



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:54 AM UTC

PDB ID : 9I3V / pdb\_00009i3v  
EMDB ID : EMD-52617  
Title : Cryo-EM structure of the human LRP2 ectodomain  
Authors : Ramanadane, K.; Coscia, F.  
Deposited on : 2025-01-24  
Resolution : 3.51 Å(reported)  
Based on initial model : 8EM4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

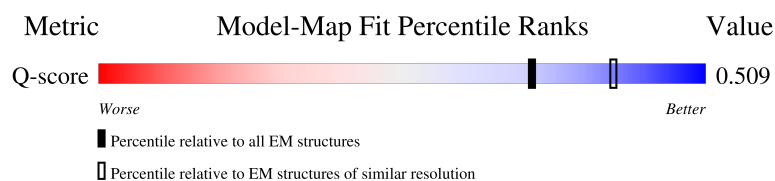
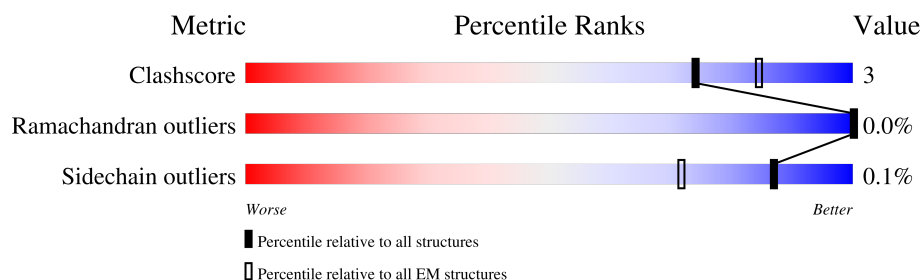
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.51 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.




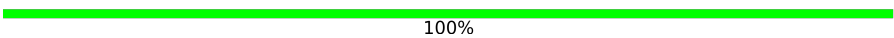
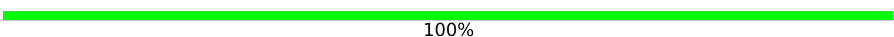

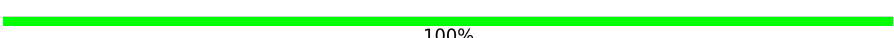
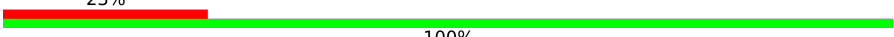
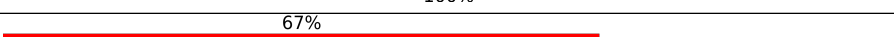
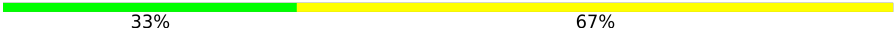


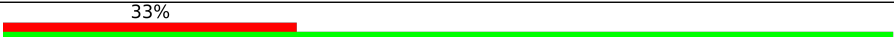
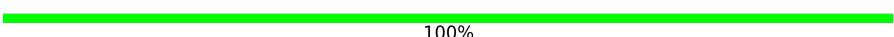
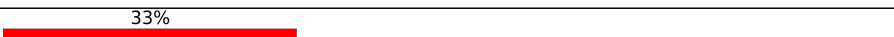
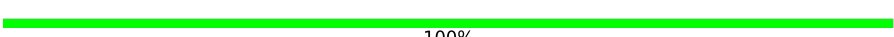
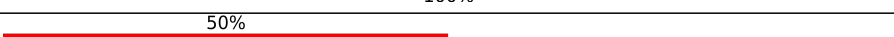

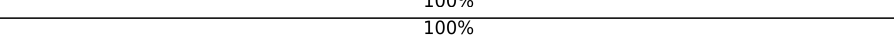

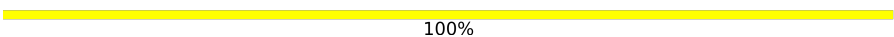
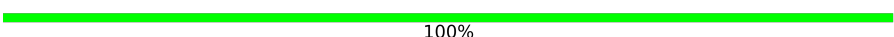
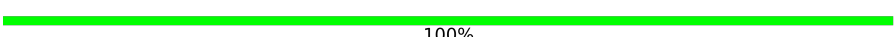
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13085 ( 3.01 - 4.01 )

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

Mol	Chain	Length	Quality of chain
1	A	4473	 5% 79% 7% 15%
1	B	4473	 1% 78% 7% 15%
2	D	10	 100%
2	E	10	 100%

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Mol	Chain	Length	Quality of chain
3	C	7	
3	F	7	
3	J	7	
4	H	12	
5	I	8	
6	G	13	
7	K	3	
7	N	3	
7	O	3	
7	P	3	
7	Q	3	
7	W	3	
7	X	3	
8	L	2	
8	M	2	
8	R	2	
8	S	2	
8	T	2	
8	U	2	
8	V	2	
8	Y	2	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NGA	B	4511	X	-	-	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 118041 atoms, of which 56764 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 Low-density lipoprotein receptor-related protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	3811	Total	C	H	N	O	S	0	0
			58095	18655	28064	5256	5817	303		
1	B	3804	Total	C	H	N	O	S	0	0
			57947	18608	27987	5241	5808	303		

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

- Molecule 2 is a protein called Unidentified peptide.

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

- Molecule 3 is a protein called Unidentified peptide.

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

- Molecule 4 is a protein called Unidentified peptide.

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

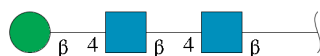
- Molecule 5 is a protein called Unidentified peptide.

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

- Molecule 6 is a protein called Unidentified peptide.

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

- Molecule 7 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.



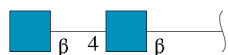
Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
7	N	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
7	O	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
7	P	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
7	Q	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
7	X	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

- Molecule 8 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
8	L	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
8	M	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
8	R	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
8	S	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
8	T	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
8	U	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
8	V	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
8	Y	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





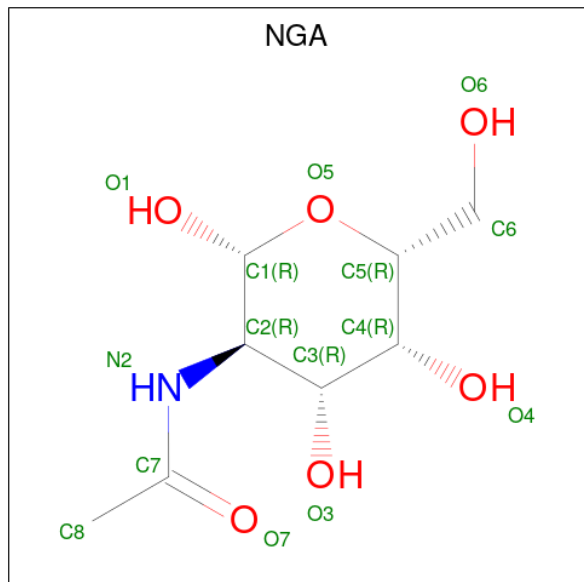
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	A	1	Total	C	H	N	O	0
			28	8	14	1	5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

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

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



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

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

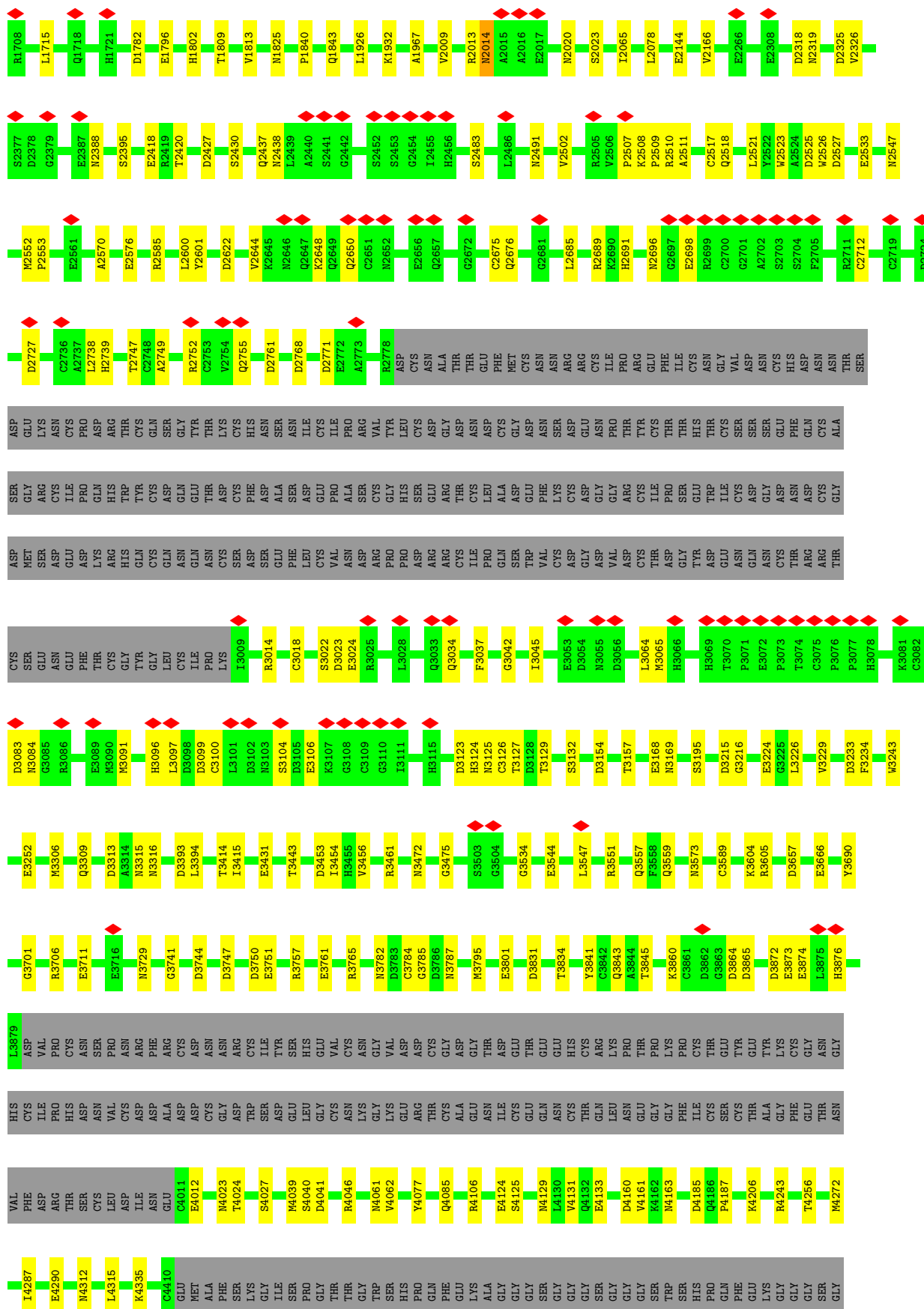
- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

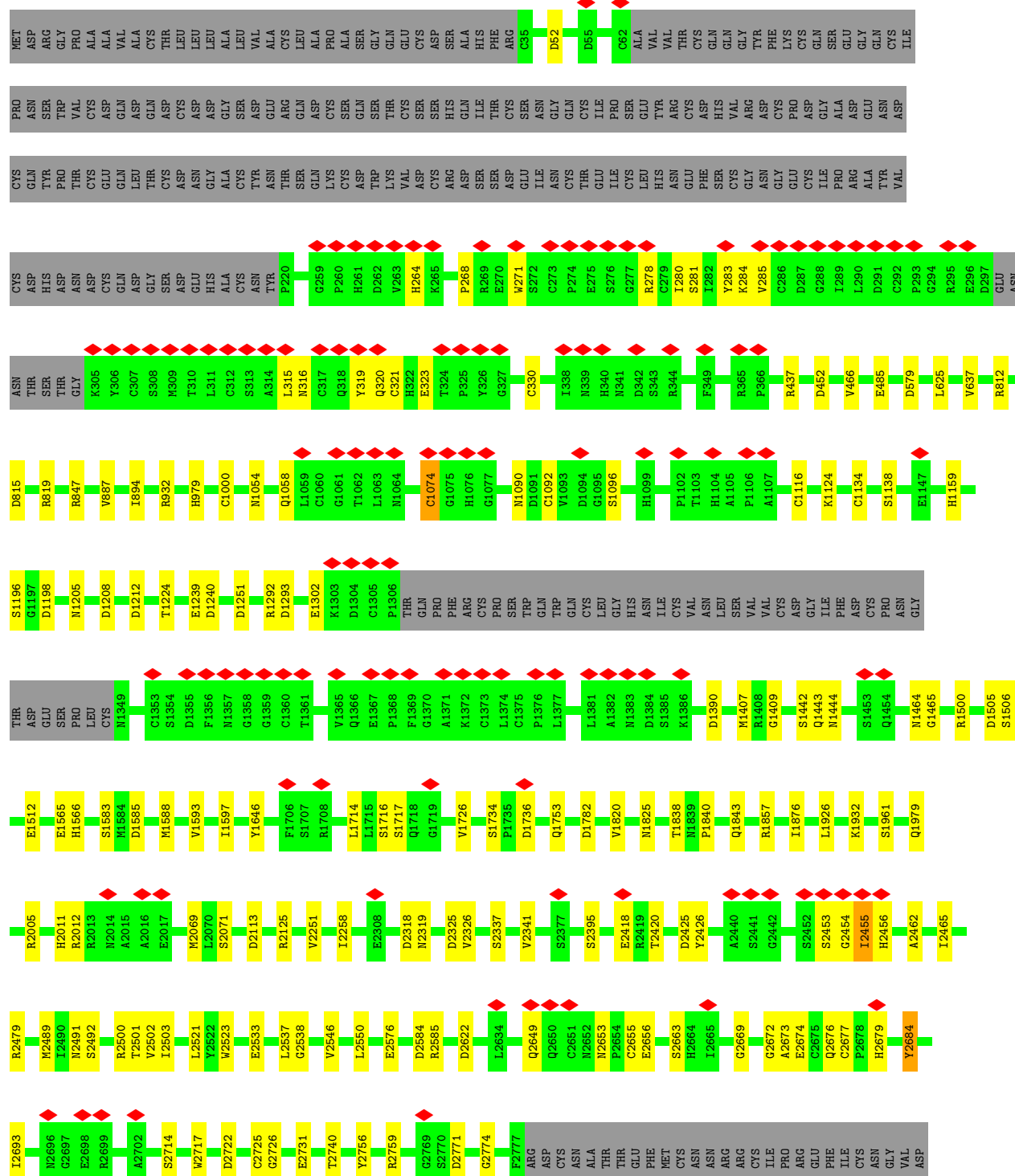
- Molecule 12 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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





Chain B:





There are no outlier residues recorded for this chain.

- Molecule 3: Unidentified peptide

Chain C:  86% 14%



- Molecule 3: Unidentified peptide

Chain F:  100%

There are no outlier residues recorded for this chain.

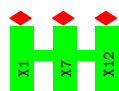
- Molecule 3: Unidentified peptide

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Unidentified peptide

Chain H:  25% 100%



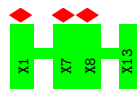
- Molecule 5: Unidentified peptide

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unidentified peptide

Chain G:  23% 100%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%





- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 67%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  67% 33%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  33% 33% 67%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  33% 100%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  33% 100%



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

Chain L:  100%



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

Chain M:  50% 100%



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

Chain R:  100%



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

Chain S:  100% 50% 50%



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

Chain T:  50% 50%



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

Chain U:  100%



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

Chain V:  100%

3AG1  
3AG2

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

Chain Y:  100%

3AG1  
3AG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	300645	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	1.330	Depositor
Minimum map value	-0.312	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.318	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: CA, NI, NGA, 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	0.15	0/30775	0.35	2/41803 (0.0%)
1	B	0.16	0/30701	0.37	6/41703 (0.0%)
All	All	0.16	0/61476	0.36	8/83506 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1224	THR	CA-C-N	7.71	131.13	120.65
1	B	1224	THR	C-N-CA	7.71	131.13	120.65
1	A	2014	ASN	CA-C-N	5.89	132.30	121.70
1	A	2014	ASN	C-N-CA	5.89	132.30	121.70
1	B	2649	GLN	CA-C-N	5.71	131.97	121.70
1	B	2649	GLN	C-N-CA	5.71	131.97	121.70
1	B	3616	PHE	CA-C-N	5.71	131.97	121.70
1	B	3616	PHE	C-N-CA	5.71	131.97	121.70

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30031	28064	28143	190	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	29960	27987	28060	191	0
2	D	50	0	12	0	0
2	E	50	0	13	0	0
3	C	35	0	9	1	0
3	F	35	0	9	0	0
3	J	35	0	10	0	0
4	H	60	0	15	0	0
5	I	40	0	11	0	0
6	G	65	0	16	0	0
7	K	39	37	34	1	0
7	N	39	37	34	1	0
7	O	39	37	34	0	0
7	P	39	37	34	1	0
7	Q	39	37	34	0	0
7	W	39	37	34	0	0
7	X	39	37	34	0	0
8	L	28	27	25	0	0
8	M	28	27	25	0	0
8	R	28	27	25	0	0
8	S	28	27	25	0	0
8	T	28	27	25	0	0
8	U	28	27	25	1	0
8	V	28	27	25	0	0
8	Y	28	27	25	0	0
9	A	154	126	143	6	0
9	B	112	112	104	0	0
10	A	56	0	52	4	0
10	B	70	0	65	3	0
11	A	12	0	0	0	0
11	B	13	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
All	All	61277	56764	57100	379	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 (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLY:O	1:A:368:ARG:NH1	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3278:ASP:OD2	1:B:3281:SER:OG	2.05	0.74
1:A:4163:ASN:OD1	1:B:3791:ARG:NH1	2.21	0.73
1:B:1961:SER:OG	1:B:1979:GLN:OE1	2.08	0.72
1:A:313:SER:O	1:A:316:ASN:ND2	2.23	0.71
1:B:1782:ASP:OD2	1:B:1825:ASN:ND2	2.24	0.70
1:B:3842:CYS:SG	1:B:3843:GLN:N	2.65	0.70
1:A:3589:CYS:O	1:A:3604:LYS:NZ	2.24	0.69
1:A:829:ARG:NH2	3:C:4:UNK:O	2.25	0.69
1:B:3491:CYS:SG	1:B:3506:THR:OG1	2.49	0.69
1:A:3472:ASN:OD1	1:A:3475:GLY:N	2.26	0.68
1:A:4024:THR:O	1:A:4027:SER:OG	2.06	0.68
1:A:3551:ARG:NH2	1:A:3557:GLN:O	2.27	0.68
1:A:4160:ASP:OD2	1:A:4163:ASN:ND2	2.26	0.68
1:B:3829:GLU:OE2	1:B:3835:ARG:NH2	2.27	0.68
9:A:4510:NAG:H83	9:A:4510:NAG:H3	1.76	0.67
1:B:1442:SER:OG	1:B:1443:GLN:OE1	2.12	0.67
1:B:316:ASN:OD1	1:B:320:GLN:NE2	2.28	0.67
1:B:1512:GLU:OE2	1:B:1646:TYR:OH	2.11	0.67
1:A:2675:CYS:SG	1:A:2676:GLN:N	2.67	0.66
1:B:3491:CYS:HG	1:B:3506:THR:HG1	1.40	0.66
1:B:3639:GLN:NE2	1:B:3640:PHE:O	2.29	0.65
1:B:4393:GLU:N	1:B:4393:GLU:OE1	2.30	0.65
1:B:3086:ARG:NH1	1:B:3087:CYS:O	2.29	0.65
1:B:2453:SER:O	1:B:2456:HIS:NE2	2.29	0.65
1:A:3224:GLU:OE2	1:A:3224:GLU:N	2.31	0.64
1:B:1205:ASN:ND2	1:B:1212:ASP:OD2	2.30	0.64
1:B:1565:GLU:OE1	1:B:1565:GLU:N	2.31	0.64
1:A:1274:SER:O	1:A:1274:SER:OG	2.16	0.64
1:A:1606:ASP:OD2	1:A:1609:ASN:ND2	2.32	0.63
1:B:3601:CYS:SG	1:B:3602:ALA:N	2.71	0.63
1:A:4312:ASN:ND2	1:B:4312:ASN:OD1	2.31	0.62
1:B:1566:HIS:ND1	1:B:1716:SER:O	2.32	0.62
1:A:2768:ASP:N	1:A:2771:ASP:OD1	2.32	0.62
1:A:3226:LEU:HD13	1:A:3229:VAL:HG11	1.82	0.62
1:A:1090:ASN:ND2	1:A:1092:CYS:O	2.33	0.61
1:A:3415:ILE:O	1:A:3461:ARG:NH1	2.33	0.61
1:B:2676:GLN:N	1:B:2676:GLN:OE1	2.34	0.61
1:B:1444:ASN:ND2	1:B:1465:GLY:O	2.33	0.61
1:A:3083:ASP:OD2	1:A:3104:SER:OG	2.18	0.61
1:A:903:ASP:OD2	1:A:905:ARG:NH2	2.34	0.60
1:A:2418:GLU:OE2	1:A:2437:GLN:NE2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1840:PRO:O	1:A:1843:GLN:NE2	2.33	0.60
1:A:3014:ARG:NE	1:A:3042:GLY:O	2.34	0.60
1:A:2648:LYS:O	1:A:2650:GLN:NE2	2.34	0.60
1:A:2013:ARG:O	1:A:2014:ASN:ND2	2.35	0.60
1:A:3657:ASP:OD2	1:A:3706:ARG:NH2	2.35	0.60
1:A:3091:MET:HE1	1:B:3111:ILE:HD11	1.84	0.59
1:A:1409:GLY:O	10:A:4514:NGA:O6	2.21	0.59
1:A:3037:PHE:N	1:A:3045:ILE:O	2.36	0.59
1:B:1054:ASN:O	1:B:1058:GLN:N	2.36	0.59
1:A:4012:GLU:OE2	1:A:4023:ASN:ND2	2.35	0.59
1:A:2576:GLU:OE2	1:A:2585:ARG:NH1	2.36	0.59
1:B:3084:ASN:ND2	1:B:3102:ASP:OD1	2.36	0.59
1:A:1479:ARG:NH2	1:A:1499:ASP:OD2	2.36	0.59
1:A:4125:SER:OG	1:A:4129:ASN:OD1	2.20	0.59
1:A:3729:ASN:N	1:A:3747:ASP:OD2	2.35	0.58
1:B:1840:PRO:O	1:B:1843:GLN:NE2	2.36	0.58
1:B:3633:ARG:NH2	1:B:3635:CYS:SG	2.76	0.58
1:B:3741:GLY:N	1:B:3751:GLU:OE1	2.37	0.58
1:A:2552:MET:HE3	1:A:2552:MET:HA	1.85	0.57
1:A:4133:GLU:OE1	1:A:4133:GLU:N	2.37	0.57
1:A:1206:ARG:NH1	1:A:1218:ASP:O	2.37	0.57
1:A:2685:LEU:HD13	1:A:2696:ASN:OD1	2.04	0.57
1:A:3084:ASN:ND2	1:A:3100:CYS:O	2.38	0.57
1:B:3014:ARG:NH2	1:B:3044:CYS:SG	2.78	0.57
1:A:1506:SER:OG	1:A:1809:THR:O	2.10	0.57
1:A:2552:MET:HE3	1:A:2553:PRO:HD2	1.86	0.57
1:A:801:THR:HG22	1:A:808:ILE:HG12	1.85	0.57
1:A:2738:LEU:O	1:A:2739:HIS:ND1	2.36	0.57
1:B:2501:THR:OG1	1:B:2677:CYS:O	2.23	0.56
1:A:2395:SER:O	1:A:2420:THR:N	2.38	0.56
1:A:2420:THR:OG1	1:A:2438:ASN:O	2.22	0.56
1:A:3129:THR:OG1	1:A:3132:SER:N	2.38	0.56
1:B:1116:CYS:SG	1:B:1138:SER:OG	2.59	0.56
1:B:1407:MET:N	1:B:1407:MET:SD	2.78	0.56
1:A:3831:ASP:OD1	1:A:3831:ASP:N	2.36	0.56
1:A:4039:MET:O	1:A:4046:ARG:NH1	2.38	0.56
1:B:437:ARG:NH1	1:B:452:ASP:OD1	2.38	0.56
1:A:2689:ARG:O	1:A:2691:HIS:ND1	2.38	0.56
1:B:3673:SER:OG	1:B:3674:SER:N	2.38	0.56
1:A:1410:SER:HA	10:A:4514:NGA:O5	2.03	0.56
1:A:2508:LYS:NZ	1:A:2533:GLU:OE2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3795:MET:N	1:A:3795:MET:HE2	2.22	0.55
1:A:3573:ASN:O	1:A:3605:ARG:NH2	2.40	0.55
1:B:2454:GLY:O	1:B:2456:HIS:N	2.40	0.55
1:B:2546:VAL:HG12	1:B:2550:LEU:HD11	1.89	0.55
1:B:3764:PHE:HB2	1:B:3777:ILE:HD11	1.87	0.55
1:B:2722:ASP:N	1:B:2731:GLU:OE2	2.38	0.55
1:A:3125:ASN:HA	9:A:4528:NAG:O7	2.07	0.55
1:A:3782:ASN:OD1	1:A:3787:ASN:ND2	2.40	0.55
1:B:3173:SER:HA	10:B:4509:NGA:O5	2.03	0.55
1:A:1796:GLU:OE2	1:A:1802:HIS:NE2	2.40	0.55
1:A:4243:ARG:NH1	1:A:4256:THR:OG1	2.40	0.55
1:A:1224:THR:HG21	10:A:4512:NGA:O7	2.07	0.55
1:B:1716:SER:OG	1:B:1717:SER:N	2.40	0.54
1:A:1239:GLU:N	1:A:1239:GLU:OE1	2.40	0.54
1:B:3521:ASN:ND2	1:B:3523:GLU:OE2	2.40	0.54
1:A:3123:ASP:OD1	1:A:3124:HIS:N	2.40	0.54
1:B:3551:ARG:NH2	1:B:3557:GLN:O	2.40	0.54
1:A:4024:THR:N	1:A:4027:SER:O	2.40	0.54
1:A:1227:PRO:O	1:A:3195:SER:OG	2.24	0.54
1:A:3168:GLU:OE1	1:A:3169:ASN:N	2.40	0.54
1:A:3782:ASN:ND2	1:A:3784:CYS:O	2.41	0.54
7:P:1:NAG:O3	7:P:2:NAG:O5	2.22	0.54
1:A:2622:ASP:N	1:A:2622:ASP:OD1	2.39	0.54
1:A:4272:MET:SD	1:A:4272:MET:N	2.81	0.54
1:A:3666:GLU:OE1	1:A:3690:TYR:OH	2.14	0.54
1:B:2318:ASP:OD1	1:B:2319:ASN:N	2.41	0.53
1:B:3146:ASP:OD2	1:B:3149:THR:OG1	2.16	0.53
1:A:2526:TRP:CZ2	1:A:2552:MET:HE1	2.44	0.53
1:A:3018:CYS:SG	1:A:3022:SER:N	2.82	0.53
1:B:264:HIS:O	1:B:278:ARG:NE	2.42	0.53
1:B:1464:ASN:OD1	1:B:1500:ARG:NH1	2.40	0.53
1:A:4085:GLN:OE1	1:A:4106:ARG:NH2	2.42	0.53
1:B:2622:ASP:OD1	1:B:2622:ASP:N	2.40	0.53
1:A:309:MET:HE2	1:A:309:MET:HA	1.91	0.53
1:A:2698:GLU:N	1:A:2698:GLU:OE1	2.42	0.53
1:A:4124:GLU:OE1	1:A:4125:SER:N	2.42	0.53
1:B:1390:ASP:OD1	1:B:1409:GLY:N	2.41	0.53
1:B:2677:CYS:O	1:B:2679:HIS:ND1	2.42	0.52
1:B:2489:MET:SD	1:B:2491:ASN:ND2	2.82	0.52
1:B:3761:GLU:N	1:B:3761:GLU:OE1	2.42	0.52
1:A:1366:GLN:NE2	1:A:1367:GLU:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3761:GLU:N	1:A:3761:GLU:OE1	2.42	0.52
1:B:3633:ARG:O	1:B:3641:ARG:NH2	2.43	0.52
1:A:3034:GLN:OE1	1:A:3034:GLN:N	2.42	0.52
1:A:3860:LYS:N	1:A:3864:ASP:OD2	2.43	0.52
8:U:1:NAG:O3	8:U:2:NAG:O5	2.25	0.52
1:A:3551:ARG:O	1:A:3559:GLN:NE2	2.41	0.52
1:A:3233:ASP:OD1	1:A:3234:PHE:N	2.42	0.52
1:A:1059:LEU:HD23	1:A:1060:CYS:O	2.09	0.52
1:B:3215:ASP:OD1	1:B:3216:GLY:N	2.43	0.52
1:B:1293:ASP:N	1:B:1302:GLU:OE2	2.41	0.51
1:B:1734:SER:OG	1:B:1736:ASP:OD1	2.23	0.51
1:B:3082:CYS:N	1:B:3086:ARG:O	2.43	0.51
1:B:4255:GLU:HG2	1:B:4266:VAL:HG22	1.91	0.51
1:B:2337:SER:O	1:B:2341:VAL:HG22	2.11	0.51
1:B:3603:ASN:ND2	1:B:3622:ASN:OD1	2.43	0.51
1:A:2491:ASN:OD1	1:A:2502:VAL:HG22	2.11	0.51
1:B:1588:MET:HE3	1:B:1588:MET:HA	1.93	0.51
1:B:1714:LEU:HD12	1:B:1726:VAL:HG11	1.92	0.51
1:B:2425:ASP:OD1	1:B:2426:TYR:N	2.43	0.51
1:B:812:ARG:NH1	1:B:815:ASP:OD2	2.44	0.51
1:B:3429:THR:HG22	1:B:3446:ASN:HB3	1.93	0.51
1:A:1583:SER:OG	1:A:1585:ASP:OD1	2.24	0.51
1:A:1926:LEU:HD12	1:A:1932:LYS:O	2.11	0.51
1:B:2653:ASN:ND2	1:B:2656:GLU:OE1	2.43	0.51
1:B:3621:ASP:OD1	1:B:3621:ASP:N	2.44	0.51
1:B:932:ARG:NH2	1:B:1208:ASP:OD2	2.44	0.51
1:B:3765:ARG:NH1	1:B:3769:GLN:OE1	2.44	0.51
1:A:1666:MET:SD	1:A:1678:VAL:HG22	2.51	0.51
1:B:1443:GLN:OE1	1:B:1443:GLN:N	2.44	0.50
1:B:2395:SER:O	1:B:2420:THR:N	2.43	0.50
1:B:2523:TRP:NE1	1:B:2533:GLU:OE2	2.44	0.50
1:B:3196:ASN:OD1	1:B:3196:ASN:N	2.45	0.50
1:B:3478:HIS:NE2	1:B:3522:ASN:O	2.44	0.50
1:A:2318:ASP:OD1	1:A:2319:ASN:N	2.45	0.50
1:B:2714:SER:HG	1:B:2717:TRP:CD1	2.30	0.50
1:A:493:MET:HE1	1:A:675:VAL:HG12	1.94	0.50
1:B:3616:PHE:HB3	1:B:3617:ASN:HA	1.94	0.50
1:B:3807:SER:OG	1:B:3808:GLY:N	2.44	0.50
1:A:911:GLU:OE1	1:A:912:GLN:N	2.45	0.49
1:A:266:CYS:SG	1:A:267:SER:N	2.86	0.49
1:A:753:SER:HB3	1:A:770:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:VAL:HG21	1:B:321:CYS:SG	2.52	0.49
1:B:466:VAL:HG12	1:B:485:GLU:OE2	2.13	0.49
1:B:3501:GLN:NE2	1:B:3504:GLY:O	2.43	0.49
1:B:3644:ASN:ND2	1:B:3662:ASP:OD1	2.45	0.49
1:B:2663:SER:O	1:B:2663:SER:OG	2.22	0.49
1:A:1277:HIS:ND1	1:A:1283:CYS:SG	2.74	0.49
1:B:3784:CYS:N	1:B:3789:ASP:OD1	2.41	0.49
1:A:3744:ASP:N	1:A:3750:ASP:OD2	2.44	0.49
1:A:3125:ASN:CG	9:A:4528:NAG:H2	2.38	0.49
1:B:3265:ILE:HD11	1:B:3301:GLY:HA2	1.94	0.49
1:B:1583:SER:OG	1:B:1585:ASP:OD1	2.26	0.49
1:B:3701:GLY:N	1:B:3711:GLU:OE1	2.43	0.49
1:A:2600:LEU:HD23	1:A:2601:TYR:N	2.28	0.48
1:B:2418:GLU:OE1	1:B:2418:GLU:N	2.45	0.48
1:B:3691:ARG:NH1	1:B:3704:ASP:O	2.46	0.48
1:A:3154:ASP:OD2	1:A:3157:THR:OG1	2.23	0.48
1:A:3843:GLN:OE1	1:A:3845:THR:OG1	2.31	0.48
1:B:3224:GLU:OE1	1:B:3224:GLU:N	2.46	0.48
1:A:2427:ASP:OD2	1:A:2430:SER:OG	2.31	0.48
1:A:3065:MET:HE2	1:A:3065:MET:N	2.28	0.48
1:A:786:VAL:HG11	1:A:789:LEU:HD21	1.95	0.48
1:A:1484:ASP:OD2	1:A:1487:GLN:NE2	2.47	0.48
1:A:2510:ARG:HB2	1:A:2526:TRP:H	1.79	0.48
1:B:3553:CYS:SG	1:B:3554:ARG:N	2.86	0.48
1:A:1206:ARG:NH1	1:A:1207:CYS:SG	2.87	0.48
1:A:3701:GLY:N	1:A:3711:GLU:OE1	2.46	0.48
1:B:2113:ASP:OD2	1:B:2125:ARG:NH1	2.47	0.48
1:B:4091:TRP:O	1:B:4328:LYS:NZ	2.43	0.48
7:N:1:NAG:O3	7:N:2:NAG:O5	2.26	0.48
1:A:3315:ASN:ND2	9:A:4510:NAG:H2	2.29	0.48
1:A:4077:TYR:O	1:A:4131:VAL:HG21	2.13	0.48
1:A:3023:ASP:OD1	1:A:3024:GLU:N	2.47	0.48
1:B:2491:ASN:OD1	1:B:2500:ARG:NH1	2.47	0.48
1:B:3585:ASP:OD1	1:B:3586:ARG:N	2.46	0.48
1:A:4290:GLU:OE1	1:A:4290:GLU:N	2.46	0.47
1:A:3215:ASP:OD1	1:A:3216:GLY:N	2.46	0.47
1:A:3872:ASP:OD1	1:A:3873:GLU:N	2.47	0.47
1:B:3828:ASP:OD1	1:B:3829:GLU:N	2.46	0.47
1:A:1034:LYS:HG2	1:A:1055:SER:HB3	1.96	0.47
1:A:4335:LYS:NZ	1:B:52:ASP:OD1	2.28	0.47
1:B:1240:ASP:OD1	1:B:1240:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3683:GLU:O	1:B:3695:LYS:NZ	2.46	0.47
1:B:2455:ILE:HG13	1:B:2456:HIS:H	1.80	0.47
1:A:1164:LEU:O	1:A:1164:LEU:HD23	2.14	0.47
1:A:3313:ASP:OD2	1:A:3316:ASN:N	2.48	0.47
1:B:2011:HIS:ND1	1:B:2012:ARG:O	2.46	0.47
1:A:1802:HIS:CE1	1:A:1813:VAL:HG22	2.50	0.47
1:A:3018:CYS:N	1:A:3023:ASP:OD2	2.48	0.47
1:A:3534:GLY:N	1:A:3544:GLU:OE1	2.46	0.47
1:B:2759:ARG:NH1	1:B:2771:ASP:O	2.47	0.47
1:B:1292:ARG:N	1:B:1302:GLU:OE2	2.47	0.47
1:B:1505:ASP:OD1	1:B:1506:SER:N	2.48	0.46
1:B:4022:ARG:NH1	1:B:4029:GLU:OE2	2.48	0.46
1:B:4243:ARG:NH1	1:B:4256:THR:OG1	2.48	0.46
1:B:4152:VAL:O	1:B:4332:ASN:ND2	2.48	0.46
1:A:3801:GLU:OE1	1:A:3801:GLU:N	2.46	0.46
1:A:4023:ASN:OD1	1:A:4024:THR:N	2.48	0.46
1:A:279:CYS:SG	1:A:280:ILE:N	2.88	0.46
1:B:3395:GLU:N	1:B:3395:GLU:OE1	2.48	0.46
1:A:1393:GLU:OE2	10:A:4514:NGA:O6	2.34	0.46
1:A:2388:ASN:ND2	1:A:2644:VAL:HG13	2.31	0.46
1:A:2508:LYS:HD3	1:A:2525:ASP:OD2	2.16	0.46
1:A:3315:ASN:CG	9:A:4510:NAG:H2	2.41	0.46
1:B:1239:GLU:OE1	1:B:1239:GLU:N	2.48	0.46
1:B:3376:ASN:OD1	1:B:3376:ASN:N	2.48	0.46
1:B:3312:VAL:HG23	1:B:3356:LYS:HB3	1.96	0.46
1:A:2517:CYS:SG	1:A:2518:GLN:N	2.85	0.46
1:B:2489:MET:HE2	1:B:2502:VAL:HG13	1.98	0.46
1:B:3009:ILE:HD12	1:B:3010:PHE:CZ	2.50	0.46
1:B:3835:ARG:O	10:B:4510:NGA:H5	2.15	0.46
1:A:1277:HIS:HD1	1:A:1283:CYS:HG	1.49	0.46
1:B:819:ARG:NE	1:B:1000:CYS:O	2.44	0.46
1:B:3055:ASN:O	1:B:3055:ASN:ND2	2.49	0.46
1:A:4024:THR:OG1	1:A:4027:SER:O	2.14	0.46
1:B:2479:ARG:NH2	1:B:2492:SER:OG	2.49	0.46
1:A:2521:LEU:HD23	1:A:2523:TRP:CE3	2.52	0.45
1:B:847:ARG:NH2	1:B:1251:ASP:OD2	2.49	0.45
1:B:2492:SER:HB3	1:B:2503:ILE:HD11	1.98	0.45
1:A:2065:ILE:HD11	1:A:2078:LEU:CD2	2.46	0.45
1:A:3097:LEU:HD23	1:A:3099:ASP:N	2.32	0.45
1:A:2325:ASP:OD1	1:A:2326:VAL:N	2.46	0.45
1:A:3453:ASP:OD1	1:A:3454:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2576:GLU:OE1	1:B:2585:ARG:NH2	2.48	0.45
1:A:1566:HIS:ND1	1:A:1715:LEU:HD23	2.32	0.45
1:B:3863:GLY:N	1:B:3873:GLU:OE1	2.46	0.45
1:A:3243:TRP:NE1	1:A:3252:GLU:OE1	2.47	0.45
1:A:3226:LEU:CD1	1:A:3229:VAL:HG11	2.46	0.45
1:B:3274:SER:O	1:B:3326:LEU:HD22	2.17	0.45
1:A:3306:MET:HE3	1:A:3309:GLN:HB3	1.99	0.45
1:B:887:VAL:HG22	1:B:894:ILE:HG12	1.99	0.45
1:A:2507:PRO:HD2	1:A:2508:LYS:HZ2	1.80	0.45
1:B:3669:GLU:OE1	1:B:3669:GLU:N	2.45	0.45
1:B:4287:ILE:HD12	1:B:4315:LEU:HD23	1.99	0.45
1:B:3105:ASP:OD1	1:B:3106:GLU:N	2.50	0.45
1:A:3393:ASP:OD1	1:A:3394:LEU:N	2.49	0.44
1:B:2725:CYS:SG	1:B:2726:GLY:N	2.90	0.44
1:A:1420:MET:HE1	1:A:1422:GLU:OE1	2.18	0.44
1:B:2655:CYS:SG	1:B:2673:ALA:HB1	2.57	0.44
1:B:3740:ASP:N	1:B:3751:GLU:OE1	2.51	0.44
1:B:1753:GLN:OE1	1:B:2005:ARG:NH2	2.51	0.44
1:B:4278:ASP:OD2	1:B:4319:ARG:NH1	2.50	0.44
1:B:4280:PHE:HB2	1:B:4320:ILE:HD13	2.00	0.44
1:B:2669:GLY:N	1:B:2672:GLY:O	2.49	0.44
1:B:3806:THR:OG1	1:B:3825:ASP:OD2	2.33	0.44
1:B:4135:ASP:O	1:B:4137:LYS:NZ	2.43	0.44
1:A:1782:ASP:OD2	1:A:1825:ASN:ND2	2.50	0.44
1:B:1593:VAL:CG1	1:B:1597:ILE:HD11	2.47	0.44
1:A:493:MET:HE1	1:A:675:VAL:CG1	2.48	0.44
1:A:3414:THR:HG21	1:A:3456:VAL:HG23	2.00	0.44
1:B:2462:ALA:HB1	1:B:2465:ILE:HD11	1.99	0.44
1:B:2584:ASP:OD1	1:B:2584:ASP:N	2.51	0.44
1:B:3265:ILE:HG22	1:B:3269:LEU:HD11	2.00	0.44
1:B:3561:SER:OG	1:B:3580:ASP:OD2	2.36	0.44
1:B:4217:GLY:O	1:B:4218:GLU:HG3	2.17	0.44
1:A:4185:ASP:OD2	1:A:4206:LYS:N	2.50	0.44
1:B:3083:ASP:OD1	1:B:3104:SER:OG	2.28	0.44
1:B:4041:ASP:OD1	1:B:4042:ARG:N	2.51	0.44
1:A:1414:SER:HA	1:A:1421:LEU:HD21	2.00	0.44
1:A:973:ALA:HB1	1:B:2756:TYR:OH	2.17	0.43
1:A:3125:ASN:HA	9:A:4528:NAG:C7	2.47	0.43
1:A:4061:ASN:OD1	1:A:4062:VAL:HG23	2.18	0.43
1:B:2325:ASP:OD1	1:B:2326:VAL:N	2.46	0.43
1:B:2740:THR:OG1	10:B:4513:NGA:H4	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2527:ASP:OD1	1:A:2527:ASP:N	2.52	0.43
1:A:3757:ARG:O	1:A:3765:ARG:NH2	2.51	0.43
1:B:625:LEU:CD2	1:B:637:VAL:HG22	2.47	0.43
1:B:3431:GLU:HG2	1:B:3443:THR:HG22	1.99	0.43
1:A:2552:MET:HG3	1:A:2570:ALA:HB3	1.99	0.43
1:B:2069:MET:O	1:B:2071:SER:N	2.50	0.43
1:A:794:ILE:HG21	1:A:972:ASN:OD1	2.18	0.43
1:A:2747:THR:HG21	1:A:2755:GLN:O	2.18	0.43
1:A:3126:CYS:SG	1:A:3127:THR:N	2.91	0.43
1:B:1838:THR:HG23	1:B:1876:ILE:HD12	2.01	0.43
1:A:3547:LEU:HD12	1:A:3547:LEU:O	2.17	0.43
1:A:4040:SER:OG	1:A:4041:ASP:N	2.52	0.43
1:B:2251:VAL:HG12	1:B:2258:ILE:HG12	2.00	0.43
1:B:3710:ASP:N	1:B:3710:ASP:OD1	2.52	0.43
1:A:466:VAL:HG12	1:A:485:GLU:OE2	2.18	0.43
1:B:3065:MET:HE2	1:B:3065:MET:C	2.43	0.43
1:B:3298:ASP:OD1	1:B:3299:LEU:N	2.47	0.43
1:B:3473:ASN:ND2	1:B:3476:CYS:O	2.50	0.43
1:B:4272:MET:SD	1:B:4272:MET:N	2.85	0.43
1:A:636:GLN:OE1	1:A:636:GLN:N	2.51	0.43
1:A:2483:SER:OG	1:A:2511:ALA:O	2.31	0.43
1:A:2749:ALA:O	1:A:2752:ARG:N	2.52	0.43
1:A:3864:ASP:N	1:A:3873:GLU:OE2	2.52	0.43
1:B:3135:CYS:SG	1:B:3143:LEU:HD11	2.59	0.43
1:B:4039:MET:O	1:B:4046:ARG:NH2	2.52	0.43
1:B:284:LYS:NZ	1:B:323:GLU:OE1	2.46	0.43
1:B:2759:ARG:NH2	1:B:2774:GLY:O	2.52	0.43
1:B:3413:ILE:CG2	1:B:3420:ILE:HD11	2.48	0.43
1:A:348:GLU:OE1	1:A:348:GLU:N	2.49	0.43
1:A:1114:TYR:N	1:A:1122:ILE:O	2.49	0.43
1:B:1074:CYS:O	1:B:1096:SER:OG	2.30	0.43
1:B:4361:GLU:N	1:B:4361:GLU:OE1	2.51	0.43
1:A:2509:PRO:O	1:A:2510:ARG:HD3	2.19	0.42
1:A:2510:ARG:HG3	1:A:2527:ASP:HA	2.00	0.42
1:B:1926:LEU:HD12	1:B:1932:LYS:O	2.19	0.42
1:B:1090:ASN:ND2	1:B:1092:CYS:O	2.52	0.42
1:B:2538:GLY:N	1:B:2674:GLU:OE2	2.52	0.42
1:B:3427:THR:O	1:B:3429:THR:HG23	2.19	0.42
1:A:3834:THR:HG22	1:A:3841:TYR:CZ	2.54	0.42
1:B:1820:VAL:O	1:B:1857:ARG:NH1	2.53	0.42
1:A:1597:ILE:HD11	1:A:1600:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3622:ASN:OD1	1:B:3622:ASN:N	2.51	0.42
1:A:3064:LEU:HA	1:A:3065:MET:HE2	2.00	0.42
1:A:3096:HIS:N	1:A:3106:GLU:OE1	2.49	0.42
1:B:3090:MET:N	1:B:3090:MET:SD	2.92	0.42
1:A:932:ARG:NH2	1:A:1208:ASP:OD2	2.53	0.42
1:A:1068:SER:OG	1:A:1069:SER:N	2.52	0.42
1:A:1536:SER:OG	1:A:1537:LYS:N	2.53	0.42
1:A:4287:ILE:HD12	1:A:4315:LEU:HD23	2.02	0.42
1:B:3703:ASP:OD1	1:B:3708:ASN:N	2.52	0.42
1:A:4161:VAL:HG22	1:A:4187:PRO:O	2.19	0.42
1:B:3232:LEU:N	1:B:3453:ASP:OD2	2.46	0.42
1:B:280:ILE:HD12	1:B:283:TYR:CZ	2.55	0.42
1:B:3236:ARG:NH1	1:B:3462:GLN:O	2.53	0.42
1:A:378:ILE:HD11	7:K:1:NAG:H82	2.02	0.42
1:A:3431:GLU:CG	1:A:3443:THR:HG22	2.50	0.42
1:B:3413:ILE:HG21	1:B:3420:ILE:HD11	2.02	0.42
1:A:3784:CYS:SG	1:A:3785:GLY:N	2.93	0.41
1:B:268:PRO:O	1:B:281:SER:N	2.51	0.41
1:A:1044:LEU:HD21	1:A:1059:LEU:HD13	2.01	0.41
1:A:3741:GLY:N	1:A:3751:GLU:OE1	2.44	0.41
1:A:2526:TRP:CH2	1:A:2552:MET:HE1	2.54	0.41
1:B:3569:GLN:N	1:B:3569:GLN:OE1	2.54	0.41
1:A:2020:ASN:H	1:A:2023:SER:HG	1.67	0.41
1:B:316:ASN:ND2	1:B:319:TYR:O	2.48	0.41
1:B:579:ASP:OD2	1:B:1159:HIS:NE2	2.49	0.41
1:B:1196:SER:OG	1:B:1198:ASP:OD1	2.35	0.41
1:B:2503:ILE:HG21	1:B:2521:LEU:CD1	2.50	0.41
1:A:1967:ALA:HB1	1:A:2009:VAL:HG23	2.03	0.41
1:B:3431:GLU:OE2	1:B:3441:ARG:NH2	2.54	0.41
1:B:3613:CYS:O	1:B:3615:THR:HG23	2.20	0.41
1:B:3514:SER:OG	1:B:3590:GLU:O	2.29	0.41
1:A:1420:MET:HE2	1:A:1420:MET:C	2.45	0.41
1:B:2684:TYR:N	1:B:2693:ILE:O	2.51	0.41
1:B:3210:ARG:NE	1:B:3219:TYR:OH	2.53	0.41
1:A:263:VAL:HG13	1:A:271:TRP:HZ2	1.85	0.41
1:A:2523:TRP:NE1	1:A:2533:GLU:OE1	2.53	0.41
1:A:3874:GLU:OE1	1:A:3876:HIS:NE2	2.52	0.41
1:B:3782:ASN:ND2	1:B:3785:GLY:O	2.49	0.41
1:A:350:ASP:OD2	1:A:353:GLN:NE2	2.54	0.41
1:A:2761:ASP:OD2	1:B:979:HIS:ND1	2.51	0.40
1:A:1264:ASN:OD1	1:A:1264:ASN:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2144:GLU:CD	1:A:2166:VAL:HG23	2.45	0.40
1:A:2547:ASN:OD1	1:A:2547:ASN:N	2.54	0.40
1:B:4161:VAL:HG22	1:B:4187:PRO:O	2.21	0.40
1:A:2712:CYS:SG	1:A:2727:ASP:N	2.92	0.40
1:B:316:ASN:ND2	1:B:330:CYS:O	2.54	0.40
1:B:3315:ASN:OD1	1:B:3315:ASN:N	2.54	0.40
1:B:4061:ASN:OD1	1:B:4062:VAL:HG23	2.22	0.40
1:A:3865:ASP:N	1:A:3873:GLU:OE2	2.53	0.40
1:B:2503:ILE:HG23	1:B:2537:LEU:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3799/4473 (85%)	3498 (92%)	300 (8%)	1 (0%)	100	100
1	B	3792/4473 (85%)	3455 (91%)	335 (9%)	2 (0%)	48	79
All	All	7591/8946 (85%)	6953 (92%)	635 (8%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3816	LYS
1	B	2455	ILE
1	A	611	GLU

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

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



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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2733/3934 (70%)	2732 (100%)	1 (0%)	100	100
1	B	3348/3934 (85%)	3340 (100%)	8 (0%)	87	85
All	All	6081/7868 (77%)	6072 (100%)	9 (0%)	87	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1079	CYS
1	B	271	TRP
1	B	315	LEU
1	B	1074	CYS
1	B	1124	LYS
1	B	1134	CYS
1	B	2684	TYR
1	B	3732	CYS
1	B	3834	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	912	GLN
1	A	925	HIS
1	A	1090	ASN
1	A	1142	ASN
1	A	1150	GLN
1	A	1263	HIS
1	A	1522	ASN
1	A	1697	GLN
1	A	1711	HIS
1	A	2211	GLN
1	A	2376	GLN
1	A	3078	HIS
1	A	3577	ASN
1	A	3738	GLN
1	A	3787	ASN
1	A	4273	ASN
1	A	4283	GLN
1	B	264	HIS

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	410	HIS
1	B	508	ASN
1	B	656	GLN
1	B	1010	HIS
1	B	1076	HIS
1	B	1264	ASN
1	B	1456	HIS
1	B	1825	ASN
1	B	1843	GLN
1	B	2211	GLN
1	B	2438	ASN
1	B	3342	HIS
1	B	3557	GLN
1	B	3799	HIS
1	B	4013	GLN
1	B	4273	ASN
1	B	4388	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 ⓘ

37 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	$\# Z  > 2$
7	NAG	K	1	7,1	14,14,15	0.27	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	K	2	7	14,14,15	0.43	0	17,19,21	0.72	0
7	BMA	K	3	7	11,11,12	0.61	0	15,15,17	0.73	0
8	NAG	L	1	1,8	14,14,15	0.27	0	17,19,21	0.44	0
8	NAG	L	2	8	14,14,15	0.17	0	17,19,21	0.42	0
8	NAG	M	1	1,8	14,14,15	0.35	0	17,19,21	0.77	0
8	NAG	M	2	8	14,14,15	0.25	0	17,19,21	0.43	0
7	NAG	N	1	7,1	14,14,15	0.24	0	17,19,21	0.61	0
7	NAG	N	2	7	14,14,15	0.22	0	17,19,21	0.44	0
7	BMA	N	3	7	11,11,12	0.52	0	15,15,17	0.69	0
7	NAG	O	1	7,1	14,14,15	0.38	0	17,19,21	0.66	0
7	NAG	O	2	7	14,14,15	0.30	0	17,19,21	0.84	1 (5%)
7	BMA	O	3	7	11,11,12	0.67	0	15,15,17	1.09	0
7	NAG	P	1	7,1	14,14,15	0.23	0	17,19,21	0.62	0
7	NAG	P	2	7	14,14,15	0.24	0	17,19,21	0.52	0
7	BMA	P	3	7	11,11,12	0.51	0	15,15,17	0.74	0
7	NAG	Q	1	7,1	14,14,15	0.40	0	17,19,21	0.49	0
7	NAG	Q	2	7	14,14,15	0.21	0	17,19,21	0.68	0
7	BMA	Q	3	7	11,11,12	0.56	0	15,15,17	0.70	0
8	NAG	R	1	1,8	14,14,15	0.42	0	17,19,21	0.63	0
8	NAG	R	2	8	14,14,15	0.35	0	17,19,21	0.55	0
8	NAG	S	1	1,8	14,14,15	0.21	0	17,19,21	0.56	0
8	NAG	S	2	8	14,14,15	0.36	0	17,19,21	0.69	1 (5%)
8	NAG	T	1	1,8	14,14,15	0.16	0	17,19,21	0.78	1 (5%)
8	NAG	T	2	8	14,14,15	0.22	0	17,19,21	0.54	0
8	NAG	U	1	1,8	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	U	2	8	14,14,15	0.22	0	17,19,21	0.53	0
8	NAG	V	1	1,8	14,14,15	0.26	0	17,19,21	0.41	0
8	NAG	V	2	8	14,14,15	0.20	0	17,19,21	0.41	0
7	NAG	W	1	7,1	14,14,15	0.23	0	17,19,21	0.59	0
7	NAG	W	2	7	14,14,15	0.20	0	17,19,21	0.45	0
7	BMA	W	3	7	11,11,12	0.51	0	15,15,17	0.67	0
7	NAG	X	1	7,1	14,14,15	0.33	0	17,19,21	0.47	0
7	NAG	X	2	7	14,14,15	0.27	0	17,19,21	0.53	0
7	BMA	X	3	7	11,11,12	0.51	0	15,15,17	0.68	0
8	NAG	Y	1	1,8	14,14,15	0.51	0	17,19,21	0.60	0
8	NAG	Y	2	8	14,14,15	0.24	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	K	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
8	NAG	L	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	L	2	8	-	0/6/23/26	0/1/1/1
8	NAG	M	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	M	2	8	-	0/6/23/26	0/1/1/1
7	NAG	N	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	1/2/19/22	0/1/1/1
7	NAG	O	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	O	2	7	-	1/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
7	NAG	P	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	4/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
8	NAG	R	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	R	2	8	-	0/6/23/26	0/1/1/1
8	NAG	S	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	S	2	8	-	4/6/23/26	0/1/1/1
8	NAG	T	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	T	2	8	-	4/6/23/26	0/1/1/1
8	NAG	U	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	U	2	8	-	4/6/23/26	0/1/1/1
8	NAG	V	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
7	NAG	W	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	W	2	7	-	2/6/23/26	0/1/1/1
7	BMA	W	3	7	-	0/2/19/22	0/1/1/1
7	NAG	X	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	4/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1
8	NAG	Y	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	1	NAG	C1-O5-C5	2.44	115.45	112.19
8	S	2	NAG	C1-O5-C5	2.08	114.98	112.19
7	O	2	NAG	C1-O5-C5	2.04	114.91	112.19

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	1	NAG	C4-C5-C6-O6
8	M	1	NAG	C4-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
8	V	2	NAG	O5-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
8	U	2	NAG	C4-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
8	L	1	NAG	O5-C5-C6-O6
8	M	1	NAG	O5-C5-C6-O6
8	S	2	NAG	O5-C5-C6-O6
8	S	2	NAG	C4-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6
8	T	1	NAG	C4-C5-C6-O6
8	V	2	NAG	C4-C5-C6-O6
8	T	2	NAG	C4-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
7	X	2	NAG	C4-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
7	K	1	NAG	O5-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	W	1	NAG	C4-C5-C6-O6
8	U	1	NAG	C4-C5-C6-O6
7	N	3	BMA	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
7	N	1	NAG	C1-C2-N2-C7
7	O	1	NAG	C1-C2-N2-C7
7	P	1	NAG	C1-C2-N2-C7
7	P	2	NAG	C1-C2-N2-C7
7	W	1	NAG	C1-C2-N2-C7
7	X	2	NAG	C1-C2-N2-C7
8	M	1	NAG	C1-C2-N2-C7
8	S	1	NAG	C1-C2-N2-C7
8	U	2	NAG	C1-C2-N2-C7
7	N	1	NAG	C4-C5-C6-O6
7	N	1	NAG	C3-C2-N2-C7
7	O	1	NAG	C3-C2-N2-C7
7	P	1	NAG	C3-C2-N2-C7
7	P	2	NAG	C3-C2-N2-C7
7	W	1	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7
8	S	1	NAG	C3-C2-N2-C7
8	S	2	NAG	C3-C2-N2-C7
8	T	1	NAG	C3-C2-N2-C7
8	T	2	NAG	C3-C2-N2-C7
8	U	2	NAG	C3-C2-N2-C7
8	Y	2	NAG	C3-C2-N2-C7
8	S	2	NAG	C1-C2-N2-C7
8	T	1	NAG	C1-C2-N2-C7
8	T	2	NAG	C1-C2-N2-C7
8	Y	2	NAG	C1-C2-N2-C7
7	O	2	NAG	C4-C5-C6-O6
8	M	1	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 4 short contacts:

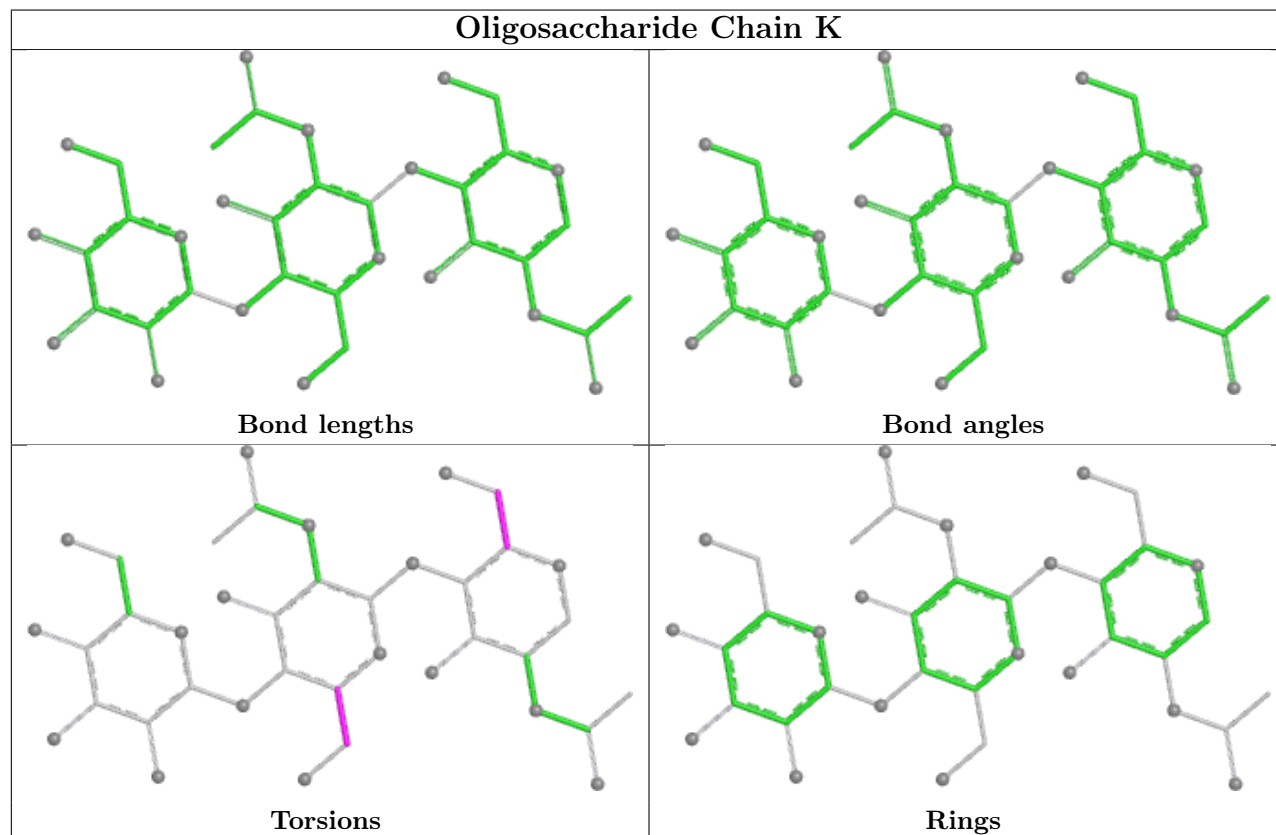
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	U	1	NAG	1	0
7	P	2	NAG	1	0
7	N	1	NAG	1	0
8	U	2	NAG	1	0
7	K	1	NAG	1	0

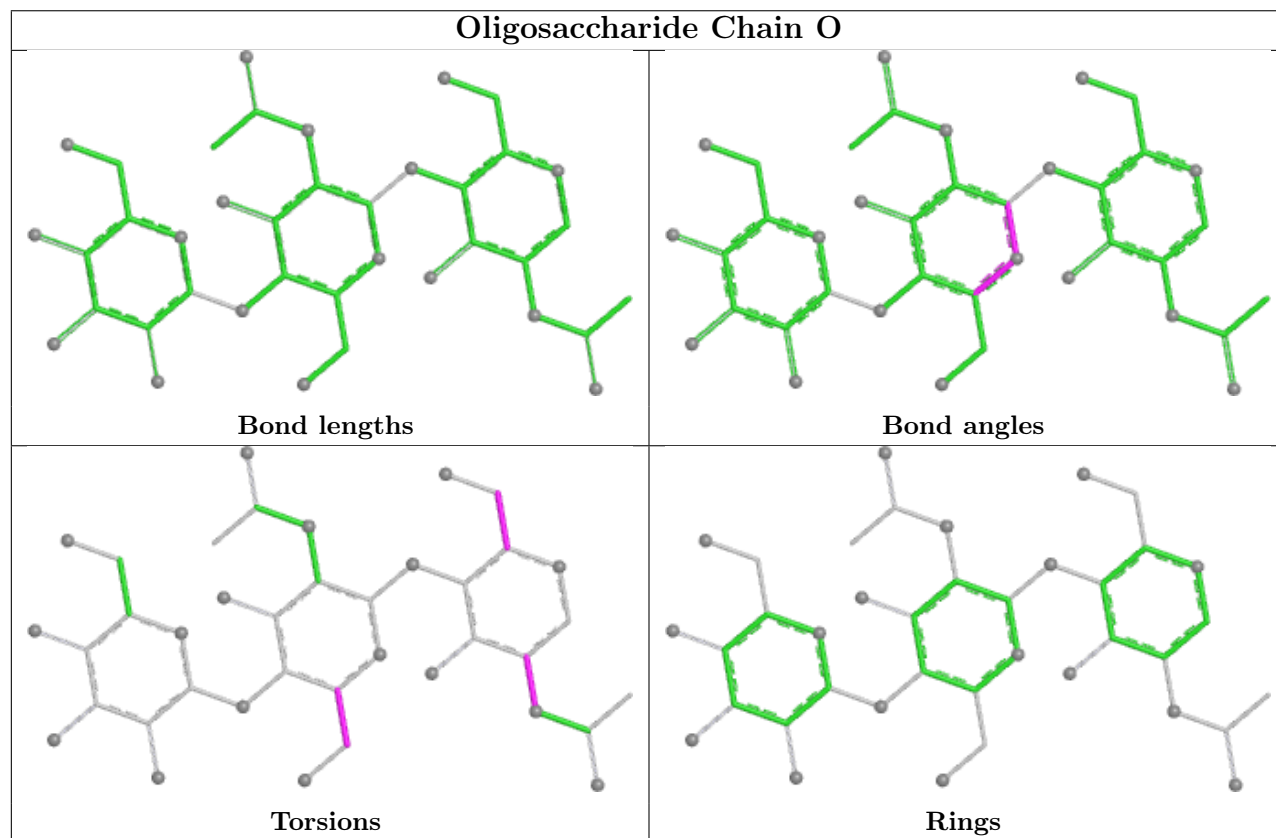
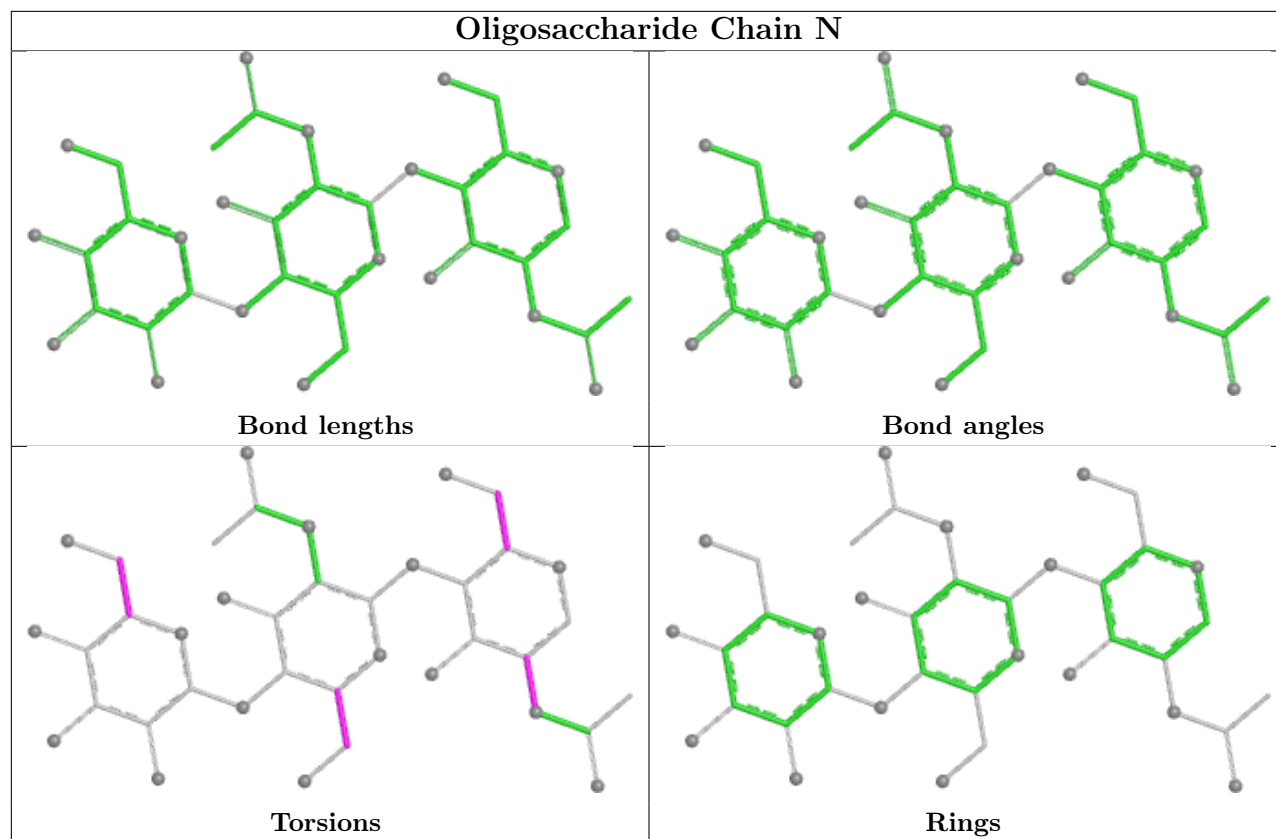
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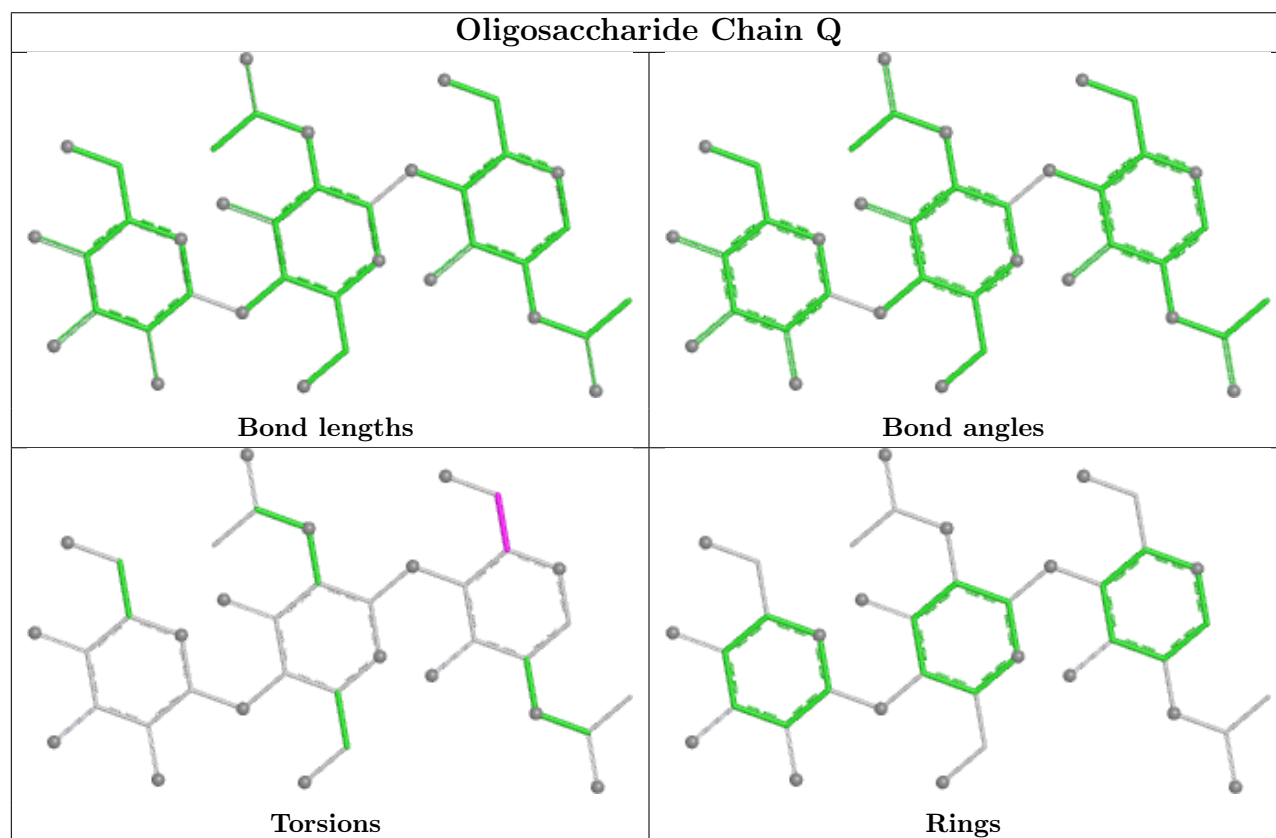
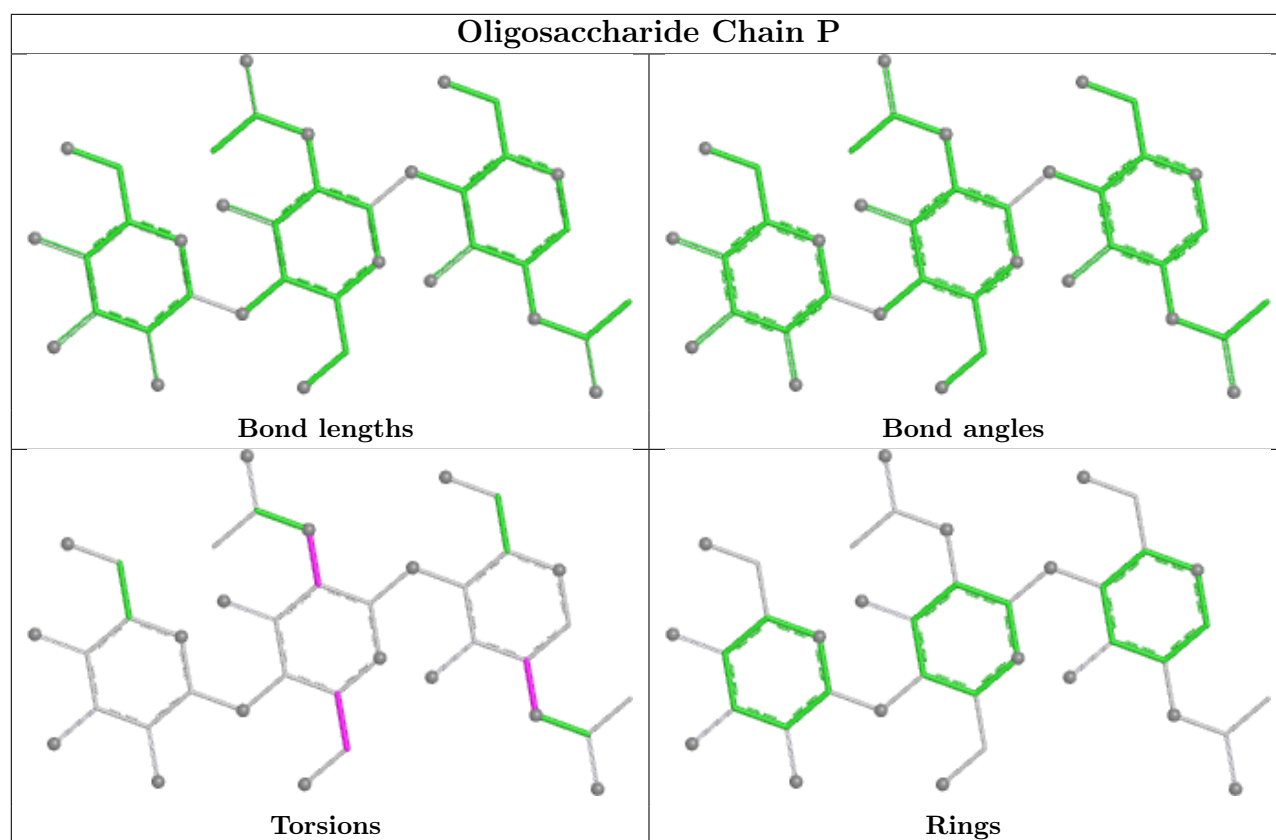
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	1	NAG	1	0
7	N	2	NAG	1	0

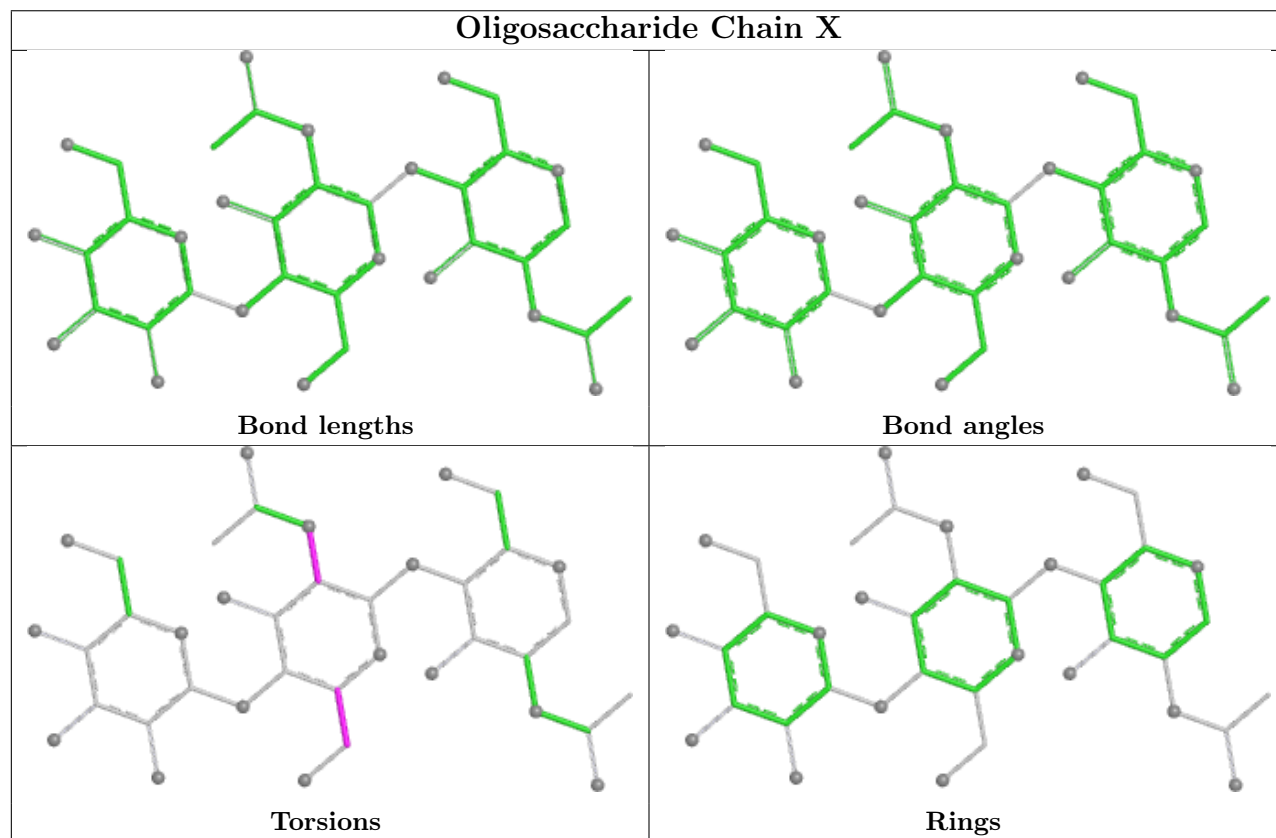
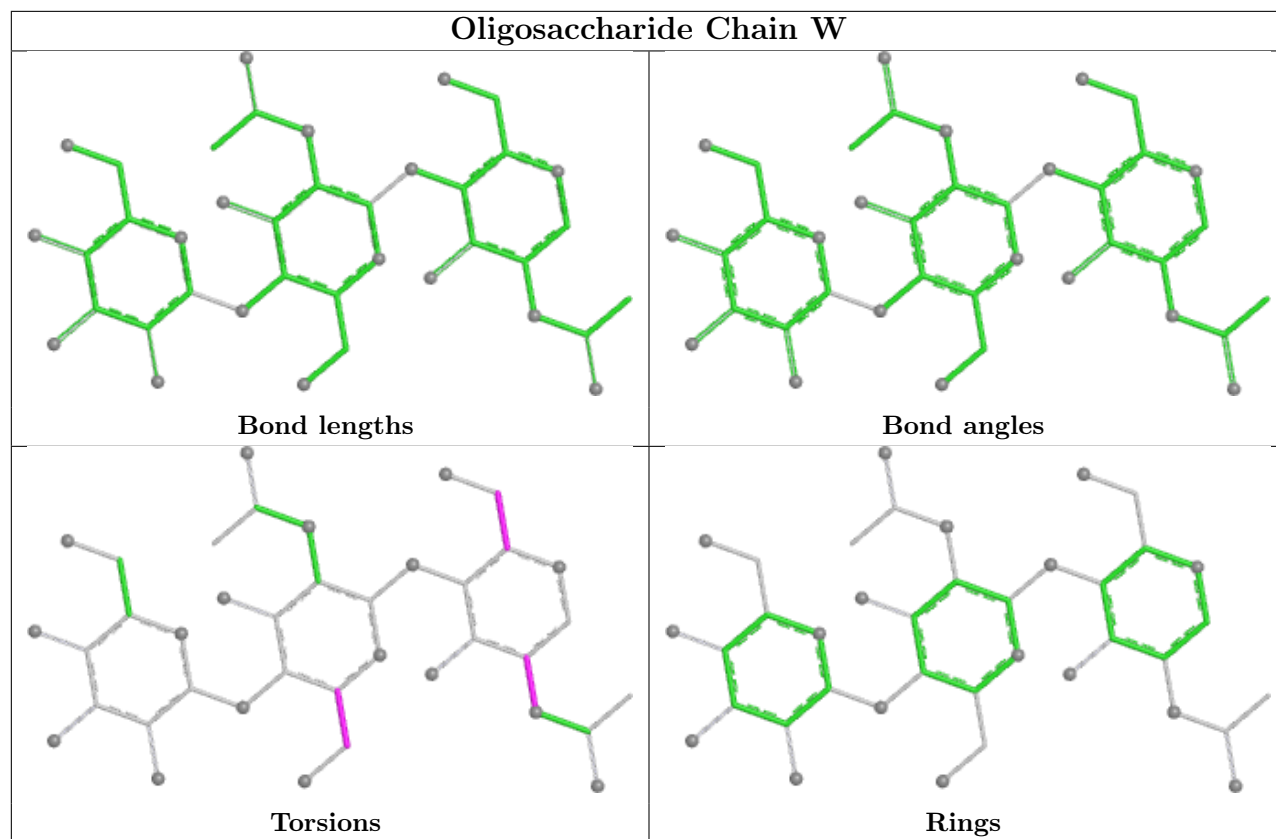
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

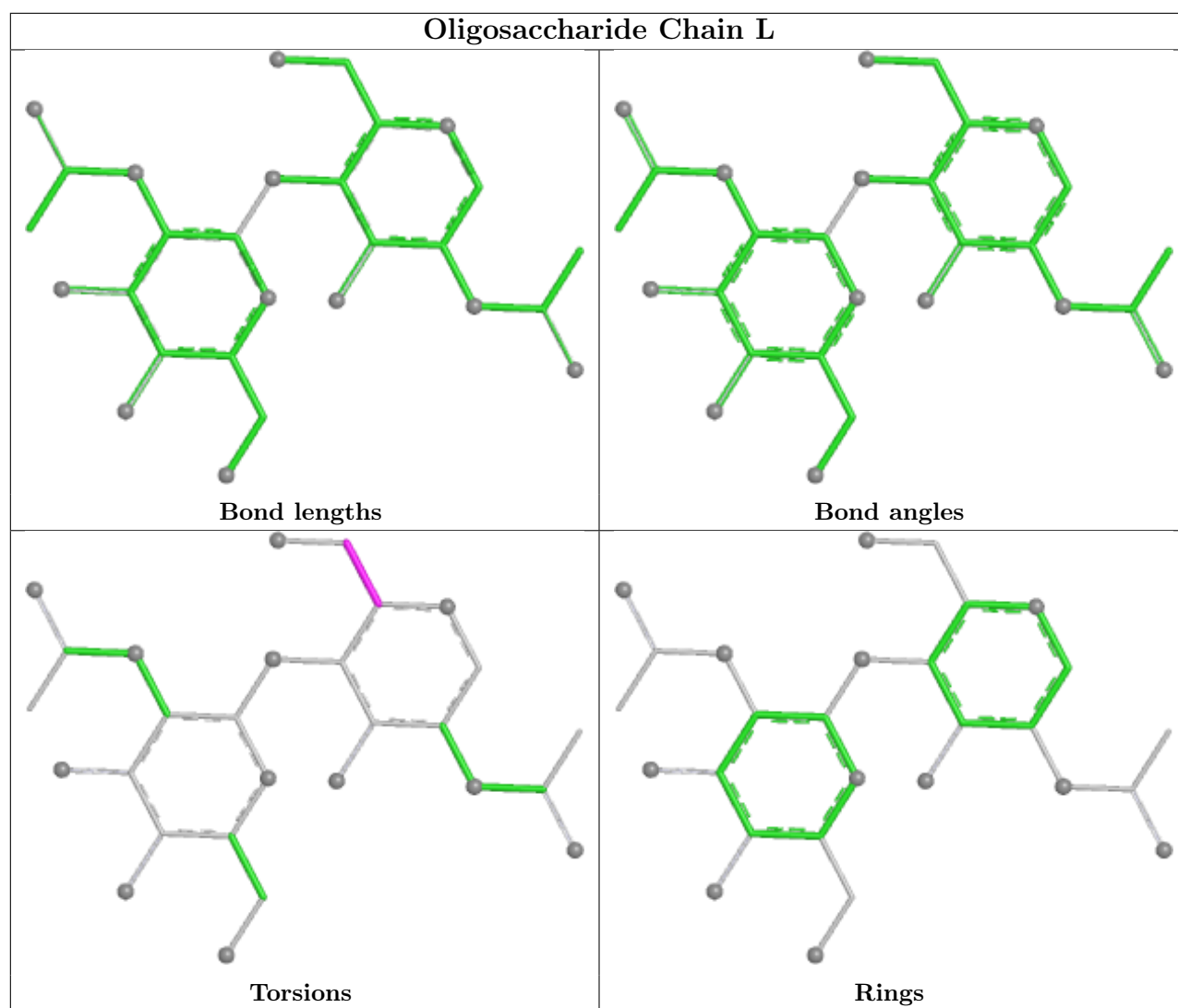


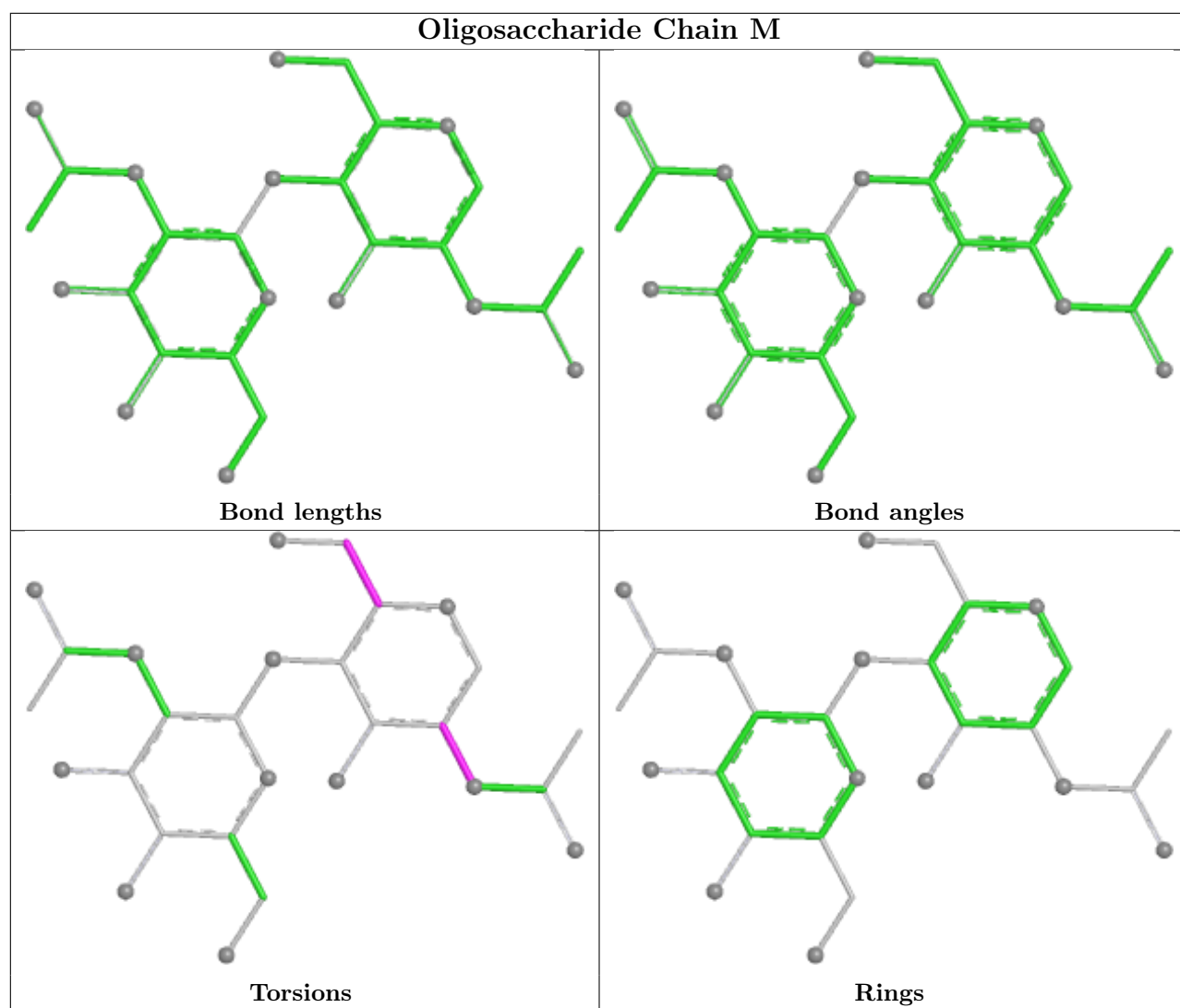


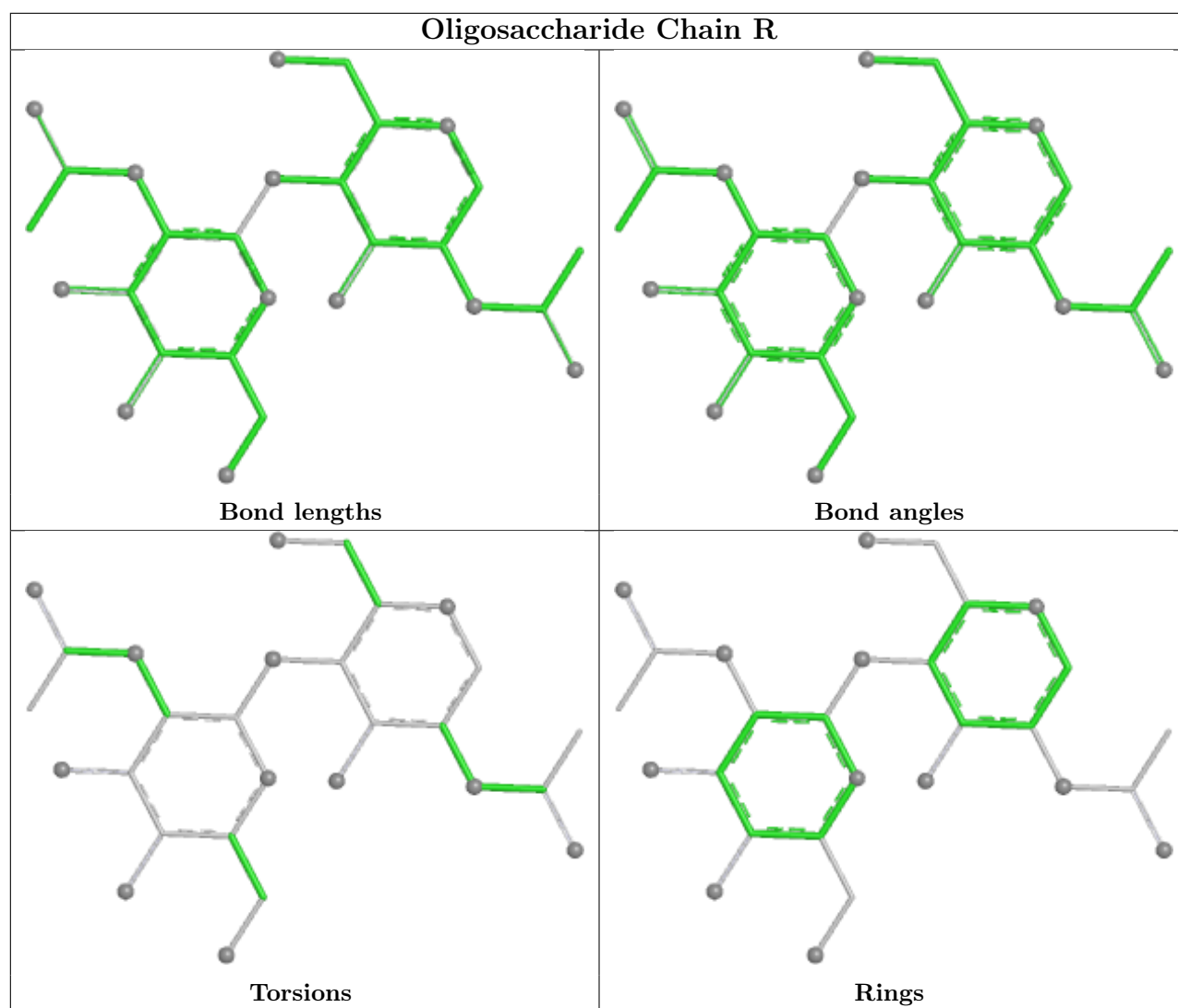


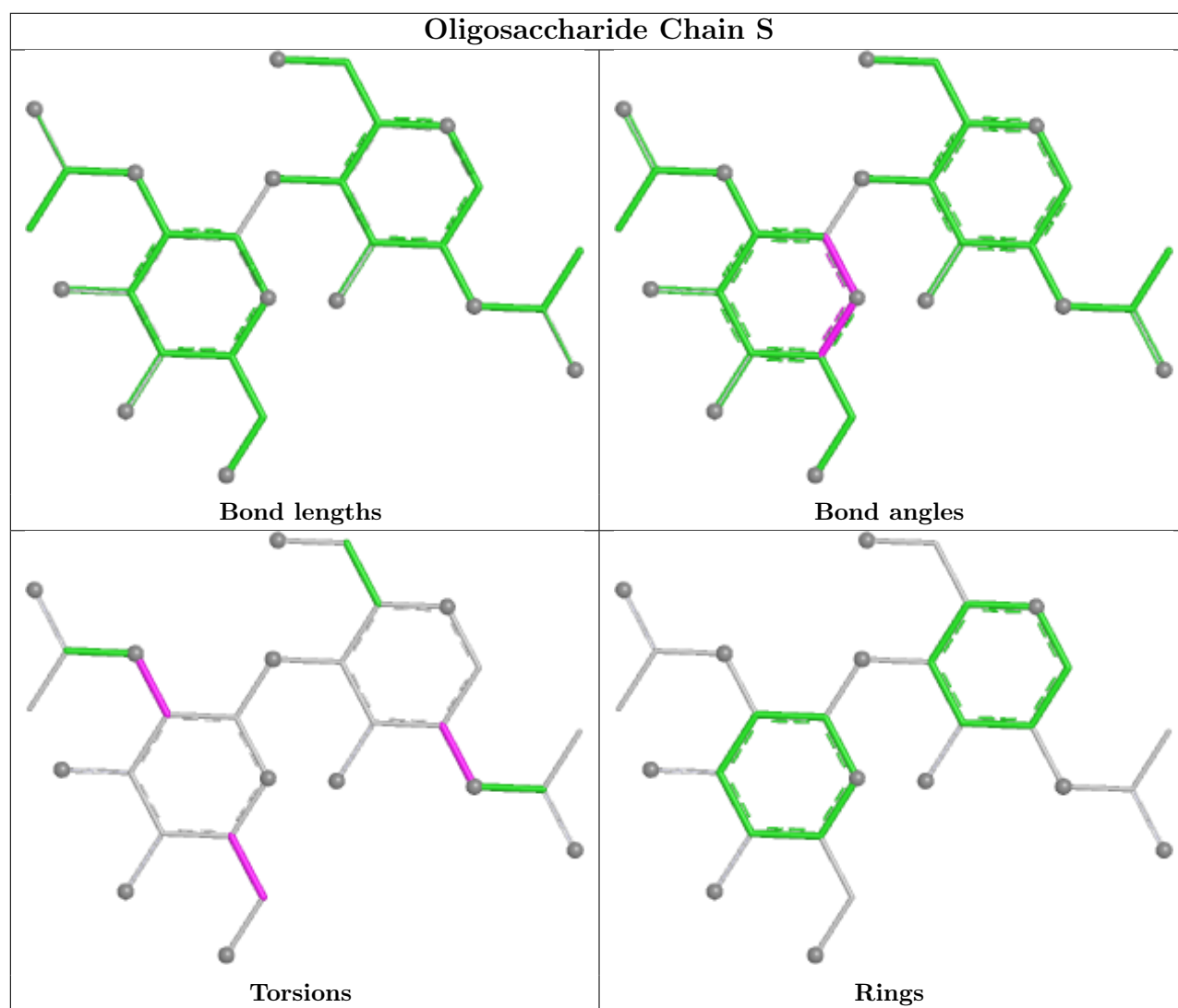


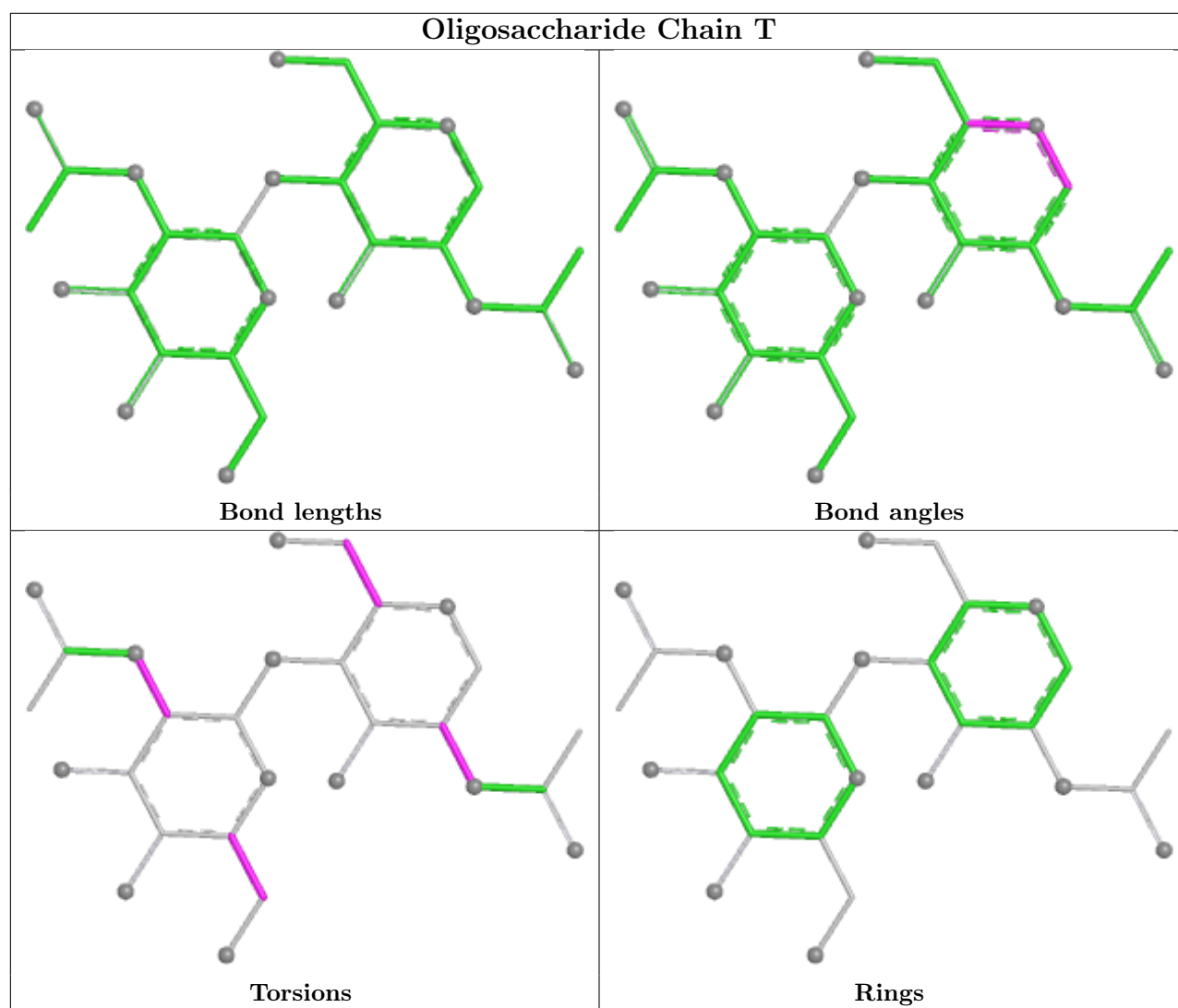


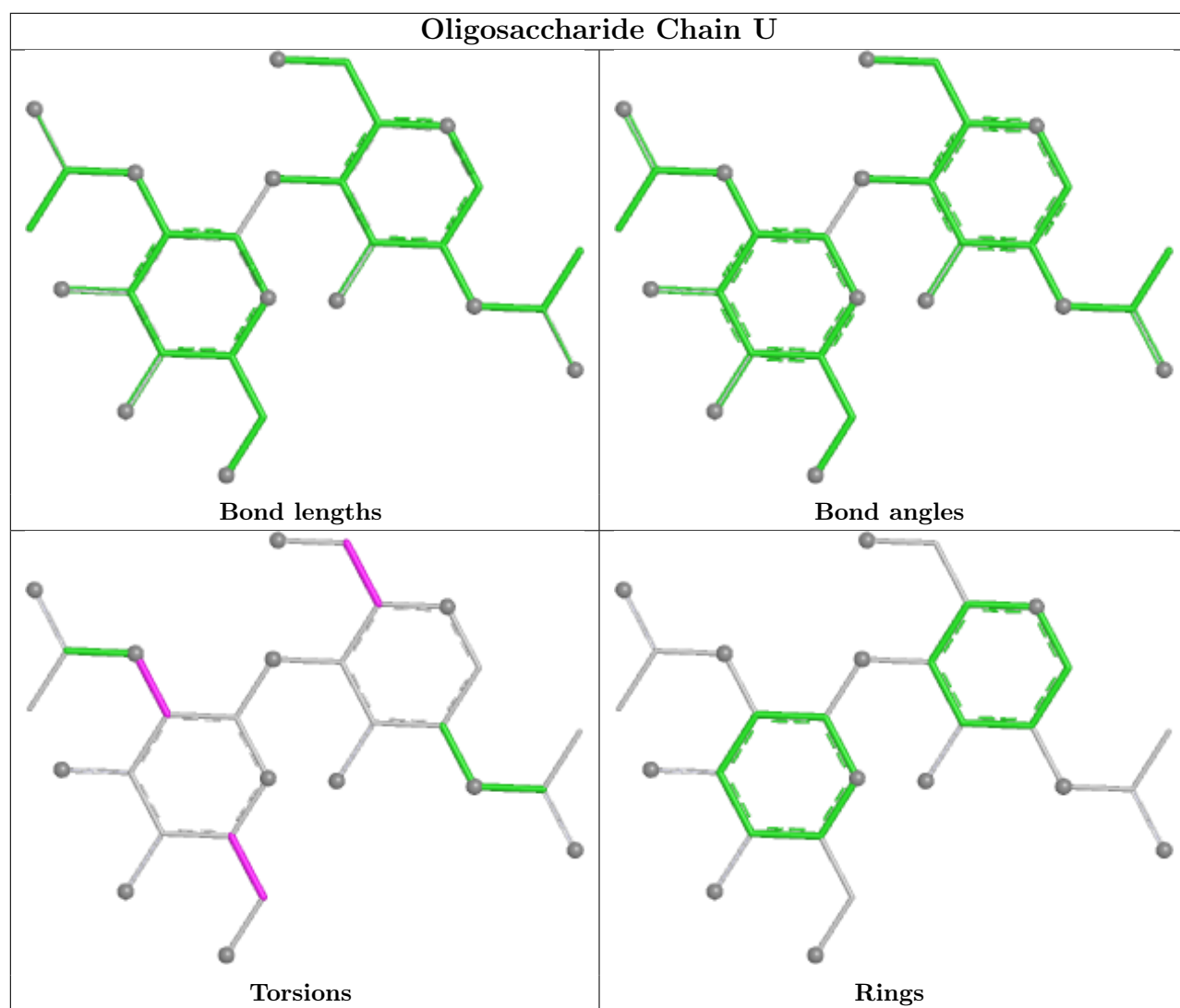




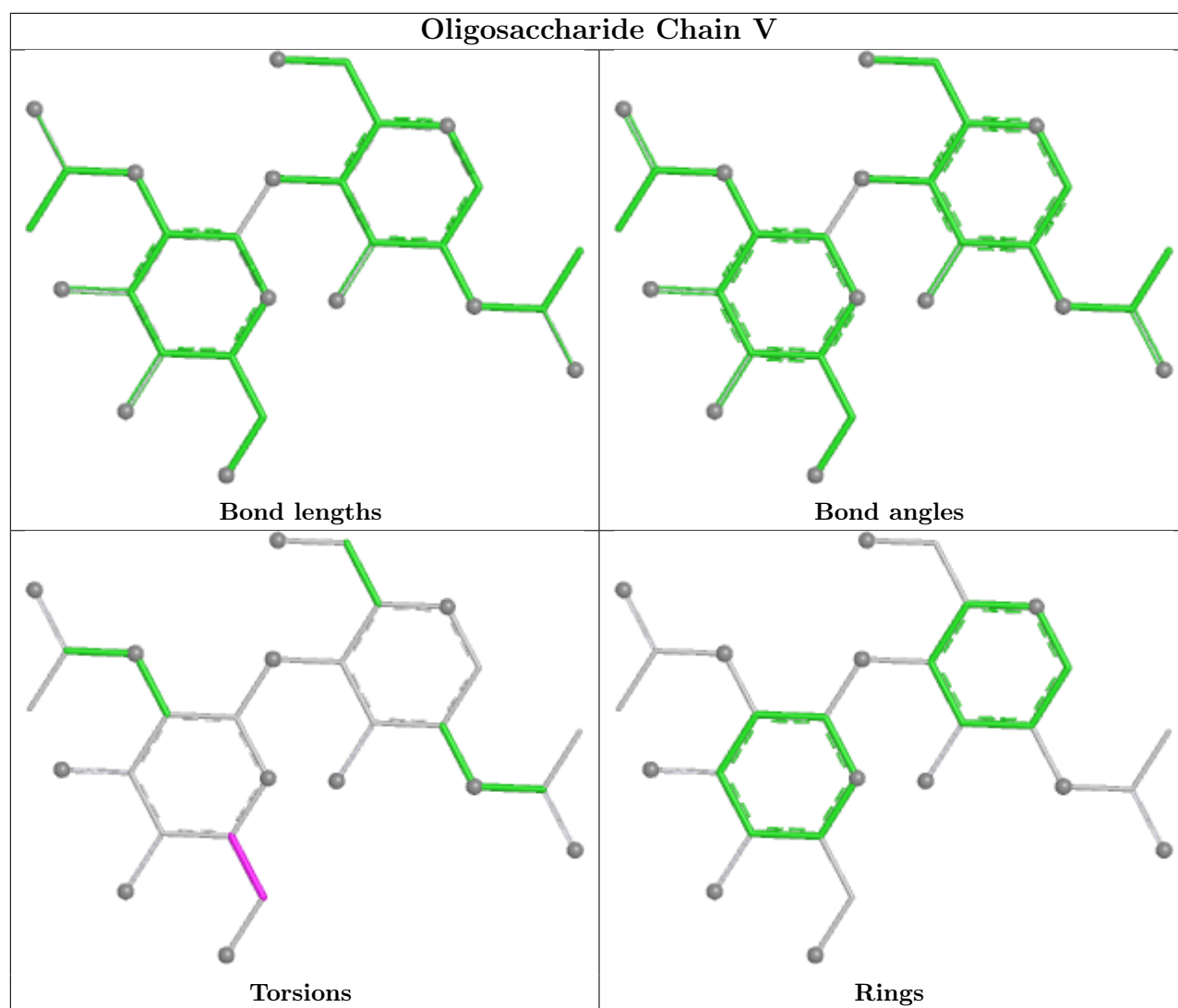


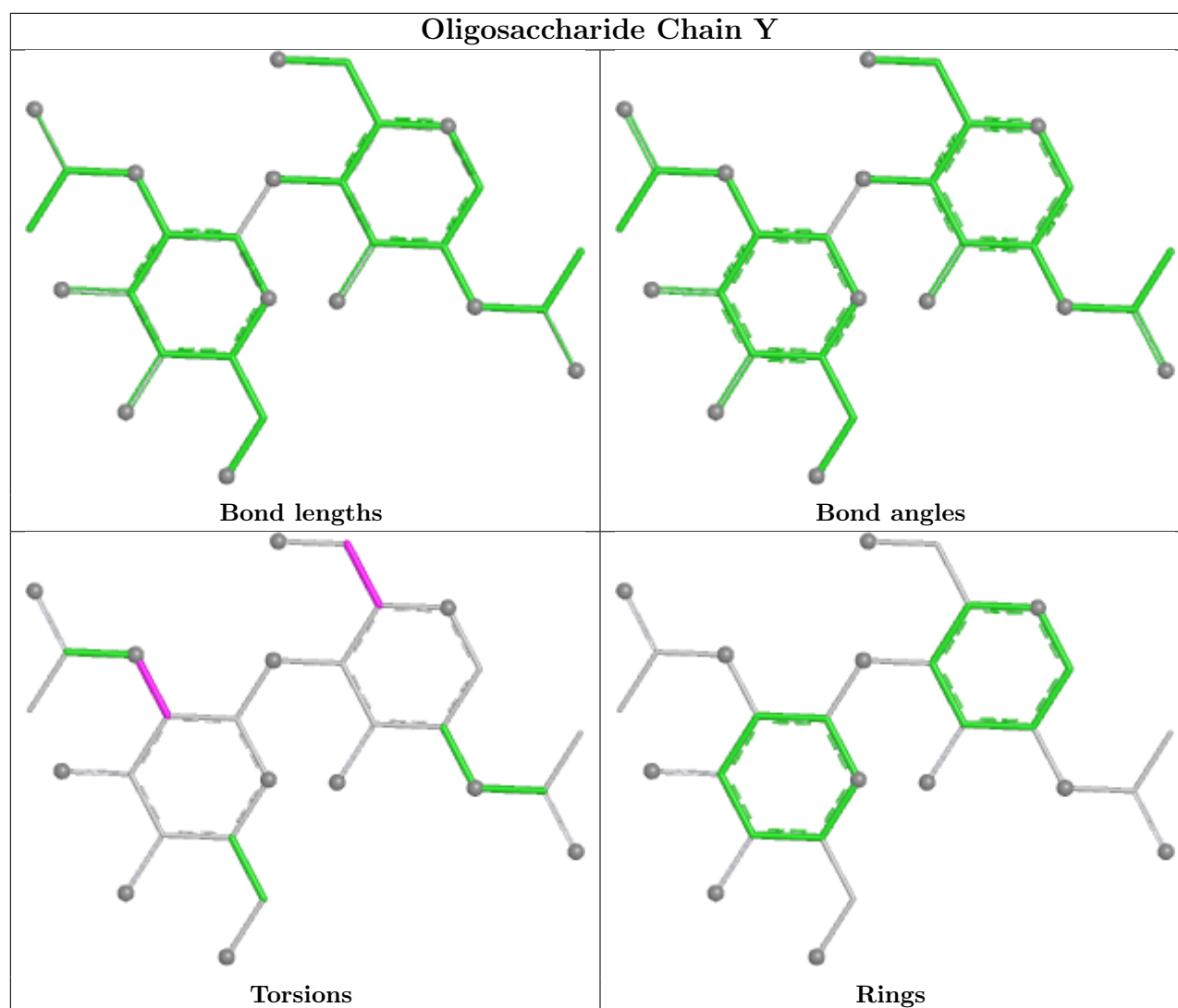












## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
9	NAG	B	4501	1	14,14,15	0.25	0	17,19,21	0.47	0
9	NAG	A	4502	1	14,14,15	0.28	0	17,19,21	0.46	0
10	NGA	A	4513	-	14,14,15	0.59	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	A	4504	1	14,14,15	0.20	0	17,19,21	0.49	0
10	NGA	A	4514	-	14,14,15	0.58	0	17,19,21	0.69	0
10	NGA	B	4512	1	14,14,15	0.59	0	17,19,21	0.63	0
10	NGA	B	4509	-	14,14,15	0.61	0	17,19,21	0.80	1 (5%)
9	NAG	A	4508	1	14,14,15	0.19	0	17,19,21	0.44	0
10	NGA	B	4510	1	14,14,15	0.55	0	17,19,21	0.66	0
9	NAG	A	4503	1	14,14,15	0.30	0	17,19,21	0.55	0
9	NAG	B	4507	1	14,14,15	0.24	0	17,19,21	0.42	0
9	NAG	B	4506	1	14,14,15	0.16	0	17,19,21	0.46	0
9	NAG	B	4502	1	14,14,15	0.24	0	17,19,21	0.41	0
9	NAG	A	4501	1	14,14,15	0.21	0	17,19,21	0.48	0
9	NAG	B	4505	-	14,14,15	0.20	0	17,19,21	0.44	0
10	NGA	A	4511	1	14,14,15	0.59	0	17,19,21	0.75	0
9	NAG	A	4510	-	14,14,15	0.35	0	17,19,21	1.02	1 (5%)
9	NAG	A	4507	1	14,14,15	0.20	0	17,19,21	0.43	0
9	NAG	A	4528	-	14,14,15	0.47	0	17,19,21	0.40	0
9	NAG	B	4504	1	14,14,15	0.24	0	17,19,21	0.44	0
9	NAG	A	4506	1	14,14,15	0.21	0	17,19,21	0.51	0
9	NAG	B	4503	-	14,14,15	0.21	0	17,19,21	0.41	0
10	NGA	B	4511	1	14,14,15	0.55	0	17,19,21	0.57	0
10	NGA	A	4512	1	14,14,15	0.56	0	17,19,21	0.73	0
10	NGA	B	4513	-	14,14,15	0.53	0	17,19,21	0.57	0
9	NAG	A	4505	-	14,14,15	0.24	0	17,19,21	0.51	0
9	NAG	B	4508	1	14,14,15	0.24	0	17,19,21	0.55	0
9	NAG	A	4509	-	14,14,15	0.20	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	4501	1	-	2/6/23/26	0/1/1/1
9	NAG	A	4502	1	-	2/6/23/26	0/1/1/1
10	NGA	A	4513	-	-	0/6/23/26	0/1/1/1
9	NAG	A	4504	1	-	2/6/23/26	0/1/1/1
10	NGA	A	4514	-	-	0/6/23/26	0/1/1/1
10	NGA	B	4512	1	-	2/6/23/26	0/1/1/1
10	NGA	B	4509	-	-	3/6/23/26	0/1/1/1
9	NAG	A	4508	1	-	0/6/23/26	0/1/1/1
10	NGA	B	4510	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	4503	1	-	2/6/23/26	0/1/1/1
9	NAG	B	4507	1	-	0/6/23/26	0/1/1/1
9	NAG	B	4506	1	-	0/6/23/26	0/1/1/1
9	NAG	B	4502	1	-	2/6/23/26	0/1/1/1
9	NAG	A	4501	1	-	2/6/23/26	0/1/1/1
9	NAG	B	4505	-	-	2/6/23/26	0/1/1/1
10	NGA	A	4511	1	-	4/6/23/26	0/1/1/1
9	NAG	A	4510	-	-	6/6/23/26	0/1/1/1
9	NAG	A	4507	1	-	1/6/23/26	0/1/1/1
9	NAG	A	4528	-	-	3/6/23/26	0/1/1/1
9	NAG	B	4504	1	-	0/6/23/26	0/1/1/1
9	NAG	A	4506	1	-	2/6/23/26	0/1/1/1
9	NAG	B	4503	-	-	2/6/23/26	0/1/1/1
10	NGA	B	4511	1	1/1/5/7	3/6/23/26	0/1/1/1
10	NGA	A	4512	1	-	4/6/23/26	0/1/1/1
10	NGA	B	4513	-	-	3/6/23/26	0/1/1/1
9	NAG	A	4505	-	-	3/6/23/26	0/1/1/1
9	NAG	B	4508	1	-	3/6/23/26	0/1/1/1
9	NAG	A	4509	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	4510	NAG	C2-N2-C7	3.32	127.35	122.90
10	B	4509	NGA	C2-N2-C7	-2.07	120.13	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	4511	NGA	C1

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	4511	NGA	C1-C2-N2-C7
10	A	4511	NGA	C8-C7-N2-C2
10	A	4511	NGA	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
10	A	4512	NGA	C1-C2-N2-C7
10	A	4512	NGA	C8-C7-N2-C2
10	A	4512	NGA	O7-C7-N2-C2
10	B	4509	NGA	C3-C2-N2-C7
10	B	4509	NGA	C8-C7-N2-C2
10	B	4509	NGA	O7-C7-N2-C2
10	B	4512	NGA	C8-C7-N2-C2
10	B	4512	NGA	O7-C7-N2-C2
10	B	4513	NGA	C3-C2-N2-C7
10	B	4513	NGA	C8-C7-N2-C2
10	B	4513	NGA	O7-C7-N2-C2
10	B	4510	NGA	C8-C7-N2-C2
10	B	4511	NGA	O7-C7-N2-C2
9	A	4501	NAG	O5-C5-C6-O6
9	A	4502	NAG	O5-C5-C6-O6
9	A	4504	NAG	O5-C5-C6-O6
9	B	4503	NAG	O5-C5-C6-O6
9	B	4501	NAG	O5-C5-C6-O6
10	B	4511	NGA	C8-C7-N2-C2
9	B	4503	NAG	C4-C5-C6-O6
9	A	4502	NAG	C4-C5-C6-O6
9	A	4504	NAG	C4-C5-C6-O6
9	B	4501	NAG	C4-C5-C6-O6
10	B	4510	NGA	O7-C7-N2-C2
9	A	4501	NAG	C4-C5-C6-O6
9	B	4502	NAG	O5-C5-C6-O6
9	A	4510	NAG	C8-C7-N2-C2
9	A	4510	NAG	O7-C7-N2-C2
9	A	4510	NAG	O5-C5-C6-O6
9	B	4505	NAG	O5-C5-C6-O6
9	B	4505	NAG	C4-C5-C6-O6
10	B	4511	NGA	O5-C5-C6-O6
10	A	4512	NGA	O5-C5-C6-O6
9	A	4507	NAG	O5-C5-C6-O6
10	A	4511	NGA	O5-C5-C6-O6
9	A	4510	NAG	C4-C5-C6-O6
9	A	4528	NAG	C3-C2-N2-C7
9	A	4528	NAG	O5-C5-C6-O6
9	B	4508	NAG	O5-C5-C6-O6
9	A	4503	NAG	C1-C2-N2-C7
9	A	4505	NAG	C1-C2-N2-C7
9	A	4506	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	A	4528	NAG	C1-C2-N2-C7
9	B	4508	NAG	C1-C2-N2-C7
9	A	4505	NAG	O5-C5-C6-O6
9	A	4503	NAG	C3-C2-N2-C7
9	A	4505	NAG	C3-C2-N2-C7
9	A	4506	NAG	C3-C2-N2-C7
9	B	4508	NAG	C3-C2-N2-C7
9	B	4502	NAG	C4-C5-C6-O6
9	A	4510	NAG	C1-C2-N2-C7
9	A	4510	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	4514	NGA	3	0
10	B	4509	NGA	1	0
10	B	4510	NGA	1	0
9	A	4510	NAG	3	0
9	A	4528	NAG	3	0
10	A	4512	NGA	1	0
10	B	4513	NGA	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

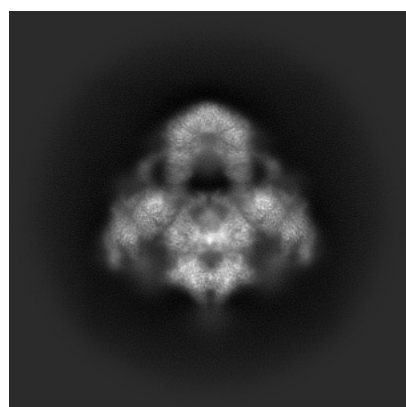
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52617. These allow visual inspection of the internal detail of the map and identification of artifacts.

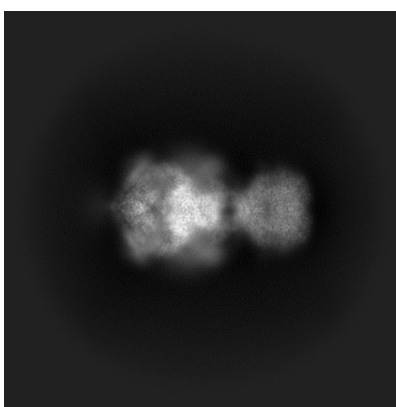
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

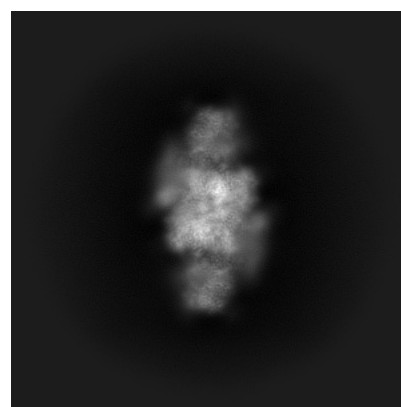
#### 6.1.1 Primary map



X



Y

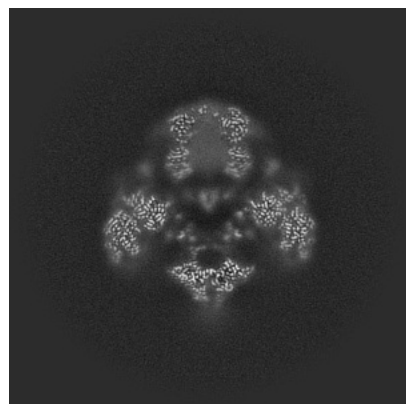


Z

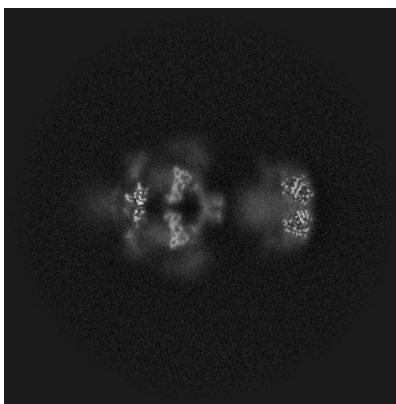
The images above show the map projected in three orthogonal directions.

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

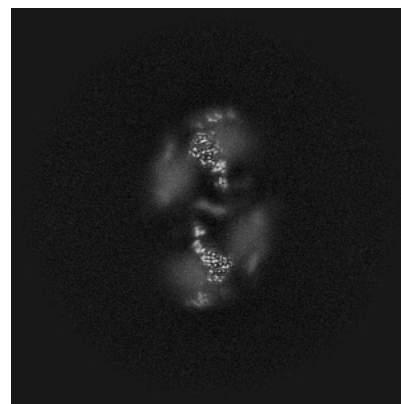
#### 6.2.1 Primary map



X Index: 280



Y Index: 280

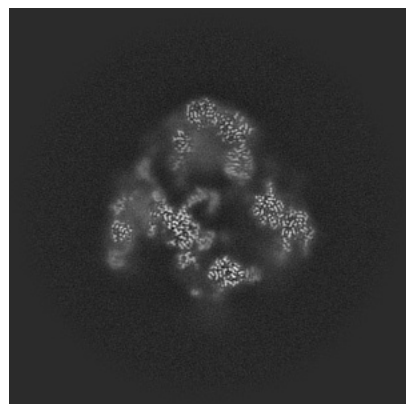


Z Index: 280

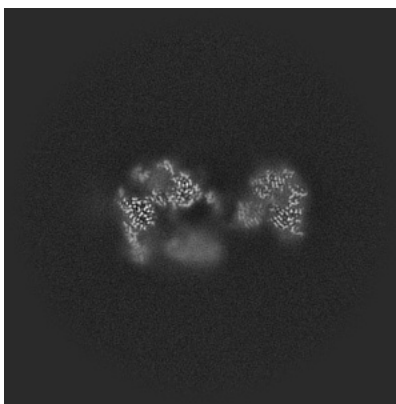
The images above show central slices of the map in three orthogonal directions.

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

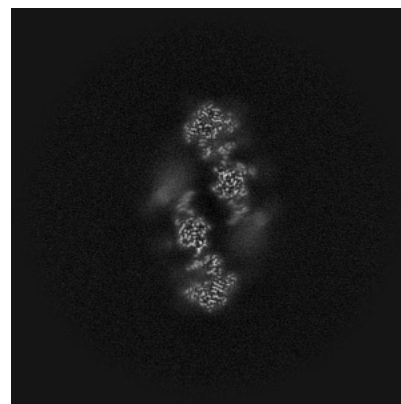
### 6.3.1 Primary map



X Index: 266



Y Index: 306

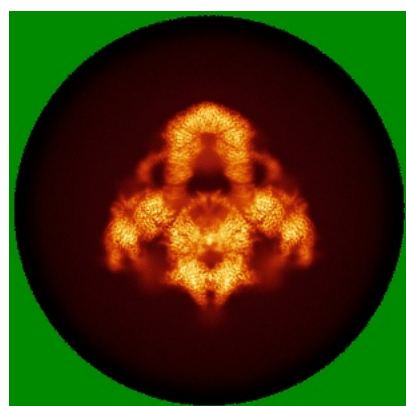


Z Index: 254

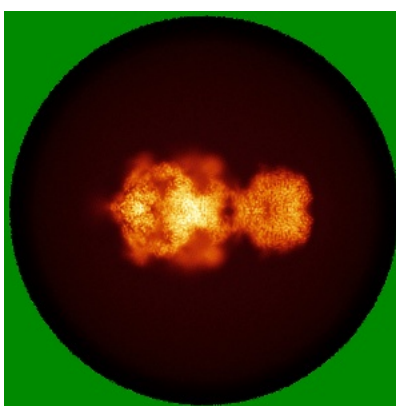
The images above show the largest variance slices of the map in three orthogonal directions.

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

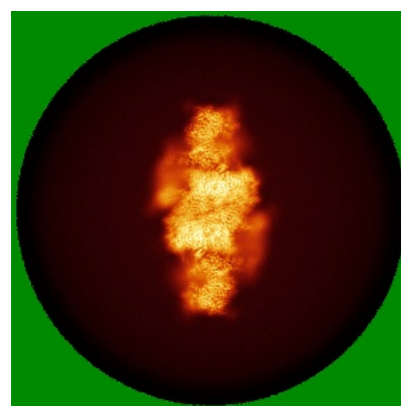
### 6.4.1 Primary map



X



Y



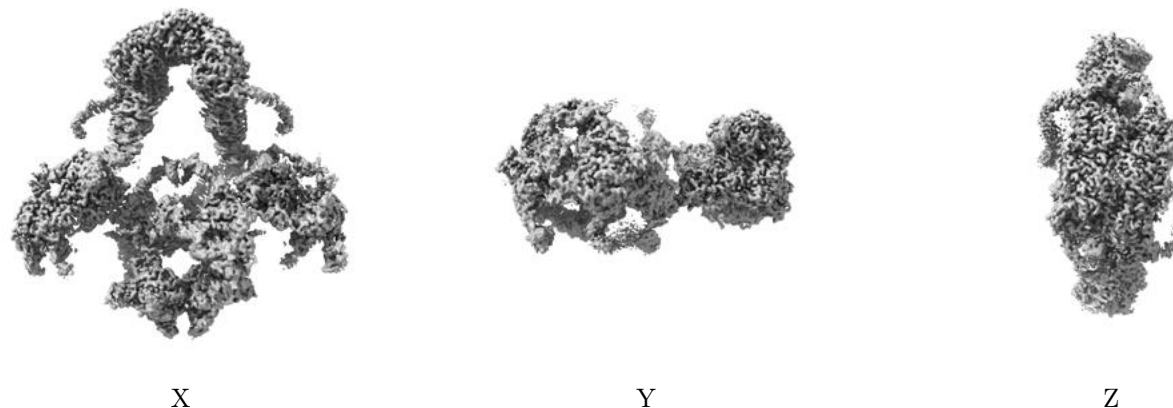
Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.318. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

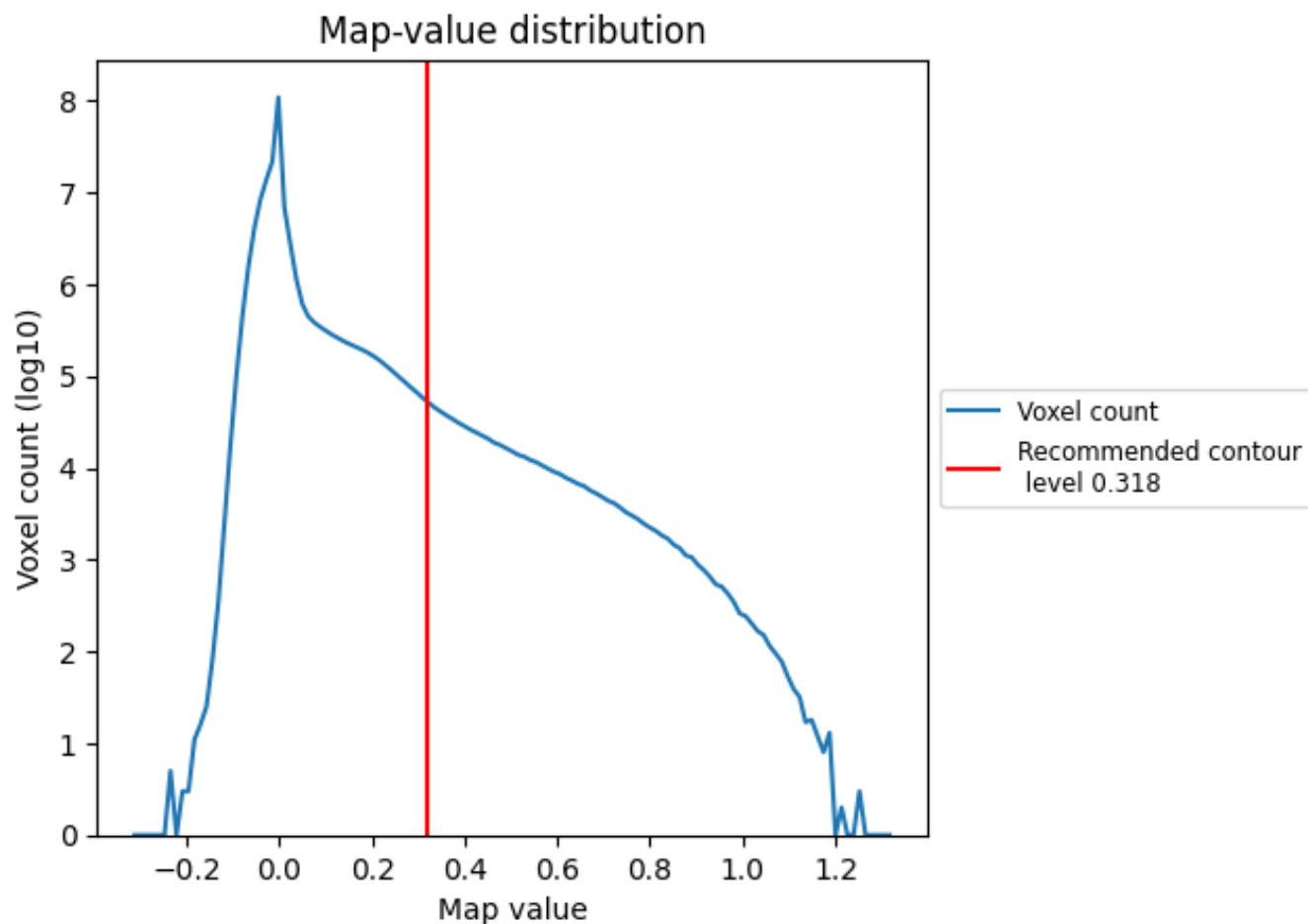
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

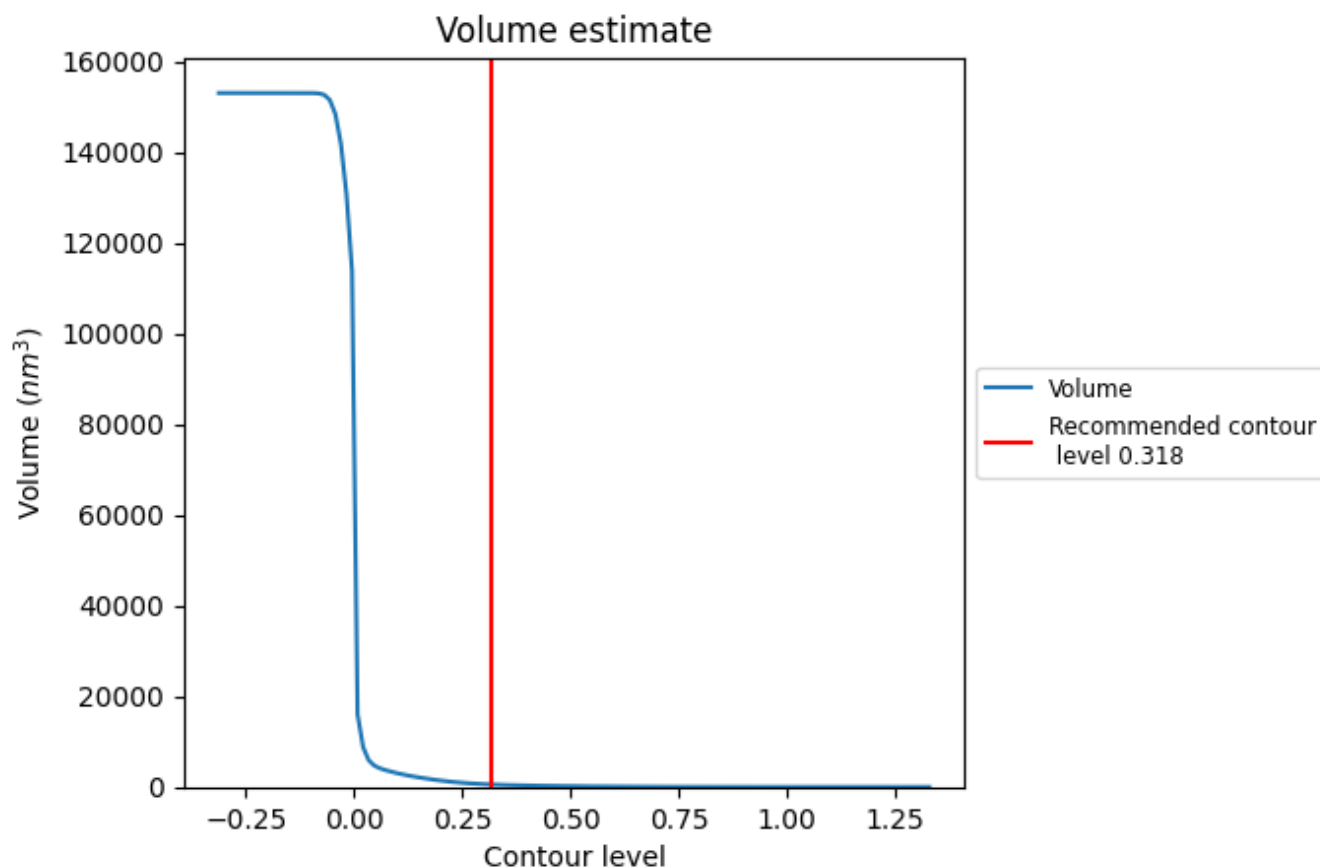
This section contains the results of statistical analysis of the map.

### 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.

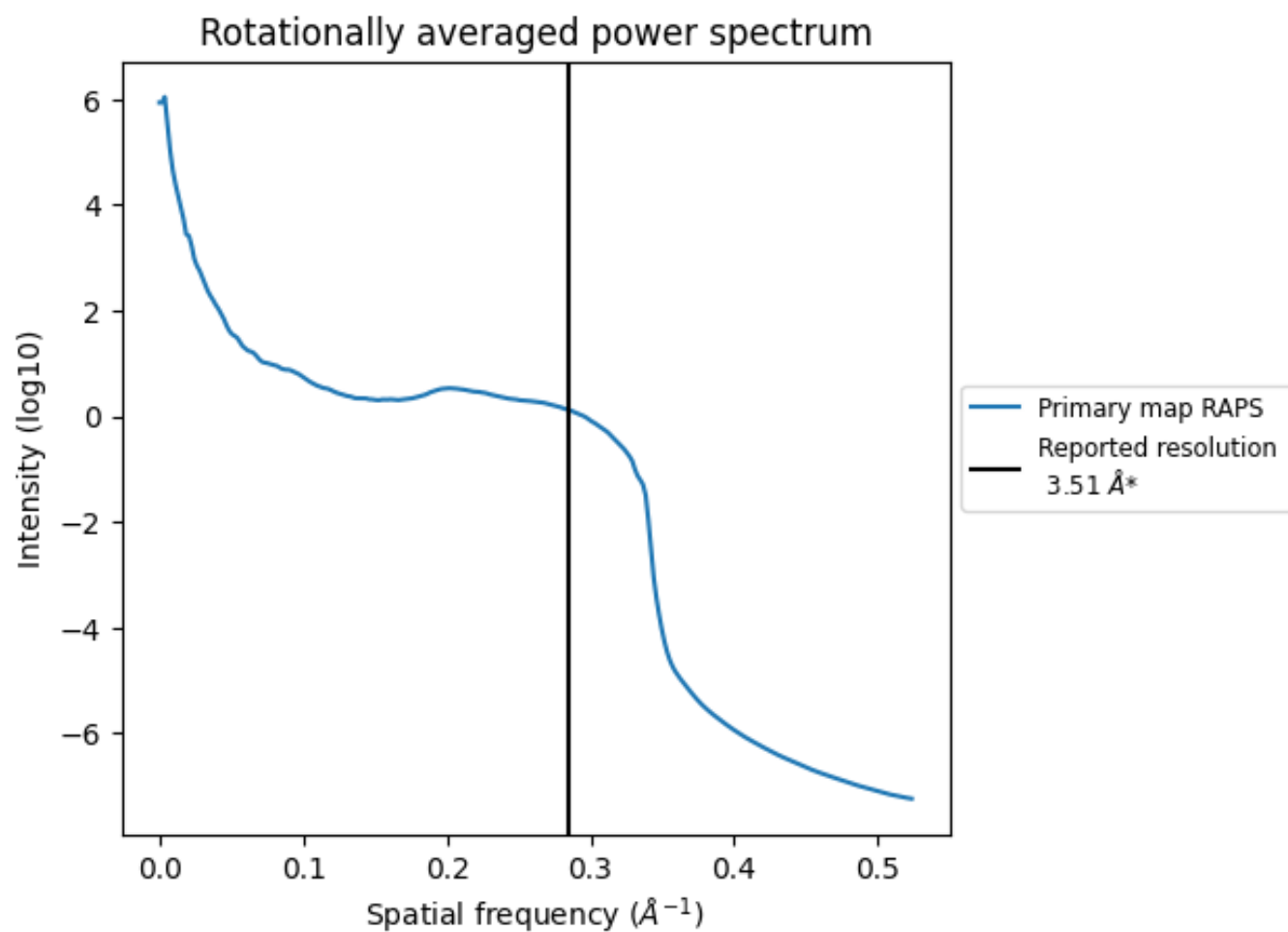
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 543 nm<sup>3</sup>; this corresponds to an approximate mass of 491 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 0.285 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

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

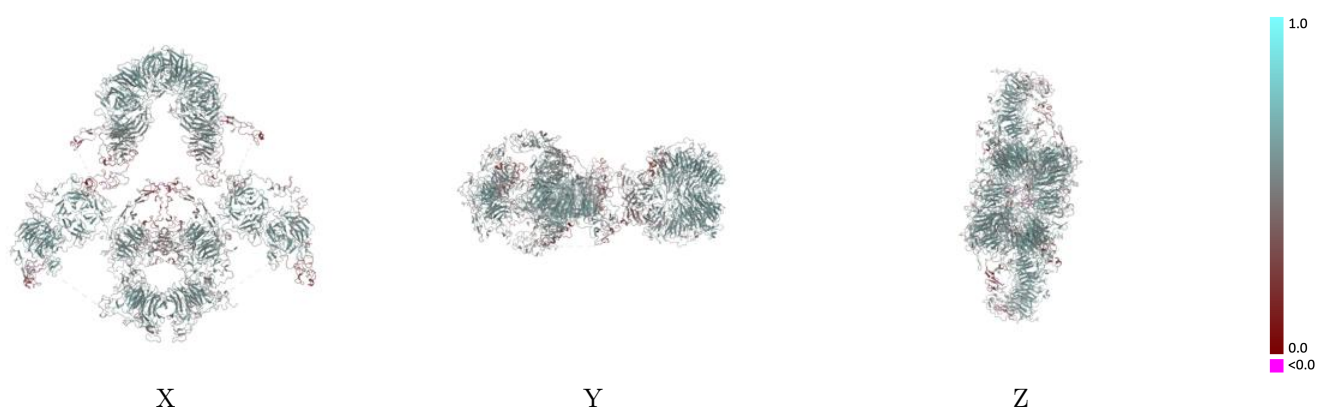
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52617 and PDB model 9I3V. Per-residue inclusion information can be found in section 3 on page 12.

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

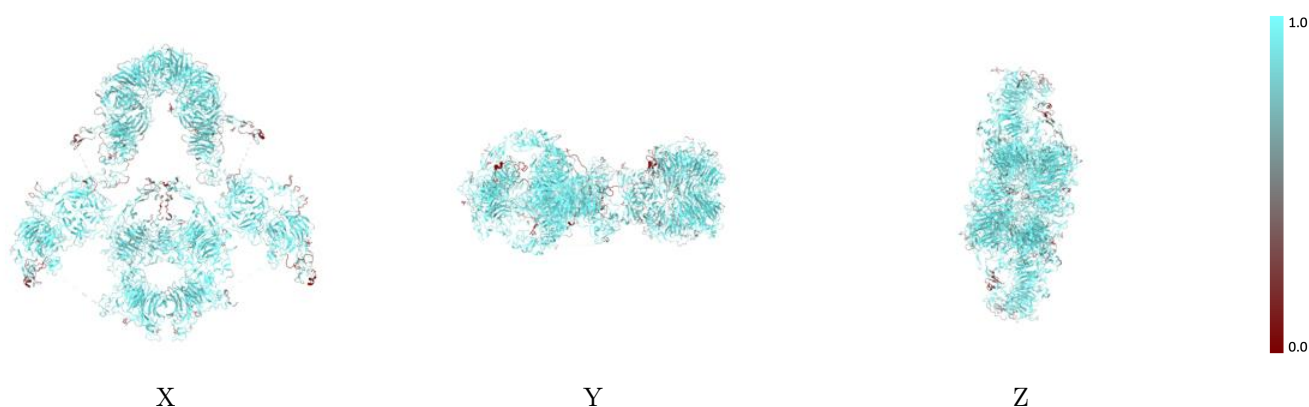
This section was not generated.

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



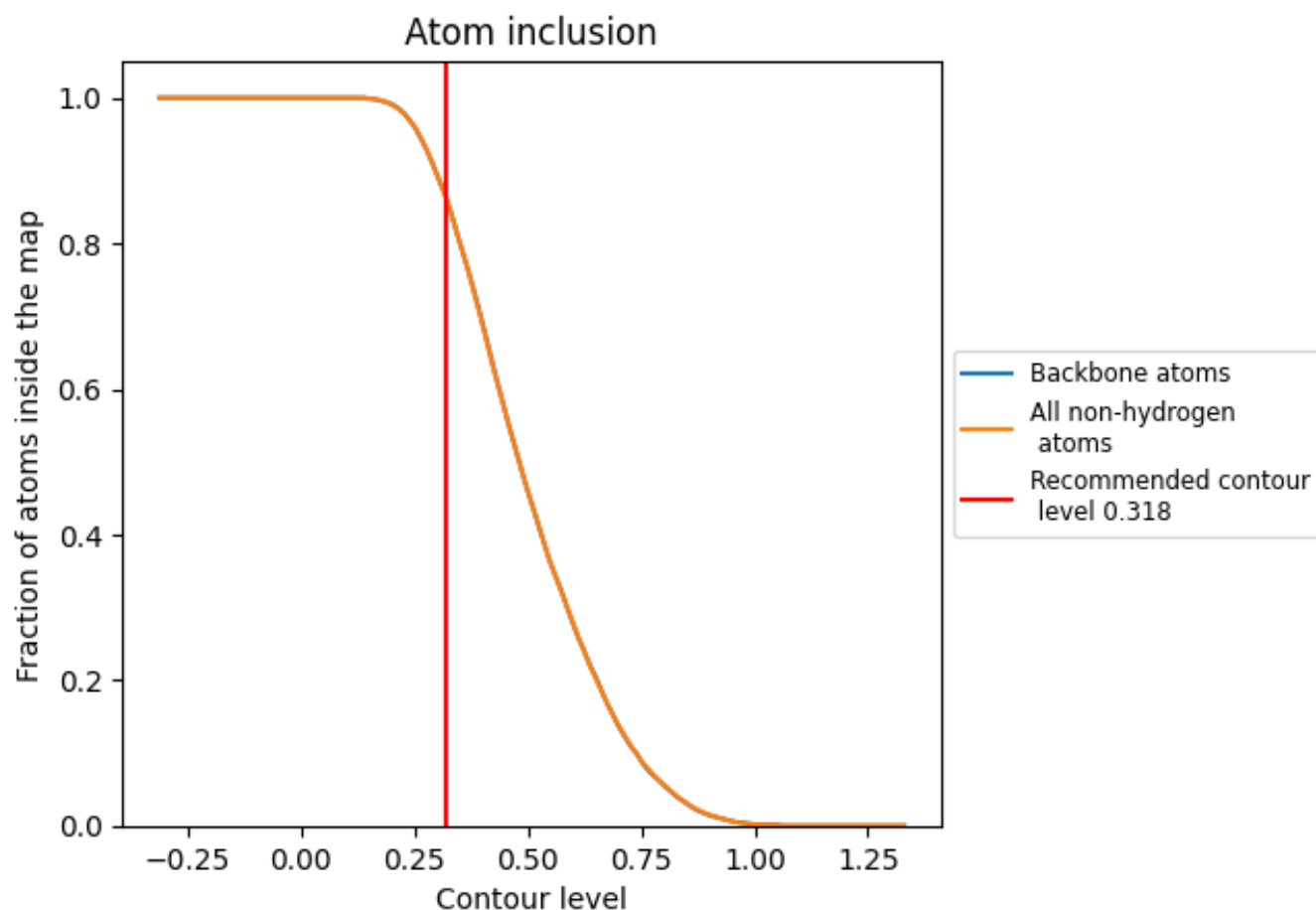
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.318).





















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.318) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8650	 0.5090
A	 0.8690	 0.5080
B	 0.8780	 0.5090
C	 0.9710	 0.5480
D	 0.9600	 0.5350
E	 1.0000	 0.5550
F	 1.0000	 0.5580
G	 0.6310	 0.5050
H	 0.6670	 0.5440
I	 0.9250	 0.5340
J	 1.0000	 0.5120
K	 0.1540	 0.3550
L	 0.7500	 0.4740
M	 0.2140	 0.3770
N	 0.7180	 0.5700
O	 0.8720	 0.4550
P	 0.6410	 0.4730
Q	 0.5130	 0.4350
R	 0.6790	 0.4350
S	 0.1790	 0.2990
T	 0.8570	 0.4080
U	 0.8930	 0.5090
V	 0.8570	 0.5050
W	 0.7950	 0.5580
X	 0.5900	 0.4790
Y	 0.7500	 0.5180

