



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 11:48 AM UTC

PDB ID : 8WHW / pdb_00008whw
EMDB ID : EMD-37550
Title : Spike Trimer of BA.2.86 with single RBD up
Authors : Yue, C.; Liu, P.
Deposited on : 2023-09-23
Resolution : 3.85 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

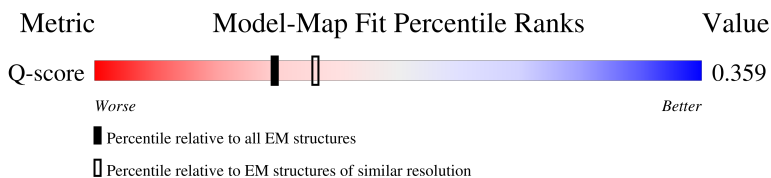
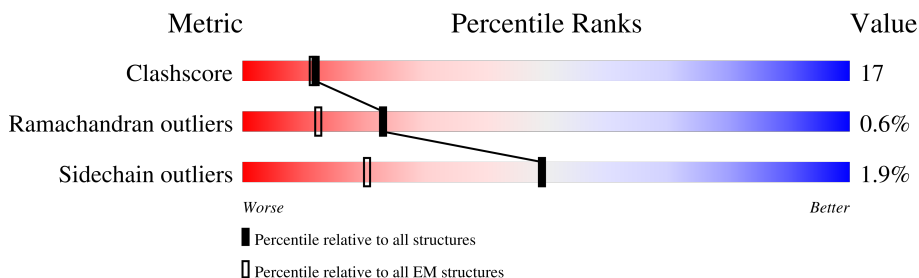
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.85 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	8989 (3.35 - 4.35)

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	1206	
1	B	1206	
1	C	1206	
2	D	2	

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

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

There are 273 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	0	MET	-	expression tag	UNP P0DTC2
A	1	PHE	-	expression tag	UNP P0DTC2
A	2	VAL	-	expression tag	UNP P0DTC2
A	3	PHE	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	VAL	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	PRO	-	expression tag	UNP P0DTC2
A	9	LEU	-	expression tag	UNP P0DTC2
A	10	VAL	-	expression tag	UNP P0DTC2
A	11	SER	-	expression tag	UNP P0DTC2
A	12	SER	-	expression tag	UNP P0DTC2
A	13	GLN	-	expression tag	UNP P0DTC2
A	14	CYS	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	MET	-	expression tag	UNP P0DTC2
A	17	PRO	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	PHE	-	expression tag	UNP P0DTC2
A	20	ASN	-	expression tag	UNP P0DTC2
A	21	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	-	expression tag	UNP P0DTC2
A	23	THR	-	expression tag	UNP P0DTC2
A	24	THR	-	expression tag	UNP P0DTC2
A	25	THR	-	expression tag	UNP P0DTC2
A	26	GLN	-	expression tag	UNP P0DTC2
A	27	SER	-	expression tag	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	216	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	HIS	VAL	variant	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	PRO	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	554	LYS	GLU	conflict	UNP P0DTC2
A	570	VAL	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	621	SER	PRO	conflict	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	conflict	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	0	MET	-	expression tag	UNP P0DTC2
B	1	PHE	-	expression tag	UNP P0DTC2
B	2	VAL	-	expression tag	UNP P0DTC2
B	3	PHE	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	VAL	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	PRO	-	expression tag	UNP P0DTC2
B	9	LEU	-	expression tag	UNP P0DTC2
B	10	VAL	-	expression tag	UNP P0DTC2
B	11	SER	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	GLN	-	expression tag	UNP P0DTC2
B	14	CYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	VAL	-	expression tag	UNP P0DTC2
B	16	MET	-	expression tag	UNP P0DTC2
B	17	PRO	-	expression tag	UNP P0DTC2
B	18	LEU	-	expression tag	UNP P0DTC2
B	19	PHE	-	expression tag	UNP P0DTC2
B	20	ASN	-	expression tag	UNP P0DTC2
B	21	LEU	-	expression tag	UNP P0DTC2
B	22	ILE	-	expression tag	UNP P0DTC2
B	23	THR	-	expression tag	UNP P0DTC2
B	24	THR	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	GLN	-	expression tag	UNP P0DTC2
B	27	SER	-	expression tag	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
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	conflict	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	variant	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	conflict	UNP P0DTC2
B	445	HIS	VAL	variant	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	0	MET	-	expression tag	UNP P0DTC2
C	1	PHE	-	expression tag	UNP P0DTC2
C	2	VAL	-	expression tag	UNP P0DTC2
C	3	PHE	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	VAL	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	PRO	-	expression tag	UNP P0DTC2
C	9	LEU	-	expression tag	UNP P0DTC2
C	10	VAL	-	expression tag	UNP P0DTC2
C	11	SER	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	GLN	-	expression tag	UNP P0DTC2
C	14	CYS	-	expression tag	UNP P0DTC2
C	15	VAL	-	expression tag	UNP P0DTC2
C	16	MET	-	expression tag	UNP P0DTC2
C	17	PRO	-	expression tag	UNP P0DTC2
C	18	LEU	-	expression tag	UNP P0DTC2
C	19	PHE	-	expression tag	UNP P0DTC2
C	20	ASN	-	expression tag	UNP P0DTC2
C	21	LEU	-	expression tag	UNP P0DTC2
C	22	ILE	-	expression tag	UNP P0DTC2
C	23	THR	-	expression tag	UNP P0DTC2
C	24	THR	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	GLN	-	expression tag	UNP P0DTC2
C	27	SER	-	expression tag	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	conflict	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	variant	UNP P0DTC2
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

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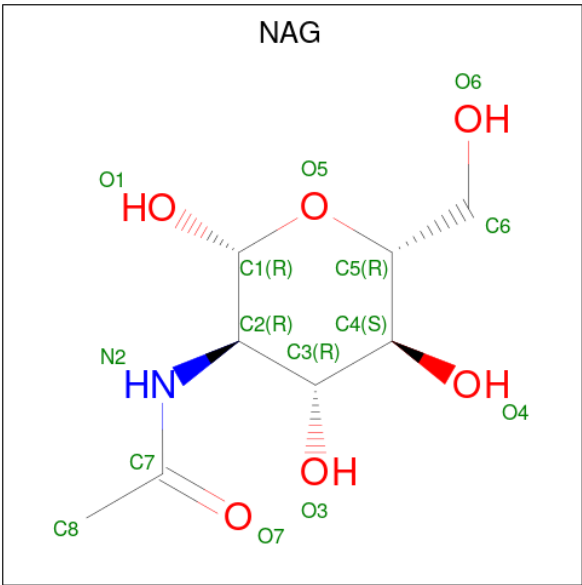
Chain	Residue	Modelled	Actual	Comment	Reference
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	HIS	VAL	variant	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	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
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2

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



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

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

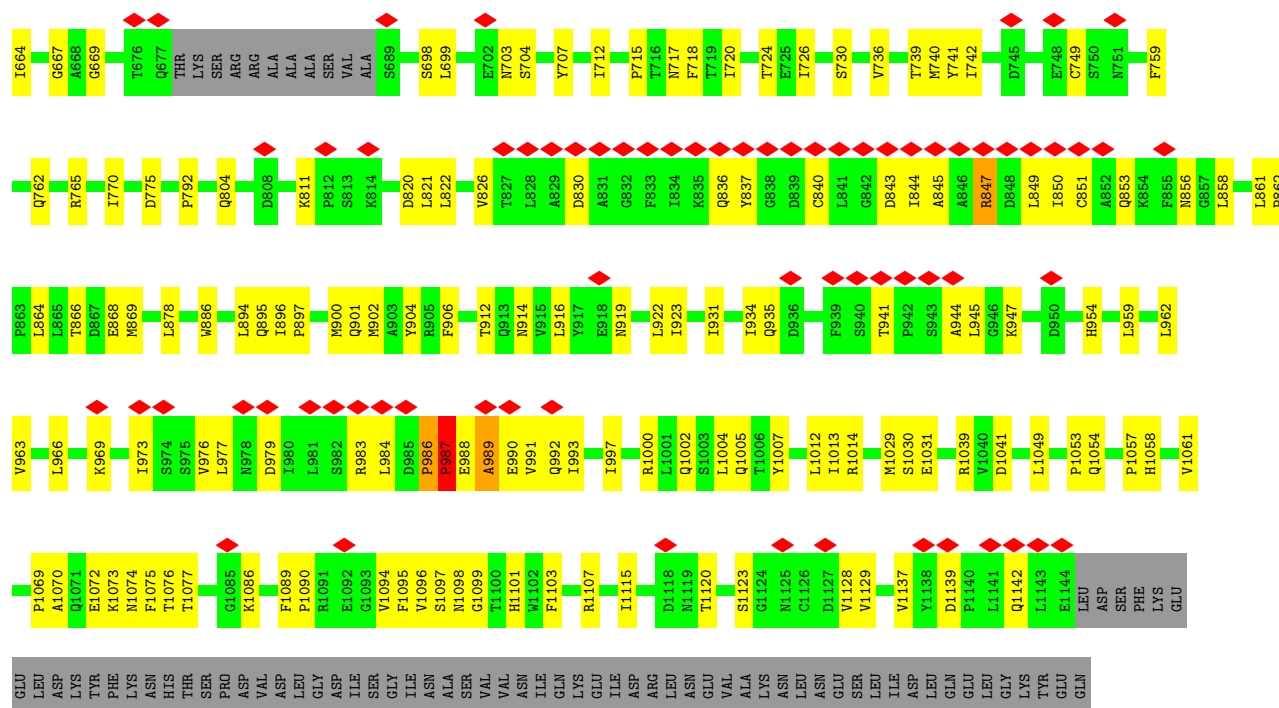


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3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

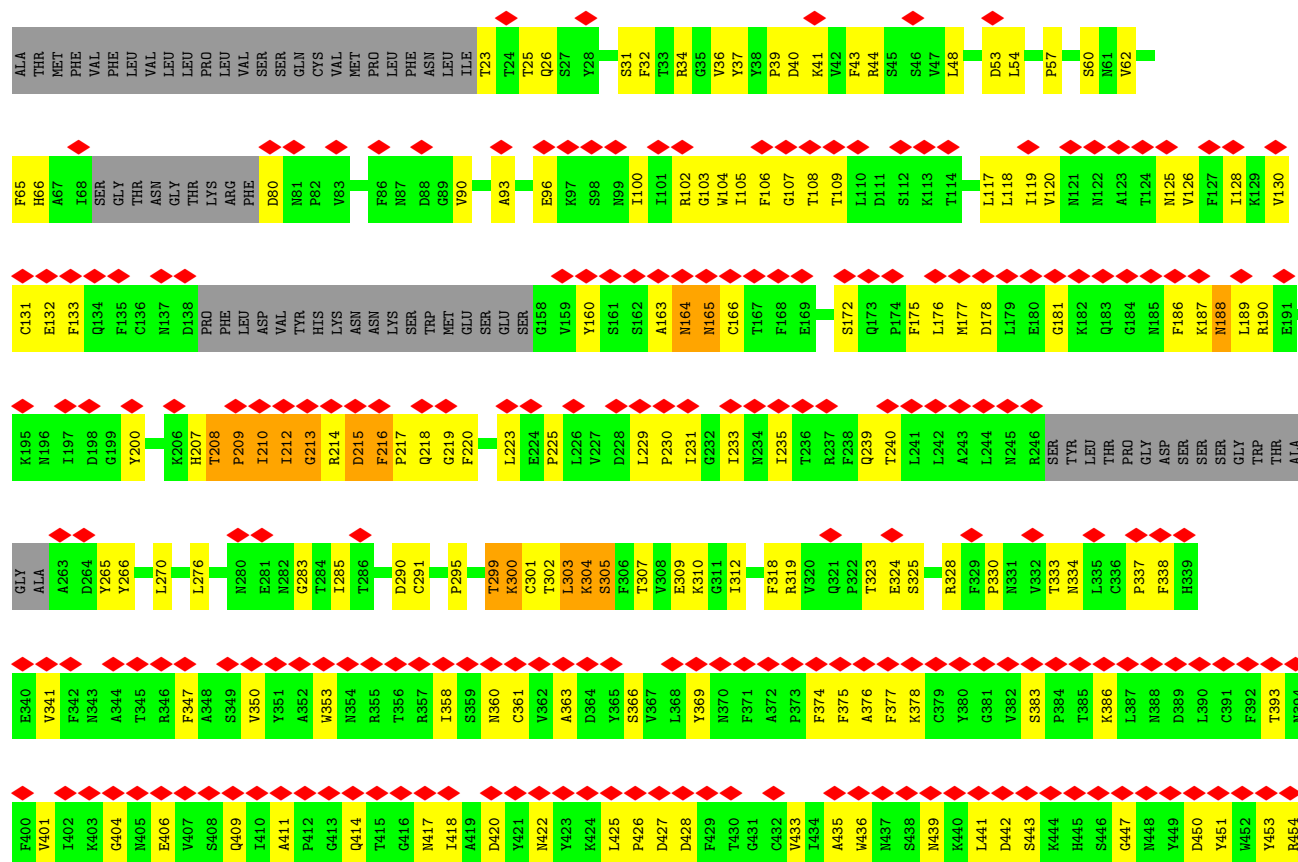
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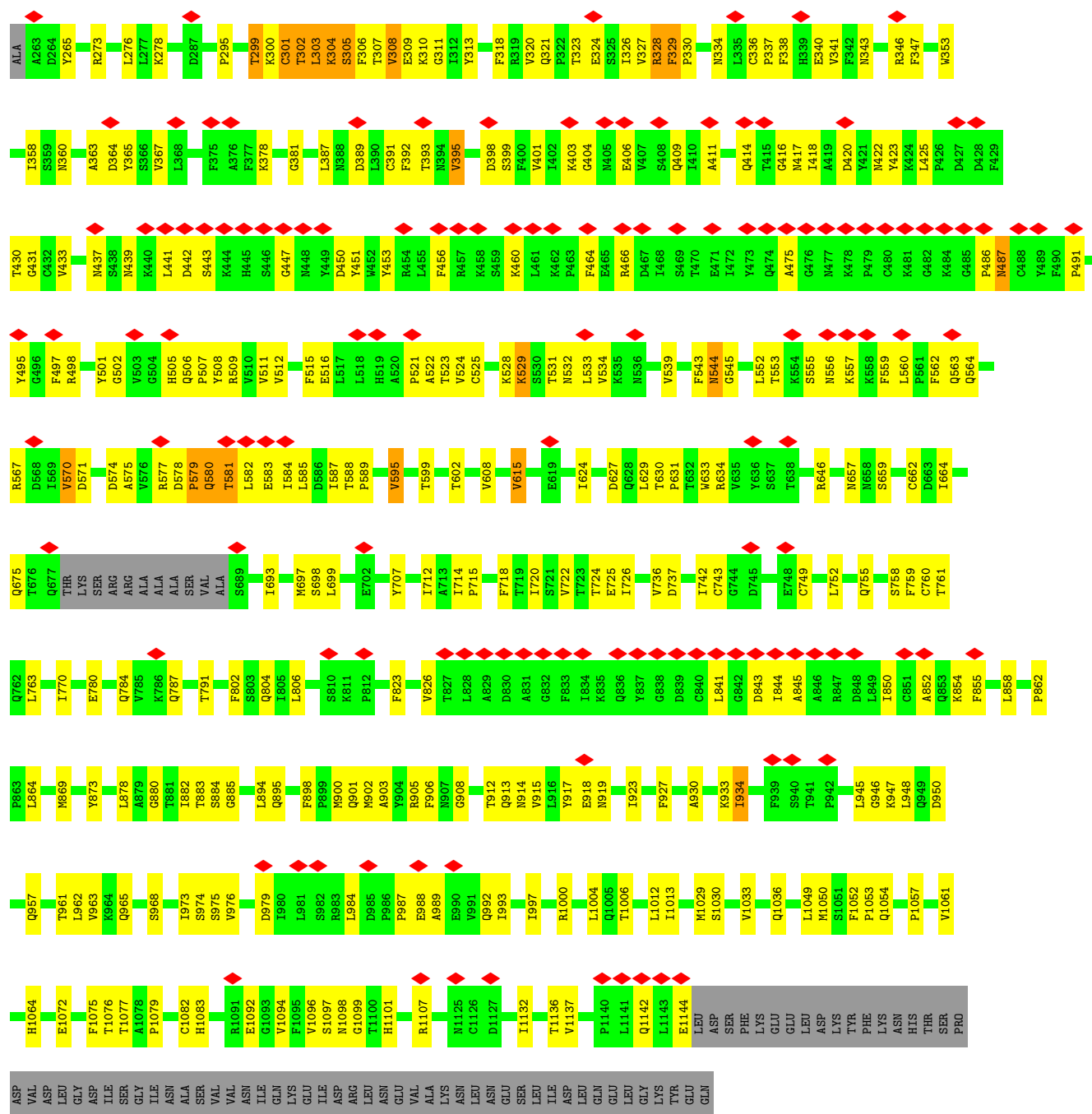
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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C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



• Molecule 1: Spike glycoprotein





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



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





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



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



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



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



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



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



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



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



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



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



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



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



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





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

Chain S:  100%



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

Chain T:  50% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50577	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.838	Depositor
Minimum map value	-0.795	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.44	Depositor
Map size ($\text{\AA}$)	320.0, 320.0, 320.0	wwPDB
Map dimensions	320, 320, 320	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: NAG, BMA

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	0.38	0/8516	0.58	4/11591 (0.0%)
1	B	0.30	0/8516	0.54	7/11591 (0.1%)
1	C	0.38	0/8516	0.59	3/11591 (0.0%)
All	All	0.36	0/25548	0.57	14/34773 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	2
All	All	0	6

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	GLN	CA-C-N	-6.70	113.74	120.10
1	A	218	GLN	C-N-CA	-6.70	113.74	120.10
1	B	213	GLY	N-CA-C	-6.56	106.68	115.21
1	A	986	PRO	N-CA-C	6.52	118.66	110.70
1	B	209	PRO	N-CA-C	-6.47	99.14	112.47
1	C	570	VAL	N-CA-C	5.70	112.30	106.21
1	A	303	LEU	N-CA-C	-5.62	106.63	112.93
1	B	1074	ASN	CA-C-N	-5.60	114.84	121.90
1	B	1074	ASN	C-N-CA	-5.60	114.84	121.90
1	B	39	PRO	CB-CA-C	-5.45	102.81	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	341	VAL	N-CA-C	-5.44	107.97	113.47
1	B	299	THR	N-CA-C	-5.25	105.25	110.97
1	C	299	THR	N-CA-C	-5.17	105.73	111.36
1	B	986	PRO	N-CA-C	5.10	116.92	110.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	847	ARG	Sidechain
1	B	567	ARG	Sidechain
1	C	328	ARG	Sidechain
1	C	466	ARG	Sidechain

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	8316	0	8101	293	0
1	B	8316	0	8102	339	0
1	C	8316	0	8104	320	0
2	D	25	0	22	1	0
2	E	25	0	22	0	0
2	F	25	0	22	0	0
2	G	25	0	22	0	0
2	H	25	0	22	2	0
2	I	25	0	22	0	0
2	J	25	0	22	0	0
2	K	25	0	22	0	0
2	L	25	0	22	0	0
2	M	25	0	22	0	0
2	N	25	0	22	0	0
2	O	25	0	22	0	0
2	P	25	0	22	0	0
2	Q	25	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	25	0	22	0	0
2	S	25	0	22	0	0
2	T	25	0	22	0	0
3	A	140	0	130	2	0
3	B	154	0	143	2	0
3	C	140	0	130	3	0
All	All	25807	0	25084	882	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 17.

All (882) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ILE:CG2	1:B:212:ILE:H	1.45	1.26
1:B:210:ILE:HG22	1:B:212:ILE:N	1.47	1.15
1:B:189:LEU:HD22	1:B:210:ILE:CD1	1.81	1.10
1:C:188:ASN:CA	1:C:209:PRO:HA	1.90	1.00
1:C:188:ASN:HA	1:C:209:PRO:CA	1.94	0.96
1:B:189:LEU:HD22	1:B:210:ILE:HD12	0.99	0.96
1:B:645:THR:HG22	1:B:647:ALA:H	1.31	0.95
1:C:188:ASN:HA	1:C:209:PRO:HA	0.97	0.94
1:B:189:LEU:CD2	1:B:210:ILE:HD12	1.96	0.89
1:B:34:ARG:HG2	1:B:216:PHE:HE1	1.38	0.88
1:B:369:TYR:HA	1:B:374:PHE:HZ	1.39	0.87
1:C:62:VAL:HG21	1:C:216:PHE:CE2	2.13	0.84
1:C:486:PRO:O	1:C:487:ASN:ND2	2.13	0.81
1:C:578:ASP:C	1:C:580:GLN:H	1.89	0.80
1:B:210:ILE:HG22	1:B:212:ILE:H	0.66	0.78
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.65	0.78
1:A:190:ARG:HB3	1:A:192:PHE:HE1	1.49	0.77
1:C:521:PRO:HG3	1:C:564:GLN:HE21	1.50	0.77
1:A:53:ASP:OD1	1:A:54:LEU:N	2.18	0.76
1:B:210:ILE:HG22	1:B:212:ILE:CG1	2.14	0.76
1:C:189:LEU:HG	1:C:208:THR:O	1.86	0.75
1:C:310:LYS:HG2	1:C:664:ILE:HD11	1.68	0.75
1:B:330:PRO:HA	1:B:579:PRO:HB2	1.67	0.75
1:A:759:PHE:HE1	1:A:1005:GLN:HE21	1.34	0.75
1:A:699:LEU:HD21	1:C:869:MET:HB2	1.69	0.74
1:C:417:ASN:O	1:C:422:ASN:ND2	2.20	0.74
1:A:895:GLN:NE2	1:B:1074:ASN:OD1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:HG22	1:B:109:THR:HG23	1.71	0.73
1:A:577:ARG:HD3	1:A:582:LEU:HD13	1.68	0.73
1:C:329:PHE:HB2	1:C:528:LYS:HG3	1.71	0.73
1:B:48:LEU:HD13	1:B:305:SER:HA	1.71	0.72
1:C:486:PRO:C	1:C:487:ASN:HD22	1.97	0.72
1:A:131:CYS:SG	1:A:132:GLU:N	2.63	0.72
1:A:214:ARG:HB2	1:A:217:PRO:HB3	1.71	0.72
1:B:96:GLU:OE1	1:B:100:ILE:N	2.23	0.72
1:C:581:THR:O	1:C:583:GLU:N	2.23	0.72
1:B:904:TYR:HE1	1:C:1107:ARG:HG2	1.54	0.71
1:C:65:PHE:HB2	1:C:265:TYR:HB3	1.72	0.71
1:A:724:THR:HB	1:A:934:ILE:HD11	1.72	0.71
1:C:96:GLU:OE1	1:C:100:ILE:N	2.24	0.71
1:C:987:PRO:HD2	1:C:988:GLU:OE2	1.92	0.70
1:B:131:CYS:SG	1:B:132:GLU:N	2.65	0.70
1:C:44:ARG:HB3	1:C:47:VAL:HG11	1.72	0.70
1:B:189:LEU:HB3	1:B:208:THR:O	1.91	0.69
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.73	0.69
1:B:731:MET:HE3	1:B:955:ASN:HD21	1.58	0.69
1:B:208:THR:O	1:B:210:ILE:N	2.26	0.69
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.75	0.69
1:A:447:GLY:HA2	1:A:498:ARG:HG3	1.74	0.69
1:A:856:ASN:HD21	1:A:963:VAL:HG13	1.57	0.69
1:A:498:ARG:H	1:A:501:TYR:HE1	1.39	0.69
1:B:31:SER:HA	1:B:216:PHE:CE2	2.27	0.69
1:B:276:LEU:HD11	1:B:304:LYS:HA	1.73	0.69
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.74	0.68
1:C:791:THR:HG21	1:C:806:LEU:HD23	1.75	0.68
1:A:861:LEU:HD12	1:A:862:PRO:HD2	1.75	0.68
1:A:866:THR:HG22	1:A:868:GLU:H	1.59	0.68
1:B:462:LYS:HD2	1:B:465:GLU:HB2	1.74	0.68
1:A:454:ARG:NH1	1:A:467:ASP:O	2.26	0.68
1:C:559:PHE:HB2	1:C:584:ILE:HD11	1.74	0.68
1:B:128:ILE:HD11	1:B:175:PHE:HZ	1.59	0.67
1:B:190:ARG:HD3	1:B:207:HIS:CE1	2.29	0.67
1:A:900:MET:SD	1:B:1077:THR:OG1	2.51	0.67
1:C:456:PHE:HB2	1:C:491:PRO:HA	1.75	0.67
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.77	0.67
1:C:128:ILE:HD11	1:C:175:PHE:HZ	1.59	0.67
1:C:131:CYS:SG	1:C:132:GLU:N	2.67	0.66
1:C:347:PHE:HD2	1:C:399:SER:HB2	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:THR:HB	1:B:210:ILE:HG13	1.76	0.66
1:C:903:ALA:HB1	1:C:913:GLN:HB3	1.78	0.66
1:B:454:ARG:NH1	1:B:467:ASP:O	2.27	0.66
1:C:555:SER:HB3	1:C:584:ILE:HG22	1.78	0.66
1:B:125:ASN:HB2	3:B:1301:NAG:H61	1.75	0.66
1:B:866:THR:H	1:B:869:MET:HE2	1.60	0.65
1:B:533:LEU:HD23	1:B:535:LYS:HE3	1.76	0.65
1:A:619:GLU:OE1	1:A:619:GLU:N	2.29	0.65
1:A:792:PRO:HG3	1:B:707:TYR:HB3	1.77	0.65
1:B:187:LYS:O	1:B:209:PRO:HA	1.95	0.65
1:A:989:ALA:O	1:A:990:GLU:C	2.40	0.65
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.32	0.65
1:B:210:ILE:HG22	1:B:212:ILE:HG13	1.78	0.65
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.79	0.64
1:C:200:TYR:HA	1:C:230:PRO:HA	1.78	0.64
1:C:34:ARG:NH2	1:C:217:PRO:O	2.30	0.64
1:C:360:ASN:H	1:C:523:THR:HB	1.61	0.64
1:C:533:LEU:HD11	1:C:552:LEU:HD12	1.77	0.64
1:B:117:LEU:HD12	1:B:118:LEU:H	1.63	0.64
1:A:406:GLU:HG2	1:A:418:ILE:HG13	1.80	0.64
1:B:422:ASN:ND2	1:B:454:ARG:O	2.23	0.64
1:A:617:CYS:HA	1:A:620:VAL:HG22	1.80	0.64
1:B:409:GLN:HE22	1:B:418:ILE:H	1.43	0.64
1:B:576:VAL:HG23	1:B:587:ILE:HD11	1.79	0.64
1:B:208:THR:HB	1:B:210:ILE:CG1	2.27	0.64
1:C:406:GLU:OE1	1:C:406:GLU:N	2.30	0.64
1:A:983:ARG:HE	1:A:984:LEU:HG	1.62	0.63
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.30	0.63
1:B:427:ASP:OD1	1:B:428:ASP:N	2.31	0.63
1:C:578:ASP:C	1:C:580:GLN:N	2.57	0.63
1:B:215:ASP:HB2	1:B:266:TYR:CE2	2.34	0.63
1:A:1074:ASN:OD1	1:C:895:GLN:NE2	2.30	0.63
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.80	0.63
1:C:311:GLY:HA2	1:C:664:ILE:HD12	1.81	0.63
1:A:358:ILE:HB	1:A:395:VAL:HB	1.80	0.63
1:A:1013:ILE:HD13	1:B:1013:ILE:HD11	1.79	0.63
1:B:773:GLU:OE2	1:B:774:GLN:NE2	2.31	0.63
1:A:239:GLN:HE21	1:A:240:THR:H	1.47	0.62
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.81	0.62
1:B:792:PRO:HG3	1:C:707:TYR:HD1	1.64	0.62
1:C:174:PRO:HG2	1:C:177:MET:HE1	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:THR:O	1:B:210:ILE:HG13	1.99	0.62
1:B:1096:VAL:O	1:B:1103:PHE:N	2.26	0.62
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.31	0.62
1:B:23:THR:N	1:B:80:ASP:OD1	2.31	0.62
1:B:34:ARG:HG2	1:B:216:PHE:CE1	2.29	0.62
1:B:32:PHE:HB3	1:B:218:GLN:OE1	2.00	0.62
1:C:229:LEU:HD23	1:C:229:LEU:H	1.64	0.62
1:C:578:ASP:N	1:C:583:GLU:O	2.22	0.62
1:C:39:PRO:HG3	1:C:55:PHE:HZ	1.64	0.62
1:B:62:VAL:HG21	1:B:216:PHE:HE2	1.64	0.62
1:C:303:LEU:O	1:C:304:LYS:C	2.42	0.62
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.34	0.61
1:A:894:LEU:HD13	1:B:715:PRO:HD3	1.81	0.61
1:B:62:VAL:HG21	1:B:216:PHE:CE2	2.35	0.61
1:C:441:LEU:HD22	1:C:509:ARG:HH12	1.65	0.61
1:B:369:TYR:HA	1:B:374:PHE:CZ	2.29	0.61
1:C:328:ARG:HD2	1:C:579:PRO:HG2	1.82	0.61
1:C:381:GLY:HA3	1:C:430:THR:HG23	1.82	0.61
1:A:96:GLU:OE1	1:A:101:ILE:HG22	2.01	0.61
1:A:977:LEU:HD11	1:A:993:ILE:HG23	1.81	0.61
1:B:303:LEU:O	1:B:304:LYS:C	2.44	0.61
1:A:271:GLN:OE1	1:A:271:GLN:N	2.34	0.61
1:B:856:ASN:HD22	1:B:966:LEU:HD13	1.65	0.61
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.34	0.61
1:C:533:LEU:HD11	1:C:552:LEU:CD1	2.31	0.61
1:B:486:PRO:O	1:B:487:ASN:ND2	2.33	0.60
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.81	0.60
1:B:902:MET:HE1	1:B:1050:MET:HE2	1.83	0.60
1:A:878:LEU:HD11	1:A:1054:GLN:HE22	1.66	0.60
1:A:108:THR:HG22	1:A:109:THR:HG23	1.83	0.60
1:C:307:THR:HA	1:C:602:THR:HG21	1.84	0.60
1:A:988:GLU:O	1:A:989:ALA:C	2.45	0.60
1:C:659:SER:HB3	1:C:698:SER:HB2	1.84	0.60
1:A:922:LEU:HD11	2:H:1:NAG:H3	1.84	0.60
1:A:329:PHE:O	1:A:580:GLN:NE2	2.31	0.60
1:B:43:PHE:HE1	1:B:283:GLY:HA3	1.66	0.60
1:C:712:ILE:HD13	1:C:1094:VAL:HG11	1.83	0.60
1:A:570:VAL:HG21	1:C:852:ALA:HB1	1.84	0.60
1:A:962:LEU:HD13	1:A:1007:TYR:HB2	1.84	0.59
1:B:312:ILE:HB	1:B:598:ILE:HG22	1.84	0.59
1:A:864:LEU:HA	1:B:667:GLY:HA2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.84	0.59
1:C:393:THR:OG1	1:C:516:GLU:OE1	2.20	0.59
1:B:577:ARG:HD3	1:B:582:LEU:HD13	1.82	0.59
1:A:57:PRO:HG3	1:A:273:ARG:HD2	1.84	0.59
1:A:912:THR:OG1	1:A:914:ASN:OD1	2.21	0.59
1:C:475:ALA:HB3	1:C:487:ASN:HB2	1.83	0.59
1:C:567:ARG:HD3	1:C:571:ASP:HA	1.85	0.59
1:C:392:PHE:HD1	1:C:524:VAL:HG23	1.66	0.59
1:C:420:ASP:HB3	1:C:460:LYS:HD2	1.85	0.59
1:B:239:GLN:NE2	1:B:240:THR:O	2.35	0.59
1:C:1142:GLN:OE1	1:C:1142:GLN:N	2.36	0.59
1:A:108:THR:HB	1:A:114:THR:HG21	1.83	0.58
1:A:914:ASN:ND2	1:B:1123:SER:OG	2.35	0.58
1:A:322:PRO:HB3	1:A:539:VAL:HA	1.84	0.58
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.84	0.58
1:A:988:GLU:O	1:A:991:VAL:N	2.28	0.58
1:B:41:LYS:HB3	1:C:563:GLN:HA	1.86	0.58
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.33	0.58
1:A:703:ASN:ND2	1:C:787:GLN:OE1	2.36	0.58
1:C:398:ASP:HB2	1:C:512:VAL:HG12	1.85	0.58
1:A:456:PHE:HB3	1:A:473:TYR:HD2	1.69	0.58
1:C:358:ILE:HB	1:C:395:VAL:HB	1.85	0.58
1:B:468:ILE:HD12	1:B:468:ILE:H	1.69	0.58
1:B:107:GLY:H	1:B:235:ILE:HG23	1.67	0.58
1:C:200:TYR:HD1	1:C:230:PRO:HB3	1.67	0.58
1:A:65:PHE:HB2	1:A:265:TYR:CD2	2.39	0.58
1:A:1115:ILE:HG12	1:A:1137:VAL:HG23	1.85	0.58
1:B:189:LEU:O	1:B:190:ARG:HG2	2.04	0.58
1:C:334:ASN:ND2	1:C:360:ASN:O	2.35	0.58
1:B:447:GLY:HA2	1:B:498:ARG:HG2	1.86	0.58
1:C:447:GLY:HA2	1:C:498:ARG:HG2	1.86	0.57
1:A:48:LEU:HD12	1:A:276:LEU:HD21	1.87	0.57
1:A:1041:ASP:HB3	1:C:1030:SER:HB3	1.86	0.57
1:C:976:VAL:HG12	1:C:979:ASP:H	1.69	0.57
1:C:806:LEU:HD12	1:C:806:LEU:H	1.69	0.57
1:B:898:PHE:HZ	1:B:1050:MET:HE1	1.69	0.57
1:A:109:THR:H	1:A:237:ARG:HD3	1.68	0.57
1:B:778:THR:HG22	1:B:865:LEU:HD12	1.86	0.57
1:C:48:LEU:HD13	1:C:305:SER:HA	1.86	0.57
1:A:712:ILE:HD13	1:A:1094:VAL:HG11	1.85	0.57
1:C:578:ASP:CG	1:C:581:THR:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.28	0.57
1:C:336:CYS:HB2	1:C:338:PHE:CE2	2.39	0.57
1:A:1031:GLU:OE2	1:B:1039:ARG:NE	2.34	0.57
1:B:328:ARG:HD3	1:B:579:PRO:HD2	1.87	0.57
1:A:32:PHE:HD2	1:A:218:GLN:HB3	1.69	0.56
1:B:117:LEU:HD12	1:B:118:LEU:N	2.20	0.56
1:A:317:ASN:ND2	1:C:737:ASP:OD2	2.38	0.56
1:A:853:GLN:HG2	1:A:858:LEU:HD23	1.87	0.56
1:A:986:PRO:O	1:A:987:PRO:C	2.48	0.56
1:A:989:ALA:O	1:A:992:GLN:N	2.38	0.56
1:B:118:LEU:HD21	1:B:120:VAL:HG12	1.87	0.56
1:B:220:PHE:HE2	1:B:285:ILE:HG22	1.71	0.56
1:B:666:ILE:HG12	1:B:671:CYS:HA	1.88	0.56
1:C:115:GLN:HE21	1:C:233:ILE:HB	1.71	0.56
1:B:178:ASP:OD1	1:B:178:ASP:N	2.37	0.56
1:B:988:GLU:O	1:B:989:ALA:C	2.48	0.56
1:B:1098:ASN:CG	1:B:1101:HIS:H	2.14	0.56
1:C:39:PRO:HG2	1:C:51:THR:HG21	1.87	0.56
1:A:375:PHE:HE2	1:A:407:VAL:HG11	1.69	0.56
1:B:596:SER:HB2	1:B:611:LEU:HD22	1.88	0.56
1:C:393:THR:HA	1:C:522:ALA:HA	1.86	0.56
1:B:638:THR:HG23	1:B:640:SER:H	1.69	0.56
1:C:131:CYS:HB3	1:C:133:PHE:CZ	2.41	0.55
1:C:1144:GLU:N	1:C:1144:GLU:OE2	2.38	0.55
1:C:453:TYR:CD1	1:C:495:TYR:HD1	2.24	0.55
1:C:736:VAL:HG22	1:C:858:LEU:HD22	1.87	0.55
1:B:104:TRP:CD1	1:B:240:THR:HG23	2.41	0.55
1:A:739:THR:OG1	1:A:740:MET:N	2.40	0.55
1:C:975:SER:O	1:C:975:SER:OG	2.25	0.55
1:A:40:ASP:OD1	1:A:42:VAL:N	2.34	0.55
1:A:119:ILE:HD12	1:A:128:ILE:HD12	1.89	0.55
1:C:102:ARG:HH12	1:C:176:LEU:HD12	1.72	0.55
1:A:121:ASN:HD21	1:A:175:PHE:HB2	1.72	0.55
1:B:215:ASP:HB2	1:B:266:TYR:HE2	1.71	0.55
1:B:103:GLY:HA3	1:B:120:VAL:HA	1.89	0.55
1:C:965:GLN:O	1:C:968:SER:OG	2.22	0.55
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.72	0.54
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.31	0.54
1:B:599:THR:HB	1:B:608:VAL:HG12	1.88	0.54
1:C:418:ILE:H	1:C:418:ILE:HD12	1.72	0.54
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:904:TYR:CE1	1:C:1107:ARG:HG2	2.40	0.54
1:B:976:VAL:HB	1:B:979:ASP:HB3	1.88	0.54
1:B:986:PRO:O	1:B:987:PRO:C	2.50	0.54
1:A:1002:GLN:HG2	1:C:759:PHE:HZ	1.73	0.54
1:B:200:TYR:HA	1:B:230:PRO:HA	1.88	0.54
1:B:1098:ASN:OD1	1:B:1101:HIS:N	2.37	0.54
1:A:904:TYR:CE2	1:B:1107:ARG:HG2	2.43	0.54
1:C:309:GLU:HG2	1:C:313:TYR:OH	2.07	0.54
1:B:338:PHE:HE2	1:B:358:ILE:HD13	1.73	0.54
1:B:894:LEU:HD13	1:C:715:PRO:HD3	1.90	0.54
1:C:720:ILE:HD12	1:C:923:ILE:HD11	1.90	0.54
1:A:44:ARG:HB3	1:A:47:VAL:HG11	1.89	0.54
1:A:121:ASN:ND2	1:A:175:PHE:HB2	2.23	0.54
1:A:342:PHE:CZ	1:A:368:LEU:HD13	2.43	0.54
1:A:843:ASP:O	1:A:845:ALA:N	2.40	0.54
1:B:323:THR:OG1	1:B:324:GLU:N	2.41	0.54
1:B:843:ASP:O	1:B:845:ALA:N	2.41	0.54
1:B:318:PHE:HZ	1:B:615:VAL:HG21	1.73	0.54
1:C:752:LEU:HD12	1:C:993:ILE:HG21	1.90	0.53
1:A:618:THR:OG1	1:A:619:GLU:OE1	2.26	0.53
1:A:900:MET:HE1	1:B:1077:THR:HG21	1.91	0.53
1:B:310:LYS:HG3	1:B:664:ILE:HD11	1.89	0.53
1:C:178:ASP:N	1:C:178:ASP:OD1	2.39	0.53
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.72	0.53
1:C:439:ASN:O	1:C:443:SER:OG	2.24	0.53
1:C:898:PHE:CZ	1:C:1050:MET:HE1	2.43	0.53
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.91	0.53
1:A:303:LEU:HD11	1:A:308:VAL:HG22	1.90	0.53
1:A:353:TRP:CD1	1:A:353:TRP:H	2.26	0.53
1:A:638:THR:N	1:A:641:ASN:OD1	2.41	0.53
1:B:130:VAL:HG21	1:B:231:ILE:HD12	1.91	0.53
1:B:457:ARG:HD3	1:B:458:LYS:N	2.23	0.53
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.42	0.53
1:A:629:LEU:HG	1:A:631:PRO:HD2	1.91	0.53
1:B:837:TYR:OH	1:C:589:PRO:O	2.25	0.53
1:C:117:LEU:HD12	1:C:118:LEU:N	2.24	0.53
1:A:178:ASP:N	1:A:178:ASP:OD1	2.40	0.53
1:A:321:GLN:NE2	1:A:630:THR:OG1	2.42	0.53
1:B:43:PHE:HD2	1:C:557:LYS:HD3	1.72	0.53
1:C:353:TRP:CD1	1:C:353:TRP:H	2.27	0.53
1:A:976:VAL:HB	1:A:979:ASP:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.91	0.53
1:B:189:LEU:C	1:B:190:ARG:HG2	2.34	0.53
1:B:290:ASP:OD1	1:B:291:CYS:N	2.40	0.53
1:B:404:GLY:HA2	1:B:508:TYR:HD2	1.74	0.53
1:C:403:LYS:HG2	1:C:505:HIS:HA	1.90	0.53
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.91	0.52
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.36	0.52
1:A:902:MET:HE1	1:A:1049:LEU:HD13	1.90	0.52
1:A:1077:THR:OG1	1:C:900:MET:HE1	2.08	0.52
1:C:389:ASP:OD1	1:C:389:ASP:N	2.41	0.52
1:B:210:ILE:CG2	1:B:212:ILE:N	2.20	0.52
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.91	0.52
1:A:410:ILE:HG13	1:A:410:ILE:O	2.08	0.52
1:B:210:ILE:HG22	1:B:212:ILE:HG12	1.91	0.52
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.92	0.52
1:C:570:VAL:O	1:C:570:VAL:HG23	2.08	0.52
1:C:843:ASP:O	1:C:845:ALA:N	2.41	0.52
1:A:830:ASP:HB3	1:A:850:ILE:HD12	1.90	0.52
1:B:65:PHE:HD2	1:B:265:TYR:CD1	2.27	0.52
1:B:210:ILE:CG2	1:B:212:ILE:CG1	2.87	0.52
1:B:319:ARG:O	1:B:630:THR:OG1	2.21	0.52
1:C:752:LEU:HD12	1:C:993:ILE:CG2	2.40	0.52
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.91	0.52
1:C:581:THR:C	1:C:583:GLU:H	2.16	0.52
1:C:858:LEU:HD12	1:C:963:VAL:HG12	1.91	0.52
1:C:993:ILE:O	1:C:997:ILE:HG12	2.10	0.52
1:B:453:TYR:HB3	1:B:495:TYR:CE1	2.43	0.52
1:C:722:VAL:HG12	1:C:934:ILE:HD12	1.90	0.52
1:A:350:VAL:HG11	1:A:418:ILE:HD12	1.91	0.52
1:B:847:ARG:NE	1:C:574:ASP:OD1	2.43	0.52
1:A:37:TYR:HB3	1:A:223:LEU:HB3	1.92	0.51
1:A:667:GLY:HA2	1:C:864:LEU:HA	1.91	0.51
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.92	0.51
1:C:595:VAL:HG21	1:C:633:TRP:HZ2	1.75	0.51
1:B:578:ASP:OD2	1:B:581:THR:N	2.42	0.51
1:B:898:PHE:CZ	1:B:1050:MET:HE1	2.44	0.51
1:C:880:GLY:O	1:C:884:SER:OG	2.23	0.51
1:B:337:PRO:HD2	1:B:358:ILE:HG23	1.92	0.51
1:B:962:LEU:HD22	1:B:1007:TYR:CG	2.46	0.51
1:C:912:THR:O	1:C:915:VAL:HG12	2.10	0.51
1:C:1075:PHE:O	1:C:1076:THR:OG1	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:LEU:HD21	1:B:613:GLN:HG3	1.93	0.51
1:A:599:THR:HB	1:A:608:VAL:HG12	1.92	0.51
1:A:765:ARG:NE	1:B:957:GLN:OE1	2.44	0.51
1:B:133:PHE:HB3	1:B:160:TYR:HB2	1.93	0.51
1:B:557:LYS:HB2	1:B:584:ILE:HD13	1.93	0.51
1:B:1075:PHE:O	1:B:1076:THR:OG1	2.21	0.51
1:C:303:LEU:HD11	1:C:308:VAL:HG13	1.93	0.51
1:A:208:THR:O	1:A:209:PRO:C	2.53	0.51
1:A:589:PRO:HB3	1:C:855:PHE:HA	1.93	0.51
1:B:210:ILE:CG2	1:B:212:ILE:HG13	2.39	0.51
1:B:399:SER:HB3	1:B:511:VAL:HG22	1.93	0.51
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.46	0.50
1:A:931:ILE:O	1:A:934:ILE:HG22	2.11	0.50
1:B:105:ILE:HG22	1:B:239:GLN:OE1	2.12	0.50
1:B:406:GLU:N	1:B:406:GLU:OE1	2.43	0.50
1:B:1005:GLN:NE2	1:C:1006:THR:OG1	2.44	0.50
1:A:231:ILE:CG2	1:A:233:ILE:HG22	2.41	0.50
1:A:303:LEU:O	1:A:304:LYS:C	2.54	0.50
1:A:373:PRO:HD2	1:A:436:TRP:CD1	2.46	0.50
1:A:578:ASP:OD2	1:A:581:THR:HG23	2.10	0.50
1:A:973:ILE:HG21	1:A:983:ARG:HH22	1.76	0.50
1:B:725:GLU:HG3	1:B:1064:HIS:CD2	2.46	0.50
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.52	0.50
1:C:276:LEU:CD1	1:C:304:LYS:HA	2.42	0.50
1:C:329:PHE:HE1	1:C:545:GLY:H	1.58	0.50
1:C:543:PHE:O	1:C:544:ASN:C	2.53	0.50
1:A:736:VAL:HG23	1:A:858:LEU:HD12	1.93	0.50
1:B:177:MET:H	1:B:207:HIS:CE1	2.30	0.50
1:B:307:THR:HA	1:B:602:THR:HG21	1.94	0.50
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.43	0.50
1:A:104:TRP:CD1	1:A:240:THR:HG23	2.46	0.50
1:A:133:PHE:HE1	1:A:135:PHE:HA	1.76	0.50
1:B:160:TYR:HE1	1:B:163:ALA:HB2	1.76	0.50
1:B:459:SER:OG	1:B:460:LYS:N	2.45	0.50
1:B:931:ILE:O	1:B:934:ILE:HG22	2.12	0.50
1:C:113:LYS:HD2	1:C:113:LYS:O	2.12	0.50
1:C:675:GLN:HG3	1:C:693:ILE:HD11	1.94	0.50
1:A:1075:PHE:HB3	1:A:1097:SER:O	2.12	0.50
1:B:629:LEU:HG	1:B:631:PRO:HD2	1.94	0.50
1:C:392:PHE:CD1	1:C:524:VAL:HG23	2.46	0.50
1:C:403:LYS:HB3	1:C:406:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ASP:O	1:C:580:GLN:N	2.44	0.50
1:A:1098:ASN:OD1	1:A:1099:GLY:N	2.45	0.50
1:B:353:TRP:H	1:B:353:TRP:CD1	2.29	0.50
1:B:598:ILE:HG21	1:B:666:ILE:HD12	1.94	0.50
1:C:30:ASN:HD21	1:C:59:PHE:HD1	1.60	0.50
1:C:200:TYR:CD1	1:C:230:PRO:HB3	2.45	0.50
1:A:840:CYS:HB2	1:B:588:THR:HG23	1.93	0.49
1:A:847:ARG:HH21	1:B:572:THR:HB	1.77	0.49
1:B:106:PHE:HB3	1:B:235:ILE:HG23	1.94	0.49
1:C:276:LEU:HD11	1:C:304:LYS:HA	1.93	0.49
1:C:758:SER:HB2	1:C:761:THR:HB	1.94	0.49
1:C:898:PHE:HZ	1:C:1050:MET:HE1	1.76	0.49
1:A:1012:LEU:HD12	1:B:1013:ILE:HG21	1.94	0.49
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.93	0.49
1:B:736:VAL:HG12	1:B:858:LEU:HG	1.94	0.49
1:B:900:MET:HE1	1:C:1077:THR:OG1	2.12	0.49
1:C:295:PRO:HG3	1:C:633:TRP:CD1	2.48	0.49
1:C:930:ALA:HA	1:C:933:LYS:HG2	1.94	0.49
1:A:659:SER:HB3	1:A:698:SER:HB2	1.94	0.49
1:A:836:GLN:O	1:A:837:TYR:C	2.56	0.49
1:B:663:ASP:HB3	1:B:673:SER:HB2	1.95	0.49
1:B:1012:LEU:HB3	1:C:1013:ILE:HD13	1.95	0.49
1:C:199:GLY:O	1:C:200:TYR:C	2.55	0.49
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.76	0.49
1:A:439:ASN:O	1:A:443:SER:OG	2.25	0.49
1:A:1098:ASN:CG	1:A:1101:HIS:H	2.20	0.49
1:B:210:ILE:O	1:B:212:ILE:C	2.54	0.49
1:B:347:PHE:HD2	1:B:399:SER:HB2	1.78	0.49
1:B:902:MET:CE	1:B:1050:MET:HE2	2.42	0.49
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.12	0.49
1:C:1098:ASN:CG	1:C:1101:HIS:H	2.19	0.49
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.94	0.49
1:A:770:ILE:HD11	1:A:1012:LEU:HD13	1.95	0.49
1:B:299:THR:O	1:B:300:LYS:C	2.56	0.49
1:B:560:LEU:HD12	1:B:560:LEU:H	1.78	0.49
1:A:720:ILE:HG13	1:A:923:ILE:HG13	1.94	0.49
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	1.93	0.49
1:B:325:SER:HB2	1:B:540:ASN:HB2	1.95	0.49
1:B:624:ILE:HG23	1:B:634:ARG:HD2	1.95	0.49
1:C:497:PHE:HA	1:C:501:TYR:HE2	1.78	0.49
1:C:749:CYS:SG	1:C:997:ILE:HD11	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ARG:HB3	1:C:47:VAL:CG1	2.41	0.48
1:C:81:ASN:ND2	1:C:240:THR:O	2.25	0.48
1:C:364:ASP:OD1	1:C:364:ASP:N	2.43	0.48
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.94	0.48
1:C:580:GLN:HG2	3:C:1310:NAG:H2	1.95	0.48
1:C:927:PHE:HZ	1:C:1052:PHE:HE2	1.61	0.48
1:C:946:GLY:O	1:C:950:ASP:HB2	2.12	0.48
1:A:34:ARG:O	1:A:56:LEU:HD23	2.12	0.48
1:A:231:ILE:HG22	1:A:233:ILE:HG22	1.94	0.48
1:A:989:ALA:C	1:A:991:VAL:N	2.67	0.48
1:A:328:ARG:NH1	1:A:578:ASP:OD1	2.46	0.48
1:B:175:PHE:O	1:B:207:HIS:CE1	2.67	0.48
1:C:588:THR:HG22	1:C:589:PRO:O	2.13	0.48
1:A:993:ILE:O	1:A:997:ILE:HG12	2.14	0.48
1:B:126:VAL:HG22	1:B:172:SER:H	1.77	0.48
1:A:280:ASN:HB2	1:A:286:THR:HG23	1.96	0.48
1:B:102:ARG:HB3	1:B:120:VAL:HG23	1.94	0.48
1:B:231:ILE:HG22	1:B:233:ILE:HG23	1.94	0.48
1:B:841:LEU:HB2	1:C:553:THR:HG21	1.96	0.48
1:B:959:LEU:O	1:B:963:VAL:HG23	2.14	0.48
1:A:320:VAL:O	1:A:590:CYS:SG	2.72	0.48
1:A:376:ALA:HB3	1:A:435:ALA:HB3	1.96	0.48
1:A:453:TYR:CD2	1:A:495:TYR:HE1	2.32	0.48
1:A:559:PHE:HB2	1:A:584:ILE:HD11	1.95	0.48
1:A:856:ASN:ND2	1:A:963:VAL:HG13	2.26	0.48
1:C:878:LEU:HD13	1:C:1053:PRO:HD2	1.96	0.48
1:A:115:GLN:NE2	1:A:165:ASN:O	2.47	0.48
1:A:393:THR:CG2	1:A:520:ALA:HB3	2.44	0.48
1:A:715:PRO:HD3	1:C:894:LEU:HD13	1.96	0.48
1:B:378:LYS:HG2	1:B:433:VAL:HG22	1.96	0.48
1:B:450:ASP:OD1	1:B:450:ASP:N	2.47	0.48
1:B:526:GLY:O	1:B:528:LYS:NZ	2.46	0.48
1:C:126:VAL:HG11	1:C:175:PHE:CE1	2.49	0.48
1:C:177:MET:H	1:C:207:HIS:CE1	2.30	0.48
1:C:902:MET:SD	1:C:1050:MET:HE2	2.53	0.48
1:C:1082:CYS:HB2	1:C:1132:ILE:HD11	1.95	0.48
1:A:43:PHE:HA	1:B:563:GLN:HE22	1.79	0.48
1:A:379:CYS:HB2	1:A:384:PRO:HD3	1.96	0.48
1:C:191:GLU:HB2	1:C:223:LEU:HD11	1.95	0.48
1:C:726:ILE:HG23	1:C:1061:VAL:HG22	1.96	0.48
1:A:234:ASN:OD1	3:A:1310:NAG:N2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:ALA:C	1:B:557:LYS:HE2	2.39	0.47
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.47	0.47
1:B:451:TYR:HB2	1:B:495:TYR:HB2	1.96	0.47
1:B:853:GLN:HG2	1:B:963:VAL:HG21	1.95	0.47
1:C:760:CYS:HA	1:C:763:LEU:HG	1.95	0.47
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.47	0.47
1:A:497:PHE:CG	1:A:507:PRO:HG3	2.49	0.47
1:B:406:GLU:HA	1:B:409:GLN:HB2	1.96	0.47
1:C:363:ALA:N	1:C:525:CYS:O	2.35	0.47
1:A:556:ASN:H	1:C:844:ILE:HG23	1.78	0.47
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.78	0.47
1:B:188:ASN:HA	1:B:209:PRO:CA	2.44	0.47
1:C:84:LEU:HB2	1:C:238:PHE:HD2	1.79	0.47
1:A:425:LEU:HD12	1:A:425:LEU:H	1.78	0.47
1:A:864:LEU:O	1:B:669:GLY:N	2.40	0.47
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.96	0.47
1:B:765:ARG:NE	1:C:957:GLN:OE1	2.47	0.47
1:B:776:LYS:HZ3	1:B:1019:ARG:HH22	1.61	0.47
1:B:975:SER:O	1:B:975:SER:OG	2.33	0.47
1:C:631:PRO:HB3	1:C:633:TRP:CH2	2.49	0.47
1:C:850:ILE:O	1:C:854:LYS:HG2	2.15	0.47
1:A:541:PHE:CZ	1:A:587:ILE:HD12	2.50	0.47
1:A:969:LYS:HE2	1:C:755:GLN:HG2	1.95	0.47
1:A:321:GLN:N	1:A:628:GLN:O	2.45	0.47
1:B:215:ASP:O	1:B:217:PRO:N	2.48	0.47
1:B:375:PHE:HD2	1:B:436:TRP:HA	1.79	0.47
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.96	0.47
1:A:42:VAL:HG11	1:B:567:ARG:HB2	1.96	0.47
1:A:265:TYR:O	1:A:266:TYR:C	2.58	0.47
1:A:715:PRO:HG3	1:A:1069:PRO:HB3	1.97	0.47
1:A:954:HIS:HB3	1:A:1014:ARG:NH1	2.29	0.47
1:A:1128:VAL:HG11	1:C:918:GLU:HG3	1.96	0.47
1:B:210:ILE:C	1:B:213:GLY:N	2.70	0.47
1:B:212:ILE:HG13	1:B:217:PRO:HB3	1.97	0.47
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.97	0.47
1:B:574:ASP:O	1:B:587:ILE:HD12	2.15	0.47
1:C:387:LEU:HD12	1:C:387:LEU:O	2.14	0.47
1:C:392:PHE:HD2	1:C:515:PHE:HB3	1.80	0.47
1:B:804:GLN:O	1:B:818:ILE:HG12	2.15	0.47
1:C:823:PHE:CD1	1:C:1057:PRO:HG3	2.50	0.47
1:A:329:PHE:HE2	1:A:528:LYS:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:C	1:B:190:ARG:CG	2.88	0.47
1:B:295:PRO:HG3	1:B:633:TRP:HD1	1.80	0.47
1:C:175:PHE:CD1	1:C:175:PHE:N	2.82	0.47
1:B:176:LEU:O	1:B:177:MET:HE2	2.15	0.46
1:B:318:PHE:HD2	1:B:629:LEU:HD11	1.81	0.46
1:B:1127:ASP:OD1	1:B:1127:ASP:N	2.47	0.46
1:C:177:MET:HB2	1:C:207:HIS:ND1	2.31	0.46
1:C:295:PRO:HG3	1:C:633:TRP:HD1	1.78	0.46
1:C:973:ILE:HG22	1:C:992:GLN:HG3	1.96	0.46
1:B:735:SER:O	1:B:735:SER:OG	2.23	0.46
1:C:103:GLY:HA3	1:C:120:VAL:HA	1.95	0.46
1:C:215:ASP:O	1:C:216:PHE:C	2.56	0.46
1:C:324:GLU:HG3	1:C:534:VAL:HG21	1.97	0.46
1:A:741:TYR:CD2	1:A:1004:LEU:HD22	2.49	0.46
1:B:358:ILE:HD12	1:B:395:VAL:HG12	1.97	0.46
1:B:420:ASP:O	1:B:461:LEU:N	2.48	0.46
1:B:588:THR:O	1:B:589:PRO:C	2.59	0.46
1:C:25:THR:HG23	1:C:66:HIS:HB2	1.98	0.46
1:C:204:TYR:CE2	1:C:225:PRO:HG3	2.50	0.46
1:C:330:PRO:HG2	1:C:525:CYS:SG	2.55	0.46
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.82	0.46
1:A:368:LEU:HD11	1:A:434:ILE:HD13	1.97	0.46
1:A:699:LEU:HD12	1:A:699:LEU:H	1.80	0.46
1:A:699:LEU:HB3	1:C:873:TYR:CZ	2.51	0.46
1:B:25:THR:HG23	1:B:66:HIS:HB2	1.96	0.46
1:B:395:VAL:HG22	1:B:515:PHE:HD1	1.81	0.46
1:B:988:GLU:O	1:B:991:VAL:N	2.41	0.46
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.48	0.46
1:C:57:PRO:HB2	1:C:60:SER:HB3	1.97	0.46
1:A:405:ASN:OD1	1:A:405:ASN:N	2.48	0.46
1:A:560:LEU:HD13	1:A:563:GLN:HE21	1.80	0.46
1:A:612:TYR:HE2	1:A:651:ILE:HD12	1.80	0.46
1:A:983:ARG:HD2	1:A:983:ARG:O	2.14	0.46
1:B:439:ASN:O	1:B:443:SER:OG	2.25	0.46
1:B:805:ILE:HD12	1:B:878:LEU:HD11	1.96	0.46
1:C:553:THR:O	1:C:585:LEU:HA	2.15	0.46
1:B:497:PHE:CG	1:B:507:PRO:HG3	2.50	0.46
1:B:595:VAL:HG21	1:B:633:TRP:HZ2	1.80	0.46
1:B:675:GLN:HG2	1:B:693:ILE:HG12	1.96	0.46
1:C:577:ARG:HA	1:C:584:ILE:HA	1.98	0.46
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:SER:HB3	1:B:1041:ASP:HB3	1.98	0.46
1:B:804:GLN:HB3	1:B:818:ILE:HD11	1.96	0.46
1:C:134:GLN:HG3	1:C:135:PHE:H	1.81	0.46
1:C:206:LYS:HB3	1:C:223:LEU:HD13	1.97	0.46
1:A:821:LEU:HD11	1:A:935:GLN:HG3	1.96	0.46
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.16	0.46
1:C:423:TYR:OH	1:C:464:PHE:HE1	1.98	0.46
1:A:105:ILE:HG13	1:A:239:GLN:HB3	1.97	0.46
1:A:265:TYR:O	1:A:265:TYR:CG	2.69	0.46
1:A:401:VAL:HG12	1:A:509:ARG:HG3	1.97	0.46
1:B:417:ASN:HD22	1:B:455:LEU:HD23	1.80	0.46
1:B:788:ILE:HG23	1:B:876:ALA:HB2	1.97	0.46
1:B:980:ILE:HA	1:B:983:ARG:HG2	1.98	0.46
1:C:321:GLN:NE2	1:C:630:THR:OG1	2.49	0.46
1:C:575:ALA:HA	1:C:585:LEU:O	2.16	0.46
1:C:323:THR:OG1	1:C:324:GLU:N	2.49	0.45
1:A:393:THR:HA	1:A:522:ALA:HA	1.98	0.45
1:B:441:LEU:HD22	1:B:509:ARG:HH12	1.80	0.45
1:B:873:TYR:CZ	1:C:699:LEU:HB3	2.51	0.45
1:A:119:ILE:O	1:A:119:ILE:HG22	2.16	0.45
1:A:176:LEU:C	1:A:177:MET:HE2	2.42	0.45
1:A:844:ILE:O	1:B:557:LYS:HG2	2.17	0.45
1:A:858:LEU:HD21	1:A:959:LEU:CD1	2.46	0.45
1:A:886:TRP:HH2	1:A:904:TYR:HB3	1.81	0.45
1:C:106:PHE:CE2	1:C:238:PHE:HD1	2.34	0.45
1:C:278:LYS:HB2	1:C:306:PHE:CE1	2.51	0.45
1:C:528:LYS:HG2	1:C:529:LYS:N	2.32	0.45
1:C:557:LYS:HB2	1:C:584:ILE:HD13	1.97	0.45
1:B:225:PRO:HG2	1:C:562:PHE:CE2	2.52	0.45
1:B:295:PRO:HG3	1:B:633:TRP:CD1	2.52	0.45
1:C:164:ASN:C	1:C:166:CYS:H	2.24	0.45
1:C:197:ILE:O	1:C:198:ASP:C	2.60	0.45
1:C:718:PHE:HE1	1:C:919:ASN:ND2	2.14	0.45
1:A:42:VAL:CG1	1:B:567:ARG:HB2	2.46	0.45
1:A:83:VAL:HG11	1:A:237:ARG:CZ	2.47	0.45
1:A:497:PHE:CD1	1:A:507:PRO:HG3	2.51	0.45
1:B:214:ARG:O	1:B:215:ASP:CB	2.65	0.45
1:C:40:ASP:CG	1:C:41:LYS:H	2.24	0.45
1:C:763:LEU:HD13	1:C:1004:LEU:HG	1.98	0.45
1:A:420:ASP:HB3	1:A:460:LYS:HD2	1.97	0.45
1:A:1123:SER:OG	1:C:914:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PRO:O	1:B:341:VAL:HG23	2.17	0.45
1:A:422:ASN:ND2	1:A:454:ARG:O	2.29	0.45
1:A:718:PHE:HE1	1:A:919:ASN:HD21	1.63	0.45
1:A:989:ALA:O	1:A:991:VAL:N	2.50	0.45
1:B:106:PHE:HB3	1:B:235:ILE:CG2	2.47	0.45
1:B:181:GLY:H	1:B:186:PHE:HD2	1.65	0.45
1:B:190:ARG:HD3	1:B:207:HIS:ND1	2.30	0.45
1:B:208:THR:C	1:B:210:ILE:N	2.75	0.45
1:B:983:ARG:HG3	1:B:984:LEU:HD13	1.99	0.45
1:C:97:LYS:HE2	1:C:184:GLY:HA3	1.99	0.45
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.98	0.45
1:A:624:ILE:HG23	1:A:634:ARG:HD2	1.98	0.45
1:B:229:LEU:HG	1:B:231:ILE:HD11	1.99	0.45
1:B:973:ILE:HD13	1:B:973:ILE:HA	1.87	0.45
1:B:1029:MET:SD	1:B:1033:VAL:HG21	2.56	0.45
1:C:1098:ASN:OD1	1:C:1099:GLY:N	2.50	0.45
1:A:365:TYR:HD2	1:A:368:LEU:HD23	1.82	0.45
1:A:403:LYS:HB3	1:A:406:GLU:OE1	2.17	0.45
1:A:886:TRP:HZ3	1:A:901:GLN:HG3	1.81	0.45
1:B:366:SER:HA	1:B:369:TYR:HB3	1.99	0.45
1:B:858:LEU:HD22	1:B:963:VAL:HG22	1.98	0.45
1:C:48:LEU:CD1	1:C:305:SER:HA	2.46	0.45
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.52	0.45
1:C:439:ASN:OD1	1:C:507:PRO:HD2	2.16	0.45
1:C:1092:GLU:OE2	1:C:1092:GLU:N	2.49	0.45
1:A:450:ASP:OD1	1:A:450:ASP:N	2.50	0.45
1:A:900:MET:HE3	1:A:900:MET:HB2	1.57	0.45
1:B:215:ASP:OD2	1:B:216:PHE:N	2.50	0.45
1:B:878:LEU:O	1:B:882:ILE:HG23	2.17	0.45
1:C:624:ILE:HA	1:C:634:ARG:HH21	1.80	0.45
1:A:109:THR:OG1	1:A:111:ASP:OD1	2.36	0.44
1:A:568:ASP:CG	1:A:569:ILE:N	2.75	0.44
1:B:409:GLN:NE2	1:B:418:ILE:H	2.14	0.44
1:B:543:PHE:CG	1:B:576:VAL:HG11	2.52	0.44
1:B:903:ALA:HB1	1:B:913:GLN:HB3	1.99	0.44
1:B:905:ARG:CZ	1:B:1050:MET:HG2	2.47	0.44
1:C:124:THR:O	1:C:174:PRO:HD3	2.17	0.44
1:C:562:PHE:CE1	1:C:563:GLN:HG2	2.52	0.44
1:C:878:LEU:O	1:C:882:ILE:HG12	2.17	0.44
1:A:858:LEU:HD21	1:A:959:LEU:HD11	1.98	0.44
1:A:1002:GLN:HG2	1:C:759:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:THR:OG1	1:B:334:ASN:N	2.49	0.44
1:C:188:ASN:OD1	1:C:188:ASN:N	2.50	0.44
1:C:365:TYR:CD2	1:C:387:LEU:HG	2.52	0.44
1:C:947:LYS:HE3	1:C:947:LYS:HB2	1.83	0.44
1:B:214:ARG:O	1:B:215:ASP:HB3	2.17	0.44
1:B:763:LEU:HD23	1:B:1004:LEU:HG	1.98	0.44
1:B:1013:ILE:HD13	1:B:1013:ILE:HA	1.74	0.44
1:A:308:VAL:H	1:A:602:THR:CG2	2.30	0.44
1:A:546:LEU:HD13	1:A:546:LEU:HA	1.87	0.44
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.50	0.44
1:C:189:LEU:HD23	1:C:210:ILE:HG12	2.00	0.44
1:B:360:ASN:O	1:B:360:ASN:ND2	2.50	0.44
1:B:383:SER:HB3	1:B:386:LYS:HB2	1.99	0.44
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.82	0.44
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.80	0.44
1:C:159:VAL:HG12	1:C:159:VAL:O	2.17	0.44
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.99	0.44
1:A:402:ILE:HG12	1:A:406:GLU:HB2	1.99	0.44
1:A:988:GLU:HG3	1:A:992:GLN:HE21	1.83	0.44
1:B:363:ALA:O	1:B:527:PRO:HD3	2.18	0.44
1:C:33:THR:HG23	1:C:58:PHE:CZ	2.52	0.44
1:C:129:LYS:HE2	1:C:169:GLU:HG3	1.99	0.44
1:C:337:PRO:O	1:C:340:GLU:N	2.50	0.44
1:A:386:LYS:HB2	1:A:386:LYS:HE3	1.93	0.44
1:B:557:LYS:HB2	1:B:584:ILE:HG21	1.99	0.44
1:B:844:ILE:HG23	1:C:556:ASN:HB2	1.99	0.44
1:C:301:CYS:O	1:C:302:THR:C	2.60	0.44
1:A:103:GLY:HA3	1:A:120:VAL:HA	2.00	0.44
1:A:338:PHE:HB3	1:A:342:PHE:CE2	2.53	0.44
1:A:456:PHE:HB2	1:A:491:PRO:HA	2.00	0.44
1:A:707:TYR:HB2	1:C:883:THR:HB	1.98	0.44
1:A:897:PRO:HA	1:B:707:TYR:CE1	2.53	0.44
1:B:215:ASP:O	1:B:216:PHE:C	2.60	0.44
1:B:309:GLU:O	1:B:310:LYS:C	2.61	0.44
1:B:471:GLU:N	1:B:491:PRO:HG3	2.33	0.44
1:B:966:LEU:HG	1:B:1000:ARG:NH2	2.33	0.44
1:A:295:PRO:HG3	1:A:633:TRP:CD1	2.52	0.44
1:A:350:VAL:HG22	1:A:422:ASN:HB3	2.00	0.44
1:A:559:PHE:HB3	1:A:577:ARG:NH2	2.33	0.44
1:A:647:ALA:HA	1:C:862:PRO:HG3	1.99	0.44
1:B:57:PRO:HB2	1:B:60:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:VAL:HG11	1:B:216:PHE:HE2	1.83	0.44
1:C:164:ASN:O	1:C:166:CYS:N	2.46	0.44
1:C:176:LEU:HD22	1:C:190:ARG:HD2	1.98	0.44
1:C:724:THR:HB	1:C:934:ILE:HD11	1.99	0.44
1:A:133:PHE:HB2	1:A:160:TYR:HB2	1.99	0.43
1:A:553:THR:HG21	1:C:841:LEU:HB2	2.00	0.43
1:B:746:SER:HB3	1:B:748:GLU:OE1	2.17	0.43
1:B:775:ASP:OD1	1:B:864:LEU:HB3	2.18	0.43
1:C:411:ALA:C	1:C:425:LEU:HD12	2.43	0.43
1:C:627:ASP:HA	1:C:634:ARG:HH22	1.83	0.43
1:A:1094:VAL:HG23	1:A:1107:ARG:HD2	1.99	0.43
1:B:131:CYS:HB3	1:B:133:PHE:CE2	2.53	0.43
1:B:529:LYS:HB2	1:B:529:LYS:HE2	1.75	0.43
1:B:776:LYS:NZ	1:B:1019:ARG:HH22	2.16	0.43
1:C:97:LYS:O	1:C:97:LYS:NZ	2.52	0.43
1:C:106:PHE:HD1	1:C:235:ILE:HD13	1.83	0.43
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.53	0.43
1:A:204:TYR:CE2	1:A:225:PRO:HG3	2.53	0.43
1:A:560:LEU:HB2	1:A:563:GLN:HG2	2.00	0.43
1:A:941:THR:HG21	1:A:944:ALA:HB2	1.99	0.43
1:B:471:GLU:H	1:B:491:PRO:HG3	1.83	0.43
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.73	0.43
1:A:1039:ARG:H	1:A:1039:ARG:HG2	1.57	0.43
1:C:780:GLU:O	1:C:784:GLN:NE2	2.49	0.43
1:A:1090:PRO:HG3	1:A:1095:PHE:CD1	2.53	0.43
1:B:360:ASN:H	1:B:523:THR:CG2	2.32	0.43
1:C:164:ASN:C	1:C:166:CYS:N	2.76	0.43
1:C:560:LEU:H	1:C:563:GLN:HG3	1.83	0.43
1:A:347:PHE:HB2	1:A:401:VAL:HG13	2.01	0.43
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.58	0.43
1:B:877:LEU:HA	1:B:877:LEU:HD23	1.77	0.43
1:C:103:GLY:C	1:C:241:LEU:HG	2.43	0.43
1:C:188:ASN:HB3	1:C:209:PRO:HG3	2.00	0.43
1:C:885:GLY:HA2	1:C:901:GLN:CD	2.43	0.43
1:A:115:GLN:OE1	1:A:130:VAL:HG12	2.18	0.43
1:A:436:TRP:HZ3	1:A:511:VAL:HG12	1.83	0.43
1:A:703:ASN:OD1	1:A:704:SER:N	2.50	0.43
1:C:401:VAL:HG21	1:C:451:TYR:CE2	2.54	0.43
1:A:357:ARG:HB2	1:A:357:ARG:CZ	2.47	0.43
1:A:364:ASP:O	1:A:367:VAL:HG22	2.18	0.43
1:A:454:ARG:HG2	1:A:492:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:CYS:HB2	1:B:588:THR:CG2	2.47	0.43
1:A:988:GLU:O	1:A:990:GLU:N	2.52	0.43
1:B:902:MET:HE2	1:B:902:MET:HA	2.01	0.43
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.34	0.43
1:C:328:ARG:HD2	1:C:579:PRO:CG	2.46	0.43
1:C:450:ASP:OD1	1:C:450:ASP:N	2.50	0.43
1:C:908:GLY:HA3	1:C:1036:GLN:HE22	1.84	0.43
1:A:555:SER:HB2	1:A:586:ASP:OD1	2.19	0.43
1:B:993:ILE:O	1:B:997:ILE:HG12	2.19	0.43
1:C:574:ASP:O	1:C:587:ILE:N	2.52	0.43
1:C:858:LEU:HD13	1:C:962:LEU:HD13	2.00	0.43
1:A:459:SER:OG	1:A:460:LYS:N	2.51	0.43
1:A:983:ARG:HH21	1:A:984:LEU:HD11	1.84	0.43
1:A:1129:VAL:HG13	1:C:917:TYR:HB3	2.01	0.43
1:B:986:PRO:HB2	1:B:987:PRO:HD3	2.01	0.43
1:C:328:ARG:HD3	1:C:579:PRO:HB2	2.01	0.43
1:C:391:CYS:HB3	1:C:522:ALA:CB	2.49	0.43
1:C:1029:MET:O	1:C:1033:VAL:HB	2.19	0.43
1:A:180:GLU:HA	1:A:186:PHE:HD2	1.84	0.42
1:A:775:ASP:OD1	1:A:864:LEU:HB3	2.19	0.42
1:A:822:LEU:HD22	1:A:945:LEU:HD21	2.01	0.42
1:B:34:ARG:CZ	1:B:217:PRO:HD2	2.48	0.42
1:B:377:PHE:O	1:B:377:PHE:CG	2.73	0.42
1:B:904:TYR:OH	1:C:1094:VAL:HG23	2.19	0.42
1:B:1098:ASN:OD1	1:B:1099:GLY:N	2.52	0.42
1:C:131:CYS:HB2	1:C:166:CYS:HB3	1.92	0.42
1:C:209:PRO:O	1:C:210:ILE:C	2.61	0.42
1:C:214:ARG:O	1:C:217:PRO:HG3	2.19	0.42
1:C:802:PHE:O	1:C:804:GLN:N	2.52	0.42
1:A:318:PHE:HZ	1:A:615:VAL:HG21	1.84	0.42
1:A:641:ASN:O	1:A:642:VAL:HG23	2.19	0.42
1:A:669:GLY:N	1:C:864:LEU:O	2.41	0.42
1:B:37:TYR:OH	1:B:54:LEU:O	2.28	0.42
1:B:105:ILE:HG13	1:B:117:LEU:O	2.19	0.42
1:B:880:GLY:O	1:B:884:SER:OG	2.27	0.42
1:B:976:VAL:O	1:B:980:ILE:HG23	2.19	0.42
1:A:125:ASN:HD22	1:A:171:VAL:HG13	1.84	0.42
1:A:730:SER:O	1:A:1058:HIS:HB3	2.19	0.42
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.53	0.42
1:A:1086:LYS:HE3	1:A:1086:LYS:HB2	1.89	0.42
1:A:1139:ASP:OD1	1:A:1142:GLN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:HG	1:B:190:ARG:H	1.85	0.42
1:B:334:ASN:CG	1:B:361:CYS:HA	2.44	0.42
1:C:62:VAL:HG11	1:C:216:PHE:CZ	2.53	0.42
1:C:378:LYS:O	1:C:433:VAL:HG12	2.19	0.42
1:A:163:ALA:HA	1:A:166:CYS:SG	2.60	0.42
1:A:369:TYR:HA	1:A:374:PHE:CE2	2.54	0.42
1:B:350:VAL:HG22	1:B:422:ASN:HB3	2.01	0.42
1:B:624:ILE:HD13	1:B:624:ILE:HA	1.87	0.42
1:C:364:ASP:O	1:C:367:VAL:HG12	2.20	0.42
1:C:714:ILE:HD12	1:C:1096:VAL:HG21	2.02	0.42
1:A:762:GLN:HA	1:A:765:ARG:NH1	2.35	0.42
1:A:1075:PHE:C	1:A:1076:THR:HG1	2.18	0.42
1:B:165:ASN:O	1:B:166:CYS:SG	2.78	0.42
1:B:426:PRO:HG3	1:B:464:PHE:CE2	2.54	0.42
1:B:731:MET:HG2	1:B:774:GLN:OE1	2.18	0.42
1:C:320:VAL:HG22	1:C:629:LEU:HD12	2.02	0.42
1:A:328:ARG:NH2	1:A:578:ASP:OD2	2.53	0.42
1:A:409:GLN:HG2	1:A:419:ALA:HB2	2.00	0.42
1:A:866:THR:O	1:A:869:MET:HG2	2.20	0.42
1:A:959:LEU:HD12	1:A:959:LEU:HA	1.74	0.42
1:C:34:ARG:NH2	1:C:219:GLY:O	2.52	0.42
1:A:904:TYR:HE2	1:B:1107:ARG:HG2	1.85	0.42
1:A:1073:LYS:HE2	1:A:1075:PHE:CZ	2.54	0.42
1:B:210:ILE:CG2	1:B:212:ILE:HG12	2.50	0.42
1:C:189:LEU:HD12	1:C:189:LEU:O	2.20	0.42
1:A:40:ASP:OD1	1:A:40:ASP:C	2.62	0.42
1:A:196:ASN:CG	1:A:235:ILE:HD12	2.44	0.42
1:B:41:LYS:HG2	1:C:562:PHE:CD2	2.55	0.42
1:B:176:LEU:HA	1:B:207:HIS:HE1	1.83	0.42
1:C:378:LYS:HA	1:C:378:LYS:HE2	2.02	0.42
1:A:1076:THR:HB	1:A:1097:SER:HB3	2.02	0.42
1:B:62:VAL:HG11	1:B:216:PHE:CE2	2.55	0.42
1:B:301:CYS:O	1:B:302:THR:C	2.62	0.42
1:B:401:VAL:HG21	1:B:451:TYR:CZ	2.54	0.42
1:B:748:GLU:OE1	1:B:749:CYS:N	2.51	0.42
1:C:580:GLN:HG2	3:C:1310:NAG:H4	2.02	0.42
1:A:403:LYS:H	1:A:495:TYR:HE2	1.68	0.42
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.81	0.42
1:A:461:LEU:HD21	1:A:467:ASP:HB2	2.01	0.42
1:B:160:TYR:CE1	1:B:163:ALA:HB2	2.54	0.42
1:B:218:GLN:OE1	1:B:218:GLN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ALA:HB3	1:B:435:ALA:HB3	2.02	0.42
1:C:502:GLY:O	1:C:506:GLN:HG2	2.20	0.42
1:A:43:PHE:N	1:B:563:GLN:OE1	2.53	0.41
1:A:660:TYR:C	1:A:698:SER:HB3	2.45	0.41
1:B:930:ALA:HA	1:B:933:LYS:HG2	2.01	0.41
1:C:403:LYS:N	1:C:495:TYR:OH	2.51	0.41
1:A:42:VAL:HG11	1:B:567:ARG:HD2	2.02	0.41
1:A:562:PHE:HD1	1:A:562:PHE:H	1.66	0.41
1:A:598:ILE:N	1:A:609:ALA:O	2.45	0.41
1:B:208:THR:HB	1:B:210:ILE:HG12	1.98	0.41
1:B:338:PHE:CE2	1:B:358:ILE:HD13	2.53	0.41
1:B:736:VAL:HG21	1:B:1004:LEU:HD11	2.02	0.41
1:B:886:TRP:CH2	1:B:904:TYR:HB3	2.55	0.41
1:C:194:PHE:HB3	1:C:201:PHE:CZ	2.55	0.41
1:C:1075:PHE:HB3	1:C:1097:SER:O	2.21	0.41
1:C:1098:ASN:OD1	1:C:1101:HIS:N	2.35	0.41
1:A:775:ASP:OD2	1:A:864:LEU:HD23	2.20	0.41
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.55	0.41
1:B:108:THR:HG21	3:B:1304:NAG:H62	2.01	0.41
1:B:325:SER:CB	1:B:540:ASN:HB2	2.51	0.41
1:B:630:THR:HB	1:B:631:PRO:HD3	2.02	0.41
1:B:806:LEU:HD23	1:B:806:LEU:HA	1.83	0.41
1:B:831:ALA:HB3	1:B:834:ILE:HG23	2.01	0.41
1:C:878:LEU:HA	1:C:878:LEU:HD12	1.75	0.41
1:A:1029:MET:HE2	1:A:1029:MET:HB2	1.90	0.41
1:A:1115:ILE:HG23	1:A:1137:VAL:HA	2.03	0.41
1:B:722:VAL:HG12	1:B:934:ILE:HD12	2.03	0.41
1:B:773:GLU:OE1	1:B:1019:ARG:HB2	2.19	0.41
1:B:900:MET:HE3	1:C:1079:PRO:HD3	2.02	0.41
1:C:105:ILE:C	1:C:106:PHE:HD2	2.28	0.41
1:A:93:ALA:HA	1:A:190:ARG:O	2.20	0.41
1:A:836:GLN:NE2	1:A:851:CYS:SG	2.94	0.41
1:A:106:PHE:HB2	1:A:117:LEU:HB3	2.03	0.41
1:B:566:GLY:N	1:B:575:ALA:O	2.54	0.41
1:B:1048:HIS:HE2	1:B:1050:MET:C	2.28	0.41
1:C:588:THR:HG23	1:C:589:PRO:HD2	2.03	0.41
1:B:26:GLN:HA	1:B:65:PHE:HD1	1.86	0.41
1:B:37:TYR:OH	1:B:53:ASP:OD1	2.39	0.41
1:B:218:GLN:O	1:B:219:GLY:C	2.61	0.41
1:C:99:ASN:HD21	1:C:102:ARG:HH11	1.68	0.41
1:C:564:GLN:OE1	1:C:577:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ASP:HB2	1:C:583:GLU:HG2	2.03	0.41
1:C:629:LEU:HD23	1:C:631:PRO:HG2	2.03	0.41
1:C:974:SER:OG	1:C:975:SER:N	2.53	0.41
1:A:37:TYR:HA	1:A:223:LEU:HB3	2.01	0.41
1:A:131:CYS:HB2	1:A:166:CYS:HB3	1.90	0.41
1:A:348:ALA:O	1:A:400:PHE:HA	2.21	0.41
1:A:355:ARG:H	2:D:1:NAG:H82	1.86	0.41
1:B:992:GLN:H	1:B:992:GLN:HG2	1.73	0.41
1:C:409:GLN:NE2	1:C:416:GLY:HA3	2.36	0.41
1:A:46:SER:O	1:A:46:SER:OG	2.35	0.41
1:A:84:LEU:HD13	1:A:84:LEU:HA	1.91	0.41
1:A:403:LYS:HE3	1:A:495:TYR:CE2	2.56	0.41
1:A:557:LYS:HG3	1:C:844:ILE:O	2.21	0.41
1:B:417:ASN:ND2	1:B:455:LEU:HD23	2.36	0.41
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.93	0.41
1:B:528:LYS:HE3	1:B:528:LYS:HB3	1.97	0.41
1:B:589:PRO:O	1:B:590:CYS:C	2.62	0.41
1:B:725:GLU:HG3	1:B:1064:HIS:HD2	1.85	0.41
1:B:833:PHE:O	1:C:646:ARG:NE	2.52	0.41
1:C:231:ILE:HG22	1:C:233:ILE:HG23	2.03	0.41
1:C:534:VAL:HG23	1:C:539:VAL:HG21	2.02	0.41
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.54	0.41
1:C:961:THR:O	1:C:965:GLN:HG2	2.21	0.41
1:C:984:LEU:HB3	1:C:989:ALA:HB2	2.02	0.41
1:C:1029:MET:HE2	1:C:1053:PRO:HB3	2.02	0.41
1:C:1083:HIS:CG	1:C:1137:VAL:HG22	2.56	0.41
1:A:424:LYS:HE3	1:A:424:LYS:HB2	1.94	0.41
1:A:717:ASN:C	1:A:1070:ALA:HB3	2.46	0.41
1:A:1089:PHE:O	1:A:1120:THR:OG1	2.27	0.41
3:A:1304:NAG:HO3	3:A:1304:NAG:HO6	1.61	0.41
1:B:188:ASN:HA	1:B:209:PRO:HA	2.02	0.41
1:B:855:PHE:HA	1:C:589:PRO:HG3	2.02	0.41
1:C:120:VAL:HG13	1:C:127:PHE:HB3	2.02	0.41
1:C:631:PRO:HB3	1:C:633:TRP:CZ3	2.56	0.41
1:C:878:LEU:HD11	1:C:1052:PHE:HB3	2.02	0.41
1:A:106:PHE:CD1	1:A:117:LEU:HD23	2.56	0.40
1:A:334:ASN:O	1:A:362:VAL:N	2.42	0.40
1:A:543:PHE:HB3	1:A:576:VAL:HG11	2.03	0.40
1:A:1096:VAL:O	1:A:1103:PHE:N	2.47	0.40
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.95	0.40
1:C:437:ASN:OD1	1:C:439:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.86	0.40
1:A:187:LYS:H	1:A:210:ILE:HB	1.85	0.40
1:A:404:GLY:HA2	1:A:508:TYR:HD2	1.86	0.40
1:A:922:LEU:HD21	2:H:1:NAG:H5	2.03	0.40
1:B:43:PHE:O	1:B:44:ARG:HD2	2.21	0.40
1:B:90:VAL:N	1:B:270:LEU:HD12	2.36	0.40
1:B:546:LEU:HD11	1:B:573:THR:HG21	2.03	0.40
1:B:631:PRO:HB3	1:B:633:TRP:CZ3	2.56	0.40
1:C:25:THR:O	1:C:65:PHE:HA	2.21	0.40
1:C:216:PHE:O	1:C:217:PRO:C	2.64	0.40
1:C:657:ASN:HB3	3:C:1305:NAG:O5	2.21	0.40
1:A:403:LYS:HG2	1:A:504:GLY:O	2.21	0.40
1:A:453:TYR:CG	1:A:495:TYR:CE1	3.09	0.40
1:A:638:THR:HG22	1:A:641:ASN:CG	2.47	0.40
1:A:947:LYS:HB2	1:A:947:LYS:HE2	1.75	0.40
1:B:543:PHE:HB3	1:B:576:VAL:HG11	2.04	0.40
1:B:765:ARG:HH22	1:C:961:THR:HG21	1.86	0.40
1:B:885:GLY:HA2	1:B:901:GLN:CD	2.46	0.40
1:B:1086:LYS:HB2	1:B:1086:LYS:HE3	1.85	0.40
1:B:1098:ASN:ND2	1:B:1101:HIS:H	2.19	0.40
1:C:324:GLU:HG2	1:C:539:VAL:HG22	2.04	0.40
1:C:346:ARG:HE	1:C:346:ARG:HA	1.86	0.40
1:C:365:TYR:CE2	1:C:387:LEU:HG	2.57	0.40
1:A:168:PHE:CZ	1:A:229:LEU:HD13	2.56	0.40
1:A:631:PRO:HB3	1:A:633:TRP:CH2	2.57	0.40
1:B:189:LEU:HG	1:B:190:ARG:N	2.36	0.40
1:B:490:PHE:CG	1:B:491:PRO:HD2	2.56	0.40
1:B:748:GLU:OE1	1:B:748:GLU:N	2.54	0.40
1:C:599:THR:HB	1:C:608:VAL:HG12	2.04	0.40
1:A:351:TYR:CE1	1:A:452:TRP:HB2	2.56	0.40
1:B:117:LEU:HD11	1:B:119:ILE:HG12	2.02	0.40
1:B:1114:ILE:HD13	1:B:1114:ILE:HA	1.94	0.40
1:C:134:GLN:HG2	1:C:162:SER:HB2	2.03	0.40
1:C:176:LEU:C	1:C:177:MET:HE2	2.47	0.40
1:C:1075:PHE:C	1:C:1076:THR:HG1	2.23	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	1053/1206 (87%)	953 (90%)	95 (9%)	5 (0%)	24	59
1	B	1053/1206 (87%)	955 (91%)	93 (9%)	5 (0%)	24	59
1	C	1053/1206 (87%)	955 (91%)	90 (8%)	8 (1%)	16	50
All	All	3159/3618 (87%)	2863 (91%)	278 (9%)	18 (1%)	23	55

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	987	PRO
1	A	989	ALA
1	B	215	ASP
1	B	304	LYS
1	C	164	ASN
1	C	582	LEU
1	A	217	PRO
1	B	164	ASN
1	B	210	ILE
1	C	304	LYS
1	C	544	ASN
1	C	580	GLN
1	A	304	LYS
1	C	165	ASN
1	C	579	PRO
1	A	218	GLN
1	B	534	VAL
1	C	210	ILE

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	925/1054 (88%)	912 (99%)	13 (1%)	59	70
1	B	925/1054 (88%)	910 (98%)	15 (2%)	55	69
1	C	925/1054 (88%)	900 (97%)	25 (3%)	39	60
All	All	2775/3162 (88%)	2722 (98%)	53 (2%)	49	66

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	62	VAL
1	A	210	ILE
1	A	300	LYS
1	A	303	LEU
1	A	304	LYS
1	A	305	SER
1	A	343	ASN
1	A	386	LYS
1	A	462	LYS
1	A	849	LEU
1	A	896	ILE
1	A	987	PRO
1	B	36	VAL
1	B	40	ASP
1	B	164	ASN
1	B	165	ASN
1	B	188	ASN
1	B	208	THR
1	B	212	ILE
1	B	216	PHE
1	B	300	LYS
1	B	303	LEU
1	B	305	SER
1	B	569	ILE
1	B	617	CYS
1	B	987	PRO
1	B	1106	GLN
1	C	54	LEU
1	C	61	ASN
1	C	216	PHE

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Mol	Chain	Res	Type
1	C	299	THR
1	C	300	LYS
1	C	301	CYS
1	C	302	THR
1	C	303	LEU
1	C	305	SER
1	C	308	VAL
1	C	326	ILE
1	C	327	VAL
1	C	329	PHE
1	C	343	ASN
1	C	395	VAL
1	C	487	ASN
1	C	511	VAL
1	C	529	LYS
1	C	531	THR
1	C	532	ASN
1	C	581	THR
1	C	595	VAL
1	C	615	VAL
1	C	934	ILE
1	C	1136	THR

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	207	HIS
1	A	239	GLN
1	A	321	GLN
1	A	505	HIS
1	A	926	GLN
1	A	965	GLN
1	A	992	GLN
1	A	1005	GLN
1	A	1054	GLN
1	B	66	HIS
1	B	207	HIS
1	B	334	ASN
1	B	388	ASN
1	B	409	GLN
1	B	506	GLN
1	B	607	GLN

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Mol	Chain	Res	Type
1	B	804	GLN
1	B	856	ASN
1	B	965	GLN
1	B	1135	ASN
1	C	66	HIS
1	C	99	ASN
1	C	134	GLN
1	C	196	ASN
1	C	207	HIS
1	C	487	ASN
1	C	505	HIS
1	C	914	ASN
1	C	978	ASN
1	C	1011	GLN
1	C	1036	GLN
1	C	1058	HIS
1	C	1119	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	0.61	1 (7%)	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	D	2	2	11,11,12	0.64	0	15,15,17	0.64	0
2	NAG	E	1	2	14,14,15	0.27	0	17,19,21	0.43	0
2	BMA	E	2	2	11,11,12	0.56	0	15,15,17	0.73	0
2	NAG	F	1	1,2	14,14,15	0.20	0	17,19,21	0.43	0
2	BMA	F	2	2	11,11,12	0.58	0	15,15,17	0.70	0
2	NAG	G	1	1,2	14,14,15	0.23	0	17,19,21	0.52	0
2	BMA	G	2	2	11,11,12	0.60	0	15,15,17	0.64	0
2	NAG	H	1	1,2	14,14,15	0.25	0	17,19,21	0.46	0
2	BMA	H	2	2	11,11,12	0.56	0	15,15,17	0.66	0
2	NAG	I	1	1,2	14,14,15	1.18	1 (7%)	17,19,21	1.12	1 (5%)
2	BMA	I	2	2	11,11,12	0.53	0	15,15,17	1.13	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.22	0	17,19,21	0.39	0
2	BMA	J	2	2	11,11,12	0.63	0	15,15,17	0.66	0
2	NAG	K	1	1,2	14,14,15	0.19	0	17,19,21	0.43	0
2	BMA	K	2	2	11,11,12	0.55	0	15,15,17	0.68	0
2	NAG	L	1	1,2	14,14,15	0.20	0	17,19,21	0.50	0
2	BMA	L	2	2	11,11,12	0.56	0	15,15,17	0.68	0
2	NAG	M	1	1,2	14,14,15	0.25	0	17,19,21	0.44	0
2	BMA	M	2	2	11,11,12	0.55	0	15,15,17	0.67	0
2	NAG	N	1	1,2	14,14,15	1.19	1 (7%)	17,19,21	1.08	1 (5%)
2	BMA	N	2	2	11,11,12	0.55	0	15,15,17	1.10	1 (6%)
2	NAG	O	1	1,2	14,14,15	0.21	0	17,19,21	0.43	0
2	BMA	O	2	2	11,11,12	0.62	0	15,15,17	0.76	0
2	NAG	P	1	1,2	14,14,15	0.26	0	17,19,21	0.40	0
2	BMA	P	2	2	11,11,12	0.55	0	15,15,17	0.65	0
2	NAG	Q	1	1,2	14,14,15	0.17	0	17,19,21	0.44	0
2	BMA	Q	2	2	11,11,12	0.58	0	15,15,17	0.66	0
2	NAG	R	1	1,2	14,14,15	0.23	0	17,19,21	0.52	0
2	BMA	R	2	2	11,11,12	0.62	0	15,15,17	0.70	0
2	NAG	S	1	1,2	14,14,15	0.22	0	17,19,21	0.44	0
2	BMA	S	2	2	11,11,12	0.53	0	15,15,17	0.67	0
2	NAG	T	1	1,2	14,14,15	1.24	1 (7%)	17,19,21	1.16	1 (5%)
2	BMA	T	2	2	11,11,12	0.54	0	15,15,17	1.13	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	1	NAG	O5-C1	-4.25	1.36	1.43
2	N	1	NAG	O5-C1	-4.09	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C1	-4.01	1.37	1.43
2	D	1	NAG	O5-C1	-2.10	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	1	NAG	C3-C4-C5	3.20	116.03	110.23
2	I	1	NAG	C3-C4-C5	3.03	115.73	110.23
2	I	2	BMA	C1-O5-C5	2.89	116.06	112.19
2	T	2	BMA	C1-O5-C5	2.88	116.04	112.19
2	N	1	NAG	C3-C4-C5	2.82	115.35	110.23
2	N	2	BMA	C1-O5-C5	2.69	115.79	112.19

There are no chirality outliers.

All (31) torsion outliers are listed below:

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

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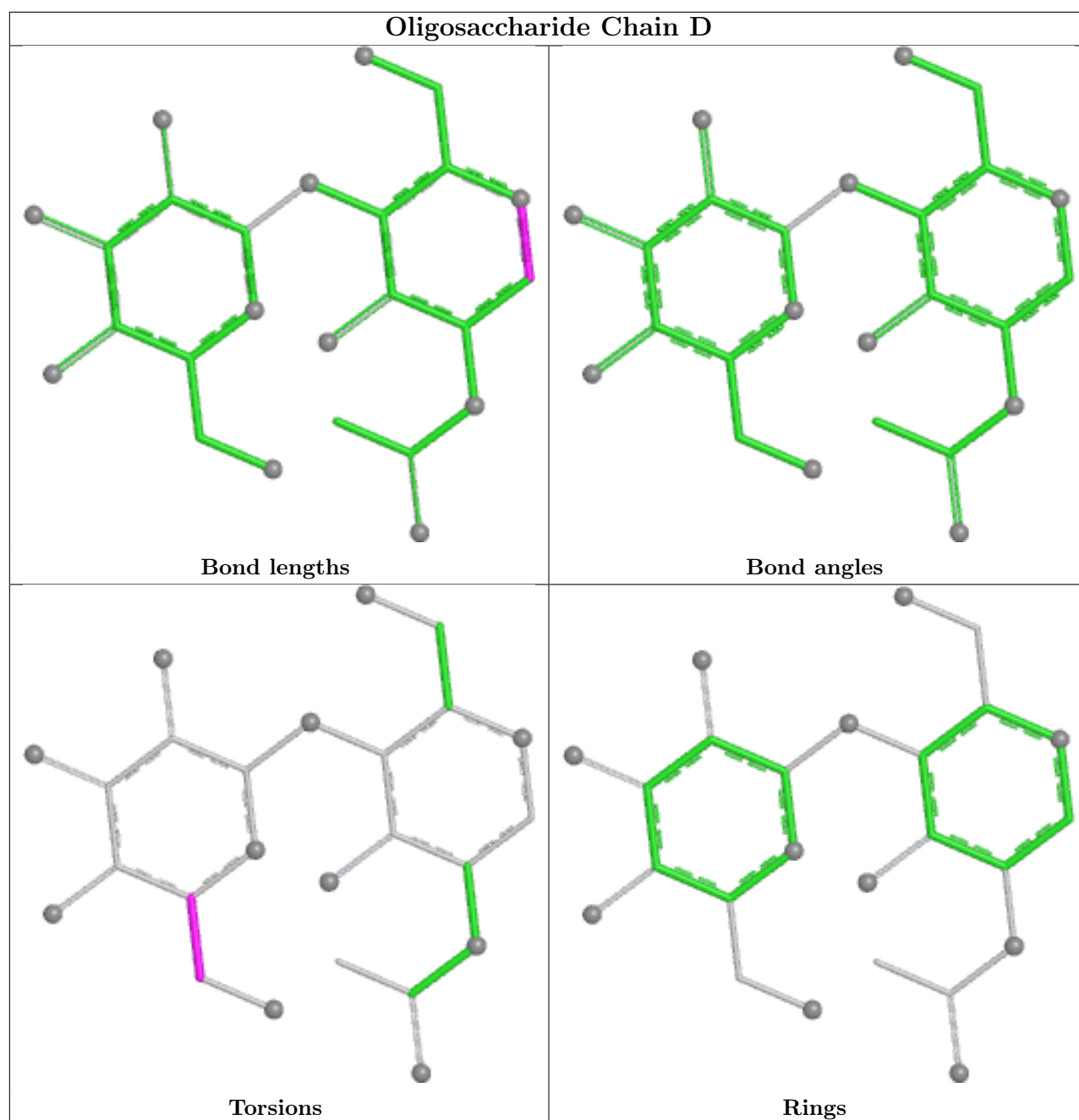
Mol	Chain	Res	Type	Atoms
2	D	2	BMA	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6

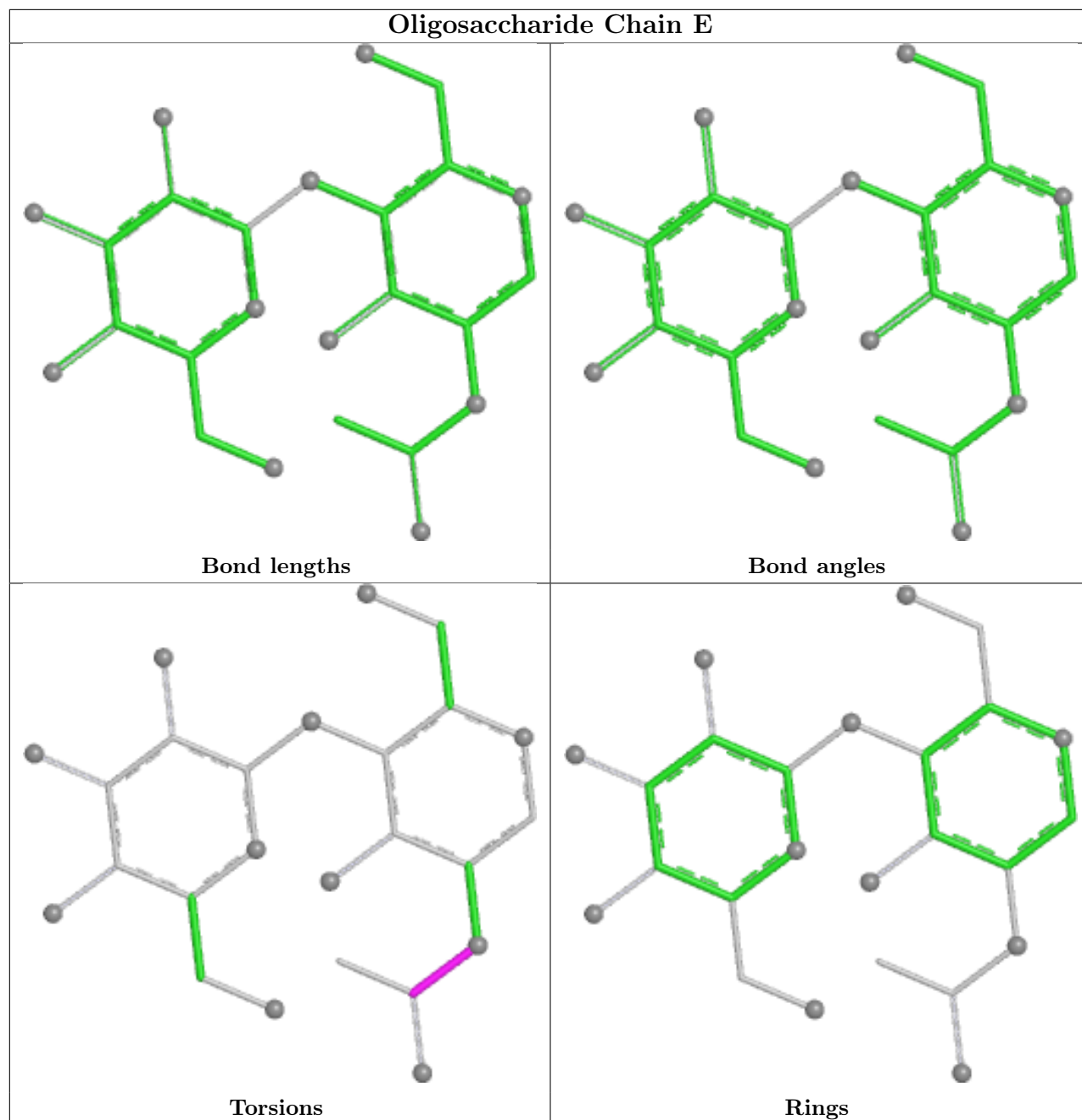
There are no ring outliers.

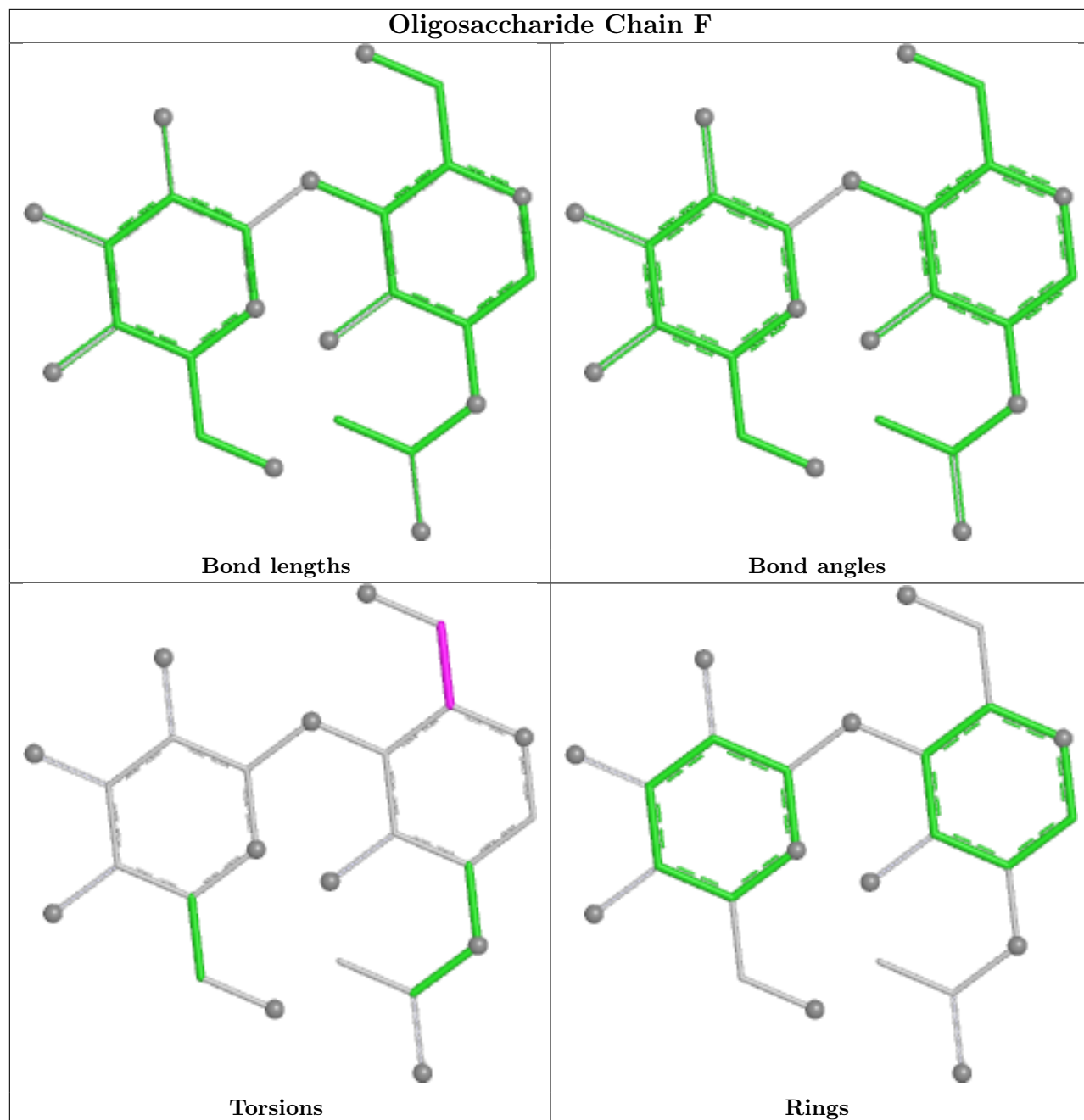
2 monomers are involved in 3 short contacts:

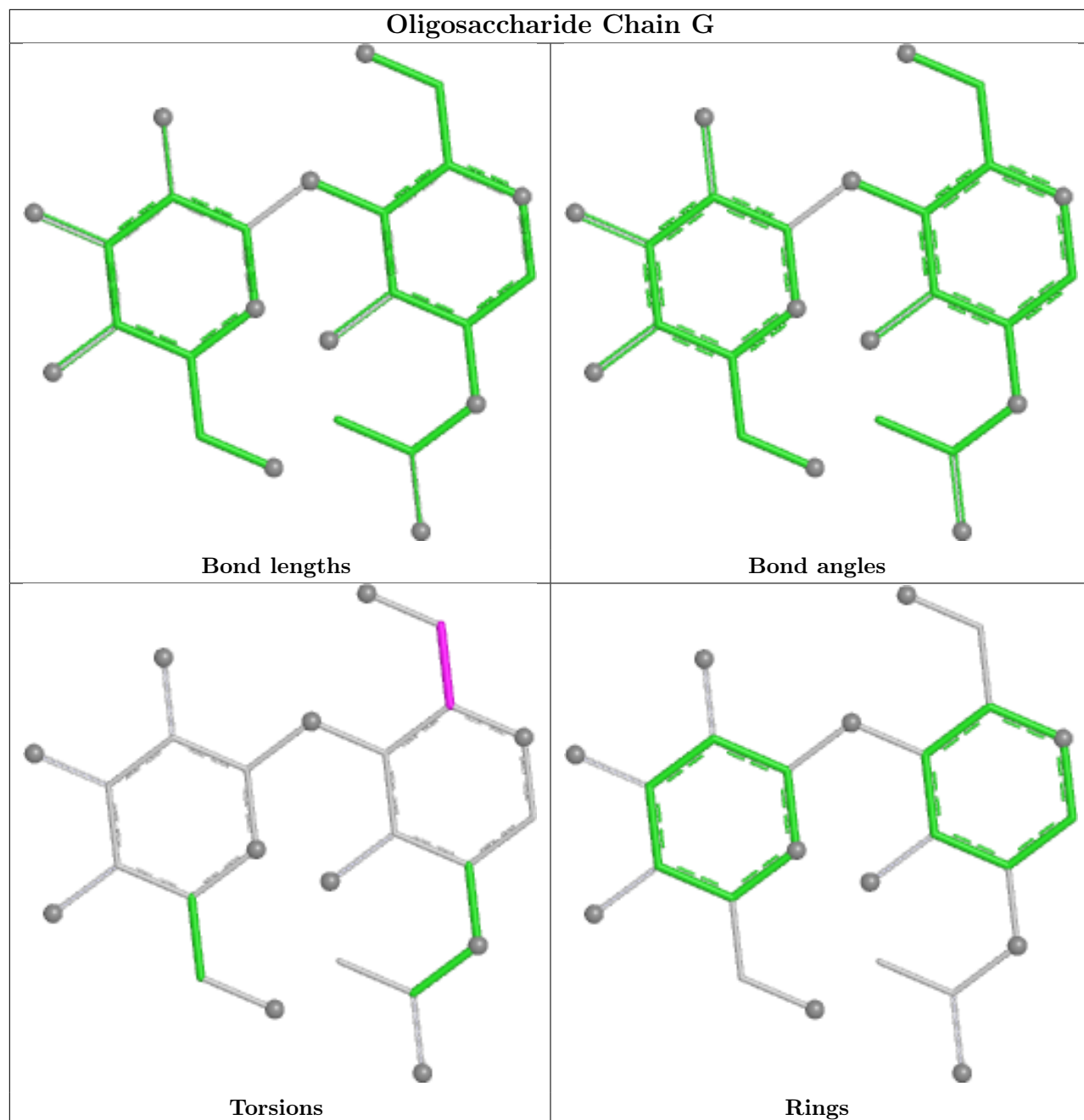
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	2	0
2	D	1	NAG	1	0

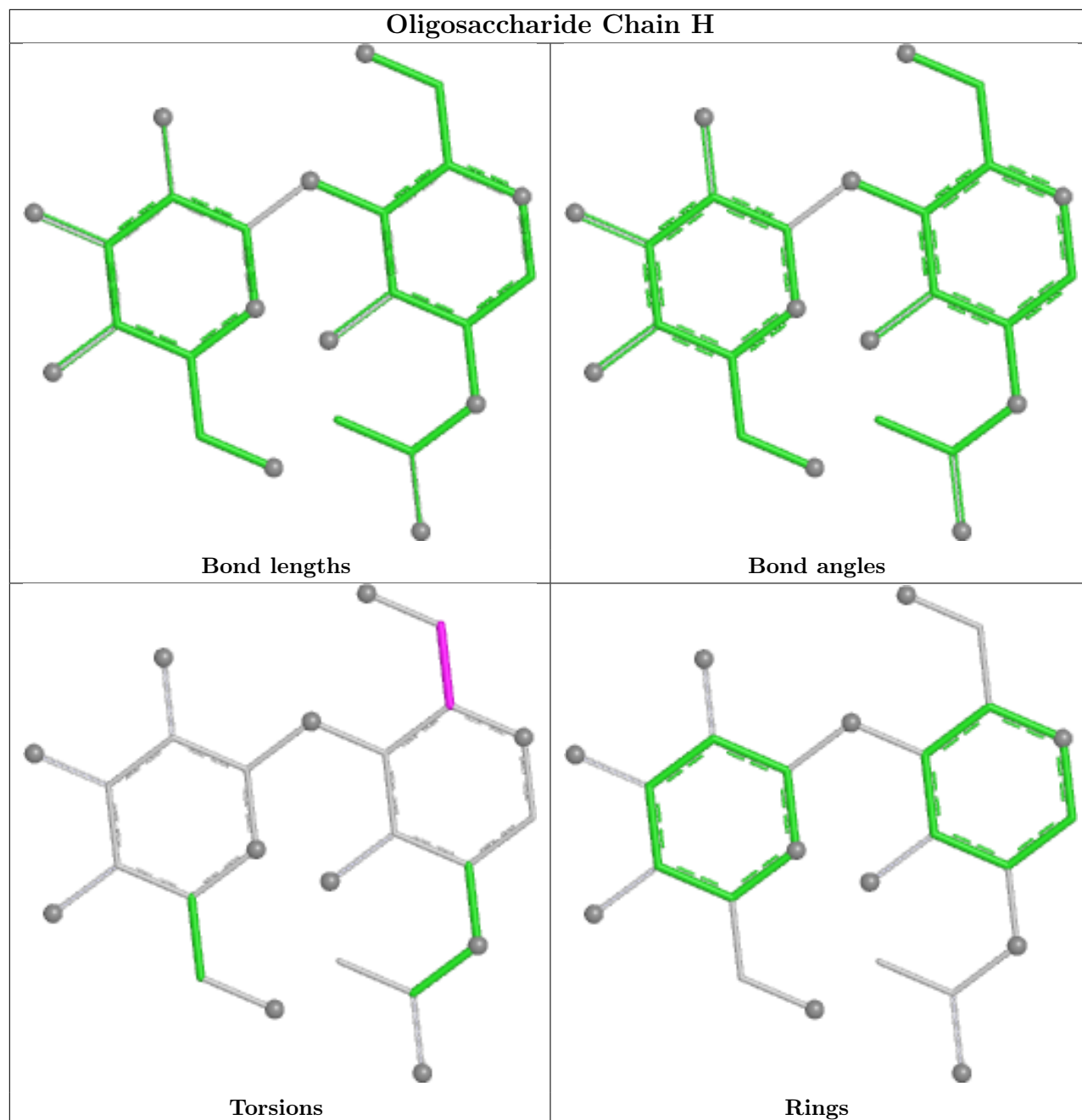
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

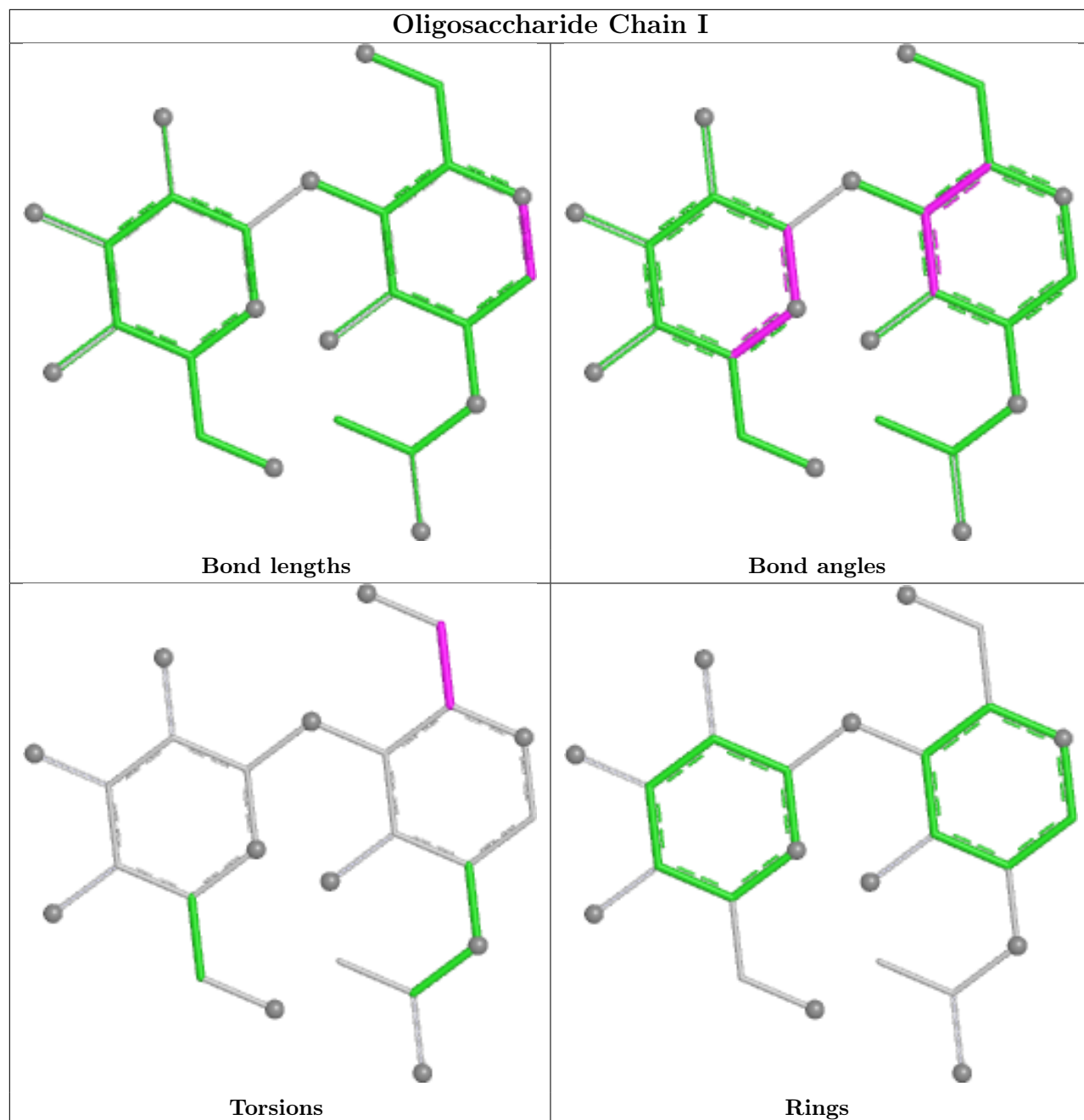


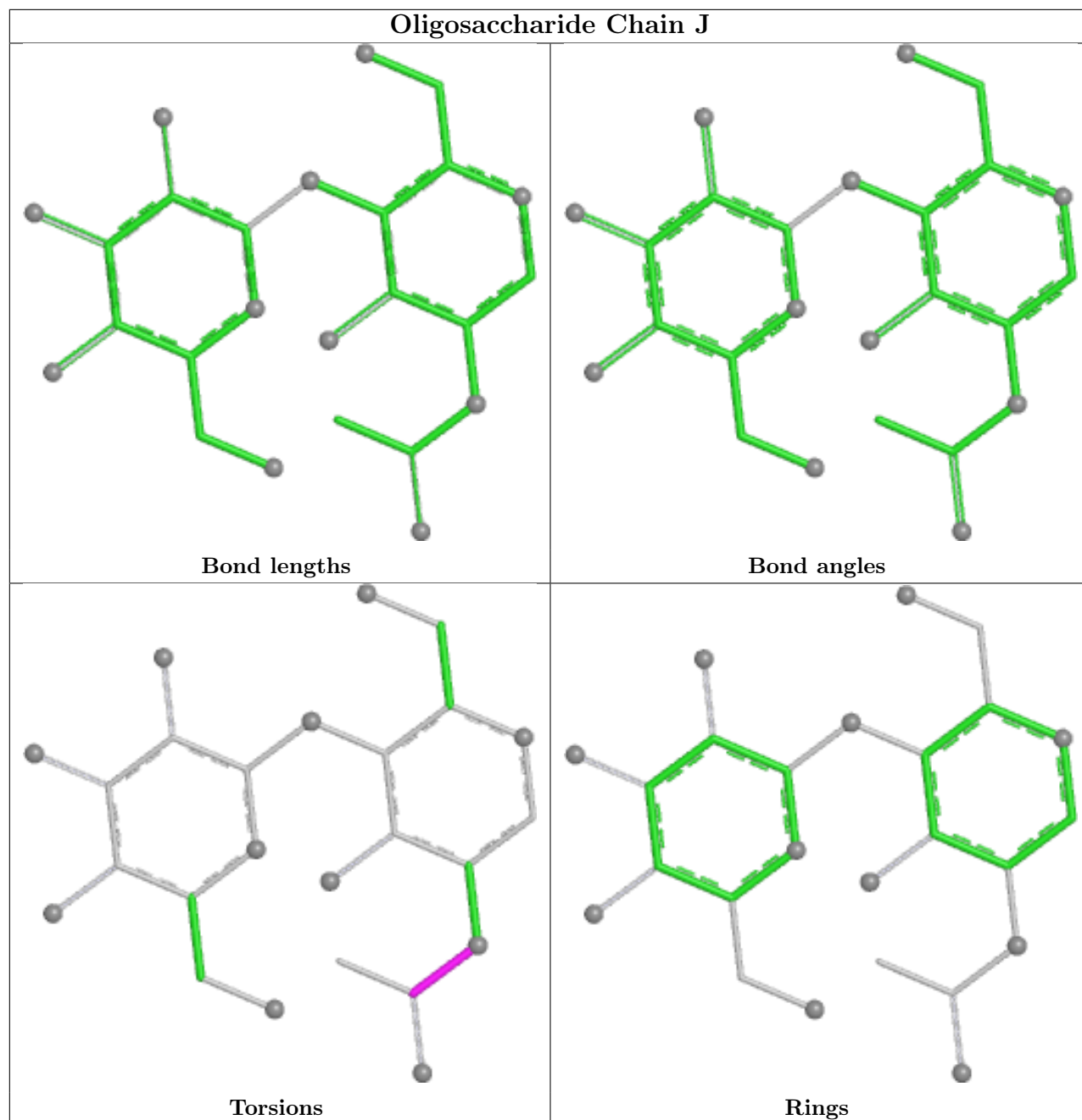


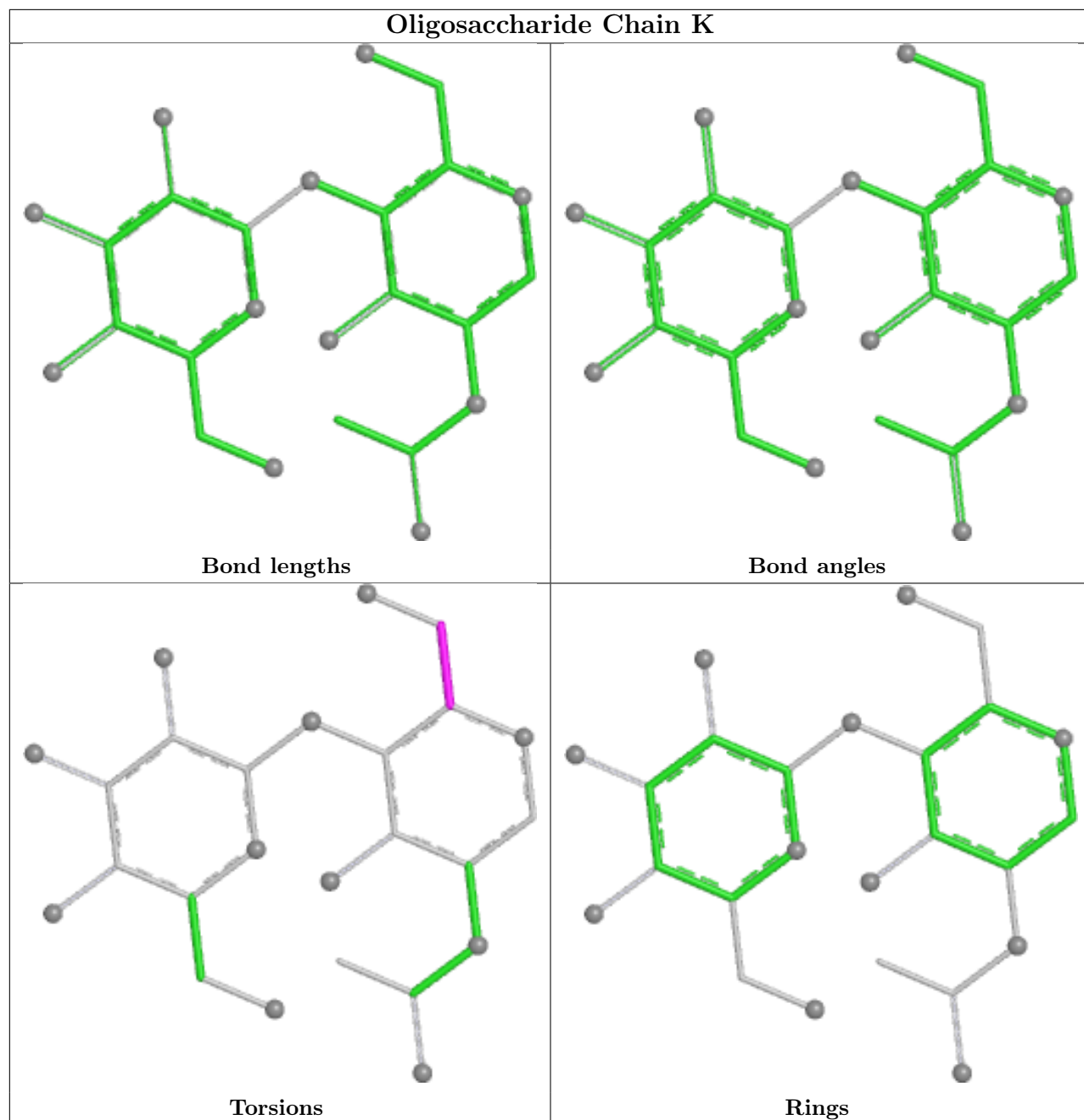


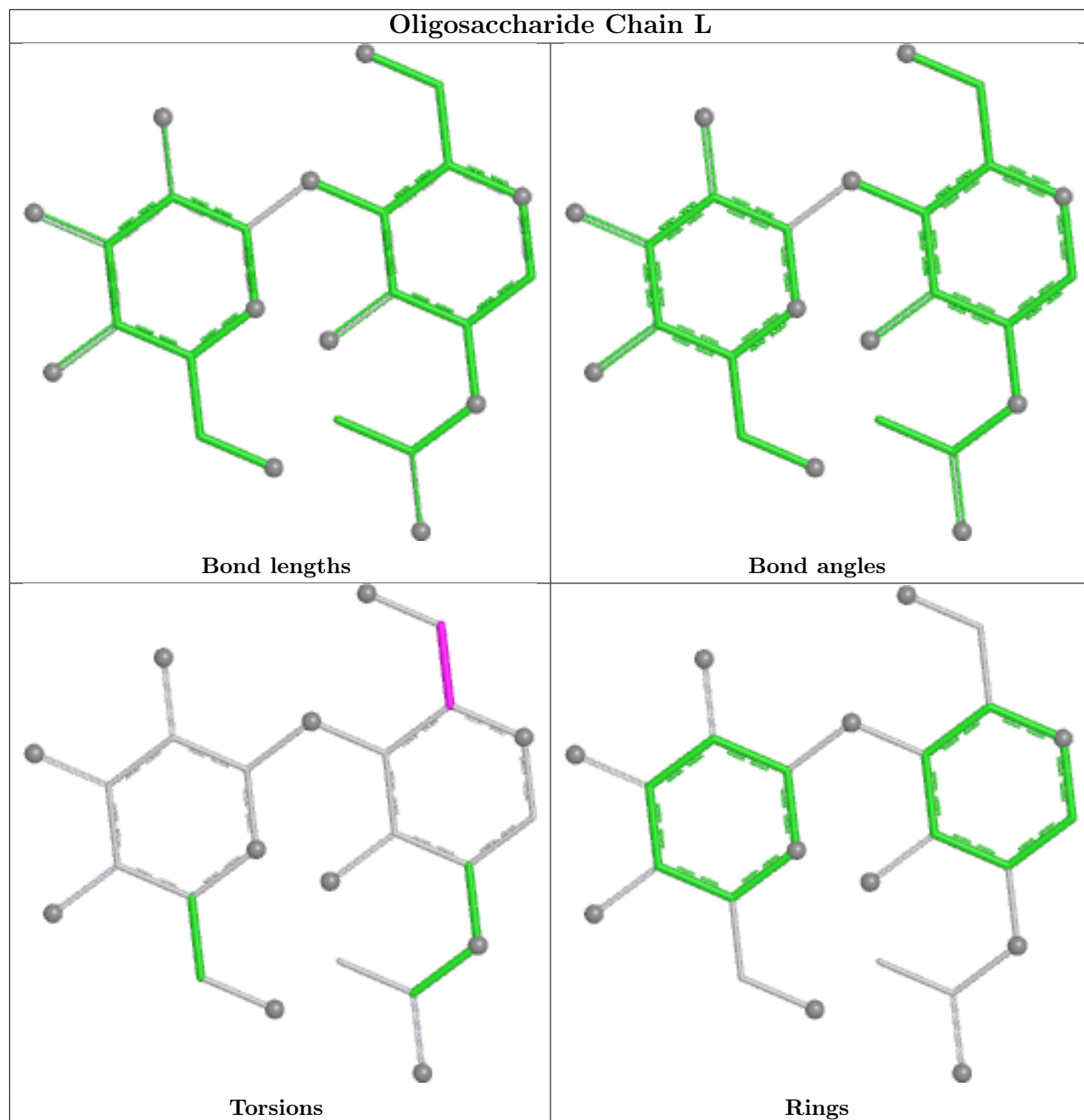


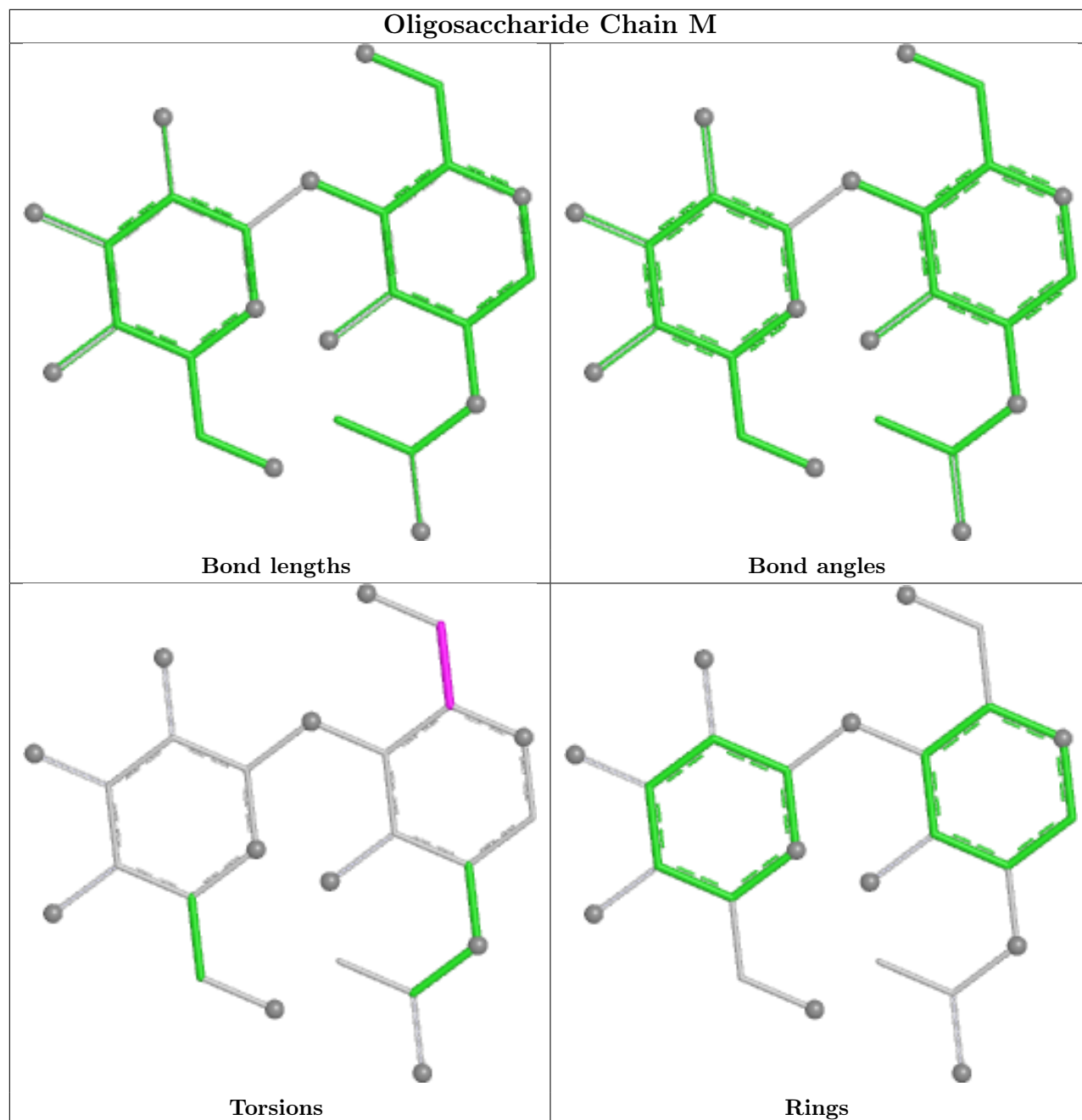


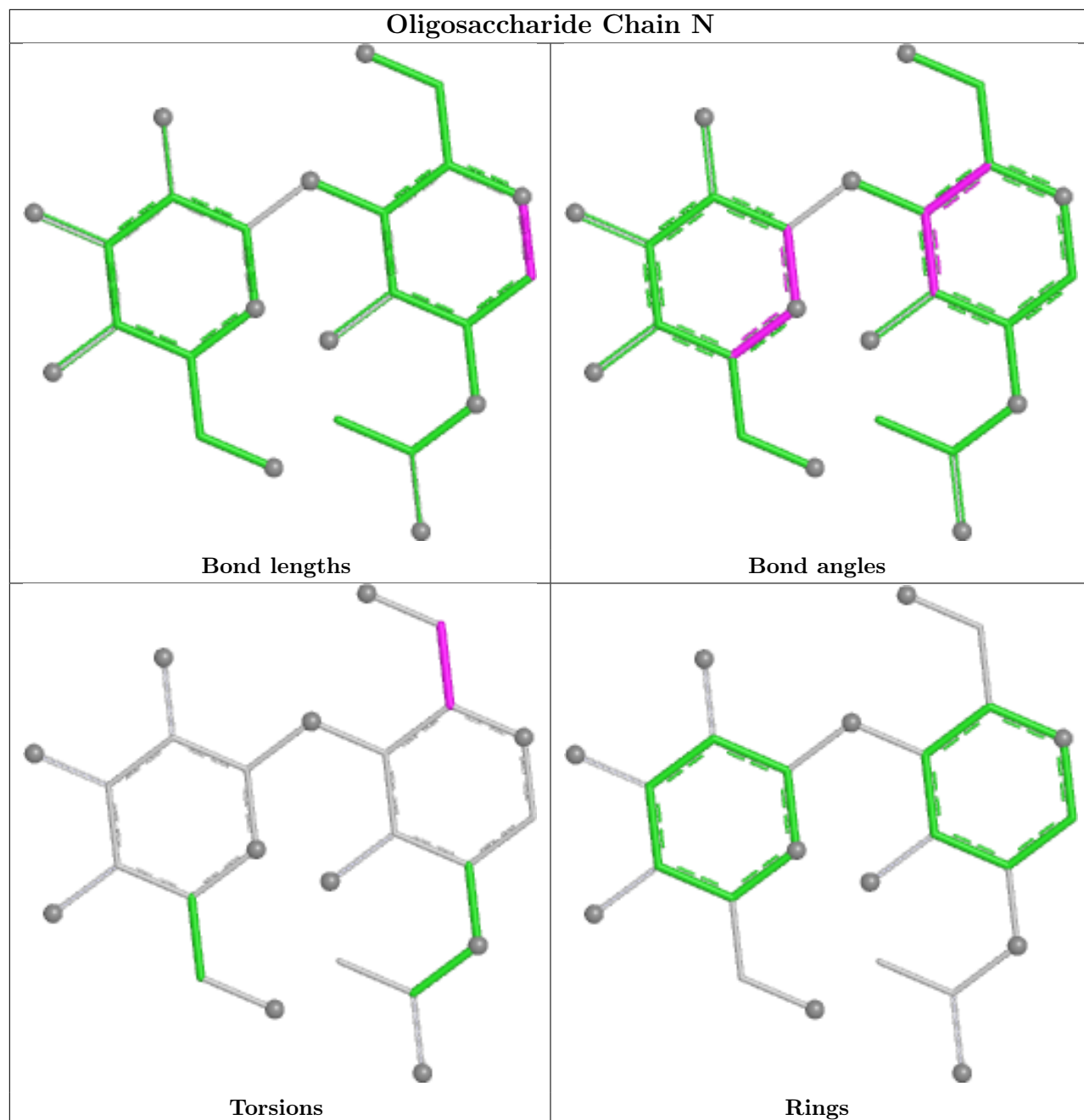


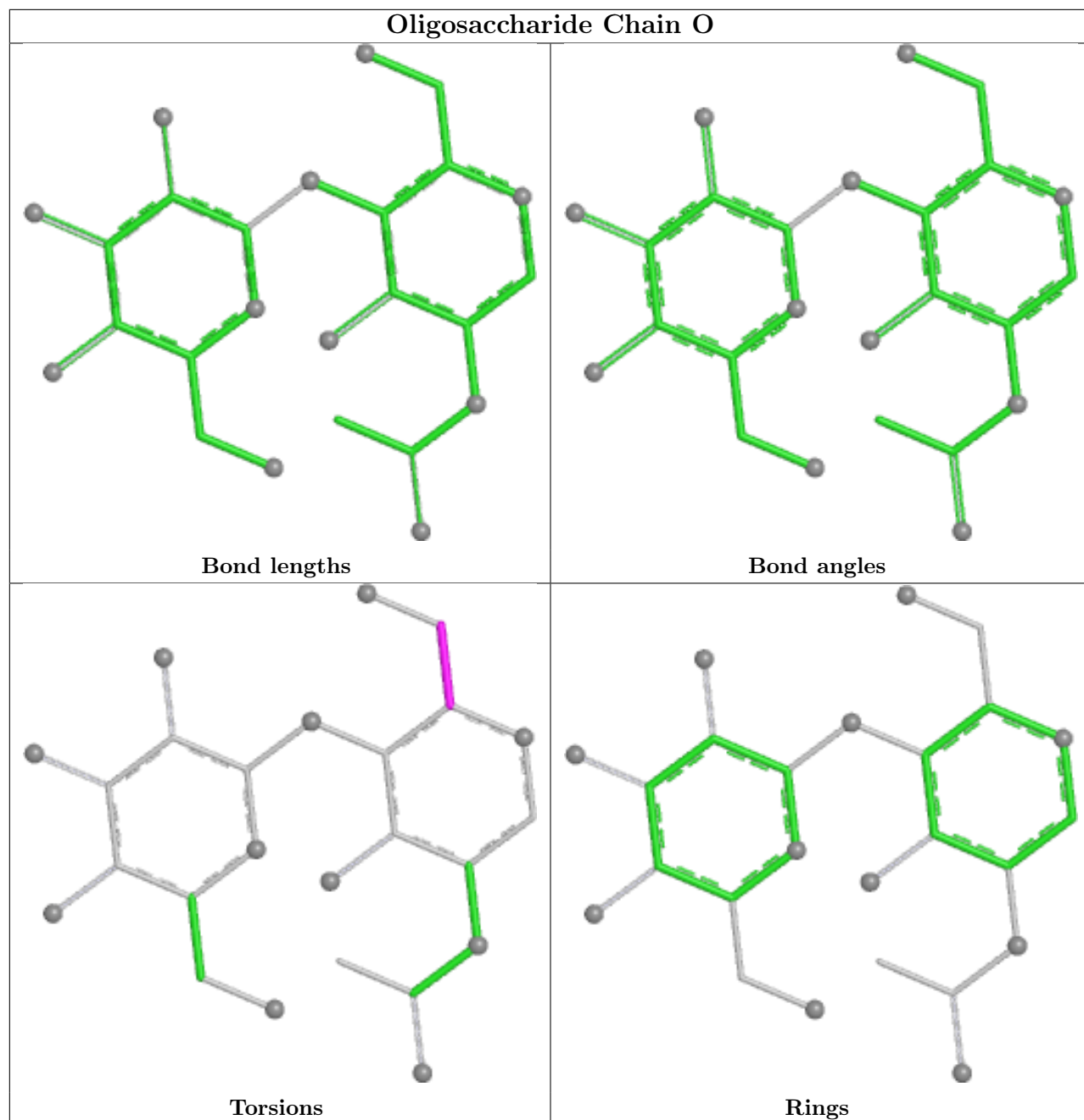


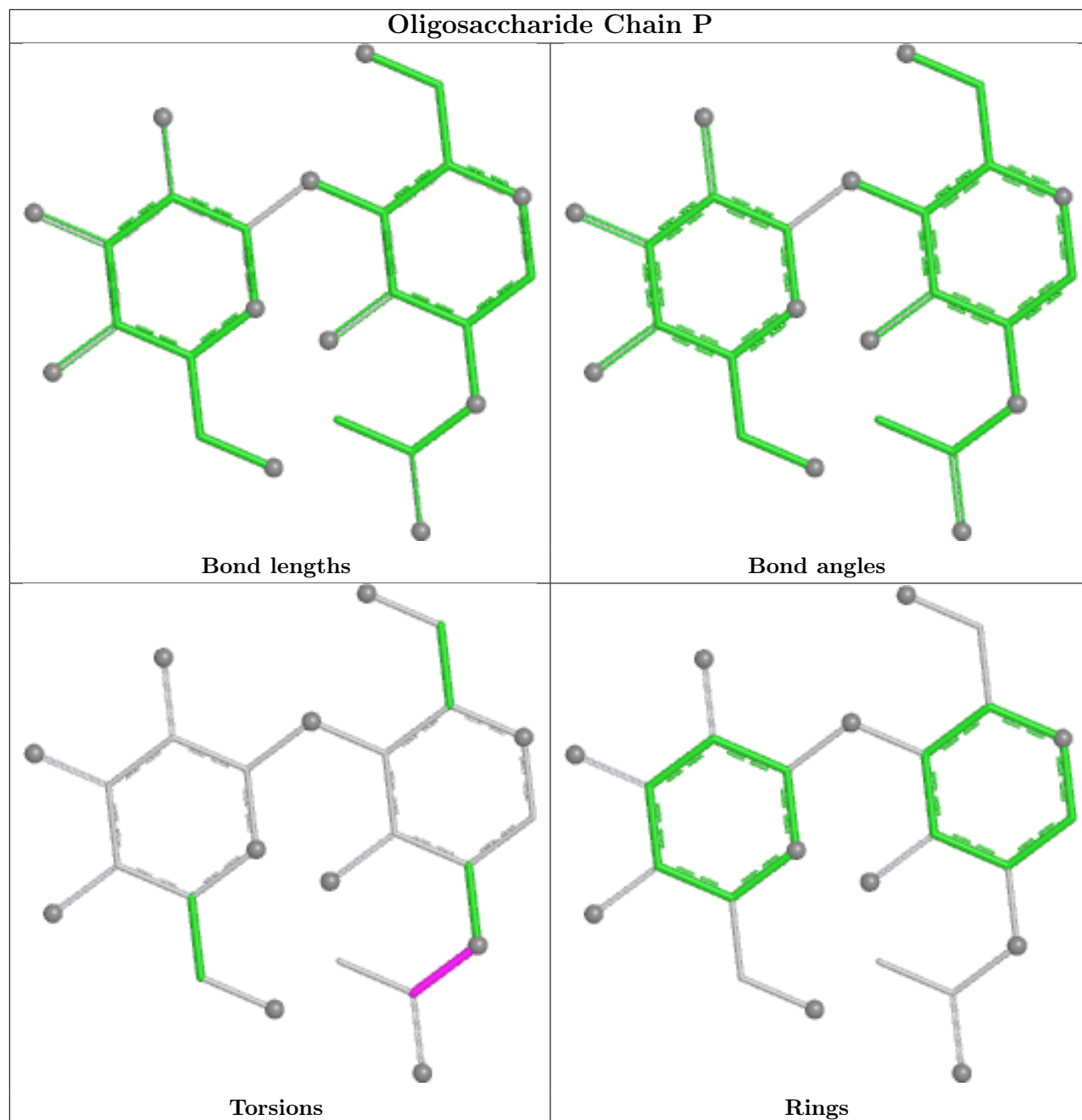


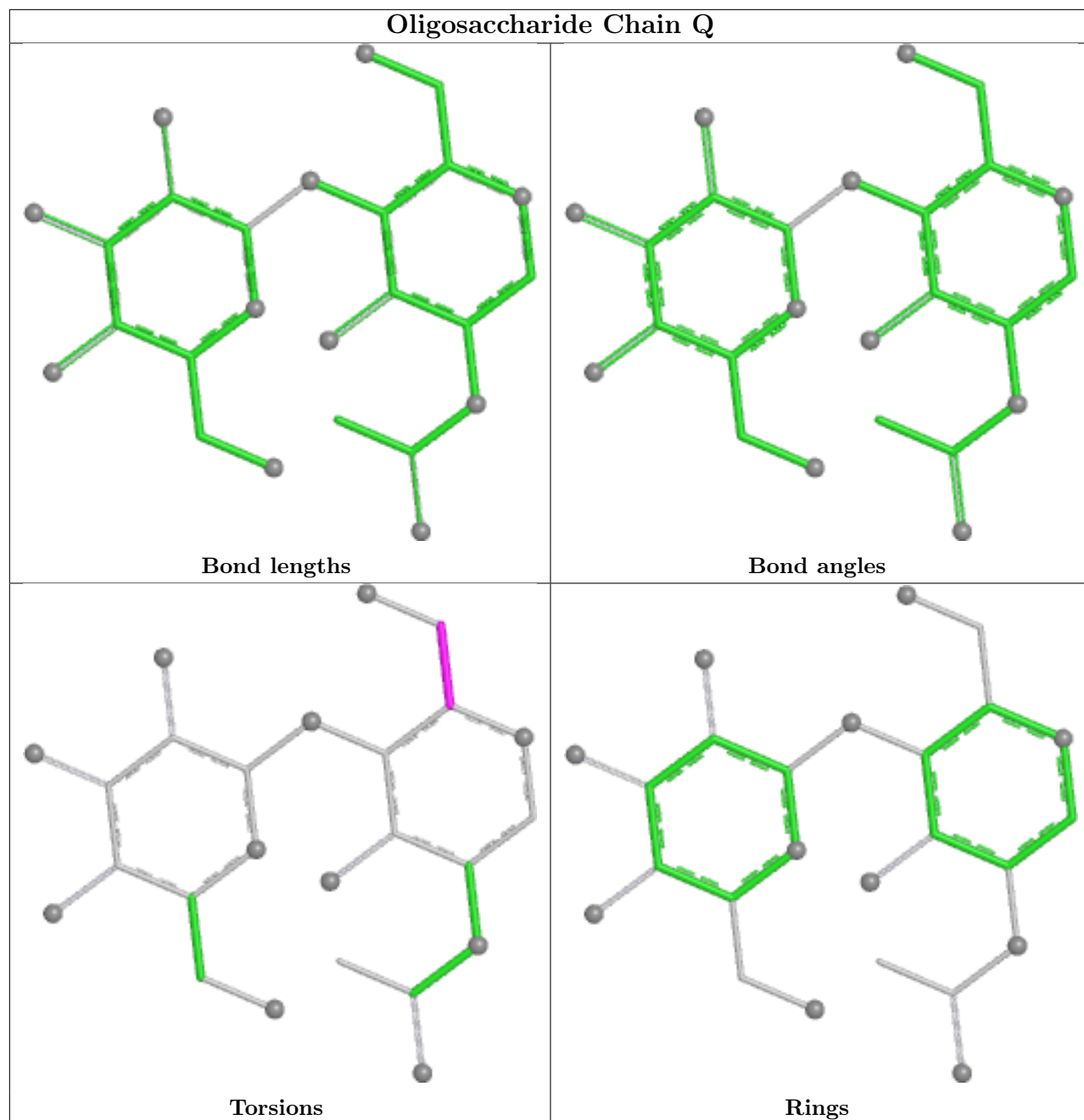


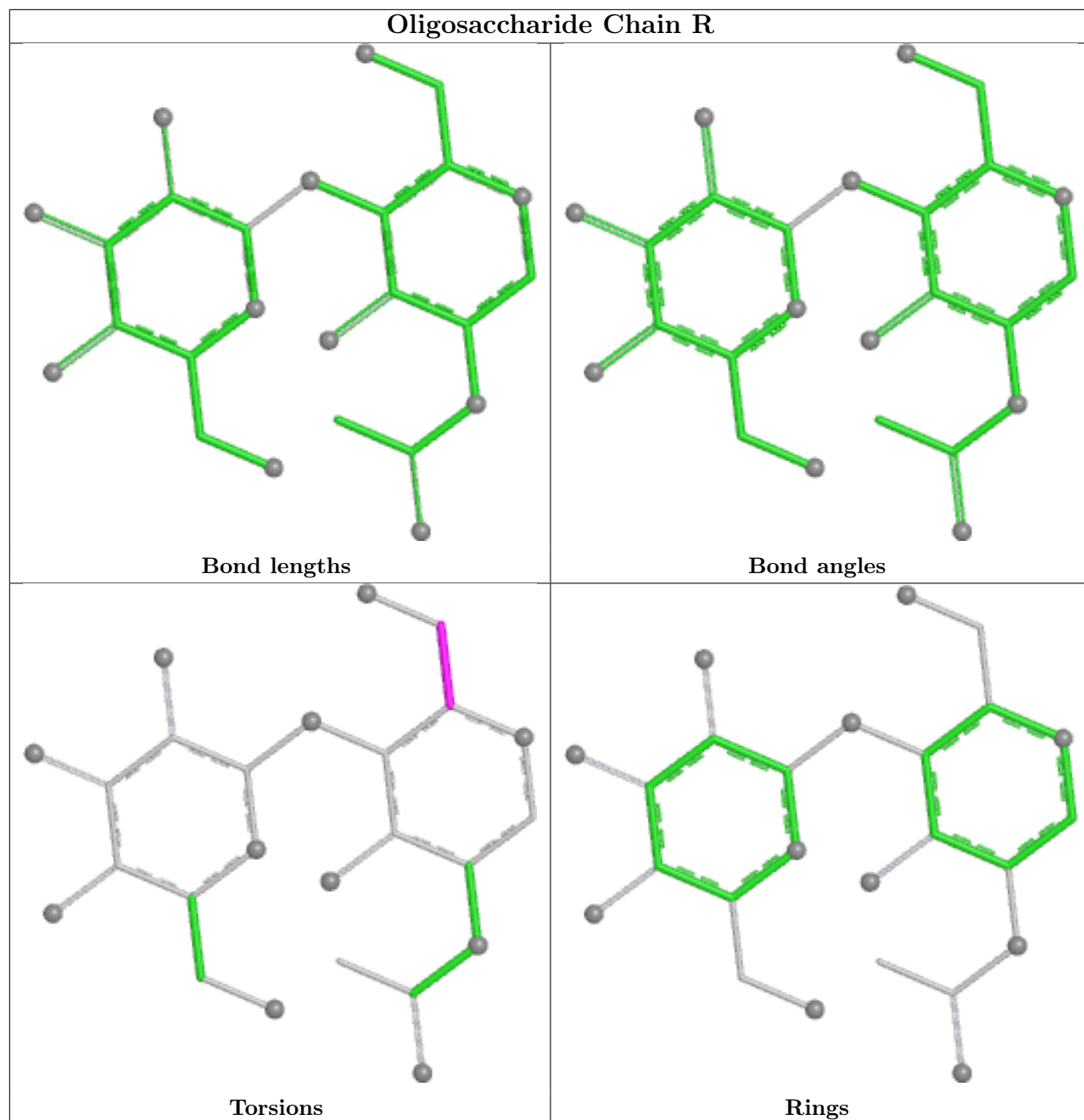


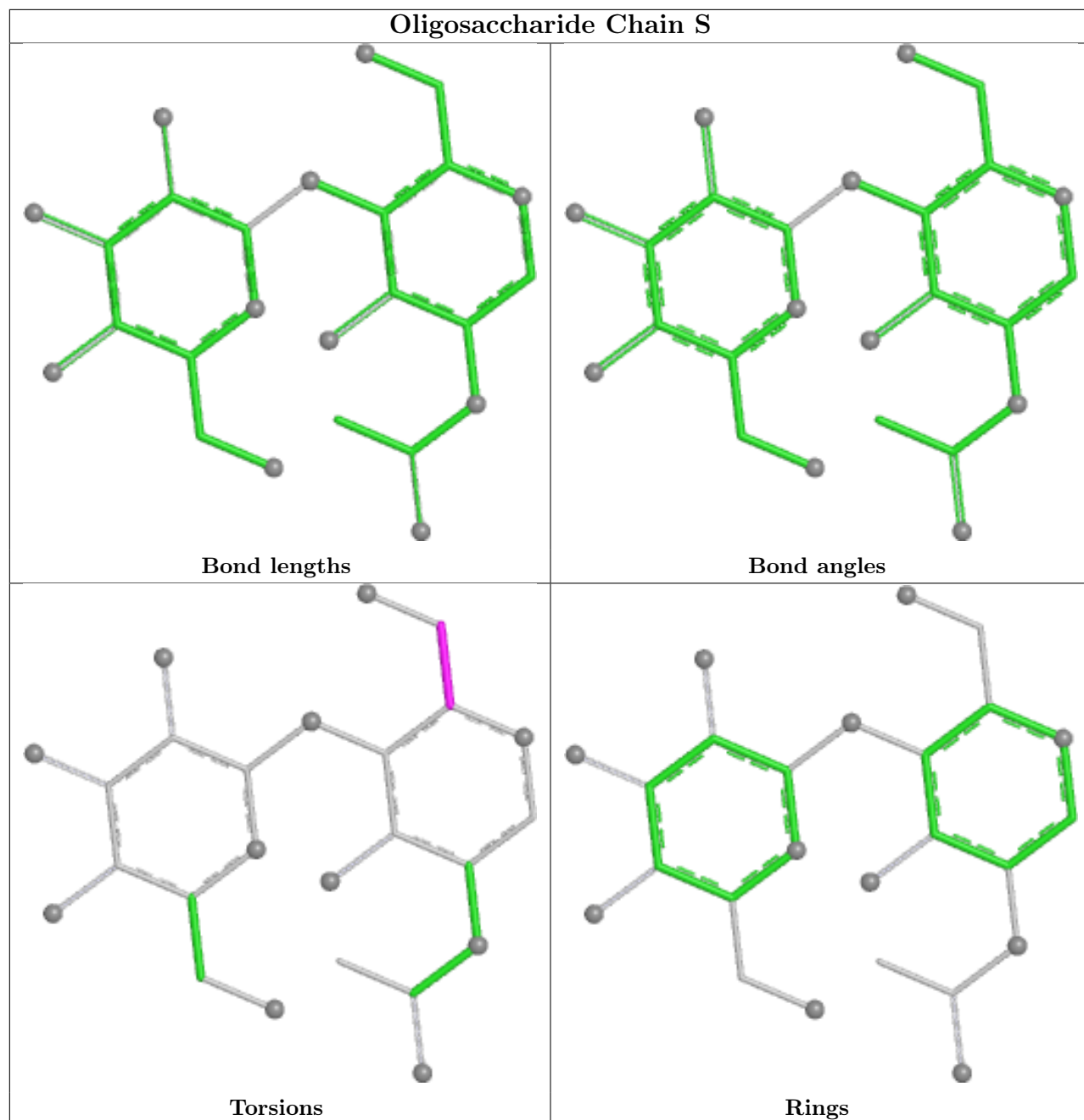


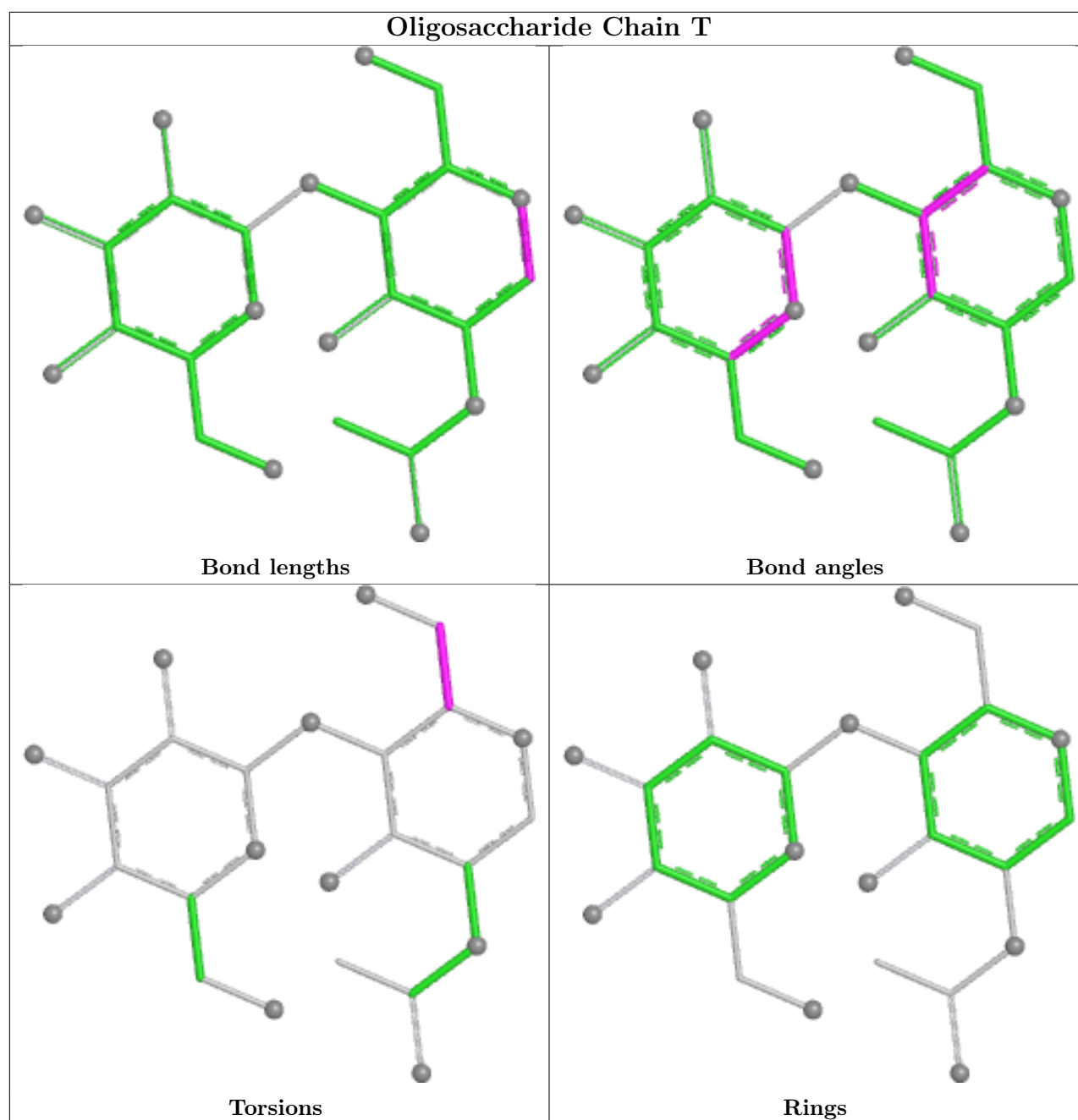












5.6 Ligand geometry [i](#)

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1301	1	14,14,15	0.38	0	17,19,21	0.78	1 (5%)
3	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	C	1302	1	14,14,15	0.37	0	17,19,21	0.42	0
3	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.45	0
3	NAG	C	1304	1	14,14,15	0.31	0	17,19,21	1.41	1 (5%)
3	NAG	A	1302	1	14,14,15	0.26	0	17,19,21	0.38	0
3	NAG	A	1307	1	14,14,15	0.19	0	17,19,21	0.52	0
3	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	C	1307	1	14,14,15	0.21	0	17,19,21	0.51	0
3	NAG	B	1309	1	14,14,15	0.27	0	17,19,21	0.55	0
3	NAG	C	1309	1	14,14,15	0.38	0	17,19,21	0.45	0
3	NAG	C	1303	1	14,14,15	0.40	0	17,19,21	0.87	2 (11%)
3	NAG	B	1311	1	14,14,15	0.29	0	17,19,21	0.46	0
3	NAG	C	1305	1	14,14,15	0.38	0	17,19,21	0.45	0
3	NAG	B	1302	1	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	A	1305	1	14,14,15	0.40	0	17,19,21	0.49	0
3	NAG	B	1310	1	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	C	1301	1	14,14,15	0.38	0	17,19,21	0.85	1 (5%)
3	NAG	A	1310	1	14,14,15	0.32	0	17,19,21	0.69	0
3	NAG	A	1301	1	14,14,15	0.19	0	17,19,21	0.49	0
3	NAG	A	1306	1	14,14,15	0.16	0	17,19,21	0.46	0
3	NAG	B	1307	1	14,14,15	0.33	0	17,19,21	0.39	0
3	NAG	B	1304	1	14,14,15	0.39	0	17,19,21	1.00	2 (11%)
3	NAG	B	1308	1	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	A	1304	1	14,14,15	0.29	0	17,19,21	1.37	1 (5%)
3	NAG	B	1303	1	14,14,15	0.42	0	17,19,21	0.58	0
3	NAG	B	1305	1	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	C	1306	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	B	1306	1	14,14,15	0.30	0	17,19,21	1.38	1 (5%)
3	NAG	C	1310	1	14,14,15	0.38	0	17,19,21	0.55	0
3	NAG	A	1308	1	14,14,15	0.58	0	17,19,21	0.91	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1304	NAG	C1-O5-C5	5.21	119.17	112.19
3	B	1306	NAG	C1-O5-C5	5.08	119.00	112.19
3	A	1304	NAG	C1-O5-C5	5.05	118.95	112.19
3	B	1304	NAG	C1-C2-N2	2.95	115.08	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1301	NAG	C2-N2-C7	2.45	126.18	122.90
3	A	1308	NAG	C1-O5-C5	2.35	115.34	112.19
3	B	1304	NAG	C2-N2-C7	2.29	125.97	122.90
3	A	1308	NAG	C3-C4-C5	2.19	114.21	110.23
3	C	1301	NAG	C1-C2-N2	2.19	113.88	110.43
3	C	1303	NAG	C1-C2-N2	2.08	113.71	110.43
3	C	1303	NAG	O5-C1-C2	-2.06	108.10	111.29

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	C8-C7-N2-C2
3	B	1303	NAG	O7-C7-N2-C2
3	B	1304	NAG	C1-C2-N2-C7
3	C	1303	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	C	1303	NAG	C8-C7-N2-C2
3	C	1303	NAG	O7-C7-N2-C2
3	A	1310	NAG	C4-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	C	1301	NAG	C8-C7-N2-C2
3	B	1309	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	C	1301	NAG	O7-C7-N2-C2
3	C	1306	NAG	O5-C5-C6-O6
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	A	1307	NAG	C8-C7-N2-C2
3	A	1307	NAG	O7-C7-N2-C2
3	A	1308	NAG	C8-C7-N2-C2
3	A	1308	NAG	O7-C7-N2-C2
3	A	1309	NAG	C8-C7-N2-C2
3	A	1309	NAG	O7-C7-N2-C2
3	B	1309	NAG	C8-C7-N2-C2
3	B	1309	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	B	1310	NAG	C8-C7-N2-C2
3	B	1310	NAG	O7-C7-N2-C2
3	C	1307	NAG	C8-C7-N2-C2
3	C	1307	NAG	O7-C7-N2-C2
3	C	1306	NAG	C4-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	B	1304	NAG	C3-C2-N2-C7
3	C	1301	NAG	C3-C2-N2-C7
3	B	1304	NAG	C8-C7-N2-C2
3	A	1305	NAG	O5-C5-C6-O6
3	B	1304	NAG	O7-C7-N2-C2
3	C	1308	NAG	C4-C5-C6-O6
3	B	1301	NAG	C3-C2-N2-C7
3	A	1307	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1303	NAG	C3-C2-N2-C7
3	C	1304	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1301	NAG	1	0
3	C	1305	NAG	1	0
3	A	1310	NAG	1	0
3	B	1304	NAG	1	0
3	A	1304	NAG	1	0
3	C	1310	NAG	2	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.

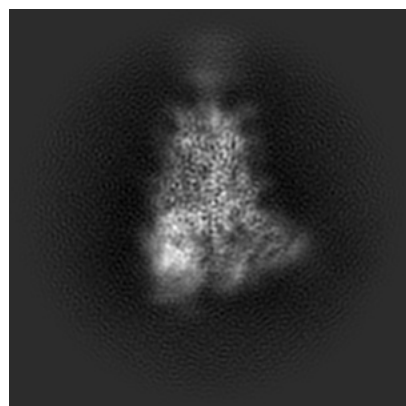
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37550. These allow visual inspection of the internal detail of the map and identification of artifacts.

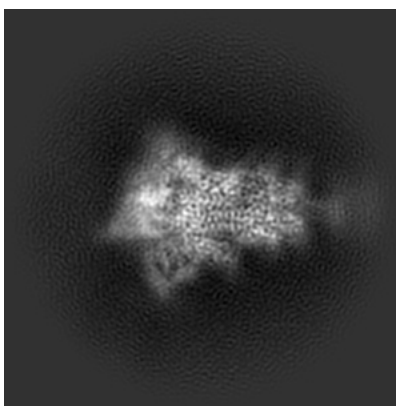
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

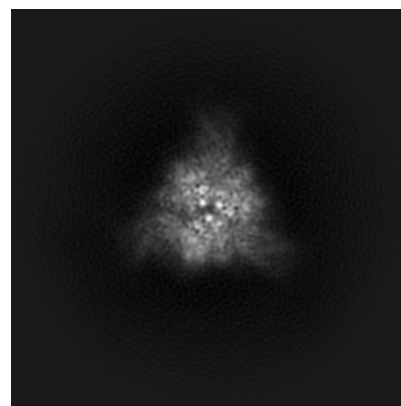
6.1.1 Primary map



X

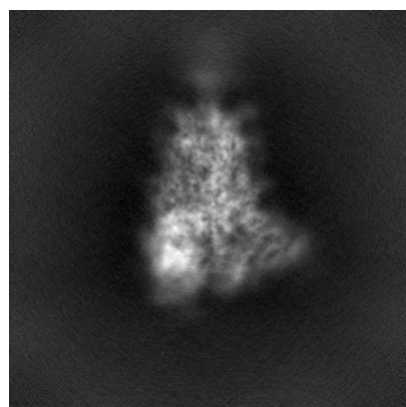


Y

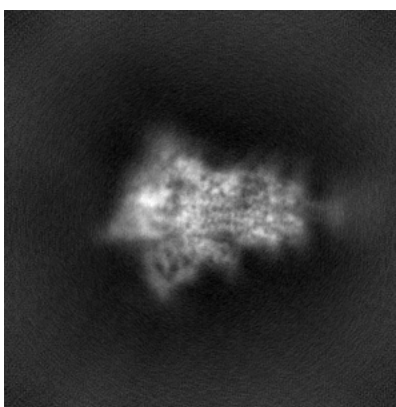


Z

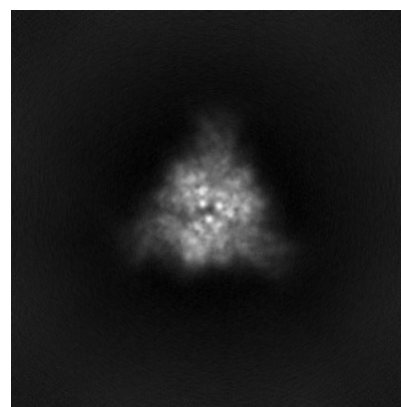
6.1.2 Raw map



X



Y

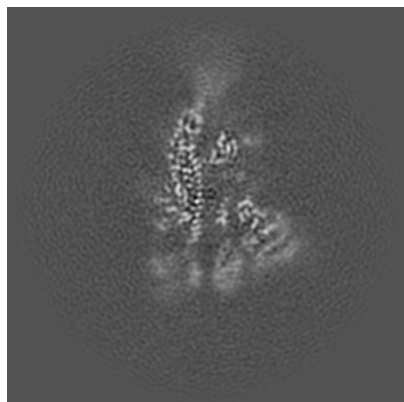


Z

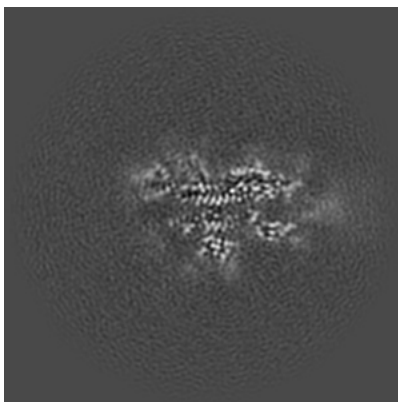
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

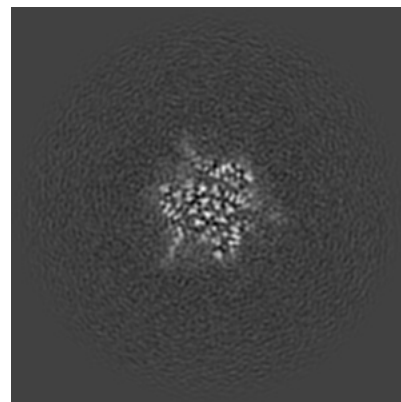
6.2.1 Primary map



X Index: 160

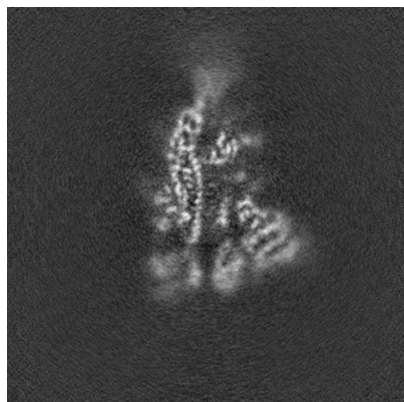


Y Index: 160

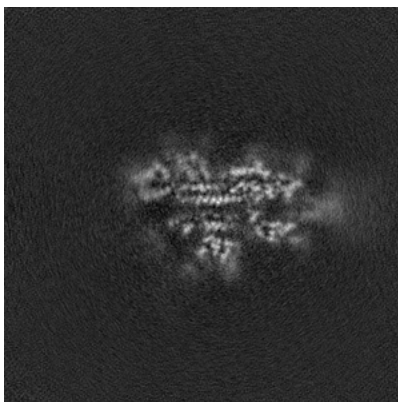


Z Index: 160

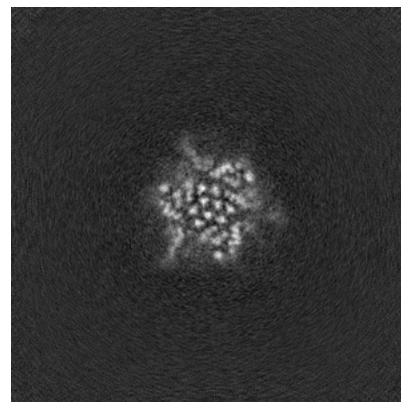
6.2.2 Raw map



X Index: 160



Y Index: 160

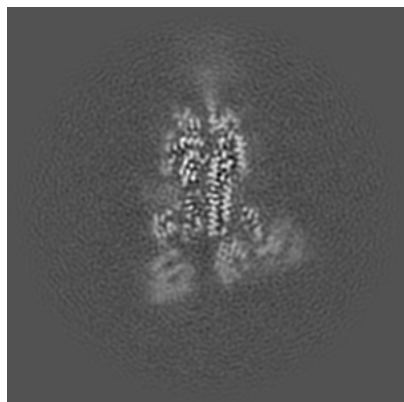


Z Index: 160

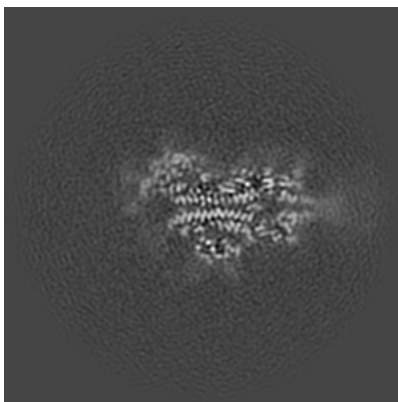
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

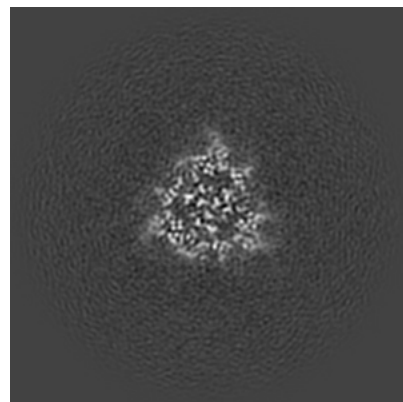
6.3.1 Primary map



X Index: 152

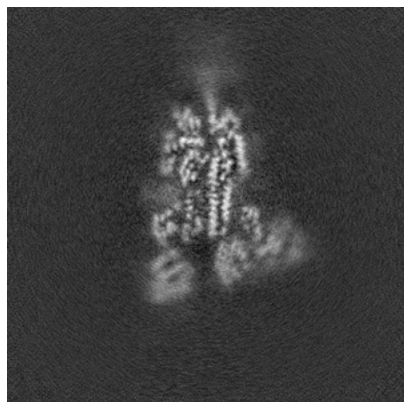


Y Index: 164

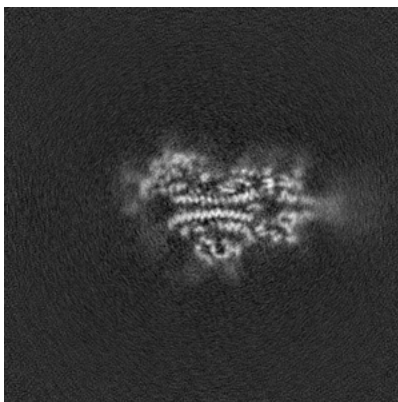


Z Index: 154

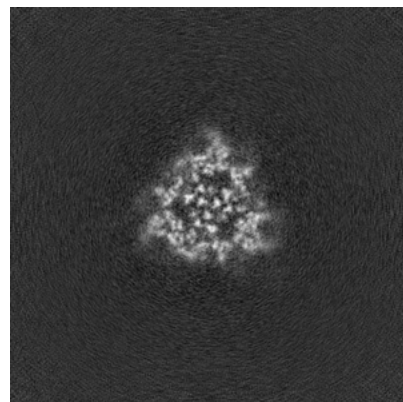
6.3.2 Raw map



X Index: 152



Y Index: 164

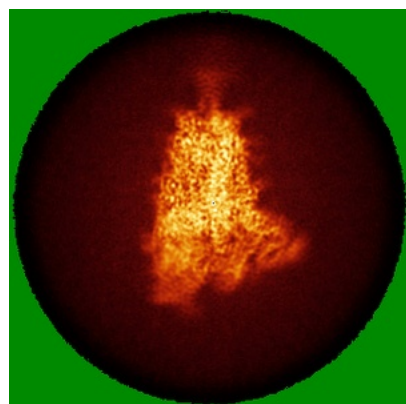


Z Index: 154

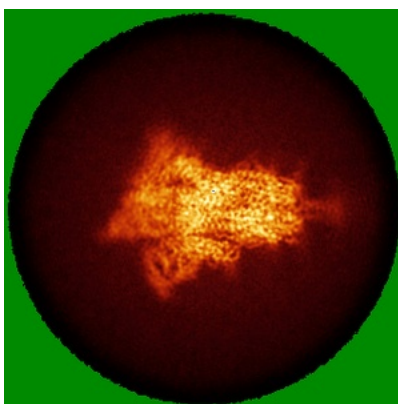
The images above show the largest variance slices of the map in three orthogonal directions.

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

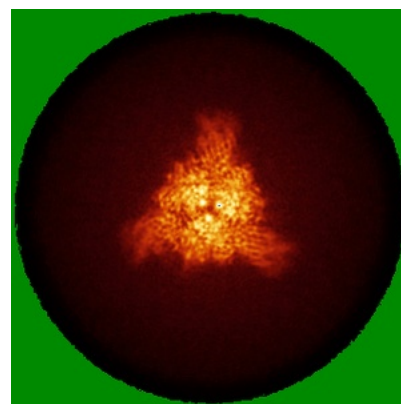
6.4.1 Primary map



X

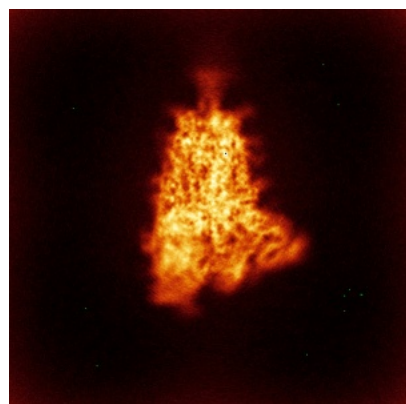


Y

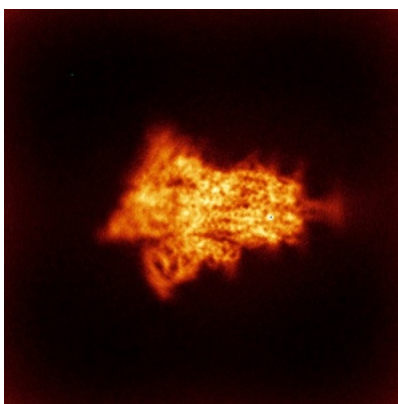


Z

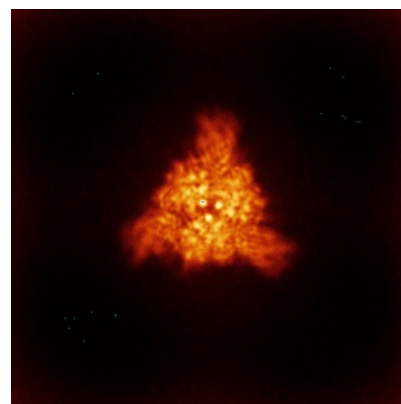
6.4.2 Raw map



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



X



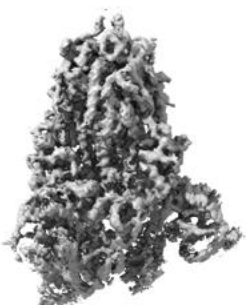
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.44. 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



X



Y



Z

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.

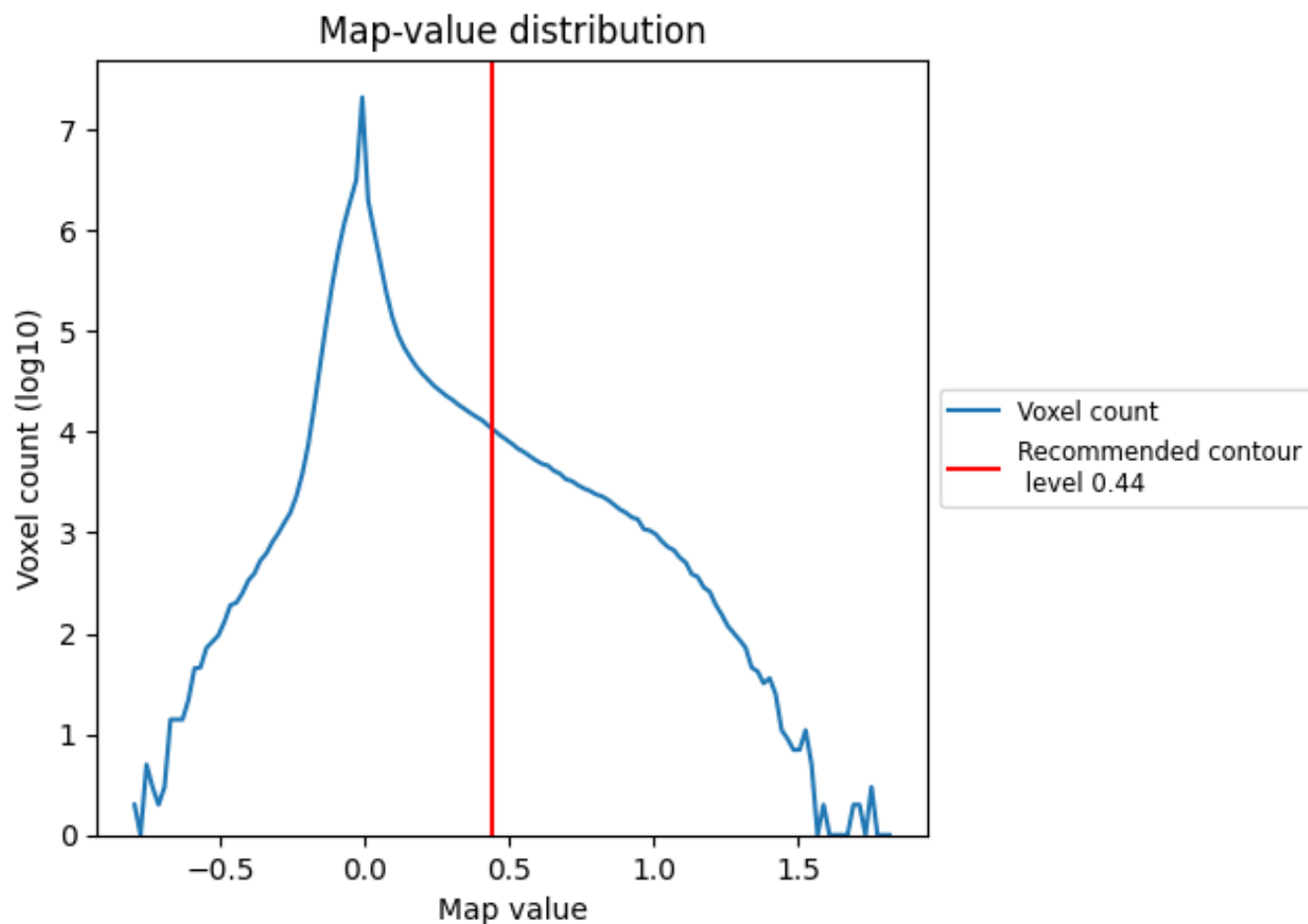
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

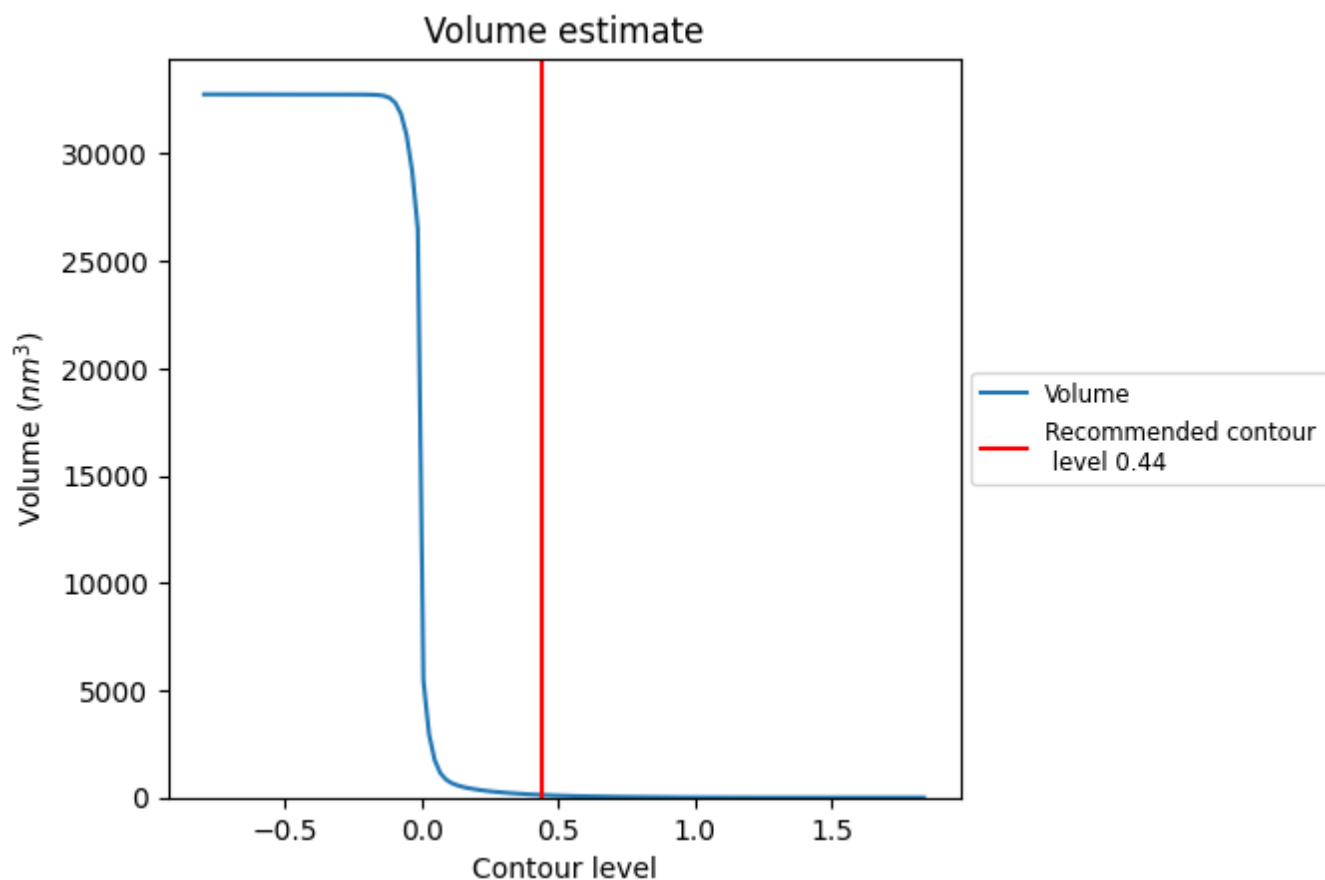
This section contains the results of statistical analysis of the map.

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.

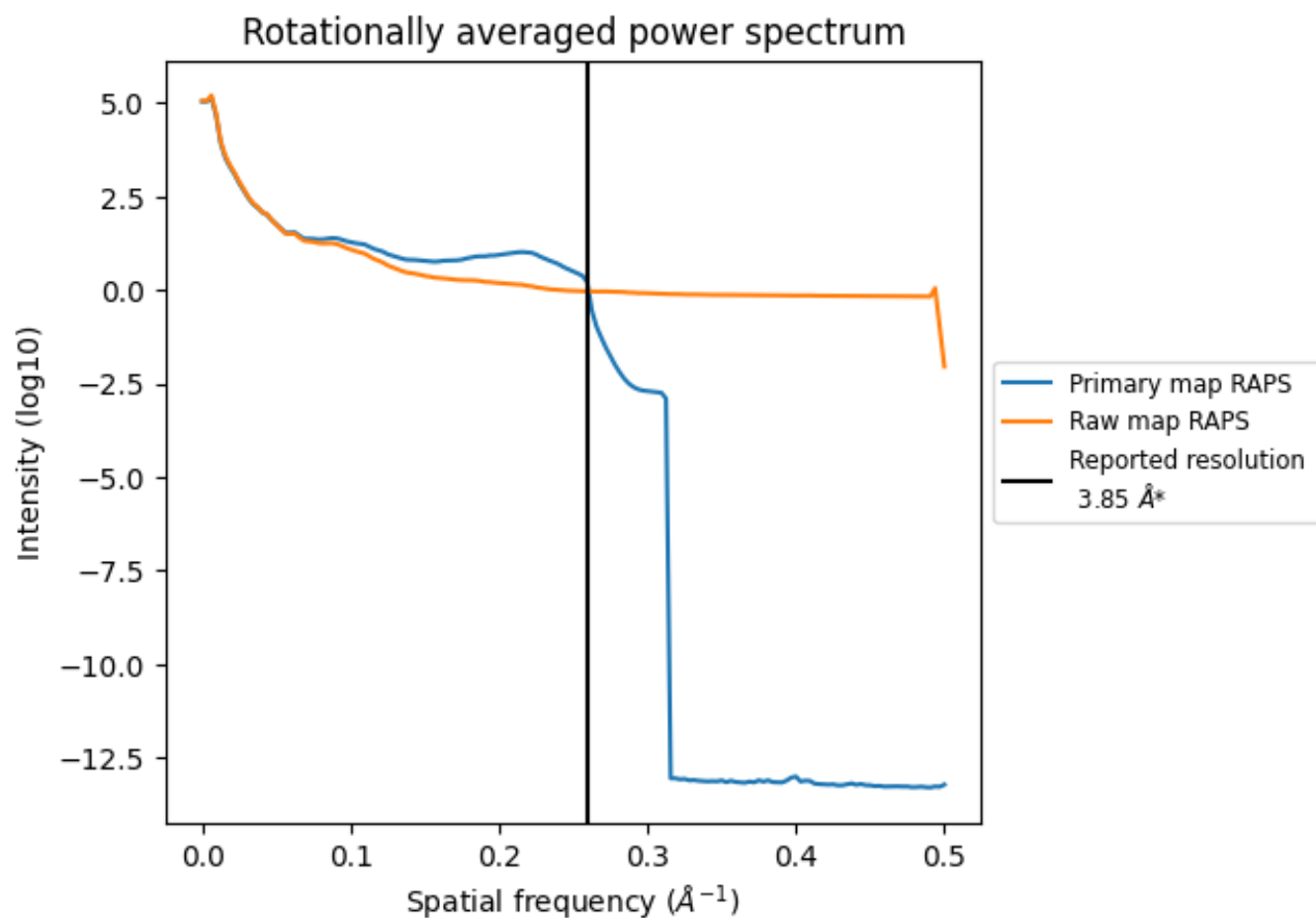
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm³; this corresponds to an approximate mass of 109 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 ⓘ

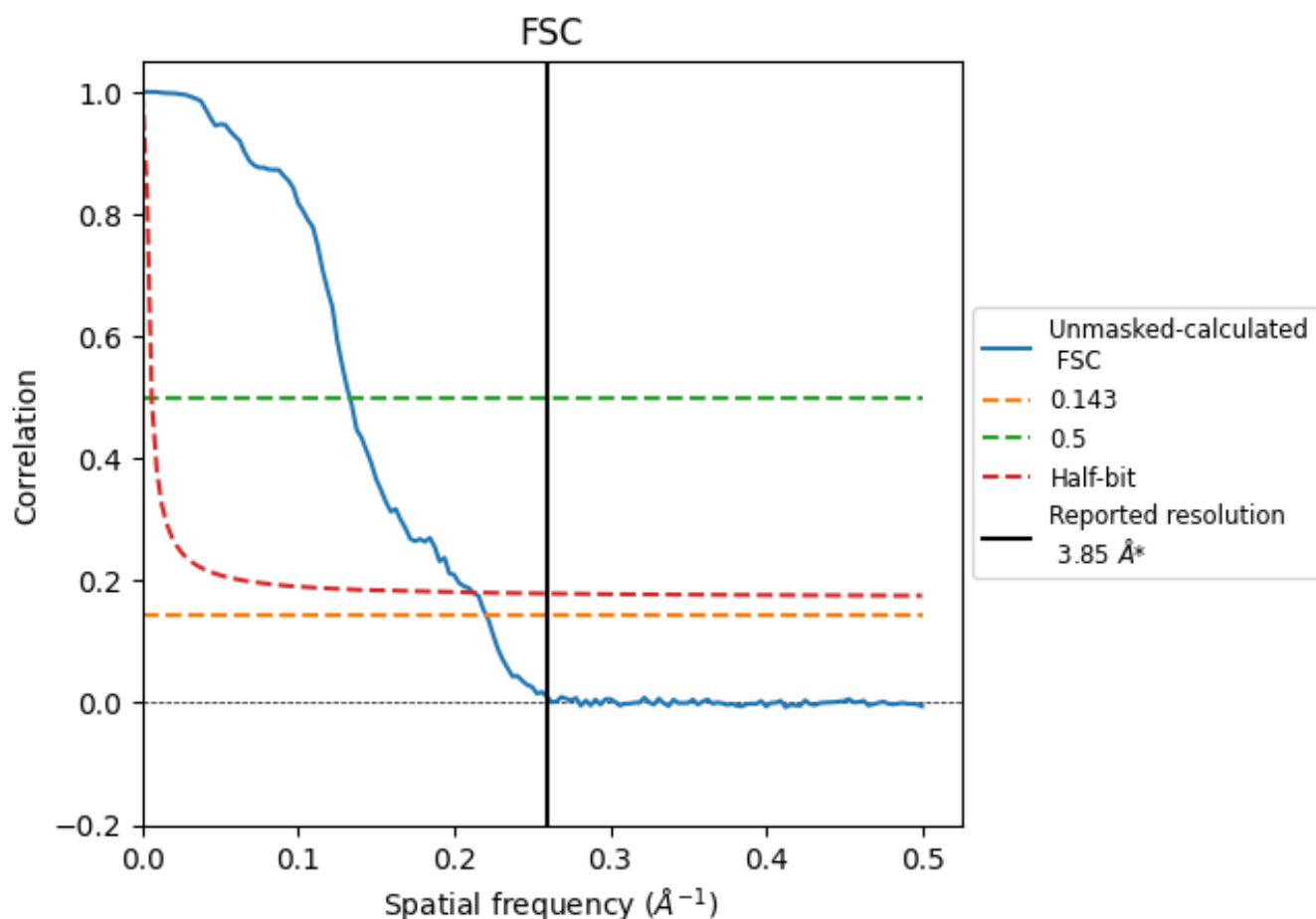


*Reported resolution corresponds to spatial frequency of 0.260 $\text{\AA}^{-1}$

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 0.260 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

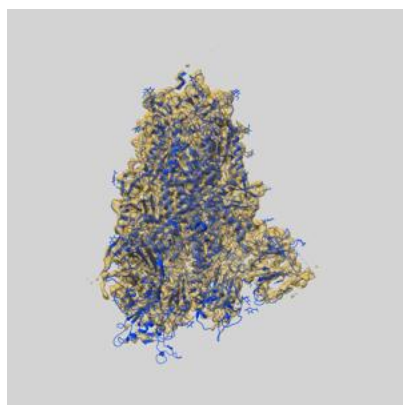
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.54	7.52	4.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.54 differs from the reported value 3.85 by more than 10 %

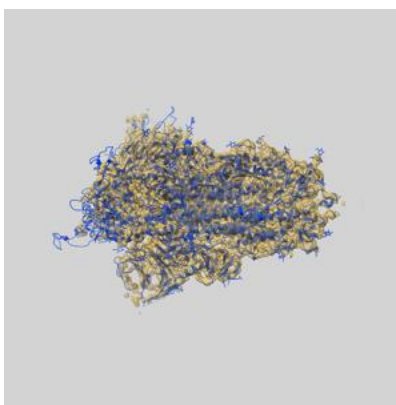
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37550 and PDB model 8WHW. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

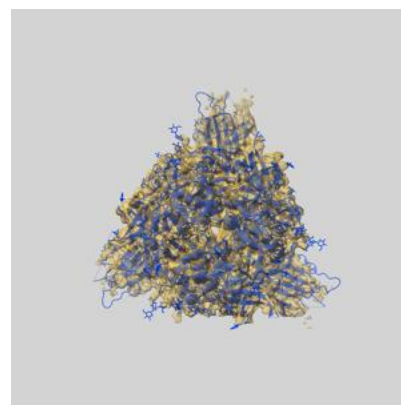
9.1 Map-model overlay [i](#)



X



Y



Z

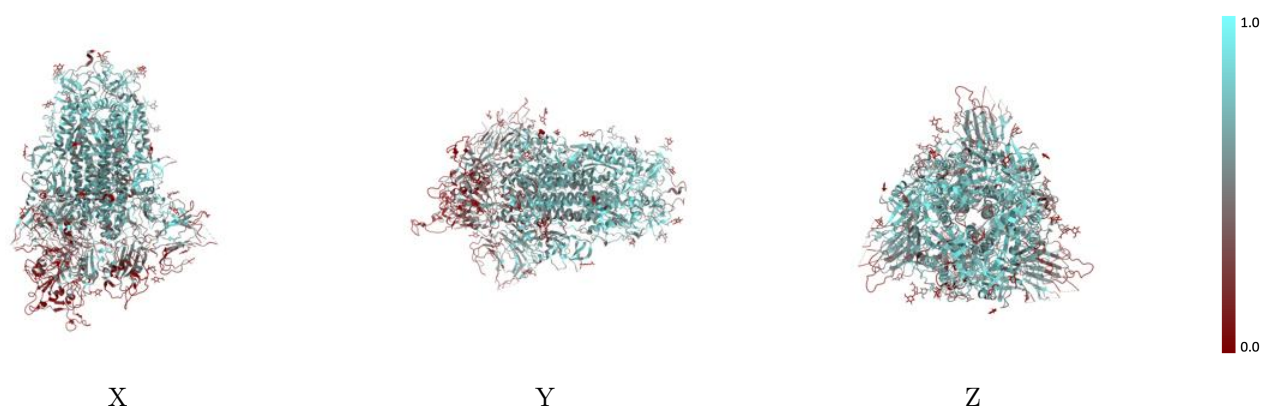
The images above show the 3D surface view of the map at the recommended contour level 0.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



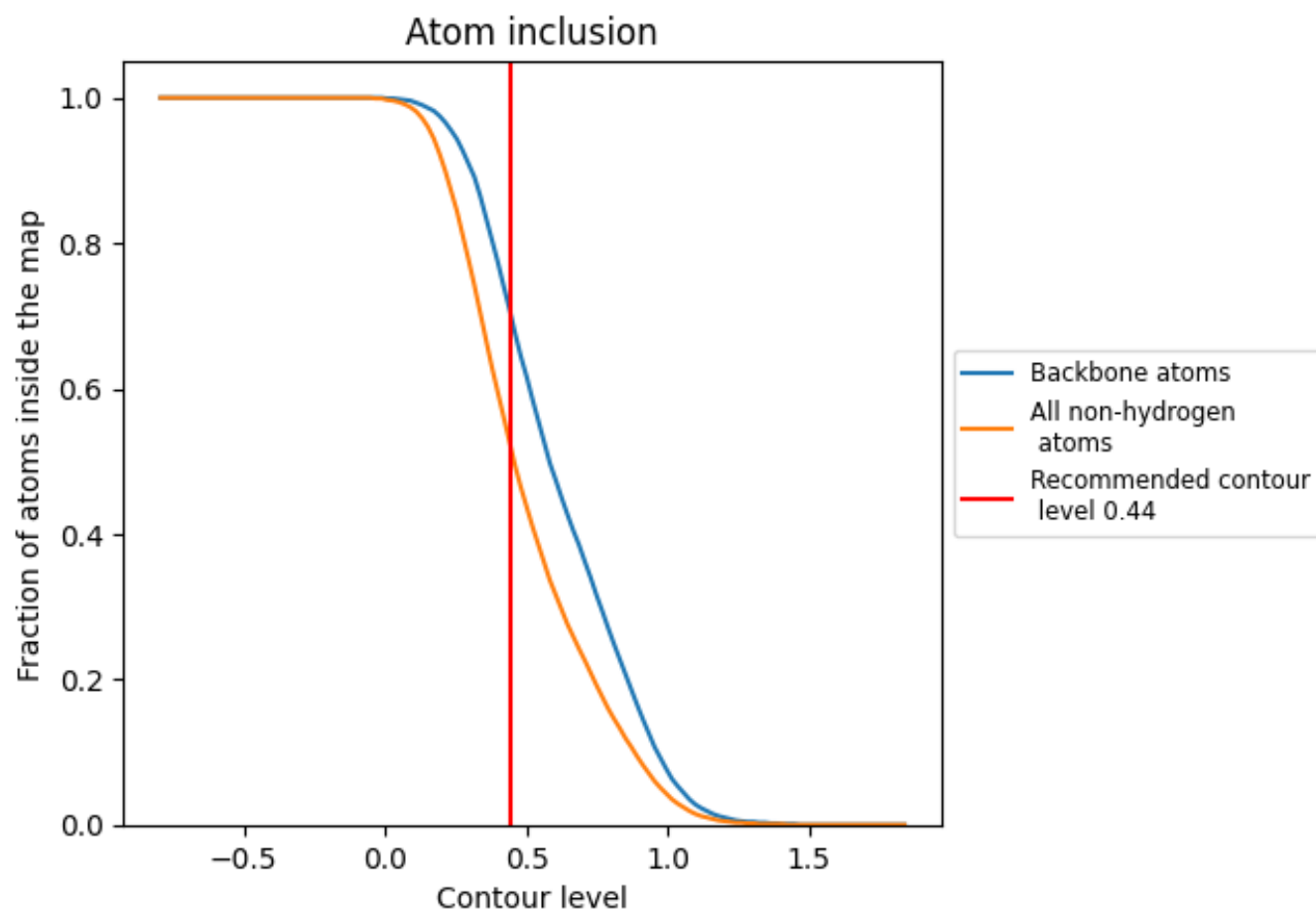
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.44).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 53% 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 (0.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5260	 0.3590
A	 0.5280	 0.3620
B	 0.4930	 0.3390
C	 0.5670	 0.3740
D	 0.0400	 0.3550
E	 0.1200	 0.3390
F	 0.2400	 0.3110
G	 0.5200	 0.4410
H	 0.4800	 0.4660
I	 0.3600	 0.3230
J	 0.0000	 0.2720
K	 0.3600	 0.3580
L	 0.4800	 0.3910
M	 0.4000	 0.4370
N	 0.3200	 0.3580
O	 0.2800	 0.4210
P	 0.1200	 0.3490
Q	 0.2800	 0.3220
R	 0.5200	 0.4160
S	 0.6000	 0.3980
T	 0.3600	 0.2130

