



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 02:35 AM UTC

PDB ID : 9QAW / pdb_00009qaw
EMDB ID : EMD-52977
Title : CryoEM structure of the human LRP2 receptor ectodomain in complex with LRPAP1
Authors : Ramanadane, K.; Coscia, F.
Deposited on : 2025-02-28
Resolution : 3.34 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:

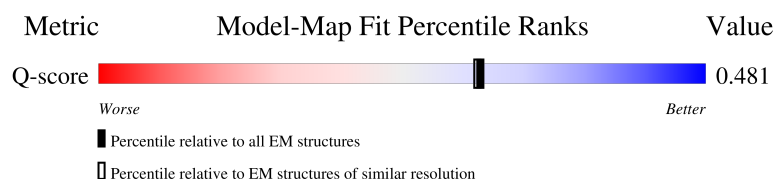
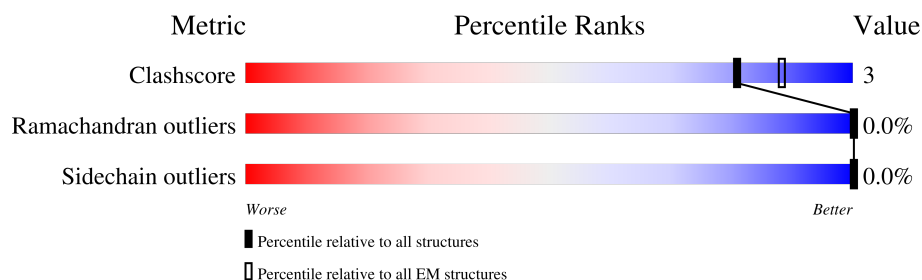
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 3.34 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	14446 (2.84 - 3.84)

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	K	344	
1	L	344	
2	A	4473	
2	B	4473	

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Mol	Chain	Length	Quality of chain
3	D	10	100%
3	E	10	100%
4	C	7	100%
4	F	7	100%
4	J	7	100%
5	H	12	100%
6	I	8	100%
7	G	13	100%
8	M	3	33% 100%
8	N	3	67% 33%
8	T	3	33% 33% 33%
8	X	3	33% 67%
8	Y	3	33% 67%
8	a	3	67% 33%
8	b	3	33% 67%
9	O	2	50% 50%
9	P	2	100%
9	Q	2	50% 50%
9	R	2	100%
9	S	2	50% 50%
9	U	2	50% 50%
9	V	2	50% 50%
9	W	2	100%
9	Z	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	M	2	X	-	-	-
9	NAG	O	2	X	-	-	-
9	NAG	P	2	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 119982 atoms, of which 56524 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 Alpha-2-macroglobulin receptor-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	L	112	Total	C	N	O	3	0
			937	581	176	180		
1	K	112	Total	C	N	O	3	0
			937	581	176	180		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	MET	-	initiating methionine	UNP P30533
L	34	SER	-	expression tag	UNP P30533
L	358	ALA	-	expression tag	UNP P30533
L	359	LEU	-	expression tag	UNP P30533
L	360	GLU	-	expression tag	UNP P30533
L	361	VAL	-	expression tag	UNP P30533
L	362	LEU	-	expression tag	UNP P30533
L	363	PHE	-	expression tag	UNP P30533
L	364	GLN	-	expression tag	UNP P30533
L	365	GLY	-	expression tag	UNP P30533
L	366	PRO	-	expression tag	UNP P30533
L	367	HIS	-	expression tag	UNP P30533
L	368	HIS	-	expression tag	UNP P30533
L	369	HIS	-	expression tag	UNP P30533
L	370	HIS	-	expression tag	UNP P30533
L	371	HIS	-	expression tag	UNP P30533
L	372	HIS	-	expression tag	UNP P30533
L	373	HIS	-	expression tag	UNP P30533
L	374	HIS	-	expression tag	UNP P30533
L	375	HIS	-	expression tag	UNP P30533
L	376	HIS	-	expression tag	UNP P30533
K	33	MET	-	initiating methionine	UNP P30533
K	34	SER	-	expression tag	UNP P30533
K	358	ALA	-	expression tag	UNP P30533
K	359	LEU	-	expression tag	UNP P30533
K	360	GLU	-	expression tag	UNP P30533

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Chain	Residue	Modelled	Actual	Comment	Reference
K	361	VAL	-	expression tag	UNP P30533
K	362	LEU	-	expression tag	UNP P30533
K	363	PHE	-	expression tag	UNP P30533
K	364	GLN	-	expression tag	UNP P30533
K	365	GLY	-	expression tag	UNP P30533
K	366	PRO	-	expression tag	UNP P30533
K	367	HIS	-	expression tag	UNP P30533
K	368	HIS	-	expression tag	UNP P30533
K	369	HIS	-	expression tag	UNP P30533
K	370	HIS	-	expression tag	UNP P30533
K	371	HIS	-	expression tag	UNP P30533
K	372	HIS	-	expression tag	UNP P30533
K	373	HIS	-	expression tag	UNP P30533
K	374	HIS	-	expression tag	UNP P30533
K	375	HIS	-	expression tag	UNP P30533
K	376	HIS	-	expression tag	UNP P30533

- Molecule 2 is a protein called Low-density lipoprotein receptor-related protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	3830	Total	C	H	N	O	S	0	0
			58178	18729	28010	5279	5854	306		
2	B	3824	Total	C	H	N	O	S	0	0
			58043	18688	27935	5268	5846	306		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4424	GLY	-	expression tag	UNP P98164
A	4425	TRP	-	expression tag	UNP P98164
A	4426	SER	-	expression tag	UNP P98164
A	4427	HIS	-	expression tag	UNP P98164
A	4428	PRO	-	expression tag	UNP P98164
A	4429	GLN	-	expression tag	UNP P98164
A	4430	PHE	-	expression tag	UNP P98164
A	4431	GLU	-	expression tag	UNP P98164
A	4432	LYS	-	expression tag	UNP P98164
A	4433	ALA	-	expression tag	UNP P98164
A	4434	GLY	-	expression tag	UNP P98164
A	4435	GLY	-	expression tag	UNP P98164
A	4436	GLY	-	expression tag	UNP P98164
A	4437	SER	-	expression tag	UNP P98164

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4438	GLY	-	expression tag	UNP P98164
A	4439	GLY	-	expression tag	UNP P98164
A	4440	GLY	-	expression tag	UNP P98164
A	4441	SER	-	expression tag	UNP P98164
A	4442	GLY	-	expression tag	UNP P98164
A	4443	GLY	-	expression tag	UNP P98164
A	4444	GLY	-	expression tag	UNP P98164
A	4445	SER	-	expression tag	UNP P98164
A	4446	TRP	-	expression tag	UNP P98164
A	4447	SER	-	expression tag	UNP P98164
A	4448	HIS	-	expression tag	UNP P98164
A	4449	PRO	-	expression tag	UNP P98164
A	4450	GLN	-	expression tag	UNP P98164
A	4451	PHE	-	expression tag	UNP P98164
A	4452	GLU	-	expression tag	UNP P98164
A	4453	LYS	-	expression tag	UNP P98164
A	4454	GLY	-	expression tag	UNP P98164
A	4455	GLY	-	expression tag	UNP P98164
A	4456	GLY	-	expression tag	UNP P98164
A	4457	SER	-	expression tag	UNP P98164
A	4458	GLY	-	expression tag	UNP P98164
A	4459	GLY	-	expression tag	UNP P98164
A	4460	GLY	-	expression tag	UNP P98164
A	4461	SER	-	expression tag	UNP P98164
A	4462	GLY	-	expression tag	UNP P98164
A	4463	GLY	-	expression tag	UNP P98164
A	4464	GLY	-	expression tag	UNP P98164
A	4465	SER	-	expression tag	UNP P98164
A	4466	TRP	-	expression tag	UNP P98164
A	4467	SER	-	expression tag	UNP P98164
A	4468	HIS	-	expression tag	UNP P98164
A	4469	PRO	-	expression tag	UNP P98164
A	4470	GLN	-	expression tag	UNP P98164
A	4471	PHE	-	expression tag	UNP P98164
A	4472	GLU	-	expression tag	UNP P98164
A	4473	LYS	-	expression tag	UNP P98164
B	4424	GLY	-	expression tag	UNP P98164
B	4425	TRP	-	expression tag	UNP P98164
B	4426	SER	-	expression tag	UNP P98164
B	4427	HIS	-	expression tag	UNP P98164
B	4428	PRO	-	expression tag	UNP P98164
B	4429	GLN	-	expression tag	UNP P98164

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4430	PHE	-	expression tag	UNP P98164
B	4431	GLU	-	expression tag	UNP P98164
B	4432	LYS	-	expression tag	UNP P98164
B	4433	ALA	-	expression tag	UNP P98164
B	4434	GLY	-	expression tag	UNP P98164
B	4435	GLY	-	expression tag	UNP P98164
B	4436	GLY	-	expression tag	UNP P98164
B	4437	SER	-	expression tag	UNP P98164
B	4438	GLY	-	expression tag	UNP P98164
B	4439	GLY	-	expression tag	UNP P98164
B	4440	GLY	-	expression tag	UNP P98164
B	4441	SER	-	expression tag	UNP P98164
B	4442	GLY	-	expression tag	UNP P98164
B	4443	GLY	-	expression tag	UNP P98164
B	4444	GLY	-	expression tag	UNP P98164
B	4445	SER	-	expression tag	UNP P98164
B	4446	TRP	-	expression tag	UNP P98164
B	4447	SER	-	expression tag	UNP P98164
B	4448	HIS	-	expression tag	UNP P98164
B	4449	PRO	-	expression tag	UNP P98164
B	4450	GLN	-	expression tag	UNP P98164
B	4451	PHE	-	expression tag	UNP P98164
B	4452	GLU	-	expression tag	UNP P98164
B	4453	LYS	-	expression tag	UNP P98164
B	4454	GLY	-	expression tag	UNP P98164
B	4455	GLY	-	expression tag	UNP P98164
B	4456	GLY	-	expression tag	UNP P98164
B	4457	SER	-	expression tag	UNP P98164
B	4458	GLY	-	expression tag	UNP P98164
B	4459	GLY	-	expression tag	UNP P98164
B	4460	GLY	-	expression tag	UNP P98164
B	4461	SER	-	expression tag	UNP P98164
B	4462	GLY	-	expression tag	UNP P98164
B	4463	GLY	-	expression tag	UNP P98164
B	4464	GLY	-	expression tag	UNP P98164
B	4465	SER	-	expression tag	UNP P98164
B	4466	TRP	-	expression tag	UNP P98164
B	4467	SER	-	expression tag	UNP P98164
B	4468	HIS	-	expression tag	UNP P98164
B	4469	PRO	-	expression tag	UNP P98164
B	4470	GLN	-	expression tag	UNP P98164
B	4471	PHE	-	expression tag	UNP P98164

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4472	GLU	-	expression tag	UNP P98164
B	4473	LYS	-	expression tag	UNP P98164

- Molecule 3 is a protein called Unidentified peptide 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	10	Total	C	N	O	0	0
			50	30	10	10		
3	E	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 4 is a protein called Unidentified peptide 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	7	Total	C	N	O	0	0
			35	21	7	7		
4	F	7	Total	C	N	O	0	0
			35	21	7	7		
4	J	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 5 is a protein called Unidentified peptide 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	12	Total	C	N	O	0	0
			60	36	12	12		

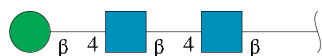
- Molecule 6 is a protein called Unidentified peptide 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 7 is a protein called Unidentified peptide 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	13	Total	C	N	O	0	0
			65	39	13	13		

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
8	N	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
8	T	3	Total	C	N	O		0	0
			39	22	2	15			
8	X	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
8	Y	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
8	a	3	Total	C	N	O		0	0
			39	22	2	15			
8	b	3	Total	C	N	O		0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



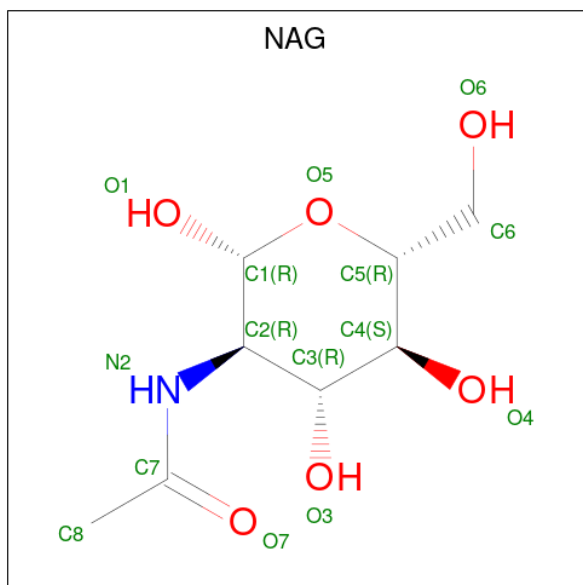
Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	2	Total	C	H	N	O	0	0
			54	16	26	2	10		
9	P	2	Total	C	H	N	O	0	0
			54	16	26	2	10		
9	Q	2	Total	C	H	N	O	0	0
			54	16	26	2	10		
9	R	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
9	S	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
9	U	2	Total	C	N	O		0	0
			28	16	2	10			
9	V	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
9	W	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



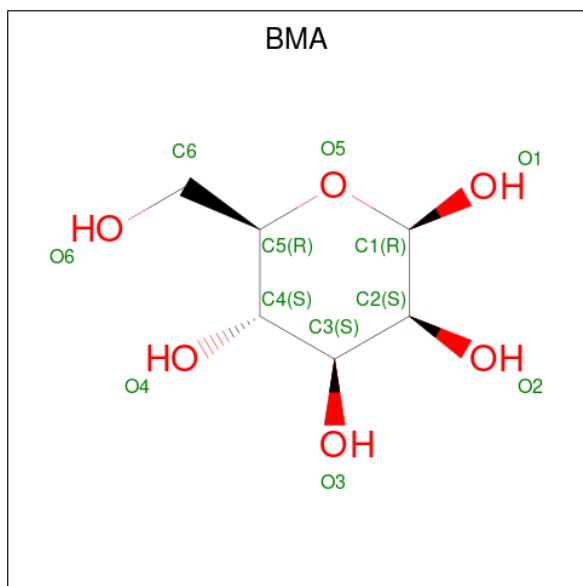
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	A	1	Total	C	N	O		0
			14	8	1	5		
10	A	1	Total	C	N	O		0
			14	8	1	5		
10	A	1	Total	C	N	O		0
			14	8	1	5		

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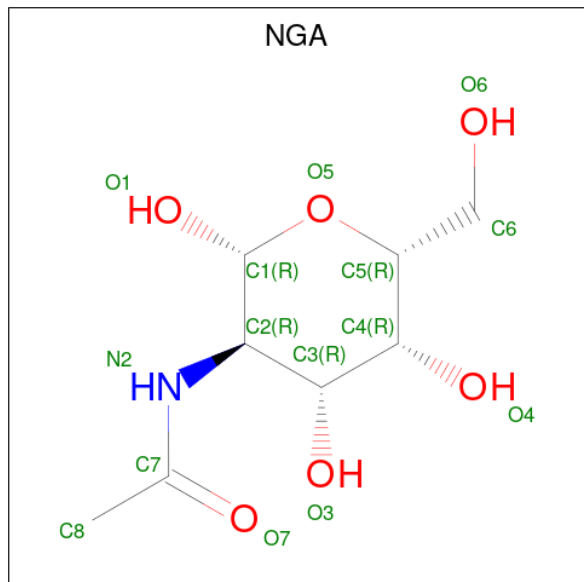
Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
10	B	1	Total	C	N	O		0
			14	8	1	5		
10	B	1	Total	C	N	O		0
			14	8	1	5		

- Molecule 11 is beta-D-mannopyranose (CCD ID: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	H	O	0
			22	6	11	5	
11	A	1	Total	C	H	O	0
			22	6	11	5	

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-galactopyranose (CCD ID: NGA) (formula: $C_8H_{15}NO_6$).



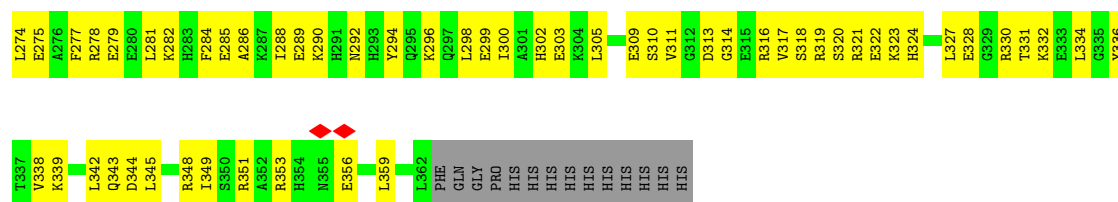
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 13 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
13	A	12	Total	Ca	0
			12	12	
13	B	13	Total	Ca	0
			13	13	

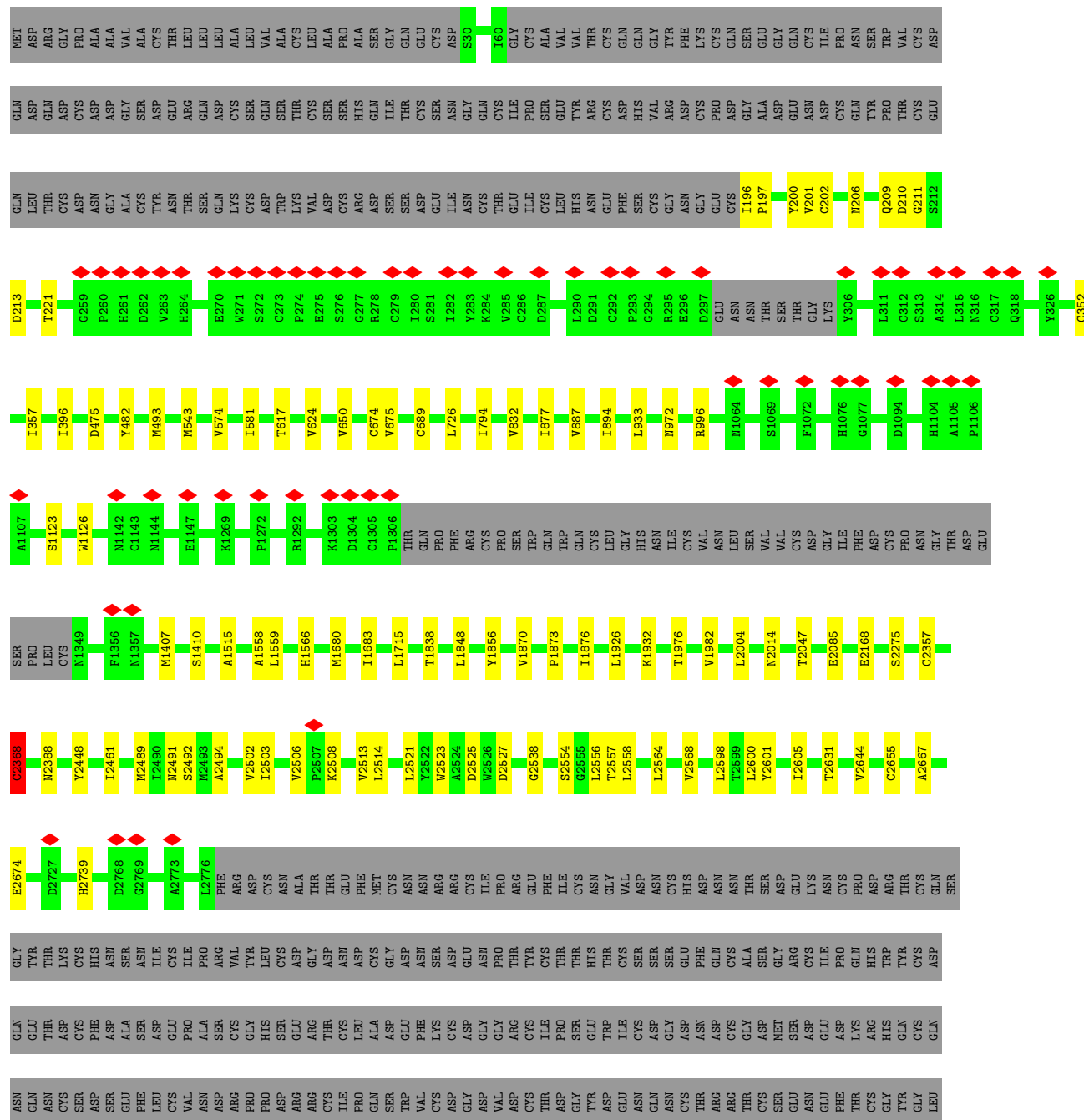
- Molecule 14 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

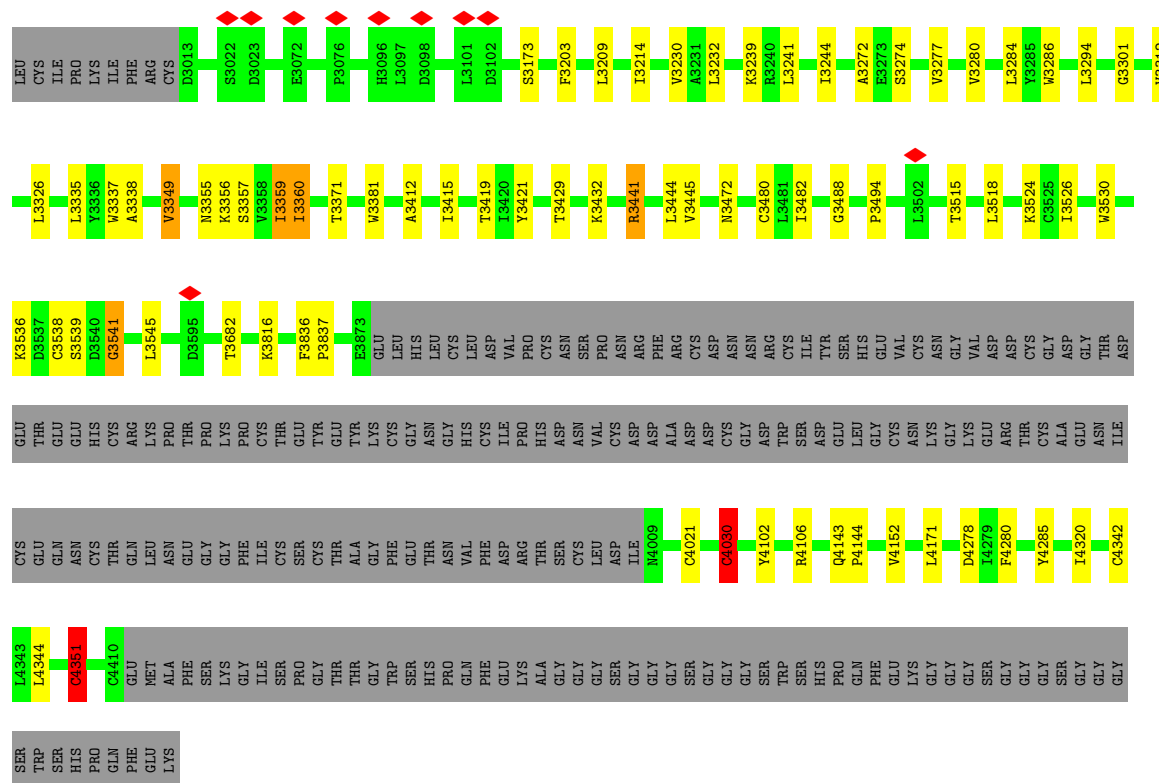
Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total 1	Ni 1	0
14	B	1	Total 1	Ni 1	0



• Molecule 2: Low-density lipoprotein receptor-related protein 2

Chain A: 83% 14%





- Molecule 3: Unidentified peptide 1

Chain D: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unidentified peptide 1

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 4: Unidentified peptide 2

Chain C: 100%

There are no outlier residues recorded for this chain.

- Molecule 4: Unidentified peptide 2

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 4: Unidentified peptide 2

Chain J: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unidentified peptide 3

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unidentified peptide 4

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Unidentified peptide 5

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 100%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  67% 33%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  33% 33% 33%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  33% 67%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  33% 67%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  67% 33%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  33% 67%

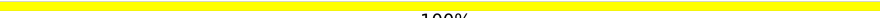


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50% 50%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	318131	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.942	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.095	Depositor
Map size (Å)	534.8, 534.8, 534.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.955, 0.955, 0.955	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, CA, NGA, NI

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	K	0.19	0/965	0.50	0/1291
1	L	0.17	0/965	0.38	0/1291
2	A	0.20	0/30915	0.37	4/41998 (0.0%)
2	B	0.22	0/30852	0.52	60/41912 (0.1%)
All	All	0.21	0/63697	0.45	64/86492 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	B	0	4
All	All	0	6

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3016	ASN	CA-C-N	11.71	143.90	121.54
2	A	3016	ASN	C-N-CA	11.71	143.90	121.54
2	B	3301	GLY	CA-C-N	10.55	142.08	121.41
2	B	3301	GLY	C-N-CA	10.55	142.08	121.41
2	B	3524	LYS	CA-C-N	10.35	141.32	121.54
2	B	3524	LYS	C-N-CA	10.35	141.32	121.54
2	B	3280	VAL	CA-C-N	10.30	141.67	121.58
2	B	3280	VAL	C-N-CA	10.30	141.67	121.58
2	B	3518	LEU	CA-C-N	10.05	142.42	122.31
2	B	3518	LEU	C-N-CA	10.05	142.42	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3349	VAL	CA-C-N	9.41	139.86	121.41
2	B	3349	VAL	C-N-CA	9.41	139.86	121.41
2	B	3359	ILE	CA-C-N	9.40	138.90	121.97
2	B	3359	ILE	C-N-CA	9.40	138.90	121.97
2	B	3480	CYS	CA-C-N	9.37	135.65	122.72
2	B	3480	CYS	C-N-CA	9.37	135.65	122.72
2	B	3274	SER	CA-C-N	9.34	134.85	120.75
2	B	3274	SER	C-N-CA	9.34	134.85	120.75
2	B	3444	LEU	CA-C-N	9.11	138.36	121.97
2	B	3444	LEU	C-N-CA	9.11	138.36	121.97
2	B	3541	GLY	CA-C-N	8.89	137.21	122.54
2	B	3541	GLY	C-N-CA	8.89	137.21	122.54
2	B	3472	ASN	CA-C-N	8.80	138.52	123.91
2	B	3472	ASN	C-N-CA	8.80	138.52	123.91
2	B	3539	SER	CA-C-N	8.45	131.60	120.28
2	B	3539	SER	C-N-CA	8.45	131.60	120.28
2	B	3338	ALA	CA-C-N	8.45	135.21	121.86
2	B	3338	ALA	C-N-CA	8.45	135.21	121.86
2	B	3494	PRO	CA-C-N	8.37	131.32	120.44
2	B	3494	PRO	C-N-CA	8.37	131.32	120.44
2	B	3357	SER	CA-C-N	8.30	132.44	120.91
2	B	3357	SER	C-N-CA	8.30	132.44	120.91
2	B	3412	ALA	CA-C-N	8.24	134.78	122.58
2	B	3412	ALA	C-N-CA	8.24	134.78	122.58
2	B	1224	THR	CA-C-N	8.20	131.80	120.65
2	B	1224	THR	C-N-CA	8.20	131.80	120.65
2	B	3538	CYS	CA-C-N	8.10	131.46	120.44
2	B	3538	CYS	C-N-CA	8.10	131.46	120.44
2	B	3203	PHE	CA-C-N	8.07	134.16	122.77
2	B	3203	PHE	C-N-CA	8.07	134.16	122.77
2	B	3545	LEU	CA-C-N	7.92	131.23	120.54
2	B	3545	LEU	C-N-CA	7.92	131.23	120.54
2	B	3445	VAL	CA-C-N	7.86	134.78	123.14
2	B	3445	VAL	C-N-CA	7.86	134.78	123.14
2	B	4351	CYS	CA-CB-SG	7.71	132.14	114.40
2	B	3415	ILE	CA-C-N	7.46	134.32	121.64
2	B	3415	ILE	C-N-CA	7.46	134.32	121.64
2	B	3441	ARG	CA-C-N	7.42	134.48	121.80
2	B	3441	ARG	C-N-CA	7.42	134.48	121.80
2	B	3381	TRP	CA-C-N	7.18	134.36	122.73
2	B	3381	TRP	C-N-CA	7.18	134.36	122.73
2	B	4144	PRO	N-CA-C	6.62	121.72	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2368	CYS	CA-CB-SG	6.30	128.90	114.40
2	A	4021	CYS	CA-CB-SG	6.01	128.23	114.40
2	B	3682	THR	OG1-CB-CG2	5.86	121.02	109.30
2	B	3419	THR	OG1-CB-CG2	5.84	120.99	109.30
2	B	3515	THR	OG1-CB-CG2	5.79	120.88	109.30
2	B	3429	THR	OG1-CB-CG2	5.72	120.74	109.30
2	B	3371	THR	OG1-CB-CG2	5.47	120.24	109.30
2	B	4030	CYS	CA-CB-SG	5.45	126.93	114.40
2	B	3371	THR	CA-CB-CG2	5.41	119.70	110.50
2	B	3359	ILE	CG1-CB-CG2	5.32	126.67	110.70
2	B	2043	CYS	CA-CB-SG	5.11	126.16	114.40
2	B	3230	VAL	CG1-CB-CG2	5.08	121.98	110.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2368	CYS	Peptide
2	A	2554	SER	Peptide
2	B	1161	CYS	Peptide
2	B	1174	CYS	Peptide
2	B	4030	CYS	Peptide
2	B	4351	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	937	0	924	98	0
1	L	937	0	924	65	0
2	A	30168	28010	28180	79	0
2	B	30108	27935	28083	80	0
3	D	50	0	12	0	0
3	E	50	0	12	0	0
4	C	35	0	10	0	0
4	F	35	0	9	0	0
4	J	35	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	60	0	15	0	0
6	I	40	0	11	0	0
7	G	65	0	16	0	0
8	M	39	37	33	0	0
8	N	39	37	34	0	0
8	T	39	0	34	1	0
8	X	39	37	34	0	0
8	Y	39	37	34	0	0
8	a	39	0	34	0	0
8	b	39	0	34	0	0
9	O	28	26	23	0	0
9	P	28	26	24	0	0
9	Q	28	26	25	0	0
9	R	28	27	25	0	0
9	S	28	27	25	2	0
9	U	28	0	25	0	0
9	V	28	27	25	2	0
9	W	28	27	25	0	0
9	Z	28	27	25	0	0
10	A	140	98	130	1	0
10	B	126	98	117	2	0
11	A	22	22	20	0	0
12	A	56	0	52	1	0
12	B	42	0	39	3	0
13	A	12	0	0	0	0
13	B	13	0	0	0	0
14	A	1	0	0	0	0
14	B	1	0	0	0	0
All	All	63458	56524	59023	319	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 3.

All (319) 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:K:269:LEU:HD23	1:K:274:LEU:HA	1.38	1.05
1:L:291:HIS:HB2	1:L:334:LEU:HD22	1.52	0.88
1:L:271:ASP:HA	1:L:274:LEU:HD12	1.58	0.84
1:L:305:LEU:HD22	1:L:321:ARG:HD3	1.59	0.84
1:K:252:PHE:HB3	1:K:258:ILE:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:617:THR:HG22	2:A:624:VAL:HG22	1.66	0.78
1:L:308:ALA:HB3	1:L:321:ARG:HH22	1.52	0.74
1:K:316:ARG:HG2	1:K:319:ARG:HE	1.54	0.72
1:L:308:ALA:HB1	1:L:317:VAL:HG22	1.72	0.71
1:L:314:GLY:HA2	1:L:317:VAL:HB	1.71	0.71
1:L:316:ARG:HG2	1:L:319:ARG:HE	1.56	0.70
2:B:201:VAL:HG12	2:B:202:CYS:H	1.56	0.70
2:B:4021:CYS:HA	2:B:4030:CYS:HB3	1.75	0.69
2:A:3226:LEU:HD13	2:A:3229:VAL:HG11	1.75	0.69
1:K:321:ARG:HG2	1:K:324:HIS:HE1	1.57	0.68
1:L:336:TYR:HA	1:L:339:LYS:HE3	1.74	0.68
1:L:307:HIS:O	1:L:311:VAL:HG12	1.94	0.68
1:K:314:GLY:HA2	1:K:317:VAL:HB	1.76	0.67
1:K:336:TYR:HA	1:K:339:LYS:HG2	1.76	0.67
1:L:291:HIS:HB2	1:L:334:LEU:CD2	2.22	0.67
1:K:316:ARG:O	1:K:319:ARG:HG3	1.94	0.66
2:A:2357:CYS:HA	2:A:2368:CYS:HB3	1.77	0.66
2:B:4342:CYS:HA	2:B:4351:CYS:HB3	1.76	0.66
1:K:275:GLU:O	1:K:279:GLU:HG2	1.96	0.65
1:L:296:LYS:O	1:L:299:GLU:HG3	1.97	0.65
2:B:212:SER:HA	2:B:215:HIS:NE2	2.13	0.64
1:K:319:ARG:O	1:K:322:GLU:HG3	1.97	0.64
1:K:268:ASN:O	1:K:270:THR:HG23	1.98	0.64
1:K:296:LYS:O	1:K:300:ILE:HG12	1.99	0.63
1:K:309:GLU:O	1:K:314:GLY:HA3	1.97	0.63
1:K:257:VAL:HG21	1:K:285[A]:GLU:HB3	1.79	0.63
1:L:333:GLU:O	1:L:337:THR:HG23	1.99	0.63
1:L:301:ALA:O	1:L:305:LEU:HG	1.99	0.62
1:K:264:ALA:HB1	1:K:269:LEU:CD2	2.29	0.62
1:K:339:LYS:HA	1:K:342:LEU:CD2	2.29	0.62
1:L:277:PHE:CE2	1:L:348:ARG:HD3	2.35	0.62
1:K:279:GLU:O	1:K:282:LYS:HG2	2.00	0.62
1:K:286:ALA:O	1:K:289:GLU:HG3	1.99	0.62
1:L:267:ALA:HA	1:L:353:ARG:HH22	1.65	0.62
1:L:298:LEU:CD1	1:L:327:LEU:HB3	2.29	0.61
1:K:257:VAL:HG21	1:K:285[B]:GLU:HB3	1.79	0.61
2:A:201:VAL:HA	2:A:213:ASP:HB3	1.81	0.61
1:K:267:ALA:HB3	1:K:269:LEU:HD13	1.83	0.61
1:K:321:ARG:HG2	1:K:324:HIS:CE1	2.36	0.60
2:A:1838:THR:HG23	2:A:1876:ILE:HD11	1.83	0.60
1:K:284:PHE:HZ	1:K:342:LEU:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2714:SER:HG	2:B:2717:TRP:CD1	2.20	0.59
1:K:298:LEU:HD23	1:K:331:THR:HG21	1.83	0.59
1:K:328:GLU:HB3	1:K:332:LYS:NZ	2.17	0.59
2:A:2557:THR:HG22	2:A:2598:LEU:HD23	1.83	0.59
1:K:275:GLU:O	1:K:278:ARG:HG2	2.01	0.59
1:K:321:ARG:HA	1:K:324:HIS:ND1	2.17	0.58
2:A:726:LEU:HD21	1:K:356:GLU:HG3	1.84	0.58
1:L:298:LEU:HD11	1:L:327:LEU:HB3	1.86	0.58
1:L:279:GLU:O	1:L:282:LYS:HG2	2.04	0.58
2:B:617:THR:HG21	2:B:646:TYR:O	2.04	0.58
1:K:314:GLY:HA2	1:K:317:VAL:CG2	2.34	0.58
1:L:324:HIS:O	1:L:328:GLU:HG3	2.04	0.57
2:A:2655:CYS:HB3	2:A:2674:GLU:OE1	2.04	0.57
2:A:197:PRO:HB2	2:A:200:TYR:CE2	2.39	0.57
1:K:264:ALA:HB1	1:K:269:LEU:HD21	1.86	0.57
1:L:261:TRP:CH2	1:L:278:ARG:HD3	2.38	0.57
1:L:328:GLU:O	1:L:332:LYS:HG2	2.04	0.57
1:L:260:LEU:CD1	1:L:281:LEU:HD11	2.34	0.57
1:L:277:PHE:O	1:L:281:LEU:HD23	2.04	0.57
1:L:302:HIS:HA	1:L:305:LEU:HG	1.86	0.57
1:L:267:ALA:HA	1:L:353:ARG:HH12	1.70	0.57
1:L:260:LEU:HD13	1:L:281:LEU:HD11	1.87	0.57
2:A:887:VAL:HG12	2:A:894:ILE:HG12	1.85	0.57
2:B:3337:TRP:CZ3	2:B:3349:VAL:HG12	2.39	0.57
1:K:313:ASP:O	1:K:317:VAL:HG23	2.05	0.57
1:K:289:GLU:HA	1:K:292:ASN:HD21	1.68	0.56
2:B:4280:PHE:HB2	2:B:4320:ILE:HD13	1.86	0.56
1:K:344:ASP:O	1:K:348:ARG:HG3	2.05	0.56
2:B:212:SER:HA	2:B:215:HIS:CD2	2.40	0.56
2:A:1407:MET:HE3	2:A:1410:SER:HB3	1.87	0.56
1:K:328:GLU:O	1:K:332:LYS:HG3	2.06	0.56
2:A:996:ARG:O	2:B:2744:THR:HG22	2.06	0.56
1:K:305:LEU:CD2	1:K:321:ARG:HB2	2.37	0.55
1:K:320:SER:HA	1:K:323:LYS:CE	2.36	0.55
1:L:338:VAL:O	1:L:342:LEU:HG	2.06	0.55
2:B:272:SER:HA	2:B:324:THR:HG21	1.88	0.55
1:L:252:PHE:HB3	1:L:256:ARG:NH2	2.21	0.55
1:K:339:LYS:HA	1:K:342:LEU:HG	1.87	0.55
2:A:396:ILE:HD12	2:A:650:VAL:HG22	1.87	0.55
2:B:396:ILE:CD1	2:B:650:VAL:HG22	2.37	0.55
1:L:334:LEU:HD23	1:L:338:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1566:HIS:ND1	2:A:1715:LEU:HD23	2.21	0.54
2:A:352:CYS:HB2	2:A:357:ILE:HG21	1.88	0.54
2:A:4021:CYS:HB3	2:A:4030:CYS:HA	1.90	0.54
2:B:2033:CYS:HA	2:B:2043:CYS:HB2	1.90	0.54
1:K:320:SER:HA	1:K:323:LYS:HE2	1.88	0.54
2:B:4278:ASP:OD2	2:B:4320:ILE:HD12	2.07	0.54
2:A:1926:LEU:HD12	2:A:1932:LYS:O	2.08	0.54
1:K:305:LEU:HD21	1:K:317:VAL:O	2.07	0.54
1:K:348:ARG:HA	1:K:351:ARG:CD	2.37	0.54
2:A:574:VAL:HG12	2:A:581:ILE:HG12	1.89	0.54
1:K:284:PHE:CZ	1:K:342:LEU:HB3	2.43	0.54
1:L:284:PHE:CE2	1:L:288:ILE:HD11	2.43	0.54
1:L:299:GLU:O	1:L:303:GLU:HG2	2.07	0.54
1:L:334:LEU:HD23	1:L:334:LEU:O	2.08	0.54
1:K:284:PHE:O	1:K:288:ILE:HG13	2.07	0.54
1:K:299:GLU:O	1:K:303:GLU:HG3	2.08	0.54
1:K:318:SER:O	1:K:321:ARG:HB3	2.08	0.54
2:A:2506:VAL:HG13	2:A:2508:LYS:O	2.07	0.53
1:K:324:HIS:O	1:K:328:GLU:HG3	2.09	0.53
2:B:4106:ARG:HG2	2:B:4143:GLN:HA	1.91	0.53
1:L:256:ARG:HD2	1:L:285[A]:GLU:OE1	2.08	0.53
1:L:339:LYS:O	1:L:343:GLN:HG2	2.08	0.53
2:B:753:SER:HB3	2:B:770:ILE:HD12	1.91	0.53
2:B:3482:ILE:HA	2:B:3488:GLY:HA2	1.89	0.53
2:A:396:ILE:CD1	2:A:650:VAL:HG22	2.39	0.53
2:B:3244:ILE:HD11	2:B:3272:ALA:HB3	1.91	0.52
1:K:254:GLU:OE2	1:K:255:PRO:HD2	2.09	0.52
1:K:305:LEU:CD2	1:K:317:VAL:HG12	2.39	0.52
2:B:1593:VAL:HG12	2:B:1597:ILE:HD11	1.91	0.52
2:B:4342:CYS:HA	2:B:4351:CYS:CB	2.40	0.52
2:A:832:VAL:HG11	2:A:877:ILE:HD12	1.92	0.52
12:B:4508:NGA:H83	12:B:4508:NGA:H3	1.92	0.52
2:B:470:GLU:OE1	2:B:486:THR:HG21	2.10	0.52
1:K:348:ARG:O	1:K:351:ARG:HD3	2.10	0.52
1:K:314:GLY:HA2	1:K:317:VAL:CB	2.39	0.52
2:A:4021:CYS:CB	2:A:4030:CYS:HA	2.40	0.52
2:A:2508:LYS:HG3	2:A:2527:ASP:HB3	1.93	0.51
2:B:3214:ILE:HD11	2:B:3421:TYR:OH	2.09	0.51
1:L:298:LEU:HD22	1:L:331:THR:HG21	1.93	0.51
10:A:4510:NAG:H83	10:A:4510:NAG:H3	1.92	0.51
2:B:794:ILE:HG21	2:B:972:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ASN:H	2:B:214:GLU:HG2	1.76	0.51
2:A:221:THR:HG21	12:A:4511:NGA:C7	2.41	0.51
1:K:348:ARG:HA	1:K:351:ARG:NE	2.26	0.51
1:L:317:VAL:O	1:L:321:ARG:HG2	2.11	0.51
1:L:330:ARG:O	1:L:333:GLU:HG3	2.10	0.51
1:K:327:LEU:HA	1:K:330:ARG:HG2	1.92	0.51
1:L:308:ALA:HB1	1:L:317:VAL:CG2	2.38	0.50
2:A:4161:VAL:HG22	2:A:4187:PRO:O	2.11	0.50
1:L:336:TYR:O	1:L:339:LYS:HG2	2.11	0.50
2:B:3536:LYS:HE3	2:B:3541:GLY:HA2	1.94	0.50
2:B:205:ASP:HB3	2:B:213:ASP:OD2	2.12	0.50
2:A:832:VAL:CG1	2:A:877:ILE:HD12	2.42	0.50
1:L:261:TRP:HH2	1:L:278:ARG:HD3	1.77	0.50
2:A:1838:THR:CG2	2:A:1876:ILE:HD11	2.41	0.50
1:K:254:GLU:O	1:K:258:ILE:HG12	2.11	0.50
1:K:339:LYS:HA	1:K:342:LEU:HD21	1.93	0.50
1:K:290:LYS:HE2	1:K:294:TYR:CZ	2.46	0.50
1:K:339:LYS:HA	1:K:342:LEU:CG	2.42	0.50
2:A:2600:LEU:HD23	2:A:2601:TYR:N	2.27	0.50
1:K:289:GLU:HA	1:K:292:ASN:ND2	2.25	0.50
1:L:348:ARG:HH21	1:L:349:ILE:HD11	1.75	0.49
1:K:342:LEU:HD12	1:K:343:GLN:N	2.27	0.49
1:L:259:ASP:O	1:L:263:LEU:HG	2.12	0.49
1:L:360:GLU:HG2	2:B:953:GLY:HA2	1.94	0.49
2:A:2513:VAL:HG23	2:A:2556:LEU:HD12	1.94	0.49
2:A:2655:CYS:HB2	2:A:2667:ALA:HB1	1.94	0.49
2:A:1982:VAL:HG11	2:B:2275:SER:HB2	1.93	0.49
2:A:2494:ALA:CB	9:S:1:NAG:H83	2.43	0.49
1:K:267:ALA:HA	1:K:353:ARG:CZ	2.42	0.49
2:A:2494:ALA:HB1	9:S:1:NAG:H83	1.93	0.49
2:B:1849:THR:HG23	2:B:2032:ILE:HG12	1.93	0.49
1:K:339:LYS:O	1:K:342:LEU:HG	2.13	0.49
1:K:261:TRP:O	1:K:264:ALA:HB3	2.12	0.49
2:A:3401:THR:HG21	2:A:3404:ASP:OD1	2.13	0.49
1:K:305:LEU:HD21	1:K:321:ARG:HB2	1.93	0.49
2:B:1848:LEU:HD12	2:B:1856:TYR:O	2.13	0.48
2:B:3173:SER:OG	12:B:4508:NGA:H82	2.12	0.48
2:B:3359:ILE:CG2	2:B:3360:ILE:HD12	2.44	0.48
1:K:281:LEU:HD23	1:K:345:LEU:HD13	1.95	0.48
2:A:2506:VAL:HG22	2:A:2508:LYS:HE2	1.95	0.48
8:T:1:NAG:H3	8:T:1:NAG:H83	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:302:HIS:ND1	1:L:305:LEU:HD12	2.29	0.48
2:A:2521:LEU:HD23	2:A:2523:TRP:CE3	2.48	0.48
2:B:562:VAL:HG22	2:B:573:TRP:HB2	1.95	0.48
1:L:254:GLU:O	1:L:258:ILE:HG12	2.14	0.48
2:A:2491:ASN:OD1	2:A:2502:VAL:HG22	2.14	0.48
2:A:2568:VAL:HG23	2:A:2598:LEU:HD22	1.96	0.48
1:L:254:GLU:HB2	1:L:255:PRO:HD3	1.97	0.47
1:K:259:ASP:O	1:K:263:LEU:HG	2.14	0.47
1:L:318:SER:O	1:L:322:GLU:HG3	2.14	0.47
1:K:252:PHE:HB3	1:K:258:ILE:CD1	2.38	0.47
1:K:305:LEU:HG	1:K:317:VAL:CG1	2.45	0.47
1:L:315:GLU:HG2	1:L:316:ARG:H	1.80	0.47
1:L:291:HIS:CB	1:L:334:LEU:HD22	2.33	0.47
1:L:284:PHE:HZ	1:L:338:VAL:HG13	1.80	0.47
1:L:298:LEU:HD12	1:L:327:LEU:HB3	1.96	0.47
2:A:2568:VAL:CG2	2:A:2598:LEU:HD22	2.45	0.47
2:B:1926:LEU:HD12	2:B:1932:LYS:O	2.15	0.47
2:B:2450:THR:O	2:B:2455:ILE:HG22	2.15	0.47
2:B:3232:LEU:HD12	2:B:3241:LEU:HD21	1.96	0.47
2:A:2513:VAL:C	2:A:2514:LEU:HD12	2.40	0.47
2:B:2747:THR:HG22	2:B:2749:ALA:H	1.80	0.47
1:K:257:VAL:CG2	1:K:285[A]:GLU:HB3	2.45	0.47
1:K:345:LEU:O	1:K:349:ILE:HG12	2.15	0.47
2:B:887:VAL:HG22	2:B:894:ILE:HG12	1.97	0.47
1:K:257:VAL:CG2	1:K:285[B]:GLU:HB3	2.45	0.47
2:A:2558:LEU:HD12	2:A:2564:LEU:O	2.15	0.46
1:L:252:PHE:O	1:L:256:ARG:HG2	2.14	0.46
1:L:253:GLU:HA	1:L:256:ARG:NH1	2.29	0.46
1:L:347:GLY:HA2	1:L:350[B]:SER:OG	2.16	0.46
1:L:347:GLY:HA2	1:L:350[A]:SER:OG	2.16	0.46
2:A:2506:VAL:CG2	2:A:2508:LYS:HE2	2.46	0.46
2:B:1059:LEU:HD12	2:B:1060:CYS:N	2.30	0.46
1:K:264:ALA:HB1	1:K:269:LEU:HD22	1.97	0.46
2:B:887:VAL:HG23	2:B:919:LEU:HD22	1.96	0.46
2:A:201:VAL:HG23	2:A:202:CYS:H	1.81	0.46
2:B:3326:LEU:HD11	2:B:3335:LEU:HD21	1.97	0.46
2:A:1870:VAL:HG22	2:A:1873:PRO:HD3	1.98	0.46
2:B:3432:LYS:O	2:B:3441:ARG:HA	2.15	0.46
2:A:674:CYS:HB3	2:A:689:CYS:HA	1.97	0.46
2:A:2503:ILE:HG23	2:A:2538:GLY:HA2	1.97	0.46
1:K:305:LEU:HG	1:K:317:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3214:ILE:HD11	2:B:3421:TYR:CZ	2.51	0.46
1:K:294:TYR:HB3	1:K:331:THR:CG2	2.46	0.46
2:A:2489:MET:H	2:A:2489:MET:HE2	1.81	0.45
1:K:281:LEU:CD2	1:K:345:LEU:HD13	2.47	0.45
1:K:298:LEU:CD2	1:K:331:THR:HG21	2.45	0.45
2:B:3836:PHE:HB2	2:B:3837:PRO:HD3	1.97	0.45
2:A:197:PRO:HB2	2:A:200:TYR:CD2	2.51	0.45
2:A:1680:MET:HB3	2:A:1683:ILE:HD11	1.98	0.45
2:A:3834:THR:HG22	2:A:3841:TYR:CZ	2.52	0.45
2:A:2357:CYS:CA	2:A:2368:CYS:HB3	2.46	0.45
2:B:3337:TRP:HZ3	2:B:3349:VAL:HG12	1.81	0.45
2:B:3349:VAL:O	2:B:3349:VAL:HG13	2.16	0.45
2:A:4188:ALA:HB3	2:A:4202:THR:OG1	2.17	0.45
2:A:209:GLN:HG2	2:A:210:ASP:N	2.31	0.45
2:A:2357:CYS:HA	2:A:2368:CYS:CB	2.44	0.45
2:B:202:CYS:HA	2:B:214:GLU:OE2	2.16	0.45
1:K:284:PHE:CE1	1:K:338:VAL:HG13	2.52	0.45
2:B:3239:LYS:HB3	9:V:1:NAG:H82	1.98	0.45
1:L:305:LEU:HD22	1:L:321:ARG:CD	2.40	0.44
2:A:482:TYR:OH	2:A:543:MET:HE2	2.17	0.44
1:K:256:ARG:O	1:K:260:LEU:HD23	2.17	0.44
2:A:1976:THR:OG1	2:A:2004:LEU:HD13	2.16	0.44
2:B:1870:VAL:HG22	2:B:1873:PRO:HD3	1.97	0.44
2:A:933:LEU:HD13	1:K:359:LEU:HD21	2.00	0.44
2:A:2492:SER:CB	2:A:2503:ILE:HD11	2.48	0.44
2:B:574:VAL:HG12	2:B:581:ILE:HG12	2.00	0.44
2:B:3286:TRP:O	2:B:3294:LEU:HD12	2.17	0.44
2:B:3277:VAL:HG22	2:B:3284:LEU:HD12	2.00	0.44
2:B:3355:ASN:ND2	10:B:4512:NAG:H4	2.32	0.44
2:B:1515:ALA:HB1	2:B:1559:LEU:HD13	2.00	0.44
2:B:3355:ASN:HD22	10:B:4512:NAG:H2	1.82	0.44
1:K:334:LEU:O	1:K:338:VAL:HG23	2.17	0.44
2:A:794:ILE:HG21	2:A:972:ASN:OD1	2.18	0.44
2:B:1593:VAL:CG1	2:B:1597:ILE:HD11	2.48	0.44
2:B:3239:LYS:CB	9:V:1:NAG:H82	2.48	0.44
1:L:322:GLU:O	1:L:326:LEU:HG	2.18	0.43
1:L:287:LYS:HE3	1:L:341:HIS:NE2	2.33	0.43
2:A:3277:VAL:HG22	2:A:3284:LEU:CD1	2.48	0.43
2:B:1111:ASP:OD1	2:B:1112:THR:HG23	2.18	0.43
1:L:305:LEU:HD11	1:L:324:HIS:CD2	2.53	0.43
2:B:2454:GLY:O	2:B:2455:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:281:LEU:O	1:K:285[A]:GLU:HG3	2.18	0.43
1:K:281:LEU:O	1:K:285[B]:GLU:HG3	2.18	0.43
1:K:310:SER:O	1:K:311:VAL:HG22	2.18	0.43
2:B:1665:VAL:HG23	2:B:1683:ILE:CD1	2.49	0.43
2:B:3244:ILE:HD11	2:B:3272:ALA:CB	2.49	0.43
1:K:305:LEU:HD13	1:K:321:ARG:HA	2.00	0.43
2:A:2598:LEU:HD11	2:A:2605:ILE:CG2	2.48	0.43
1:L:332:LYS:HA	1:L:332:LYS:HE2	2.00	0.43
2:A:4287:ILE:HD12	2:A:4315:LEU:HD23	2.01	0.43
2:B:2455:ILE:HG13	2:B:2456:HIS:N	2.34	0.43
2:B:4152:VAL:HG23	2:B:4344:LEU:HD11	2.01	0.43
2:B:4285:TYR:CD1	2:B:4320:ILE:HD11	2.54	0.43
1:K:275:GLU:HA	1:K:278:ARG:HG2	2.01	0.43
1:K:298:LEU:HD12	1:K:299:GLU:N	2.33	0.43
1:L:268:ASN:C	1:L:269:LEU:HD22	2.44	0.42
1:K:288:ILE:HG12	1:K:338:VAL:CG1	2.49	0.42
2:B:209:GLN:HG2	2:B:210:ASP:N	2.33	0.42
2:B:221:THR:OG1	12:B:4509:NGA:H2	2.19	0.42
1:K:277:PHE:O	1:K:281:LEU:HG	2.19	0.42
1:K:299:GLU:HG2	1:K:303:GLU:OE2	2.19	0.42
1:L:287:LYS:HD3	1:L:337:THR:OG1	2.19	0.42
2:B:205:ASP:H	2:B:214:GLU:CD	2.28	0.42
1:K:262:ASP:HA	1:K:265:GLN:OE1	2.19	0.42
2:A:206:ASN:HB2	2:A:211:GLY:HA2	2.00	0.42
2:B:3312:VAL:HG12	2:B:3356:LYS:HD3	2.02	0.42
1:K:267:ALA:HB3	1:K:269:LEU:CD1	2.49	0.42
1:L:359:LEU:HD23	1:L:359:LEU:O	2.20	0.42
1:K:254:GLU:OE1	1:K:256:ARG:HB2	2.19	0.42
1:K:269:LEU:O	1:K:273:GLU:HB2	2.19	0.42
1:K:330:ARG:O	1:K:334:LEU:HD23	2.19	0.42
1:L:296:LYS:O	1:L:300:ILE:HG22	2.19	0.42
2:A:196:ILE:HB	2:A:197:PRO:HD2	2.02	0.42
2:A:493:MET:HE3	2:A:675:VAL:HG11	2.02	0.42
2:B:2487:ASN:HB3	2:B:2489:MET:HE3	2.02	0.42
2:A:1558:ALA:C	2:A:1559:LEU:HD12	2.44	0.42
2:A:2506:VAL:HG22	2:A:2508:LYS:H	1.84	0.42
2:A:4156:ILE:HG23	2:A:4171:LEU:HD23	2.02	0.42
1:K:302:HIS:HB2	1:K:324:HIS:CD2	2.55	0.42
1:L:308:ALA:HB2	1:L:316:ARG:HH22	1.84	0.41
2:A:1515:ALA:HB1	2:A:1559:LEU:HD13	2.02	0.41
2:B:3536:LYS:CE	2:B:3541:GLY:HA2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:ILE:HG13	2:B:198:ARG:HD3	2.02	0.41
2:B:4102:TYR:OH	2:B:4171:LEU:HD22	2.19	0.41
2:B:3209:LEU:HD23	2:B:3232:LEU:HD13	2.02	0.41
1:K:305:LEU:HD11	1:K:320:SER:OG	2.20	0.41
2:A:2388:ASN:ND2	2:A:2644:VAL:HG13	2.36	0.41
1:K:269:LEU:HD23	1:K:274:LEU:HD12	2.02	0.41
2:B:564:LEU:CD2	2:B:571:VAL:HG22	2.50	0.41
2:A:1848:LEU:HD12	2:A:1856:TYR:O	2.20	0.41
2:A:2275:SER:HB2	2:B:1982:VAL:HG11	2.02	0.41
2:B:508:ASN:HA	2:B:532:LEU:HD12	2.03	0.41
2:B:2251:VAL:HG12	2:B:2258:ILE:HG12	2.01	0.41
1:K:336:TYR:HA	1:K:339:LYS:HE3	2.03	0.41
2:A:2168:GLU:OE1	2:A:2631:THR:HG22	2.21	0.41
2:A:2388:ASN:HD21	2:A:2644:VAL:HG13	1.85	0.41
2:A:2448:TYR:CE1	2:A:2461:ILE:HD11	2.56	0.40
2:B:2033:CYS:HA	2:B:2043:CYS:CB	2.50	0.40
1:K:336:TYR:CA	1:K:339:LYS:HG2	2.48	0.40
1:K:309:GLU:HG3	1:K:314:GLY:O	2.21	0.40
2:B:964:ASP:HB3	2:B:967:ILE:HD12	2.03	0.40
1:K:267:ALA:HA	1:K:353:ARG:NH2	2.36	0.40
2:A:1123:SER:HG	2:A:1126:TRP:CG	2.39	0.40
2:A:2047:THR:HG23	2:A:2085:GLU:HB2	2.02	0.40
2:A:2508:LYS:HG2	2:A:2525:ASP:CB	2.51	0.40
2:B:3526:ILE:HG23	2:B:3530:TRP:CE3	2.57	0.40
1:K:353:ARG:HG2	1:K:353:ARG:HH11	1.85	0.40
2:A:475:ASP:OD1	2:A:543:MET:HE1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	113/344 (33%)	101 (89%)	12 (11%)	0	100	100
1	L	113/344 (33%)	107 (95%)	6 (5%)	0	100	100
2	A	3818/4473 (85%)	3504 (92%)	313 (8%)	1 (0%)	100	100
2	B	3812/4473 (85%)	3452 (91%)	358 (9%)	2 (0%)	48	76
All	All	7856/9634 (82%)	7164 (91%)	689 (9%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2739	HIS
2	B	3360	ILE
2	B	3816	LYS

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	K	101/308 (33%)	101 (100%)	0	100	100
1	L	101/308 (33%)	97 (96%)	4 (4%)	28	55
2	A	3372/3934 (86%)	3371 (100%)	1 (0%)	100	100
2	B	3365/3934 (86%)	3365 (100%)	0	100	100
All	All	6939/8484 (82%)	6934 (100%)	5 (0%)	100	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	285[A]	GLU
1	L	285[B]	GLU
1	L	350[A]	SER
1	L	350[B]	SER
2	A	2014	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	265	GLN
1	L	324	HIS
2	A	32	HIS
2	A	316	ASN
2	A	678	HIS
2	A	860	HIS
2	A	915	HIS
2	A	959	HIS
2	A	1010	HIS
2	A	1191	GLN
2	A	1253	HIS
2	A	1349	ASN
2	A	1762	ASN
2	A	1790	GLN
2	A	1843	GLN
2	A	2000	ASN
2	A	2211	GLN
2	A	2381	ASN
2	A	2402	HIS
2	A	2613	GLN
2	A	3569	GLN
2	A	3629	HIS
2	A	4297	GLN
2	B	372	HIS
2	B	410	HIS
2	B	489	ASN
2	B	656	GLN
2	B	912	GLN
2	B	1191	GLN
2	B	1216	ASN
2	B	1285	HIS
2	B	1576	HIS
2	B	1609	ASN
2	B	1675	ASN
2	B	1920	HIS
2	B	1969	HIS
2	B	2211	GLN
2	B	2302	GLN
2	B	2309	ASN
2	B	2344	ASN
2	B	2613	GLN
2	B	2619	ASN
2	B	3303	HIS

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Mol	Chain	Res	Type
2	B	3342	HIS
2	B	3355	ASN
2	B	3629	HIS
2	B	4020	HIS
2	B	4061	ASN
2	B	4298	ASN
2	B	4336	GLN
1	K	283	HIS
1	K	297	GLN
1	K	343	GLN

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 ⓘ

39 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	$\# Z > 2$
8	NAG	M	1	2,8	14,14,15	0.75	0	17,19,21	2.45	7 (41%)
8	NAG	M	2	8	14,14,15	0.89	1 (7%)	17,19,21	2.68	5 (29%)
8	BMA	M	3	8	11,11,12	0.84	0	15,15,17	2.06	3 (20%)
8	NAG	N	1	2,8	14,14,15	0.73	0	17,19,21	1.01	0
8	NAG	N	2	8	14,14,15	0.73	0	17,19,21	1.00	0
8	BMA	N	3	8	11,11,12	0.81	0	15,15,17	1.87	2 (13%)
9	NAG	O	1	2,9	14,14,15	0.77	0	17,19,21	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	O	2	9	14,14,15	0.73	0	17,19,21	2.81	8 (47%)
9	NAG	P	1	2,9	14,14,15	0.73	0	17,19,21	1.18	3 (17%)
9	NAG	P	2	9	14,14,15	0.77	0	17,19,21	2.11	5 (29%)
9	NAG	Q	1	2,9	14,14,15	0.80	0	17,19,21	1.03	1 (5%)
9	NAG	Q	2	9	14,14,15	0.74	0	17,19,21	0.94	0
9	NAG	R	1	2,9	14,14,15	0.77	0	17,19,21	1.06	1 (5%)
9	NAG	R	2	9	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
9	NAG	S	1	2,9	14,14,15	0.70	0	17,19,21	1.21	2 (11%)
9	NAG	S	2	9	14,14,15	0.73	0	17,19,21	1.18	2 (11%)
8	NAG	T	1	2,8	14,14,15	0.73	0	17,19,21	1.69	1 (5%)
8	NAG	T	2	8	14,14,15	0.75	0	17,19,21	0.86	0
8	BMA	T	3	8	11,11,12	0.82	0	15,15,17	1.80	3 (20%)
9	NAG	U	1	2,9	14,14,15	0.78	0	17,19,21	0.90	1 (5%)
9	NAG	U	2	9	14,14,15	0.74	0	17,19,21	0.82	0
9	NAG	V	1	2,9	14,14,15	0.82	0	17,19,21	1.13	3 (17%)
9	NAG	V	2	9	14,14,15	0.73	0	17,19,21	0.98	0
9	NAG	W	1	2,9	14,14,15	0.76	0	17,19,21	0.97	0
9	NAG	W	2	9	14,14,15	0.74	0	17,19,21	0.97	0
8	NAG	X	1	2,8	14,14,15	0.74	0	17,19,21	1.02	1 (5%)
8	NAG	X	2	8	14,14,15	0.72	0	17,19,21	0.97	0
8	BMA	X	3	8	11,11,12	0.83	0	15,15,17	2.06	3 (20%)
8	NAG	Y	1	2,8	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
8	NAG	Y	2	8	14,14,15	0.72	0	17,19,21	1.01	0
8	BMA	Y	3	8	11,11,12	0.80	0	15,15,17	1.96	3 (20%)
9	NAG	Z	1	2,9	14,14,15	0.83	0	17,19,21	1.26	2 (11%)
9	NAG	Z	2	9	14,14,15	0.69	0	17,19,21	1.73	2 (11%)
8	NAG	a	1	8	14,14,15	0.76	0	17,19,21	0.80	0
8	NAG	a	2	8	14,14,15	0.75	0	17,19,21	0.73	0
8	BMA	a	3	8	11,11,12	0.82	0	15,15,17	1.85	3 (20%)
8	NAG	b	1	2,8	14,14,15	0.82	0	17,19,21	0.86	0
8	NAG	b	2	8	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
8	BMA	b	3	8	11,11,12	0.83	0	15,15,17	1.82	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
8	NAG	M	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	M	2	8	1/1/7/7	1/6/23/26	0/1/1/1
8	BMA	M	3	8	-	0/2/19/22	0/1/1/1
8	NAG	N	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	N	2	8	-	0/6/23/26	0/1/1/1
8	BMA	N	3	8	-	1/2/19/22	0/1/1/1
9	NAG	O	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	O	2	9	2/2/7/7	0/6/23/26	0/1/1/1
9	NAG	P	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	P	2	9	1/1/7/7	3/6/23/26	0/1/1/1
9	NAG	Q	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	0/6/23/26	0/1/1/1
9	NAG	R	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	R	2	9	-	0/6/23/26	0/1/1/1
9	NAG	S	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	S	2	9	-	3/6/23/26	0/1/1/1
8	NAG	T	1	2,8	-	5/6/23/26	0/1/1/1
8	NAG	T	2	8	-	3/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	U	2	9	-	3/6/23/26	0/1/1/1
9	NAG	V	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	V	2	9	-	3/6/23/26	0/1/1/1
9	NAG	W	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	W	2	9	-	0/6/23/26	0/1/1/1
8	NAG	X	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	0/2/19/22	0/1/1/1
8	NAG	Y	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	3/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
9	NAG	Z	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	1/6/23/26	0/1/1/1
8	NAG	a	1	8	-	2/6/23/26	0/1/1/1
8	NAG	a	2	8	-	0/6/23/26	0/1/1/1
8	BMA	a	3	8	-	0/2/19/22	0/1/1/1
8	NAG	b	1	2,8	-	1/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	BMA	b	3	8	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	2	NAG	C1-C2	2.78	1.56	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1	NAG	C2-N2-C7	6.89	132.13	122.90
8	M	2	NAG	C1-C2-N2	6.72	121.02	110.43
8	M	2	NAG	C1-O5-C5	6.69	121.16	112.19
8	M	3	BMA	C1-O5-C5	6.20	120.49	112.19
8	X	3	BMA	C1-O5-C5	6.14	120.42	112.19
8	Y	3	BMA	C1-O5-C5	5.77	119.92	112.19
8	N	3	BMA	C1-O5-C5	5.76	119.90	112.19
8	b	3	BMA	C1-O5-C5	5.55	119.62	112.19
8	T	1	NAG	C2-N2-C7	5.50	130.27	122.90
9	Z	2	NAG	C2-N2-C7	5.42	130.17	122.90
9	O	2	NAG	O4-C4-C5	5.27	122.30	109.32
8	a	3	BMA	C1-O5-C5	5.25	119.22	112.19
9	O	2	NAG	O3-C3-C4	5.16	122.54	110.38
9	P	2	NAG	O4-C4-C5	5.03	121.71	109.32
9	P	2	NAG	C3-C4-C5	4.96	119.23	110.23
8	T	3	BMA	C1-O5-C5	4.93	118.79	112.19
9	O	2	NAG	C4-C3-C2	4.75	117.98	111.02
9	O	2	NAG	C3-C4-C5	4.31	118.05	110.23
9	O	2	NAG	O3-C3-C2	3.99	117.68	109.40
8	M	1	NAG	O4-C4-C5	3.56	118.09	109.32
9	O	2	NAG	O4-C4-C3	3.13	117.75	110.38
8	M	1	NAG	C8-C7-N2	3.09	121.24	116.12
9	S	2	NAG	C1-O5-C5	3.08	116.31	112.19
9	O	1	NAG	O5-C1-C2	-3.04	106.59	111.29
8	M	2	NAG	C2-N2-C7	3.03	126.96	122.90
8	M	1	NAG	C1-C2-N2	3.00	115.17	110.43
9	P	2	NAG	O4-C4-C3	2.89	117.20	110.38
9	R	1	NAG	O5-C1-C2	-2.88	106.83	111.29
9	Z	1	NAG	O5-C1-C2	-2.84	106.89	111.29
9	S	1	NAG	O5-C1-C2	-2.82	106.93	111.29
9	Z	2	NAG	O7-C7-N2	2.77	126.88	121.98
8	M	1	NAG	O5-C1-C2	-2.73	107.06	111.29
9	P	1	NAG	O5-C1-C2	-2.68	107.14	111.29
8	X	3	BMA	C3-C4-C5	2.56	114.87	110.23
8	b	2	NAG	O5-C1-C2	-2.50	107.42	111.29
9	Z	1	NAG	O4-C4-C3	-2.49	104.50	110.38
9	U	1	NAG	O5-C1-C2	-2.47	107.47	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	3	BMA	C3-C4-C5	2.46	114.69	110.23
8	T	3	BMA	C3-C4-C5	2.44	114.66	110.23
8	M	2	NAG	O5-C1-C2	2.42	115.03	111.29
9	S	1	NAG	C2-N2-C7	2.39	126.10	122.90
9	Q	1	NAG	O5-C1-C2	-2.37	107.62	111.29
8	a	3	BMA	C3-C4-C5	2.37	114.53	110.23
8	M	1	NAG	O4-C4-C3	-2.30	104.95	110.38
9	S	2	NAG	C2-N2-C7	2.27	125.95	122.90
8	Y	3	BMA	C3-C4-C5	2.25	114.31	110.23
8	T	3	BMA	O4-C4-C3	-2.21	105.18	110.38
9	P	1	NAG	C4-C3-C2	-2.20	107.79	111.02
9	O	2	NAG	C1-O5-C5	2.19	115.12	112.19
8	Y	3	BMA	O4-C4-C3	-2.16	105.28	110.38
9	P	2	NAG	O5-C1-C2	-2.16	107.95	111.29
8	M	3	BMA	C2-C3-C4	2.14	114.63	110.86
9	V	1	NAG	C1-O5-C5	2.14	115.05	112.19
8	M	1	NAG	O7-C7-C8	-2.12	118.28	122.05
9	V	1	NAG	C2-N2-C7	2.12	125.74	122.90
8	M	2	NAG	C3-C4-C5	-2.12	106.39	110.23
8	X	3	BMA	O4-C4-C3	-2.12	105.39	110.38
9	P	1	NAG	C2-N2-C7	2.10	125.71	122.90
9	V	1	NAG	O5-C1-C2	-2.06	108.11	111.29
8	X	1	NAG	C2-N2-C7	2.05	125.65	122.90
8	Y	1	NAG	O5-C1-C2	-2.05	108.12	111.29
8	a	3	BMA	O4-C4-C3	-2.05	105.54	110.38
8	N	3	BMA	O4-C4-C3	-2.05	105.55	110.38
9	R	2	NAG	C1-O5-C5	2.02	114.89	112.19
9	O	2	NAG	O5-C1-C2	-2.01	108.18	111.29
9	P	2	NAG	C2-N2-C7	2.01	125.59	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	M	2	NAG	C2
9	O	2	NAG	C4
9	O	2	NAG	C3
9	P	2	NAG	C4

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	M	2	NAG	C3-C2-N2-C7
9	Z	2	NAG	C3-C2-N2-C7
8	a	1	NAG	O5-C5-C6-O6
8	M	1	NAG	C8-C7-N2-C2
8	M	1	NAG	O7-C7-N2-C2
8	T	1	NAG	C8-C7-N2-C2
8	T	1	NAG	O7-C7-N2-C2
8	T	2	NAG	C8-C7-N2-C2
8	T	2	NAG	O7-C7-N2-C2
9	U	2	NAG	C8-C7-N2-C2
9	U	2	NAG	O7-C7-N2-C2
8	a	1	NAG	C4-C5-C6-O6
8	N	3	BMA	O5-C5-C6-O6
9	Z	1	NAG	O5-C5-C6-O6
8	b	1	NAG	O5-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
9	S	2	NAG	O5-C5-C6-O6
9	U	2	NAG	O5-C5-C6-O6
9	P	2	NAG	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	Q	1	NAG	O5-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
9	U	1	NAG	O5-C5-C6-O6
8	N	1	NAG	C1-C2-N2-C7
8	X	1	NAG	C1-C2-N2-C7
8	Y	2	NAG	C1-C2-N2-C7
9	O	1	NAG	C1-C2-N2-C7
9	P	2	NAG	C1-C2-N2-C7
9	V	2	NAG	C1-C2-N2-C7
8	Y	2	NAG	C3-C2-N2-C7
8	b	2	NAG	C3-C2-N2-C7
9	O	1	NAG	C3-C2-N2-C7
9	P	1	NAG	C3-C2-N2-C7
9	P	2	NAG	C3-C2-N2-C7
9	S	1	NAG	C3-C2-N2-C7
9	S	2	NAG	C3-C2-N2-C7
9	V	1	NAG	C3-C2-N2-C7
9	V	2	NAG	C3-C2-N2-C7
8	b	3	BMA	O5-C5-C6-O6
9	Z	1	NAG	C4-C5-C6-O6
8	T	1	NAG	C1-C2-N2-C7

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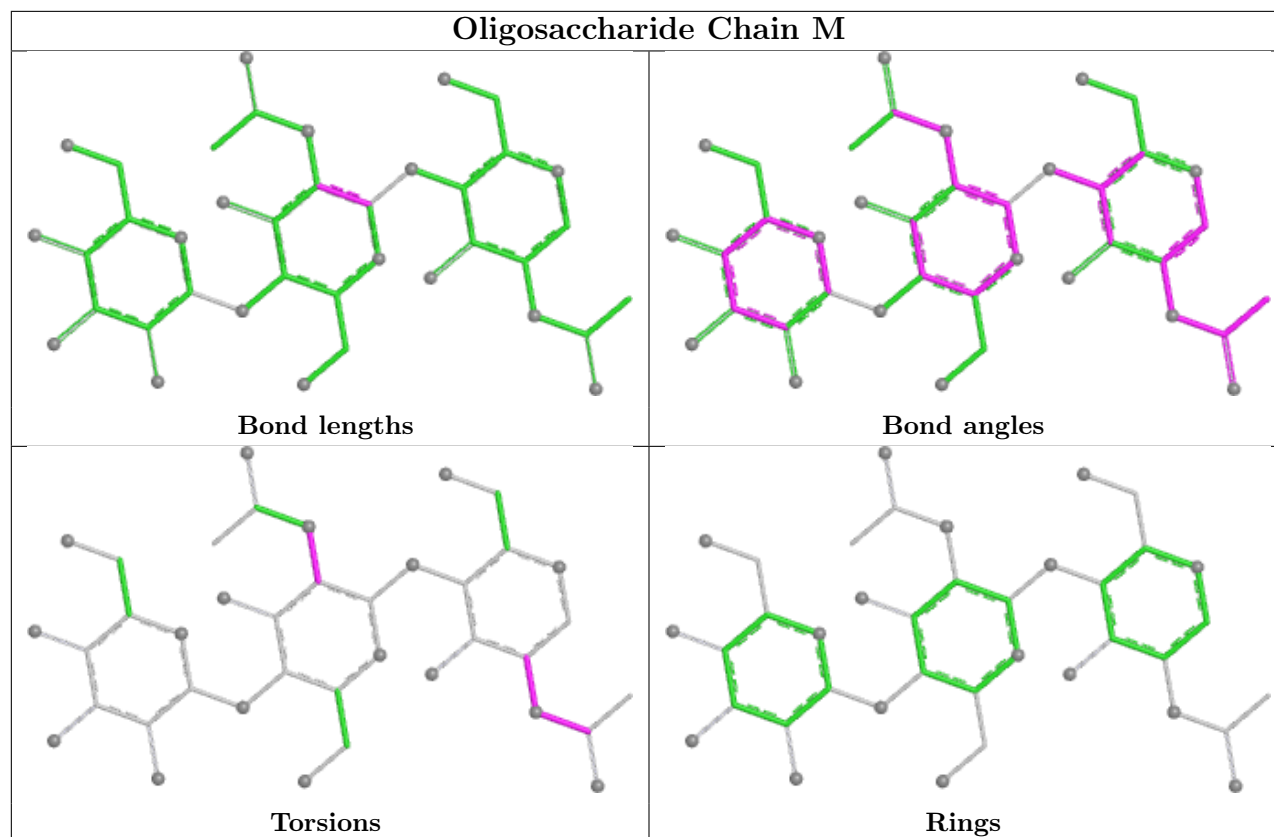
Mol	Chain	Res	Type	Atoms
8	b	2	NAG	C1-C2-N2-C7
9	P	1	NAG	C1-C2-N2-C7
9	S	1	NAG	C1-C2-N2-C7
9	S	2	NAG	C1-C2-N2-C7
9	V	1	NAG	C1-C2-N2-C7
8	N	1	NAG	C3-C2-N2-C7
8	T	1	NAG	C3-C2-N2-C7
8	X	1	NAG	C3-C2-N2-C7

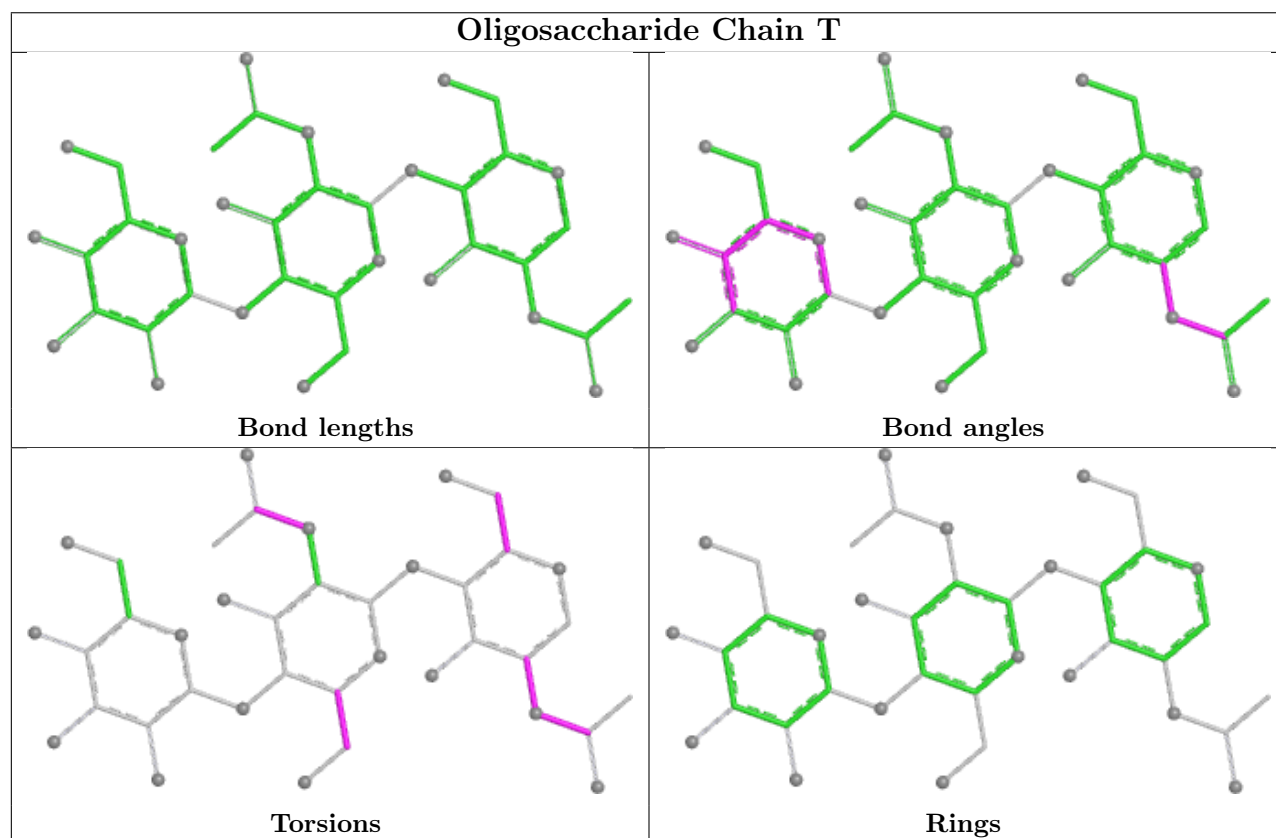
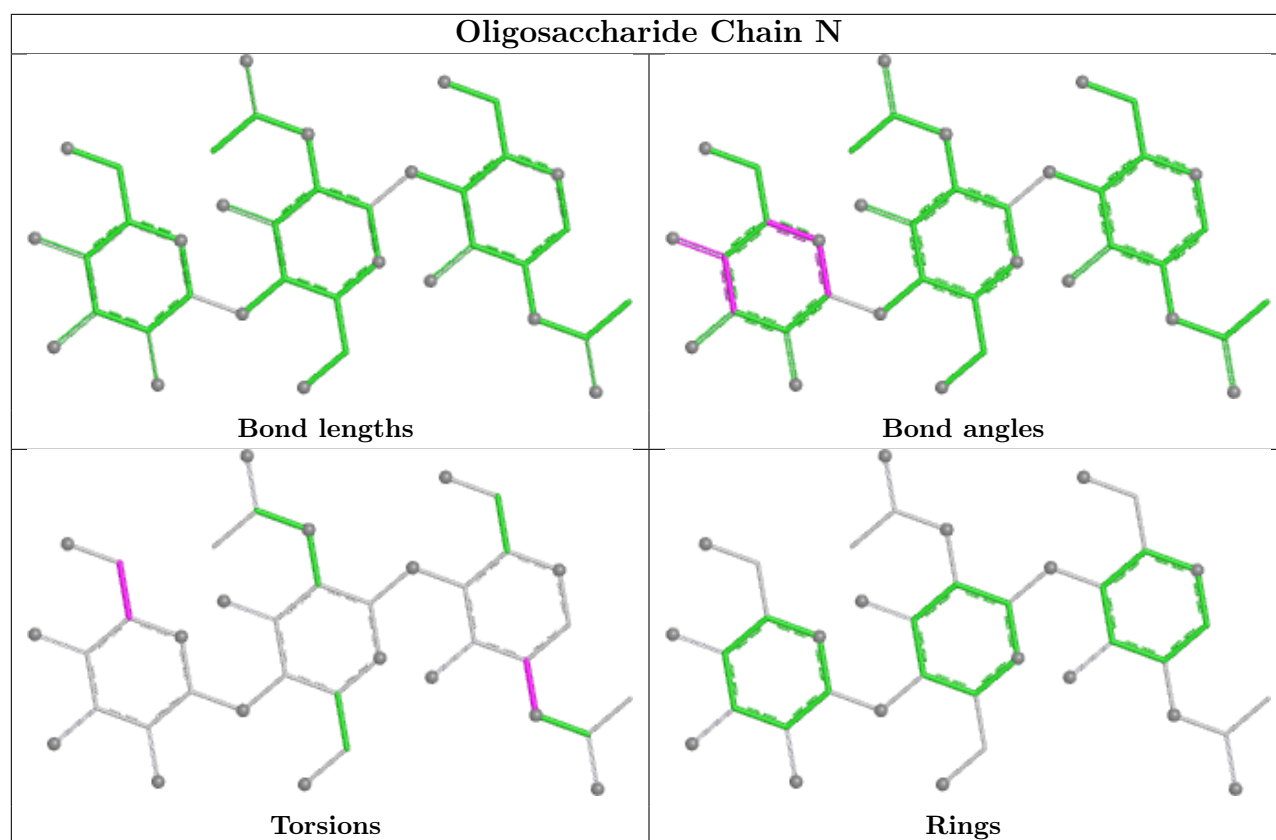
There are no ring outliers.

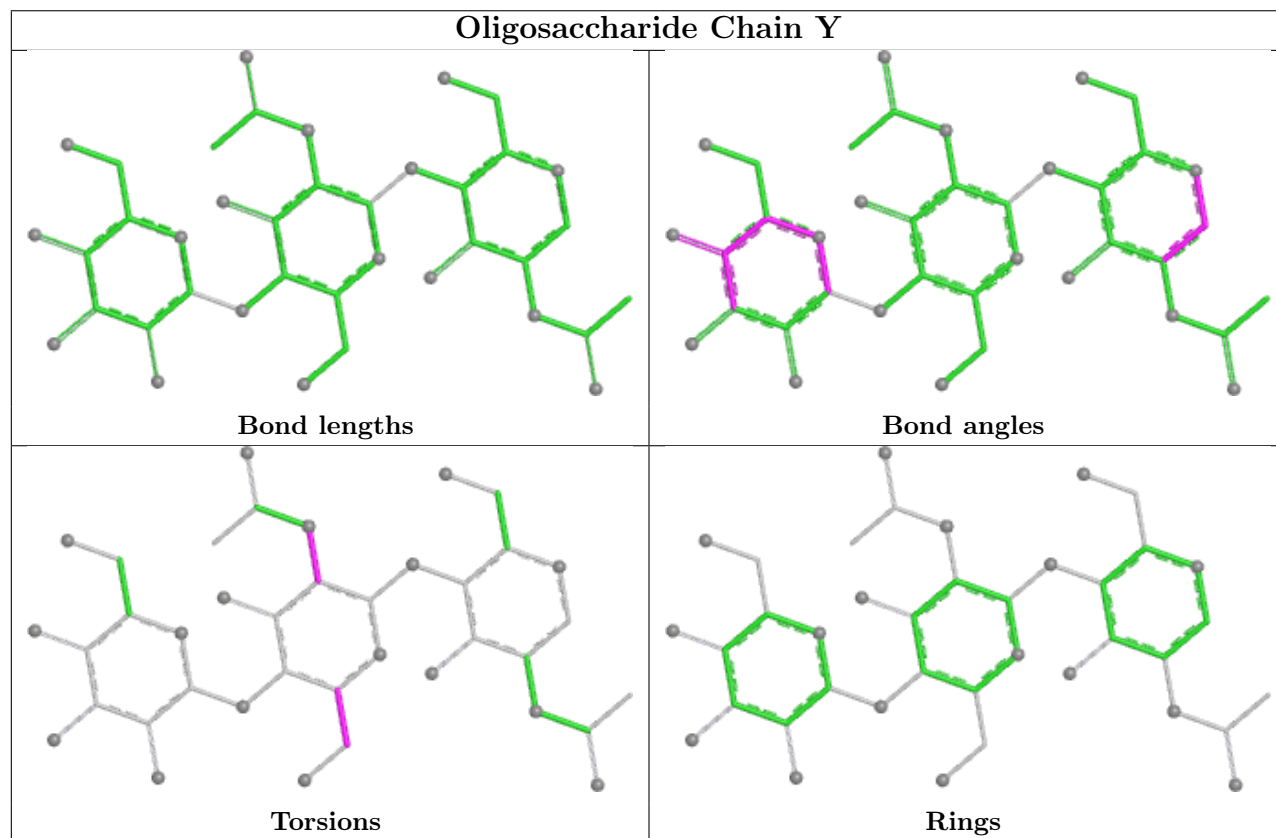
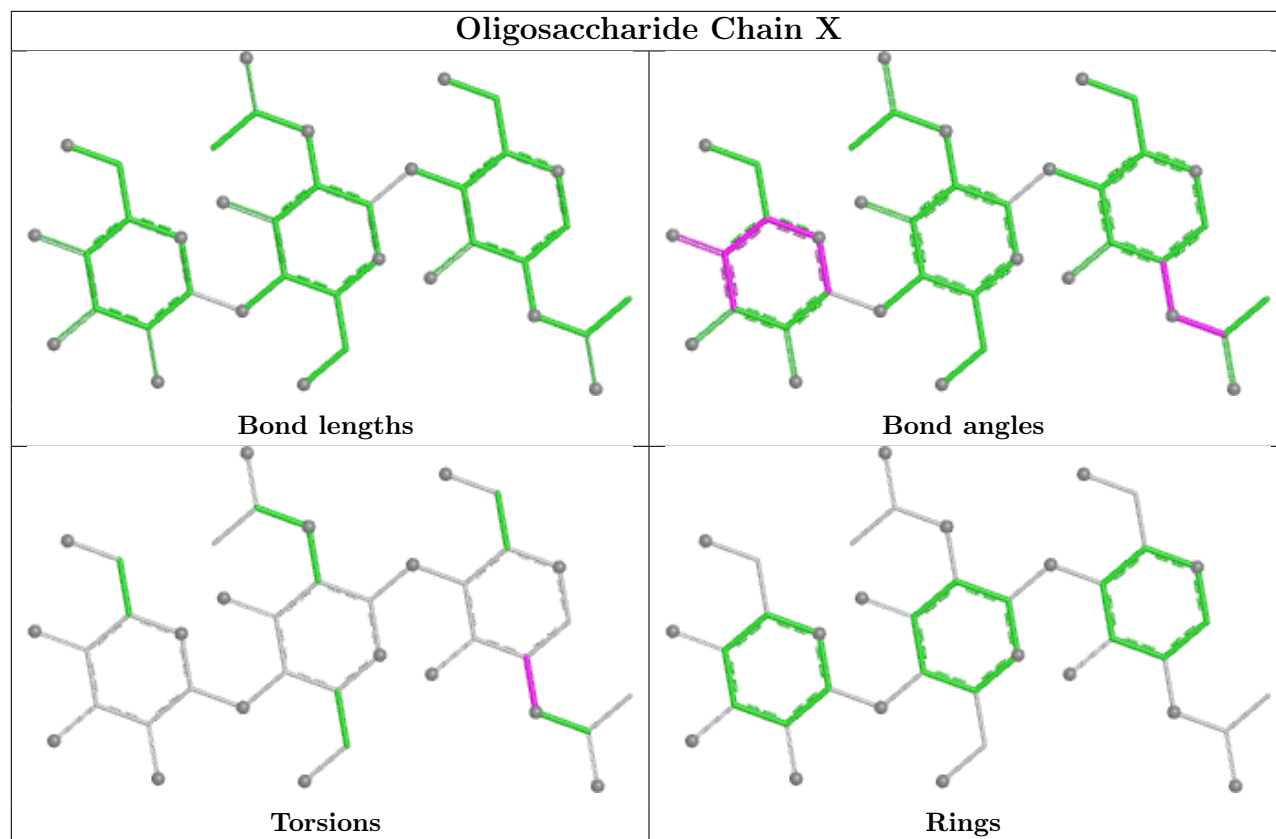
3 monomers are involved in 5 short contacts:

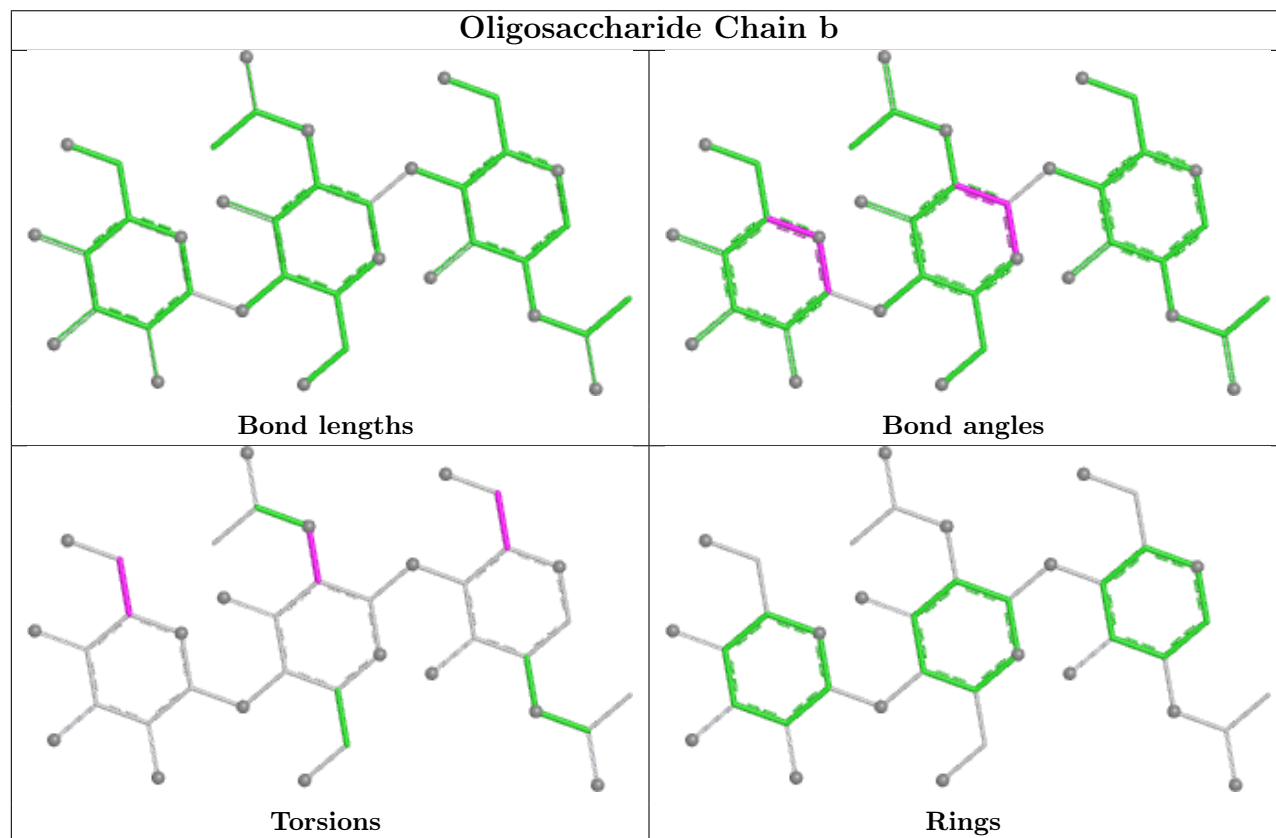
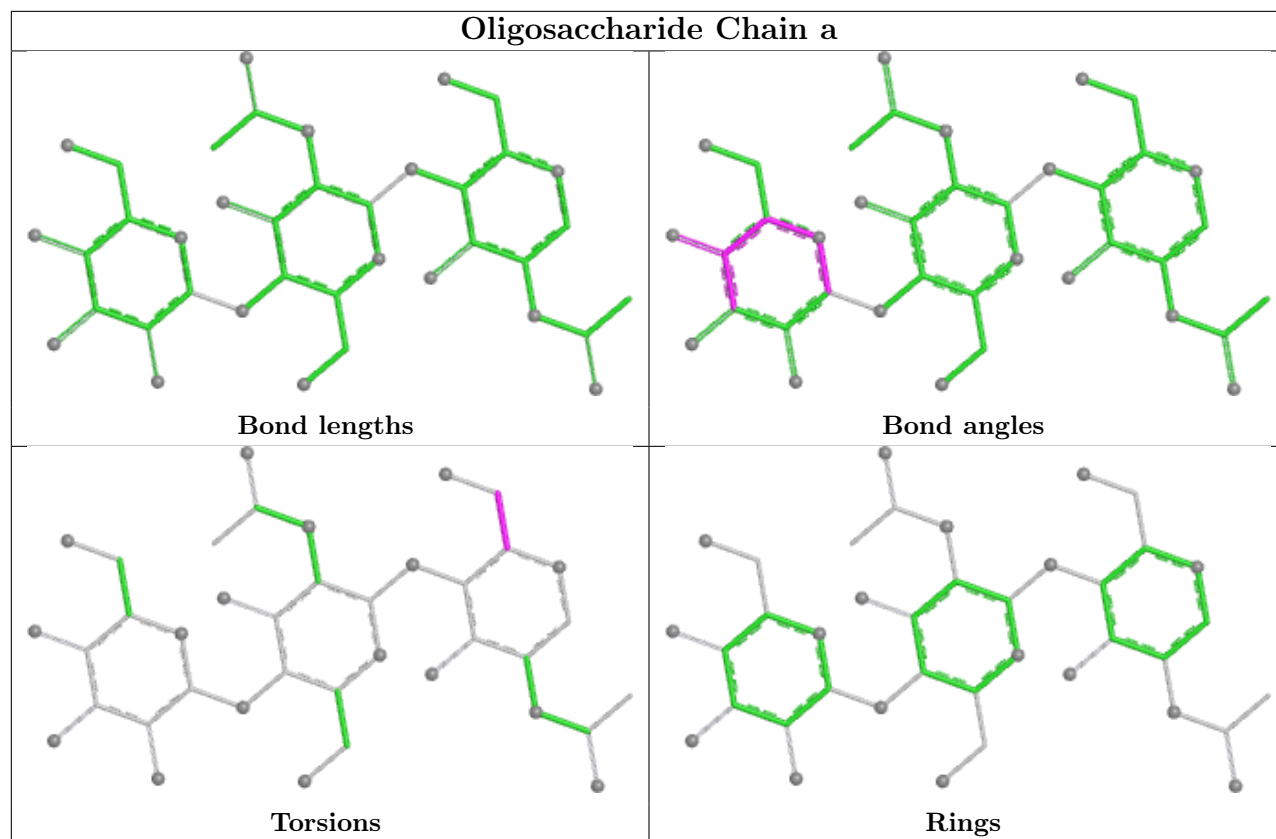
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	NAG	2	0
8	T	1	NAG	1	0
9	S	1	NAG	2	0

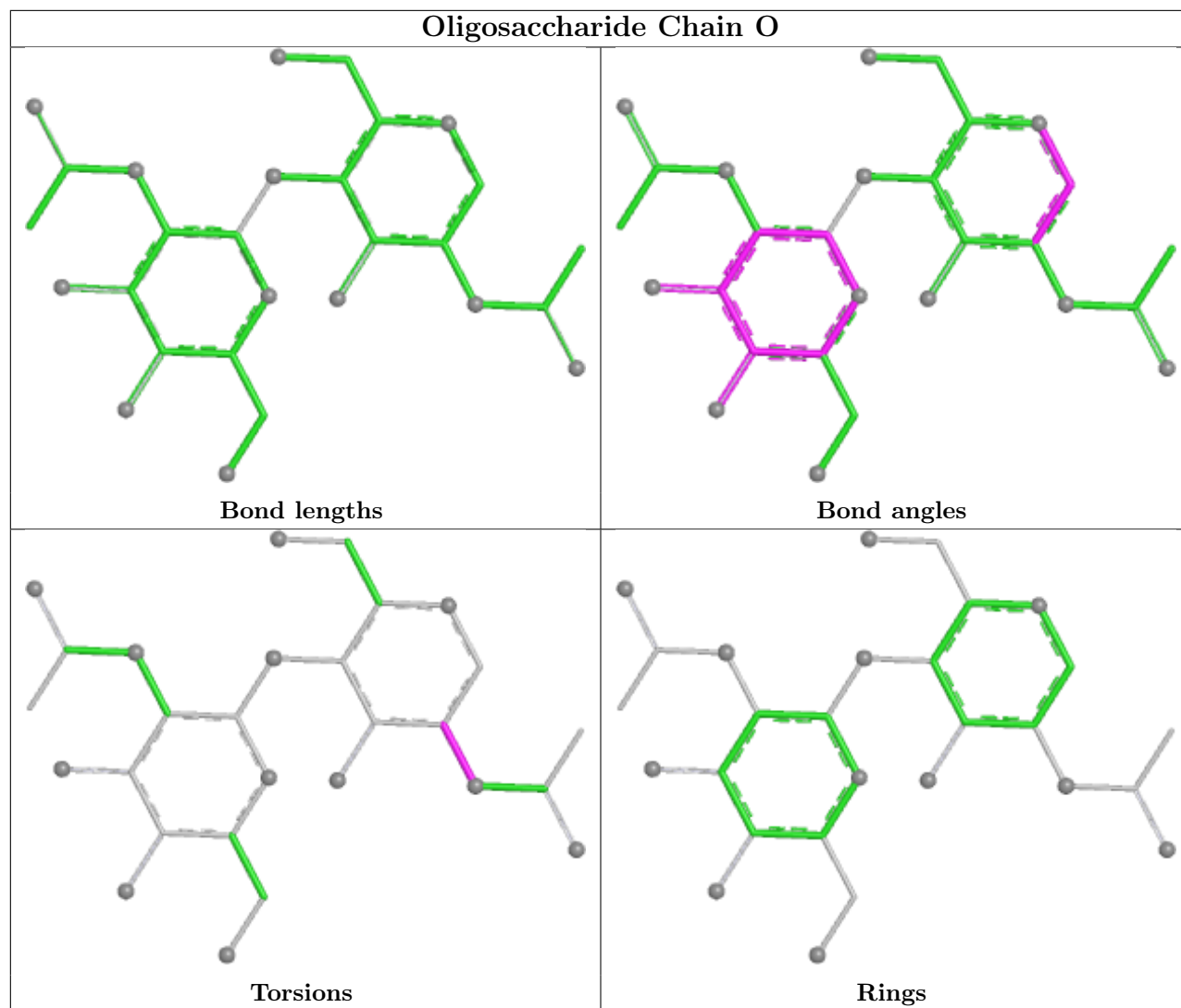
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

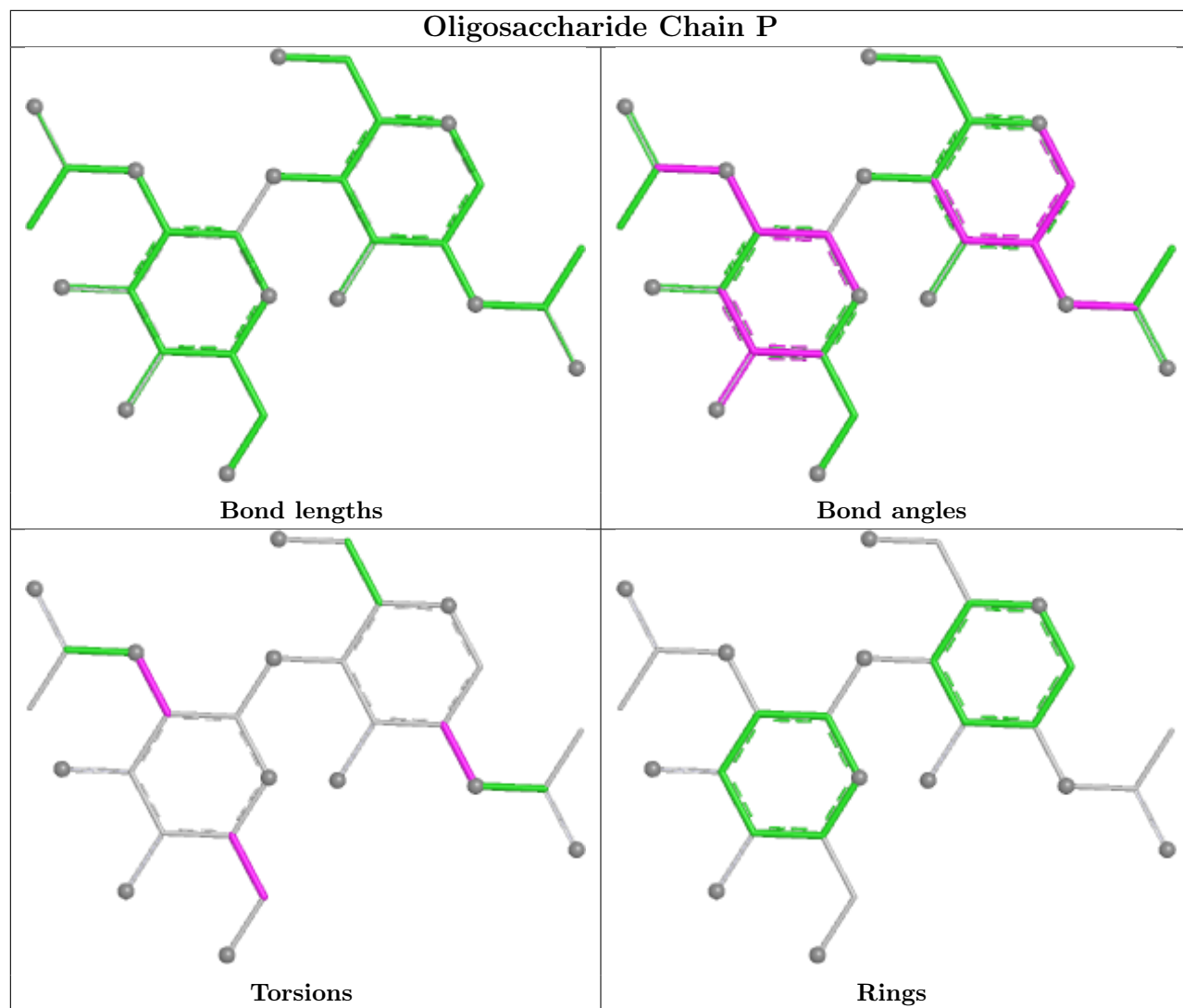


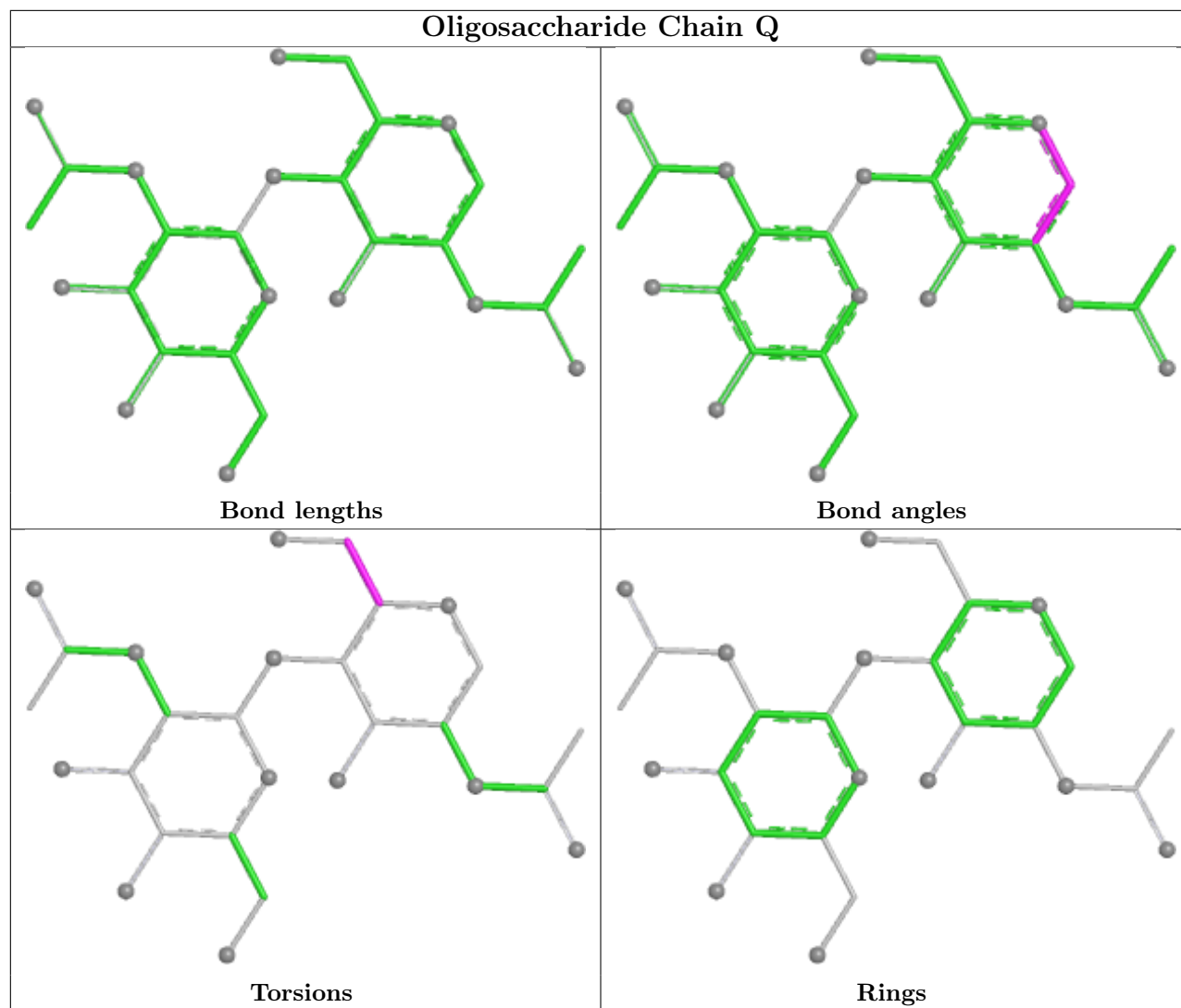


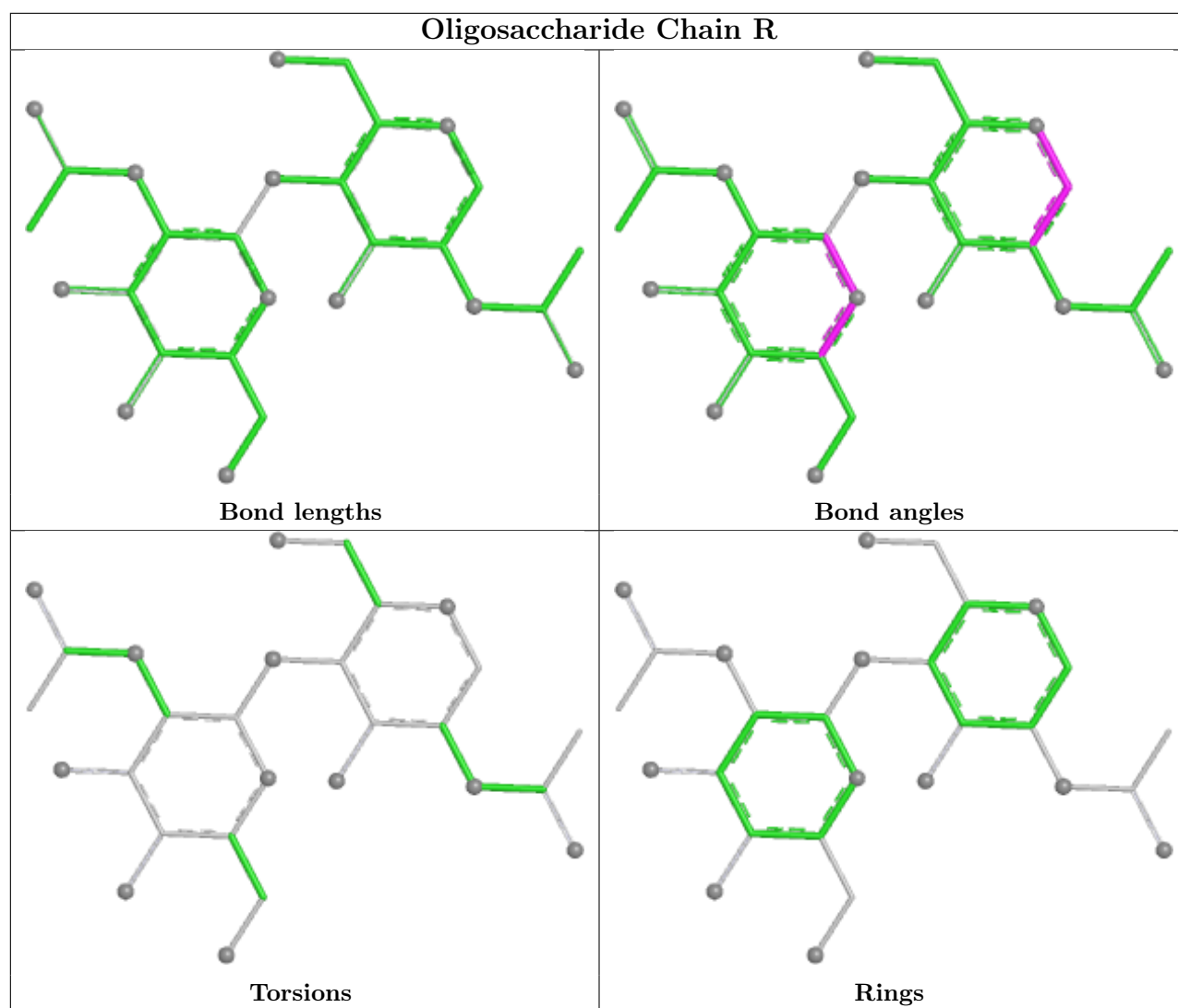


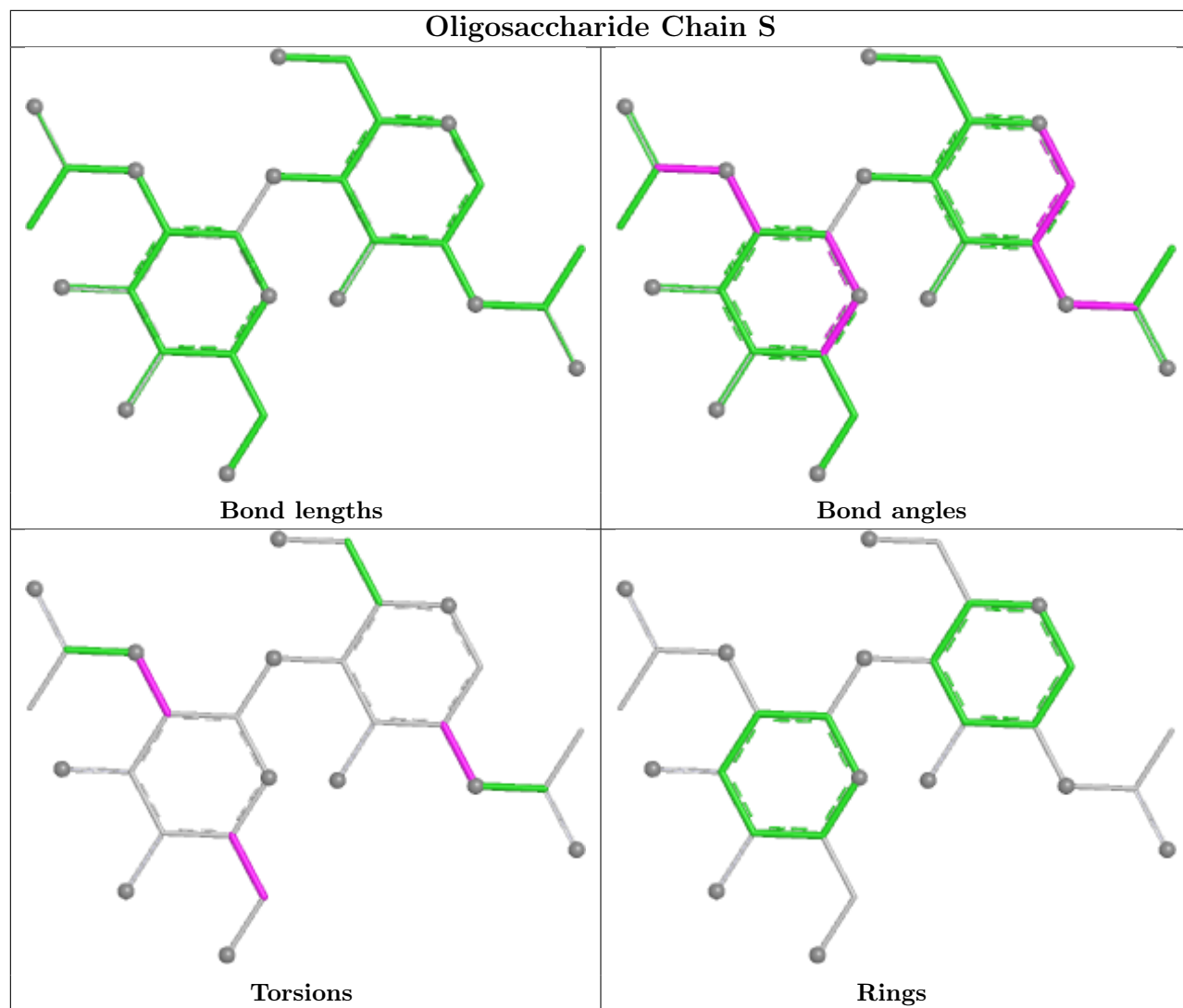


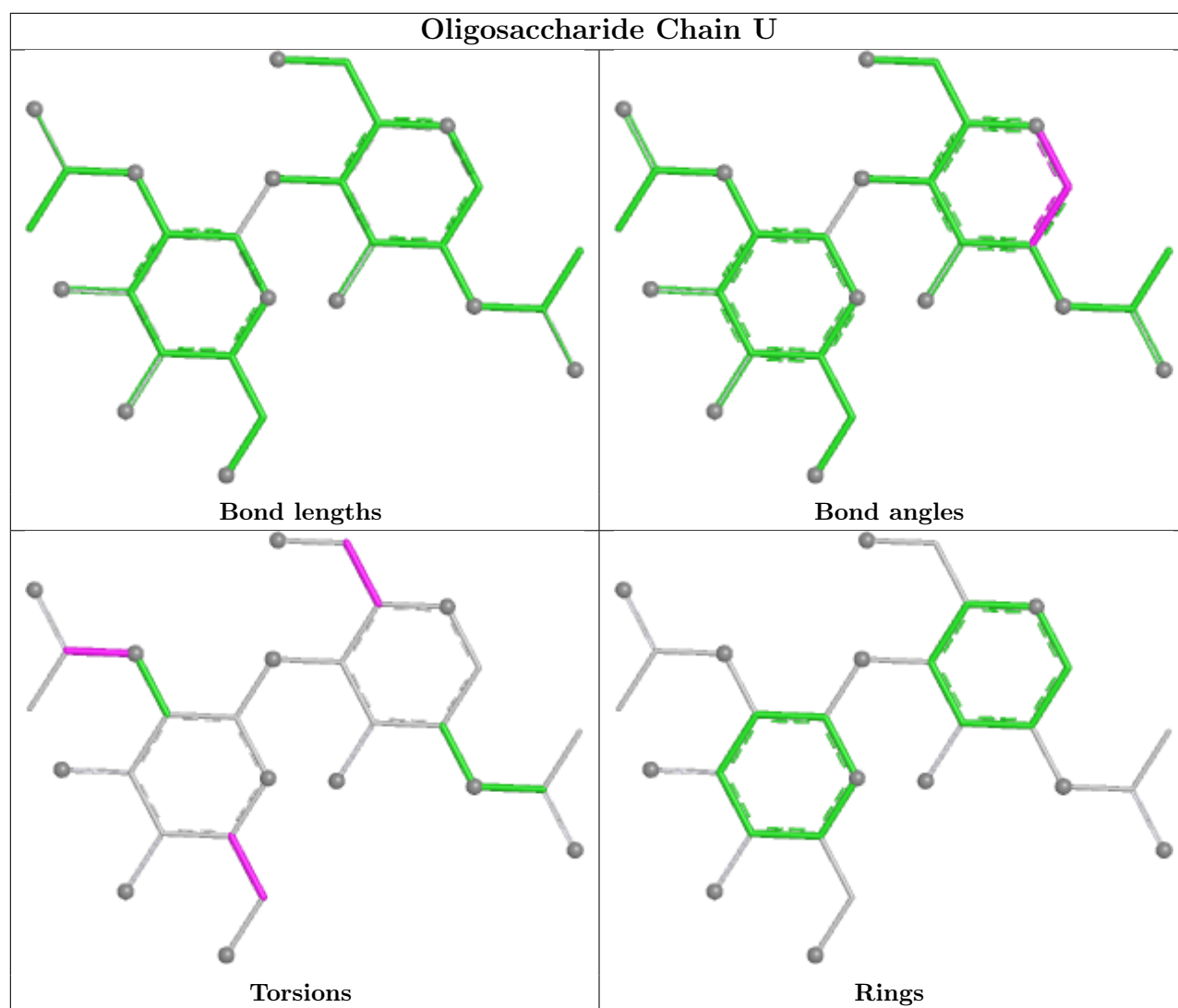


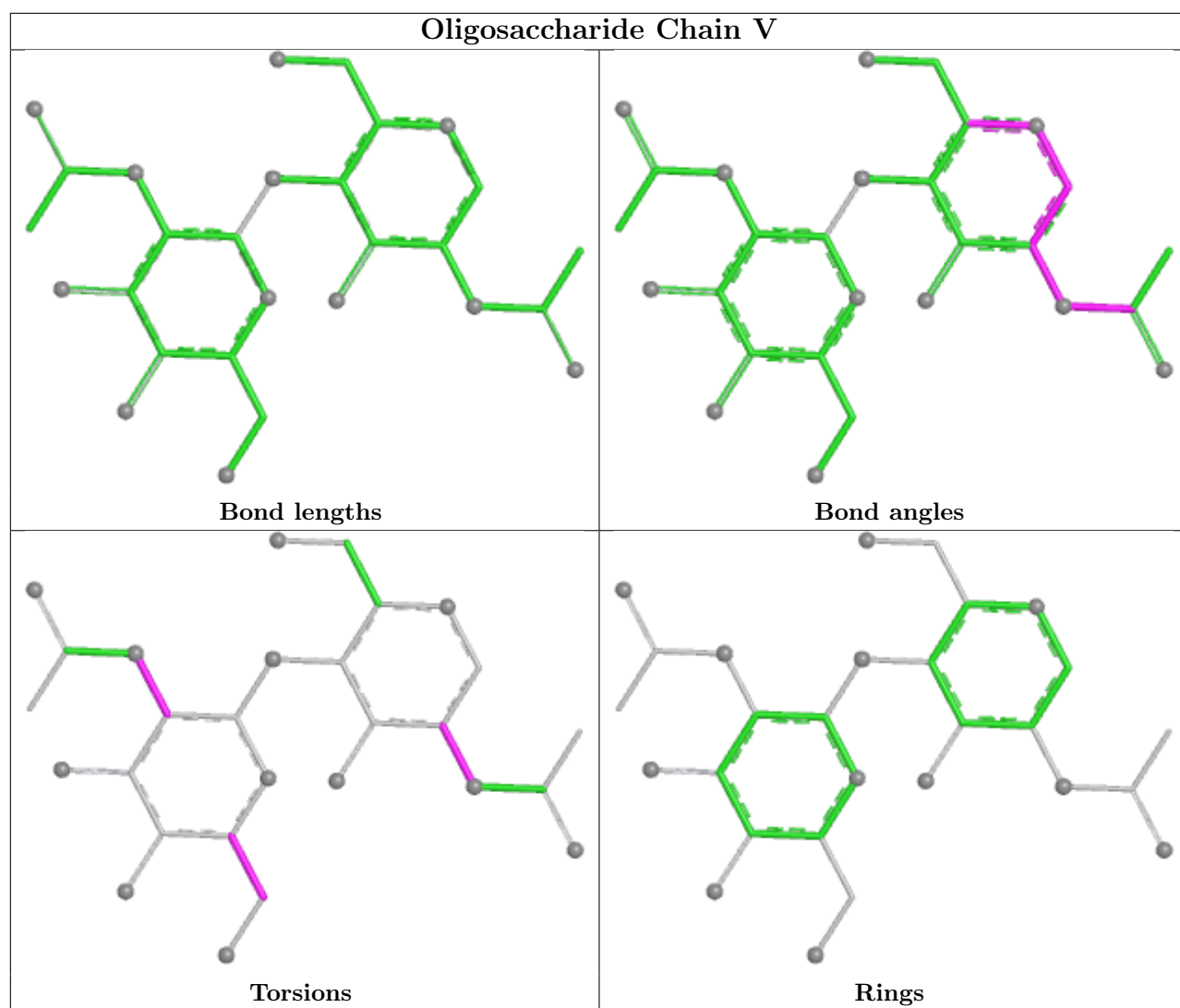


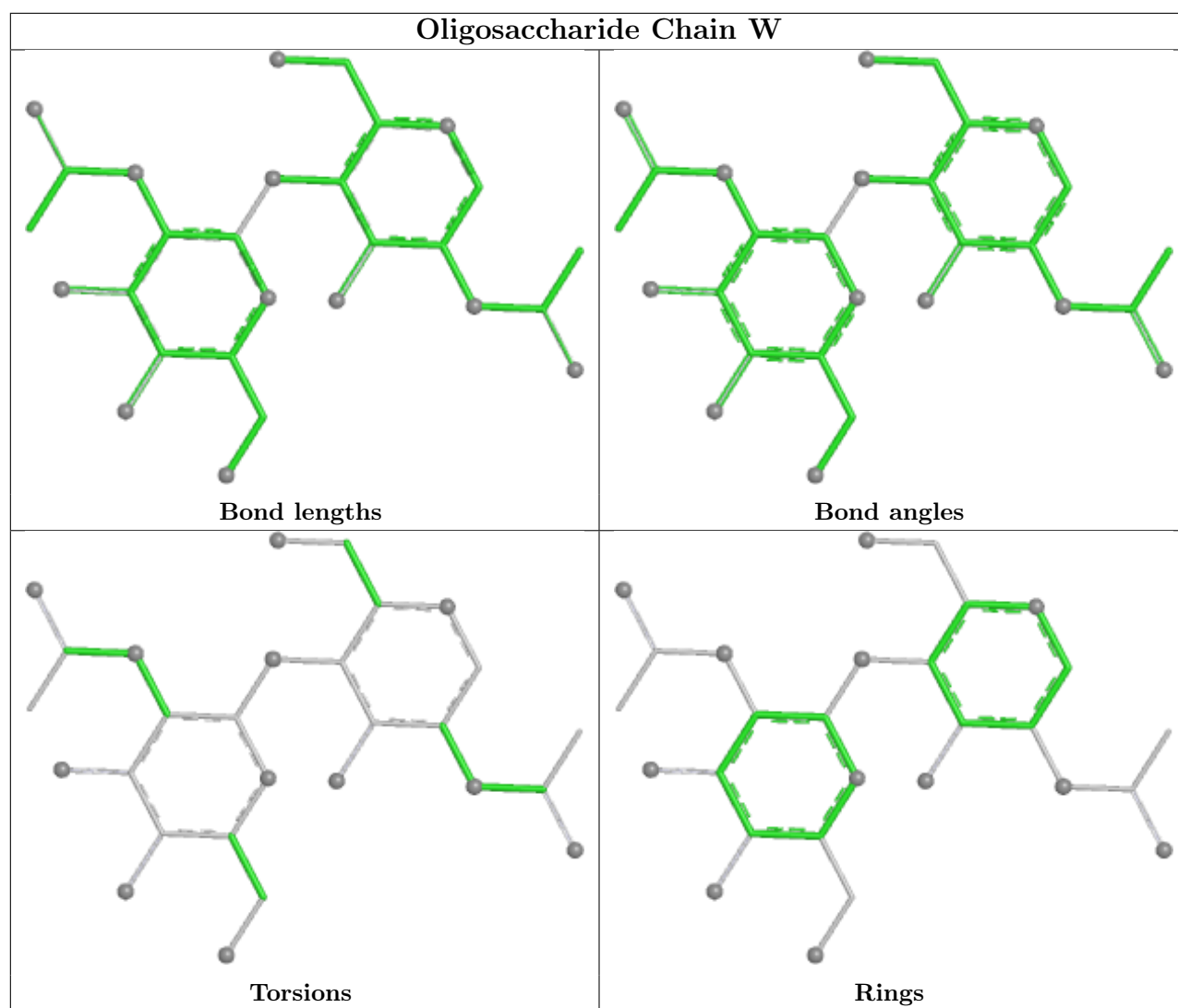


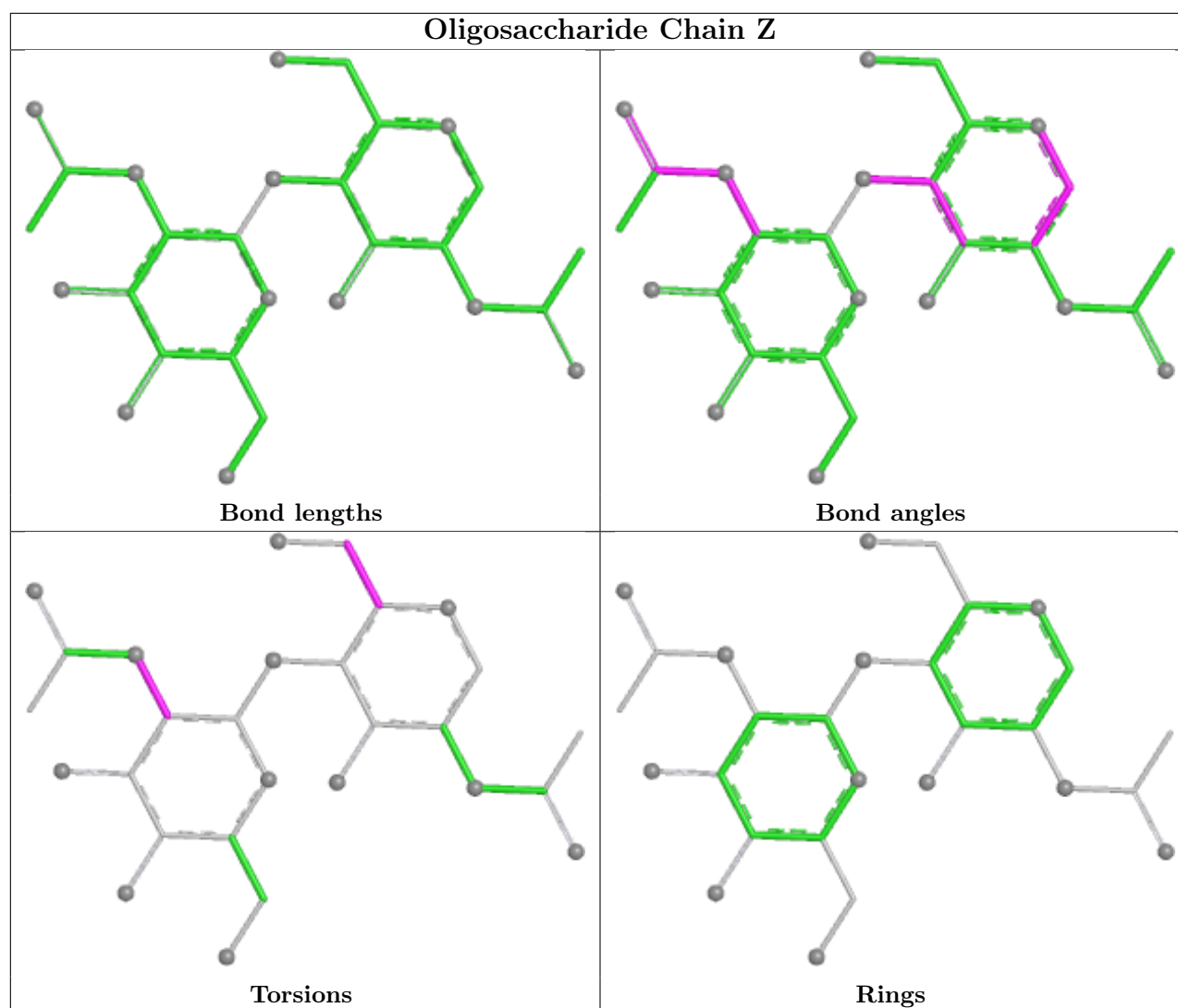












5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 27 are monoatomic - leaving 28 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	$\# Z > 2$
11	BMA	A	4505	-	11,11,12	0.87	0	15,15,17	2.09	4 (26%)
10	NAG	B	4512	-	14,14,15	0.75	0	17,19,21	0.73	0
10	NAG	B	4511	-	14,14,15	0.73	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	A	4501	2	14,14,15	0.73	0	17,19,21	0.99	1 (5%)
10	NAG	B	4505	2	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
10	NAG	B	4501	2	14,14,15	0.75	0	17,19,21	0.89	0
10	NAG	A	4503	2	14,14,15	0.72	0	17,19,21	0.94	0
12	NGA	A	4513	-	14,14,15	0.83	0	17,19,21	0.81	0
10	NAG	B	4502	2	14,14,15	0.78	0	17,19,21	0.89	0
10	NAG	A	4506	-	14,14,15	0.72	0	17,19,21	0.89	1 (5%)
12	NGA	B	4508	-	14,14,15	0.82	0	17,19,21	1.63	1 (5%)
10	NAG	A	4507	2	14,14,15	0.72	0	17,19,21	0.90	0
12	NGA	A	4512	2	14,14,15	0.81	0	17,19,21	0.76	0
10	NAG	B	4506	2	14,14,15	0.73	0	17,19,21	0.76	0
12	NGA	A	4511	2	14,14,15	0.85	0	17,19,21	0.86	0
10	NAG	A	4508	2	14,14,15	0.75	0	17,19,21	0.82	0
12	NGA	A	4514	-	14,14,15	0.84	0	17,19,21	0.78	0
10	NAG	A	4515	2	14,14,15	0.75	0	17,19,21	0.82	0
10	NAG	A	4510	-	14,14,15	0.73	0	17,19,21	1.60	1 (5%)
10	NAG	A	4509	-	14,14,15	0.74	0	17,19,21	0.80	0
10	NAG	A	4516	2	14,14,15	0.74	0	17,19,21	0.81	0
10	NAG	B	4503	2	14,14,15	0.71	0	17,19,21	0.87	0
10	NAG	B	4504	-	14,14,15	0.72	0	17,19,21	0.82	0
12	NGA	B	4509	-	14,14,15	0.81	0	17,19,21	0.87	0
10	NAG	B	4507	2	14,14,15	0.76	0	17,19,21	1.00	1 (5%)
12	NGA	B	4510	2	14,14,15	0.81	0	17,19,21	0.81	0
11	BMA	A	4504	-	11,11,12	0.86	0	15,15,17	1.82	1 (6%)
10	NAG	A	4502	2	14,14,15	0.75	0	17,19,21	0.99	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
11	BMA	A	4505	-	-	0/2/19/22	0/1/1/1
10	NAG	B	4512	-	-	2/6/23/26	0/1/1/1
10	NAG	B	4511	-	-	0/6/23/26	0/1/1/1
10	NAG	A	4501	2	-	0/6/23/26	0/1/1/1
10	NAG	B	4505	2	-	0/6/23/26	0/1/1/1
10	NAG	B	4501	2	-	0/6/23/26	0/1/1/1
10	NAG	A	4503	2	-	0/6/23/26	0/1/1/1
12	NGA	A	4513	-	-	0/6/23/26	0/1/1/1
10	NAG	B	4502	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	4506	-	-	2/6/23/26	0/1/1/1
12	NGA	B	4508	-	-	4/6/23/26	0/1/1/1
10	NAG	A	4507	2	-	0/6/23/26	0/1/1/1
12	NGA	A	4512	2	-	1/6/23/26	0/1/1/1
10	NAG	B	4506	2	-	0/6/23/26	0/1/1/1
12	NGA	A	4511	2	-	1/6/23/26	0/1/1/1
10	NAG	A	4508	2	-	0/6/23/26	0/1/1/1
12	NGA	A	4514	-	-	0/6/23/26	0/1/1/1
10	NAG	A	4515	2	-	0/6/23/26	0/1/1/1
10	NAG	A	4510	-	-	4/6/23/26	0/1/1/1
10	NAG	A	4509	-	-	0/6/23/26	0/1/1/1
10	NAG	A	4516	2	-	2/6/23/26	0/1/1/1
10	NAG	B	4503	2	-	0/6/23/26	0/1/1/1
10	NAG	B	4504	-	-	0/6/23/26	0/1/1/1
12	NGA	B	4509	-	-	2/6/23/26	0/1/1/1
10	NAG	B	4507	2	-	3/6/23/26	0/1/1/1
12	NGA	B	4510	2	-	0/6/23/26	0/1/1/1
11	BMA	A	4504	-	-	1/2/19/22	0/1/1/1
10	NAG	A	4502	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	4505	BMA	C1-O5-C5	5.97	120.19	112.19
12	B	4508	NGA	C2-N2-C7	5.96	130.89	122.90
10	A	4510	NAG	C2-N2-C7	5.51	130.29	122.90
11	A	4504	BMA	C1-O5-C5	5.45	119.48	112.19
11	A	4505	BMA	C3-C4-C5	3.08	115.83	110.23
10	A	4501	NAG	O5-C1-C2	-2.33	107.69	111.29
11	A	4505	BMA	C2-C3-C4	2.22	114.76	110.86
10	B	4505	NAG	O5-C1-C2	-2.15	107.96	111.29
11	A	4505	BMA	O4-C4-C3	-2.11	105.40	110.38
10	A	4502	NAG	C2-N2-C7	2.10	125.72	122.90
10	A	4506	NAG	C2-N2-C7	2.06	125.67	122.90
10	B	4507	NAG	C2-N2-C7	2.03	125.62	122.90

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	4509	NGA	O5-C5-C6-O6
12	B	4509	NGA	C4-C5-C6-O6
10	A	4510	NAG	C8-C7-N2-C2
10	A	4510	NAG	O7-C7-N2-C2
10	A	4516	NAG	C8-C7-N2-C2
10	A	4516	NAG	O7-C7-N2-C2
10	B	4512	NAG	C8-C7-N2-C2
10	B	4512	NAG	O7-C7-N2-C2
12	B	4508	NGA	C8-C7-N2-C2
12	B	4508	NGA	O7-C7-N2-C2
10	B	4507	NAG	O5-C5-C6-O6
12	A	4511	NGA	O5-C5-C6-O6
10	B	4502	NAG	O5-C5-C6-O6
10	A	4502	NAG	C1-C2-N2-C7
10	A	4506	NAG	C1-C2-N2-C7
10	B	4507	NAG	C1-C2-N2-C7
10	A	4502	NAG	C3-C2-N2-C7
12	B	4508	NGA	C3-C2-N2-C7
11	A	4504	BMA	O5-C5-C6-O6
10	A	4510	NAG	C1-C2-N2-C7
12	B	4508	NGA	C1-C2-N2-C7
12	A	4512	NGA	C4-C5-C6-O6
10	A	4506	NAG	C3-C2-N2-C7
10	A	4510	NAG	C3-C2-N2-C7
10	B	4507	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	4512	NAG	2	0
12	B	4508	NGA	2	0
12	A	4511	NGA	1	0
10	A	4510	NAG	1	0
12	B	4509	NGA	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

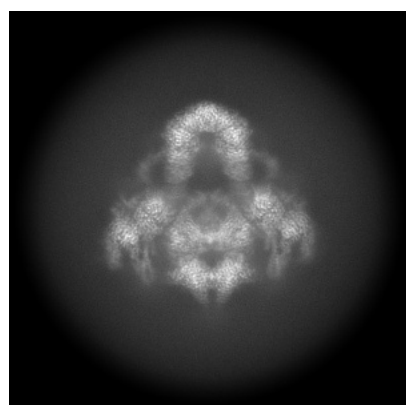
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52977. These allow visual inspection of the internal detail of the map and identification of artifacts.

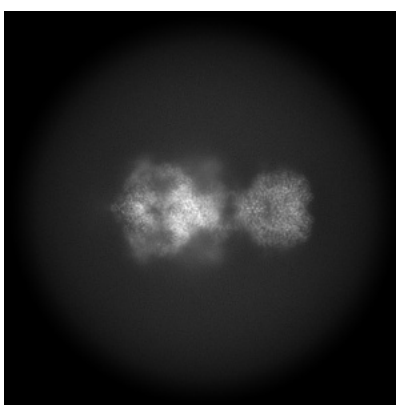
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

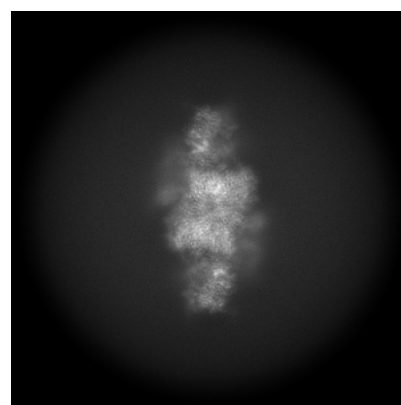
6.1.1 Primary map



X



Y

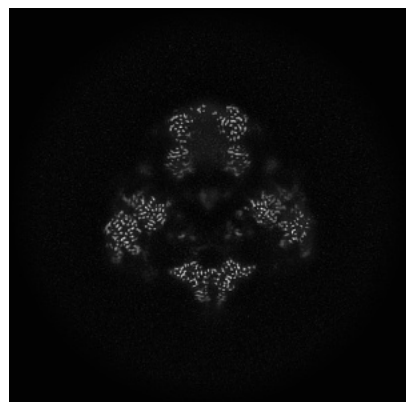


Z

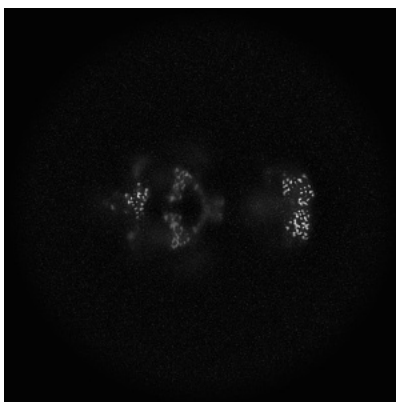
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

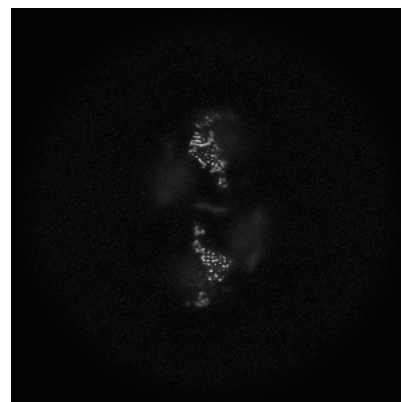
6.2.1 Primary map



X Index: 280



Y Index: 280

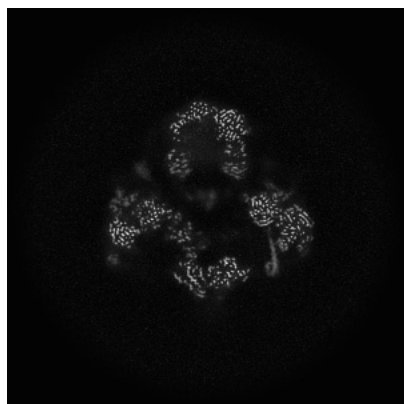


Z Index: 280

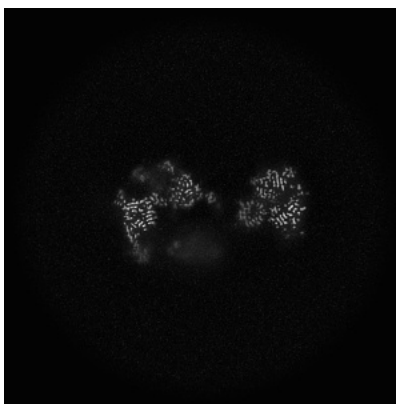
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

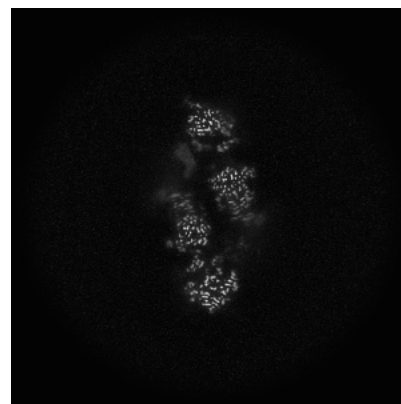
6.3.1 Primary map



X Index: 274



Y Index: 306

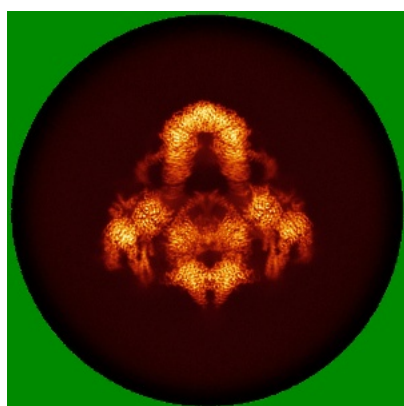


Z Index: 248

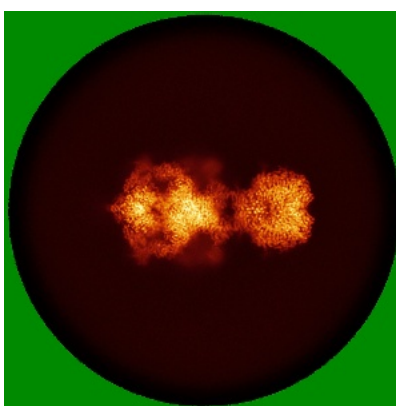
The images above show the largest variance slices of the map in three orthogonal directions.

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

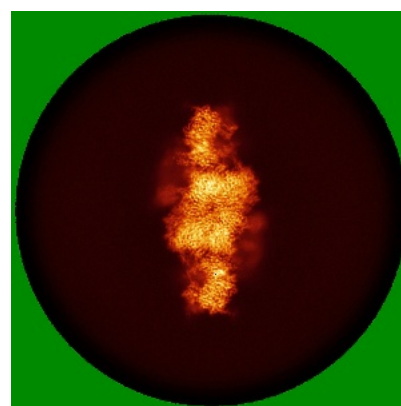
6.4.1 Primary map



X



Y

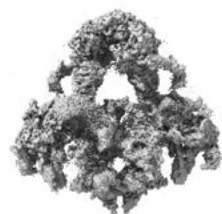


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

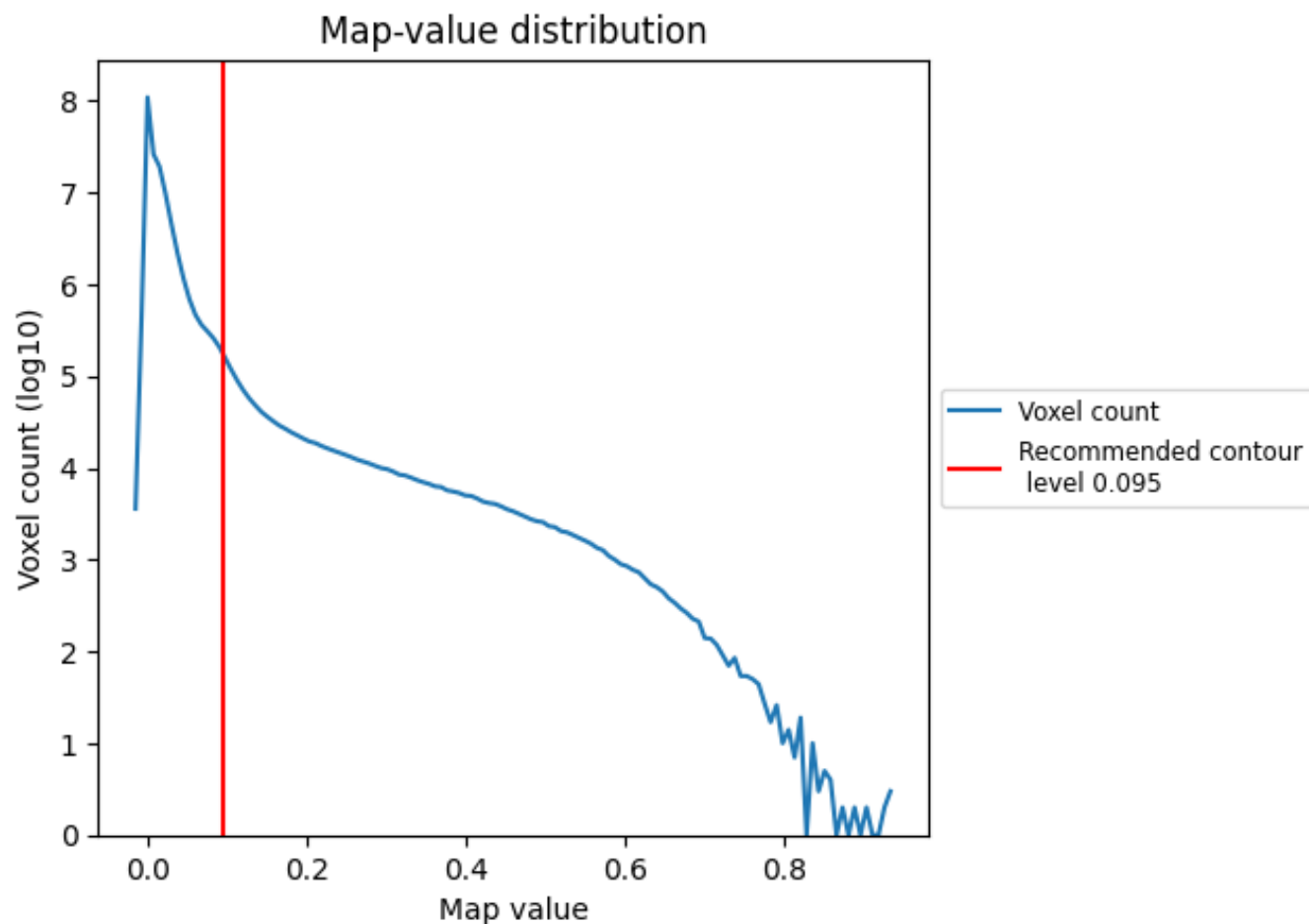
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

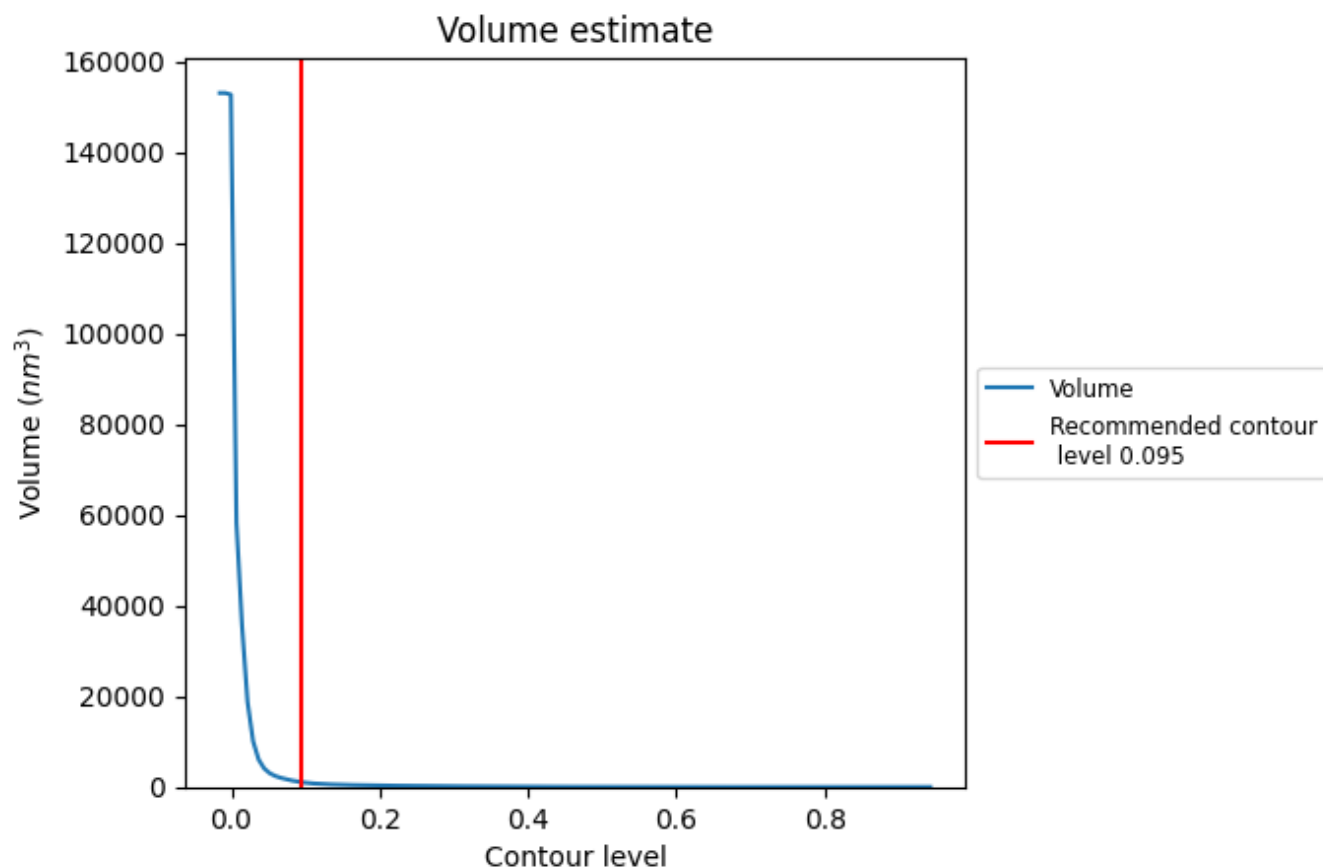
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

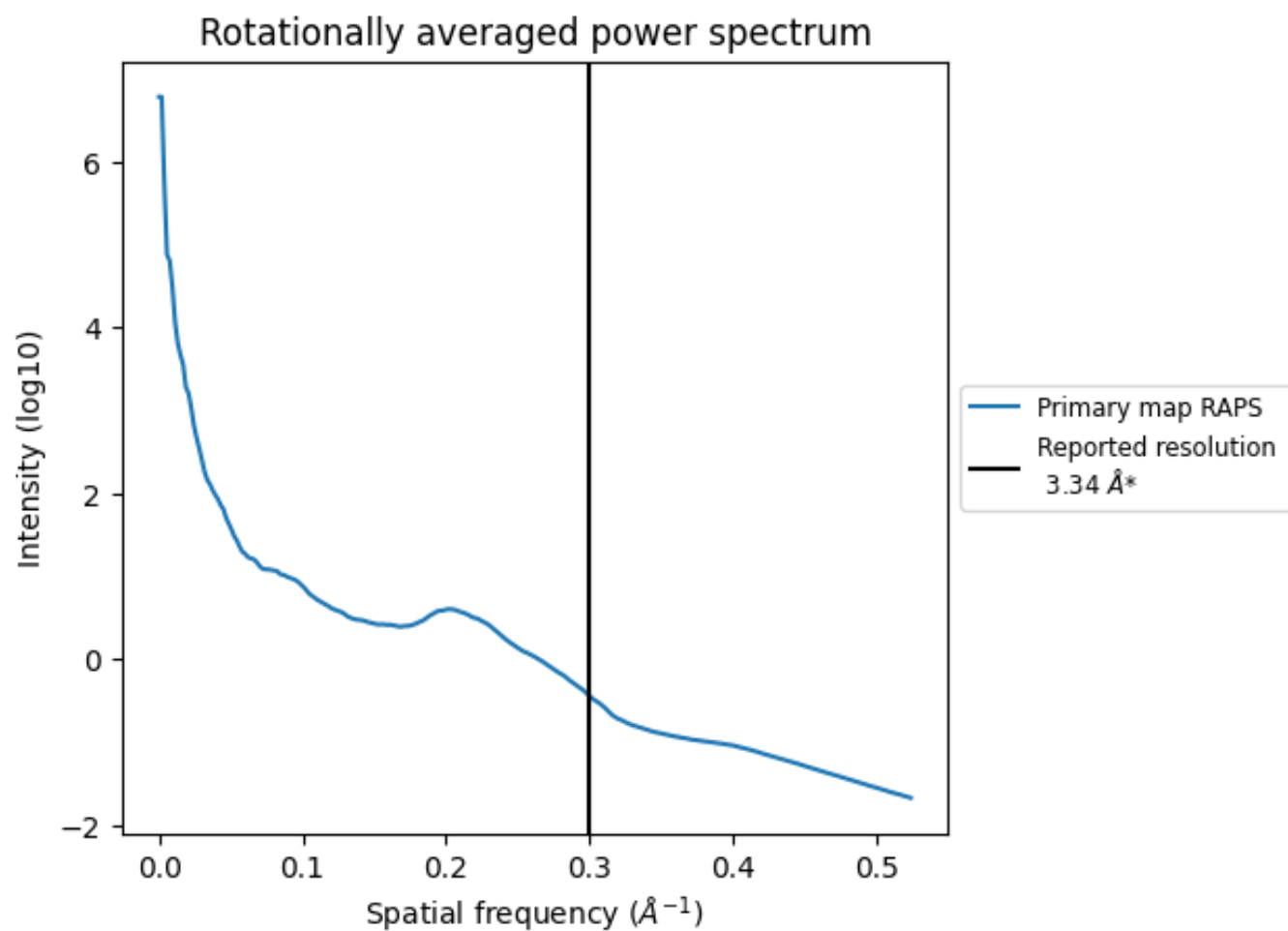
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1040 nm³; this corresponds to an approximate mass of 939 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 0.299 Å⁻¹

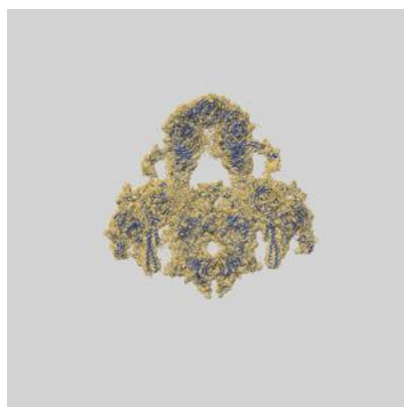
8 Fourier-Shell correlation ⓘ

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

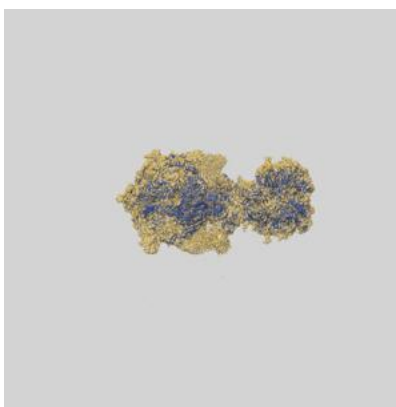
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52977 and PDB model 9QAW. Per-residue inclusion information can be found in section [3](#) on page [15](#).

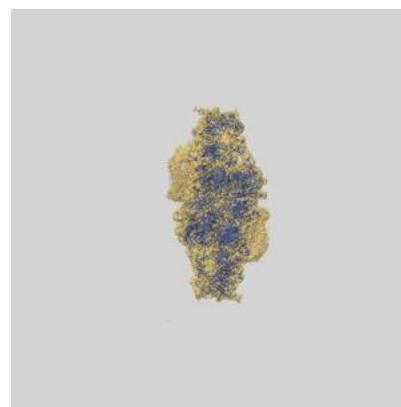
9.1 Map-model overlay [i](#)



X



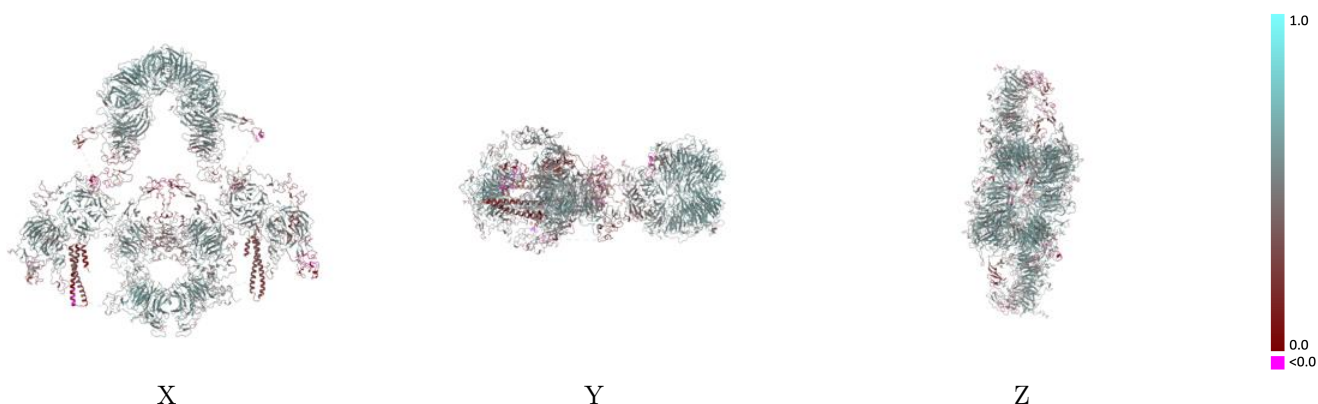
Y



Z

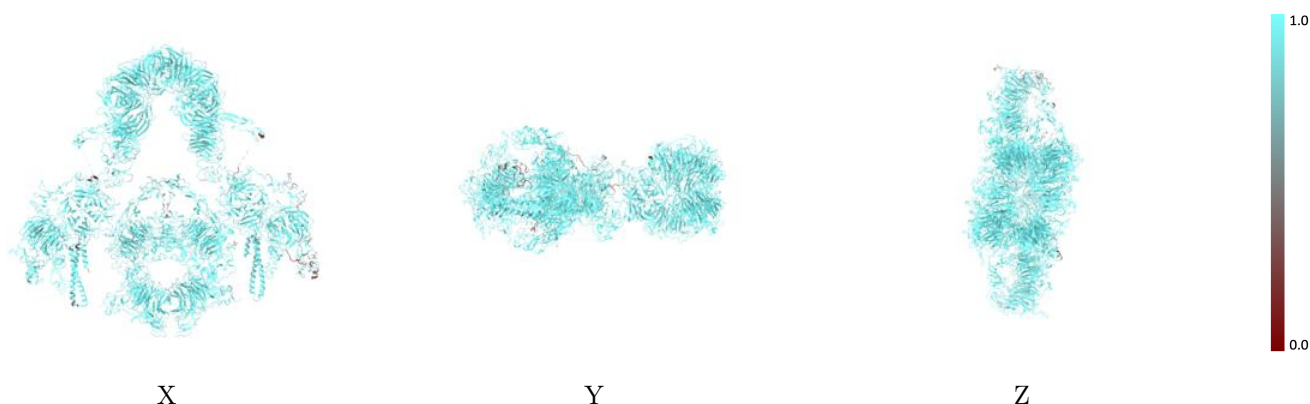
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



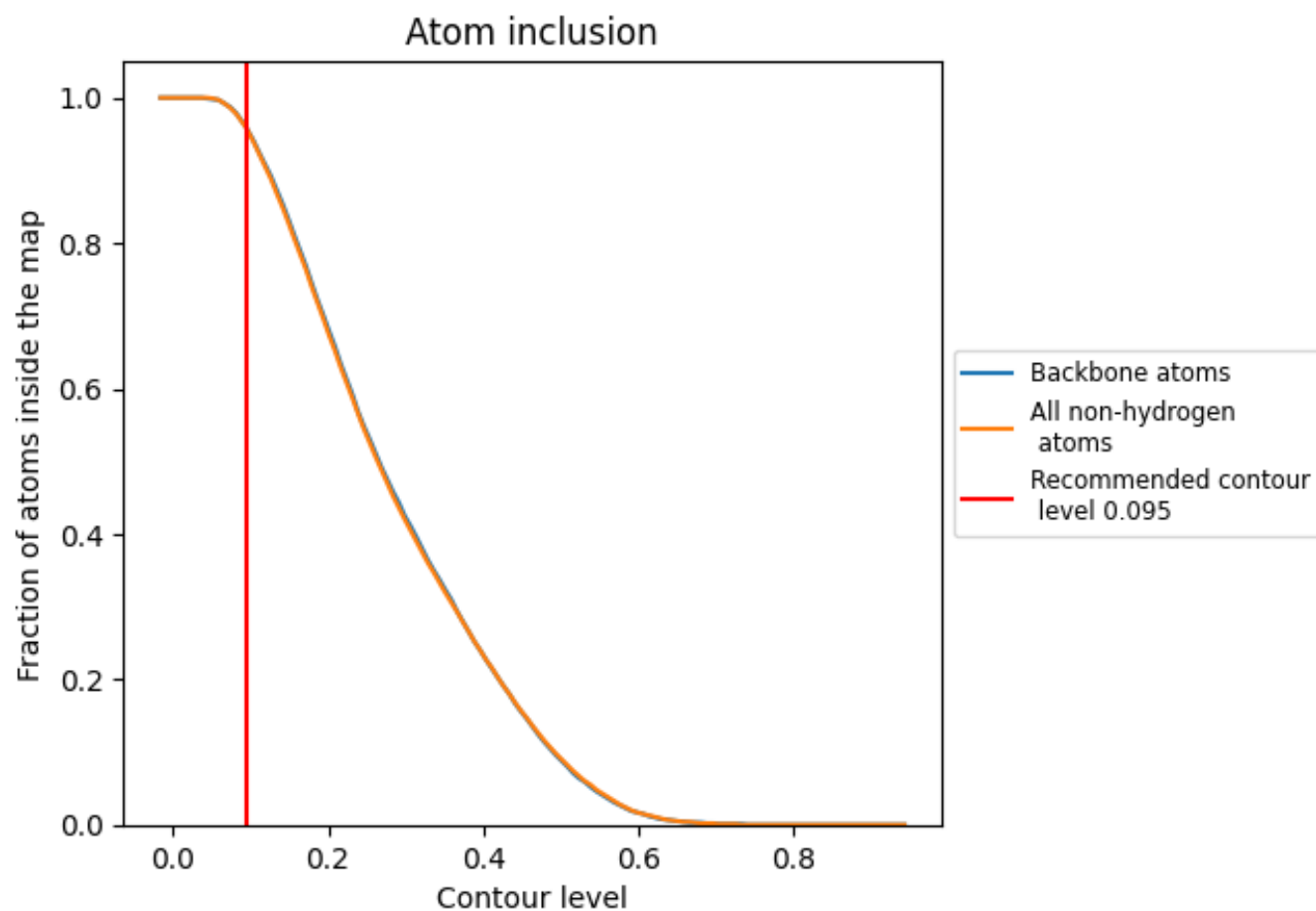
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.095).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.4810
A	 0.9530	 0.4830
B	 0.9720	 0.4930
C	 0.9430	 0.4370
D	 1.0000	 0.4480
E	 1.0000	 0.4990
F	 0.9710	 0.5290
G	 0.9850	 0.4910
H	 1.0000	 0.5380
I	 1.0000	 0.5320
J	 1.0000	 0.4900
K	 0.9180	 0.2650
L	 0.8900	 0.2420
M	 0.4360	 0.0870
N	 1.0000	 0.5520
O	 0.8930	 0.4070
P	 1.0000	 0.5060
Q	 0.9640	 0.5590
R	 0.8570	 0.3740
S	 0.6790	 0.2250
T	 1.0000	 0.4460
U	 1.0000	 0.5000
V	 0.8930	 0.4150
W	 0.9640	 0.4670
X	 0.9740	 0.5460
Y	 0.9230	 0.4590
Z	 0.9290	 0.5050
a	 0.9490	 0.4100
b	 0.9740	 0.4800

