



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:48 AM UTC

PDB ID : 8XZ8 / pdb_00008xz8
EMDB ID : EMD-38789
Title : BA.2.86 Spike in complex with bovine ACE2 (bound 1 ACE2)
Authors : Yue, C.; Liu, P.
Deposited on : 2024-01-21
Resolution : 3.65 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

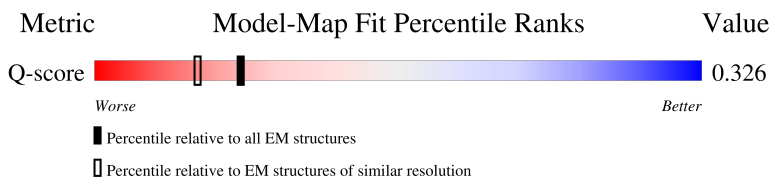
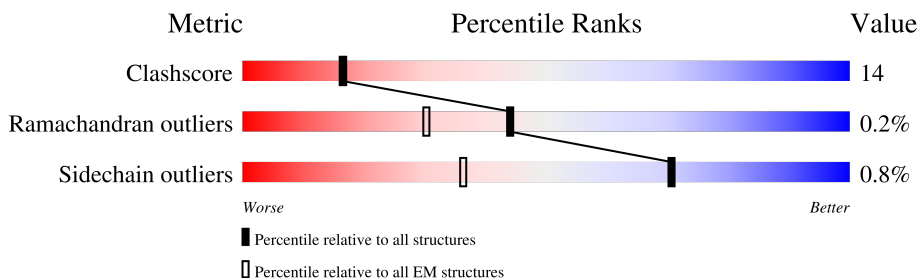
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.65 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	11564 (3.15 - 4.15)

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	804	
2	B	1206	
2	C	1206	
2	D	1206	

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Mol	Chain	Length	Quality of chain
3	E	2	 50% 100%
3	F	2	 100%
3	G	2	 100%
3	H	2	 100%
3	I	2	 100%
3	J	2	 100%
3	K	2	 100%
3	L	2	 100%
3	M	2	 100%
3	N	2	 100%
3	O	2	 100%
3	P	2	 100%
3	Q	2	 100%
3	R	2	 100%
3	S	2	 100%
3	T	2	 100%
3	U	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30785 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	596	Total	C	N	O	S	0	0
			4906	3136	815	925	30		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		
2	C	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		
2	D	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		

There are 219 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	16	MET	-	insertion	UNP P0DTC2
B	17	PRO	-	insertion	UNP P0DTC2
B	18	LEU	-	insertion	UNP P0DTC2
B	19	PHE	-	insertion	UNP P0DTC2
B	22	ILE	THR	conflict	UNP P0DTC2
B	24	THR	ARG	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	variant	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	conflict	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	683	ALA	ARG	conflict	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	16	MET	-	insertion	UNP P0DTC2
C	17	PRO	-	insertion	UNP P0DTC2
C	18	LEU	-	insertion	UNP P0DTC2
C	19	PHE	-	insertion	UNP P0DTC2
C	22	ILE	THR	conflict	UNP P0DTC2
C	24	THR	ARG	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	variant	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	conflict	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2
D	-2	ALA	-	expression tag	UNP P0DTC2
D	-1	THR	-	expression tag	UNP P0DTC2
D	16	MET	-	insertion	UNP P0DTC2
D	17	PRO	-	insertion	UNP P0DTC2
D	18	LEU	-	insertion	UNP P0DTC2
D	19	PHE	-	insertion	UNP P0DTC2
D	22	ILE	THR	conflict	UNP P0DTC2
D	24	THR	ARG	conflict	UNP P0DTC2
D	?	-	LEU	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	27	SER	ALA	variant	UNP P0DTC2
D	50	LEU	SER	conflict	UNP P0DTC2
D	?	-	HIS	deletion	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	127	PHE	VAL	conflict	UNP P0DTC2
D	143	ASP	GLY	variant	UNP P0DTC2
D	?	-	TYR	deletion	UNP P0DTC2
D	157	SER	PHE	conflict	UNP P0DTC2
D	158	GLY	ARG	conflict	UNP P0DTC2
D	?	-	ASN	deletion	UNP P0DTC2
D	212	ILE	LEU	variant	UNP P0DTC2
D	213	GLY	VAL	variant	UNP P0DTC2
D	216	PHE	LEU	variant	UNP P0DTC2
D	245	ASN	HIS	conflict	UNP P0DTC2
D	264	ASP	ALA	conflict	UNP P0DTC2
D	332	VAL	ILE	conflict	UNP P0DTC2
D	339	HIS	GLY	conflict	UNP P0DTC2
D	356	THR	LYS	conflict	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	403	LYS	ARG	conflict	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	445	HIS	VAL	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	446	SER	GLY	variant	UNP P0DTC2
D	450	ASP	ASN	conflict	UNP P0DTC2
D	452	TRP	LEU	conflict	UNP P0DTC2
D	460	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	481	LYS	ASN	conflict	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	484	LYS	GLU	variant	UNP P0DTC2
D	486	PRO	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2
D	554	LYS	GLU	conflict	UNP P0DTC2
D	570	VAL	ALA	conflict	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	621	SER	PRO	conflict	UNP P0DTC2
D	655	TYR	HIS	variant	UNP P0DTC2
D	679	LYS	ASN	variant	UNP P0DTC2
D	681	ARG	PRO	variant	UNP P0DTC2
D	683	ALA	ARG	conflict	UNP P0DTC2
D	685	ALA	ARG	conflict	UNP P0DTC2
D	764	LYS	ASN	variant	UNP P0DTC2
D	796	TYR	ASP	variant	UNP P0DTC2
D	817	PRO	PHE	conflict	UNP P0DTC2
D	892	PRO	ALA	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	939	PHE	SER	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2
D	954	HIS	GLN	variant	UNP P0DTC2
D	969	LYS	ASN	variant	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1143	LEU	PRO	conflict	UNP P0DTC2

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			25	14	1	10		
3	F	2	Total	C	N	O	0	0
			25	14	1	10		
3	G	2	Total	C	N	O	0	0
			25	14	1	10		
3	H	2	Total	C	N	O	0	0
			25	14	1	10		
3	I	2	Total	C	N	O	0	0
			25	14	1	10		
3	J	2	Total	C	N	O	0	0
			25	14	1	10		
3	K	2	Total	C	N	O	0	0
			25	14	1	10		
3	L	2	Total	C	N	O	0	0
			25	14	1	10		
3	M	2	Total	C	N	O	0	0
			25	14	1	10		
3	N	2	Total	C	N	O	0	0
			25	14	1	10		
3	O	2	Total	C	N	O	0	0
			25	14	1	10		
3	P	2	Total	C	N	O	0	0
			25	14	1	10		
3	Q	2	Total	C	N	O	0	0
			25	14	1	10		
3	R	2	Total	C	N	O	0	0
			25	14	1	10		
3	S	2	Total	C	N	O	0	0
			25	14	1	10		
3	T	2	Total	C	N	O	0	0
			25	14	1	10		
3	U	2	Total	C	N	O	0	0
			25	14	1	10		

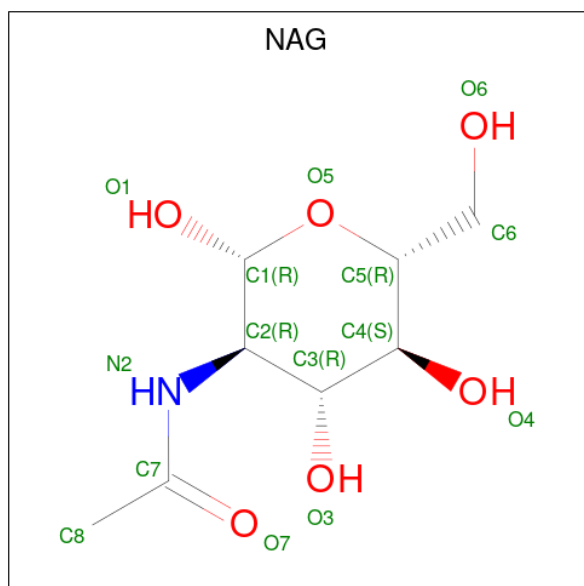
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Cl	0
			1	1	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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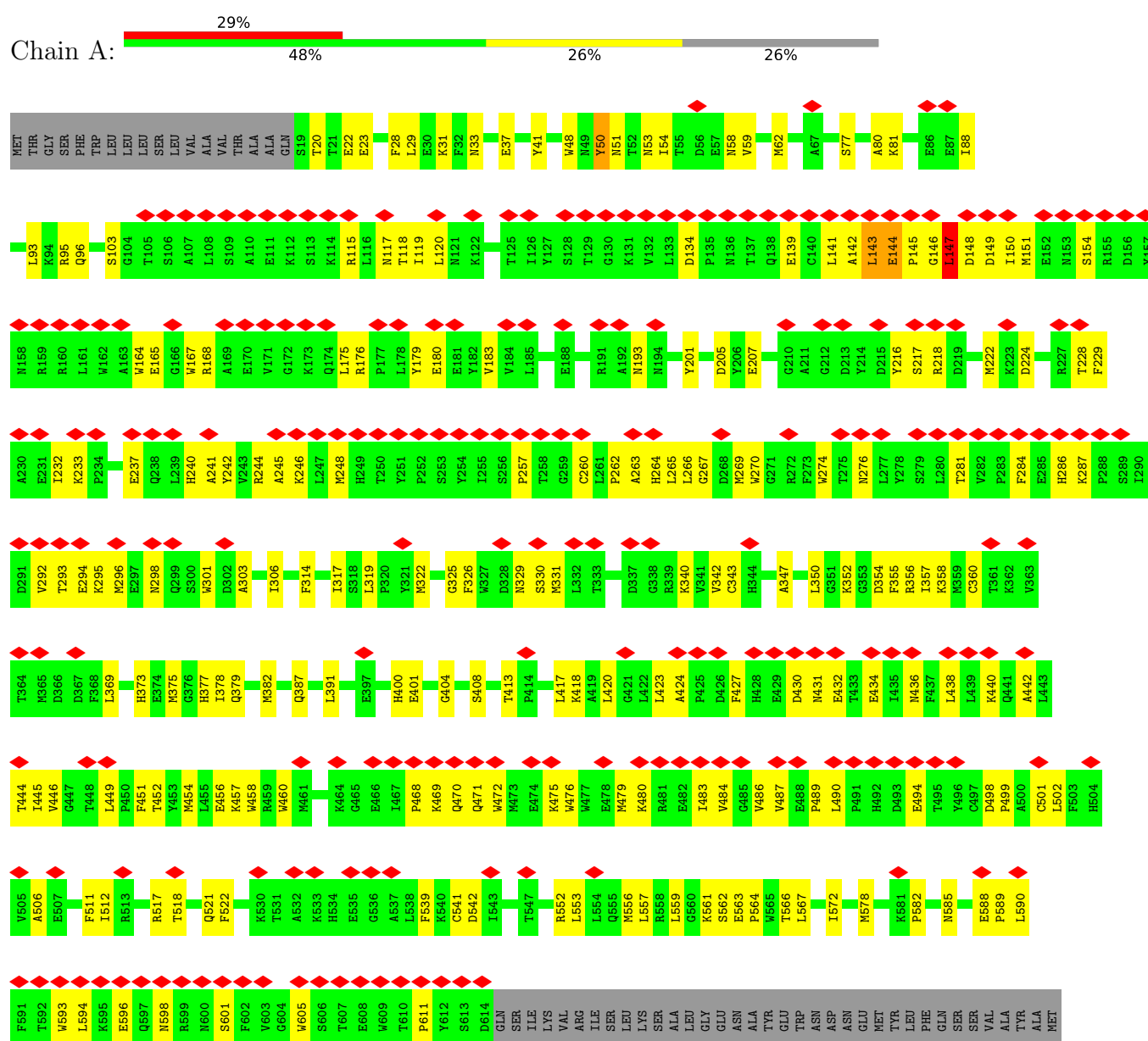
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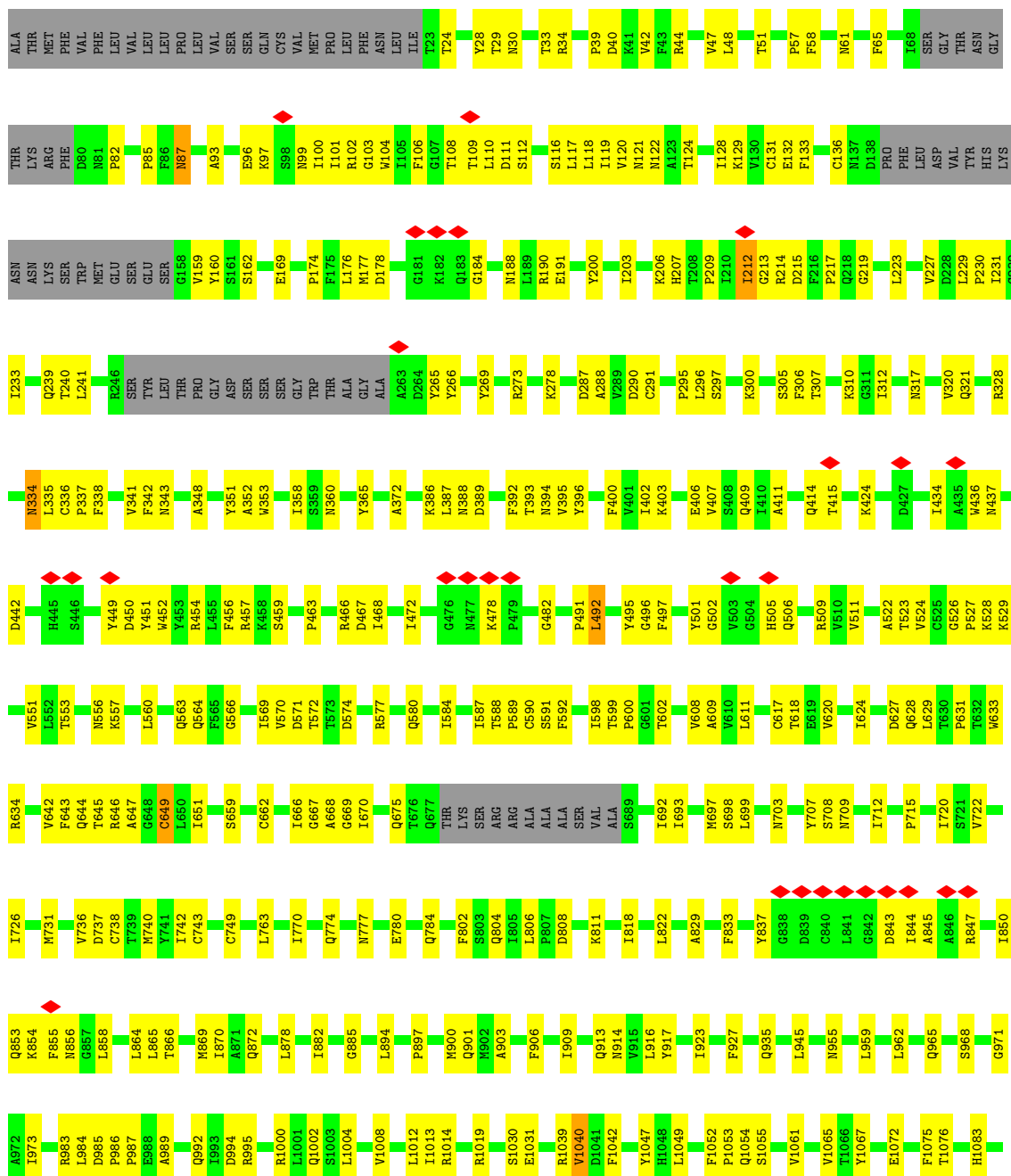
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

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

- Molecule 1: Angiotensin-converting enzyme





ARG	LEU	ASN	GLU	VAL	ALA	LYS	ASN	LEU	ASN	GLU	SER	LEU	ILE	ASP	LEU	GLN	GLU	LEU	GLY	LYS	TYR	GLU	GLN					
V1094	F1095	V1096	S1097	M1098	G1099	T1100	H1101	Q1106	F1109	V1110	E1111	I1115	V1137	E1144	LEU	ASP	SER	PHE	LYS	GLU	GLU	LEU	LEU	ASP	LYS	TYR	GLU	GLN

• Molecule 2: Spike glycoprotein

Chain D:  59% 28% 12%

ALA	THR	MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	LEU	VAL	SER	SER	GLN	CYS	VAL	MET	PRO	LEU	PHE	ASN	LEU	THR	GLY	THR	LYS		
ARG	PHE	D80	N81	N87	A93	S94	E96	I100	I101	R102	I105	T108	T109	D111	L118	L119	V120	N121	T124	N125	V126	F127	I128	K129	C131	E132	F133	Q134	
ARG	PHE	D80	N81	N87	A93	S94	E96	I100	I101	R102	I105	T108	T109	D111	L118	L119	V120	N121	T124	N125	V126	F127	I128	K129	C131	E132	F133	Q134	
TRP	THR	ALA	ALA	A263	D264	Y265	Y266	R273	Y279	D287	A288	Y289	D290	C291	D294	P295	L296	S297	K300	L303	K304	S305	F306	T307	V308	E309	K310	G311	
R357	I358	S359	N360	C361	V362	A363	D364	Y365	S366	V367	L368	Y369	N370	F371	F374	F375	A376	G381	V382	S383	P384	K385	K386	L387	N388	D389	L390	T393	
K440	L441	D442	S443	K444	H445	S446	G447	N448	Y449	D450	R454	R457	V459	D570	D571	K462	E465	R466	D467	L468	Y489	L492	G496	F497	R498	D499	T500	Y501	G502
T547	S555	N556	K557	K558	F559	L560	P561	F562	O563	R567	D568	V569	D570	D571	D574	R577	D578	P579	O580	T584	T587	T588	P589	G594	V595	L598	T599	P600	G601
N641	Q644	T645	R646	A647	G648	G649	L650	N657	N658	S659	C662	D663	V670	L671	L672	A672	Q675	P676	Q677	THR	LYS	SER	ARG	ARG	ALA	ALA	ALA	VAL	ALA
H731	V736	M740	Y741	I742	C749	F759	C760	L763	L767	I770	Q774	T778	Q787	L788	P792	Q913	N914	V915	L916	S803	Q804	L805	L806	S816	E819	D820	L821	L822	F823
L864	L865	M869	L870	Y873	T874	S875	A876	L877	L878	I882	L894	P897	M900	Q901	M902	A903	F906	T912	Q913	N914	V915	L916	S803	Q804	L805	L806	S816	E819	D820
V976	D979	L984	D985	P986	P987	E988	A989	E990	I993	I997	Q1002	L1004	Q1005	T1006	Y1007	M1008	T1009	L1012	I1013	R1014	A1015	M1028	S1030	E1031	C1032	V1033	R1039	V1040	L1049
H1083	V1096	S1097	N1098	G1099	V1102	E988	A989	E990	I1115	S1123	V1128	V1137	E1144	LEU	ASP	SER	PHE	LYS	GLU	GLU	LEU	LEU	ASP	LYS	TYR	PHE	LYS	ASN	HIS
LEU	ASP	SER	PHE	LYS	GLU	GLU	LEU	GLN	GLN	VAL	MET	PRO	LEU	GLY	LEU	ASP	TYR	GLU	GLN										

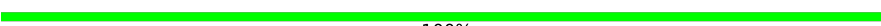
ARG
LEU
ASN
GLU
VAL
ALA
LYS
ASN
LEU
ASN
GLU
SER
LEU
ILE
ASP
LEU
GLN
GLU
LEU
GLY
LYS
TYR
GLU
GLN

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50%
100%

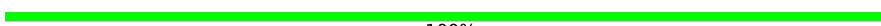

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

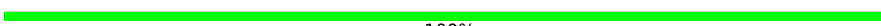
MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

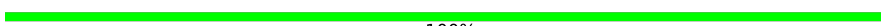
MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

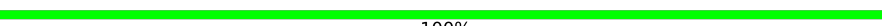
MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

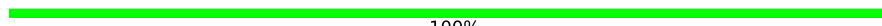
MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

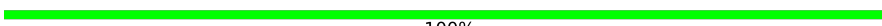


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

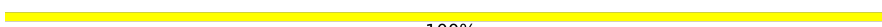


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

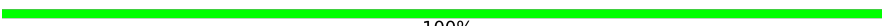


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

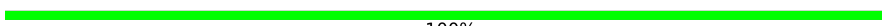


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

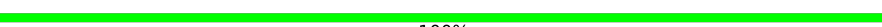


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

MAG1
BMA2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89392	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.635	Depositor
Minimum map value	-0.630	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	360.0, 360.0, 360.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.20	0/5043	0.40	0/6838
2	B	0.16	0/8516	0.39	1/11591 (0.0%)
2	C	0.15	0/8516	0.37	0/11591
2	D	0.16	0/8516	0.39	2/11591 (0.0%)
All	All	0.16	0/30591	0.39	3/41611 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	570	VAL	N-CA-C	5.79	112.41	106.21
2	D	979	ASP	CA-CB-CG	5.37	117.97	112.60
2	B	527	PRO	N-CA-C	5.04	122.84	112.47

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	4906	0	4691	149	0
2	B	8316	0	8103	246	0
2	C	8316	0	8104	257	0
2	D	8316	0	8104	273	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	25	0	22	0	0
3	F	25	0	22	0	0
3	G	25	0	22	0	0
3	H	25	0	22	0	0
3	I	25	0	22	0	0
3	J	25	0	22	0	0
3	K	25	0	22	0	0
3	L	25	0	22	0	0
3	M	25	0	22	0	0
3	N	25	0	22	0	0
3	O	25	0	22	0	0
3	P	25	0	22	0	0
3	Q	25	0	22	0	0
3	R	25	0	22	0	0
3	S	25	0	22	0	0
3	T	25	0	22	0	0
3	U	25	0	22	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	70	0	65	0	0
6	B	154	0	140	1	0
6	C	140	0	130	1	0
6	D	140	0	130	3	0
All	All	30785	0	29841	855	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 14.

All (855) 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)
2:B:334:ASN:OD1	2:B:362:VAL:HG13	1.58	1.00
2:D:617:CYS:HA	2:D:620:VAL:HG12	1.56	0.88
2:C:212:ILE:HG22	2:C:213:GLY:H	1.39	0.87
2:C:777:ASN:HD21	2:C:1019:ARG:HA	1.45	0.82
2:C:352:ALA:HA	2:C:466:ARG:HD2	1.59	0.82
1:A:293:THR:HA	1:A:296:MET:HE2	1.59	0.81
2:D:188:ASN:HA	2:D:209:PRO:HA	1.63	0.80
1:A:483:ILE:HG23	1:A:484:VAL:HG23	1.64	0.80
1:A:454:MET:HE2	1:A:484:VAL:HG21	1.64	0.79
2:C:644:GLN:HA	2:C:649:CYS:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:PRO:HG2	2:B:429:PHE:HB2	1.66	0.77
2:C:351:TYR:CE2	2:C:452:TRP:HB2	2.19	0.77
2:B:984:LEU:HB3	2:B:989:ALA:HB2	1.66	0.76
2:D:310:LYS:HG2	2:D:664:ILE:HD11	1.68	0.76
2:B:276:LEU:HD11	2:B:304:LYS:HA	1.68	0.75
2:D:555:SER:HB3	2:D:584:ILE:HG22	1.67	0.75
2:B:830:ASP:HB2	2:B:850:ILE:HD12	1.68	0.74
2:D:559:PHE:HB2	2:D:584:ILE:HD11	1.71	0.73
1:A:457:LYS:HD2	1:A:460:TRP:HD1	1.53	0.73
2:D:329:PHE:HB2	2:D:528:LYS:HG3	1.70	0.73
1:A:54:ILE:HG21	1:A:340:LYS:HE3	1.69	0.73
2:B:735:SER:HB3	2:B:861:LEU:HD11	1.70	0.73
1:A:451:PHE:HA	1:A:454:MET:HE3	1.71	0.72
2:B:726:ILE:HG12	2:B:1061:VAL:HG22	1.70	0.72
2:D:65:PHE:HB2	2:D:265:TYR:HB2	1.71	0.72
2:C:617:CYS:HA	2:C:620:VAL:HG12	1.71	0.72
2:B:646:ARG:HG3	2:C:833:PHE:HB2	1.72	0.72
1:A:248:MET:HE1	1:A:257:PRO:HA	1.73	0.71
2:B:1013:ILE:HG21	2:C:1012:LEU:HD12	1.70	0.71
2:D:311:GLY:HA2	2:D:664:ILE:HD12	1.73	0.70
1:A:53:ASN:O	1:A:58:ASN:ND2	2.23	0.70
2:D:339:HIS:O	2:D:343:ASN:HB2	1.90	0.70
2:D:131:CYS:SG	2:D:132:GLU:N	2.63	0.70
2:D:200:TYR:HA	2:D:230:PRO:HA	1.74	0.70
2:B:108:THR:HG22	2:B:109:THR:HG23	1.74	0.70
2:C:131:CYS:SG	2:C:132:GLU:N	2.57	0.70
2:B:575:ALA:HB1	2:B:584:ILE:HD11	1.74	0.70
2:D:454:ARG:NH1	2:D:467:ASP:O	2.23	0.70
2:C:903:ALA:HB1	2:C:913:GLN:HB3	1.72	0.69
2:C:858:LEU:HD11	2:C:962:LEU:HD13	1.74	0.69
2:C:65:PHE:HB2	2:C:265:TYR:HB3	1.75	0.69
2:B:569:ILE:HD12	2:B:569:ILE:H	1.57	0.69
2:D:557:LYS:HB2	2:D:584:ILE:HG21	1.74	0.69
2:B:777:ASN:HD21	2:B:1019:ARG:HA	1.58	0.68
2:C:556:ASN:HB2	2:D:844:ILE:HG23	1.75	0.68
2:B:617:CYS:HA	2:B:620:VAL:HG12	1.76	0.68
2:B:501:TYR:O	2:B:506:GLN:NE2	2.26	0.68
2:D:659:SER:HB3	2:D:698:SER:HB3	1.75	0.68
2:B:65:PHE:HB2	2:B:265:TYR:HB3	1.74	0.68
2:C:659:SER:HB3	2:C:698:SER:HB2	1.76	0.68
2:D:503:VAL:O	2:D:508:TYR:OH	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:LEU:O	2:B:577:ARG:NH2	2.27	0.67
2:C:627:ASP:HA	2:C:634:ARG:HH22	1.58	0.67
2:D:802:PHE:HB3	2:D:806:LEU:HD13	1.77	0.67
2:D:742:ILE:HG22	2:D:997:ILE:HD12	1.75	0.66
2:B:724:THR:HB	2:B:934:ILE:HD11	1.78	0.66
2:B:900:MET:SD	2:D:1077:THR:OG1	2.52	0.66
2:C:34:ARG:NH1	2:C:191:GLU:OE2	2.27	0.66
2:C:522:ALA:H	2:C:544:ASN:HD21	1.42	0.66
2:C:360:ASN:H	2:C:523:THR:HB	1.60	0.66
2:B:433:VAL:HG12	2:B:512:VAL:HG13	1.76	0.65
2:B:844:ILE:HG23	2:D:556:ASN:HB3	1.78	0.65
2:B:1041:ASP:HB3	2:C:1030:SER:HB3	1.78	0.65
2:B:330:PRO:O	2:B:331:ASN:C	2.40	0.65
2:C:624:ILE:HA	2:C:634:ARG:HH21	1.61	0.65
2:C:351:TYR:HE2	2:C:452:TRP:HB2	1.62	0.65
2:D:560:LEU:HD22	2:D:562:PHE:HD1	1.59	0.65
2:B:485:GLY:H	2:B:488:CYS:HB2	1.60	0.65
2:C:296:LEU:O	2:C:300:LYS:HG3	1.97	0.65
2:C:34:ARG:NH2	2:C:219:GLY:O	2.30	0.65
2:D:310:LYS:HG3	2:D:600:PRO:HA	1.79	0.64
1:A:325:GLY:O	1:A:329:ASN:ND2	2.30	0.64
2:B:912:THR:OG1	2:B:914:ASN:OD1	2.15	0.64
2:D:365:TYR:HA	2:D:368:LEU:HD23	1.79	0.64
2:B:131:CYS:SG	2:B:132:GLU:N	2.71	0.64
1:A:424:ALA:HB3	1:A:427:PHE:HE1	1.62	0.64
2:D:105:ILE:HG23	2:D:241:LEU:HD11	1.79	0.64
2:D:804:GLN:NE2	2:D:935:GLN:OE1	2.31	0.64
2:B:802:PHE:HB3	2:B:806:LEU:HD23	1.79	0.64
2:D:644:GLN:HA	2:D:649:CYS:HB2	1.79	0.64
2:D:720:ILE:HD12	2:D:923:ILE:HD11	1.79	0.64
1:A:479:MET:O	1:A:483:ILE:HG22	1.98	0.63
2:B:1077:THR:OG1	2:C:900:MET:SD	2.57	0.63
2:C:328:ARG:NE	2:C:580:GLN:OE1	2.30	0.63
2:B:354:ASN:HA	6:B:1310:NAG:H83	1.81	0.63
2:C:985:ASP:OD1	2:C:986:PRO:HD2	1.99	0.63
2:D:442:ASP:OD1	2:D:509:ARG:NH2	2.31	0.63
2:B:778:THR:HG22	2:B:865:LEU:HD12	1.81	0.63
2:C:646:ARG:HB2	2:C:668:ALA:HB1	1.80	0.63
2:B:290:ASP:OD1	2:B:291:CYS:N	2.32	0.63
2:C:411:ALA:HB3	2:C:414:GLN:HG3	1.81	0.63
2:C:1076:THR:HB	2:C:1097:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:667:GLY:HA2	2:D:864:LEU:HA	1.80	0.62
2:D:447:GLY:HA2	2:D:499:PRO:HD2	1.81	0.62
1:A:331:MET:H	1:A:358:LYS:HE3	1.64	0.62
2:B:353:TRP:HE1	2:B:466:ARG:HB2	1.65	0.62
1:A:489:PRO:HA	1:A:611:PRO:HG2	1.82	0.62
2:B:1075:PHE:O	2:B:1076:THR:OG1	2.18	0.62
2:C:454:ARG:HG2	2:C:492:LEU:HB3	1.82	0.62
2:D:443:SER:HB2	2:D:499:PRO:HA	1.82	0.62
2:C:34:ARG:NH2	2:C:217:PRO:O	2.33	0.62
2:C:802:PHE:HB3	2:C:806:LEU:HD13	1.82	0.62
2:B:858:LEU:HD11	2:B:962:LEU:HD23	1.83	0.61
2:C:865:LEU:HD22	2:C:869:MET:HE2	1.82	0.61
2:D:927:PHE:HZ	2:D:1052:PHE:HE2	1.48	0.61
2:D:290:ASP:OD1	2:D:291:CYS:N	2.33	0.61
2:C:176:LEU:HD22	2:C:190:ARG:HD2	1.83	0.61
2:C:454:ARG:NH1	2:C:467:ASP:O	2.28	0.61
2:D:736:VAL:HG11	2:D:1004:LEU:HD11	1.81	0.61
1:A:95:ARG:HH22	1:A:564:PRO:HG3	1.65	0.61
2:B:833:PHE:HB2	2:D:646:ARG:HG2	1.82	0.61
2:B:902:MET:HE1	2:B:1049:LEU:HD13	1.81	0.61
2:D:462:LYS:HB2	2:D:465:GLU:HG3	1.81	0.61
2:D:627:ASP:HA	2:D:634:ARG:HH22	1.65	0.61
2:D:1075:PHE:O	2:D:1076:THR:OG1	2.19	0.61
2:B:85:PRO:HA	2:B:237:ARG:HE	1.66	0.61
1:A:451:PHE:HE2	1:A:502:LEU:HD21	1.66	0.61
2:D:129:LYS:HG3	2:D:133:PHE:HZ	1.66	0.61
2:C:48:LEU:HD13	2:C:305:SER:HA	1.83	0.61
2:D:624:ILE:HA	2:D:634:ARG:HH21	1.66	0.60
1:A:287:LYS:HZ3	1:A:430:ASP:HB3	1.66	0.60
2:C:229:LEU:HD12	2:C:230:PRO:HD2	1.82	0.60
2:C:731:MET:SD	2:C:955:ASN:ND2	2.73	0.60
2:C:742:ILE:O	2:C:1000:ARG:NH1	2.33	0.60
1:A:287:LYS:HG3	1:A:432:GLU:HB2	1.84	0.60
2:D:439:ASN:O	2:D:443:SER:OG	2.19	0.60
2:B:312:ILE:HB	2:B:598:ILE:HG22	1.84	0.60
1:A:240:HIS:HB3	1:A:244:ARG:HH21	1.67	0.60
2:B:400:PHE:HB2	2:B:510:VAL:HG13	1.83	0.60
2:C:450:ASP:OD1	2:C:450:ASP:N	2.35	0.60
2:C:804:GLN:NE2	2:C:935:GLN:OE1	2.31	0.60
2:D:599:THR:HB	2:D:608:VAL:HG12	1.83	0.60
2:D:763:LEU:HD11	2:D:1004:LEU:HG	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1075:PHE:O	2:C:1076:THR:OG1	2.16	0.60
2:B:334:ASN:OD1	2:B:334:ASN:C	2.45	0.60
2:C:116:SER:N	2:C:131:CYS:O	2.24	0.59
2:C:780:GLU:O	2:C:784:GLN:NE2	2.35	0.59
2:B:325:SER:HB2	2:B:540:ASN:HD22	1.67	0.59
2:D:763:LEU:HG	2:D:1008:VAL:HG21	1.82	0.59
1:A:262:PRO:HD2	1:A:265:LEU:HD12	1.82	0.59
2:B:327:VAL:HG12	2:B:542:ASN:HB3	1.84	0.59
2:D:369:TYR:HA	2:D:374:PHE:HE2	1.67	0.59
1:A:242:TYR:OH	1:A:594:LEU:O	2.15	0.59
1:A:88:ILE:HD11	1:A:93:LEU:HB3	1.84	0.59
2:B:96:GLU:OE1	2:B:100:ILE:N	2.28	0.59
2:D:81:ASN:ND2	2:D:240:THR:O	2.29	0.59
2:D:406:GLU:HA	2:D:409:GLN:HB3	1.85	0.59
2:D:560:LEU:HD22	2:D:562:PHE:CD1	2.37	0.59
2:B:577:ARG:HD3	2:B:582:LEU:HD13	1.84	0.59
2:B:699:LEU:HD13	2:C:872:GLN:HG2	1.84	0.59
2:C:643:PHE:HE2	2:C:670:ILE:HG13	1.68	0.59
2:C:290:ASP:OD1	2:C:291:CYS:N	2.36	0.59
2:C:590:CYS:O	2:D:837:TYR:OH	2.15	0.59
1:A:142:ALA:O	1:A:144:GLU:N	2.35	0.59
1:A:480:LYS:HB3	1:A:486:VAL:HB	1.84	0.59
2:D:984:LEU:HB3	2:D:989:ALA:HB2	1.85	0.58
2:C:987:PRO:HG2	2:D:413:GLY:HA3	1.84	0.58
2:D:96:GLU:OE1	2:D:100:ILE:N	2.34	0.58
1:A:522:PHE:HB3	1:A:582:PRO:HB2	1.85	0.58
2:B:589:PRO:HB3	2:C:855:PHE:HA	1.85	0.58
2:B:1076:THR:HB	2:B:1097:SER:HB3	1.85	0.58
2:C:39:PRO:HG2	2:C:51:THR:HG21	1.85	0.58
1:A:436:ASN:O	1:A:440:LYS:HG2	2.04	0.58
2:C:627:ASP:OD1	2:C:634:ARG:NH1	2.35	0.58
2:D:124:THR:OG1	6:D:1301:NAG:O7	2.21	0.58
2:B:117:LEU:HD13	2:B:130:VAL:HG22	1.85	0.58
2:C:321:GLN:N	2:C:628:GLN:O	2.36	0.58
2:C:296:LEU:HB3	2:C:608:VAL:HG11	1.84	0.58
1:A:552:ARG:NH2	1:A:572:ILE:O	2.37	0.58
2:C:442:ASP:OD1	2:C:509:ARG:NH2	2.34	0.57
2:D:1009:THR:O	2:D:1013:ILE:HG12	2.03	0.57
2:C:178:ASP:OD1	2:C:178:ASP:N	2.37	0.57
2:C:212:ILE:HG22	2:C:213:GLY:N	2.17	0.57
2:C:609:ALA:HB2	2:C:692:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:595:VAL:HG21	2:D:633:TRP:HH2	1.69	0.57
2:C:703:ASN:ND2	2:D:787:GLN:OE1	2.38	0.57
2:C:456:PHE:HB2	2:C:491:PRO:HA	1.86	0.57
1:A:141:LEU:HD22	1:A:146:GLY:HA3	1.86	0.57
2:D:381:GLY:HA3	2:D:430:THR:HG23	1.86	0.57
2:D:1002:GLN:O	2:D:1006:THR:HG23	2.05	0.57
2:B:112:SER:HB2	2:B:134:GLN:HA	1.86	0.57
2:B:502:GLY:O	2:B:504:GLY:N	2.35	0.57
2:D:454:ARG:HG2	2:D:492:LEU:HB3	1.86	0.57
2:D:856:ASN:HD22	2:D:966:LEU:HD12	1.68	0.57
1:A:242:TYR:CE2	1:A:594:LEU:HB3	2.40	0.56
1:A:598:ASN:OD1	1:A:601:SER:OG	2.23	0.56
2:C:177:MET:SD	2:C:177:MET:N	2.78	0.56
2:D:353:TRP:H	2:D:353:TRP:CD1	2.24	0.56
1:A:387:GLN:NE2	1:A:559:LEU:O	2.34	0.56
2:B:205:SER:HB3	2:B:226:LEU:HG	1.86	0.56
2:B:230:PRO:HG2	2:D:357:ARG:HD2	1.87	0.56
2:C:566:GLY:HA2	2:D:43:PHE:H	1.70	0.56
2:B:393:THR:HG21	2:B:520:ALA:HB3	1.88	0.56
2:D:363:ALA:N	2:D:525:CYS:O	2.37	0.56
2:D:450:ASP:OD1	2:D:450:ASP:N	2.36	0.56
2:D:930:ALA:HA	2:D:933:LYS:HG2	1.88	0.56
1:A:292:VAL:HA	1:A:295:LYS:HD2	1.88	0.56
2:C:118:LEU:C	2:C:119:ILE:HD13	2.30	0.56
2:D:185:ASN:OD1	2:D:212:ILE:HG22	2.06	0.56
2:B:320:VAL:N	2:B:591:SER:OG	2.39	0.56
2:C:406:GLU:HA	2:C:409:GLN:HB3	1.88	0.56
2:C:731:MET:HG3	2:C:774:GLN:HE22	1.70	0.56
2:C:971:GLY:O	2:C:995:ARG:NH1	2.38	0.56
1:A:246:LYS:HD3	1:A:281:THR:HA	1.87	0.56
1:A:267:GLY:O	1:A:276:ASN:ND2	2.37	0.56
2:B:856:ASN:OD1	2:B:966:LEU:HD12	2.05	0.56
2:D:126:VAL:HG22	2:D:172:SER:H	1.69	0.56
2:C:312:ILE:HG13	2:C:598:ILE:HG12	1.88	0.56
2:C:389:ASP:OD1	2:C:389:ASP:N	2.38	0.56
1:A:350:LEU:HB2	1:A:354:ASP:O	2.06	0.55
2:C:337:PRO:HD2	2:C:358:ILE:HG23	1.87	0.55
2:C:599:THR:HB	2:C:608:VAL:HG12	1.87	0.55
1:A:301:TRP:HE1	1:A:306:ILE:HG13	1.71	0.55
2:B:319:ARG:HE	2:C:740:MET:HE2	1.72	0.55
2:D:177:MET:HE2	2:D:177:MET:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:OD1	1:A:150:ILE:N	2.39	0.55
2:B:307:THR:HA	2:B:602:THR:HG21	1.87	0.55
2:D:120:VAL:HG13	2:D:127:PHE:HB3	1.88	0.55
2:D:945:LEU:HD12	2:D:948:LEU:HD12	1.88	0.55
1:A:375:MET:HE3	1:A:375:MET:HA	1.88	0.55
2:B:826:VAL:HB	2:B:1057:PRO:HG2	1.88	0.55
2:D:912:THR:OG1	2:D:914:ASN:OD1	2.17	0.55
2:D:976:VAL:HG12	2:D:979:ASP:H	1.72	0.55
1:A:438:LEU:HD21	1:A:590:LEU:HB2	1.88	0.55
2:B:1098:ASN:OD1	2:B:1101:HIS:N	2.39	0.55
2:D:326:ILE:HG13	2:D:539:VAL:HG11	1.89	0.55
1:A:357:ILE:C	1:A:358:LYS:HZ2	2.13	0.55
2:C:526:GLY:O	2:C:528:LYS:NZ	2.39	0.55
2:B:599:THR:HB	2:B:608:VAL:HG12	1.87	0.55
2:D:580:GLN:OE1	6:D:1310:NAG:O3	2.25	0.55
2:D:598:ILE:HD12	2:D:650:LEU:HD21	1.89	0.55
2:D:328:ARG:NH1	2:D:544:ASN:OD1	2.39	0.55
1:A:217:SER:OG	1:A:218:ARG:N	2.40	0.55
2:D:718:PHE:HE2	2:D:923:ILE:HD13	1.71	0.55
2:C:386:LYS:NZ	2:D:985:ASP:OD1	2.40	0.55
2:C:403:LYS:HE2	2:C:495:TYR:HE1	1.72	0.55
2:C:454:ARG:HH22	2:C:467:ASP:HB3	1.71	0.55
2:B:855:PHE:HB2	2:D:589:PRO:HG3	1.89	0.54
2:B:909:ILE:HD13	2:B:1049:LEU:HD21	1.89	0.54
2:C:589:PRO:HG3	2:D:855:PHE:HA	1.89	0.54
2:B:348:ALA:HB3	2:B:354:ASN:HB2	1.88	0.54
2:C:133:PHE:HA	2:C:162:SER:HB2	1.89	0.54
2:C:577:ARG:HA	2:C:584:ILE:HA	1.87	0.54
1:A:470:GLN:HA	1:A:494:GLU:HG2	1.90	0.54
2:B:1075:PHE:HB3	2:B:1097:SER:O	2.07	0.54
2:C:731:MET:HE1	2:C:1014:ARG:HB3	1.89	0.54
2:B:421:TYR:HA	2:B:457:ARG:HH21	1.73	0.54
2:B:667:GLY:HA2	2:C:864:LEU:HA	1.89	0.54
2:C:278:LYS:HG2	2:C:287:ASP:H	1.72	0.54
1:A:387:GLN:NE2	1:A:562:SER:OG	2.41	0.54
2:B:132:GLU:N	2:B:166:CYS:SG	2.67	0.54
2:D:645:THR:HG23	2:D:647:ALA:H	1.71	0.54
1:A:175:LEU:O	1:A:175:LEU:HD23	2.07	0.54
2:C:927:PHE:HZ	2:C:1052:PHE:HE2	1.54	0.54
2:C:93:ALA:HB3	2:C:266:TYR:HB2	1.90	0.54
2:D:48:LEU:HD13	2:D:305:SER:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:816:SER:H	2:D:819:GLU:HG3	1.72	0.54
1:A:472:TRP:N	1:A:494:GLU:OE1	2.41	0.54
1:A:476:TRP:CE3	1:A:499:PRO:HG2	2.43	0.54
2:C:40:ASP:N	2:C:40:ASP:OD1	2.40	0.54
2:C:707:TYR:HD2	2:D:792:PRO:HG3	1.72	0.54
2:D:307:THR:HA	2:D:602:THR:HG21	1.89	0.54
2:D:406:GLU:N	2:D:406:GLU:OE1	2.41	0.54
1:A:452:THR:HG23	1:A:511:PHE:HB3	1.90	0.53
1:A:117:ASN:HA	1:A:120:LEU:HD23	1.89	0.53
2:B:202:LYS:HZ1	2:B:225:PRO:HB3	1.73	0.53
2:D:662:CYS:HB2	2:D:697:MET:HE3	1.91	0.53
1:A:413:THR:OG1	1:A:542:ASP:OD1	2.21	0.53
2:B:941:THR:HG21	2:B:944:ALA:HB2	1.90	0.53
2:C:722:VAL:HG22	2:C:1065:VAL:HG22	1.91	0.53
1:A:475:LYS:HG3	1:A:479:MET:HE2	1.91	0.53
2:B:93:ALA:HB3	2:B:266:TYR:HB2	1.91	0.53
2:B:241:LEU:HD12	2:B:242:LEU:H	1.72	0.53
2:C:342:PHE:HZ	2:C:434:ILE:HG21	1.72	0.53
2:C:388:ASN:HB3	2:C:527:PRO:HD2	1.90	0.53
1:A:326:PHE:CE1	1:A:355:PHE:HB2	2.44	0.53
2:B:454:ARG:HG2	2:B:492:LEU:HG	1.89	0.53
2:C:353:TRP:CD1	2:C:353:TRP:H	2.26	0.53
2:C:843:ASP:O	2:C:845:ALA:N	2.41	0.53
1:A:207:GLU:OE2	1:A:218:ARG:NE	2.38	0.53
1:A:245:ALA:HA	1:A:248:MET:HG3	1.90	0.53
2:B:126:VAL:HG22	2:B:172:SER:H	1.74	0.53
2:C:551:VAL:HB	2:C:588:THR:HB	1.91	0.53
2:D:334:ASN:ND2	2:D:360:ASN:O	2.40	0.53
2:B:411:ALA:HB3	2:B:414:GLN:HG3	1.91	0.53
2:C:320:VAL:N	2:C:591:SER:OG	2.41	0.53
1:A:326:PHE:HE1	1:A:355:PHE:HB2	1.74	0.53
2:D:906:PHE:CD2	2:D:916:LEU:HB2	2.43	0.53
1:A:48:TRP:HD1	1:A:350:LEU:HD21	1.72	0.52
1:A:469:LYS:HD3	1:A:472:TRP:CD1	2.44	0.52
2:B:357:ARG:NH2	2:B:359:SER:OG	2.40	0.52
1:A:262:PRO:HG3	1:A:611:PRO:HG3	1.91	0.52
1:A:296:MET:HB2	1:A:301:TRP:HB2	1.91	0.52
2:B:729:VAL:HG11	2:B:781:VAL:HG11	1.91	0.52
2:D:93:ALA:HB3	2:D:266:TYR:HB2	1.91	0.52
1:A:20:THR:OG1	1:A:23:GLU:OE1	2.26	0.52
1:A:51:ASN:ND2	1:A:342:VAL:O	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:ILE:HG12	2:B:239:GLN:HB2	1.90	0.52
2:C:715:PRO:HD3	2:D:894:LEU:HD13	1.92	0.52
2:D:34:ARG:NH2	2:D:217:PRO:O	2.42	0.52
2:B:715:PRO:HD3	2:C:894:LEU:HD13	1.90	0.52
2:B:590:CYS:O	2:C:837:TYR:OH	2.20	0.52
2:D:326:ILE:HD11	2:D:534:VAL:HG12	1.92	0.52
2:D:560:LEU:H	2:D:563:GLN:HG3	1.74	0.52
1:A:29:LEU:HD11	1:A:96:GLN:HB3	1.90	0.52
2:C:1040:VAL:C	2:C:1042:PHE:H	2.18	0.52
1:A:264:HIS:ND1	1:A:489:PRO:HG2	2.24	0.52
2:B:230:PRO:O	2:D:396:TYR:OH	2.27	0.52
2:B:971:GLY:O	2:B:995:ARG:NH1	2.42	0.52
2:D:431:GLY:HA2	2:D:515:PHE:CD2	2.45	0.52
1:A:146:GLY:O	1:A:148:ASP:N	2.43	0.52
1:A:322:MET:HE3	1:A:326:PHE:CG	2.45	0.52
2:B:200:TYR:HA	2:B:230:PRO:HA	1.92	0.52
2:D:557:LYS:HB2	2:D:584:ILE:HD13	1.92	0.52
1:A:117:ASN:OD1	1:A:118:THR:N	2.42	0.52
2:B:31:SER:OG	2:B:60:SER:N	2.42	0.52
2:B:574:ASP:O	2:B:587:ILE:N	2.43	0.52
2:B:1027:THR:O	2:B:1031:GLU:HG3	2.10	0.52
2:B:841:LEU:HD23	2:B:841:LEU:H	1.75	0.52
2:B:897:PRO:HG2	2:B:900:MET:HG3	1.92	0.52
2:B:350:VAL:HG11	2:B:422:ASN:HD22	1.75	0.51
2:B:384:PRO:HG2	2:D:489:TYR:CZ	2.45	0.51
2:C:117:LEU:HD22	2:C:119:ILE:HD11	1.91	0.51
2:D:130:VAL:HG21	2:D:231:ILE:HD12	1.92	0.51
2:D:351:TYR:HE2	2:D:468:ILE:HG13	1.75	0.51
2:D:367:VAL:O	2:D:371:PHE:HB2	2.10	0.51
1:A:77:SER:O	1:A:81:LYS:HG2	2.09	0.51
2:B:176:LEU:C	2:B:177:MET:HE2	2.35	0.51
2:B:334:ASN:OD1	2:B:362:VAL:CG1	2.46	0.51
2:B:886:TRP:HB3	2:B:1035:GLY:HA2	1.93	0.51
2:D:714:ILE:HD12	2:D:1096:VAL:HG21	1.91	0.51
2:B:358:ILE:HB	2:B:395:VAL:HB	1.91	0.51
2:B:1029:MET:O	2:B:1033:VAL:HB	2.10	0.51
2:D:559:PHE:H	2:D:584:ILE:HD11	1.75	0.51
2:D:897:PRO:HG2	2:D:900:MET:SD	2.51	0.51
1:A:165:GLU:HG3	1:A:490:LEU:HD12	1.91	0.51
2:C:712:ILE:HD13	2:C:1094:VAL:HG11	1.92	0.51
2:B:112:SER:HA	2:B:132:GLU:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1075:PHE:HB3	2:C:1097:SER:O	2.11	0.51
2:B:894:LEU:HD13	2:D:715:PRO:HD3	1.91	0.51
2:C:589:PRO:O	2:D:837:TYR:OH	2.29	0.51
2:D:34:ARG:NH1	2:D:191:GLU:OE2	2.41	0.51
2:D:749:CYS:SG	2:D:997:ILE:HD11	2.50	0.51
1:A:431:ASN:O	1:A:434:GLU:HG3	2.10	0.51
2:B:756:TYR:OH	2:B:994:ASP:OD1	2.25	0.51
2:C:973:ILE:HG12	2:C:992:GLN:HE21	1.76	0.51
2:D:133:PHE:HA	2:D:162:SER:HB2	1.93	0.51
2:C:352:ALA:HB2	2:C:468:ILE:HD12	1.93	0.51
2:D:731:MET:HE1	2:D:1015:ALA:HA	1.93	0.51
2:B:330:PRO:HA	2:B:579:PRO:HB2	1.92	0.51
2:B:629:LEU:HG	2:B:631:PRO:HD2	1.93	0.50
2:C:903:ALA:HB2	2:C:916:LEU:HD22	1.93	0.50
2:B:722:VAL:HG22	2:B:1065:VAL:HG22	1.94	0.50
2:B:403:LYS:HD2	2:B:505:HIS:HB3	1.92	0.50
2:B:1098:ASN:CG	2:B:1101:HIS:H	2.18	0.50
2:C:214:ARG:HG3	2:C:215:ASP:H	1.76	0.50
2:C:853:GLN:HB2	2:C:858:LEU:HB2	1.94	0.50
2:D:360:ASN:H	2:D:523:THR:HB	1.75	0.50
2:D:1076:THR:HB	2:D:1097:SER:HB3	1.93	0.50
2:B:699:LEU:HD21	2:C:869:MET:HB2	1.93	0.50
2:C:472:ILE:HA	2:C:491:PRO:HD3	1.93	0.50
1:A:585:ASN:HA	1:A:588:GLU:HG2	1.94	0.50
2:B:406:GLU:HA	2:B:409:GLN:HB3	1.93	0.50
2:C:592:PHE:CZ	2:D:740:MET:HB2	2.47	0.50
2:C:986:PRO:HA	2:C:989:ALA:HB3	1.94	0.50
2:B:204:TYR:HA	2:B:225:PRO:HA	1.92	0.50
2:B:600:PRO:HD3	2:B:692:ILE:HD11	1.94	0.50
2:D:118:LEU:HG	2:D:120:VAL:HG12	1.94	0.50
1:A:22:GLU:N	1:A:22:GLU:OE1	2.43	0.49
1:A:418:LYS:HG2	1:A:423:LEU:HD22	1.94	0.49
2:C:206:LYS:HB3	2:C:223:LEU:HD13	1.94	0.49
2:C:300:LYS:HZ1	2:C:306:PHE:C	2.20	0.49
2:C:336:CYS:HB2	2:C:338:PHE:CE2	2.47	0.49
2:C:1013:ILE:HD13	2:D:1012:LEU:HB3	1.93	0.49
2:D:287:ASP:OD1	2:D:288:ALA:N	2.45	0.49
2:D:376:ALA:HB3	2:D:435:ALA:HB3	1.94	0.49
2:B:916:LEU:HD12	2:B:923:ILE:HG21	1.93	0.49
1:A:48:TRP:CD1	1:A:350:LEU:HD21	2.47	0.49
2:C:737:ASP:OD1	2:C:738:CYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:ASN:HA	2:C:209:PRO:HA	1.94	0.49
2:C:563:GLN:HA	2:D:41:LYS:HB3	1.94	0.49
2:C:909:ILE:HG12	2:C:1047:TYR:HB3	1.93	0.49
2:D:295:PRO:HG3	2:D:633:TRP:CE3	2.48	0.49
2:D:843:ASP:O	2:D:845:ALA:N	2.45	0.49
2:B:81:ASN:HD21	2:B:239:GLN:HB3	1.77	0.49
2:B:886:TRP:HZ3	2:B:905:ARG:HD3	1.78	0.49
2:B:965:GLN:O	2:B:968:SER:OG	2.30	0.49
2:C:878:LEU:O	2:C:882:ILE:HG23	2.12	0.49
2:D:740:MET:HE2	2:D:740:MET:HA	1.95	0.49
2:C:457:ARG:NE	2:C:459:SER:O	2.45	0.49
2:C:736:VAL:HG11	2:C:1004:LEU:HD11	1.94	0.49
2:D:617:CYS:O	2:D:621:SER:CB	2.61	0.49
2:D:874:THR:HG21	2:D:1054:GLN:HA	1.94	0.49
1:A:444:THR:HG23	1:A:445:ILE:HG12	1.95	0.49
2:B:448:ASN:HB3	2:B:497:PHE:HB2	1.95	0.49
2:D:305:SER:OG	2:D:306:PHE:N	2.46	0.49
2:D:337:PRO:HD2	2:D:358:ILE:HG23	1.95	0.49
1:A:563:GLU:HG3	1:A:567:LEU:HD23	1.94	0.49
2:B:193:VAL:HG13	2:B:204:TYR:HD1	1.78	0.49
2:B:612:TYR:O	2:B:648:GLY:HA3	2.13	0.49
2:D:617:CYS:O	2:D:621:SER:N	2.42	0.49
2:B:299:THR:O	2:B:303:LEU:HG	2.12	0.49
2:C:44:ARG:HD3	2:C:47:VAL:HG11	1.95	0.49
2:C:858:LEU:HD21	2:C:962:LEU:HD22	1.95	0.49
2:C:104:TRP:CD1	2:C:240:THR:HG23	2.48	0.48
2:C:763:LEU:HD22	2:C:1008:VAL:HG21	1.94	0.48
2:D:37:TYR:OH	2:D:54:LEU:O	2.24	0.48
2:D:57:PRO:HG3	2:D:273:ARG:HD2	1.95	0.48
2:D:328:ARG:HH21	2:D:580:GLN:CD	2.21	0.48
1:A:391:LEU:HA	1:A:561:LYS:HB2	1.95	0.48
2:B:42:VAL:CG1	2:D:567:ARG:HB2	2.44	0.48
2:B:459:SER:OG	2:B:460:LYS:N	2.45	0.48
2:B:983:ARG:HA	2:D:390:LEU:HD21	1.95	0.48
2:D:30:ASN:HD21	2:D:59:PHE:HD1	1.62	0.48
2:D:87:ASN:OD1	2:D:87:ASN:N	2.45	0.48
2:D:209:PRO:C	2:D:210:ILE:HG13	2.38	0.48
2:D:303:LEU:HD12	2:D:308:VAL:HG12	1.96	0.48
2:D:1029:MET:O	2:D:1033:VAL:HB	2.13	0.48
2:C:449:TYR:HA	2:C:496:GLY:HA2	1.96	0.48
2:D:795:LYS:HE3	2:D:806:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:HB3	1:A:498:ASP:OD1	2.13	0.48
1:A:229:PHE:O	1:A:233:LYS:HG2	2.13	0.48
2:C:983:ARG:HG2	2:C:984:LEU:HD12	1.95	0.48
2:B:969:LYS:NZ	2:B:973:ILE:O	2.46	0.48
2:C:102:ARG:HH21	2:C:122:ASN:HA	1.78	0.48
1:A:541:CYS:SG	1:A:542:ASP:N	2.86	0.48
2:C:457:ARG:NH1	2:C:467:ASP:OD2	2.46	0.48
2:D:176:LEU:C	2:D:177:MET:HE2	2.39	0.48
1:A:458:TRP:HB3	1:A:476:TRP:CE2	2.49	0.48
2:B:326:ILE:HG23	2:B:539:VAL:HG21	1.95	0.48
2:C:200:TYR:HA	2:C:230:PRO:HA	1.96	0.48
2:C:822:LEU:HD22	2:C:945:LEU:HD11	1.95	0.48
2:D:633:TRP:CD1	2:D:633:TRP:H	2.31	0.48
1:A:134:ASP:N	1:A:139:GLU:OE2	2.41	0.48
2:B:376:ALA:HB3	2:B:435:ALA:HB3	1.96	0.48
2:B:574:ASP:OD2	2:C:847:ARG:N	2.35	0.48
2:B:707:TYR:HE1	2:C:897:PRO:HA	1.79	0.48
2:D:403:LYS:O	2:D:407:VAL:HG23	2.14	0.48
2:B:624:ILE:HD11	2:B:629:LEU:HD22	1.95	0.48
1:A:216:TYR:CE1	1:A:566:THR:HG21	2.49	0.48
1:A:458:TRP:HB3	1:A:476:TRP:CZ2	2.49	0.48
1:A:539:PHE:HE2	1:A:589:PRO:HG2	1.79	0.48
2:B:666:ILE:HG12	2:B:671:CYS:HA	1.94	0.48
2:B:896:ILE:HG12	2:D:712:ILE:HG13	1.95	0.48
2:D:385:THR:OG1	2:D:386:LYS:N	2.47	0.48
2:D:770:ILE:HD11	2:D:1012:LEU:HD23	1.96	0.48
1:A:356:ARG:HB2	1:A:358:LYS:HZ1	1.79	0.47
2:B:822:LEU:HD22	2:B:945:LEU:HD21	1.95	0.47
2:D:194:PHE:HD1	2:D:203:ILE:HG13	1.79	0.47
2:C:858:LEU:HD12	2:C:959:LEU:HD22	1.95	0.47
2:D:878:LEU:O	2:D:882:ILE:HG23	2.14	0.47
1:A:144:GLU:H	1:A:145:PRO:HD2	1.78	0.47
1:A:476:TRP:HE3	1:A:499:PRO:HG2	1.79	0.47
2:B:978:ASN:HB3	2:D:547:THR:HG23	1.96	0.47
2:C:662:CYS:SG	2:C:697:MET:HE3	2.54	0.47
1:A:468:PRO:HD2	1:A:471:GLN:NE2	2.29	0.47
2:B:985:ASP:OD2	2:D:383:SER:OG	2.20	0.47
2:B:990:GLU:OE2	2:B:990:GLU:N	2.46	0.47
1:A:553:LEU:O	1:A:557:LEU:HG	2.14	0.47
2:C:564:GLN:OE1	2:C:577:ARG:NH1	2.47	0.47
2:D:741:TYR:HD2	2:D:1004:LEU:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ALA:O	1:A:244:ARG:HG2	2.15	0.47
2:B:305:SER:OG	2:B:306:PHE:N	2.47	0.47
2:B:350:VAL:HG11	2:B:418:ILE:HD11	1.97	0.47
2:C:29:THR:OG1	2:C:30:ASN:N	2.48	0.47
2:B:191:GLU:O	2:B:205:SER:HA	2.14	0.47
2:B:843:ASP:O	2:B:845:ALA:N	2.46	0.47
2:D:594:GLY:O	2:D:613:GLN:N	2.38	0.47
2:D:666:ILE:HD11	2:D:672:ALA:HB2	1.97	0.47
2:D:1073:LYS:HB2	2:D:1075:PHE:CZ	2.50	0.47
2:D:1075:PHE:HB3	2:D:1097:SER:O	2.15	0.47
2:D:1098:ASN:OD1	2:D:1099:GLY:N	2.48	0.47
1:A:50:TYR:CE1	1:A:59:VAL:HA	2.50	0.47
1:A:322:MET:HE1	1:A:375:MET:HE1	1.97	0.47
2:B:396:TYR:HB2	2:B:514:SER:HB3	1.95	0.47
2:B:473:TYR:HD2	2:B:489:TYR:HB2	1.80	0.47
2:B:125:ASN:ND2	2:B:172:SER:O	2.46	0.47
2:B:353:TRP:CD1	2:B:353:TRP:H	2.33	0.47
2:B:906:PHE:CD2	2:B:916:LEU:HB2	2.50	0.47
2:C:112:SER:HA	2:C:132:GLU:HG2	1.96	0.47
2:C:295:PRO:HG3	2:C:633:TRP:CD1	2.50	0.47
2:C:472:ILE:HD13	2:C:482:GLY:O	2.14	0.47
2:C:866:THR:OG1	2:C:869:MET:HG2	2.15	0.47
1:A:303:ALA:O	1:A:306:ILE:HG22	2.15	0.46
2:B:113:LYS:HB3	2:B:113:LYS:HE2	1.71	0.46
2:C:231:ILE:HG22	2:C:233:ILE:HG23	1.98	0.46
2:C:906:PHE:HA	2:C:909:ILE:HG22	1.97	0.46
2:D:229:LEU:HD23	2:D:229:LEU:H	1.81	0.46
2:D:969:LYS:HE3	2:D:974:SER:HA	1.97	0.46
1:A:417:LEU:HB3	1:A:423:LEU:HB2	1.98	0.46
2:B:1039:ARG:NE	2:C:1031:GLU:OE2	2.46	0.46
2:C:290:ASP:O	2:C:297:SER:HB3	2.15	0.46
2:C:1039:ARG:NE	2:D:1031:GLU:OE2	2.48	0.46
2:C:1083:HIS:HB2	2:C:1137:VAL:HG12	1.97	0.46
2:D:131:CYS:HB2	2:D:166:CYS:HB3	1.76	0.46
2:D:496:GLY:O	2:D:501:TYR:OH	2.18	0.46
2:B:26:GLN:HE22	2:B:82:PRO:HG3	1.80	0.46
2:B:328:ARG:HG3	2:B:579:PRO:HG2	1.98	0.46
2:B:570:VAL:HG23	2:B:572:THR:HG23	1.97	0.46
2:B:931:ILE:O	2:B:934:ILE:HG22	2.15	0.46
2:D:441:LEU:HD22	2:D:509:ARG:HH12	1.80	0.46
2:D:568:ASP:OD1	2:D:568:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ALA:N	1:A:487:VAL:O	2.45	0.46
2:B:294:ASP:OD2	2:B:296:LEU:HB3	2.16	0.46
2:B:386:LYS:NZ	2:D:457:ARG:O	2.41	0.46
2:C:829:ALA:O	2:C:850:ILE:HD11	2.15	0.46
2:C:1002:GLN:HG3	2:D:759:PHE:HZ	1.80	0.46
2:B:317:ASN:HA	2:B:594:GLY:HA2	1.98	0.46
2:B:914:ASN:ND2	2:D:1123:SER:OG	2.48	0.46
2:C:553:THR:HG21	2:D:841:LEU:HB2	1.97	0.46
2:C:878:LEU:HD11	2:C:1052:PHE:HB3	1.96	0.46
2:C:906:PHE:CD2	2:C:916:LEU:HB2	2.50	0.46
1:A:442:ALA:O	1:A:446:VAL:HG22	2.15	0.46
1:A:456:GLU:HG3	1:A:460:TRP:NE1	2.30	0.46
2:B:1098:ASN:OD1	2:B:1099:GLY:N	2.49	0.46
2:C:85:PRO:O	2:C:269:TYR:OH	2.29	0.46
2:C:502:GLY:O	2:C:506:GLN:HG2	2.15	0.46
2:D:389:ASP:OD1	2:D:389:ASP:N	2.45	0.46
2:D:650:LEU:HD23	2:D:650:LEU:HA	1.83	0.46
1:A:33:ASN:O	1:A:37:GLU:HG2	2.16	0.46
2:B:225:PRO:HG2	2:D:562:PHE:CE2	2.51	0.46
2:D:303:LEU:H	2:D:303:LEU:HG	1.54	0.46
2:B:322:PRO:HB3	2:B:539:VAL:HA	1.97	0.46
2:B:847:ARG:NH2	2:D:587:ILE:O	2.47	0.46
2:C:119:ILE:HD12	2:C:128:ILE:HG23	1.98	0.46
2:B:556:ASN:H	2:C:844:ILE:HG23	1.81	0.46
2:C:743:CYS:HB3	2:C:749:CYS:HB3	1.82	0.46
2:D:444:LYS:HG2	2:D:448:ASN:HB2	1.97	0.46
2:D:848:ASP:OD1	2:D:848:ASP:N	2.48	0.46
2:B:328:ARG:HD3	2:B:530:SER:HB3	1.97	0.45
2:C:914:ASN:HD21	2:C:1111:GLU:CD	2.24	0.45
2:D:328:ARG:NH1	2:D:579:PRO:HG2	2.31	0.45
1:A:193:ASN:HB3	1:A:201:TYR:HE2	1.81	0.45
2:B:457:ARG:CZ	2:B:461:LEU:HG	2.47	0.45
2:B:1129:VAL:HG13	2:C:917:TYR:HB3	1.97	0.45
2:D:337:PRO:O	2:D:341:VAL:HG23	2.16	0.45
2:D:448:ASN:H	2:D:498:ARG:HG2	1.80	0.45
2:B:132:GLU:OE1	2:B:165:ASN:ND2	2.43	0.45
2:B:792:PRO:HG3	2:D:707:TYR:HD2	1.82	0.45
2:B:878:LEU:O	2:B:882:ILE:HG23	2.16	0.45
2:D:1083:HIS:HB2	2:D:1137:VAL:HG12	1.98	0.45
1:A:456:GLU:HG2	1:A:512:ILE:HG13	1.98	0.45
2:B:384:PRO:HG2	2:D:489:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:878:LEU:HA	2:B:881:THR:HG22	1.99	0.45
2:C:96:GLU:OE1	2:C:100:ILE:N	2.40	0.45
2:C:307:THR:HA	2:C:602:THR:HG21	1.99	0.45
2:D:57:PRO:HB2	2:D:60:SER:HB3	1.98	0.45
1:A:314:PHE:HD1	1:A:319:LEU:HD12	1.82	0.45
2:B:178:ASP:OD1	2:B:178:ASP:N	2.49	0.45
2:C:334:ASN:OD1	2:C:334:ASN:N	2.48	0.45
2:C:850:ILE:O	2:C:853:GLN:HG2	2.17	0.45
2:D:778:THR:HG22	2:D:865:LEU:HD12	1.98	0.45
1:A:343:CYS:HB2	1:A:360:CYS:N	2.32	0.45
2:C:87:ASN:O	2:C:87:ASN:ND2	2.48	0.45
2:C:358:ILE:HB	2:C:395:VAL:HB	1.99	0.45
2:C:853:GLN:HB2	2:C:858:LEU:CB	2.46	0.45
2:C:965:GLN:O	2:C:968:SER:OG	2.31	0.45
2:D:178:ASP:OD1	2:D:178:ASP:N	2.50	0.45
2:D:617:CYS:O	2:D:621:SER:HB2	2.17	0.45
2:B:560:LEU:HD12	2:B:562:PHE:HE1	1.81	0.45
2:C:770:ILE:HD11	2:C:1012:LEU:HD13	1.98	0.45
2:B:206:LYS:HD2	2:B:222:ALA:O	2.17	0.45
2:C:310:LYS:HG3	2:C:600:PRO:HA	1.99	0.45
2:C:402:ILE:HB	2:C:406:GLU:HB3	1.99	0.45
1:A:518:THR:O	1:A:521:GLN:HG3	2.16	0.45
2:C:436:TRP:HZ3	2:C:511:VAL:HG22	1.81	0.45
2:C:570:VAL:O	2:C:572:THR:HG23	2.17	0.45
2:C:629:LEU:HD23	2:C:631:PRO:HG2	1.98	0.45
2:C:699:LEU:HB3	2:D:873:TYR:CZ	2.52	0.45
2:D:105:ILE:HG22	2:D:118:LEU:HD13	1.99	0.45
2:D:294:ASP:OD1	2:D:295:PRO:HD2	2.16	0.45
2:D:398:ASP:OD2	2:D:423:TYR:OH	2.32	0.45
1:A:294:GLU:CD	1:A:295:LYS:HG3	2.42	0.45
2:B:1072:GLU:N	2:B:1072:GLU:OE1	2.50	0.45
2:C:101:ILE:HG23	2:C:241:LEU:O	2.17	0.45
2:D:173:GLN:HG2	2:D:174:PRO:HD2	1.99	0.45
2:D:577:ARG:HA	2:D:584:ILE:HA	1.99	0.45
2:D:941:THR:HG21	2:D:944:ALA:HB2	1.99	0.45
1:A:179:TYR:O	1:A:183:VAL:HG23	2.18	0.44
1:A:502:LEU:O	1:A:506:ALA:HB2	2.17	0.44
2:B:42:VAL:HG11	2:D:567:ARG:HE	1.82	0.44
2:D:318:PHE:HD2	2:D:629:LEU:HD11	1.82	0.44
1:A:292:VAL:HG12	1:A:295:LYS:HD2	2.00	0.44
2:B:37:TYR:HA	2:B:223:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:731:MET:HE1	2:B:1014:ARG:HB3	1.98	0.44
2:C:365:TYR:CZ	2:C:387:LEU:HG	2.53	0.44
2:C:770:ILE:O	2:C:774:GLN:HG3	2.17	0.44
2:D:109:THR:OG1	2:D:111:ASP:OD1	2.36	0.44
1:A:244:ARG:HH12	1:A:260:CYS:HA	1.82	0.44
1:A:270:TRP:CD2	1:A:502:LEU:HG	2.52	0.44
1:A:326:PHE:O	1:A:330:SER:OG	2.18	0.44
2:B:336:CYS:SG	2:B:337:PRO:HD2	2.57	0.44
2:B:954:HIS:HB3	2:B:1014:ARG:NH1	2.32	0.44
2:D:321:GLN:N	2:D:628:GLN:O	2.35	0.44
2:D:534:VAL:HG13	2:D:539:VAL:HG21	1.99	0.44
2:D:788:ILE:HG23	2:D:876:ALA:HB2	2.00	0.44
2:D:903:ALA:HB1	2:D:913:GLN:HB3	1.97	0.44
2:B:567:ARG:HD2	2:C:42:VAL:HG11	2.00	0.44
2:B:802:PHE:CD1	2:B:805:ILE:HD11	2.53	0.44
1:A:81:LYS:NZ	1:A:103:SER:HB3	2.32	0.44
2:B:342:PHE:CE1	2:B:511:VAL:HG11	2.52	0.44
2:B:445:HIS:O	2:B:446:SER:OG	2.30	0.44
2:C:190:ARG:HD3	2:C:207:HIS:CE1	2.52	0.44
2:C:403:LYS:O	2:C:407:VAL:HG23	2.17	0.44
2:D:497:PHE:CE1	2:D:507:PRO:HA	2.52	0.44
2:C:108:THR:O	2:C:109:THR:OG1	2.36	0.44
2:C:437:ASN:HD21	2:C:506:GLN:HB3	1.82	0.44
2:C:1075:PHE:HB2	2:C:1096:VAL:HG22	2.00	0.44
2:C:1106:GLN:HB2	2:C:1109:PHE:O	2.17	0.44
2:D:108:THR:O	2:D:109:THR:OG1	2.36	0.44
2:D:229:LEU:HD12	2:D:231:ILE:HD11	2.00	0.44
2:D:962:LEU:HD12	2:D:1007:TYR:CG	2.52	0.44
1:A:295:LYS:O	1:A:298:ASN:HB2	2.18	0.44
2:B:555:SER:HB3	2:B:584:ILE:HG23	1.99	0.44
2:D:131:CYS:HB3	2:D:133:PHE:CE1	2.52	0.44
2:D:365:TYR:CE2	2:D:387:LEU:HG	2.53	0.44
1:A:164:TRP:NE1	1:A:269:MET:O	2.50	0.44
2:C:850:ILE:O	2:C:854:LYS:HG2	2.18	0.44
2:C:854:LYS:HA	2:C:854:LYS:HD2	1.83	0.44
2:D:44:ARG:HB3	2:D:47:VAL:HG11	1.99	0.44
2:D:821:LEU:HD11	2:D:935:GLN:HG3	2.00	0.44
2:D:822:LEU:HD22	2:D:945:LEU:HD11	1.99	0.44
2:C:365:TYR:CE1	2:C:387:LEU:HG	2.52	0.44
2:D:567:ARG:HD3	2:D:571:ASP:HA	2.00	0.44
2:D:985:ASP:HB3	2:D:987:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1049:LEU:HD11	2:D:1067:TYR:HB2	2.00	0.44
2:C:342:PHE:HE2	2:C:372:ALA:HB2	1.83	0.43
2:D:969:LYS:HE2	2:D:969:LYS:HB3	1.74	0.43
2:B:30:ASN:HB3	2:B:32:PHE:CE1	2.52	0.43
2:B:296:LEU:HB2	2:B:608:VAL:HG11	2.00	0.43
2:B:533:LEU:HD23	2:B:535:LYS:HE3	1.99	0.43
2:D:402:ILE:HD11	2:D:510:VAL:HG21	2.00	0.43
2:B:643:PHE:O	2:B:649:CYS:HA	2.18	0.43
2:B:763:LEU:HD11	2:B:1004:LEU:HG	2.00	0.43
2:C:574:ASP:O	2:C:587:ILE:N	2.48	0.43
2:C:642:VAL:HG22	2:C:651:ILE:HD13	2.00	0.43
2:D:537:LYS:HE2	2:D:537:LYS:HB2	1.75	0.43
2:B:190:ARG:HD3	2:B:207:HIS:CE1	2.52	0.43
2:B:290:ASP:O	2:B:297:SER:HB3	2.18	0.43
2:B:631:PRO:O	2:B:634:ARG:NH2	2.51	0.43
2:C:24:THR:HG21	2:C:82:PRO:HG3	2.00	0.43
2:C:870:ILE:HG22	2:C:1055:SER:HB2	1.99	0.43
2:B:300:LYS:HG2	2:B:305:SER:O	2.19	0.43
2:B:568:ASP:OD1	2:B:572:THR:OG1	2.24	0.43
2:C:611:LEU:HD22	2:C:666:ILE:HG23	2.01	0.43
2:D:95:THR:HB	2:D:189:LEU:HG	2.00	0.43
2:D:975:SER:O	2:D:975:SER:OG	2.30	0.43
1:A:446:VAL:HA	1:A:449:LEU:HD23	1.99	0.43
1:A:556:MET:HB2	1:A:556:MET:HE3	1.87	0.43
2:B:276:LEU:HB3	2:B:289:VAL:HG23	2.00	0.43
2:B:318:PHE:HD2	2:B:629:LEU:HD11	1.84	0.43
2:C:33:THR:HG23	2:C:58:PHE:CZ	2.53	0.43
2:C:393:THR:OG1	2:C:394:ASN:N	2.51	0.43
2:C:1031:GLU:OE1	2:C:1039:ARG:HD3	2.19	0.43
1:A:31:LYS:HG3	2:B:489:TYR:HD2	1.83	0.43
1:A:41:TYR:HE2	1:A:352:LYS:HB2	1.84	0.43
2:C:720:ILE:HD12	2:C:923:ILE:HG23	2.01	0.43
2:D:822:LEU:HD11	2:D:1061:VAL:HG11	2.01	0.43
2:D:990:GLU:HA	2:D:993:ILE:HG22	2.00	0.43
1:A:260:CYS:HB2	1:A:487:VAL:HG23	2.01	0.43
2:C:569:ILE:HG23	2:D:47:VAL:HG23	2.00	0.43
2:C:1098:ASN:CG	2:C:1101:HIS:H	2.26	0.43
2:B:347:PHE:HD2	2:B:399:SER:HB2	1.84	0.43
2:C:124:THR:O	2:C:174:PRO:HD3	2.19	0.43
2:D:111:ASP:HA	2:D:134:GLN:O	2.19	0.43
2:D:418:ILE:HG23	2:D:422:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:870:ILE:HG22	2:D:1055:SER:HB2	2.00	0.43
1:A:237:GLU:HG2	1:A:605:TRP:CH2	2.54	0.43
2:B:437:ASN:HA	2:B:508:TYR:HD1	1.84	0.43
2:C:119:ILE:HG22	2:C:119:ILE:O	2.19	0.43
2:C:348:ALA:O	2:C:400:PHE:HA	2.19	0.43
2:C:666:ILE:HB	2:C:670:ILE:O	2.19	0.43
2:C:708:SER:OG	2:C:709:ASN:N	2.52	0.43
1:A:266:LEU:HD12	1:A:274:TRP:NE1	2.34	0.42
2:B:748:GLU:HG3	2:B:981:LEU:HD11	2.01	0.42
2:C:392:PHE:HD1	2:C:524:VAL:HG13	1.84	0.42
2:C:403:LYS:HG2	2:C:505:HIS:HA	2.01	0.42
2:C:645:THR:HG23	2:C:647:ALA:H	1.84	0.42
2:C:818:ILE:HB	2:C:1054:GLN:OE1	2.20	0.42
2:D:188:ASN:N	2:D:188:ASN:OD1	2.51	0.42
2:D:767:LEU:HD23	2:D:767:LEU:HA	1.86	0.42
2:D:1050:MET:HE3	2:D:1050:MET:HB2	1.78	0.42
2:B:334:ASN:O	2:B:335:LEU:HD22	2.18	0.42
2:B:403:LYS:HB3	2:B:505:HIS:HA	2.01	0.42
2:B:616:ASN:O	2:B:619:GLU:HB2	2.19	0.42
2:C:627:ASP:HA	2:C:634:ARG:NH2	2.29	0.42
2:D:290:ASP:O	2:D:297:SER:HB3	2.19	0.42
2:D:770:ILE:O	2:D:774:GLN:HG2	2.18	0.42
2:B:529:LYS:HD2	2:B:529:LYS:HA	1.45	0.42
2:B:918:GLU:HG2	2:D:1128:VAL:HG21	2.01	0.42
2:B:1031:GLU:OE2	2:D:1039:ARG:NE	2.32	0.42
2:C:906:PHE:HE1	2:C:1049:LEU:HD11	1.84	0.42
2:B:303:LEU:O	2:B:304:LYS:C	2.63	0.42
2:B:497:PHE:CE2	2:B:507:PRO:HB3	2.54	0.42
2:C:317:ASN:OD1	2:C:317:ASN:N	2.52	0.42
2:C:1098:ASN:OD1	2:C:1099:GLY:N	2.52	0.42
2:D:338:PHE:HB3	2:D:368:LEU:HD11	2.01	0.42
1:A:420:LEU:HD12	1:A:420:LEU:HA	1.87	0.42
2:B:559:PHE:HB3	2:B:577:ARG:NH2	2.34	0.42
2:C:97:LYS:HE2	2:C:184:GLY:HA3	2.02	0.42
2:C:424:LYS:HG3	2:C:463:PRO:HA	2.01	0.42
2:C:571:ASP:HB2	2:D:967:SER:OG	2.19	0.42
2:D:406:GLU:HG2	2:D:418:ILE:HD12	2.02	0.42
2:D:708:SER:OG	2:D:709:ASN:N	2.52	0.42
2:B:948:LEU:HD22	2:B:1059:GLY:HA3	2.01	0.42
2:C:478:LYS:HE3	2:C:478:LYS:HB2	1.93	0.42
2:C:497:PHE:HA	2:C:501:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:393:THR:OG1	2:D:516:GLU:OE1	2.37	0.42
1:A:142:ALA:C	1:A:144:GLU:H	2.24	0.42
1:A:222:MET:HE1	1:A:460:TRP:CD1	2.55	0.42
2:B:276:LEU:CD1	2:B:304:LYS:HA	2.45	0.42
2:B:295:PRO:O	2:B:299:THR:HG22	2.20	0.42
2:B:389:ASP:OD1	2:B:389:ASP:N	2.46	0.42
2:B:818:ILE:O	2:B:822:LEU:HG	2.20	0.42
2:B:886:TRP:CZ3	2:B:905:ARG:HD3	2.55	0.42
2:D:422:ASN:ND2	2:D:454:ARG:O	2.30	0.42
2:D:902:MET:HB3	2:D:916:LEU:HD11	2.02	0.42
1:A:205:ASP:N	1:A:205:ASP:OD1	2.52	0.42
1:A:322:MET:HE3	1:A:326:PHE:CD1	2.55	0.42
2:B:34:ARG:NH2	2:B:219:GLY:O	2.53	0.42
2:B:315:THR:OG1	2:B:316:SER:N	2.53	0.42
2:C:102:ARG:HH12	2:C:176:LEU:HD12	1.85	0.42
2:C:110:LEU:HD11	2:C:239:GLN:HG3	2.00	0.42
2:D:726:ILE:HD13	2:D:1061:VAL:HG23	2.02	0.42
2:B:877:LEU:HA	2:B:877:LEU:HD23	1.85	0.42
2:B:905:ARG:O	2:B:909:ILE:HG23	2.20	0.42
2:C:669:GLY:HA2	2:D:869:MET:CE	2.49	0.42
2:D:188:ASN:HD21	2:D:190:ARG:HH21	1.66	0.42
1:A:222:MET:HE1	1:A:460:TRP:NE1	2.35	0.42
1:A:373:HIS:HA	1:A:404:GLY:O	2.20	0.42
2:B:662:CYS:HB2	2:B:697:MET:SD	2.60	0.42
2:B:638:THR:HG23	2:B:640:SER:H	1.85	0.41
2:D:124:THR:O	2:D:174:PRO:HD3	2.20	0.41
2:D:300:LYS:HG2	2:D:305:SER:O	2.19	0.41
2:D:574:ASP:O	2:D:587:ILE:N	2.49	0.41
1:A:28:PHE:CE2	1:A:80:ALA:HB2	2.55	0.41
1:A:167:TRP:CH2	1:A:501:CYS:HB3	2.55	0.41
1:A:352:LYS:HG2	2:B:505:HIS:CG	2.55	0.41
1:A:502:LEU:O	1:A:506:ALA:CB	2.68	0.41
2:B:398:ASP:HB3	2:B:400:PHE:HE1	1.85	0.41
2:B:837:TYR:OH	2:D:589:PRO:O	2.33	0.41
2:B:854:LYS:HA	2:B:854:LYS:HD2	1.88	0.41
2:B:900:MET:HE2	2:B:900:MET:HB3	1.90	0.41
2:C:109:THR:OG1	2:C:111:ASP:OD1	2.27	0.41
2:C:442:ASP:HB3	2:C:451:TYR:HE2	1.85	0.41
2:D:498:ARG:O	2:D:499:PRO:C	2.63	0.41
2:D:641:ASN:OD1	2:D:641:ASN:N	2.53	0.41
2:D:823:PHE:CD1	2:D:1057:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLU:HB3	1:A:517:ARG:HD2	2.03	0.41
2:B:104:TRP:HB2	2:B:119:ILE:HD13	2.01	0.41
2:B:188:ASN:HA	2:B:209:PRO:HA	2.02	0.41
2:B:350:VAL:HG23	2:B:400:PHE:CE2	2.55	0.41
2:B:399:SER:C	2:B:400:PHE:HD1	2.29	0.41
2:B:708:SER:OG	2:B:709:ASN:N	2.52	0.41
2:C:396:TYR:OH	2:D:230:PRO:HB2	2.20	0.41
2:C:618:THR:OG1	6:C:1305:NAG:O6	2.30	0.41
2:D:947:LYS:HE2	2:D:947:LYS:HB3	1.79	0.41
1:A:151:MET:HB2	1:A:164:TRP:CH2	2.55	0.41
1:A:228:THR:O	1:A:232:ILE:HB	2.20	0.41
2:B:57:PRO:HB2	2:B:60:SER:HB3	2.03	0.41
2:C:129:LYS:HE3	2:C:169:GLU:OE2	2.20	0.41
2:C:403:LYS:HE2	2:C:495:TYR:CE1	2.55	0.41
2:D:570:VAL:HG23	2:D:570:VAL:O	2.19	0.41
2:D:1097:SER:HB2	2:D:1102:TRP:CE3	2.55	0.41
2:D:1097:SER:HB2	2:D:1102:TRP:CD2	2.55	0.41
2:D:1115:ILE:HG22	2:D:1137:VAL:HG23	2.02	0.41
1:A:62:MET:C	1:A:62:MET:HE3	2.46	0.41
1:A:317:ILE:HD12	1:A:317:ILE:HA	1.81	0.41
2:B:231:ILE:HG22	2:B:233:ILE:HG23	2.02	0.41
2:B:475:ALA:HB3	2:B:489:TYR:HE1	1.85	0.41
2:C:106:PHE:HB2	2:C:117:LEU:HB2	2.01	0.41
2:C:203:ILE:HG22	2:C:227:VAL:O	2.20	0.41
2:D:108:THR:HG22	2:D:236:THR:HB	2.02	0.41
2:D:856:ASN:OD1	2:D:856:ASN:N	2.51	0.41
1:A:260:CYS:HB2	1:A:487:VAL:CG2	2.50	0.41
2:B:119:ILE:HG23	2:B:128:ILE:HD12	2.02	0.41
2:B:398:ASP:O	2:B:511:VAL:HA	2.20	0.41
2:B:588:THR:HG22	2:B:589:PRO:HD2	2.02	0.41
2:C:136:CYS:HB2	2:C:159:VAL:O	2.20	0.41
2:C:1040:VAL:O	2:C:1042:PHE:N	2.52	0.41
2:C:1115:ILE:HG22	2:C:1137:VAL:HG23	2.03	0.41
2:D:836:GLN:NE2	2:D:850:ILE:HB	2.35	0.41
1:A:233:LYS:O	1:A:237:GLU:HG3	2.20	0.41
1:A:593:TRP:O	1:A:596:GLU:HG3	2.20	0.41
2:C:337:PRO:O	2:C:341:VAL:HG23	2.20	0.41
2:C:529:LYS:HD2	2:C:529:LYS:HA	1.80	0.41
2:C:697:MET:HE2	2:C:697:MET:HB3	1.92	0.41
2:C:1047:TYR:O	2:C:1067:TYR:N	2.47	0.41
2:D:101:ILE:O	2:D:102:ARG:NH1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:CYS:HB3	2:D:133:PHE:CZ	2.56	0.41
2:D:386:LYS:O	2:D:390:LEU:HD11	2.21	0.41
2:D:436:TRP:NE1	2:D:438:SER:OG	2.54	0.41
1:A:115:ARG:O	1:A:119:ILE:HG13	2.21	0.41
2:B:202:LYS:HA	2:B:202:LYS:HD2	1.68	0.41
2:B:323:THR:OG1	2:B:324:GLU:N	2.54	0.41
2:C:57:PRO:HG3	2:C:273:ARG:HD2	2.03	0.41
2:C:853:GLN:HA	2:C:856:ASN:OD1	2.20	0.41
2:D:121:ASN:N	2:D:121:ASN:ND2	2.68	0.41
1:A:224:ASP:O	1:A:228:THR:HG23	2.21	0.41
1:A:377:HIS:O	1:A:400:HIS:NE2	2.41	0.41
1:A:578:MET:HE2	1:A:578:MET:HB2	1.98	0.41
2:B:193:VAL:HG13	2:B:204:TYR:CD1	2.54	0.41
2:B:309:GLU:O	2:B:313:TYR:OH	2.25	0.41
2:B:906:PHE:HE1	2:B:1067:TYR:CD2	2.39	0.41
2:C:99:ASN:ND2	2:C:101:ILE:O	2.48	0.41
2:C:121:ASN:OD1	2:C:121:ASN:N	2.53	0.41
2:C:415:THR:HG23	2:D:385:THR:HA	2.03	0.41
2:C:560:LEU:H	2:C:563:GLN:HG3	1.86	0.41
2:C:669:GLY:O	2:C:670:ILE:HD13	2.20	0.41
2:C:1053:PRO:O	2:C:1054:GLN:NE2	2.41	0.41
2:D:38:TYR:CE2	2:D:224:GLU:HG3	2.56	0.41
2:D:47:VAL:HG12	2:D:279:TYR:HB2	2.02	0.41
2:D:675:GLN:HG3	2:D:693:ILE:HD11	2.02	0.41
2:D:741:TYR:CD2	2:D:1004:LEU:HD22	2.56	0.41
2:B:734:THR:O	2:B:767:LEU:HD12	2.21	0.41
2:C:28:TYR:HD2	2:C:61:ASN:HB2	1.86	0.41
2:C:557:LYS:HD3	2:D:43:PHE:CD2	2.56	0.41
2:D:318:PHE:HZ	2:D:615:VAL:HG21	1.86	0.41
2:D:334:ASN:O	2:D:362:VAL:N	2.52	0.41
2:B:338:PHE:HD1	2:B:338:PHE:HA	1.78	0.40
2:B:743:CYS:HB3	2:B:749:CYS:HB3	1.95	0.40
2:B:904:TYR:CE2	2:D:1107:ARG:HG2	2.56	0.40
2:C:103:GLY:HA3	2:C:120:VAL:HA	2.02	0.40
2:C:133:PHE:HB3	2:C:160:TYR:HB2	2.02	0.40
2:C:669:GLY:HA2	2:D:869:MET:HE1	2.02	0.40
2:B:959:LEU:O	2:B:963:VAL:HG23	2.22	0.40
2:B:997:ILE:O	2:B:1001:LEU:HB2	2.21	0.40
2:B:1040:VAL:HG13	2:C:1030:SER:O	2.22	0.40
2:C:631:PRO:HB3	2:C:633:TRP:CH2	2.55	0.40
2:C:726:ILE:HD12	2:C:1061:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:808:ASP:HB3	2:C:811:LYS:HD2	2.03	0.40
2:D:657:ASN:HB3	6:D:1306:NAG:O5	2.21	0.40
1:A:379:GLN:HA	1:A:382:MET:HG3	2.02	0.40
2:B:409:GLN:HE21	2:B:409:GLN:HB2	1.71	0.40
2:C:675:GLN:HB2	2:C:693:ILE:HG12	2.04	0.40
2:C:885:GLY:HA2	2:C:901:GLN:CD	2.47	0.40
2:D:398:ASP:HB2	2:D:512:VAL:HG12	2.03	0.40
2:D:705:VAL:HG12	2:D:707:TYR:H	1.87	0.40
1:A:369:LEU:HD13	1:A:408:SER:HB2	2.03	0.40
2:B:86:PHE:CD2	2:B:90:VAL:HG23	2.57	0.40
2:B:177:MET:H	2:B:207:HIS:CE1	2.40	0.40
2:B:766:ALA:O	2:B:770:ILE:HG12	2.21	0.40
2:B:1034:LEU:O	2:D:1040:VAL:HG21	2.22	0.40
2:C:287:ASP:OD1	2:C:288:ALA:N	2.53	0.40
2:C:1072:GLU:OE1	2:C:1072:GLU:N	2.55	0.40
2:D:209:PRO:O	2:D:210:ILE:HG13	2.21	0.40
2:D:1072:GLU:N	2:D:1072:GLU:OE1	2.55	0.40
1:A:146:GLY:O	1:A:147:LEU:C	2.64	0.40
1:A:150:ILE:O	1:A:154:SER:OG	2.34	0.40
1:A:176:ARG:O	1:A:180:GLU:HG3	2.22	0.40
1:A:284:PHE:CE1	1:A:286:HIS:HB2	2.56	0.40
1:A:347:ALA:HB1	1:A:378:ILE:HD11	2.04	0.40
1:A:522:PHE:HD1	1:A:522:PHE:HA	1.73	0.40
2:B:990:GLU:HA	2:B:993:ILE:HB	2.04	0.40
2:C:131:CYS:HB3	2:C:133:PHE:CZ	2.56	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	594/804 (74%)	570 (96%)	21 (4%)	3 (0%)	24 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1053/1206 (87%)	969 (92%)	82 (8%)	2 (0%)	43	70
2	C	1053/1206 (87%)	965 (92%)	87 (8%)	1 (0%)	48	78
2	D	1053/1206 (87%)	978 (93%)	73 (7%)	2 (0%)	43	70
All	All	3753/4422 (85%)	3482 (93%)	263 (7%)	8 (0%)	44	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	212	ILE
2	D	210	ILE
2	D	499	PRO
1	A	147	LEU
2	B	331	ASN
1	A	143	LEU
1	A	144	GLU
2	B	534	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	525/711 (74%)	522 (99%)	3 (1%)	78	78
2	B	925/1054 (88%)	920 (100%)	5 (0%)	81	79
2	C	925/1054 (88%)	917 (99%)	8 (1%)	70	73
2	D	925/1054 (88%)	914 (99%)	11 (1%)	63	70
All	All	3300/3873 (85%)	3273 (99%)	27 (1%)	70	74

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	TYR
1	A	143	LEU
1	A	147	LEU

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Mol	Chain	Res	Type
2	B	303	LEU
2	B	304	LYS
2	B	528	LYS
2	B	529	LYS
2	B	613	GLN
2	C	87	ASN
2	C	334	ASN
2	C	335	LEU
2	C	343	ASN
2	C	492	LEU
2	C	649	CYS
2	C	994	ASP
2	C	1040	VAL
2	D	61	ASN
2	D	121	ASN
2	D	210	ILE
2	D	212	ILE
2	D	303	LEU
2	D	343	ASN
2	D	617	CYS
2	D	699	LEU
2	D	760	CYS
2	D	763	LEU
2	D	968	SER

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

Mol	Chain	Res	Type
1	A	89	GLN
1	A	174	GLN
1	A	193	ASN
1	A	387	GLN
1	A	441	GLN
1	A	571	ASN
2	B	26	GLN
2	B	66	HIS
2	B	185	ASN
2	B	188	ASN
2	B	196	ASN
2	B	207	HIS
2	B	218	GLN
2	B	388	ASN

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Mol	Chain	Res	Type
2	B	437	ASN
2	B	613	GLN
2	B	644	GLN
2	B	777	ASN
2	B	965	GLN
2	B	1011	GLN
2	C	271	GLN
2	C	321	GLN
2	C	360	ASN
2	C	437	ASN
2	C	965	GLN
2	D	121	ASN
2	D	439	ASN
2	D	540	ASN
2	D	913	GLN
2	D	954	HIS
2	D	955	ASN
2	D	992	GLN
2	D	1054	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

34 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
3	NAG	E	1	2,3	14,14,15	0.21	0	17,19,21	0.43	0
3	BMA	E	2	3	11,11,12	0.58	0	15,15,17	0.73	0
3	NAG	F	1	2,3	14,14,15	0.22	0	17,19,21	0.43	0
3	BMA	F	2	3	11,11,12	0.58	0	15,15,17	0.73	0
3	NAG	G	1	2,3	14,14,15	0.31	0	17,19,21	0.51	0
3	BMA	G	2	3	11,11,12	0.58	0	15,15,17	0.66	0
3	NAG	H	1	2,3	14,14,15	0.22	0	17,19,21	0.44	0
3	BMA	H	2	3	11,11,12	0.59	0	15,15,17	0.71	0
3	NAG	I	1	2,3	14,14,15	0.86	1 (7%)	17,19,21	0.91	1 (5%)
3	BMA	I	2	3	11,11,12	0.55	0	15,15,17	1.13	1 (6%)
3	NAG	J	1	2,3	14,14,15	0.26	0	17,19,21	0.41	0
3	BMA	J	2	3	11,11,12	0.60	0	15,15,17	0.77	0
3	NAG	K	1	2,3	14,14,15	0.22	0	17,19,21	0.43	0
3	BMA	K	2	3	11,11,12	0.60	0	15,15,17	0.65	0
3	NAG	L	1	2,3	14,14,15	0.23	0	17,19,21	0.45	0
3	BMA	L	2	3	11,11,12	0.60	0	15,15,17	0.71	0
3	NAG	M	1	2,3	14,14,15	0.27	0	17,19,21	0.48	0
3	BMA	M	2	3	11,11,12	0.59	0	15,15,17	0.65	0
3	NAG	N	1	2,3	14,14,15	0.23	0	17,19,21	0.47	0
3	BMA	N	2	3	11,11,12	0.57	0	15,15,17	0.68	0
3	NAG	O	1	2,3	14,14,15	0.91	1 (7%)	17,19,21	0.95	1 (5%)
3	BMA	O	2	3	11,11,12	0.52	0	15,15,17	1.02	1 (6%)
3	NAG	P	1	2,3	14,14,15	0.26	0	17,19,21	0.41	0
3	BMA	P	2	3	11,11,12	0.56	0	15,15,17	0.72	0
3	NAG	Q	1	2,3	14,14,15	0.22	0	17,19,21	0.42	0
3	BMA	Q	2	3	11,11,12	0.55	0	15,15,17	0.68	0
3	NAG	R	1	2,3	14,14,15	0.20	0	17,19,21	0.43	0
3	BMA	R	2	3	11,11,12	0.56	0	15,15,17	0.75	0
3	NAG	S	1	2,3	14,14,15	0.27	0	17,19,21	0.49	0
3	BMA	S	2	3	11,11,12	0.57	0	15,15,17	0.69	0
3	NAG	T	1	2,3	14,14,15	0.25	0	17,19,21	0.47	0
3	BMA	T	2	3	11,11,12	0.60	0	15,15,17	0.70	0
3	NAG	U	1	2,3	14,14,15	1.20	1 (7%)	17,19,21	1.23	1 (5%)
3	BMA	U	2	3	11,11,12	0.58	0	15,15,17	1.15	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	E	2	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	G	2	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	2,3	-	1/6/23/26	0/1/1/1
3	BMA	H	2	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	I	2	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	2,3	-	1/6/23/26	0/1/1/1
3	BMA	J	2	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	K	2	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	L	2	3	-	0/2/19/22	0/1/1/1
3	NAG	M	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	M	2	3	-	1/2/19/22	0/1/1/1
3	NAG	N	1	2,3	-	0/6/23/26	0/1/1/1
3	BMA	N	2	3	-	0/2/19/22	0/1/1/1
3	NAG	O	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	O	2	3	-	0/2/19/22	0/1/1/1
3	NAG	P	1	2,3	-	1/6/23/26	0/1/1/1
3	BMA	P	2	3	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	Q	2	3	-	0/2/19/22	0/1/1/1
3	NAG	R	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	R	2	3	-	1/2/19/22	0/1/1/1
3	NAG	S	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	S	2	3	-	0/2/19/22	0/1/1/1
3	NAG	T	1	2,3	-	0/6/23/26	0/1/1/1
3	BMA	T	2	3	-	0/2/19/22	0/1/1/1
3	NAG	U	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	U	2	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1	NAG	O5-C1	-4.09	1.36	1.43
3	O	1	NAG	O5-C1	-3.12	1.38	1.43
3	I	1	NAG	O5-C1	-2.97	1.38	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	1	NAG	C3-C4-C5	3.47	116.52	110.23
3	U	2	BMA	C1-O5-C5	2.78	115.91	112.19
3	I	2	BMA	C1-O5-C5	2.77	115.89	112.19
3	O	2	BMA	C1-O5-C5	2.55	115.61	112.19
3	O	1	NAG	C3-C4-C5	2.43	114.64	110.23
3	I	1	NAG	C3-C4-C5	2.26	114.33	110.23

There are no chirality outliers.

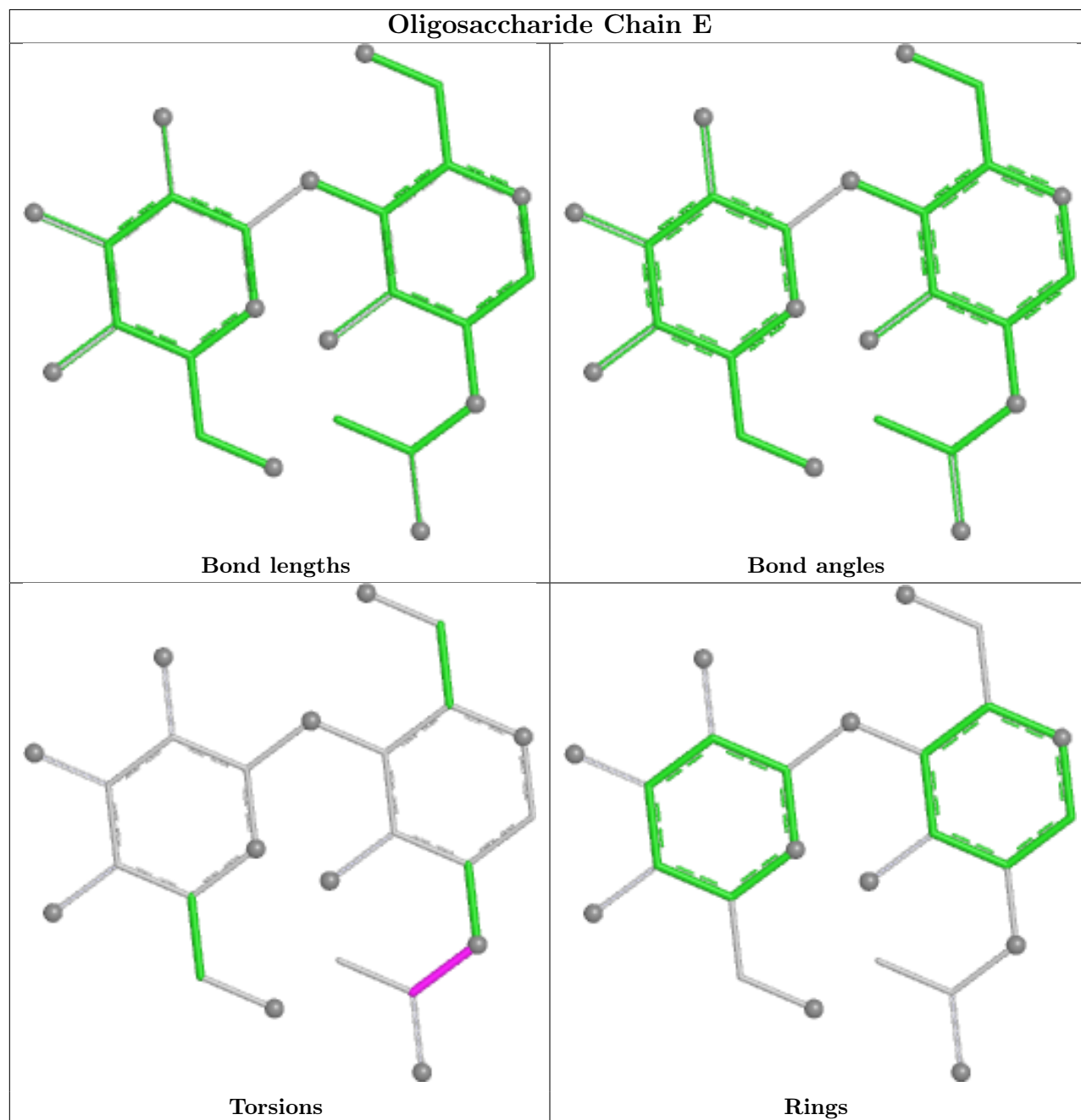
All (29) torsion outliers are listed below:

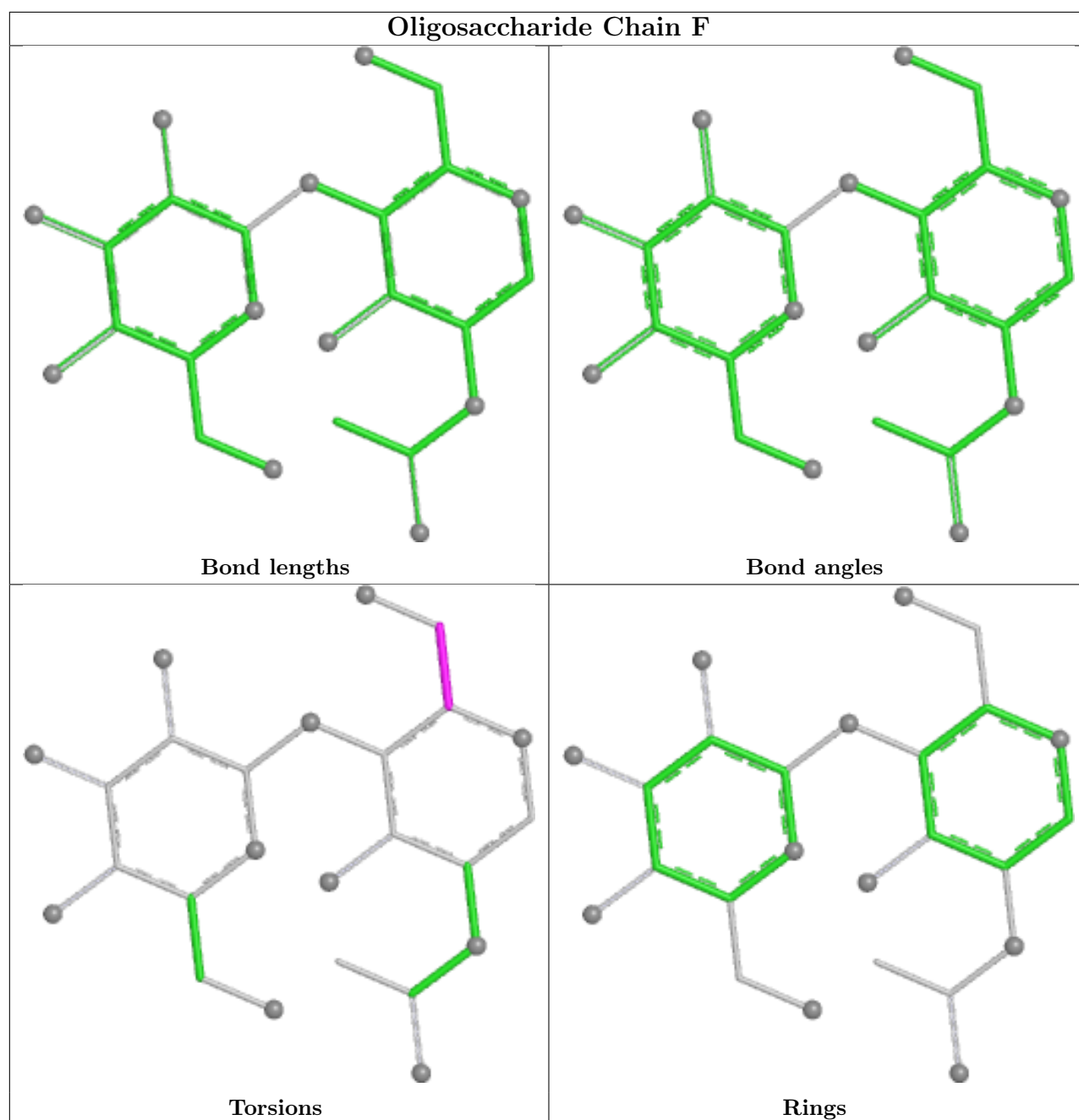
Mol	Chain	Res	Type	Atoms
3	L	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	S	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	R	2	BMA	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	M	2	BMA	O5-C5-C6-O6

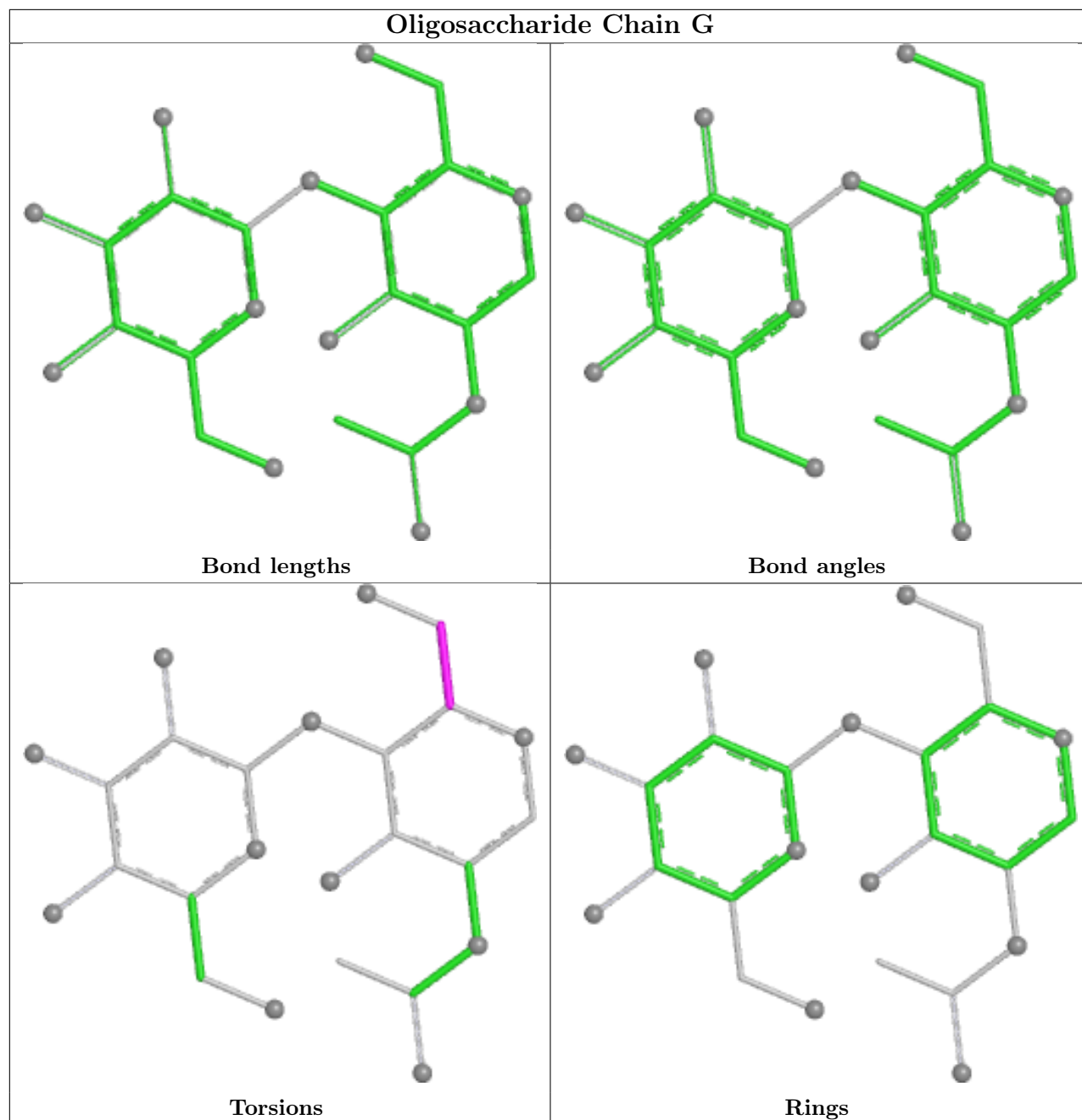
There are no ring outliers.

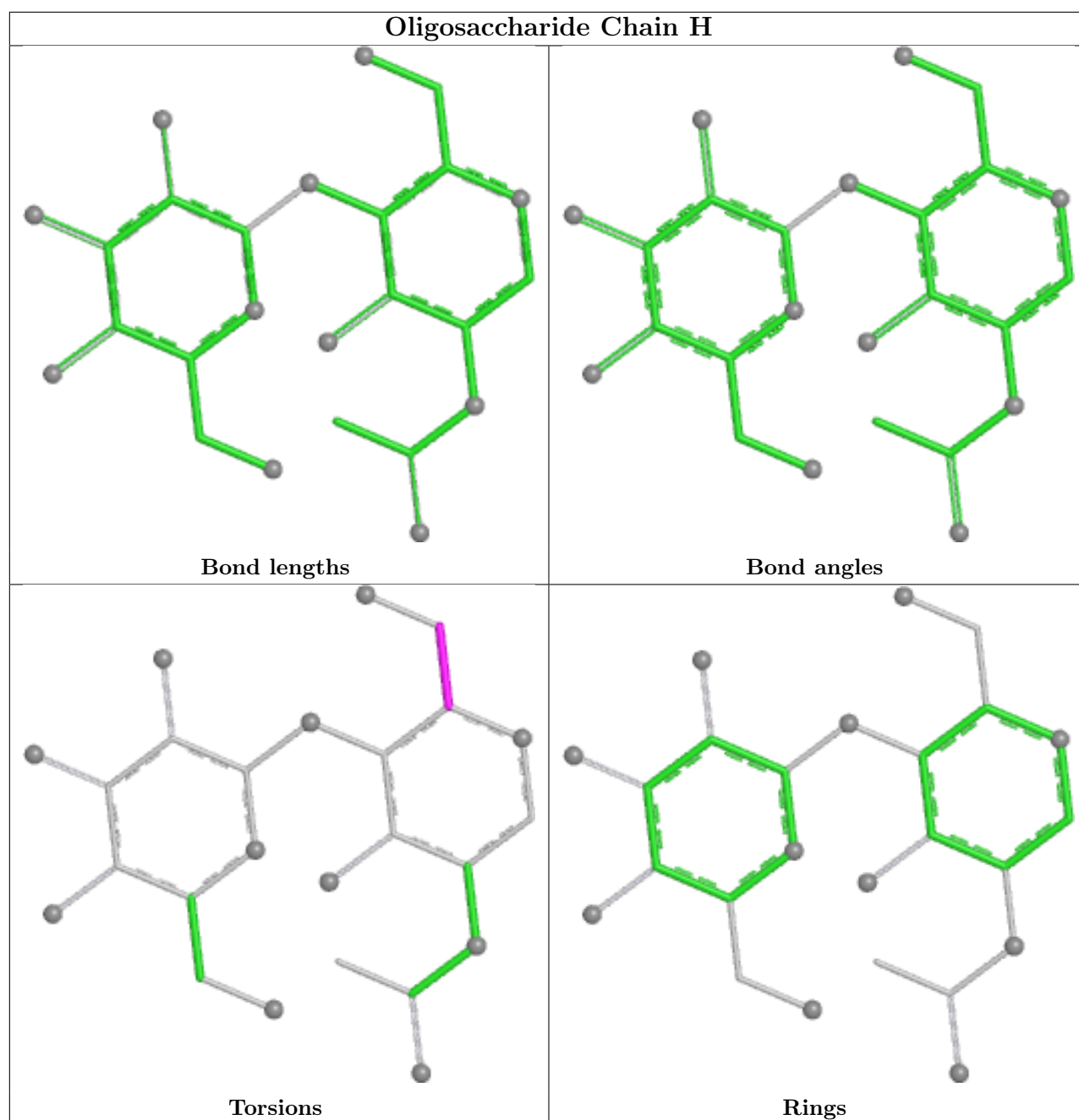
No monomer is involved in short contacts.

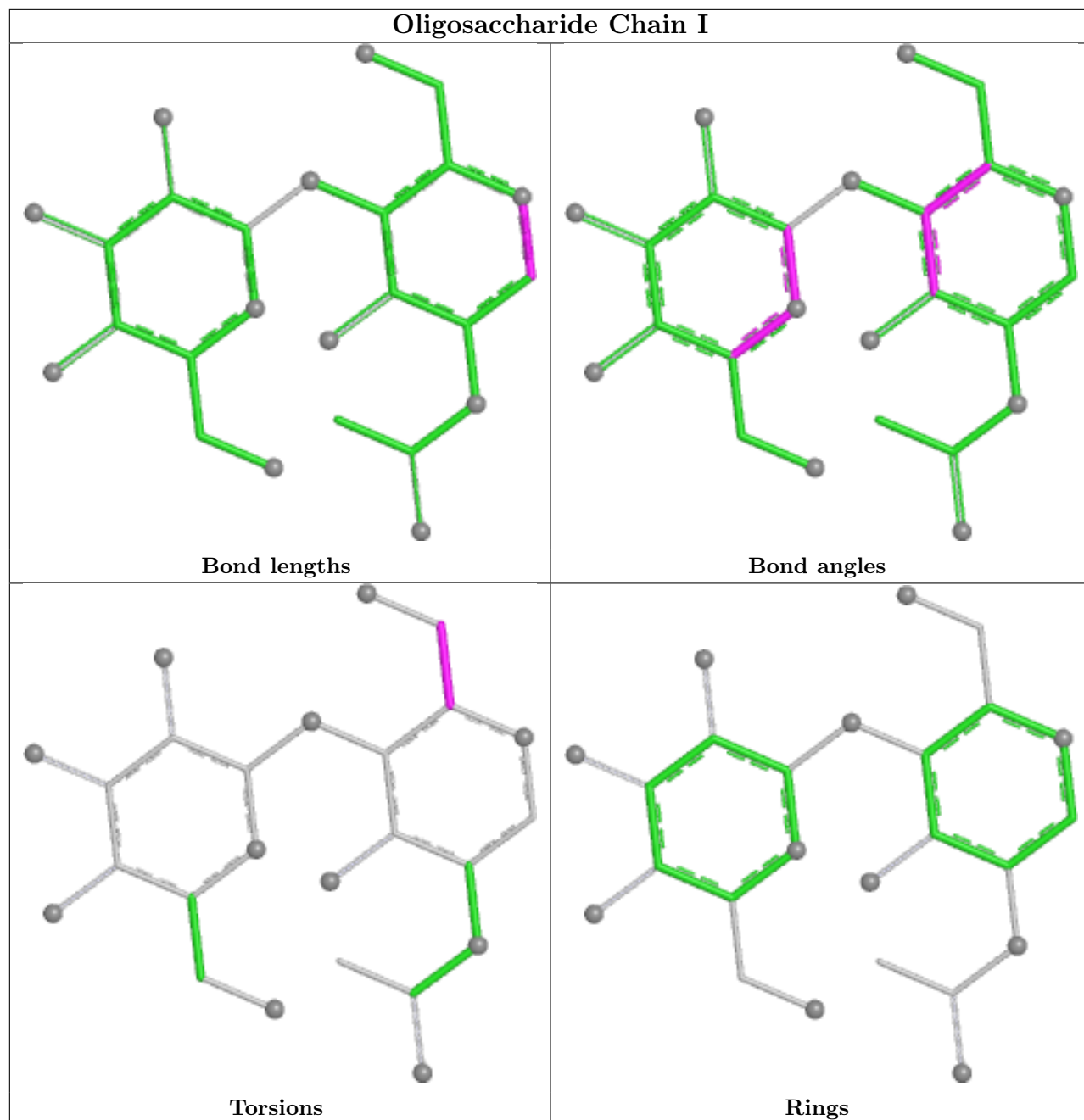
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

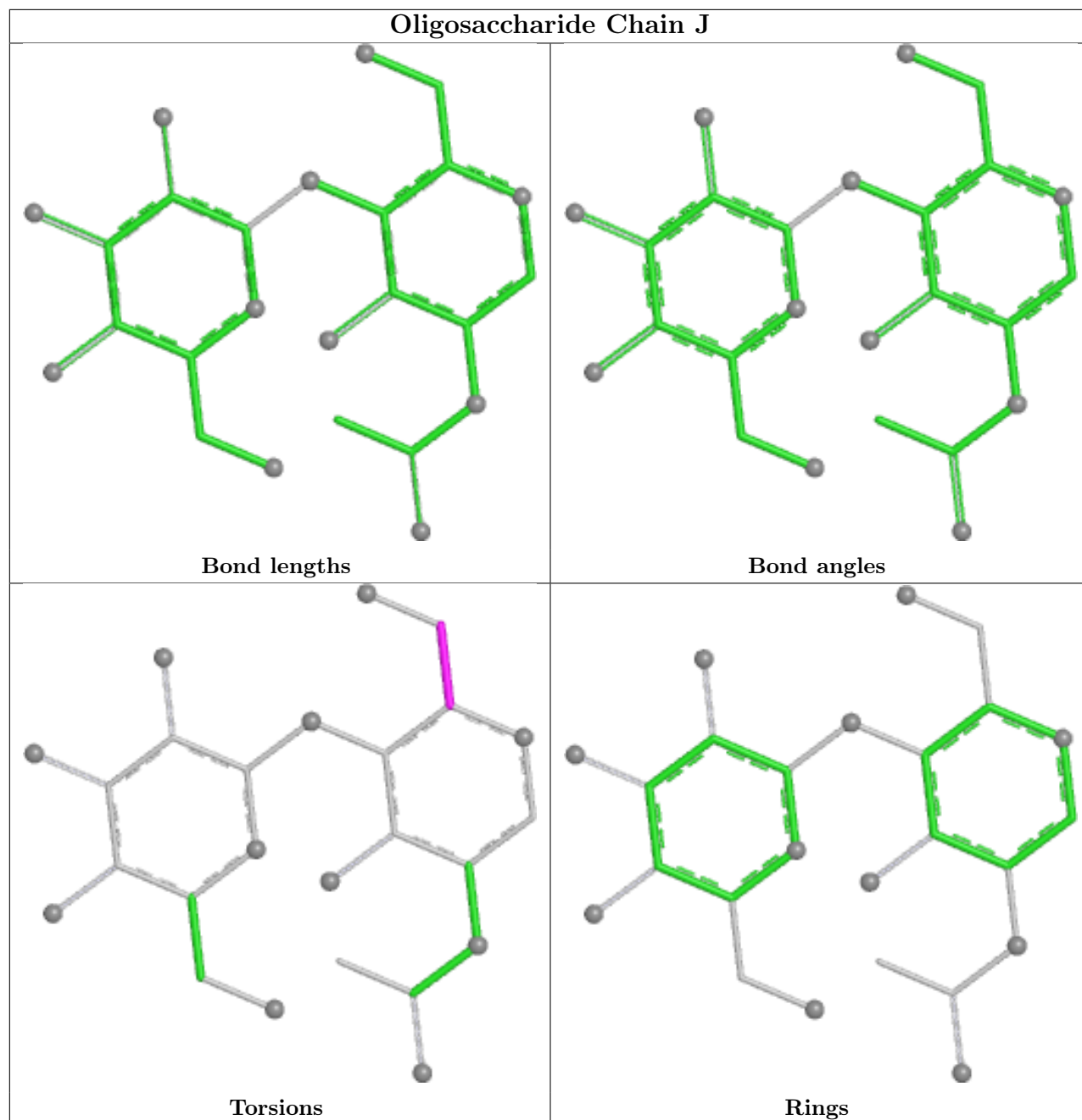


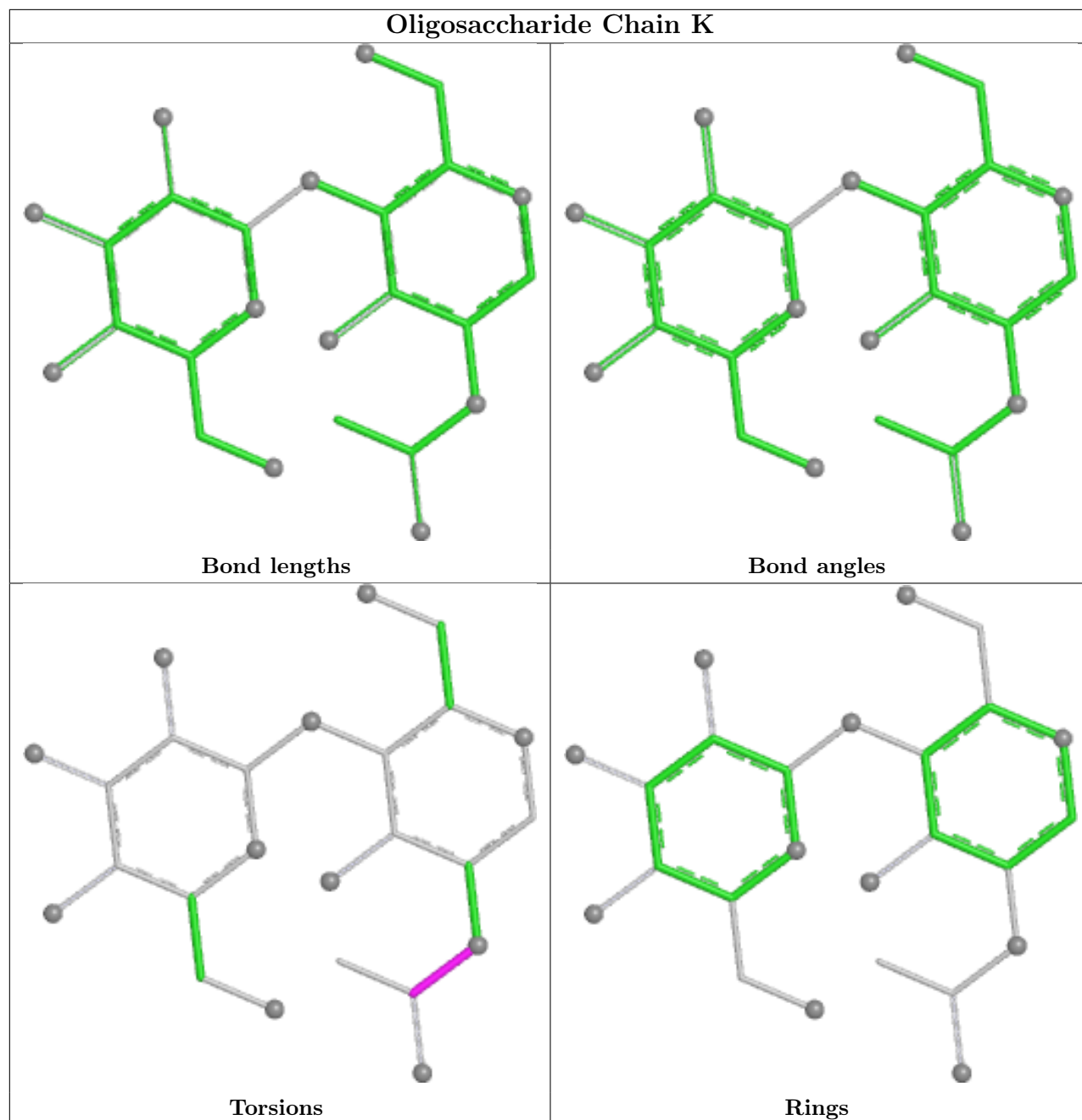


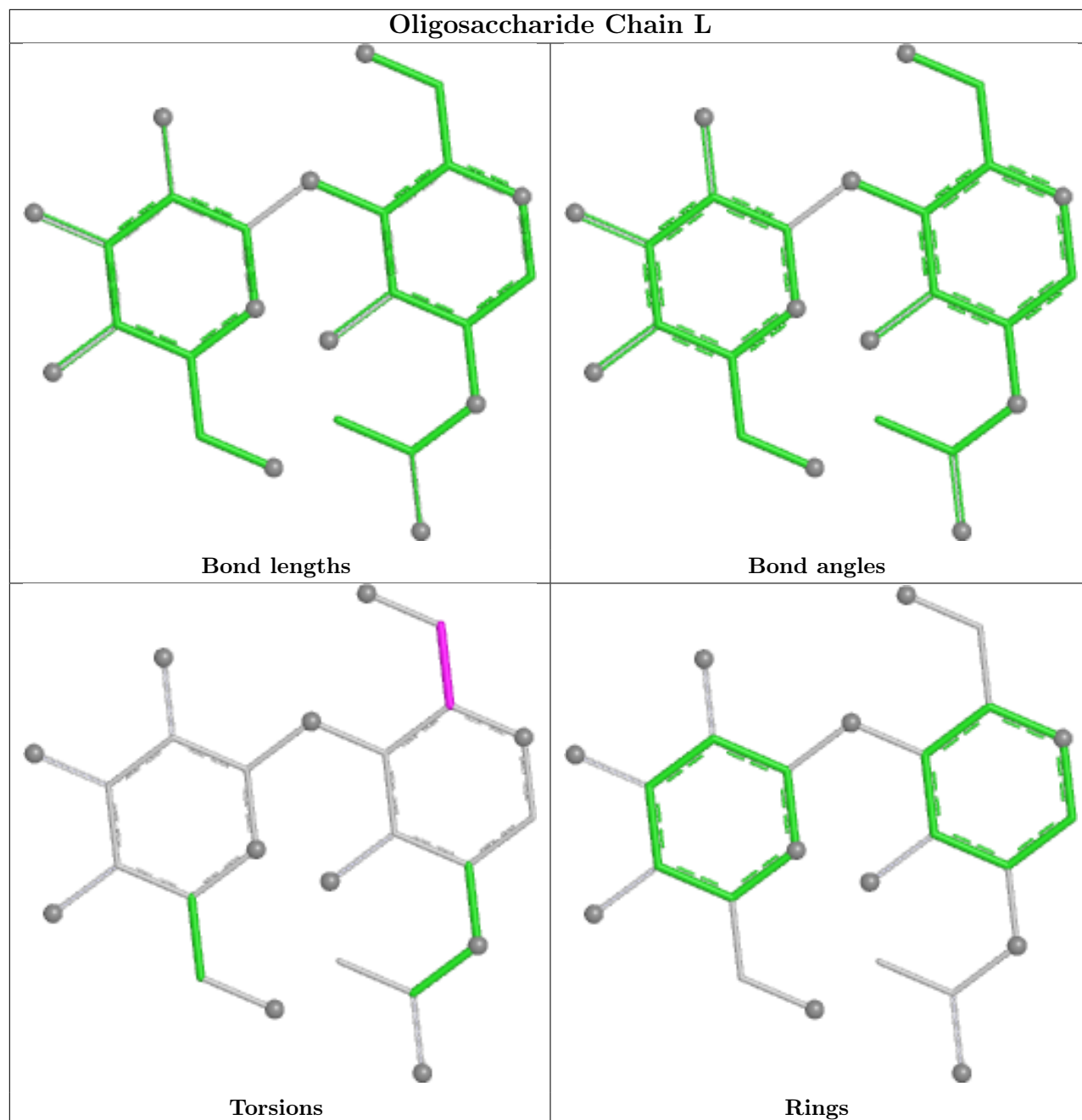


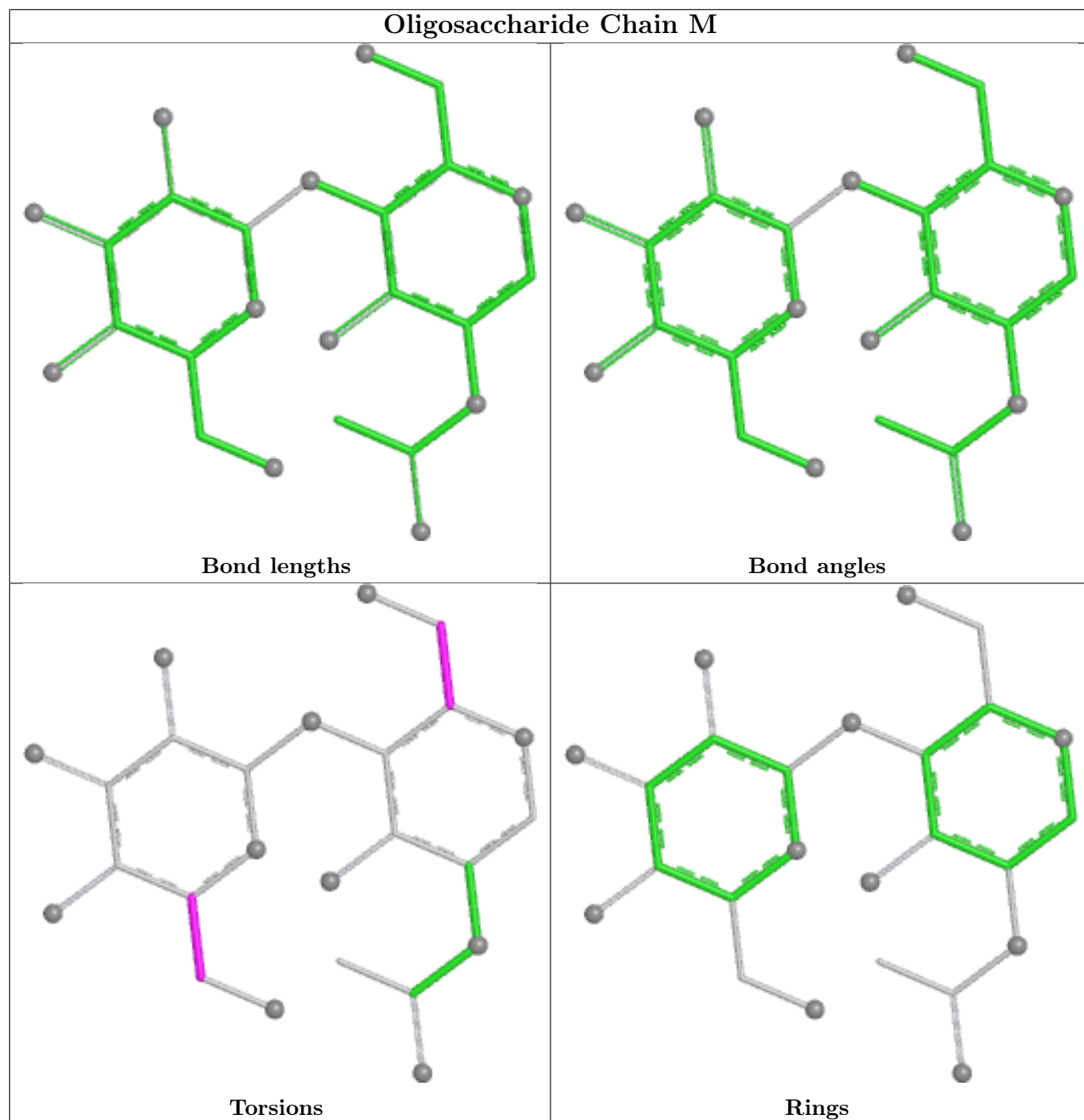


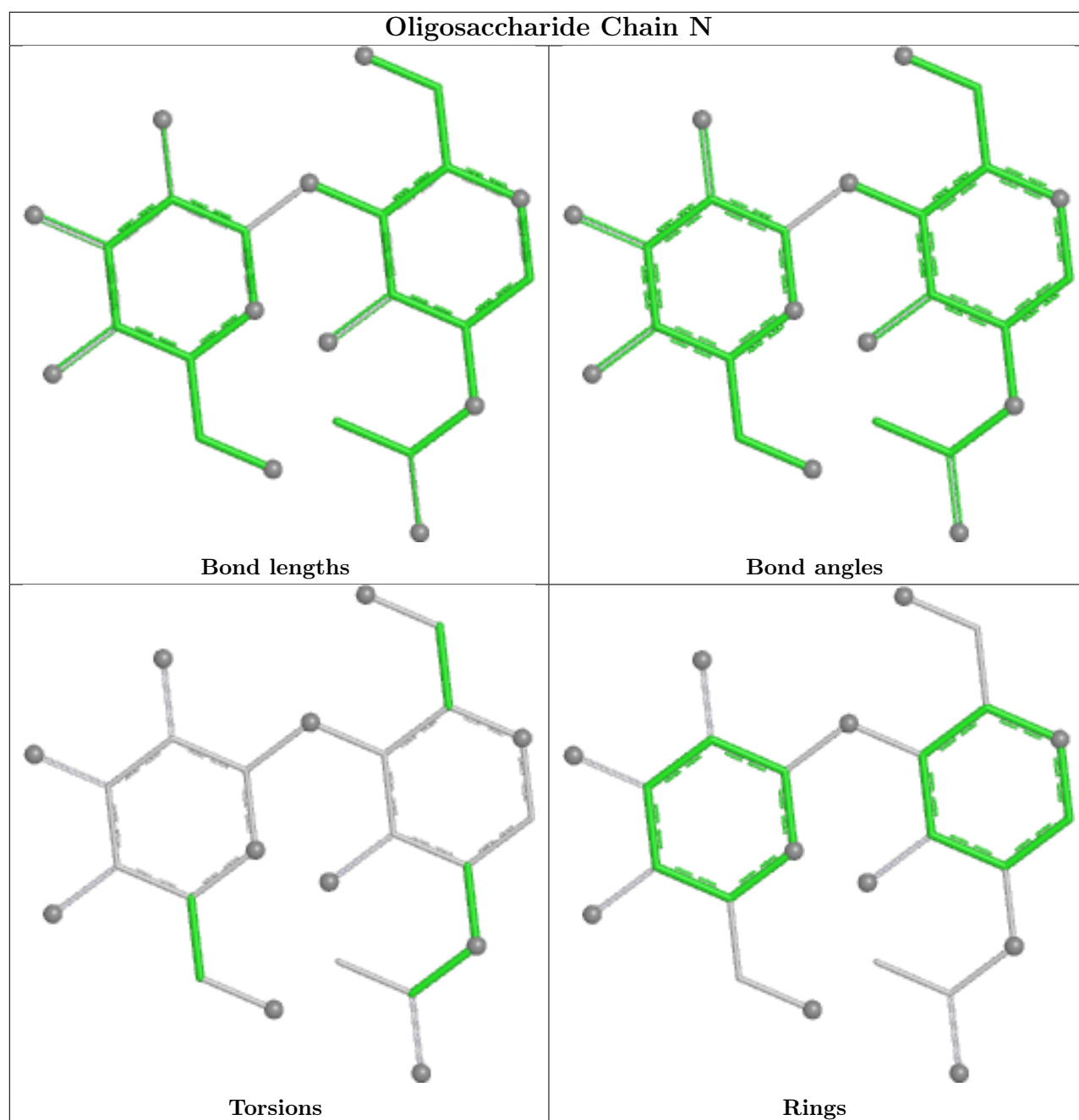


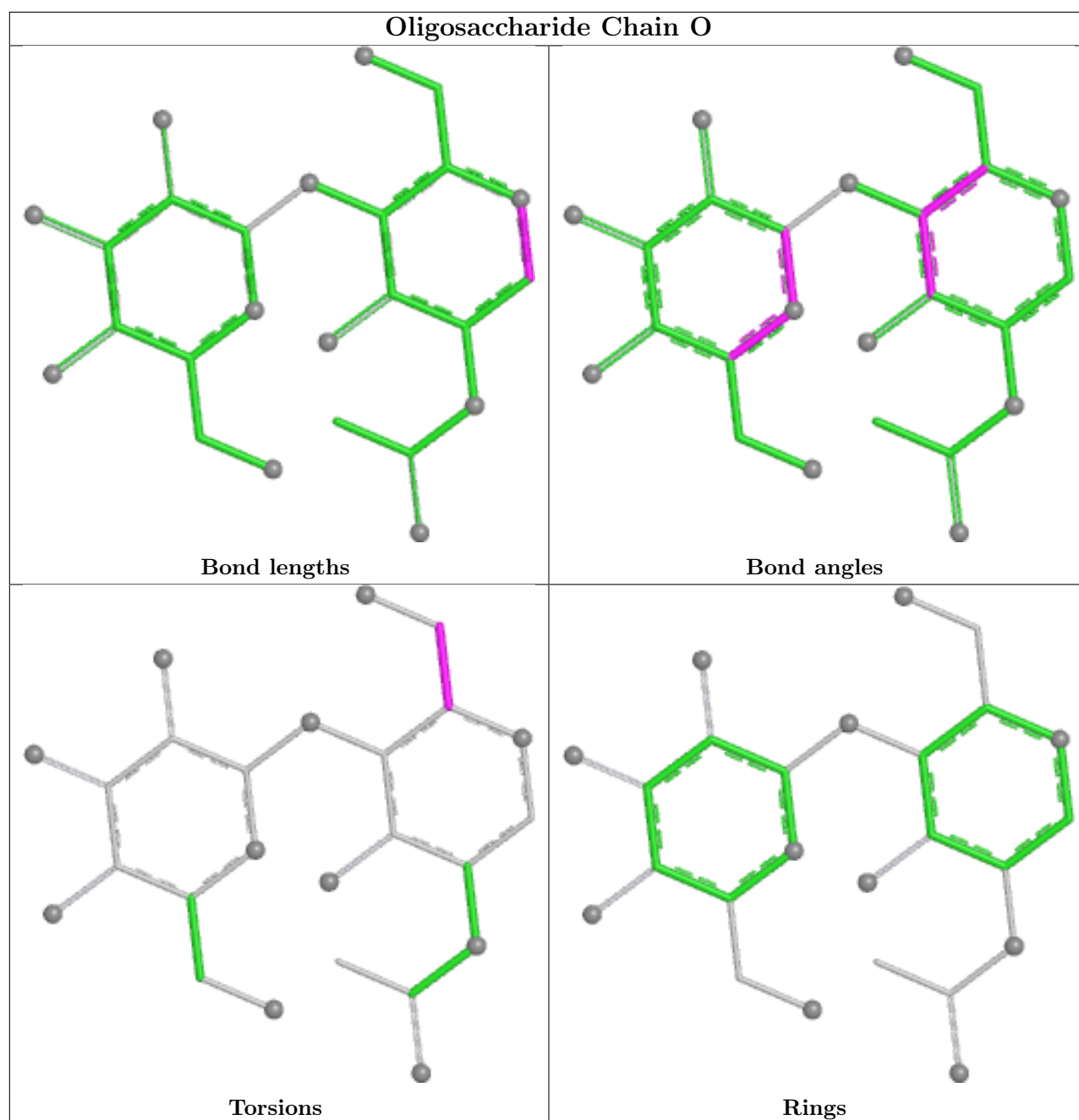


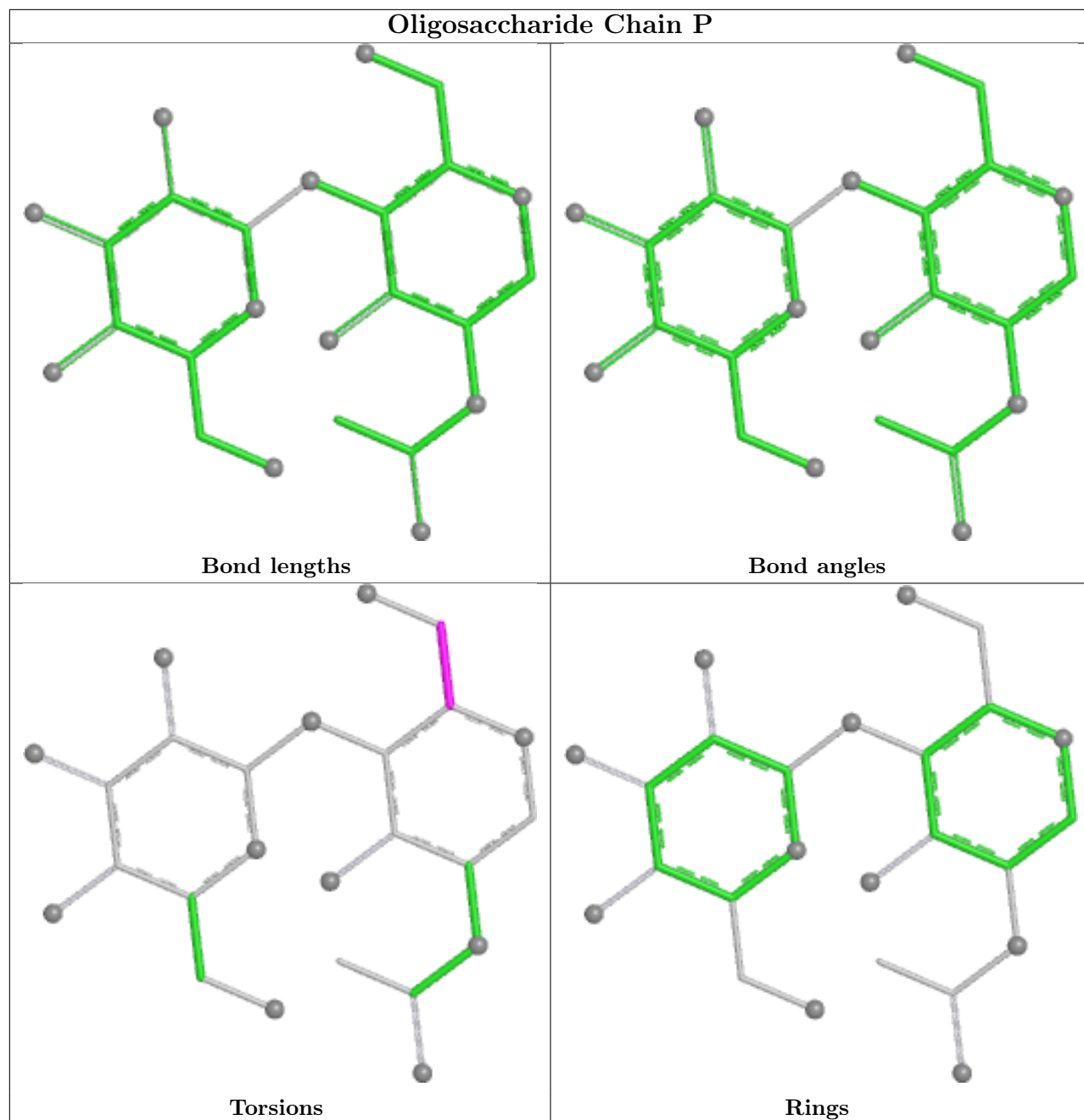


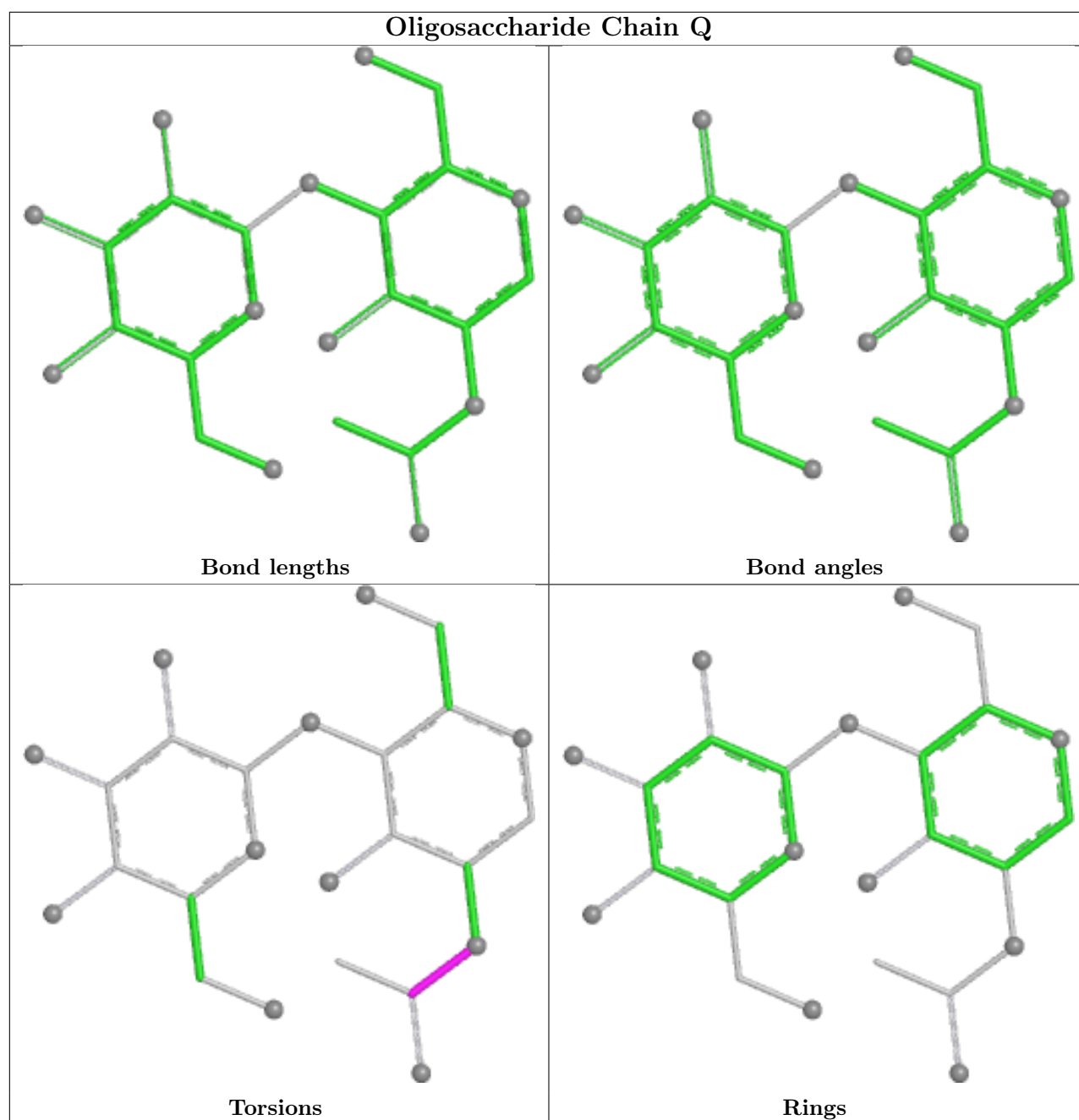


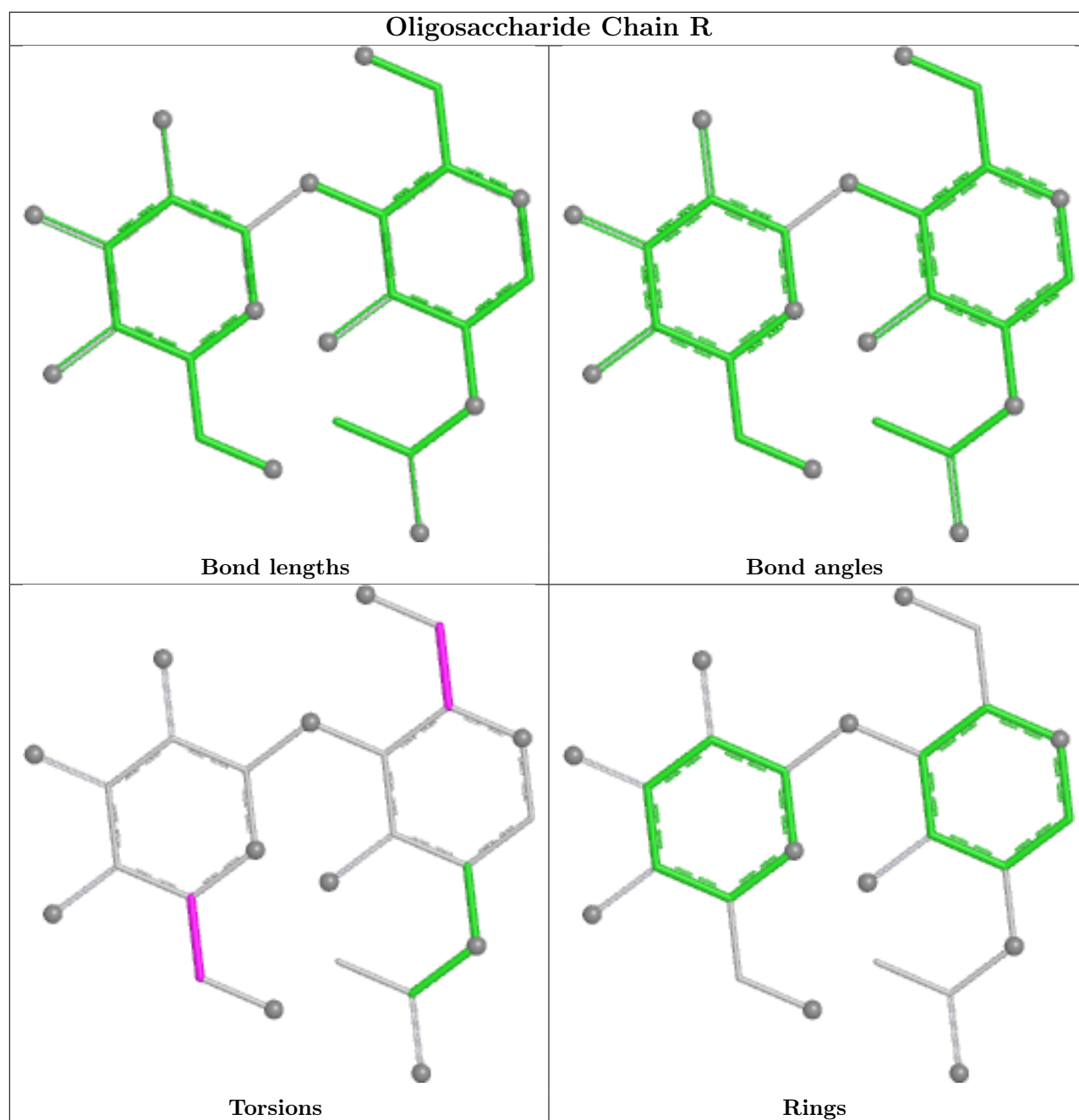


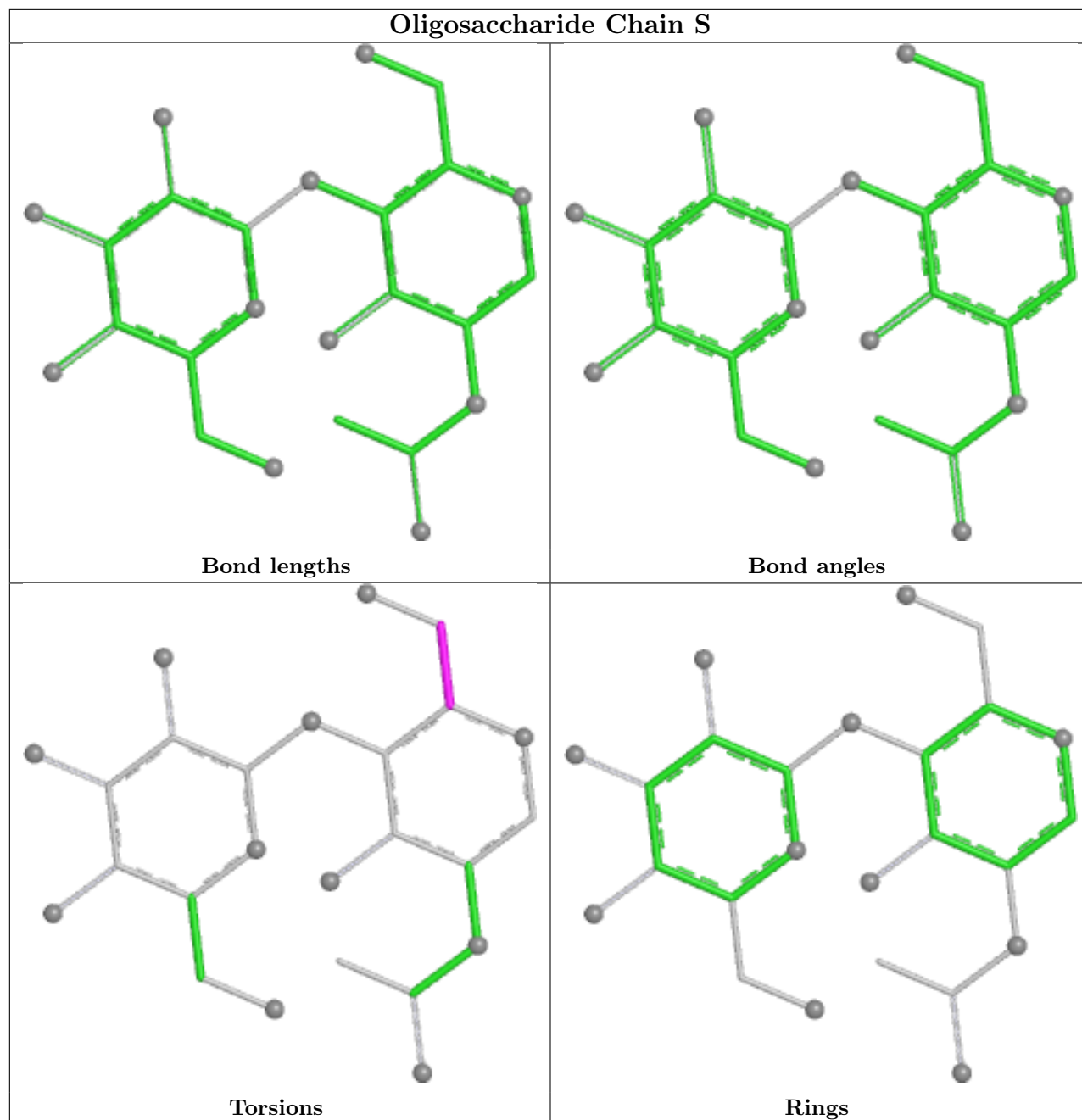


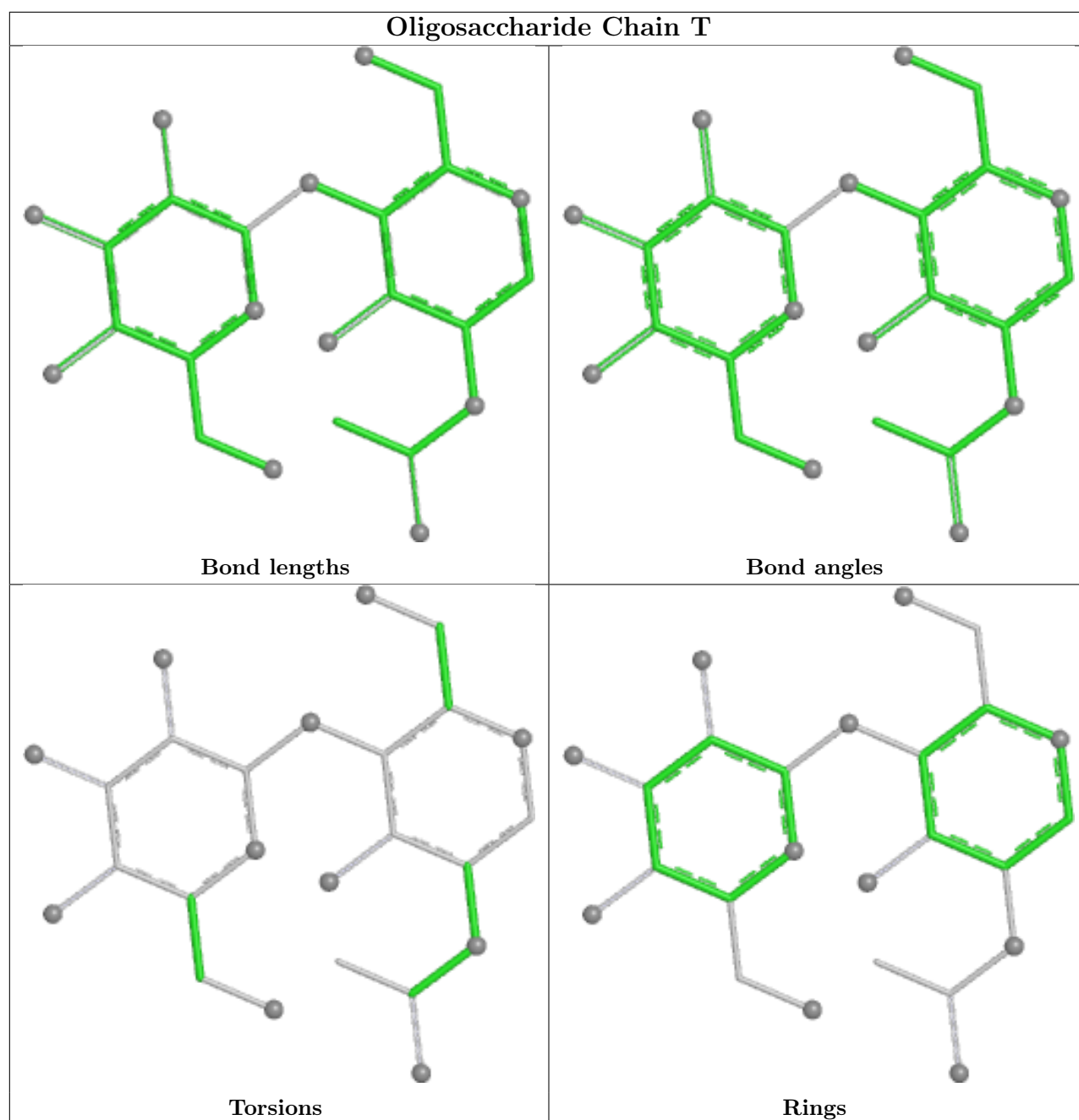


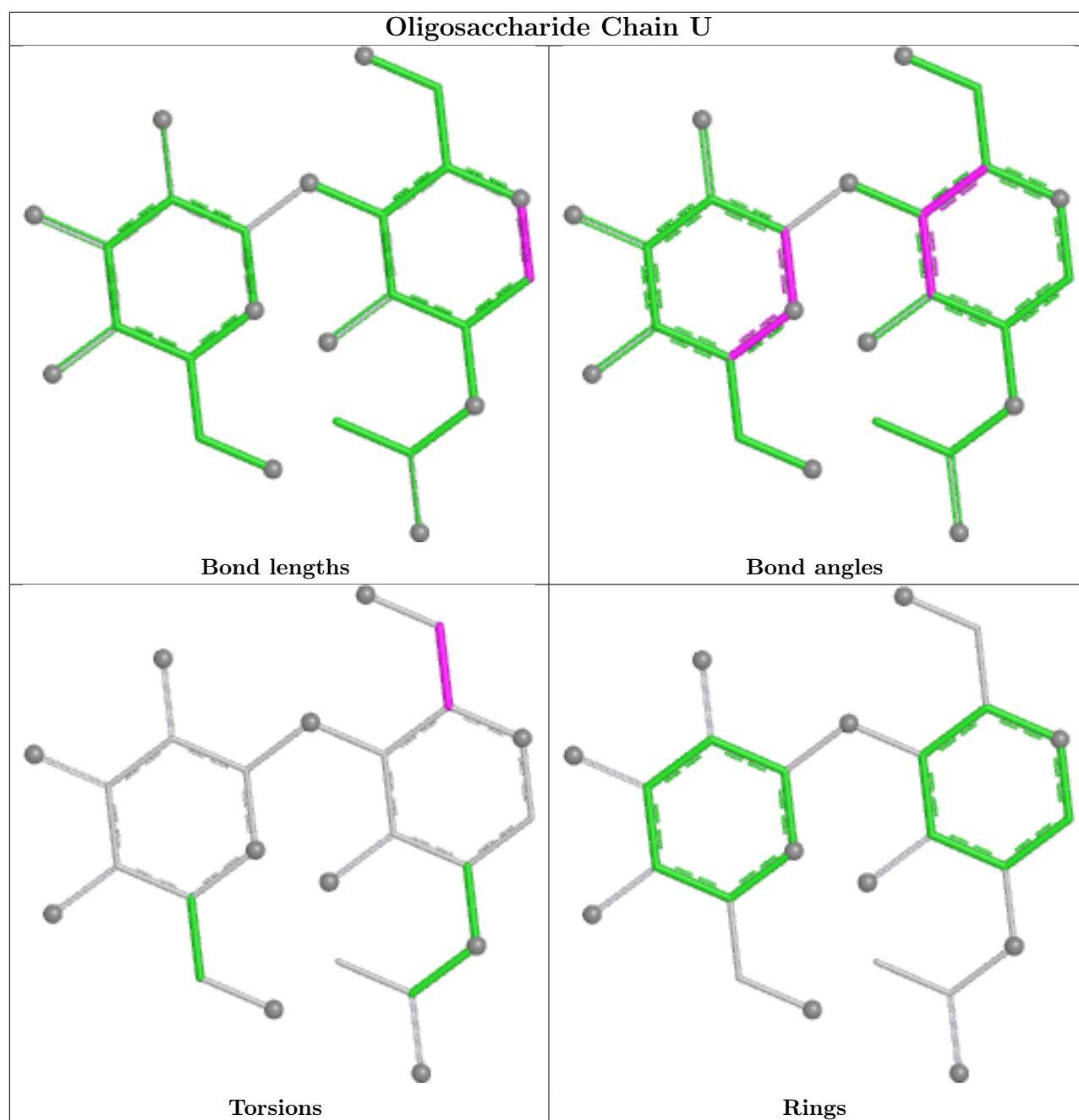












5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 for Mogul analysis.

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	D	1303	2	14,14,15	0.43	0	17,19,21	0.51	0
6	NAG	A	904	1	14,14,15	0.85	1 (7%)	17,19,21	1.52	3 (17%)
6	NAG	C	1307	2	14,14,15	0.25	0	17,19,21	0.46	0
6	NAG	B	1302	2	14,14,15	0.24	0	17,19,21	0.40	0
6	NAG	B	1308	2	14,14,15	0.20	0	17,19,21	0.44	0
6	NAG	B	1305	2	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	C	1304	2	14,14,15	0.25	0	17,19,21	0.38	0
6	NAG	D	1309	2	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	B	1309	2	14,14,15	0.35	0	17,19,21	0.62	1 (5%)
6	NAG	D	1302	2	14,14,15	0.27	0	17,19,21	0.45	0
6	NAG	C	1306	2	14,14,15	0.35	0	17,19,21	0.42	0
6	NAG	D	1307	2	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	A	905	1	14,14,15	0.27	0	17,19,21	0.52	0
6	NAG	C	1308	2	14,14,15	0.29	0	17,19,21	0.61	1 (5%)
6	NAG	B	1301	2	14,14,15	0.30	0	17,19,21	0.56	0
6	NAG	B	1304	2	14,14,15	0.24	0	17,19,21	0.40	0
6	NAG	B	1307	2	14,14,15	0.40	0	17,19,21	0.42	0
6	NAG	A	906	1	14,14,15	0.23	0	17,19,21	0.42	0
6	NAG	C	1309	2	14,14,15	0.20	0	17,19,21	0.44	0
6	NAG	D	1308	2	14,14,15	0.33	0	17,19,21	0.62	1 (5%)
6	NAG	B	1306	2	14,14,15	0.35	0	17,19,21	1.36	1 (5%)
6	NAG	B	1311	2	14,14,15	0.31	0	17,19,21	0.49	0
6	NAG	D	1305	2	14,14,15	0.31	0	17,19,21	1.40	2 (11%)
6	NAG	D	1304	2	14,14,15	0.26	0	17,19,21	0.36	0
6	NAG	B	1303	2	14,14,15	0.21	0	17,19,21	0.47	0
6	NAG	C	1310	2	14,14,15	0.41	0	17,19,21	0.42	0
6	NAG	D	1306	2	14,14,15	0.37	0	17,19,21	0.42	0
6	NAG	B	1310	-	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	C	1301	2	14,14,15	0.26	0	17,19,21	0.57	0
6	NAG	C	1305	2	14,14,15	0.29	0	17,19,21	1.37	1 (5%)
6	NAG	D	1301	2	14,14,15	0.27	0	17,19,21	0.59	0
6	NAG	C	1302	2	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	A	902	1	14,14,15	0.36	0	17,19,21	0.38	0
6	NAG	D	1310	2	14,14,15	0.29	0	17,19,21	0.40	0
6	NAG	A	903	1	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	C	1303	2	14,14,15	1.08	2 (14%)	17,19,21	0.89	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
6	NAG	D	1303	2	-	2/6/23/26	0/1/1/1
6	NAG	A	904	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1307	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	2	-	1/6/23/26	0/1/1/1
6	NAG	B	1308	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1305	2	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	2	-	1/6/23/26	0/1/1/1
6	NAG	D	1309	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1309	2	-	4/6/23/26	0/1/1/1
6	NAG	D	1302	2	-	2/6/23/26	0/1/1/1
6	NAG	C	1306	2	-	0/6/23/26	0/1/1/1
6	NAG	D	1307	2	-	2/6/23/26	0/1/1/1
6	NAG	A	905	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1308	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1301	2	-	4/6/23/26	0/1/1/1
6	NAG	B	1304	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	2	-	2/6/23/26	0/1/1/1
6	NAG	A	906	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1309	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1308	2	-	4/6/23/26	0/1/1/1
6	NAG	B	1306	2	-	0/6/23/26	0/1/1/1
6	NAG	B	1311	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1305	2	-	0/6/23/26	0/1/1/1
6	NAG	D	1304	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1303	2	-	4/6/23/26	0/1/1/1
6	NAG	C	1310	2	-	4/6/23/26	0/1/1/1
6	NAG	D	1306	2	-	2/6/23/26	0/1/1/1
6	NAG	B	1310	-	-	3/6/23/26	0/1/1/1
6	NAG	C	1301	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1305	2	-	0/6/23/26	0/1/1/1
6	NAG	D	1301	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1302	2	-	0/6/23/26	0/1/1/1
6	NAG	A	902	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1310	2	-	4/6/23/26	0/1/1/1
6	NAG	A	903	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1303	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1303	NAG	C1-C2	3.21	1.56	1.52
6	A	904	NAG	C1-C2	2.61	1.55	1.52
6	C	1303	NAG	O5-C1	2.41	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1305	NAG	C1-O5-C5	5.04	118.94	112.19
6	B	1306	NAG	C1-O5-C5	4.98	118.86	112.19
6	C	1305	NAG	C1-O5-C5	4.96	118.83	112.19
6	A	904	NAG	C1-O5-C5	4.68	118.45	112.19
6	C	1303	NAG	C1-O5-C5	3.10	116.33	112.19
6	A	904	NAG	C2-N2-C7	2.46	126.20	122.90
6	A	904	NAG	C1-C2-N2	2.25	113.97	110.43
6	B	1309	NAG	C1-O5-C5	2.10	115.01	112.19
6	D	1308	NAG	C1-O5-C5	2.10	115.00	112.19
6	D	1305	NAG	C3-C4-C5	2.09	114.02	110.23
6	C	1308	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	904	NAG	C1-C2-N2-C7
6	A	906	NAG	C4-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	D	1310	NAG	C4-C5-C6-O6
6	D	1307	NAG	O5-C5-C6-O6
6	D	1308	NAG	C4-C5-C6-O6
6	B	1311	NAG	O5-C5-C6-O6
6	D	1308	NAG	O5-C5-C6-O6
6	A	906	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	B	1303	NAG	C4-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	C	1310	NAG	C4-C5-C6-O6
6	D	1303	NAG	C4-C5-C6-O6
6	C	1309	NAG	O5-C5-C6-O6
6	D	1309	NAG	O5-C5-C6-O6
6	D	1310	NAG	O5-C5-C6-O6
6	B	1309	NAG	C4-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	1307	NAG	O5-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	B	1311	NAG	C4-C5-C6-O6
6	D	1307	NAG	C4-C5-C6-O6
6	B	1308	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	C	1310	NAG	O5-C5-C6-O6
6	B	1309	NAG	O5-C5-C6-O6
6	D	1302	NAG	O5-C5-C6-O6
6	A	905	NAG	C4-C5-C6-O6
6	B	1307	NAG	C4-C5-C6-O6
6	B	1308	NAG	C4-C5-C6-O6
6	D	1306	NAG	O5-C5-C6-O6
6	C	1309	NAG	C4-C5-C6-O6
6	D	1303	NAG	O5-C5-C6-O6
6	D	1302	NAG	C4-C5-C6-O6
6	D	1309	NAG	C4-C5-C6-O6
6	A	905	NAG	O5-C5-C6-O6
6	A	906	NAG	C8-C7-N2-C2
6	A	906	NAG	O7-C7-N2-C2
6	B	1303	NAG	C8-C7-N2-C2
6	B	1303	NAG	O7-C7-N2-C2
6	B	1309	NAG	C8-C7-N2-C2
6	B	1309	NAG	O7-C7-N2-C2
6	B	1310	NAG	C8-C7-N2-C2
6	B	1310	NAG	O7-C7-N2-C2
6	C	1308	NAG	C8-C7-N2-C2
6	C	1308	NAG	O7-C7-N2-C2
6	C	1310	NAG	C8-C7-N2-C2
6	C	1310	NAG	O7-C7-N2-C2
6	D	1308	NAG	C8-C7-N2-C2
6	D	1308	NAG	O7-C7-N2-C2
6	D	1310	NAG	C8-C7-N2-C2
6	D	1310	NAG	O7-C7-N2-C2
6	D	1304	NAG	O5-C5-C6-O6
6	D	1306	NAG	C4-C5-C6-O6
6	D	1301	NAG	O5-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	B	1305	NAG	C4-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	C	1307	NAG	C4-C5-C6-O6
6	A	905	NAG	C1-C2-N2-C7
6	B	1301	NAG	C1-C2-N2-C7
6	C	1307	NAG	O5-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	A	905	NAG	C3-C2-N2-C7
6	C	1301	NAG	C3-C2-N2-C7
6	D	1301	NAG	C3-C2-N2-C7
6	D	1304	NAG	C4-C5-C6-O6
6	C	1301	NAG	C1-C2-N2-C7
6	D	1301	NAG	C1-C2-N2-C7
6	B	1301	NAG	C3-C2-N2-C7
6	B	1310	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1306	NAG	1	0
6	B	1310	NAG	1	0
6	C	1305	NAG	1	0
6	D	1301	NAG	1	0
6	D	1310	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

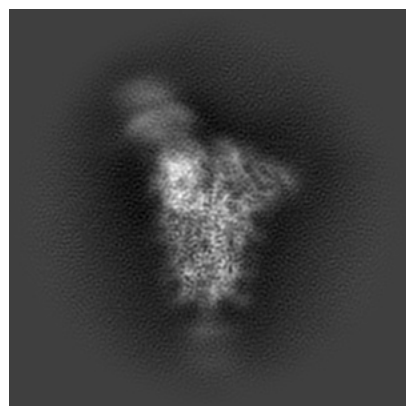
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38789. These allow visual inspection of the internal detail of the map and identification of artifacts.

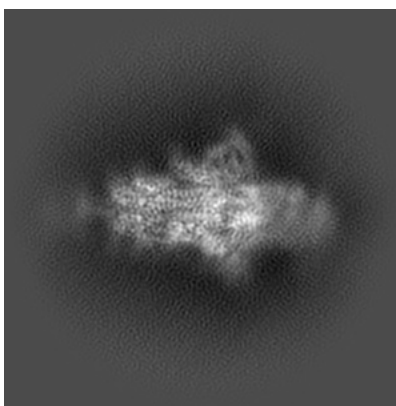
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

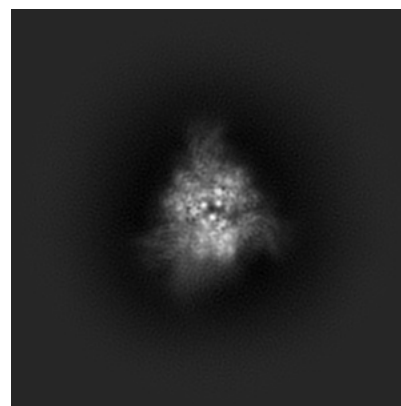
6.1.1 Primary map



X

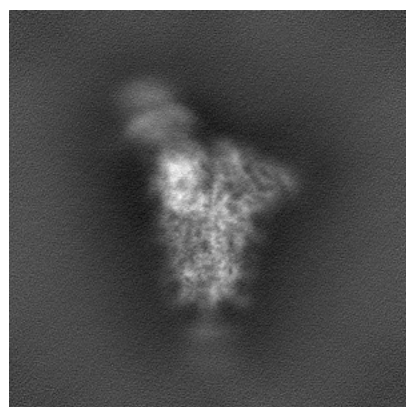


Y

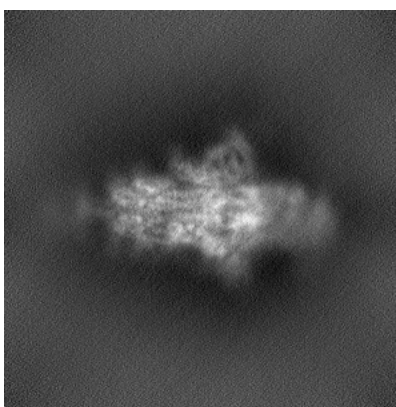


Z

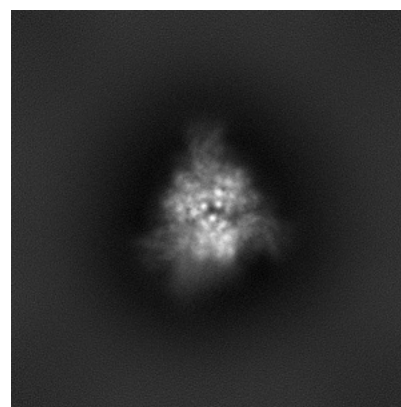
6.1.2 Raw map



X



Y

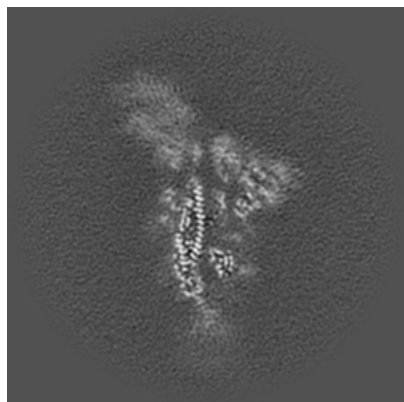


Z

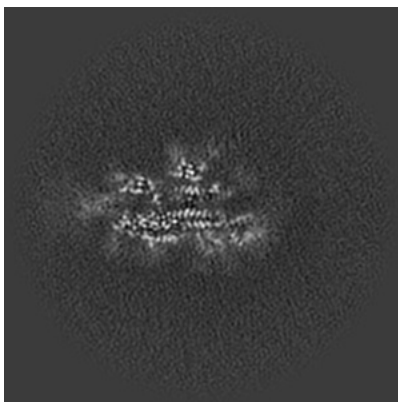
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

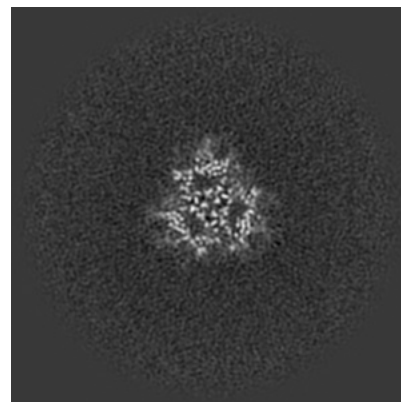
6.2.1 Primary map



X Index: 180

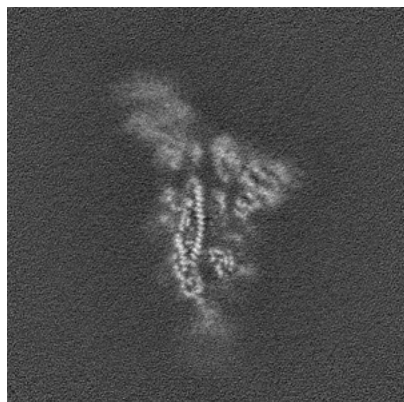


Y Index: 180



Z Index: 180

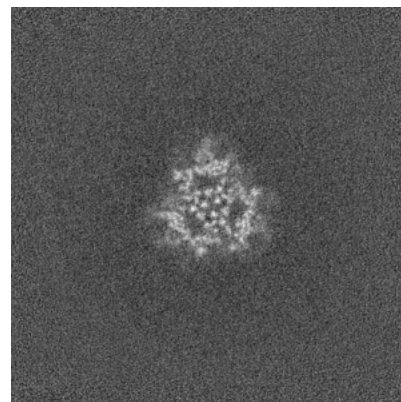
6.2.2 Raw map



X Index: 180



Y Index: 180

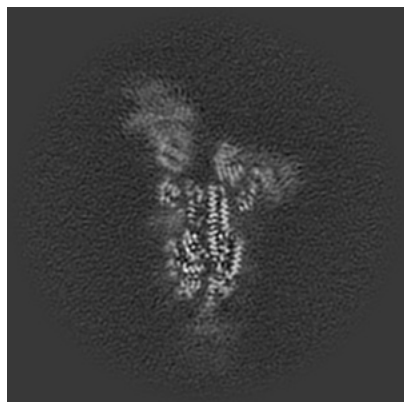


Z Index: 180

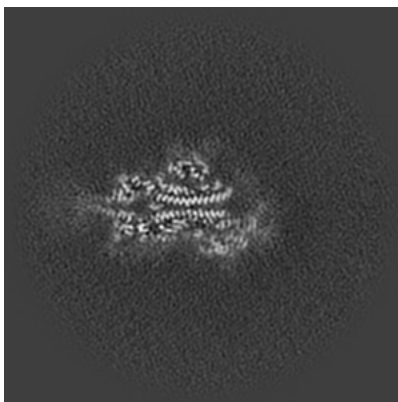
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

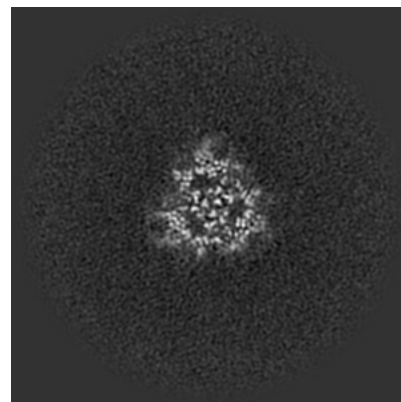
6.3.1 Primary map



X Index: 187

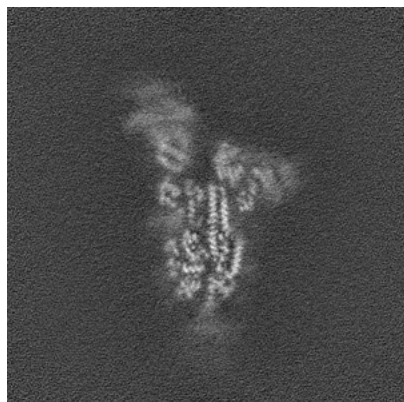


Y Index: 184

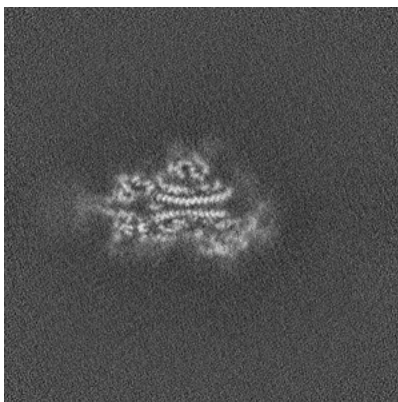


Z Index: 181

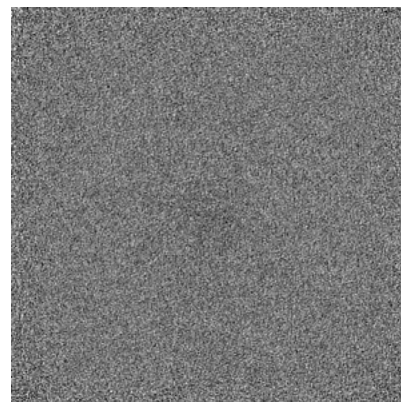
6.3.2 Raw map



X Index: 187



Y Index: 184

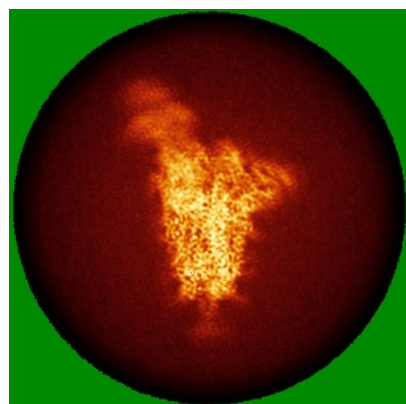


Z Index: 0

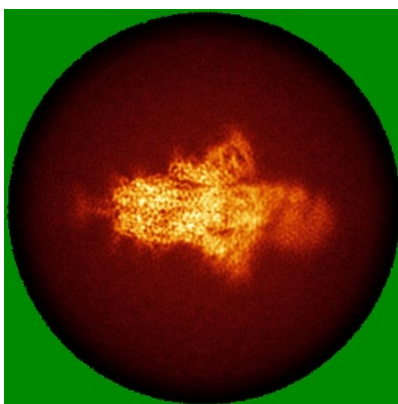
The images above show the largest variance slices of the map in three orthogonal directions.

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

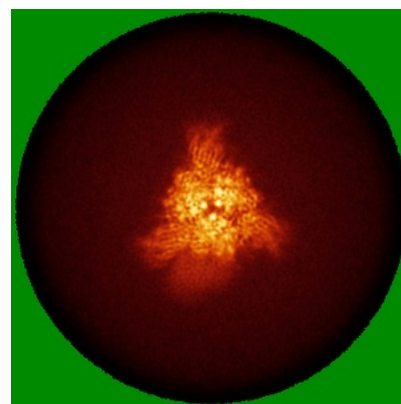
6.4.1 Primary map



X

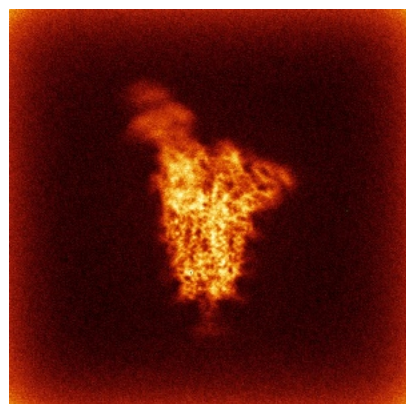


Y

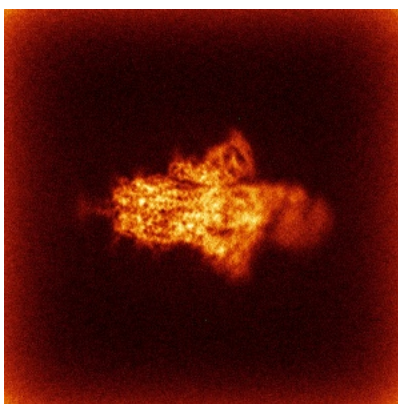


Z

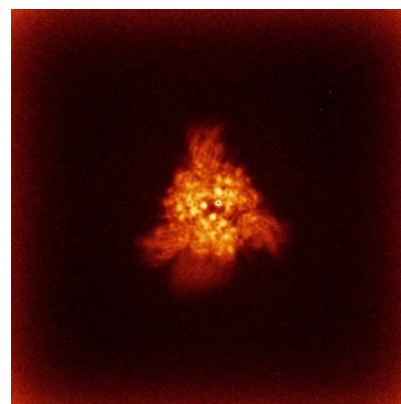
6.4.2 Raw map



X



Y

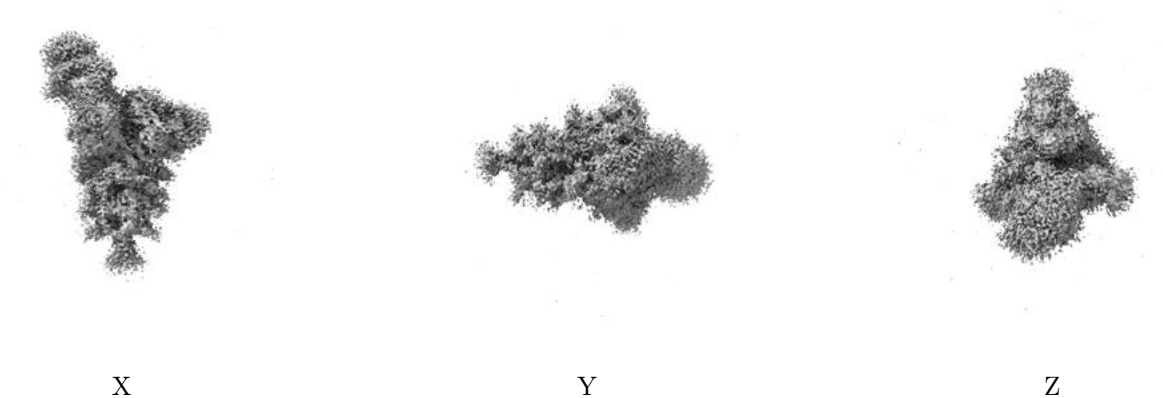


Z

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

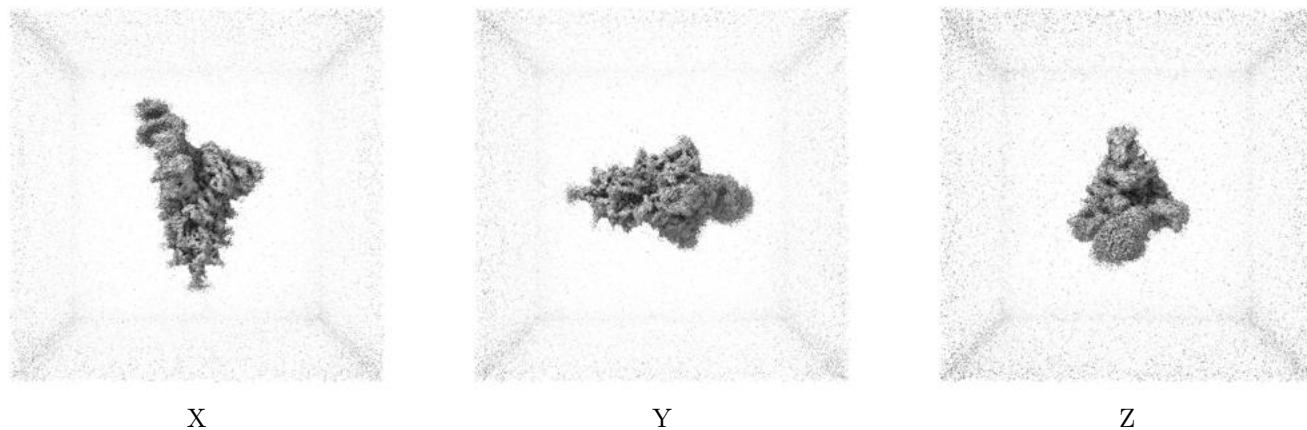
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

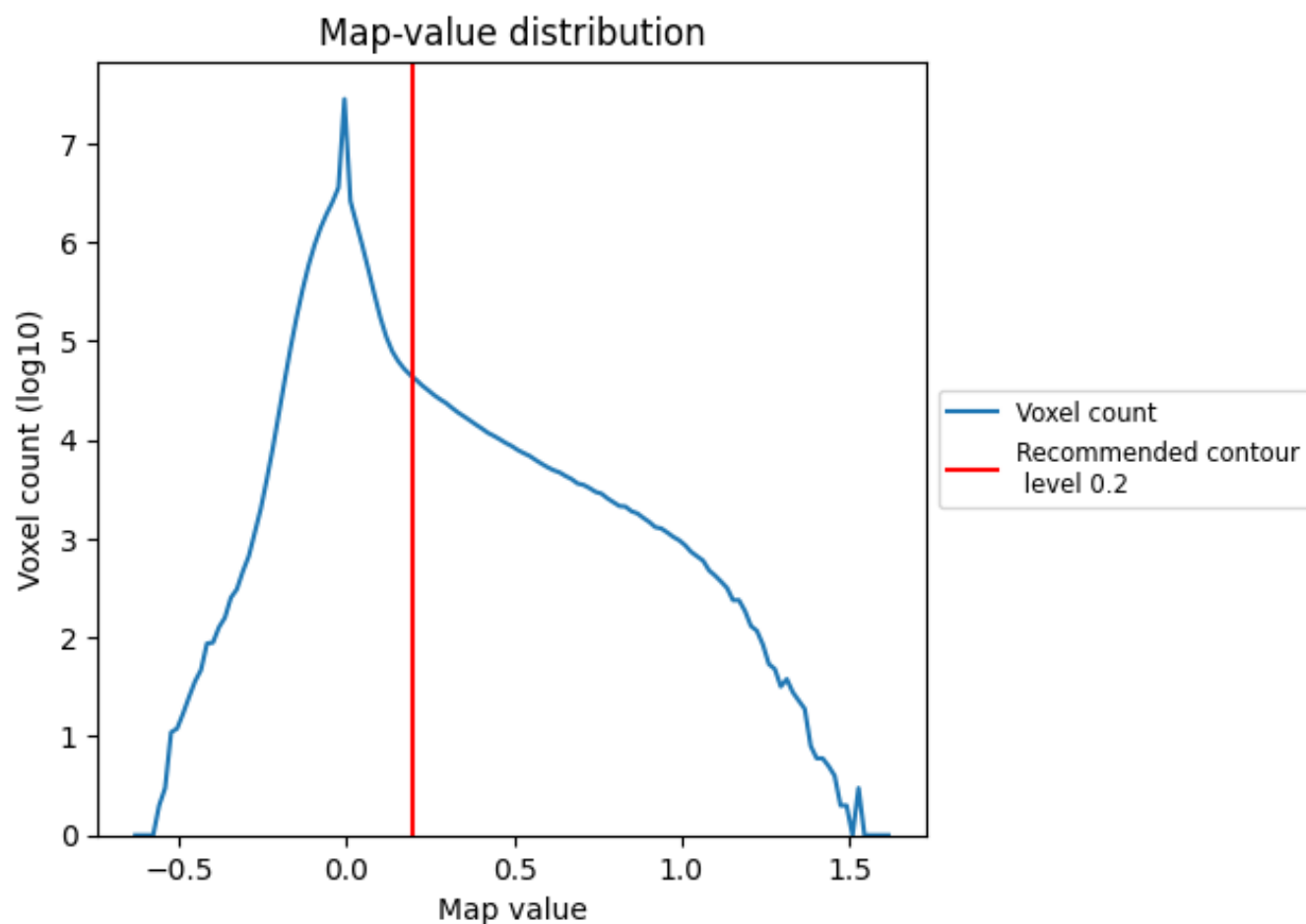
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

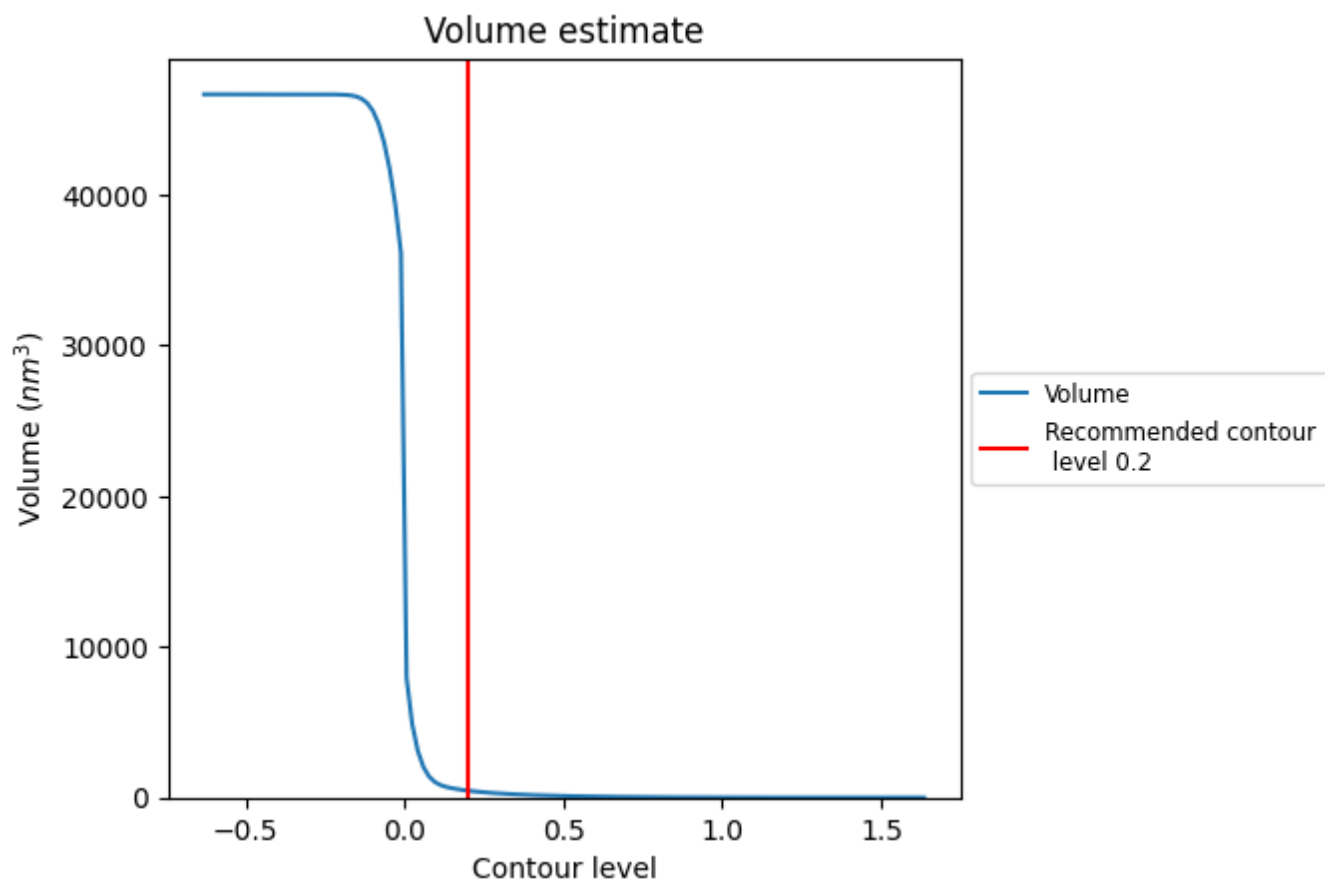
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

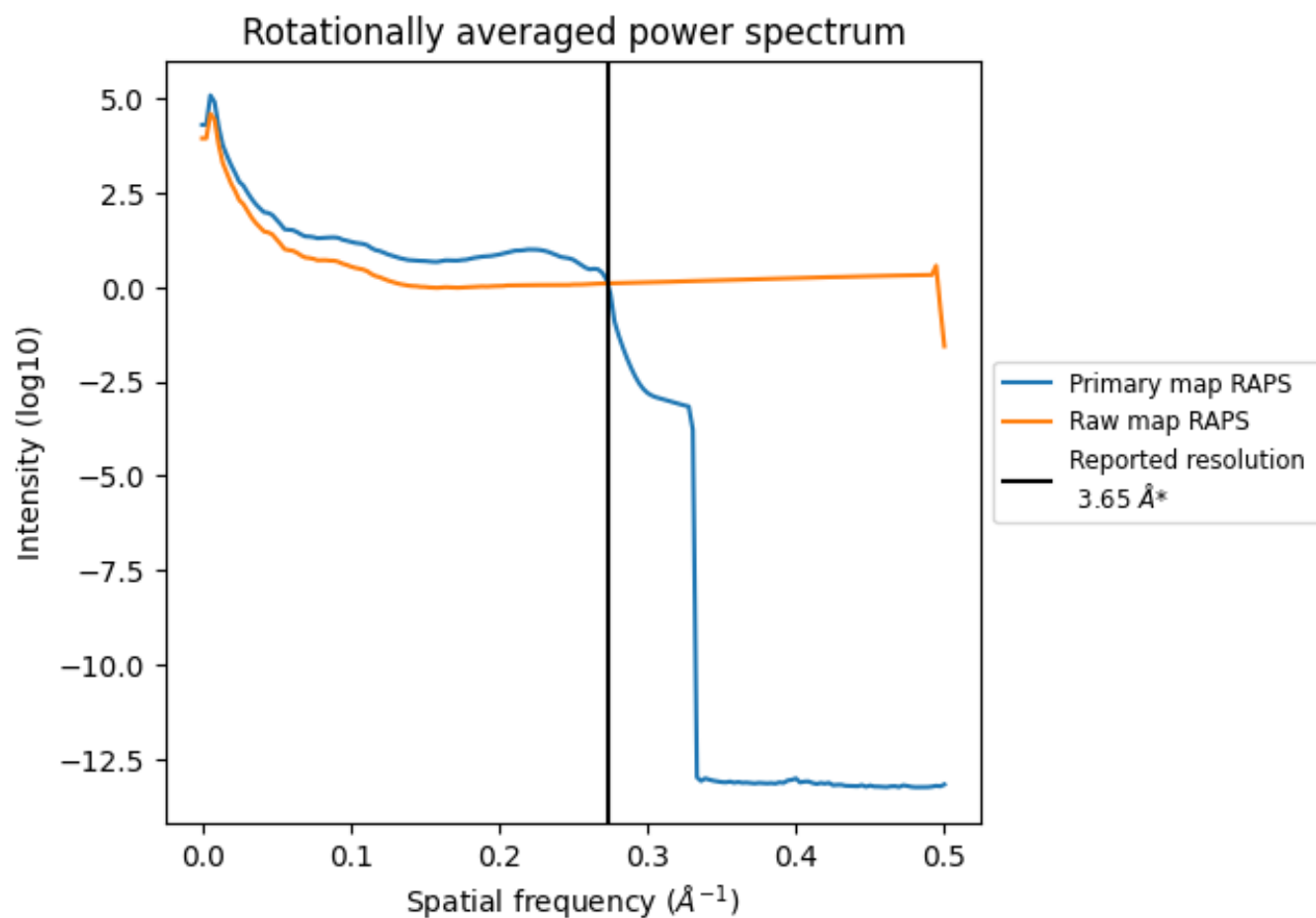
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 458 nm³; this corresponds to an approximate mass of 414 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 ⓘ

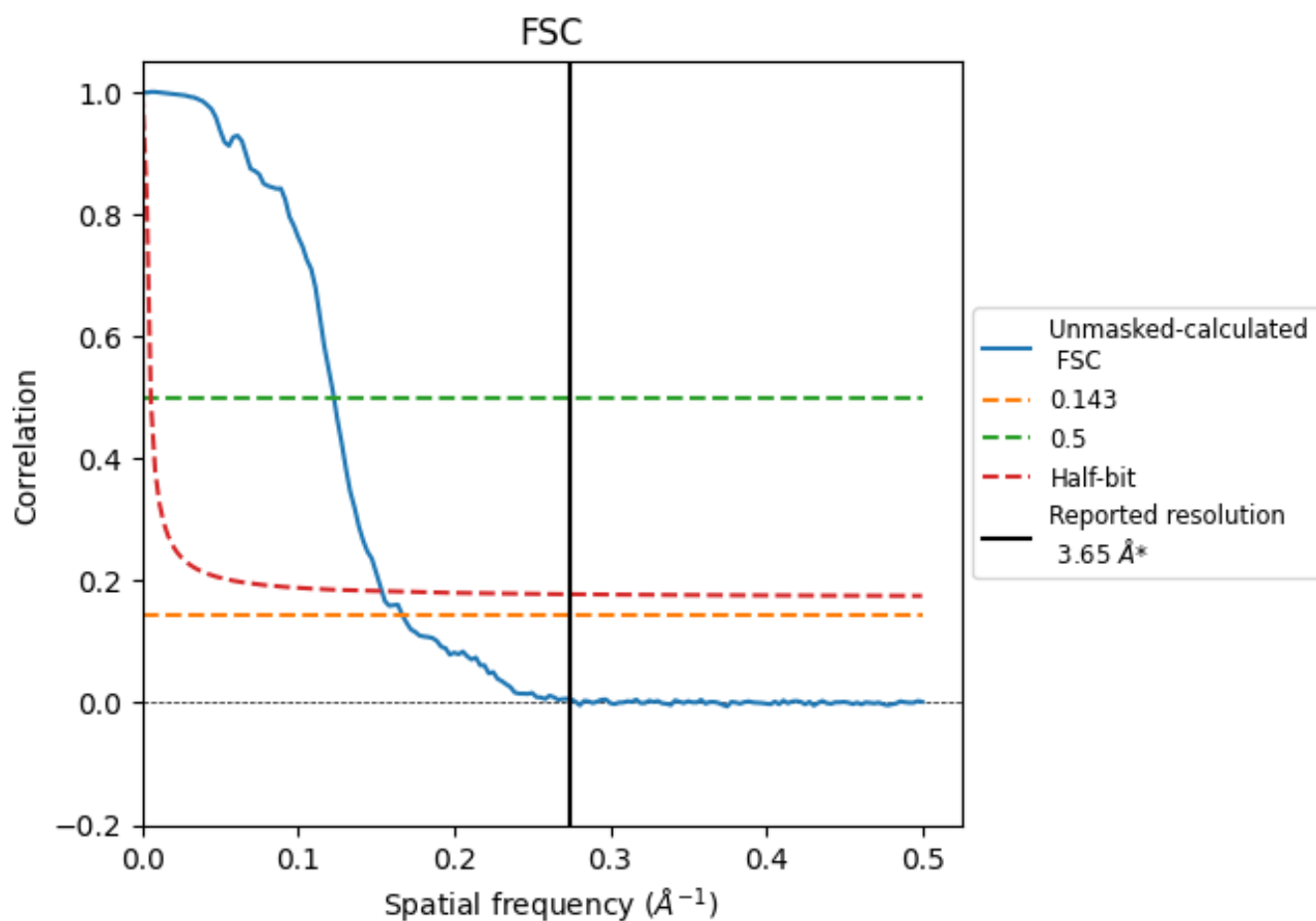


*Reported resolution corresponds to spatial frequency of 0.274 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.274 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

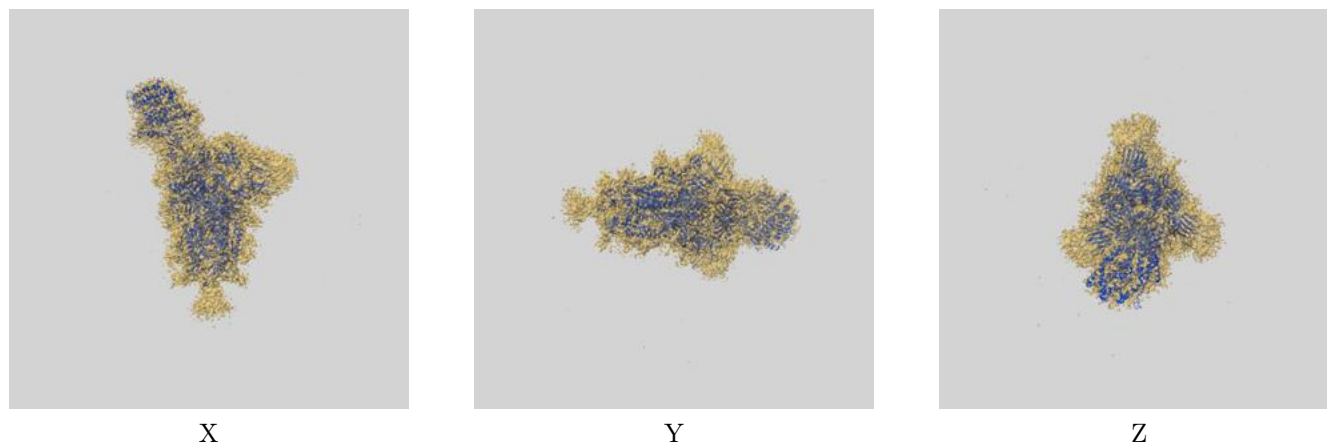
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.00	8.14	6.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.00 differs from the reported value 3.65 by more than 10 %

9 Map-model fit [i](#)

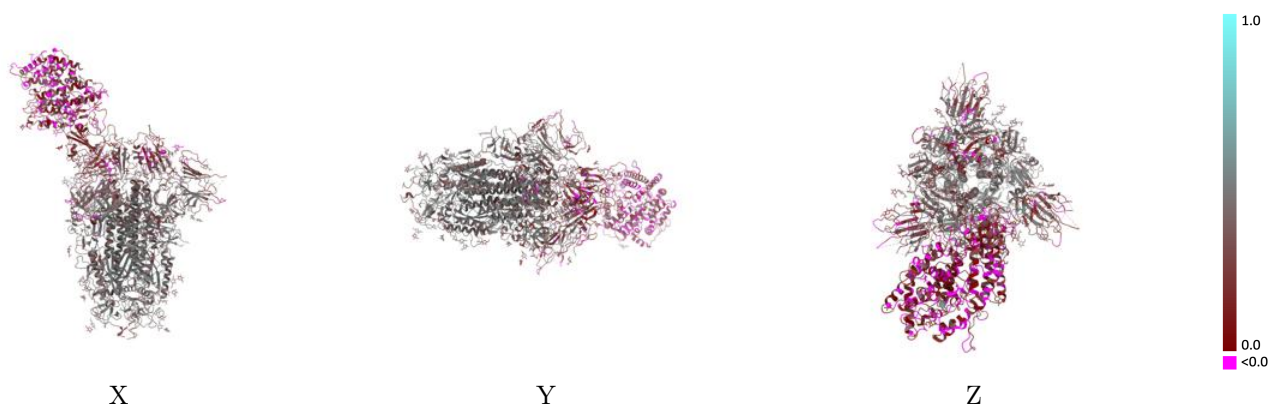
This section contains information regarding the fit between EMDB map EMD-38789 and PDB model 8XZ8. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



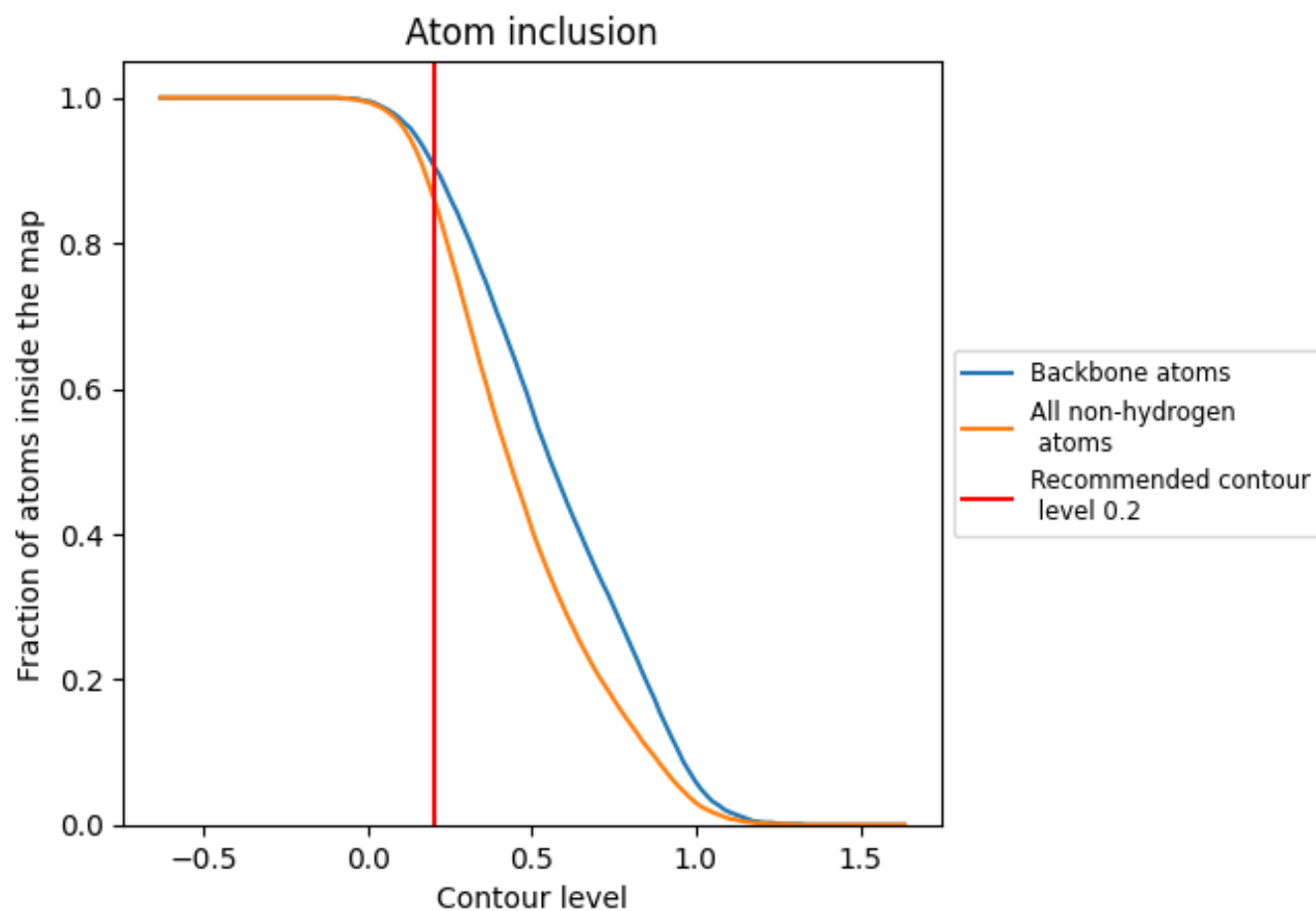
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.3260
A	 0.5330	 0.1050
B	 0.9290	 0.3510
C	 0.9170	 0.3610
D	 0.9380	 0.3920
E	 0.7200	 0.2370
F	 0.9200	 0.4060
G	 1.0000	 0.3850
H	 0.8800	 0.3830
I	 0.9200	 0.3140
J	 0.9200	 0.3820
K	 0.8400	 0.4060
L	 0.9200	 0.4020
M	 1.0000	 0.3730
N	 1.0000	 0.4350
O	 0.9200	 0.3080
P	 0.9600	 0.3850
Q	 0.9200	 0.4030
R	 0.8800	 0.3820
S	 0.9200	 0.3500
T	 0.9600	 0.3930
U	 0.8400	 0.2970

