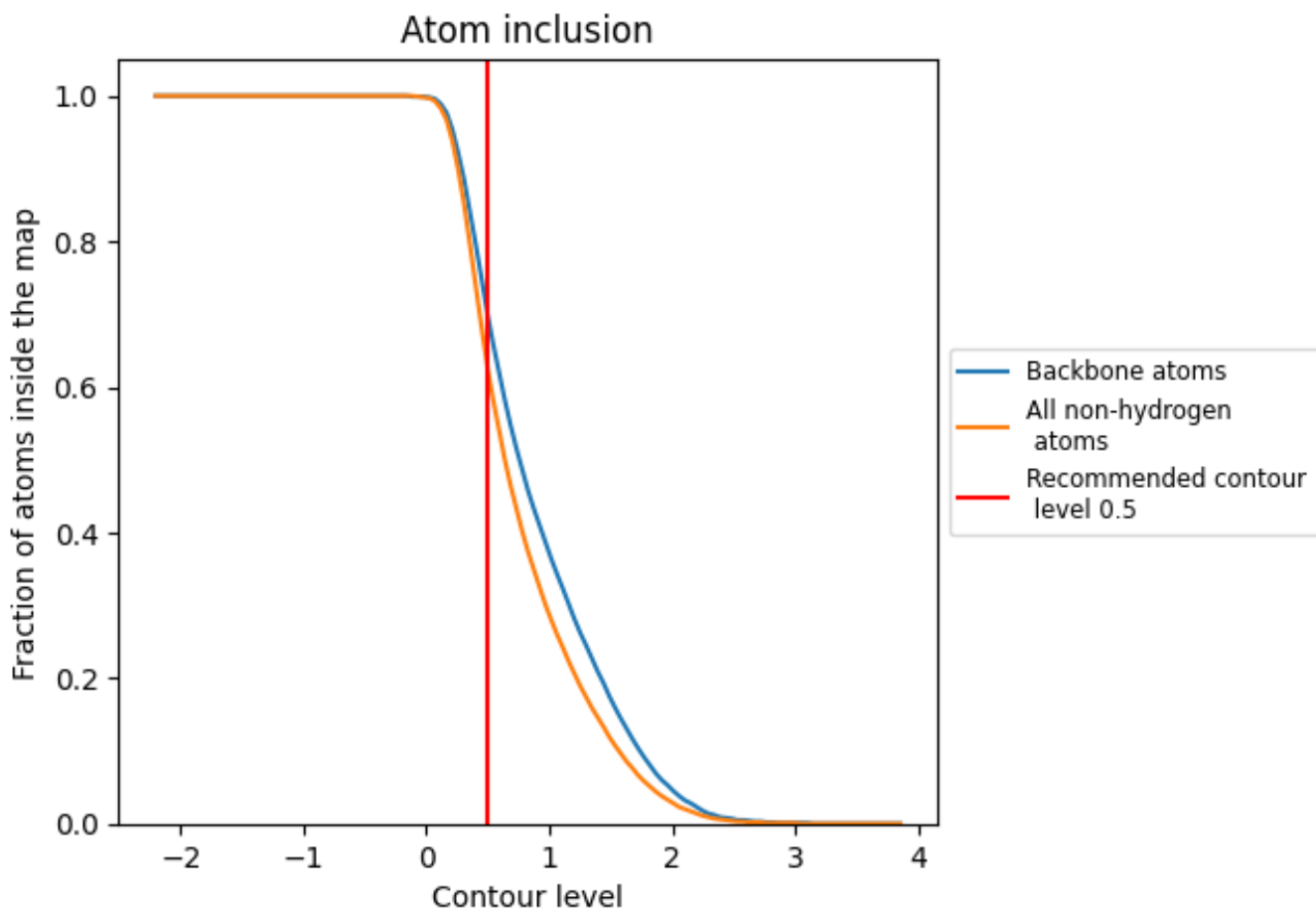
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 62% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6240	 0.3550
A	 0.6690	 0.3730
B	 0.7800	 0.4260
C	 0.6810	 0.3720
D	 0.6790	 0.4600
E	 0.3930	 0.4030
F	 0.7140	 0.4400
G	 0.6190	 0.3350
H	 0.0280	 0.1040
I	 0.0060	 0.1160
J	 0.4990	 0.2950
K	 0.0080	 0.0880
L	 0.0180	 0.1020
M	 0.5130	 0.3510
N	 0.2050	 0.1540
O	 0.0000	 0.1990
P	 0.1070	 0.2540
Q	 0.7500	 0.4340
R	 0.0000	 0.1790
S	 0.7860	 0.4500
T	 0.4100	 0.2690
U	 0.3850	 0.2940
V	 0.0000	 0.2610
W	 0.8570	 0.4760
X	 0.2140	 0.2960
Y	 0.7140	 0.4050
Z	 0.4870	 0.3500
a	 0.1790	 0.1560

