



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:57 PM UTC

PDB ID : 8DOK / pdb_00008dok
EMDB ID : EMD-27596
Title : Cryo-EM structure of T/F100 SOSIP.664 HIV-1 Env trimer in complex with 8ANC195 and 10-1074
Authors : Chen, Y.; Zhou, F.; Huang, R.; Tolbert, W.; Pazgier, M.
Deposited on : 2022-07-13
Resolution : 3.20 Å(reported)
Based on initial model : 8CZZ

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

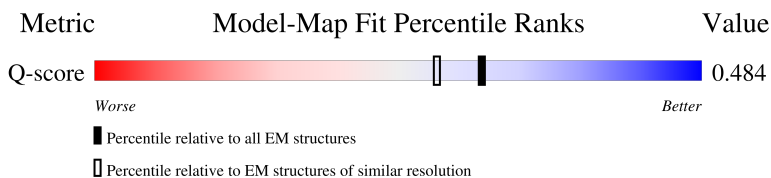
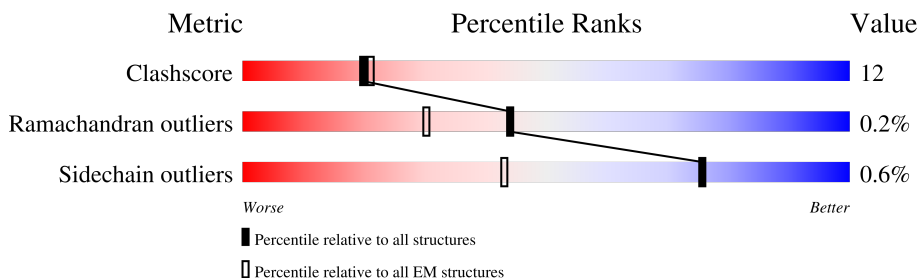
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

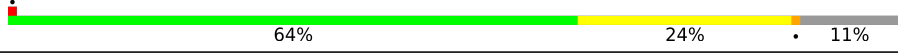
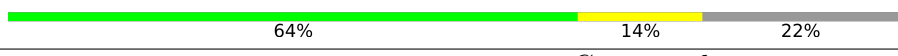
The reported resolution of this entry is 3.20 Å.

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.



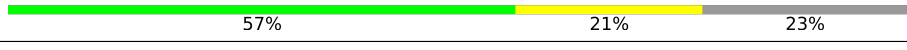
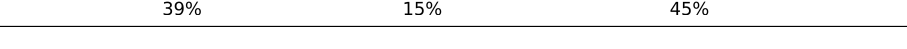
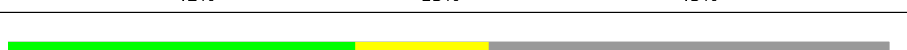
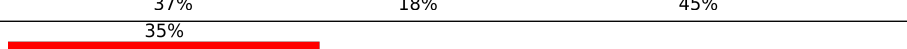
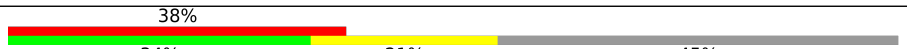
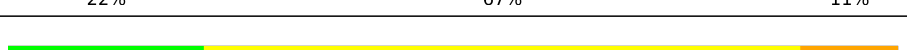
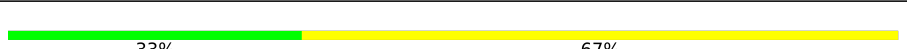
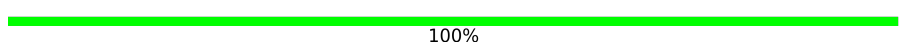
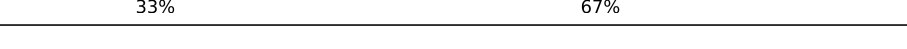
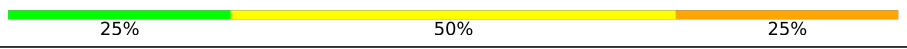
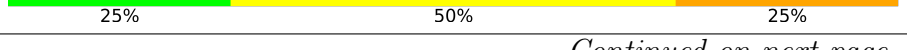
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	486	
1	E	486	
1	I	486	
2	B	155	

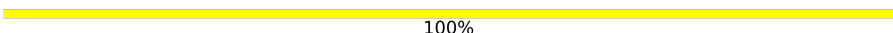
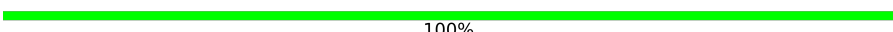
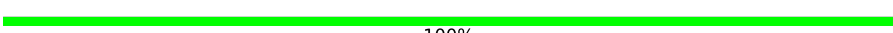
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Mol	Chain	Length	Quality of chain
2	F	155	
2	J	155	
3	C	238	
3	G	238	
3	K	238	
4	D	215	
4	H	215	
4	L	215	
5	M	238	
5	O	238	
5	Q	238	
6	N	214	
6	P	214	
6	R	214	
7	S	9	
7	i	9	
8	T	3	
8	W	3	
8	X	3	
8	g	3	
8	h	3	
8	r	3	
8	s	3	
9	U	4	
9	b	4	

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Mol	Chain	Length	Quality of chain
9	m	4	 50% 50%
10	V	2	 100%
10	l	2	 100%
10	p	2	 50% 50%
10	q	2	 100%
11	Y	10	 30% 60% 10%
12	Z	6	 17% 50% 50%
13	j	5	 40% 60%

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
14	NAG	A	1009	-	-	X	-
9	NAG	m	1	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 25844 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CRF-1_AE T/F100 Env gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	437	Total	C	N	O	S	0	0
			3458	2184	611	636	27		
1	E	435	Total	C	N	O	S	0	0
			3442	2175	609	631	27		
1	I	434	Total	C	N	O	S	0	0
			3438	2173	608	630	27		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	CYS	ALA	conflict	UNP A0A140EMT3
A	508	ARG	-	expression tag	UNP A0A140EMT3
A	509	ARG	-	expression tag	UNP A0A140EMT3
A	510	ARG	-	expression tag	UNP A0A140EMT3
A	511	ARG	-	expression tag	UNP A0A140EMT3
A	512	ARG	-	expression tag	UNP A0A140EMT3
A	513	ARG	-	expression tag	UNP A0A140EMT3
E	501	CYS	ALA	conflict	UNP A0A140EMT3
E	508	ARG	-	expression tag	UNP A0A140EMT3
E	509	ARG	-	expression tag	UNP A0A140EMT3
E	510	ARG	-	expression tag	UNP A0A140EMT3
E	511	ARG	-	expression tag	UNP A0A140EMT3
E	512	ARG	-	expression tag	UNP A0A140EMT3
E	513	ARG	-	expression tag	UNP A0A140EMT3
I	501	CYS	ALA	conflict	UNP A0A140EMT3
I	508	ARG	-	expression tag	UNP A0A140EMT3
I	509	ARG	-	expression tag	UNP A0A140EMT3
I	510	ARG	-	expression tag	UNP A0A140EMT3
I	511	ARG	-	expression tag	UNP A0A140EMT3
I	512	ARG	-	expression tag	UNP A0A140EMT3
I	513	ARG	-	expression tag	UNP A0A140EMT3

- Molecule 2 is a protein called CRF-1_AE T/F100 HIV-1 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	121	Total	C	N	O	S	0	0
			970	619	162	184	5		
2	F	117	Total	C	N	O	S	0	0
			939	599	157	178	5		
2	J	120	Total	C	N	O	S	0	0
			966	617	161	183	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP A0A6C0ZY47
B	605	CYS	THR	conflict	UNP A0A6C0ZY47
B	665	ALA	-	expression tag	UNP A0A6C0ZY47
B	666	ALA	-	expression tag	UNP A0A6C0ZY47
F	559	PRO	ILE	conflict	UNP A0A6C0ZY47
F	605	CYS	THR	conflict	UNP A0A6C0ZY47
F	665	ALA	-	expression tag	UNP A0A6C0ZY47
F	666	ALA	-	expression tag	UNP A0A6C0ZY47
J	559	PRO	ILE	conflict	UNP A0A6C0ZY47
J	605	CYS	THR	conflict	UNP A0A6C0ZY47
J	665	ALA	-	expression tag	UNP A0A6C0ZY47
J	666	ALA	-	expression tag	UNP A0A6C0ZY47

- Molecule 3 is a protein called Heavy chain of 8ANC195.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	130	Total	C	N	O	S	0	0
			1003	636	174	190	3		
3	G	130	Total	C	N	O	S	0	0
			1003	636	174	190	3		
3	K	130	Total	C	N	O	S	0	0
			1003	636	174	190	3		

- Molecule 4 is a protein called Light chain of 8ANC195.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	107	Total	C	N	O	S	0	0
			814	510	143	158	3		
4	H	108	Total	C	N	O	S	0	0
			823	516	145	159	3		
4	L	108	Total	C	N	O	S	0	0
			823	516	145	159	3		

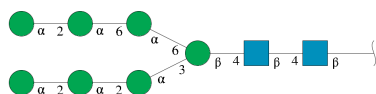
- Molecule 5 is a protein called Heavy chain of 10-1074.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	131	Total	C	N	O	S	0	0
			1030	651	173	202	4		
5	O	131	Total	C	N	O	S	0	0
			1030	651	173	202	4		
5	Q	131	Total	C	N	O	S	0	0
			1030	651	173	202	4		

- Molecule 6 is a protein called Light chain of 10-1074.

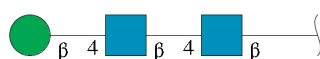
Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
6	P	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
6	R	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]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	S	9	Total	C	N	O	0	0
			105	58	2	45		
7	i	9	Total	C	N	O	0	0
			105	58	2	45		

- 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	T	3	Total	C	N	O	0	0
			39	22	2	15		
8	W	3	Total	C	N	O	0	0
			39	22	2	15		
8	X	3	Total	C	N	O	0	0
			39	22	2	15		
8	g	3	Total	C	N	O	0	0
			39	22	2	15		
8	h	3	Total	C	N	O	0	0
			39	22	2	15		
8	r	3	Total	C	N	O	0	0
			39	22	2	15		
8	s	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-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	4	Total	C	N	O	0	0
			56	32	4	20		
9	b	4	Total	C	N	O	0	0
			56	32	4	20		
9	m	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



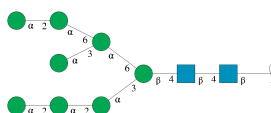
Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	2	Total	C	N	O	0	0
			28	16	2	10		
10	l	2	Total	C	N	O	0	0
			28	16	2	10		

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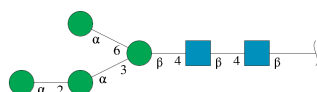
Mol	Chain	Residues	Atoms				AltConf	Trace
10	p	2	Total	C	N	O	0	0
			28	16	2	10		
10	q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



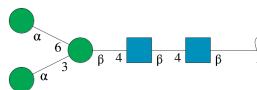
Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



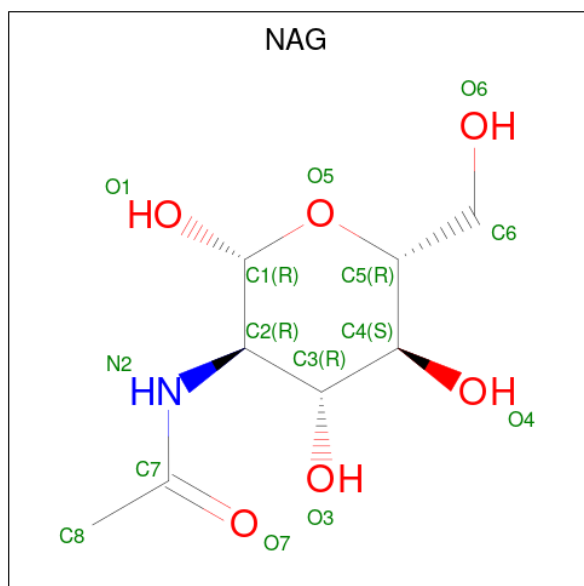
Mol	Chain	Residues	Atoms				AltConf	Trace
12	Z	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
13	j	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				AltConf
14	B	1	Total 14	C 8	N 1	O 5	0
14	B	1	Total 14	C 8	N 1	O 5	0
14	C	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	F	1	Total 14	C 8	N 1	O 5	0
14	F	1	Total 14	C 8	N 1	O 5	0
14	F	1	Total 14	C 8	N 1	O 5	0
14	G	1	Total 14	C 8	N 1	O 5	0
14	I	1	Total 14	C 8	N 1	O 5	0
14	I	1	Total 14	C 8	N 1	O 5	0

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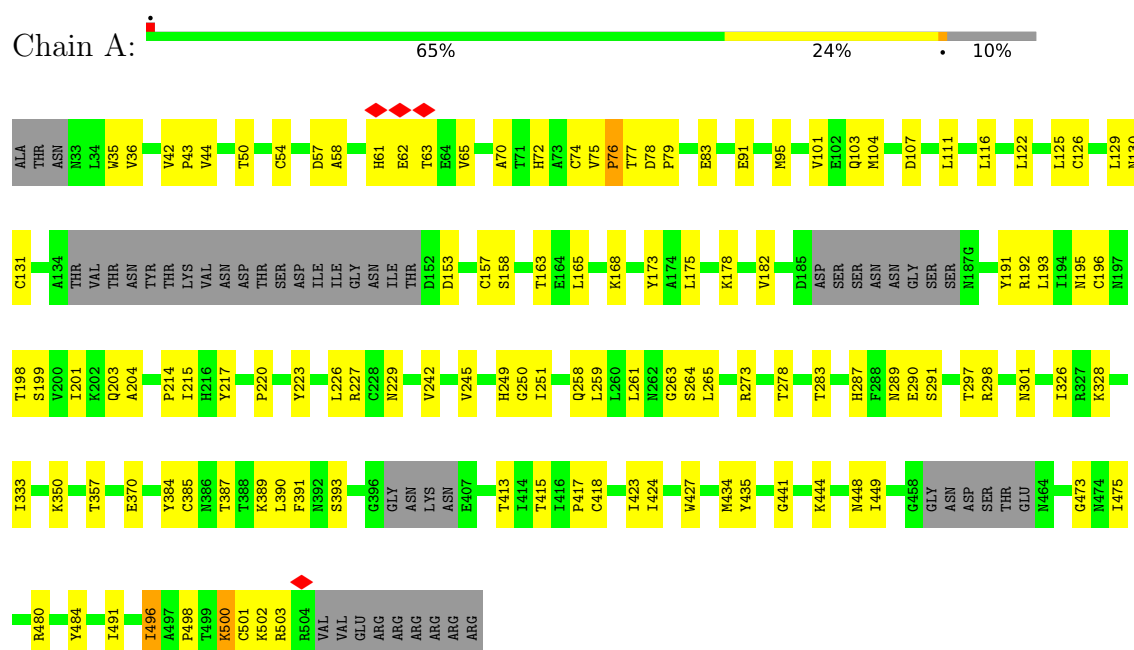
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Mol	Chain	Residues	Atoms				AltConf
14	I	1	Total	C	N	O	0
			14	8	1	5	
14	I	1	Total	C	N	O	0
			14	8	1	5	
14	I	1	Total	C	N	O	0
			14	8	1	5	
14	I	1	Total	C	N	O	0
			14	8	1	5	
14	I	1	Total	C	N	O	0
			14	8	1	5	
14	I	1	Total	C	N	O	0
			14	8	1	5	
14	J	1	Total	C	N	O	0
			14	8	1	5	
14	J	1	Total	C	N	O	0
			14	8	1	5	
14	J	1	Total	C	N	O	0
			14	8	1	5	
14	K	1	Total	C	N	O	0
			14	8	1	5	

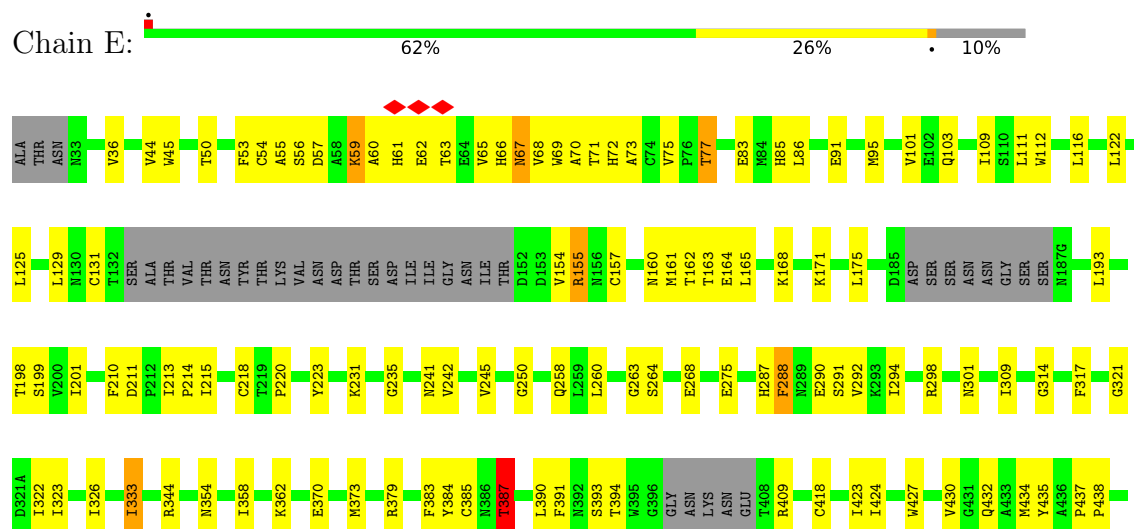
3 Residue-property plots

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

• Molecule 1: CRF-1_AE T/F100 Env gp120



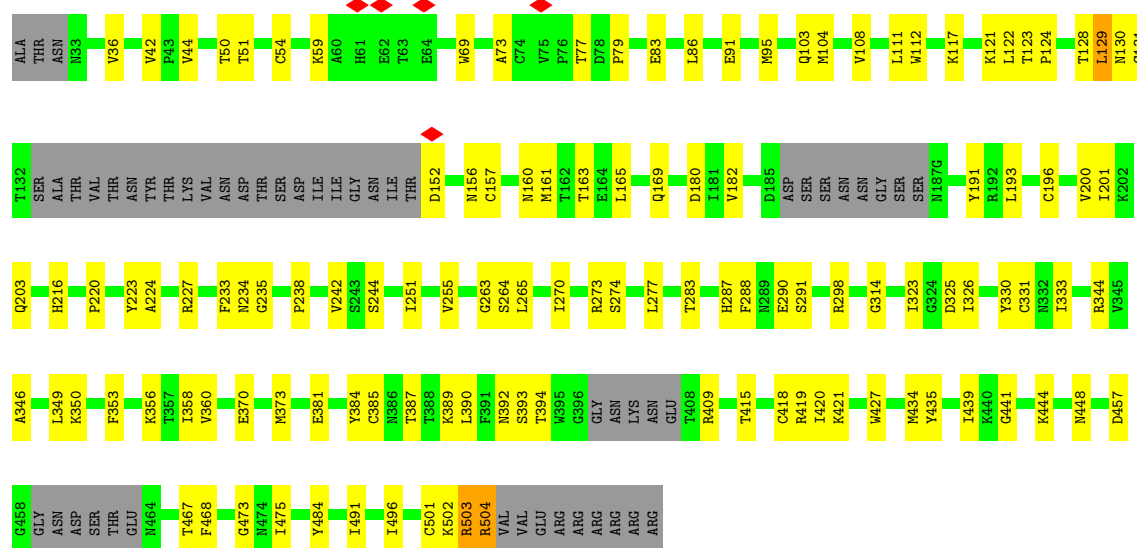
• Molecule 1: CRF-1_AE T/F100 Env gp120





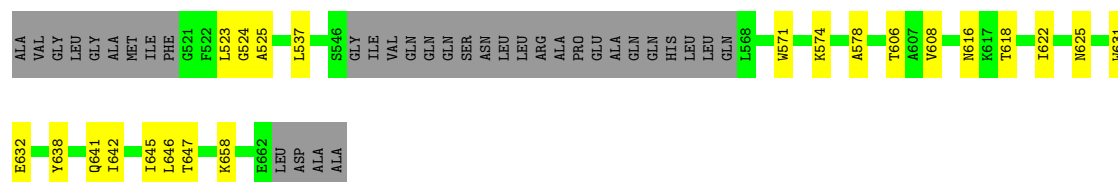
• Molecule 1: CRF-1_AE T/F100 Env gp120

Chain I: 64% 24% 11%



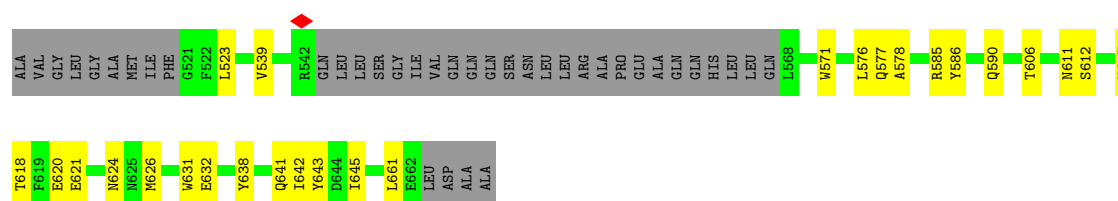
• Molecule 2: CRF-1_AE T/F100 HIV-1 gp41

Chain B: 64% 14% 22%



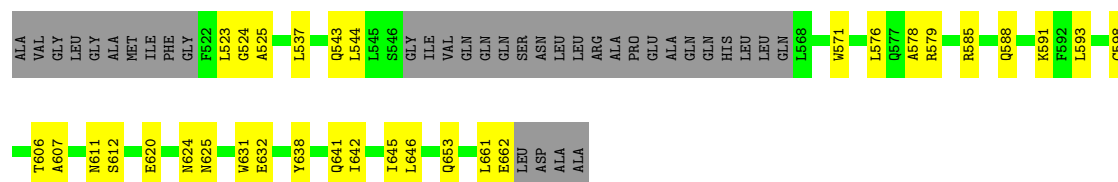
• Molecule 2: CRF-1_AE T/F100 HIV-1 gp41

Chain F: 59% 17% 25%

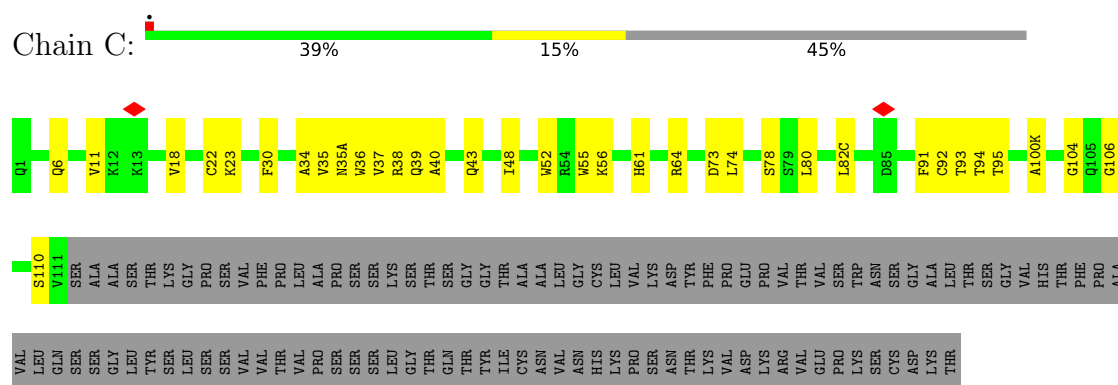


• Molecule 2: CRF-1_AE T/F100 HIV-1 gp41

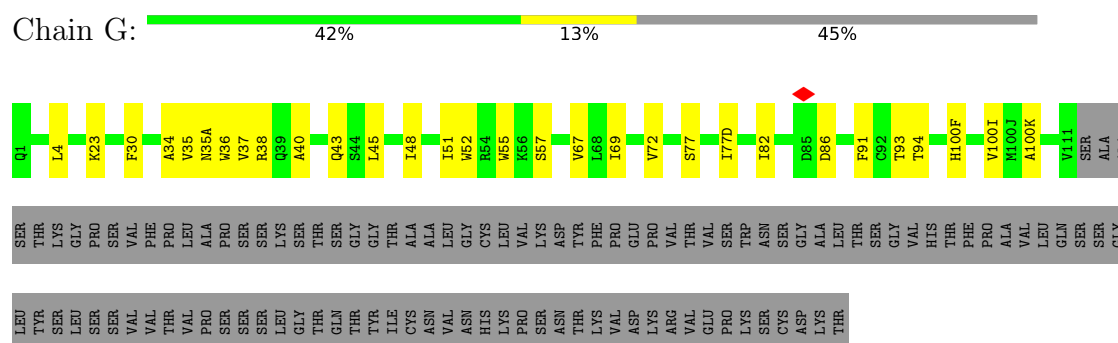
Chain J: 57% 21% 23%



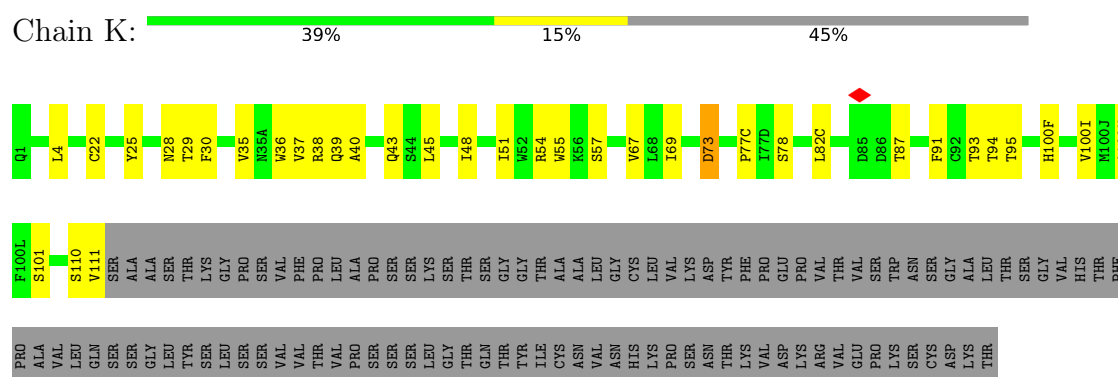
• Molecule 3: Heavy chain of 8ANC195



• Molecule 3: Heavy chain of 8ANC195

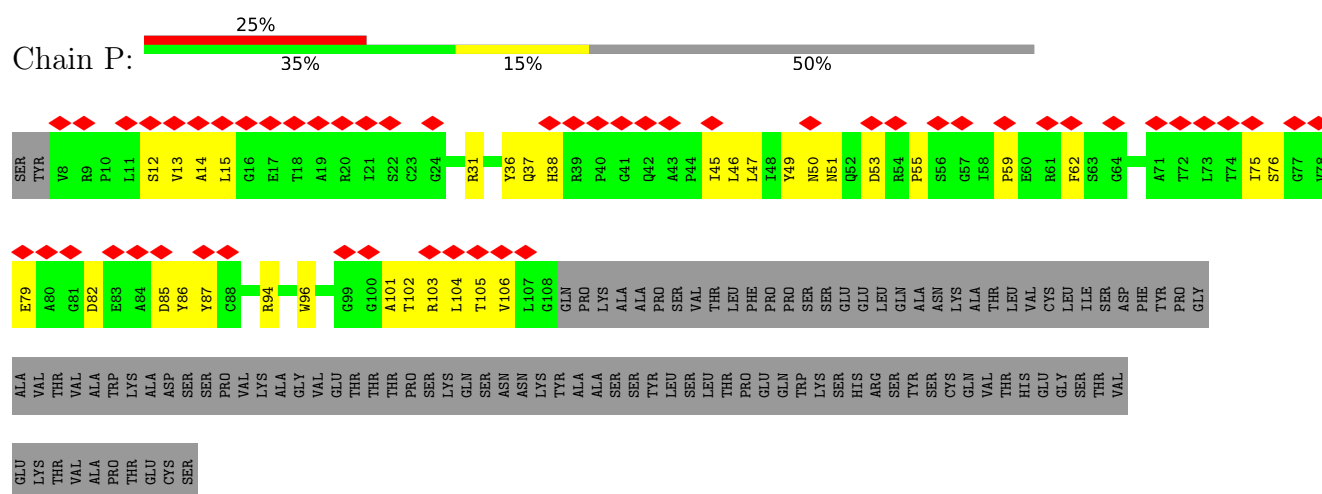


• Molecule 3: Heavy chain of 8ANC195

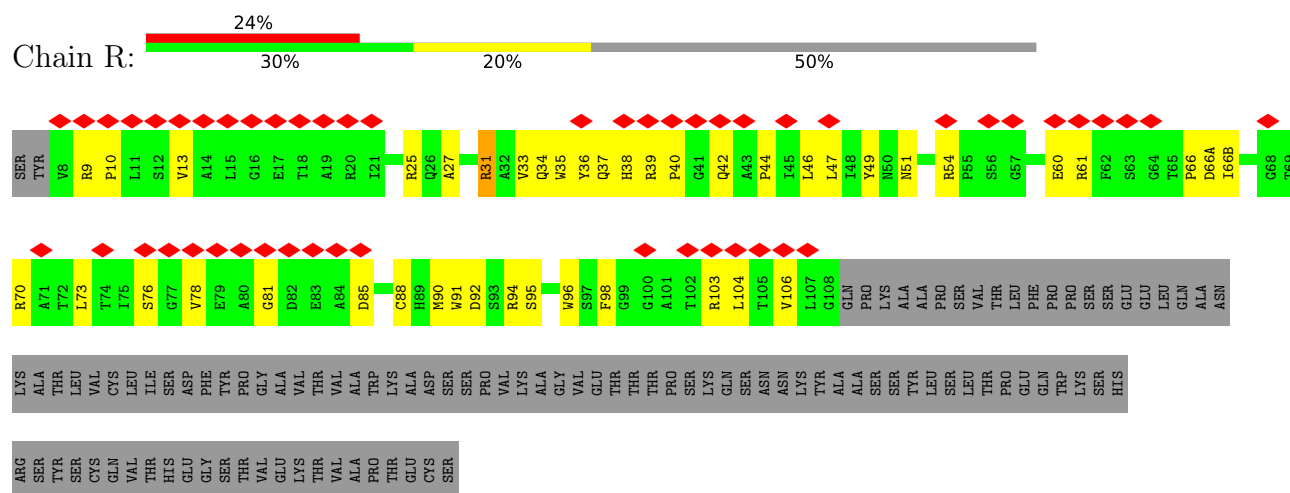


• Molecule 4: Light chain of 8ANC195





• Molecule 6: Light chain of 10-1074



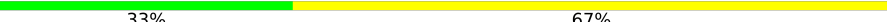
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

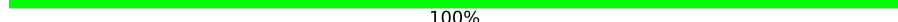


- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  33% 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 W:  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 X:  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 g:  33% 67%

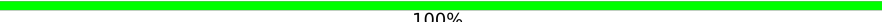


- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  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 r:  100%

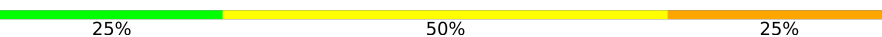


- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  67% 33%

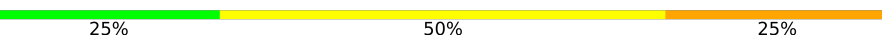


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  25% 50% 25%



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

Chain b:  25% 50% 25%

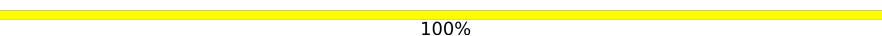


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  50% 50%

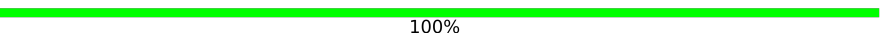


- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q: 100%



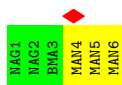
- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 30% 60% 10%



- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 17% 50% 50%



- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j: 40% 60%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	476274	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	60241	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.679	Depositor
Minimum map value	-1.184	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	268.91998, 268.91998, 268.91998	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8299999, 0.8299999, 0.8299999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/3535	0.61	3/4795 (0.1%)
1	E	0.47	1/3519 (0.0%)	0.70	10/4773 (0.2%)
1	I	0.45	4/3515 (0.1%)	0.59	5/4768 (0.1%)
2	B	0.27	0/989	0.48	1/1341 (0.1%)
2	F	0.21	0/958	0.38	0/1299
2	J	0.44	0/985	0.47	0/1336
3	C	0.17	0/1030	0.35	0/1403
3	G	0.20	0/1030	0.37	0/1403
3	K	0.17	0/1030	0.36	0/1403
4	D	0.36	0/832	0.49	1/1130 (0.1%)
4	H	0.28	0/841	0.55	3/1141 (0.3%)
4	L	0.35	0/841	0.46	0/1141
5	M	0.12	0/1055	0.30	0/1436
5	O	0.12	0/1055	0.33	0/1436
5	Q	0.19	0/1055	0.38	0/1436
6	N	0.18	0/845	0.41	1/1148 (0.1%)
6	P	0.18	0/845	0.41	1/1148 (0.1%)
6	R	0.22	0/845	0.46	0/1148
All	All	0.34	5/24805 (0.0%)	0.52	25/33685 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	331	CYS	C-N	-9.22	1.20	1.33
1	E	70	ALA	CA-C	-7.04	1.44	1.53
1	I	156	ASN	C-N	-6.79	1.23	1.33
1	I	130	ASN	C-N	6.21	1.41	1.33
1	I	129	LEU	C-O	-5.13	1.17	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	HIS	N-CA-C	-10.90	100.01	113.97
4	H	7	SER	N-CA-C	8.58	124.13	112.55
1	E	432	GLN	N-CA-C	8.53	122.67	109.96
1	I	263	GLY	CA-C-O	-8.00	114.28	122.28
1	A	263	GLY	CA-C-O	-6.95	114.97	122.47
2	B	524	GLY	N-CA-C	6.59	120.15	112.50
1	I	387	THR	CA-CB-OG1	-6.45	99.92	109.60
1	E	57	ASP	N-CA-C	6.33	119.67	109.79
1	E	288	PHE	CB-CA-C	-6.09	99.24	109.48
6	P	76	SER	N-CA-C	-5.93	100.55	108.19
1	E	387	THR	CA-C-N	5.85	129.20	120.31
1	E	387	THR	C-N-CA	5.85	129.20	120.31
1	I	288	PHE	CB-CA-C	-5.82	99.71	109.48
4	H	8	PRO	CA-C-O	-5.82	117.01	121.31
4	D	10	THR	N-CA-C	-5.72	100.60	109.24
1	E	288	PHE	CA-CB-CG	5.59	119.39	113.80
1	E	263	GLY	CA-C-O	-5.57	114.66	122.51
1	I	288	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	500	LYS	N-CA-C	5.41	117.46	110.65
6	N	67	PHE	N-CA-C	-5.36	101.03	109.50
1	E	387	THR	N-CA-CB	-5.30	102.48	111.17
1	E	59	LYS	N-CA-C	-5.23	102.31	110.10
1	E	77	THR	CB-CA-C	-5.21	98.82	110.19
4	H	7	SER	O-C-N	-5.17	116.30	120.38
1	I	501	CYS	N-CA-C	5.09	117.81	110.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3398	102	0
1	E	3442	0	3385	114	0
1	I	3438	0	3381	99	0
2	B	970	0	950	25	0
2	F	939	0	915	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	966	0	947	41	0
3	C	1003	0	973	25	0
3	G	1003	0	973	22	0
3	K	1003	0	973	26	0
4	D	814	0	787	15	0
4	H	823	0	800	20	0
4	L	823	0	800	19	0
5	M	1030	0	995	31	0
5	O	1030	0	995	32	0
5	Q	1030	0	995	39	0
6	N	824	0	788	25	0
6	P	824	0	788	26	0
6	R	824	0	788	30	0
7	S	105	0	88	1	0
7	i	105	0	88	1	0
8	T	39	0	34	0	0
8	W	39	0	34	0	0
8	X	39	0	34	2	0
8	g	39	0	34	2	0
8	h	39	0	34	2	0
8	r	39	0	34	0	0
8	s	39	0	34	1	0
9	U	56	0	49	2	0
9	b	56	0	49	6	0
9	m	56	0	49	15	0
10	V	28	0	25	0	0
10	l	28	0	25	0	0
10	p	28	0	25	1	0
10	q	28	0	25	0	0
11	Y	116	0	97	1	0
12	Z	72	0	61	0	0
13	j	61	0	52	1	0
14	A	140	0	130	10	0
14	B	28	0	26	1	0
14	C	14	0	13	0	0
14	E	168	0	156	8	0
14	F	42	0	39	1	0
14	G	14	0	13	0	0
14	I	126	0	117	2	0
14	J	42	0	39	2	0
14	K	14	0	13	0	0
All	All	25844	0	25048	630	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (630) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:523:LEU:HD12	2:J:523:LEU:O	1.52	1.08
4:L:7:SER:HB3	4:L:8:PRO:HD3	1.30	1.08
1:E:290:GLU:HG3	14:E:608:NAG:H62	1.42	1.02
4:L:11:LEU:CD2	4:L:19:VAL:HG23	1.89	1.01
1:I:330:TYR:HE2	9:m:1:NAG:H82	1.27	0.98
1:E:444:LYS:HZ1	9:b:1:NAG:H81	1.30	0.96
1:E:444:LYS:NZ	9:b:1:NAG:H81	1.82	0.95
1:I:504:ARG:HG3	2:J:653:GLN:OE1	1.68	0.93
4:L:11:LEU:HD23	4:L:19:VAL:HG21	1.51	0.93
4:L:11:LEU:CD2	4:L:19:VAL:CG2	2.47	0.92
1:A:261:LEU:HD23	1:A:449:ILE:HG22	1.52	0.91
1:I:504:ARG:HB2	2:J:653:GLN:OE1	1.71	0.91
1:E:112:TRP:CG	1:E:427:TRP:HZ3	1.89	0.90
1:E:155:ARG:HG3	1:E:155:ARG:HH11	1.38	0.88
4:L:11:LEU:HD23	4:L:19:VAL:CG2	2.04	0.88
1:A:192:ARG:HH21	14:A:1009:NAG:H82	1.38	0.87
1:E:175:LEU:HD21	14:E:607:NAG:H82	1.55	0.87
1:E:290:GLU:HG3	14:E:608:NAG:C6	2.06	0.85
1:A:261:LEU:CD2	1:A:449:ILE:HG22	2.07	0.85
1:I:330:TYR:CE2	9:m:1:NAG:H82	2.13	0.84
4:L:11:LEU:HD21	4:L:19:VAL:HG23	1.61	0.82
1:E:160:ASN:HB3	14:E:601:NAG:HN2	1.43	0.82
1:A:57:ASP:OD2	1:A:58:ALA:N	2.14	0.81
1:A:77:THR:O	1:A:79:PRO:HD3	1.80	0.81
1:A:491:ILE:HD13	2:B:523:LEU:CD1	2.14	0.78
1:E:112:TRP:CG	1:E:427:TRP:CZ3	2.72	0.78
1:I:95:MET:HE1	1:I:273:ARG:HB3	1.65	0.77
2:J:524:GLY:O	2:J:525:ALA:HB3	1.84	0.77
1:A:297:THR:HG22	1:A:444:LYS:HG3	1.66	0.77
1:A:491:ILE:HD13	2:B:523:LEU:HD13	1.67	0.76
1:E:112:TRP:CD2	1:E:427:TRP:HZ3	2.04	0.76
2:B:625:ASN:HB3	14:B:702:NAG:HN2	1.50	0.76
4:H:8:PRO:HB2	4:H:11:LEU:HD23	1.67	0.76
5:M:37:ILE:HB	5:M:91:TYR:HB2	1.68	0.76
1:E:444:LYS:NZ	9:b:1:NAG:C8	2.50	0.75
1:I:504:ARG:CG	2:J:653:GLN:OE1	2.33	0.74
1:E:109:ILE:HD13	1:E:430:VAL:CG1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:444:LYS:NZ	9:m:1:NAG:O7	2.21	0.74
4:L:7:SER:CB	4:L:8:PRO:HD3	2.13	0.74
1:I:244:SER:HB2	2:J:523:LEU:HD11	1.69	0.74
1:I:504:ARG:CB	2:J:653:GLN:OE1	2.35	0.73
6:R:85:ASP:HB3	6:R:103:ARG:HD2	1.69	0.73
1:A:75:VAL:O	1:A:76:PRO:C	2.30	0.73
4:D:7:SER:HB2	4:D:8:PRO:HD3	1.71	0.73
2:J:625:ASN:HB3	14:J:703:NAG:HN2	1.54	0.73
1:E:109:ILE:HD13	1:E:430:VAL:HG12	1.71	0.72
1:I:291:SER:HB2	1:I:448:ASN:HB3	1.71	0.72
1:E:394:THR:O	1:E:409:ARG:NH2	2.23	0.71
5:M:100:ARG:NH1	9:U:4:NAG:O7	2.22	0.71
1:A:264:SER:O	1:A:287:HIS:NE2	2.20	0.70
1:I:504:ARG:HB2	2:J:653:GLN:CD	2.16	0.70
1:A:491:ILE:HG12	2:B:523:LEU:HD11	1.73	0.70
1:A:61:HIS:HE1	1:A:70:ALA:HA	1.57	0.70
1:E:198:THR:O	1:I:314:GLY:HA3	1.93	0.69
1:E:290:GLU:OE2	1:E:344:ARG:NH1	2.24	0.69
1:I:491:ILE:O	2:J:585:ARG:NH2	2.26	0.69
1:E:290:GLU:CG	14:E:608:NAG:H62	2.20	0.69
1:I:330:TYR:HE2	9:m:1:NAG:C8	2.04	0.69
5:Q:35:THR:OG1	5:Q:47:TRP:NE1	2.26	0.69
6:R:33:VAL:HG12	6:R:90:MET:HA	1.76	0.68
4:D:4:MET:HE3	4:D:25:ALA:HB2	1.75	0.67
1:E:333:ILE:HG13	1:E:390:LEU:HD21	1.77	0.66
1:A:491:ILE:CD1	2:B:523:LEU:CD1	2.74	0.66
6:N:23:CYS:O	6:N:70:ARG:NH2	2.29	0.66
6:P:79:GLU:HG2	6:P:82:ASP:HB2	1.77	0.66
1:A:198:THR:O	1:E:314:GLY:HA3	1.95	0.66
1:A:389:LYS:NZ	1:A:415:THR:O	2.28	0.66
5:O:39:GLN:HB2	5:O:45:LEU:HD12	1.77	0.66
4:D:7:SER:CB	4:D:8:PRO:HD3	2.26	0.65
1:E:161:MET:HG2	1:E:162:THR:H	1.60	0.65
5:M:67:VAL:HG12	5:M:82:LEU:HG	1.79	0.65
2:J:523:LEU:O	2:J:523:LEU:CD1	2.37	0.65
4:H:31:ASN:ND2	8:h:1:NAG:H82	2.12	0.65
1:I:503:ARG:HH11	1:I:504:ARG:HE	1.44	0.64
3:C:40:ALA:HB3	3:C:43:GLN:HB2	1.77	0.64
5:M:29:MET:HE1	5:M:73:THR:HA	1.79	0.64
1:A:491:ILE:CD1	2:B:523:LEU:HD13	2.27	0.64
3:G:100(F):HIS:HE2	4:H:92:ASP:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:82:ASP:HB3	6:N:104:LEU:HD13	1.80	0.64
4:D:46:LEU:HD23	4:D:55:LEU:HD11	1.80	0.64
1:E:160:ASN:HB3	14:E:601:NAG:N2	2.11	0.64
1:E:155:ARG:HG3	1:E:155:ARG:NH1	2.06	0.64
1:I:298:ARG:NH2	1:I:441:GLY:O	2.30	0.64
1:I:330:TYR:CE2	9:m:1:NAG:C8	2.81	0.64
5:M:51:ILE:HA	5:M:57:ALA:HA	1.79	0.64
5:Q:5:GLN:HA	5:Q:105:LYS:HZ3	1.63	0.63
3:C:11:VAL:HG22	3:C:110:SER:HB2	1.79	0.63
1:I:50:THR:O	1:I:103:GLN:NE2	2.31	0.63
1:A:491:ILE:CG1	2:B:523:LEU:HD11	2.27	0.63
1:E:95:MET:HG2	1:E:235:GLY:O	1.98	0.63
1:A:289:ASN:OD1	1:A:290:GLU:N	2.32	0.63
5:Q:75:LYS:HB2	5:Q:77:GLN:HG2	1.81	0.63
6:R:31:ARG:HH21	6:R:51:ASN:HD21	1.45	0.63
3:C:22:CYS:HB3	3:C:78:SER:HB3	1.81	0.62
1:A:129:LEU:HD11	1:A:193:LEU:HD12	1.81	0.62
1:A:220:PRO:HB3	2:B:578:ALA:HB1	1.81	0.62
3:C:6:GLN:HE21	3:C:92:CYS:HB3	1.64	0.62
2:B:638:TYR:O	2:B:642:ILE:HG13	1.99	0.62
1:I:290:GLU:OE2	1:I:344:ARG:NH1	2.33	0.62
3:C:6:GLN:HE22	3:C:104:GLY:HA3	1.64	0.61
6:P:13:VAL:HG12	6:P:104:LEU:HD11	1.82	0.61
1:A:44:VAL:HG21	2:B:632:GLU:HG3	1.82	0.61
1:I:182:VAL:HG11	10:p:1:NAG:H62	1.82	0.61
1:I:163:THR:HG23	1:I:165:LEU:H	1.64	0.61
6:P:37:GLN:HE21	6:P:45:ILE:HG12	1.66	0.60
2:B:647:THR:HG21	2:F:539:VAL:HG13	1.83	0.60
1:E:116:LEU:HD21	1:E:434:MET:HB3	1.84	0.60
1:I:264:SER:O	1:I:287:HIS:NE2	2.30	0.60
1:E:288:PHE:HB3	1:E:290:GLU:O	2.00	0.60
1:E:322:ILE:O	6:P:94:ARG:NH2	2.35	0.60
1:A:77:THR:O	1:A:79:PRO:CD	2.47	0.60
1:A:301:ASN:HB3	14:A:1004:NAG:O5	2.02	0.60
4:H:8:PRO:CB	4:H:11:LEU:HD23	2.32	0.60
5:M:51:ILE:HD12	5:M:69:ILE:HG23	1.84	0.60
5:M:6:GLU:HA	5:M:22:CYS:HA	1.85	0.59
1:A:116:LEU:HD21	1:A:434:MET:HE3	1.83	0.59
3:C:18:VAL:HG12	3:C:82(C):LEU:HD11	1.84	0.59
1:A:50:THR:O	1:A:103:GLN:NE2	2.36	0.59
1:E:61:HIS:CD2	1:E:72:HIS:HB3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HB2	1:A:201:ILE:HG13	1.84	0.59
1:I:373:MET:HE2	14:I:608:NAG:H83	1.84	0.59
1:E:424:ILE:HD11	1:E:434:MET:HE2	1.85	0.59
5:Q:100:ARG:HH12	9:m:4:NAG:H4	1.68	0.59
1:A:175:LEU:HD11	14:A:1006:NAG:H82	1.85	0.58
1:A:424:ILE:HB	1:A:434:MET:HG2	1.85	0.58
1:E:131:CYS:HA	1:E:157:CYS:HA	1.86	0.58
1:A:74:CYS:O	1:A:76:PRO:O	2.21	0.58
5:Q:67:VAL:HG12	5:Q:82:LEU:HG	1.84	0.58
3:G:40:ALA:HB3	3:G:43:GLN:HB2	1.84	0.58
6:R:34:GLN:OE1	6:R:91:TRP:NE1	2.37	0.58
1:E:358:ILE:HD12	1:E:468:PHE:HE1	1.69	0.58
1:E:490:GLN:HG3	2:F:585:ARG:HH12	1.67	0.58
2:J:524:GLY:O	2:J:525:ALA:CB	2.49	0.58
1:E:201:ILE:HD12	1:E:435:TYR:HB2	1.85	0.58
6:R:38:HIS:HA	6:R:44:PRO:HB3	1.84	0.58
1:A:61:HIS:O	1:A:65:VAL:N	2.34	0.58
1:I:238:PRO:HG3	3:K:54:ARG:HG2	1.84	0.58
3:K:38:ARG:HB2	3:K:48:ILE:HD11	1.85	0.58
5:O:69:ILE:HD11	5:O:80:LEU:HD12	1.85	0.58
4:L:7:SER:HB3	4:L:8:PRO:CD	2.19	0.57
1:A:192:ARG:NH2	14:A:1009:NAG:H82	2.14	0.57
4:H:35:TRP:HB2	4:H:48:ILE:HB	1.85	0.57
1:E:83:GLU:HG2	1:E:245:VAL:HG12	1.84	0.57
14:F:702:NAG:H5	4:H:28:SER:HB2	1.86	0.57
1:E:387:THR:O	1:E:387:THR:HG23	2.04	0.57
3:C:73:ASP:OD2	7:S:1:NAG:O3	2.22	0.56
2:J:638:TYR:O	2:J:642:ILE:HG13	2.05	0.56
1:A:75:VAL:C	1:A:76:PRO:O	2.46	0.56
1:A:289:ASN:OD1	1:A:290:GLU:HG2	2.05	0.56
1:A:370:GLU:HG3	1:A:384:TYR:HE2	1.71	0.56
1:I:244:SER:CB	2:J:523:LEU:HD11	2.35	0.56
3:K:35:VAL:HG12	3:K:94:THR:HG22	1.88	0.56
5:Q:72:ASP:OD2	5:Q:77:GLN:NE2	2.33	0.56
6:R:27:ALA:CB	6:R:31:ARG:HG2	2.35	0.56
1:E:198:THR:OG1	1:E:199:SER:N	2.33	0.56
6:N:46:LEU:HG	6:N:55:PRO:HG2	1.87	0.56
5:Q:100:ARG:NH1	9:m:4:NAG:H2	2.21	0.56
1:I:394:THR:O	1:I:409:ARG:NH2	2.38	0.56
1:E:112:TRP:CD2	1:E:427:TRP:CZ3	2.91	0.56
1:E:220:PRO:HB3	2:F:578:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:31:ASN:HD22	8:h:1:NAG:H82	1.70	0.56
1:I:504:ARG:HB2	2:J:653:GLN:NE2	2.21	0.56
5:Q:83:THR:HG22	5:Q:86:ASP:HB2	1.88	0.56
4:D:6:GLN:HE22	4:D:87:TYR:HA	1.70	0.56
1:I:86:LEU:HD11	2:J:523:LEU:HD13	1.87	0.56
1:A:227:ARG:HH21	1:A:229:ASN:HD21	1.53	0.56
1:A:328:LYS:HE3	1:A:417:PRO:HB3	1.88	0.56
5:O:60:ASN:HB2	5:O:63:LEU:HD23	1.87	0.56
1:E:91:GLU:HB3	1:E:242:VAL:HG11	1.87	0.56
6:P:85:ASP:HA	6:P:103:ARG:HB3	1.88	0.55
1:A:36:VAL:HG13	1:A:496:ILE:HG23	1.88	0.55
1:A:491:ILE:CD1	2:B:523:LEU:HD11	2.36	0.55
1:I:503:ARG:NH1	1:I:504:ARG:HE	2.03	0.55
1:A:192:ARG:NH2	14:A:1009:NAG:C7	2.69	0.55
1:E:370:GLU:HG3	1:E:384:TYR:HE2	1.71	0.55
1:A:192:ARG:HH21	14:A:1009:NAG:C8	2.17	0.55
6:N:49:TYR:HD2	6:N:55:PRO:HG3	1.71	0.55
1:E:290:GLU:OE2	1:E:344:ARG:NH2	2.40	0.55
5:M:47:TRP:HB2	6:N:98:PHE:HE1	1.72	0.55
1:I:325:ASP:OD1	1:I:325:ASP:O	2.24	0.55
1:I:389:LYS:NZ	1:I:415:THR:O	2.31	0.54
2:J:588:GLN:HA	2:J:591:LYS:HD3	1.89	0.54
6:R:47:LEU:HD12	6:R:73:LEU:HD21	1.89	0.54
1:E:56:SER:O	1:E:77:THR:HG23	2.07	0.54
1:A:204:ALA:HB2	1:A:434:MET:HE2	1.88	0.54
1:E:44:VAL:HG21	2:F:632:GLU:HG3	1.88	0.54
1:E:67:ASN:C	1:E:69:TRP:N	2.63	0.54
1:I:220:PRO:HG3	2:J:578:ALA:HB1	1.89	0.54
5:Q:6:GLU:HA	5:Q:22:CYS:HA	1.89	0.54
1:A:168:LYS:NZ	1:I:128:THR:OG1	2.41	0.54
6:N:10:PRO:HB3	6:N:103:ARG:HB2	1.89	0.54
1:A:122:LEU:HB3	1:A:125:LEU:HD21	1.89	0.54
3:G:35:VAL:HG12	3:G:94:THR:HG22	1.89	0.54
3:K:73:ASP:OD1	3:K:73:ASP:N	2.37	0.54
1:A:498:PRO:HD3	2:B:631:TRP:CZ2	2.43	0.53
6:N:85:ASP:HB3	6:N:103:ARG:HG2	1.90	0.53
6:R:92:ASP:HB2	6:R:95:SER:HB2	1.90	0.53
5:M:53:ASP:O	5:M:71:ARG:NH2	2.39	0.53
5:Q:36:TRP:CE2	5:Q:80:LEU:HB2	2.43	0.53
9:U:2:NAG:H62	9:U:3:NAG:H83	1.91	0.53
9:b:2:NAG:H61	9:b:3:NAG:N2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:VAL:HG12	3:C:94:THR:HG22	1.90	0.53
4:L:46:LEU:HD23	4:L:55:LEU:HD11	1.90	0.53
6:R:37:GLN:NE2	6:R:38:HIS:O	2.42	0.53
6:N:18:THR:OG1	6:N:20:ARG:NH1	2.40	0.53
5:Q:35:THR:HA	5:Q:50:TYR:HA	1.90	0.53
2:B:606:THR:HG21	2:B:646:LEU:HG	1.90	0.53
1:I:124:PRO:HB2	1:I:161:MET:HE2	1.89	0.53
1:I:203:GLN:HG3	1:I:435:TYR:HD2	1.73	0.53
1:I:255:VAL:HG13	1:I:475:ILE:HD11	1.90	0.53
5:O:49:GLY:HA2	6:P:96:TRP:HZ3	1.73	0.53
1:A:104:MET:HG3	1:A:217:TYR:OH	2.09	0.53
1:A:214:PRO:HB3	1:A:250:GLY:HA3	1.90	0.53
1:E:36:VAL:HG13	1:E:496:ILE:HG23	1.91	0.53
1:I:44:VAL:HG21	2:J:632:GLU:HG3	1.90	0.53
1:E:294:ILE:HD12	1:E:333:ILE:CD1	2.39	0.53
3:K:100(F):HIS:NE2	4:L:91:TYR:O	2.41	0.53
6:N:33:VAL:HG22	6:N:51:ASN:HB2	1.91	0.53
5:O:53:ASP:HA	5:O:71:ARG:HH22	1.74	0.53
5:O:100(A):ILE:HG22	5:O:100(J):PHE:HB3	1.90	0.53
6:R:61:ARG:HD2	6:R:76:SER:HB3	1.91	0.53
1:I:326:ILE:HG13	6:R:94:ARG:HD3	1.91	0.53
3:C:6:GLN:HB3	3:C:107:THR:HG23	1.91	0.52
5:O:34:TRP:HB2	5:O:51:ILE:HG23	1.91	0.52
5:Q:38:ARG:NH2	5:Q:86:ASP:OD1	2.41	0.52
1:E:109:ILE:HD13	1:E:430:VAL:HG11	1.90	0.52
1:E:214:PRO:HB3	1:E:250:GLY:HA3	1.90	0.52
1:I:330:TYR:OH	9:m:1:NAG:H83	2.08	0.52
1:I:457:ASP:HB3	1:I:467:THR:HB	1.91	0.52
5:Q:6:GLU:HG2	5:Q:22:CYS:HB3	1.91	0.52
3:C:22:CYS:N	3:C:78:SER:O	2.41	0.52
5:M:7:SER:N	5:M:21:THR:O	2.40	0.52
1:E:65:VAL:O	1:E:66:HIS:C	2.52	0.52
3:K:87:THR:HG23	3:K:110:SER:HA	1.91	0.52
2:F:641:GLN:O	2:F:645:ILE:HG12	2.10	0.52
1:I:95:MET:HB2	1:I:235:GLY:O	2.10	0.52
1:E:55:ALA:HA	1:E:75:VAL:O	2.09	0.52
3:K:100(F):HIS:HE2	4:L:92:ASP:HA	1.74	0.52
1:I:265:LEU:HD21	1:I:291:SER:HB3	1.92	0.52
5:O:36:TRP:CE2	5:O:80:LEU:HB2	2.45	0.52
5:Q:37:ILE:HG12	5:Q:47:TRP:HD1	1.74	0.52
1:A:131:CYS:HA	1:A:157:CYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:ILE:CD1	1:E:430:VAL:HG11	2.40	0.51
1:E:129:LEU:HD11	1:E:193:LEU:HD12	1.93	0.51
1:E:496:ILE:HD11	2:F:643:TYR:HE1	1.75	0.51
6:P:31:ARG:O	6:P:51:ASN:ND2	2.42	0.51
3:G:4:LEU:HD21	3:G:94:THR:HG23	1.92	0.51
5:M:60:ASN:HB3	5:M:63:LEU:HD13	1.91	0.51
4:L:31:ASN:ND2	8:s:1:NAG:H82	2.25	0.51
6:N:34:GLN:HB2	6:N:89:HIS:HB3	1.93	0.51
1:E:67:ASN:O	1:E:68:VAL:C	2.54	0.51
1:E:85:HIS:NE2	1:E:241:ASN:HB2	2.26	0.51
1:I:504:ARG:CB	2:J:653:GLN:CD	2.83	0.51
5:M:15:SER:HA	5:M:82(B):SER:HA	1.93	0.51
6:R:25:ARG:O	6:R:70:ARG:NH1	2.43	0.51
6:R:39:ARG:HG2	6:R:42:GLN:HB2	1.92	0.51
1:E:496:ILE:O	2:F:631:TRP:NE1	2.33	0.51
4:H:29:ILE:HB	4:H:71:PHE:HZ	1.75	0.51
5:M:103:TRP:HB3	6:N:44:PRO:HD2	1.92	0.51
5:O:7:SER:HB2	5:O:21:THR:HB	1.93	0.51
1:A:70:ALA:HB3	1:A:111:LEU:HD22	1.92	0.51
1:A:75:VAL:HB	1:A:76:PRO:HD3	1.93	0.51
1:A:283:THR:HG21	1:A:473:GLY:HA2	1.93	0.51
1:A:413:THR:HG23	14:A:1003:NAG:H81	1.93	0.51
1:E:444:LYS:HZ3	9:b:1:NAG:C8	2.23	0.51
5:O:45:LEU:HD22	6:P:38:HIS:CD2	2.46	0.51
5:Q:95:ALA:HB1	5:Q:100(N):TYR:HB3	1.92	0.51
4:D:92:ASP:OD2	4:D:93:THR:HG23	2.10	0.51
1:I:333:ILE:HD13	1:I:390:LEU:HD21	1.93	0.51
4:D:4:MET:SD	4:D:90:GLN:HB3	2.51	0.50
3:G:37:VAL:HG11	3:G:45:LEU:HD23	1.93	0.50
3:K:73:ASP:HA	3:K:77(C):PRO:HB3	1.94	0.50
3:K:95:THR:HG22	3:K:101:SER:H	1.76	0.50
6:R:66:PRO:HB2	6:R:66(B):ILE:HG13	1.92	0.50
1:A:198:THR:OG1	1:A:199:SER:N	2.45	0.50
1:I:323:ILE:O	1:I:323:ILE:HG22	2.10	0.50
4:H:20:ARG:HG2	4:H:74:THR:HG22	1.92	0.50
1:I:381:GLU:HG2	1:I:439:ILE:HG12	1.94	0.50
1:A:203:GLN:HG3	1:A:435:TYR:HD2	1.75	0.50
1:E:155:ARG:NH1	1:E:155:ARG:CG	2.73	0.50
3:G:51:ILE:HG12	3:G:57:SER:HB3	1.93	0.50
5:Q:28:SER:O	5:Q:30:ASN:ND2	2.44	0.50
1:A:249:HIS:O	1:A:251:ILE:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:TRP:HE1	1:A:475:ILE:HG21	1.77	0.50
1:A:427:TRP:NE1	1:A:475:ILE:HG21	2.27	0.50
1:E:264:SER:O	1:E:287:HIS:NE2	2.23	0.50
3:C:6:GLN:OE1	3:C:106:GLY:N	2.31	0.50
1:I:95:MET:SD	1:I:484:TYR:HB2	2.52	0.50
1:I:129:LEU:HD11	1:I:193:LEU:HD12	1.93	0.50
5:M:18:LEU:HB2	5:M:82:LEU:HB2	1.92	0.50
6:R:37:GLN:NE2	6:R:81:GLY:O	2.44	0.50
2:J:624:ASN:HB3	14:J:703:NAG:H82	1.94	0.49
3:K:51:ILE:HG12	3:K:57:SER:HB3	1.92	0.49
5:O:12:VAL:HG11	5:O:18:LEU:HD12	1.93	0.49
5:O:36:TRP:CG	5:O:80:LEU:HD13	2.47	0.49
1:I:270:ILE:HD12	1:I:344:ARG:HB3	1.94	0.49
3:K:67:VAL:O	7:i:9:MAN:O4	2.23	0.49
1:A:111:LEU:HD11	2:B:571:TRP:CZ2	2.47	0.49
6:N:38:HIS:HA	6:N:44:PRO:HB3	1.94	0.49
3:K:40:ALA:HB3	3:K:43:GLN:HB3	1.94	0.49
5:O:84:PRO:HB3	5:O:111:VAL:HG21	1.93	0.49
5:Q:100(E):VAL:HG22	9:m:2:NAG:H81	1.94	0.49
1:A:258:GLN:OE1	1:A:387:THR:OG1	2.23	0.49
2:F:620:GLU:O	2:F:624:ASN:HB2	2.12	0.49
5:Q:100(D):VAL:HA	9:m:2:NAG:H83	1.93	0.49
1:E:258:GLN:OE1	1:E:387:THR:HG21	2.13	0.49
1:E:323:ILE:O	1:E:323:ILE:HG13	2.12	0.49
2:F:611:ASN:OD1	2:F:612:SER:N	2.46	0.49
5:O:67:VAL:HG22	5:O:82:LEU:HG	1.95	0.49
5:Q:47:TRP:HB2	6:R:98:PHE:HE1	1.78	0.49
5:Q:100:ARG:HD2	9:m:4:NAG:H83	1.93	0.49
1:I:51:THR:HA	1:I:103:GLN:HE22	1.77	0.49
5:O:31:ASN:OD1	5:O:32:TYR:N	2.44	0.49
1:E:71:THR:CB	1:E:213:ILE:HD11	2.42	0.48
1:E:301:ASN:HB3	14:E:604:NAG:O5	2.13	0.48
1:I:350:LYS:NZ	1:I:356:LYS:O	2.46	0.48
6:P:46:LEU:HD11	6:P:55:PRO:HG3	1.94	0.48
6:P:59:PRO:HD2	6:P:62:PHE:HE2	1.78	0.48
1:A:35:TRP:CZ2	1:A:502:LYS:HG3	2.49	0.48
1:A:192:ARG:NH2	14:A:1009:NAG:C8	2.76	0.48
1:E:67:ASN:ND2	1:E:211:ASP:O	2.36	0.48
6:N:39:ARG:HE	6:N:40:PRO:HD2	1.78	0.48
5:Q:38:ARG:NH1	5:Q:46:GLU:OE1	2.46	0.48
1:E:373:MET:SD	14:E:609:NAG:H83	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:47:TRP:HZ2	5:M:50:TYR:HD2	1.62	0.48
5:Q:55:GLU:OE2	5:Q:71:ARG:NH2	2.47	0.48
5:M:11:LEU:HB3	5:M:112:SER:HB3	1.95	0.48
1:A:101:VAL:HG11	1:A:480:ARG:NH1	2.29	0.48
3:G:72:VAL:HG22	11:Y:5:MAN:H61	1.94	0.48
1:I:121:LYS:HE3	1:I:200:VAL:HG11	1.95	0.48
4:L:22:SER:HB2	4:L:72:THR:HG22	1.95	0.48
1:A:370:GLU:HG3	1:A:384:TYR:CE2	2.48	0.48
1:I:131:CYS:HA	1:I:157:CYS:HA	1.95	0.48
1:I:496:ILE:O	2:J:631:TRP:NE1	2.38	0.48
3:K:22:CYS:N	3:K:78:SER:O	2.41	0.48
1:E:56:SER:C	1:E:77:THR:HG23	2.38	0.48
2:J:593:LEU:HG	2:J:598:CYS:O	2.14	0.48
3:K:22:CYS:HB3	3:K:78:SER:HB3	1.95	0.48
1:A:83:GLU:HG2	1:A:245:VAL:HG12	1.95	0.47
1:A:496:ILE:HG21	2:B:642:ILE:HG21	1.95	0.47
2:B:618:THR:O	2:B:622:ILE:HG13	2.13	0.47
6:P:12:SER:HB2	6:P:105:THR:H	1.78	0.47
1:A:36:VAL:HG11	2:B:646:LEU:HD11	1.96	0.47
4:D:31:ASN:ND2	8:X:1:NAG:H82	2.28	0.47
1:I:503:ARG:NH1	1:I:504:ARG:NE	2.62	0.47
3:K:95:THR:HG21	3:K:100(K):ALA:O	2.14	0.47
4:D:29:ILE:HB	4:D:71:PHE:HZ	1.80	0.47
3:G:38:ARG:HB3	3:G:48:ILE:HD11	1.96	0.47
1:I:91:GLU:HB3	1:I:242:VAL:HG21	1.96	0.47
1:I:503:ARG:O	2:J:607:ALA:HB2	2.14	0.47
4:L:45:ARG:HH22	4:L:59:PRO:HD3	1.78	0.47
6:P:75:ILE:HG13	6:P:104:LEU:HD22	1.96	0.47
1:A:259:LEU:HD21	1:A:391:PHE:HZ	1.78	0.47
1:A:480:ARG:O	1:A:484:TYR:HB3	2.14	0.47
3:C:30:PHE:HB2	3:C:55:TRP:CH2	2.49	0.47
3:C:38:ARG:HB3	3:C:48:ILE:HD11	1.96	0.47
1:E:160:ASN:HA	1:E:171:LYS:HA	1.96	0.47
1:I:86:LEU:HD21	2:J:523:LEU:HD12	1.96	0.47
6:P:79:GLU:H	6:P:82:ASP:HB3	1.79	0.47
1:E:391:PHE:CD2	1:E:470:PRO:HG3	2.50	0.47
1:I:152:ASP:HB3	1:I:419:ARG:HE	1.79	0.47
1:E:73:ALA:HB3	2:F:571:TRP:HD1	1.79	0.47
1:I:129:LEU:HD11	1:I:193:LEU:CD1	2.45	0.47
5:Q:12:VAL:O	5:Q:112:SER:N	2.48	0.47
5:Q:58:THR:HG22	6:R:96:TRP:HH2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:HB2	1:A:191:TYR:CD1	2.50	0.47
1:A:503:ARG:HB3	2:J:661:LEU:HD13	1.97	0.47
1:E:385:CYS:HA	1:E:418:CYS:HA	1.96	0.47
3:G:100(K):ALA:HB2	4:H:91:TYR:CE1	2.49	0.47
2:J:641:GLN:O	2:J:645:ILE:HG12	2.14	0.47
6:N:37:GLN:HB2	6:N:47:LEU:HD21	1.97	0.47
5:O:13:LYS:HB2	5:O:16:GLU:HG3	1.96	0.47
5:O:15:SER:HA	5:O:82(B):SER:HA	1.97	0.47
1:E:45:TRP:CD1	1:E:489:VAL:HG21	2.50	0.47
1:I:86:LEU:HD21	2:J:523:LEU:CD1	2.45	0.47
5:O:22:CYS:SG	5:O:78:LEU:HB2	2.54	0.47
6:R:27:ALA:HB1	6:R:31:ARG:HG2	1.97	0.47
3:G:23:LYS:HG2	3:G:77(D):ILE:HG12	1.97	0.47
1:E:163:THR:HG22	1:E:164:GLU:N	2.30	0.46
1:I:180:ASP:OD2	1:I:421:LYS:HG3	2.15	0.46
2:B:641:GLN:O	2:B:645:ILE:HG12	2.16	0.46
4:D:31:ASN:HD22	8:X:1:NAG:H82	1.81	0.46
1:E:129:LEU:HD11	1:E:193:LEU:CD1	2.45	0.46
3:G:45:LEU:HD21	4:H:44:PRO:HG2	1.96	0.46
5:Q:29:MET:SD	5:Q:30:ASN:N	2.88	0.46
1:E:292:VAL:O	1:E:449:ILE:N	2.36	0.46
6:R:54:ARG:NH1	6:R:60:GLU:HA	2.29	0.46
9:m:1:NAG:H83	9:m:1:NAG:H3	1.97	0.46
1:A:333:ILE:HD13	1:A:390:LEU:HD21	1.98	0.46
1:E:165:LEU:HD12	1:E:168:LYS:HD2	1.97	0.46
1:E:291:SER:HB2	1:E:448:ASN:HB3	1.98	0.46
1:I:283:THR:HG21	1:I:473:GLY:H	1.80	0.46
5:Q:3:GLN:O	5:Q:25:SER:N	2.44	0.46
1:E:370:GLU:HG3	1:E:384:TYR:CE2	2.48	0.46
1:I:50:THR:HG21	1:I:223:TYR:CZ	2.50	0.46
5:M:50:TYR:O	5:M:58:THR:N	2.48	0.46
5:O:18:LEU:HD11	5:O:109:VAL:HG21	1.96	0.46
5:Q:34:TRP:CD1	5:Q:94:THR:HG22	2.50	0.46
1:A:91:GLU:HB3	1:A:242:VAL:HG21	1.97	0.46
1:A:158:SER:HB3	1:A:173:TYR:CE1	2.51	0.46
2:B:606:THR:HG22	2:B:608:VAL:H	1.81	0.46
2:J:611:ASN:OD1	2:J:612:SER:N	2.49	0.46
3:C:39:GLN:OE1	4:D:38:GLN:NE2	2.38	0.46
1:I:358:ILE:HD12	1:I:468:PHE:HE1	1.81	0.46
3:C:61:HIS:HA	3:C:64:ARG:HG3	1.98	0.46
1:E:193:LEU:HD23	1:E:423:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:8:PRO:O	4:L:102:THR:HG23	2.16	0.46
5:M:11:LEU:HD22	5:M:112:SER:HB3	1.98	0.46
5:M:37:ILE:HG13	5:M:103:TRP:CZ3	2.51	0.46
5:O:36:TRP:CE3	5:O:80:LEU:HD22	2.51	0.46
1:A:42:VAL:HG12	2:B:537:LEU:HD21	1.98	0.46
2:F:618:THR:HG23	2:F:621:GLU:H	1.80	0.46
5:M:35:THR:HG23	5:M:93:ALA:HB3	1.96	0.46
6:N:38:HIS:HB2	6:N:87:TYR:HE2	1.81	0.46
6:P:31:ARG:HH11	6:P:51:ASN:HD21	1.63	0.46
6:P:47:LEU:HD23	6:P:62:PHE:HB3	1.98	0.46
5:Q:38:ARG:HG2	5:Q:88:ALA:HB3	1.96	0.46
5:Q:87:THR:HG21	5:Q:111:VAL:HG13	1.98	0.46
1:E:161:MET:HE1	1:E:309:ILE:HG22	1.98	0.46
1:I:224:ALA:HB2	1:I:491:ILE:HD11	1.98	0.46
1:E:496:ILE:HG21	2:F:642:ILE:HG21	1.98	0.45
1:A:163:THR:HG23	1:A:165:LEU:H	1.79	0.45
4:H:7:SER:HB3	4:H:22:SER:HB3	1.98	0.45
1:I:77:THR:O	1:I:79:PRO:HD3	2.16	0.45
3:G:35:VAL:HA	3:G:93:THR:O	2.17	0.45
2:J:606:THR:HG21	2:J:646:LEU:HD22	1.98	0.45
1:A:61:HIS:CE1	1:A:70:ALA:HA	2.43	0.45
1:A:500:LYS:O	2:J:662:GLU:HG2	2.17	0.45
1:A:501:CYS:SG	2:J:661:LEU:CD1	3.04	0.45
1:E:50:THR:HG21	1:E:223:TYR:CZ	2.52	0.45
3:G:30:PHE:HB2	3:G:55:TRP:CH2	2.51	0.45
4:H:7:SER:HB3	4:H:8:PRO:HD3	1.98	0.45
1:A:62:GLU:O	1:A:63:THR:HG22	2.16	0.45
3:G:67:VAL:HG23	3:G:82:ILE:HD13	1.98	0.45
4:H:61:ARG:HD2	4:H:82:ASP:OD2	2.17	0.45
1:I:233:PHE:C	1:I:235:GLY:H	2.25	0.45
1:I:349:LEU:O	1:I:353:PHE:HB2	2.17	0.45
3:K:28:ASN:OD1	3:K:29:THR:N	2.48	0.45
1:E:111:LEU:HD11	2:F:571:TRP:CZ2	2.51	0.45
6:R:36:TYR:HA	6:R:46:LEU:HA	1.98	0.45
1:A:387:THR:HG22	1:A:390:LEU:HD12	1.98	0.45
1:E:354:ASN:OD1	3:G:77:SER:OG	2.30	0.45
2:F:576:LEU:HD23	2:J:576:LEU:HD21	1.98	0.45
3:G:35(A):ASN:O	3:G:93:THR:OG1	2.34	0.45
1:I:104:MET:HE1	1:I:251:ILE:HG22	1.98	0.45
1:I:434:MET:HE2	1:I:434:MET:HB3	1.80	0.45
5:M:34:TRP:CE3	5:M:78:LEU:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:HH22	14:A:1009:NAG:C7	2.29	0.45
3:C:39:GLN:NE2	4:D:38:GLN:OE1	2.43	0.45
1:I:108:VAL:O	1:I:112:TRP:HD1	1.99	0.45
6:N:61:ARG:CZ	6:N:76:SER:HB3	2.47	0.45
5:O:70:SER:HB2	5:O:81:LYS:NZ	2.32	0.45
5:O:100(A):ILE:HG13	9:b:3:NAG:H5	1.98	0.45
1:E:480:ARG:O	1:E:484:TYR:HB3	2.16	0.44
4:H:80:ALA:HA	4:H:83:PHE:HD1	1.82	0.44
1:I:385:CYS:HA	1:I:418:CYS:HA	1.99	0.44
3:K:36:TRP:CD1	3:K:69:ILE:HD12	2.52	0.44
1:I:392:ASN:HD21	14:I:609:NAG:H4	1.82	0.44
3:K:37:VAL:HG23	3:K:91:PHE:HB2	2.00	0.44
6:R:66(A):ASP:OD1	9:m:4:NAG:H61	2.17	0.44
1:I:42:VAL:HG12	2:J:537:LEU:HD21	1.99	0.44
5:O:29:MET:SD	5:O:73:THR:HA	2.57	0.44
1:A:291:SER:HB2	1:A:448:ASN:HB3	1.99	0.44
1:E:86:LEU:HD21	2:F:523:LEU:HD23	1.99	0.44
3:C:37:VAL:HG23	3:C:91:PHE:HB2	1.99	0.44
1:E:59:LYS:HB3	1:E:62:GLU:HA	1.98	0.44
1:E:210:PHE:CZ	1:E:434:MET:HE1	2.53	0.44
5:O:29:MET:HA	5:O:34:TRP:HZ2	1.82	0.44
6:P:14:ALA:HA	6:P:106:VAL:HG22	2.00	0.44
5:Q:35:THR:HG21	5:Q:100(P):MET:HE1	2.00	0.44
6:R:10:PRO:HA	6:R:103:ARG:HB2	2.00	0.44
6:R:27:ALA:HB2	6:R:31:ARG:HG2	2.00	0.44
6:R:34:GLN:HA	6:R:49:TYR:HA	2.00	0.44
1:A:182:VAL:HG11	14:A:1009:NAG:H81	1.99	0.44
3:C:36:TRP:CG	3:C:80:LEU:HD13	2.53	0.44
2:F:661:LEU:HD21	1:I:503:ARG:HG2	1.99	0.44
1:I:330:TYR:OH	9:m:1:NAG:C8	2.66	0.44
5:M:28:SER:HB3	5:M:31:ASN:HB3	1.99	0.44
1:A:298:ARG:NH2	1:A:441:GLY:O	2.51	0.43
1:E:50:THR:O	1:E:103:GLN:NE2	2.49	0.43
1:A:50:THR:HG21	1:A:223:TYR:CZ	2.53	0.43
1:A:265:LEU:H	1:A:265:LEU:HD23	1.83	0.43
1:E:161:MET:HB3	1:E:161:MET:HE2	1.65	0.43
3:G:100(I):VAL:HG12	4:H:91:TYR:HB2	1.98	0.43
1:A:54:CYS:SG	1:A:215:ILE:HG23	2.58	0.43
1:A:278:THR:HG23	3:C:74:LEU:HD22	2.00	0.43
1:E:112:TRP:CD1	1:E:427:TRP:HZ3	2.35	0.43
2:J:543:GLN:HG3	2:J:544:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:39:GLN:NE2	4:L:38:GLN:OE1	2.39	0.43
6:P:38:HIS:CE1	6:P:87:TYR:HB2	2.53	0.43
6:R:78:VAL:HG11	6:R:106:VAL:HG21	2.00	0.43
3:C:6:GLN:NE2	3:C:104:GLY:HA3	2.30	0.43
3:C:34:ALA:HB2	3:C:52:TRP:HD1	1.82	0.43
1:I:95:MET:CB	1:I:235:GLY:O	2.65	0.43
1:I:370:GLU:HG2	1:I:384:TYR:CE2	2.54	0.43
1:I:427:TRP:NE1	1:I:475:ILE:HG12	2.34	0.43
3:C:56:LYS:HE2	3:C:56:LYS:HB3	1.87	0.43
1:E:125:LEU:HD11	1:E:317:PHE:CE1	2.54	0.43
1:I:73:ALA:HB3	2:J:571:TRP:HD1	1.84	0.43
1:I:503:ARG:HD2	1:I:503:ARG:HA	1.71	0.43
6:N:37:GLN:NE2	6:N:81:GLY:O	2.52	0.43
6:R:39:ARG:HE	6:R:40:PRO:HD2	1.83	0.43
1:E:54:CYS:SG	1:E:215:ILE:HG23	2.59	0.43
1:E:231:LYS:HD3	1:E:268:GLU:OE1	2.18	0.43
1:I:69:TRP:HA	1:I:111:LEU:HD13	2.00	0.43
5:M:6:GLU:OE2	5:M:6:GLU:N	2.52	0.43
5:M:21:THR:CG2	5:M:77:GLN:HB3	2.49	0.43
5:M:95:ALA:HB1	5:M:100(N):TYR:HB3	2.01	0.43
5:O:43:LYS:HE2	5:O:43:LYS:HB3	1.86	0.43
3:K:35:VAL:HA	3:K:93:THR:O	2.17	0.43
6:N:53:ASP:OD1	6:N:53:ASP:N	2.51	0.43
6:P:36:TYR:HB2	6:P:38:HIS:HE1	1.84	0.43
1:E:326:ILE:HG13	1:E:326:ILE:O	2.19	0.43
1:E:491:ILE:O	2:F:585:ARG:NH2	2.50	0.43
5:M:12:VAL:HG11	5:M:18:LEU:HG	2.01	0.43
5:M:100(P):MET:HB2	6:N:36:TYR:CE1	2.54	0.43
5:O:27:ASP:HB2	5:O:31:ASN:HD21	1.83	0.43
1:E:154:VAL:HG21	1:E:175:LEU:HD23	2.01	0.42
2:F:617:LYS:HE2	2:F:626:MET:HE1	2.00	0.42
1:I:122:LEU:HB2	1:I:201:ILE:O	2.19	0.42
5:Q:23:SER:HA	5:Q:77:GLN:HA	2.01	0.42
6:R:35:TRP:CE2	6:R:73:LEU:HB2	2.54	0.42
1:A:501:CYS:SG	2:J:661:LEU:HD12	2.59	0.42
4:D:32:TRP:HB2	4:D:92:ASP:HB2	2.01	0.42
1:E:446:LEU:O	8:g:1:NAG:H5	2.19	0.42
1:I:160:ASN:HB3	1:I:169:GLN:NE2	2.34	0.42
1:I:504:ARG:HB2	2:J:653:GLN:HE22	1.83	0.42
6:P:50:ASN:HB3	6:P:53:ASP:HB2	2.01	0.42
9:m:3:NAG:O3	9:m:4:NAG:O5	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:SD	1:A:273:ARG:HD3	2.60	0.42
1:A:226:LEU:HD13	1:A:242:VAL:HG11	2.01	0.42
6:P:46:LEU:HD13	6:P:49:TYR:HB3	2.01	0.42
2:B:658:LYS:HG2	1:E:501:CYS:SG	2.60	0.42
1:I:131:CYS:HB2	1:I:191:TYR:CD1	2.55	0.42
3:K:25:TYR:CD2	13:j:2:NAG:H2	2.55	0.42
5:O:38:ARG:HH12	5:O:86:ASP:HB2	1.84	0.42
1:A:43:PRO:HG2	2:B:525:ALA:O	2.19	0.42
1:A:326:ILE:O	1:A:326:ILE:HG13	2.19	0.42
3:C:95:THR:HG21	3:C:100(K):ALA:O	2.19	0.42
1:E:59:LYS:HG3	1:E:63:THR:HG23	2.02	0.42
1:E:379:ARG:HD2	8:g:3:BMA:H5	2.00	0.42
6:R:35:TRP:CH2	6:R:88:CYS:HB2	2.55	0.42
1:E:95:MET:SD	1:E:235:GLY:HA3	2.60	0.42
1:E:298:ARG:HB2	1:E:383:PHE:HZ	1.84	0.42
1:I:36:VAL:HG13	1:I:496:ILE:HG23	2.02	0.42
1:I:83:GLU:OE2	1:I:227:ARG:NH1	2.52	0.42
1:I:111:LEU:HD11	2:J:571:TRP:CZ2	2.54	0.42
6:N:85:ASP:OD1	6:N:85:ASP:N	2.51	0.42
6:P:75:ILE:HD12	6:P:82:ASP:OD1	2.20	0.42
5:Q:37:ILE:HB	5:Q:91:TYR:HB2	2.01	0.42
1:A:107:ASP:OD2	2:B:574:LYS:NZ	2.46	0.42
4:H:4:MET:HE2	4:H:23:CYS:SG	2.59	0.42
1:I:117:LYS:HB3	1:I:117:LYS:HE3	1.70	0.42
5:O:38:ARG:O	5:O:46:GLU:HB3	2.19	0.42
6:P:37:GLN:HB3	6:P:47:LEU:HD11	2.00	0.42
6:P:86:TYR:N	6:P:102:THR:O	2.45	0.42
6:R:9:ARG:HA	6:R:10:PRO:HD3	1.92	0.42
2:F:577:GLN:OE1	2:J:579:ARG:NH2	2.53	0.42
3:K:82(C):LEU:HD21	3:K:111:VAL:HG21	2.01	0.42
5:M:29:MET:HE3	5:M:76:ASN:HA	2.01	0.42
1:A:104:MET:HE1	1:A:251:ILE:HG22	2.01	0.41
1:I:360:VAL:HG12	1:I:394:THR:OG1	2.20	0.41
1:A:195:ASN:HB2	1:A:423:ILE:HG21	2.02	0.41
1:E:53:PHE:CE2	1:E:218:CYS:HB2	2.55	0.41
6:P:12:SER:HA	6:P:104:LEU:HD12	2.01	0.41
3:G:38:ARG:HH22	3:G:86:ASP:HA	1.86	0.41
1:I:420:ILE:HD12	1:I:420:ILE:H	1.85	0.41
1:A:61:HIS:HB3	1:A:65:VAL:O	2.21	0.41
1:A:350:LYS:NZ	1:A:357:THR:HA	2.36	0.41
1:E:36:VAL:O	2:F:606:THR:OG1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:586:TYR:O	2:F:590:GLN:HG2	2.20	0.41
4:L:7:SER:O	4:L:9:SER:N	2.48	0.41
5:M:100:ARG:HH21	6:N:30:SER:HB2	1.85	0.41
1:E:101:VAL:HG11	1:E:480:ARG:NH1	2.36	0.41
1:E:275:GLU:O	1:E:275:GLU:HG3	2.21	0.41
1:E:290:GLU:OE2	1:E:344:ARG:CZ	2.69	0.41
3:G:100(F):HIS:NE2	4:H:91:TYR:O	2.51	0.41
5:O:36:TRP:HB3	5:O:48:ILE:HD11	2.02	0.41
6:P:85:ASP:HB3	6:P:101:ALA:HB1	2.02	0.41
6:R:13:VAL:HB	6:R:104:LEU:HG	2.02	0.41
6:P:15:LEU:HD12	6:P:106:VAL:HG11	2.02	0.41
1:A:130:ASN:HB3	1:A:158:SER:OG	2.19	0.41
1:A:153:ASP:HA	1:A:178:LYS:HD2	2.02	0.41
4:D:88:CYS:O	4:D:99:GLY:N	2.47	0.41
1:E:198:THR:O	1:I:314:GLY:CA	2.68	0.41
3:G:34:ALA:HB2	3:G:52:TRP:HD1	1.86	0.41
1:I:123:THR:HG23	1:I:124:PRO:HD3	2.03	0.41
3:K:30:PHE:HB2	3:K:55:TRP:CH2	2.55	0.41
6:N:78:VAL:HG21	6:N:106:VAL:HG21	2.03	0.41
5:O:34:TRP:CD2	5:O:78:LEU:HD11	2.56	0.41
5:O:83:THR:HG22	5:O:86:ASP:OD2	2.20	0.41
5:Q:34:TRP:O	5:Q:51:ILE:N	2.53	0.41
3:C:35(A):ASN:HB2	3:C:93:THR:OG1	2.21	0.41
1:E:175:LEU:HD13	1:E:321:GLY:O	2.21	0.41
4:H:49:TYR:O	4:H:53:ALA:HB3	2.21	0.41
1:I:54:CYS:HA	1:I:216:HIS:O	2.21	0.41
6:N:39:ARG:NH2	6:N:84:ALA:HB2	2.36	0.41
5:Q:70:SER:HB2	5:Q:81:LYS:NZ	2.36	0.41
1:A:283:THR:HG21	1:A:473:GLY:CA	2.50	0.40
1:E:62:GLU:O	1:E:65:VAL:HG12	2.21	0.40
1:E:437:PRO:HA	1:E:438:PRO:HD3	1.96	0.40
6:N:31:ARG:NH2	6:N:69:THR:HG23	2.36	0.40
2:F:638:TYR:O	2:F:642:ILE:HG13	2.22	0.40
3:G:37:VAL:O	3:G:91:PHE:N	2.43	0.40
4:H:55:LEU:HD23	4:H:56:GLY:O	2.21	0.40
1:E:122:LEU:HD23	1:E:125:LEU:HD12	2.03	0.40
1:E:362:LYS:HB3	1:E:469:ARG:NH1	2.37	0.40
3:G:36:TRP:CD1	3:G:69:ILE:HD12	2.56	0.40
1:I:274:SER:HB3	1:I:277:LEU:HD23	2.03	0.40
1:I:346:ALA:O	1:I:350:LYS:HG3	2.20	0.40
3:K:4:LEU:HD12	3:K:22:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:65:THR:OG1	6:N:71:ALA:HA	2.21	0.40
5:Q:17:THR:HA	5:Q:82:LEU:O	2.22	0.40
5:Q:39:GLN:HB2	5:Q:45:LEU:HD12	2.04	0.40
1:E:60:ALA:O	1:E:61:HIS:C	2.64	0.40
1:I:59:LYS:HD2	1:I:59:LYS:HA	1.89	0.40
2:J:620:GLU:HB2	2:J:624:ASN:ND2	2.37	0.40
3:K:100(I):VAL:HG12	4:L:91:TYR:HB2	2.04	0.40
5:M:69:ILE:HB	5:M:80:LEU:HD23	2.02	0.40
5:O:86:ASP:OD1	5:O:87:THR:N	2.55	0.40
5:Q:36:TRP:CG	5:Q:80:LEU:HD13	2.56	0.40
5:Q:83:THR:HG23	5:Q:86:ASP:H	1.86	0.40
1:A:42:VAL:HA	1:A:43:PRO:HD3	1.94	0.40
1:A:385:CYS:HA	1:A:418:CYS:HA	2.03	0.40
2:B:616:ASN:HD22	4:D:28:SER:HB3	1.87	0.40
3:C:23:LYS:HB3	3:C:23:LYS:HE2	1.86	0.40
1:E:260:LEU:HD13	1:E:481:ASN:HD22	1.87	0.40
3:K:45:LEU:HD21	4:L:44:PRO:HG2	2.03	0.40
5:M:2:VAL:HG22	5:M:27:ASP:HB2	2.03	0.40
5:Q:100(B):TYR:CD2	5:Q:100(B):TYR:N	2.90	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	427/486 (88%)	402 (94%)	24 (6%)	1 (0%)	43	73
1	E	425/486 (87%)	406 (96%)	19 (4%)	0	100	100
1	I	424/486 (87%)	402 (95%)	21 (5%)	1 (0%)	43	73
2	B	117/155 (76%)	112 (96%)	5 (4%)	0	100	100
2	F	113/155 (73%)	109 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	116/155 (75%)	111 (96%)	5 (4%)	0	100	100
3	C	128/238 (54%)	124 (97%)	4 (3%)	0	100	100
3	G	128/238 (54%)	125 (98%)	3 (2%)	0	100	100
3	K	128/238 (54%)	124 (97%)	4 (3%)	0	100	100
4	D	105/215 (49%)	101 (96%)	4 (4%)	0	100	100
4	H	106/215 (49%)	102 (96%)	3 (3%)	1 (1%)	14	47
4	L	106/215 (49%)	101 (95%)	3 (3%)	2 (2%)	6	33
5	M	129/238 (54%)	129 (100%)	0	0	100	100
5	O	129/238 (54%)	129 (100%)	0	0	100	100
5	Q	129/238 (54%)	124 (96%)	5 (4%)	0	100	100
6	N	105/214 (49%)	104 (99%)	1 (1%)	0	100	100
6	P	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
6	R	105/214 (49%)	101 (96%)	4 (4%)	0	100	100
All	All	3025/4638 (65%)	2906 (96%)	114 (4%)	5 (0%)	44	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	9	SER
4	L	9	SER
1	I	234	ASN
4	L	7	SER
1	A	78	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/434 (90%)	385 (99%)	5 (1%)	61	78
1	E	388/434 (89%)	383 (99%)	5 (1%)	61	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	388/434 (89%)	383 (99%)	5 (1%)	61	78
2	B	105/130 (81%)	105 (100%)	0	100	100
2	F	101/130 (78%)	101 (100%)	0	100	100
2	J	105/130 (81%)	105 (100%)	0	100	100
3	C	111/204 (54%)	111 (100%)	0	100	100
3	G	111/204 (54%)	111 (100%)	0	100	100
3	K	111/204 (54%)	110 (99%)	1 (1%)	70	81
4	D	85/182 (47%)	85 (100%)	0	100	100
4	H	86/182 (47%)	86 (100%)	0	100	100
4	L	86/182 (47%)	86 (100%)	0	100	100
5	M	115/208 (55%)	115 (100%)	0	100	100
5	O	115/208 (55%)	115 (100%)	0	100	100
5	Q	115/208 (55%)	115 (100%)	0	100	100
6	N	85/178 (48%)	85 (100%)	0	100	100
6	P	85/178 (48%)	85 (100%)	0	100	100
6	R	85/178 (48%)	84 (99%)	1 (1%)	63	79
All	All	2667/4008 (66%)	2650 (99%)	17 (1%)	76	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	PRO
1	A	126	CYS
1	A	196	CYS
1	A	393	SER
1	A	496	ILE
1	E	67	ASN
1	E	155	ARG
1	E	333	ILE
1	E	387	THR
1	E	393	SER
1	I	196	CYS
1	I	393	SER
1	I	502	LYS
1	I	503	ARG
1	I	504	ARG

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Mol	Chain	Res	Type
3	K	73	ASP
6	R	31	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	354	ASN
1	A	432	GLN
1	A	464	ASN
2	B	540	GLN
2	B	588	GLN
4	D	6	GLN
4	D	31	ASN
1	E	82	GLN
1	E	280	ASN
1	E	302	ASN
1	E	464	ASN
1	E	481	ASN
1	E	490	GLN
1	I	114	GLN
2	J	540	GLN
2	J	543	GLN
2	J	624	ASN
3	K	3	HIS
4	L	31	ASN
6	N	50	ASN
5	O	1	GLN
6	P	37	GLN
6	P	38	HIS
6	P	51	ASN
5	Q	1	GLN
5	Q	3	GLN
6	R	37	GLN
6	R	51	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 ⓘ

80 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	S	1	7,1	14,14,15	0.44	0	17,19,21	0.82	1 (5%)
7	NAG	S	2	7	14,14,15	0.26	0	17,19,21	0.45	0
7	BMA	S	3	7	11,11,12	0.60	0	15,15,17	0.83	0
7	MAN	S	4	7	11,11,12	0.59	0	15,15,17	0.94	2 (13%)
7	MAN	S	5	7	11,11,12	0.60	0	15,15,17	1.00	2 (13%)
7	MAN	S	6	7	11,11,12	0.54	0	15,15,17	1.03	2 (13%)
7	MAN	S	7	7	11,11,12	0.59	0	15,15,17	1.10	2 (13%)
7	MAN	S	8	7	11,11,12	0.57	0	15,15,17	1.06	2 (13%)
7	MAN	S	9	7	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
8	NAG	T	1	8,1	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
8	NAG	T	2	8	14,14,15	0.42	0	17,19,21	0.75	0
8	BMA	T	3	8	11,11,12	0.35	0	15,15,17	0.98	1 (6%)
9	NAG	U	1	9,1	14,14,15	0.35	0	17,19,21	0.52	0
9	NAG	U	2	9	14,14,15	0.26	0	17,19,21	0.44	0
9	NAG	U	3	9	14,14,15	0.60	0	17,19,21	0.58	0
9	NAG	U	4	9	14,14,15	0.95	1 (7%)	17,19,21	1.27	1 (5%)
10	NAG	V	1	10,1	14,14,15	0.50	0	17,19,21	1.06	2 (11%)
10	NAG	V	2	10	14,14,15	0.36	0	17,19,21	1.03	1 (5%)
8	NAG	W	1	8,1	14,14,15	0.24	0	17,19,21	0.55	0
8	NAG	W	2	8	14,14,15	0.21	0	17,19,21	0.39	0
8	BMA	W	3	8	11,11,12	0.52	0	15,15,17	0.63	0
8	NAG	X	1	8,2	14,14,15	0.21	0	17,19,21	0.74	1 (5%)
8	NAG	X	2	8	14,14,15	0.25	0	17,19,21	0.44	0
8	BMA	X	3	8	11,11,12	0.54	0	15,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	Y	1	1,11	14,14,15	0.14	0	17,19,21	0.55	0
11	MAN	Y	10	11	11,11,12	0.59	0	15,15,17	0.96	2 (13%)
11	NAG	Y	2	11	14,14,15	0.33	0	17,19,21	0.49	0
11	BMA	Y	3	11	11,11,12	0.55	0	15,15,17	0.78	0
11	MAN	Y	4	11	11,11,12	0.54	0	15,15,17	0.97	2 (13%)
11	MAN	Y	5	11	11,11,12	0.59	0	15,15,17	1.05	2 (13%)
11	MAN	Y	6	11	11,11,12	0.51	0	15,15,17	1.02	2 (13%)
11	MAN	Y	7	11	11,11,12	0.56	0	15,15,17	1.13	2 (13%)
11	MAN	Y	8	11	11,11,12	0.57	0	15,15,17	1.03	2 (13%)
11	MAN	Y	9	11	11,11,12	0.54	0	15,15,17	0.96	2 (13%)
12	NAG	Z	1	12,1	14,14,15	0.28	0	17,19,21	0.42	0
12	NAG	Z	2	12	14,14,15	0.20	0	17,19,21	0.47	0
12	BMA	Z	3	12	11,11,12	0.44	0	15,15,17	0.74	0
12	MAN	Z	4	12	11,11,12	0.77	0	15,15,17	1.19	2 (13%)
12	MAN	Z	5	12	11,11,12	0.77	0	15,15,17	1.31	2 (13%)
12	MAN	Z	6	12	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
9	NAG	b	1	9,1	14,14,15	0.34	0	17,19,21	0.46	0
9	NAG	b	2	9	14,14,15	0.34	0	17,19,21	0.61	0
9	NAG	b	3	9	14,14,15	0.98	1 (7%)	17,19,21	1.44	1 (5%)
9	NAG	b	4	9	14,14,15	0.33	0	17,19,21	0.61	0
8	NAG	g	1	8,1	14,14,15	0.25	0	17,19,21	0.55	0
8	NAG	g	2	8	14,14,15	0.22	0	17,19,21	0.39	0
8	BMA	g	3	8	11,11,12	0.53	0	15,15,17	0.64	0
8	NAG	h	1	8,2	14,14,15	0.23	0	17,19,21	0.64	1 (5%)
8	NAG	h	2	8	14,14,15	0.28	0	17,19,21	0.43	0
8	BMA	h	3	8	11,11,12	0.55	0	15,15,17	0.71	0
7	NAG	i	1	7,1	14,14,15	0.17	0	17,19,21	0.62	1 (5%)
7	NAG	i	2	7	14,14,15	0.35	0	17,19,21	0.50	0
7	BMA	i	3	7	11,11,12	0.56	0	15,15,17	0.78	0
7	MAN	i	4	7	11,11,12	0.52	0	15,15,17	0.95	2 (13%)
7	MAN	i	5	7	11,11,12	0.60	0	15,15,17	1.11	2 (13%)
7	MAN	i	6	7	11,11,12	0.54	0	15,15,17	0.93	2 (13%)
7	MAN	i	7	7	11,11,12	0.60	0	15,15,17	1.07	2 (13%)
7	MAN	i	8	7	11,11,12	0.60	0	15,15,17	1.03	2 (13%)
7	MAN	i	9	7	11,11,12	0.54	0	15,15,17	0.98	2 (13%)
13	NAG	j	1	13,1	14,14,15	0.39	0	17,19,21	0.45	0
13	NAG	j	2	13	14,14,15	0.19	0	17,19,21	0.49	0
13	BMA	j	3	13	11,11,12	0.46	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	j	4	13	11,11,12	0.72	0	15,15,17	1.08	2 (13%)
13	MAN	j	5	13	11,11,12	0.67	0	15,15,17	0.86	1 (6%)
10	NAG	l	1	10,1	14,14,15	0.27	0	17,19,21	0.44	0
10	NAG	l	2	10	14,14,15	0.21	0	17,19,21	0.46	0
9	NAG	m	1	9,1	14,14,15	0.55	0	17,19,21	1.56	2 (11%)
9	NAG	m	2	9	14,14,15	0.38	0	17,19,21	0.48	0
9	NAG	m	3	9	14,14,15	0.20	0	17,19,21	0.68	1 (5%)
9	NAG	m	4	9	14,14,15	0.33	0	17,19,21	0.48	0
10	NAG	p	1	10,1	14,14,15	0.24	0	17,19,21	0.45	0
10	NAG	p	2	10	14,14,15	0.24	0	17,19,21	0.42	0
10	NAG	q	1	10,1	14,14,15	0.23	0	17,19,21	0.49	0
10	NAG	q	2	10	14,14,15	0.27	0	17,19,21	0.42	0
8	NAG	r	1	8,1	14,14,15	0.26	0	17,19,21	0.53	0
8	NAG	r	2	8	14,14,15	0.22	0	17,19,21	0.39	0
8	BMA	r	3	8	11,11,12	0.53	0	15,15,17	0.65	0
8	NAG	s	1	8,2	14,14,15	0.25	0	17,19,21	0.66	1 (5%)
8	NAG	s	2	8	14,14,15	0.29	0	17,19,21	0.43	0
8	BMA	s	3	8	11,11,12	0.57	0	15,15,17	0.71	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	S	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
7	MAN	S	4	7	-	0/2/19/22	0/1/1/1
7	MAN	S	5	7	-	2/2/19/22	0/1/1/1
7	MAN	S	6	7	-	0/2/19/22	0/1/1/1
7	MAN	S	7	7	-	0/2/19/22	0/1/1/1
7	MAN	S	8	7	-	0/2/19/22	0/1/1/1
7	MAN	S	9	7	-	0/2/19/22	0/1/1/1
8	NAG	T	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	4/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	U	2	9	-	0/6/23/26	0/1/1/1
9	NAG	U	3	9	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	U	4	9	-	1/6/23/26	0/1/1/1
10	NAG	V	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	V	2	10	-	0/6/23/26	0/1/1/1
8	NAG	W	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
8	BMA	W	3	8	-	0/2/19/22	0/1/1/1
8	NAG	X	1	8,2	-	1/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	1/2/19/22	0/1/1/1
11	NAG	Y	1	1,11	-	1/6/23/26	0/1/1/1
11	MAN	Y	10	11	-	2/2/19/22	0/1/1/1
11	NAG	Y	2	11	-	0/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	5	11	-	2/2/19/22	0/1/1/1
11	MAN	Y	6	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	7	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	8	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	9	11	-	0/2/19/22	0/1/1/1
12	NAG	Z	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	Z	2	12	-	2/6/23/26	0/1/1/1
12	BMA	Z	3	12	-	2/2/19/22	0/1/1/1
12	MAN	Z	4	12	-	0/2/19/22	0/1/1/1
12	MAN	Z	5	12	-	0/2/19/22	0/1/1/1
12	MAN	Z	6	12	-	0/2/19/22	0/1/1/1
9	NAG	b	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	b	2	9	-	2/6/23/26	0/1/1/1
9	NAG	b	3	9	-	2/6/23/26	0/1/1/1
9	NAG	b	4	9	-	4/6/23/26	0/1/1/1
8	NAG	g	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	g	2	8	-	2/6/23/26	0/1/1/1
8	BMA	g	3	8	-	0/2/19/22	0/1/1/1
8	NAG	h	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	h	2	8	-	0/6/23/26	0/1/1/1
8	BMA	h	3	8	-	1/2/19/22	0/1/1/1
7	NAG	i	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	i	2	7	-	0/6/23/26	0/1/1/1
7	BMA	i	3	7	-	0/2/19/22	0/1/1/1
7	MAN	i	4	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	i	5	7	-	2/2/19/22	0/1/1/1
7	MAN	i	6	7	-	1/2/19/22	0/1/1/1
7	MAN	i	7	7	-	0/2/19/22	0/1/1/1
7	MAN	i	8	7	-	0/2/19/22	0/1/1/1
7	MAN	i	9	7	-	0/2/19/22	0/1/1/1
13	NAG	j	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	j	2	13	-	2/6/23/26	0/1/1/1
13	BMA	j	3	13	-	0/2/19/22	0/1/1/1
13	MAN	j	4	13	-	0/2/19/22	0/1/1/1
13	MAN	j	5	13	-	0/2/19/22	0/1/1/1
10	NAG	l	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	l	2	10	-	0/6/23/26	0/1/1/1
9	NAG	m	1	9,1	-	6/6/23/26	0/1/1/1
9	NAG	m	2	9	-	4/6/23/26	0/1/1/1
9	NAG	m	3	9	-	2/6/23/26	0/1/1/1
9	NAG	m	4	9	-	4/6/23/26	0/1/1/1
10	NAG	p	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	p	2	10	-	2/6/23/26	0/1/1/1
10	NAG	q	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	q	2	10	-	0/6/23/26	0/1/1/1
8	NAG	r	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	r	2	8	-	2/6/23/26	0/1/1/1
8	BMA	r	3	8	-	0/2/19/22	0/1/1/1
8	NAG	s	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	s	2	8	-	0/6/23/26	0/1/1/1
8	BMA	s	3	8	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	3	NAG	O5-C1	3.53	1.49	1.43
9	U	4	NAG	O5-C1	3.35	1.49	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	3	NAG	C1-O5-C5	5.60	119.69	112.19
9	U	4	NAG	C1-O5-C5	4.97	118.85	112.19
9	m	1	NAG	C2-N2-C7	4.89	129.46	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	5	MAN	C1-O5-C5	3.54	116.93	112.19
12	Z	4	MAN	C1-O5-C5	3.03	116.25	112.19
11	Y	7	MAN	C1-O5-C5	2.97	116.17	112.19
7	S	7	MAN	C1-O5-C5	2.93	116.11	112.19
11	Y	6	MAN	C1-O5-C5	2.83	115.98	112.19
7	S	6	MAN	C1-O5-C5	2.81	115.95	112.19
13	j	4	MAN	C1-O5-C5	2.78	115.91	112.19
7	S	1	NAG	C1-O5-C5	2.78	115.91	112.19
7	i	5	MAN	C1-O5-C5	2.77	115.89	112.19
9	m	1	NAG	C1-C2-N2	2.75	114.77	110.43
7	S	8	MAN	C1-O5-C5	2.75	115.87	112.19
7	i	7	MAN	C1-O5-C5	2.69	115.79	112.19
11	Y	5	MAN	C1-O5-C5	2.63	115.72	112.19
11	Y	8	MAN	C1-O5-C5	2.63	115.71	112.19
8	X	1	NAG	C1-O5-C5	2.62	115.70	112.19
7	i	8	MAN	C1-O5-C5	2.56	115.62	112.19
12	Z	6	MAN	C1-O5-C5	2.52	115.56	112.19
7	S	8	MAN	O2-C2-C3	-2.52	104.94	110.15
7	i	8	MAN	O2-C2-C3	-2.50	104.96	110.15
7	S	5	MAN	C1-O5-C5	2.48	115.51	112.19
11	Y	8	MAN	O2-C2-C3	-2.43	105.11	110.15
11	Y	4	MAN	C1-O5-C5	2.39	115.39	112.19
10	V	2	NAG	C2-N2-C7	-2.39	119.69	122.90
11	Y	9	MAN	C1-O5-C5	2.39	115.39	112.19
7	i	4	MAN	C1-O5-C5	2.38	115.38	112.19
7	i	7	MAN	O2-C2-C3	-2.32	105.34	110.15
7	i	9	MAN	C1-O5-C5	2.32	115.30	112.19
7	S	4	MAN	O2-C2-C3	-2.31	105.36	110.15
7	i	6	MAN	C1-O5-C5	2.31	115.28	112.19
9	m	3	NAG	C1-O5-C5	2.30	115.27	112.19
7	S	7	MAN	O2-C2-C3	-2.29	105.40	110.15
11	Y	6	MAN	O2-C2-C3	-2.28	105.42	110.15
11	Y	7	MAN	O2-C2-C3	-2.28	105.42	110.15
8	s	1	NAG	C1-O5-C5	2.27	115.22	112.19
11	Y	9	MAN	O2-C2-C3	-2.26	105.48	110.15
7	i	4	MAN	O2-C2-C3	-2.25	105.50	110.15
11	Y	10	MAN	C1-O5-C5	2.24	115.19	112.19
7	i	9	MAN	O2-C2-C3	-2.24	105.51	110.15
12	Z	6	MAN	O2-C2-C3	-2.23	105.53	110.15
12	Z	5	MAN	O2-C2-C3	-2.22	105.55	110.15
7	S	6	MAN	O2-C2-C3	-2.20	105.59	110.15
7	S	9	MAN	O2-C2-C3	-2.20	105.59	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	MAN	O2-C2-C3	-2.20	105.60	110.15
7	S	9	MAN	C1-O5-C5	2.19	115.12	112.19
13	j	5	MAN	O2-C2-C3	-2.17	105.65	110.15
12	Z	4	MAN	O2-C2-C3	-2.17	105.65	110.15
10	V	1	NAG	C2-N2-C7	2.17	125.81	122.90
7	S	4	MAN	C1-O5-C5	2.17	115.09	112.19
11	Y	5	MAN	O2-C2-C3	-2.17	105.66	110.15
7	i	6	MAN	O2-C2-C3	-2.16	105.67	110.15
7	i	5	MAN	O2-C2-C3	-2.16	105.69	110.15
8	h	1	NAG	C1-O5-C5	2.15	115.07	112.19
8	T	3	BMA	O6-C6-C5	-2.15	104.00	111.33
7	S	5	MAN	O2-C2-C3	-2.15	105.70	110.15
11	Y	10	MAN	O2-C2-C3	-2.15	105.71	110.15
10	V	1	NAG	O5-C1-C2	-2.14	107.98	111.29
7	i	1	NAG	C1-O5-C5	2.06	114.94	112.19
13	j	4	MAN	O2-C2-C3	-2.04	105.93	110.15
8	T	1	NAG	O3-C3-C2	-2.03	105.17	109.40

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	V	1	NAG	C3-C2-N2-C7
10	V	1	NAG	C8-C7-N2-C2
10	V	1	NAG	O7-C7-N2-C2
8	W	1	NAG	O5-C5-C6-O6
11	Y	5	MAN	C4-C5-C6-O6
8	r	1	NAG	O5-C5-C6-O6
13	j	2	NAG	O5-C5-C6-O6
10	q	1	NAG	O5-C5-C6-O6
8	g	2	NAG	O5-C5-C6-O6
9	b	4	NAG	O5-C5-C6-O6
7	i	5	MAN	C4-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
8	W	2	NAG	O5-C5-C6-O6
8	r	2	NAG	O5-C5-C6-O6
9	U	3	NAG	O5-C5-C6-O6
8	r	1	NAG	C4-C5-C6-O6
10	p	1	NAG	O5-C5-C6-O6
7	S	5	MAN	C4-C5-C6-O6
11	Y	5	MAN	O5-C5-C6-O6
10	p	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	Z	2	NAG	O5-C5-C6-O6
10	q	1	NAG	C4-C5-C6-O6
9	m	4	NAG	O5-C5-C6-O6
9	b	3	NAG	O5-C5-C6-O6
8	T	1	NAG	C8-C7-N2-C2
8	T	1	NAG	O7-C7-N2-C2
10	p	2	NAG	O5-C5-C6-O6
8	W	1	NAG	C4-C5-C6-O6
13	j	2	NAG	C4-C5-C6-O6
7	i	5	MAN	O5-C5-C6-O6
12	Z	3	BMA	O5-C5-C6-O6
7	S	5	MAN	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
8	r	2	NAG	C4-C5-C6-O6
12	Z	2	NAG	C4-C5-C6-O6
8	g	2	NAG	C4-C5-C6-O6
8	W	2	NAG	C4-C5-C6-O6
9	b	4	NAG	C4-C5-C6-O6
9	m	3	NAG	O5-C5-C6-O6
9	U	3	NAG	C4-C5-C6-O6
10	p	1	NAG	C4-C5-C6-O6
12	Z	3	BMA	C4-C5-C6-O6
7	i	1	NAG	O5-C5-C6-O6
8	g	1	NAG	C4-C5-C6-O6
9	b	3	NAG	C4-C5-C6-O6
9	U	3	NAG	C8-C7-N2-C2
9	U	3	NAG	O7-C7-N2-C2
9	m	1	NAG	C8-C7-N2-C2
9	m	1	NAG	O7-C7-N2-C2
9	m	2	NAG	C8-C7-N2-C2
9	m	2	NAG	O7-C7-N2-C2
9	m	4	NAG	C8-C7-N2-C2
9	m	4	NAG	O7-C7-N2-C2
10	l	1	NAG	C8-C7-N2-C2
10	l	1	NAG	O7-C7-N2-C2
9	m	4	NAG	C4-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6
8	s	1	NAG	O5-C5-C6-O6
8	s	1	NAG	C4-C5-C6-O6
9	m	1	NAG	C4-C5-C6-O6
9	m	3	NAG	C4-C5-C6-O6
11	Y	10	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	i	1	NAG	C4-C5-C6-O6
8	h	1	NAG	C4-C5-C6-O6
8	X	3	BMA	O5-C5-C6-O6
8	h	1	NAG	O5-C5-C6-O6
8	h	3	BMA	O5-C5-C6-O6
9	m	1	NAG	O5-C5-C6-O6
8	X	1	NAG	O5-C5-C6-O6
9	U	4	NAG	C4-C5-C6-O6
8	s	3	BMA	O5-C5-C6-O6
9	b	2	NAG	C1-C2-N2-C7
9	m	1	NAG	C1-C2-N2-C7
8	T	2	NAG	C4-C5-C6-O6
11	Y	1	NAG	O5-C5-C6-O6
7	i	6	MAN	O5-C5-C6-O6
9	b	2	NAG	C3-C2-N2-C7
9	b	4	NAG	C3-C2-N2-C7
9	m	1	NAG	C3-C2-N2-C7
8	T	2	NAG	C8-C7-N2-C2
9	m	2	NAG	C4-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
11	Y	10	MAN	C4-C5-C6-O6
7	S	2	NAG	C1-C2-N2-C7
9	b	4	NAG	C1-C2-N2-C7
8	T	2	NAG	O7-C7-N2-C2
8	T	2	NAG	O5-C5-C6-O6
9	m	2	NAG	O5-C5-C6-O6

There are no ring outliers.

20 monomers are involved in 35 short contacts:

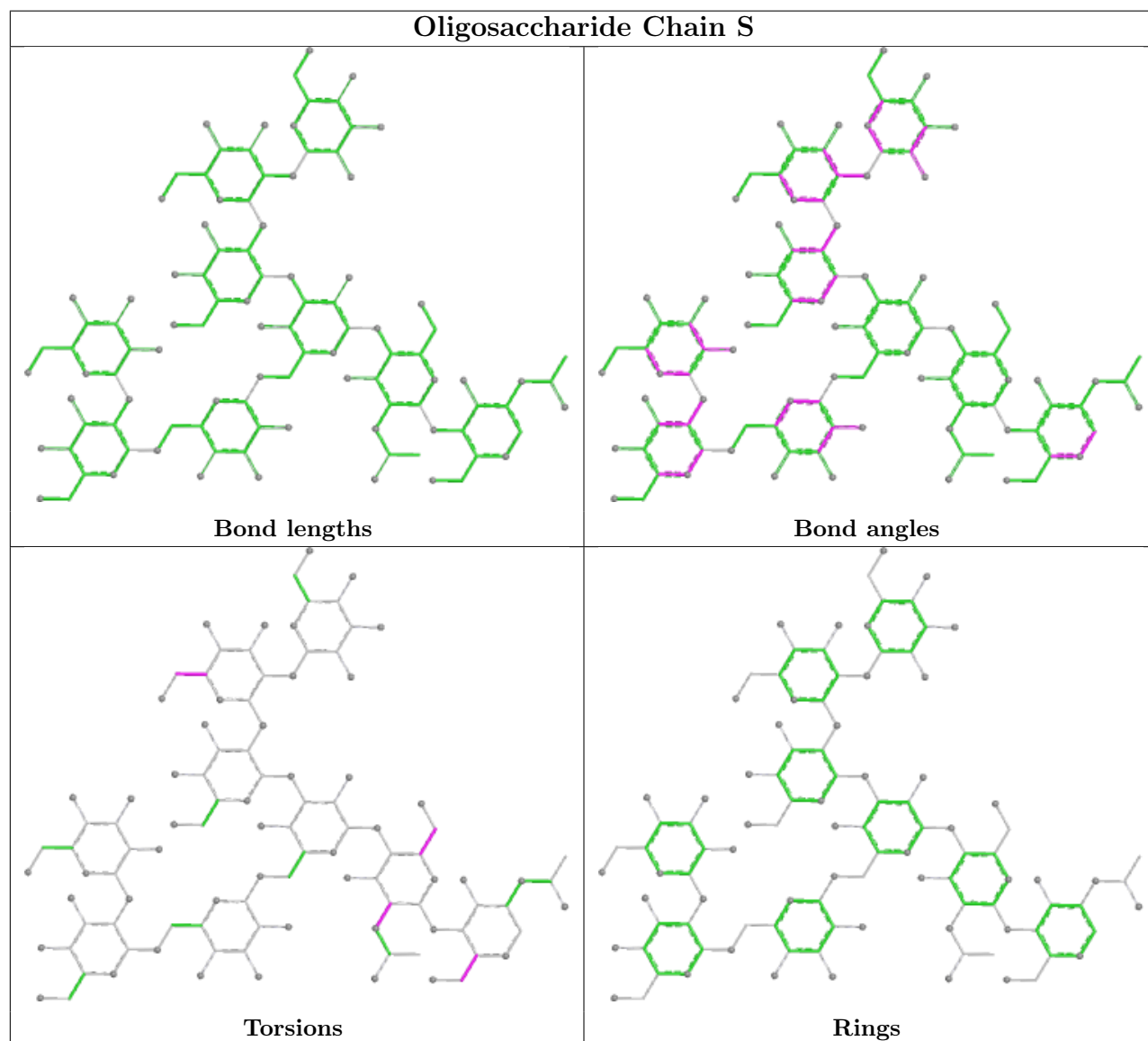
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	U	2	NAG	1	0
9	m	1	NAG	8	0
8	X	1	NAG	2	0
11	Y	5	MAN	1	0
8	s	1	NAG	1	0
8	g	3	BMA	1	0
9	U	3	NAG	1	0
9	m	3	NAG	1	0
9	b	3	NAG	2	0
9	b	2	NAG	1	0
9	U	4	NAG	1	0

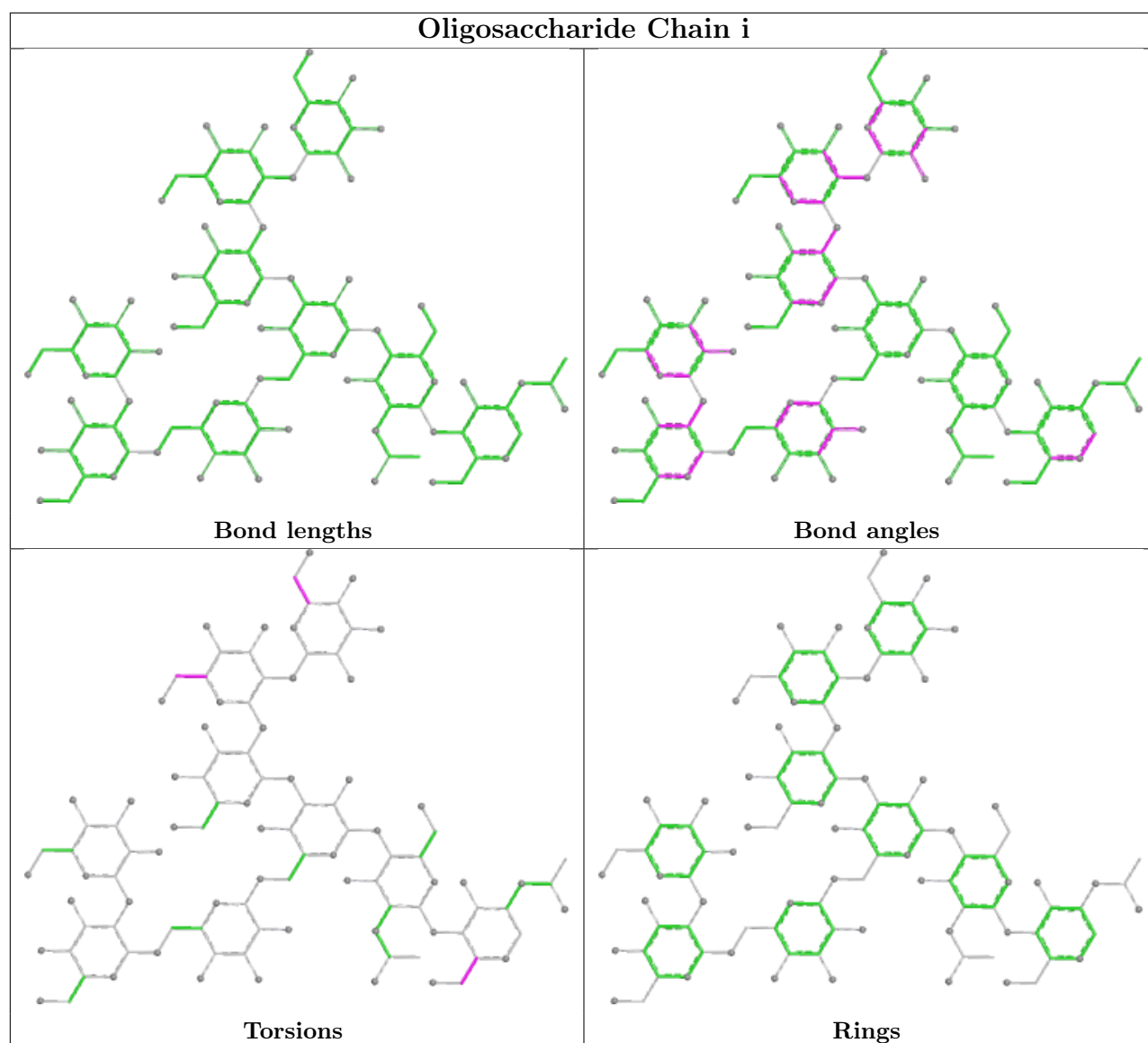
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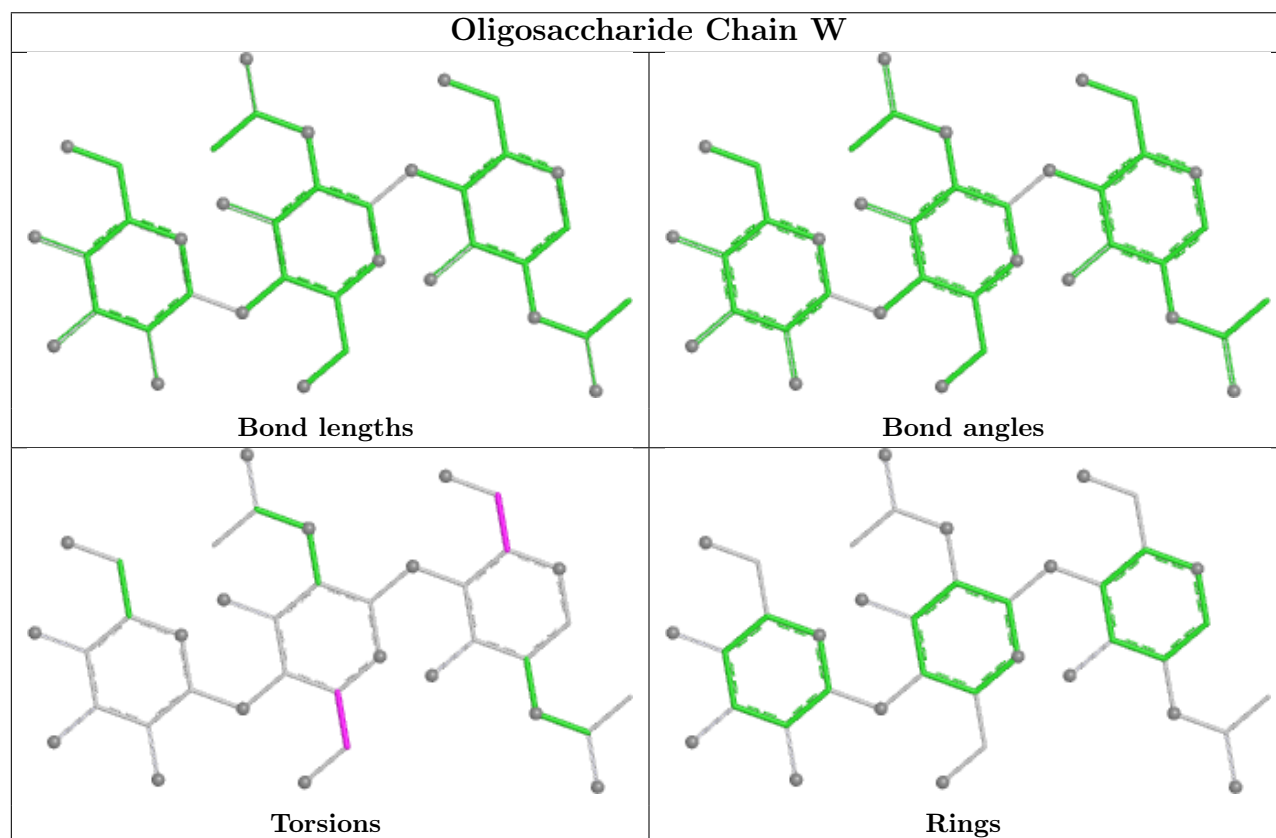
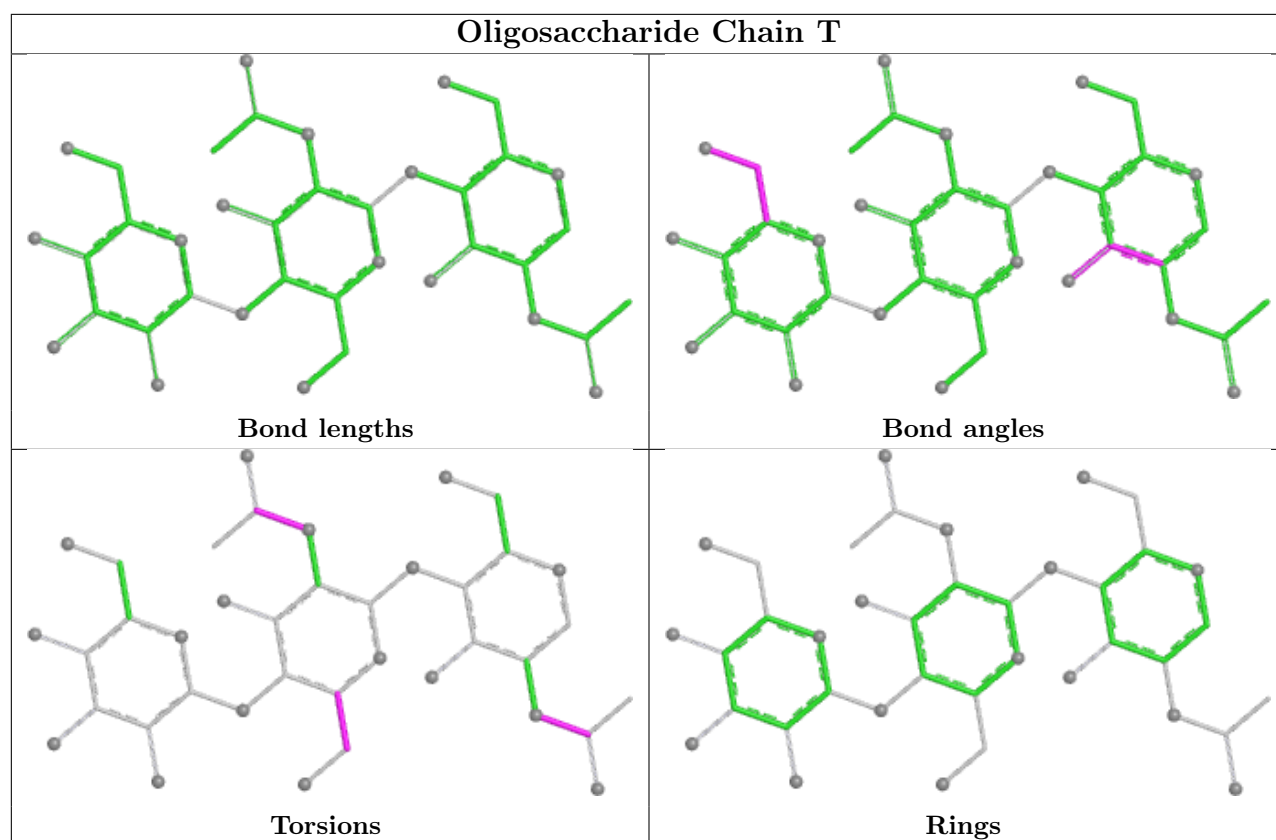
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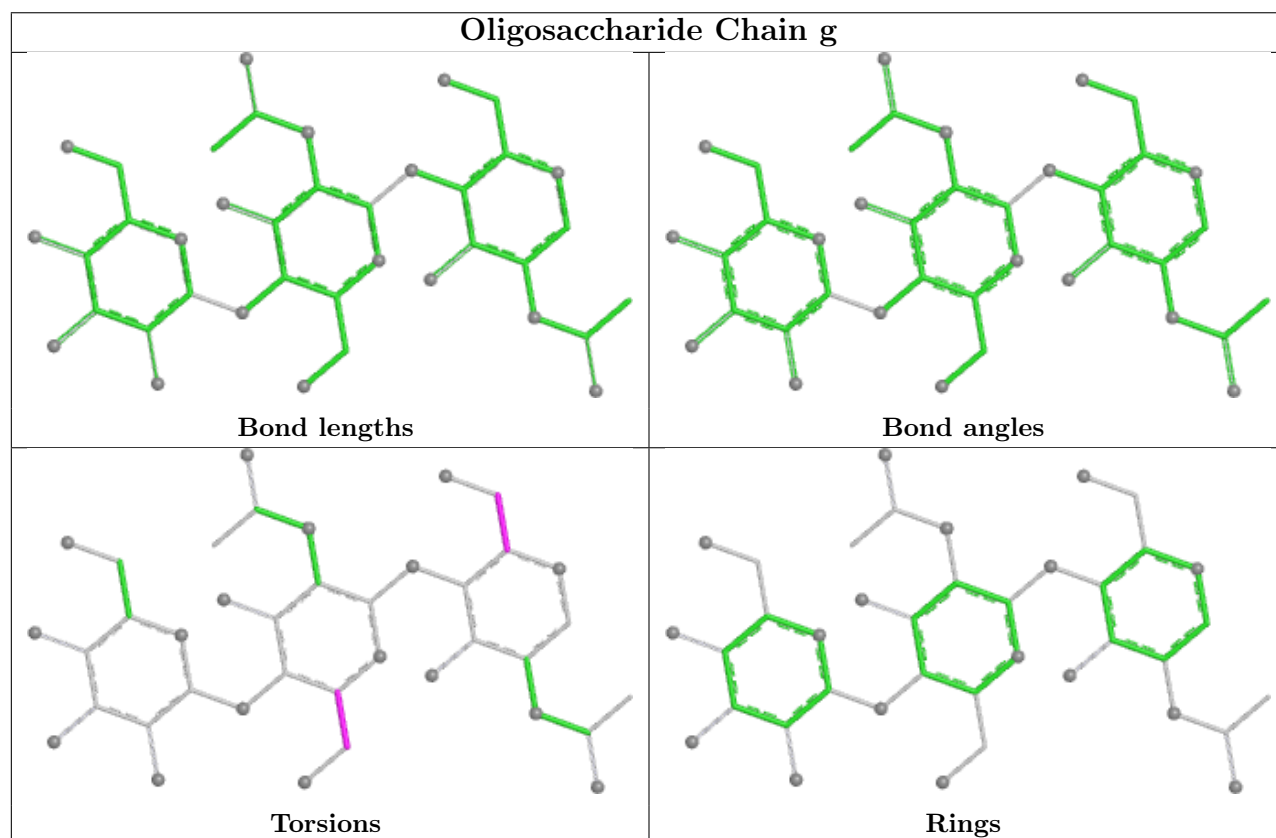
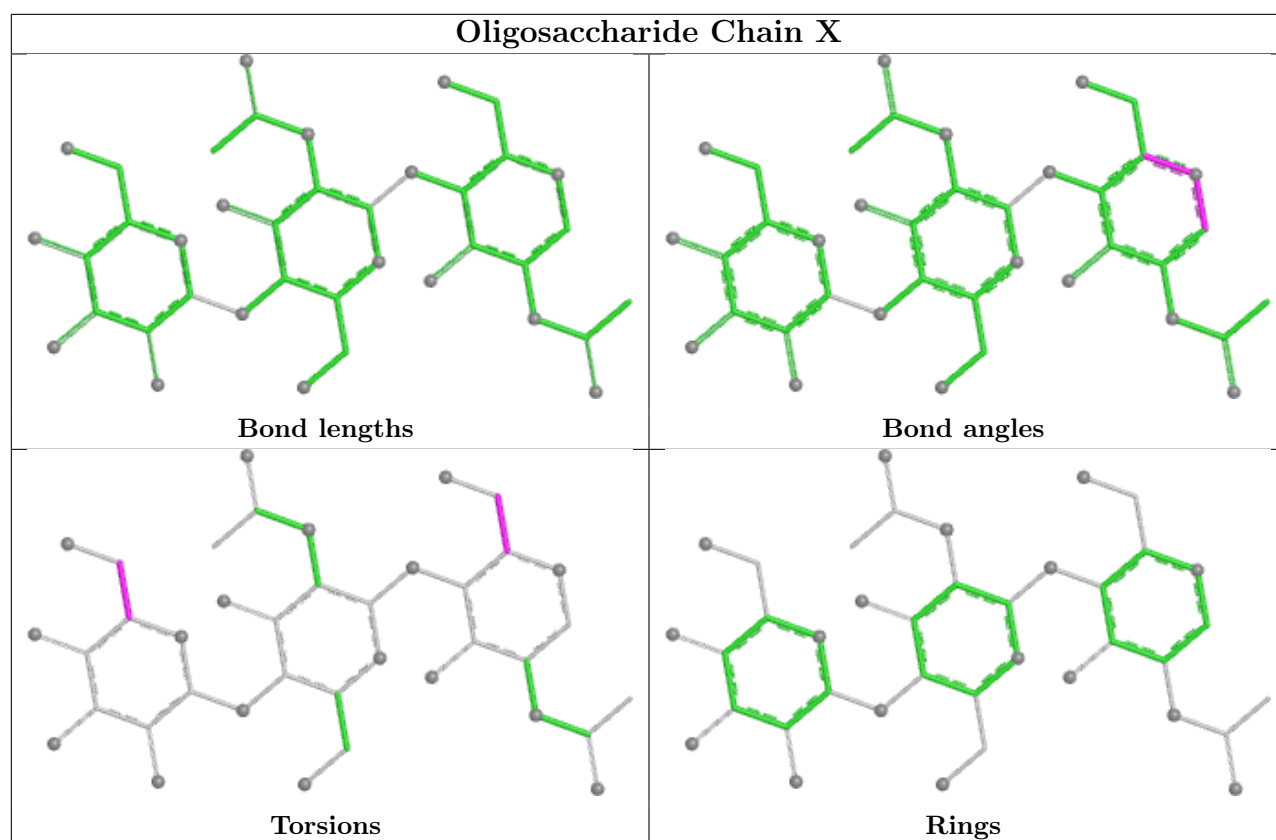
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	g	1	NAG	1	0
10	p	1	NAG	1	0
8	h	1	NAG	2	0
7	i	9	MAN	1	0
7	S	1	NAG	1	0
9	m	2	NAG	2	0
9	m	4	NAG	5	0
13	j	2	NAG	1	0
9	b	1	NAG	4	0

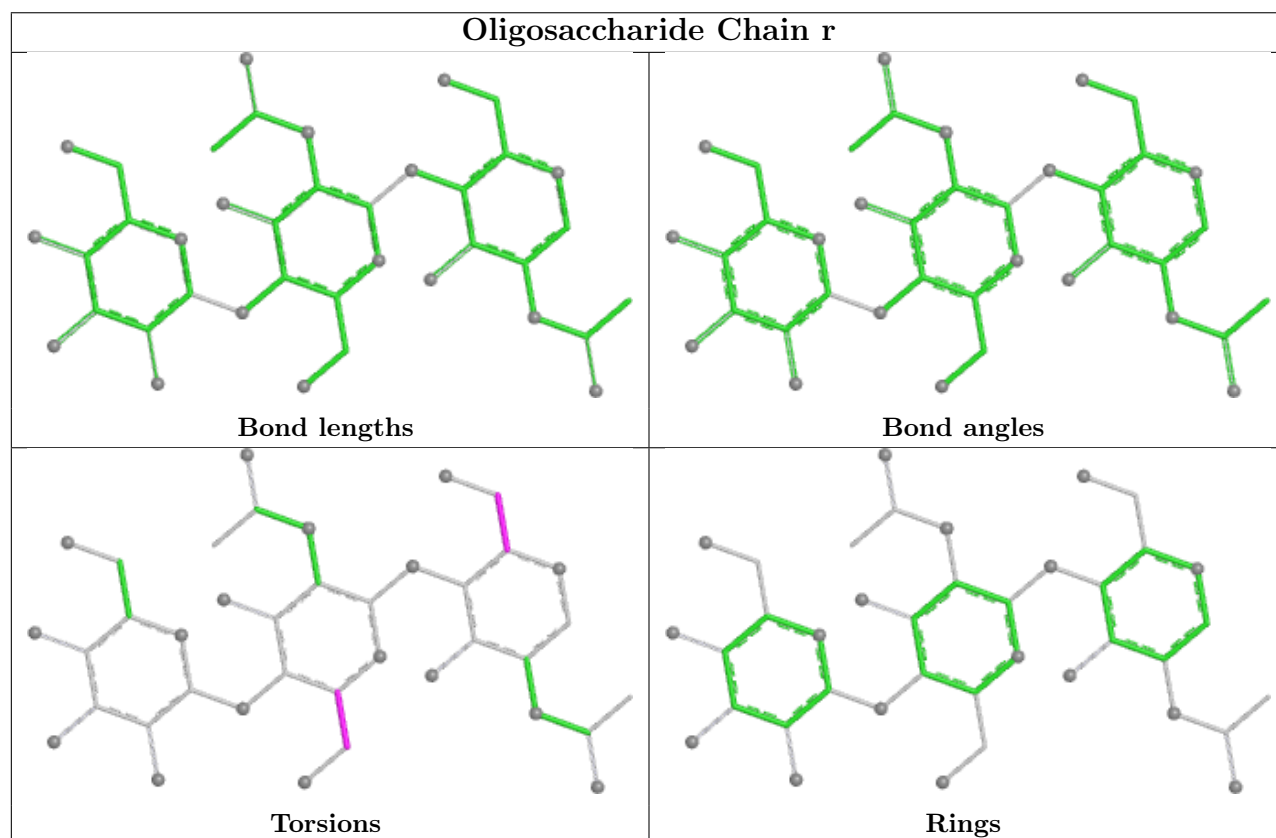
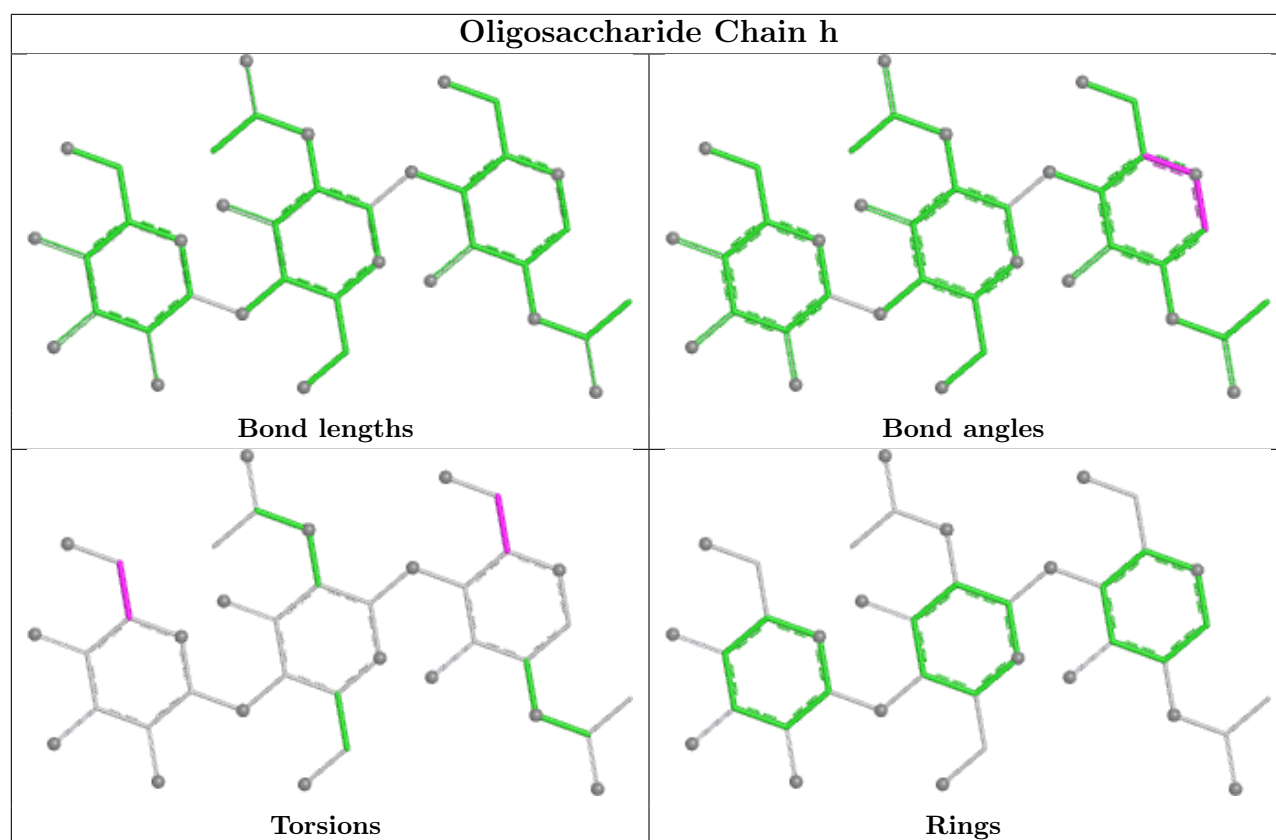
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

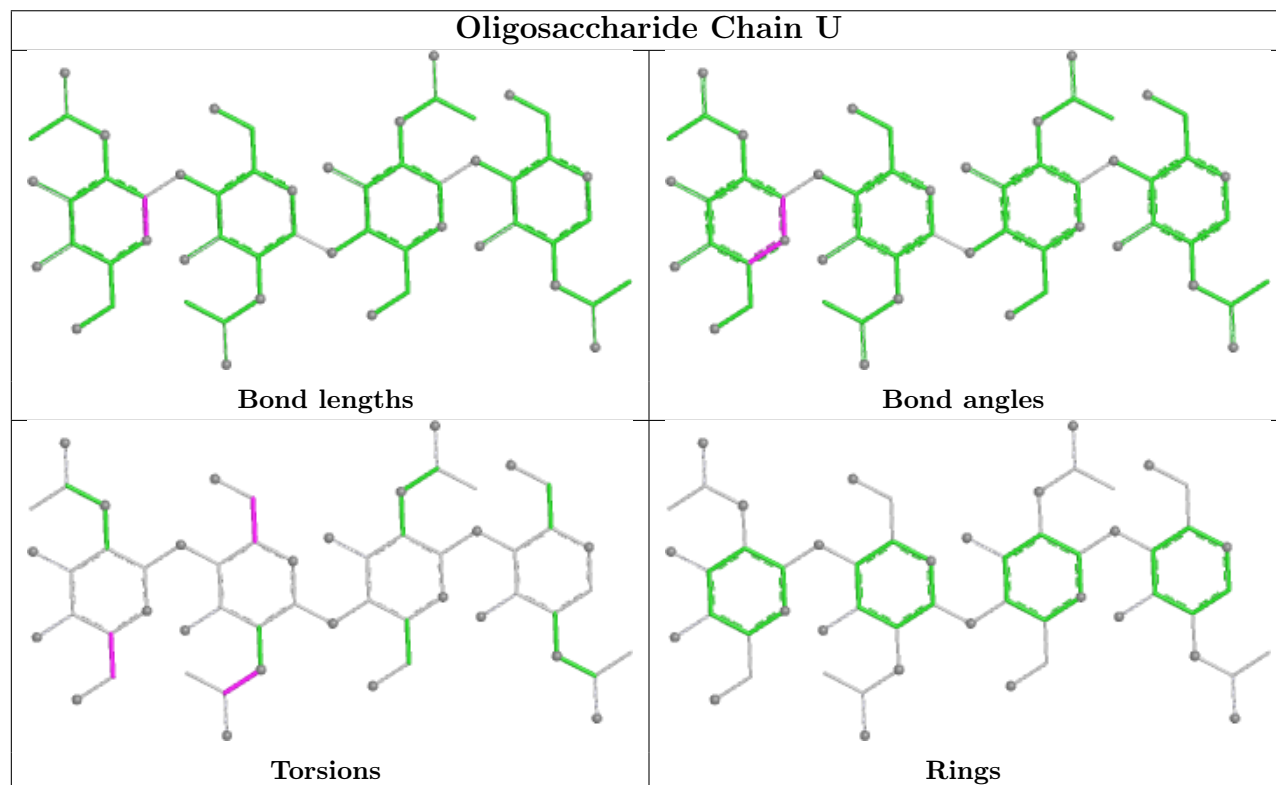
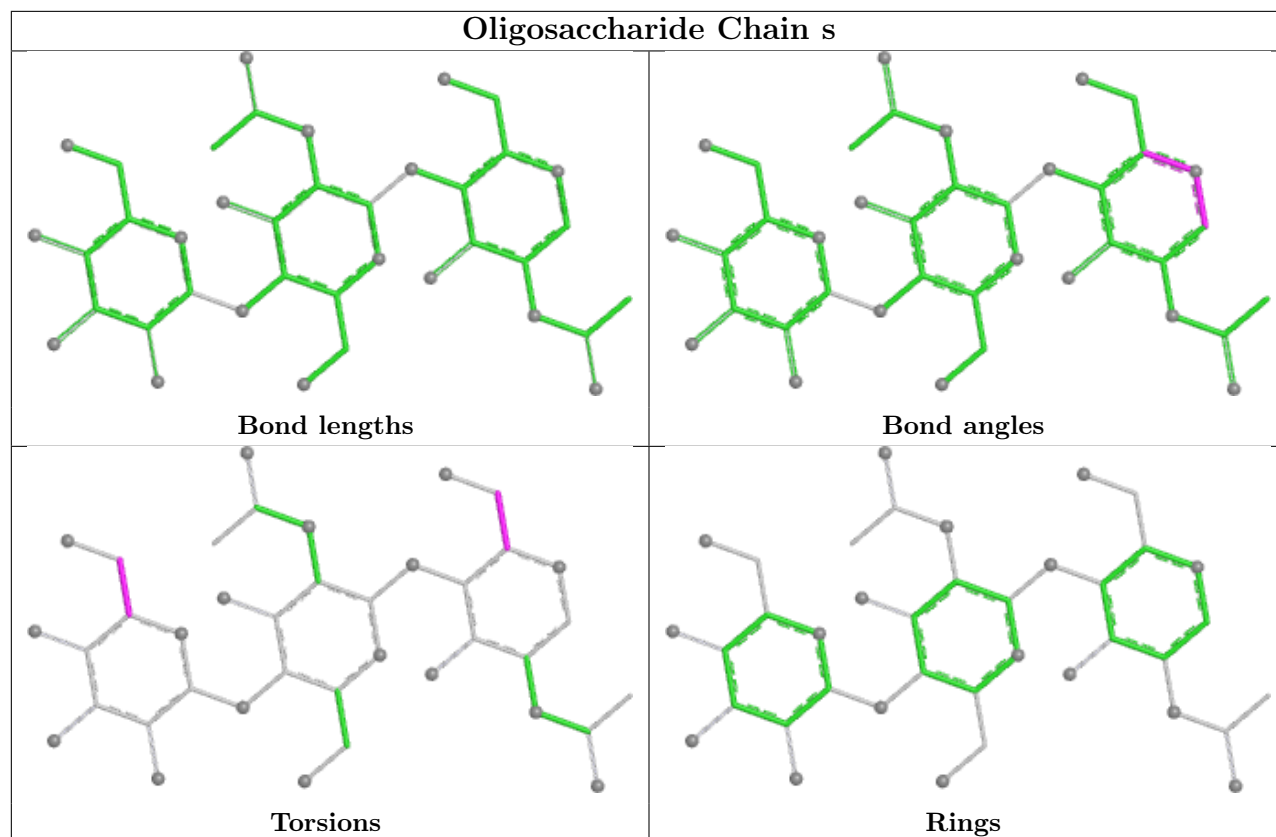


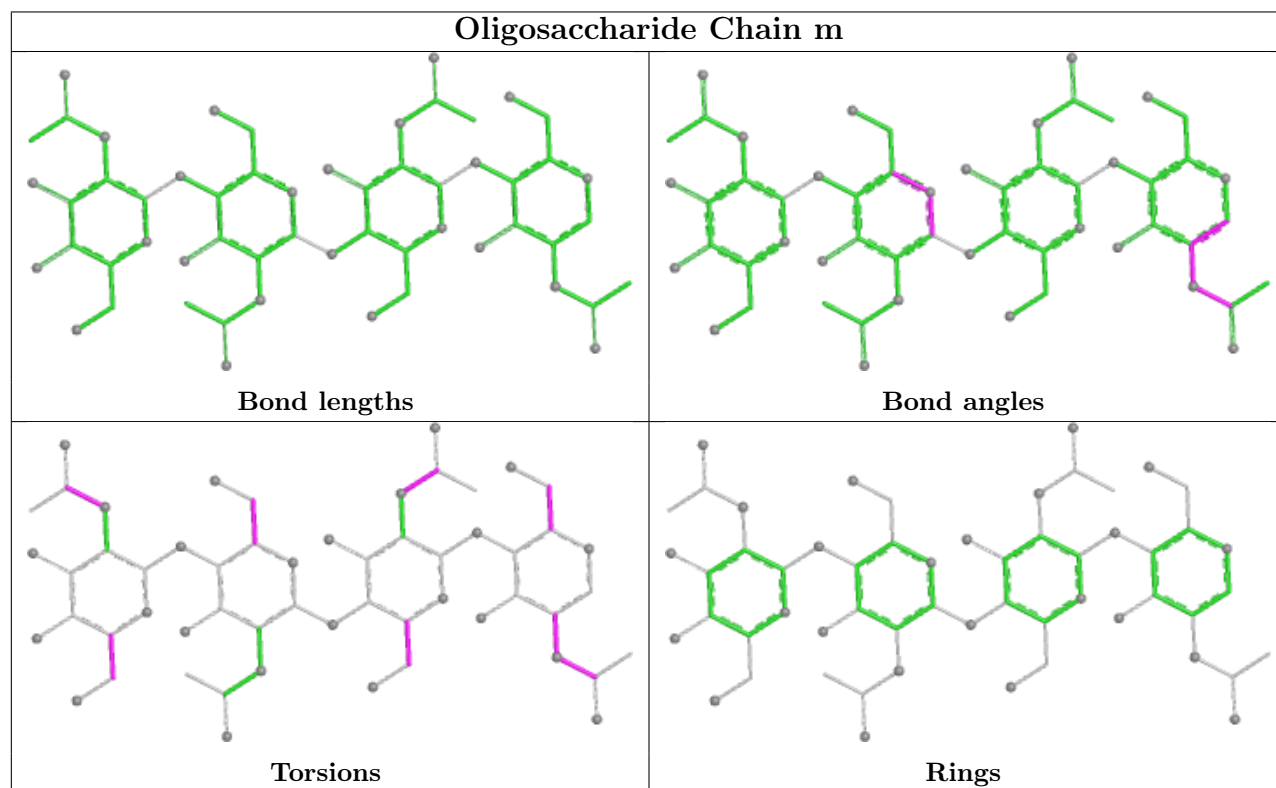
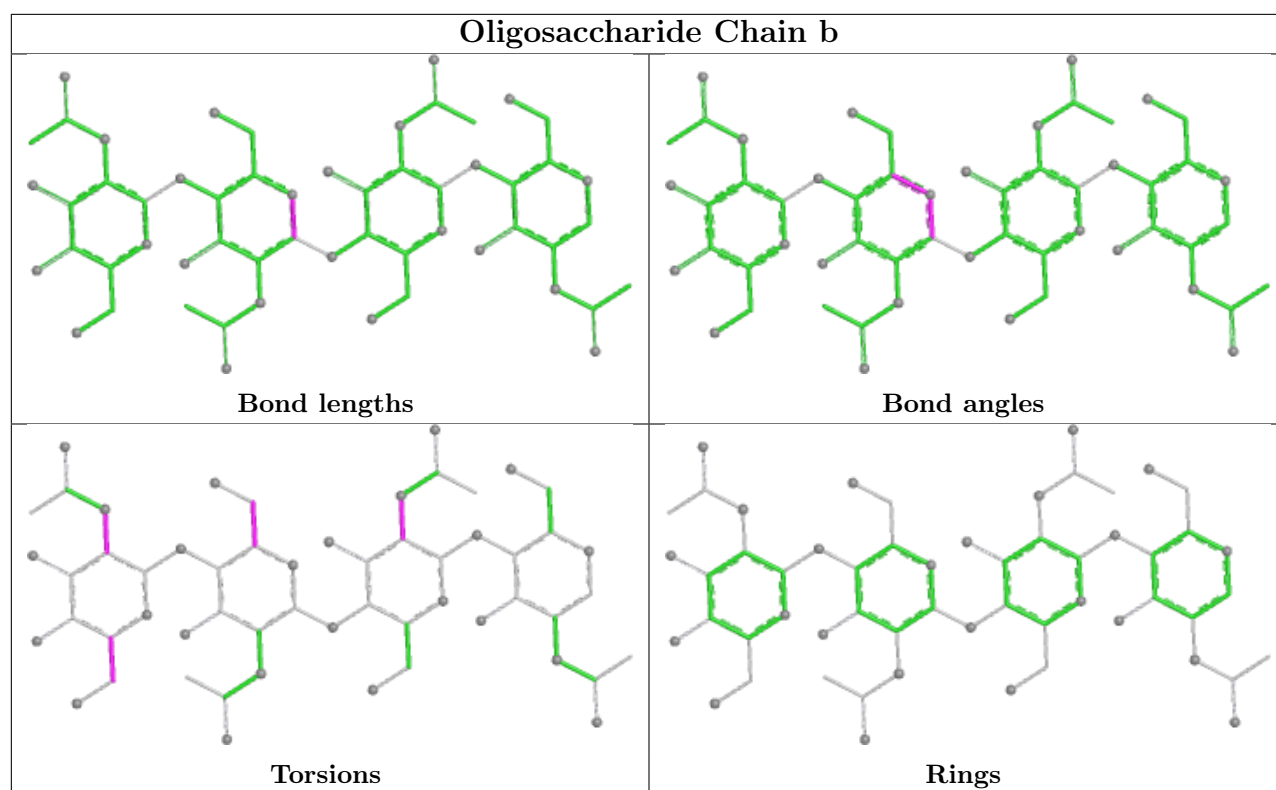


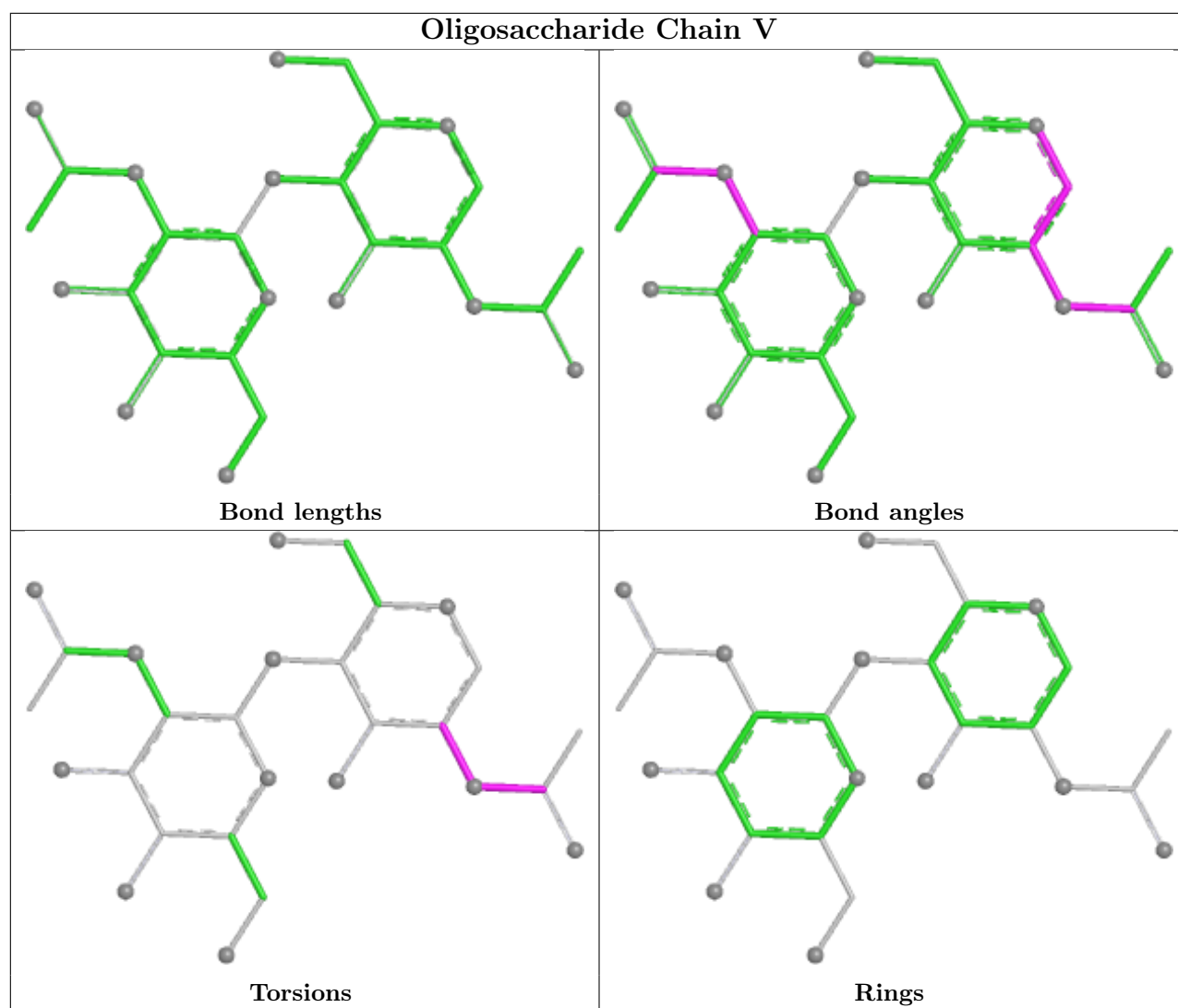


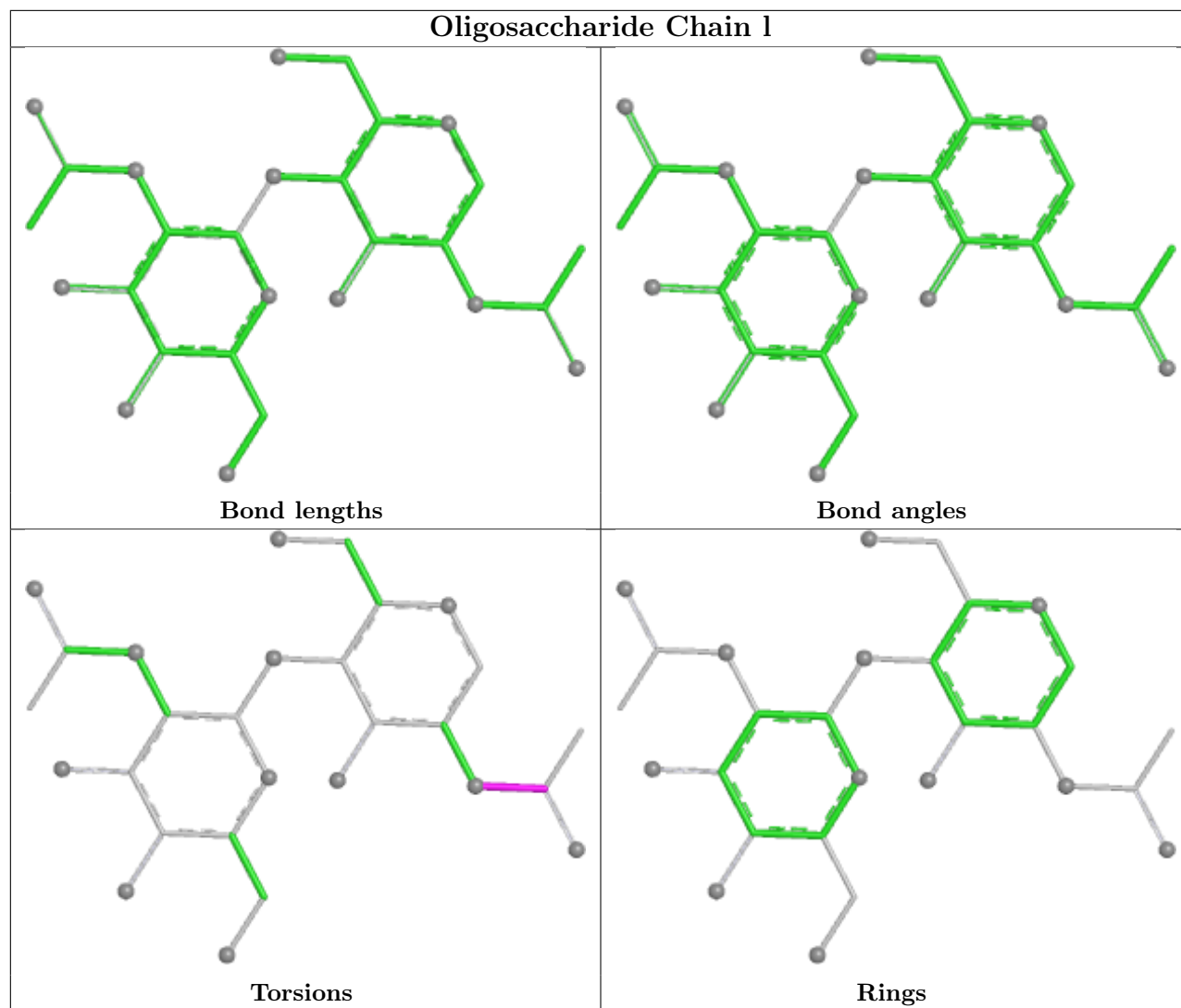


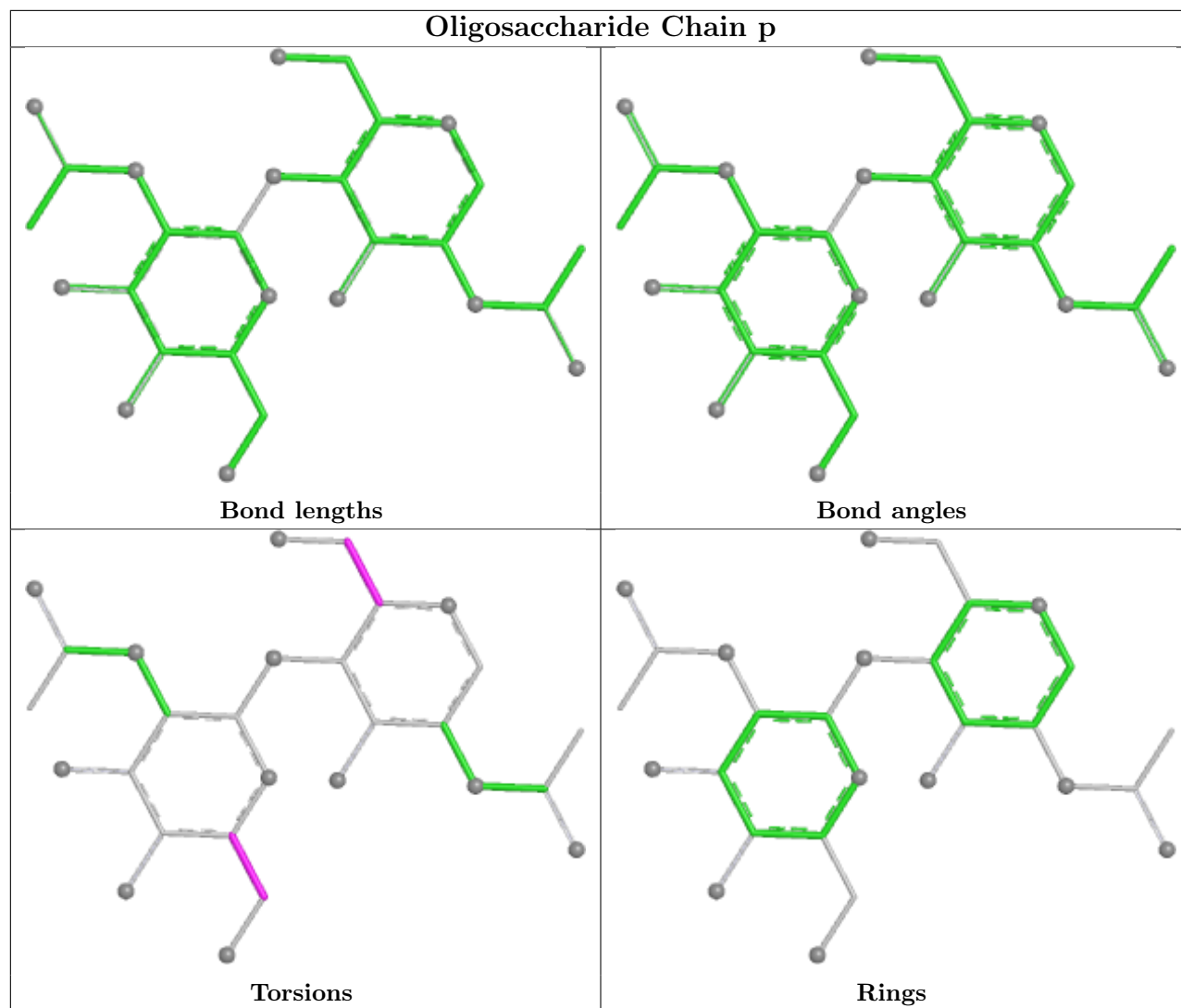


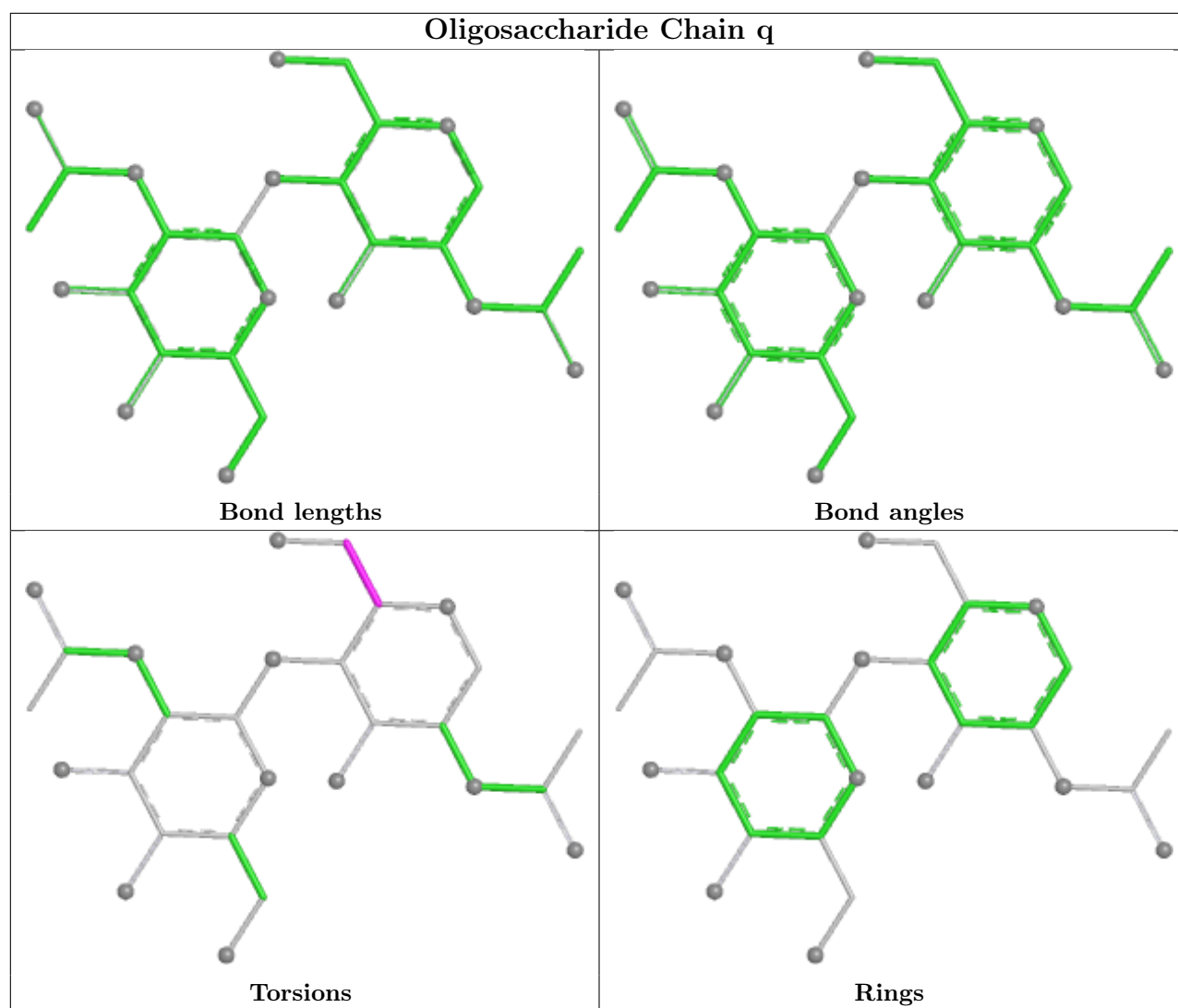


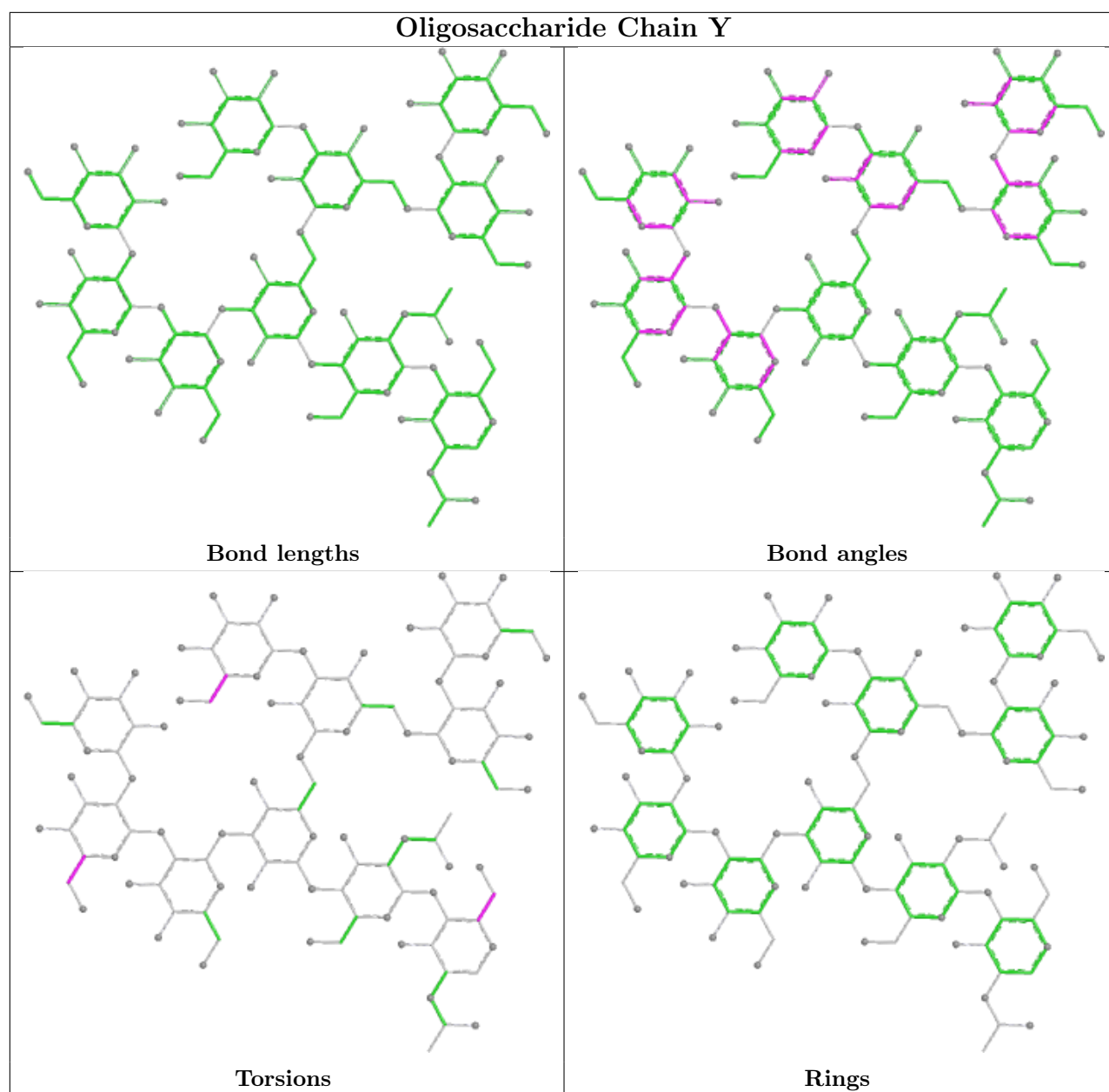


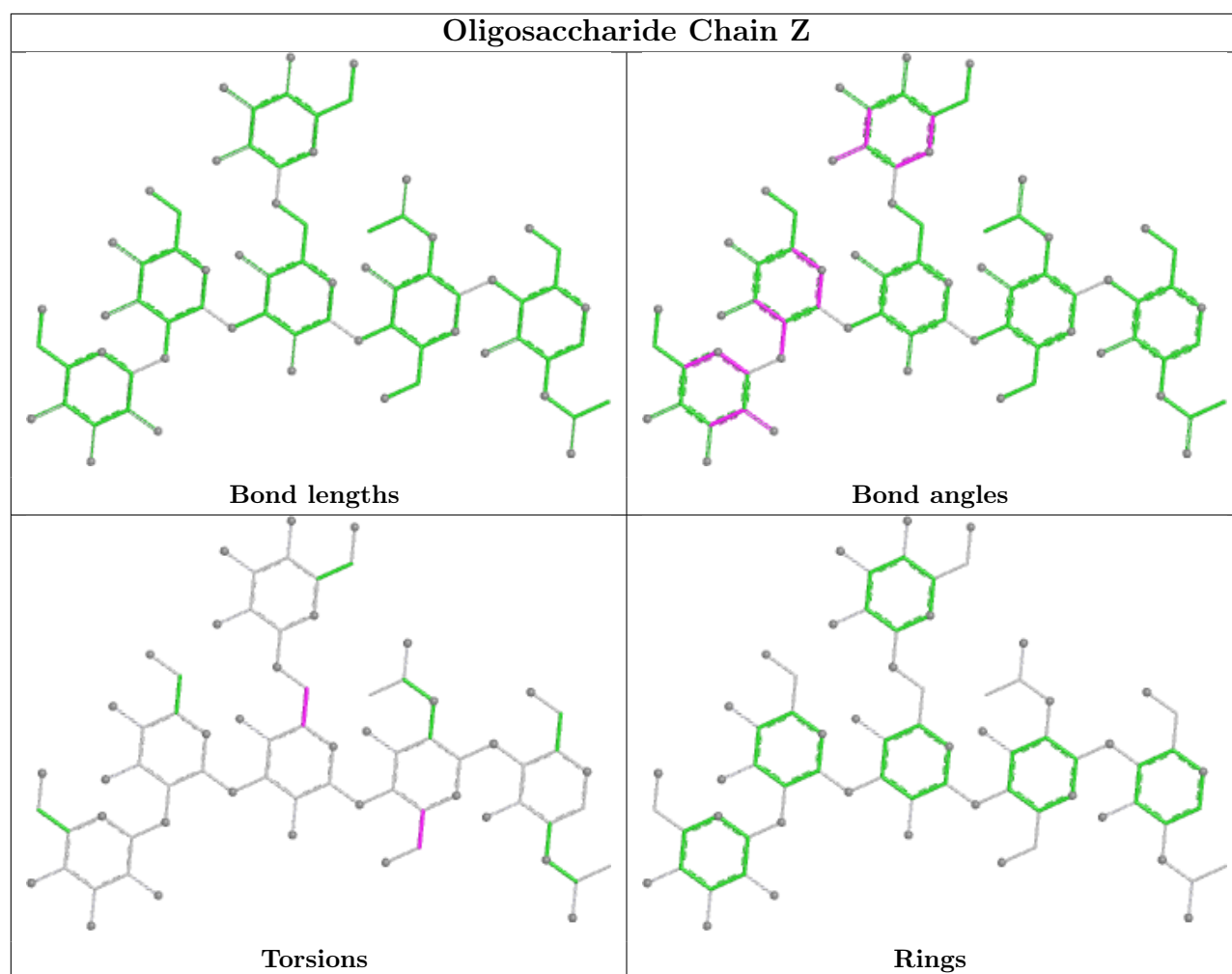


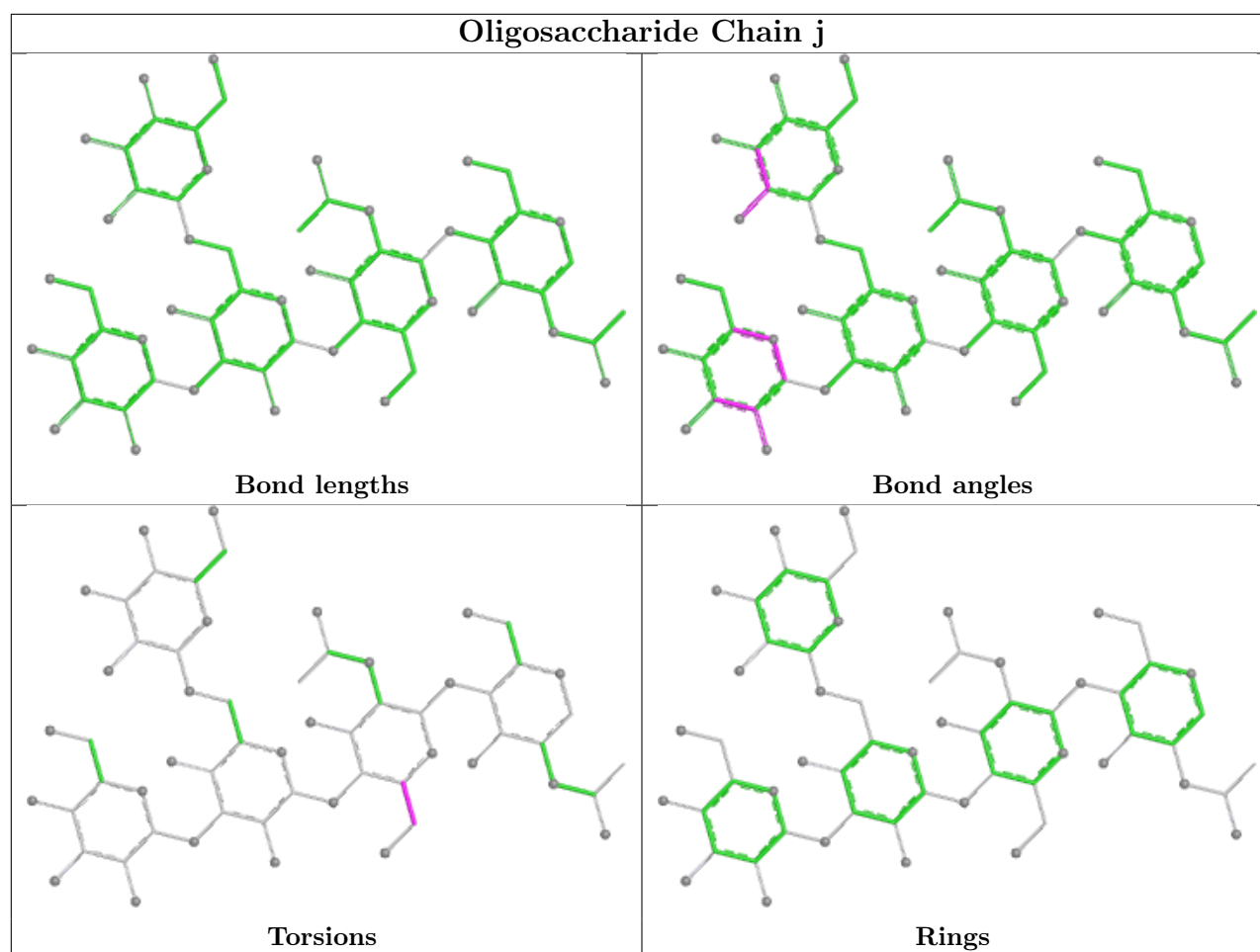












5.6 Ligand geometry [i](#)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	NAG	E	607	1	14,14,15	0.17	0	17,19,21	0.53	0
14	NAG	I	604	1	14,14,15	0.47	0	17,19,21	0.37	0
14	NAG	A	1005	1	14,14,15	0.28	0	17,19,21	0.50	0
14	NAG	E	612	1	14,14,15	0.32	0	17,19,21	0.37	0
14	NAG	I	607	1	14,14,15	0.19	0	17,19,21	0.49	0
14	NAG	F	703	2	14,14,15	0.22	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	E	601	1	14,14,15	0.58	0	17,19,21	0.58	0
14	NAG	E	608	1	14,14,15	0.92	1 (7%)	17,19,21	1.34	1 (5%)
14	NAG	I	602	1	14,14,15	0.25	0	17,19,21	0.53	0
14	NAG	J	701	2	14,14,15	0.30	0	17,19,21	0.46	0
14	NAG	B	701	2	14,14,15	0.21	0	17,19,21	0.44	0
14	NAG	E	610	1	14,14,15	0.21	0	17,19,21	0.44	0
14	NAG	E	603	1	14,14,15	0.21	0	17,19,21	0.46	0
14	NAG	F	701	2	14,14,15	0.19	0	17,19,21	0.44	0
14	NAG	A	1002	1	14,14,15	0.37	0	17,19,21	0.67	1 (5%)
14	NAG	I	601	1	14,14,15	0.22	0	17,19,21	0.45	0
14	NAG	A	1001	1	14,14,15	0.25	0	17,19,21	0.44	0
14	NAG	E	605	1	14,14,15	0.26	0	17,19,21	0.50	0
14	NAG	A	1007	1	14,14,15	0.35	0	17,19,21	1.28	3 (17%)
14	NAG	B	702	2	14,14,15	0.60	1 (7%)	17,19,21	0.63	0
14	NAG	C	301	3	14,14,15	0.31	0	17,19,21	0.38	0
14	NAG	F	702	2	14,14,15	0.24	0	17,19,21	0.49	0
14	NAG	E	609	1	14,14,15	0.17	0	17,19,21	0.58	0
14	NAG	I	603	1	14,14,15	0.21	0	17,19,21	0.45	0
14	NAG	I	605	1	14,14,15	0.21	0	17,19,21	0.43	0
14	NAG	J	703	2	14,14,15	0.40	0	17,19,21	0.55	0
14	NAG	A	1008	1	14,14,15	0.42	0	17,19,21	0.38	0
14	NAG	E	611	1	14,14,15	0.23	0	17,19,21	0.46	0
14	NAG	A	1010	1	14,14,15	0.23	0	17,19,21	0.50	0
14	NAG	I	609	1	14,14,15	0.87	2 (14%)	17,19,21	1.00	1 (5%)
14	NAG	A	1009	1	14,14,15	0.44	0	17,19,21	0.52	0
14	NAG	A	1004	1	14,14,15	0.33	0	17,19,21	0.45	0
14	NAG	E	606	1	14,14,15	0.39	0	17,19,21	0.36	0
14	NAG	E	604	1	14,14,15	0.32	0	17,19,21	0.41	0
14	NAG	K	301	3	14,14,15	0.34	0	17,19,21	0.44	0
14	NAG	A	1003	1	14,14,15	0.21	0	17,19,21	0.44	0
14	NAG	A	1006	1	14,14,15	0.17	0	17,19,21	0.52	0
14	NAG	J	702	2	14,14,15	0.34	0	17,19,21	0.41	0
14	NAG	I	608	1	14,14,15	0.21	0	17,19,21	0.57	0
14	NAG	I	606	1	14,14,15	0.27	0	17,19,21	0.39	0
14	NAG	G	301	3	14,14,15	0.25	0	17,19,21	0.43	0
14	NAG	E	602	1	14,14,15	0.37	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
14	NAG	E	607	1	-	2/6/23/26	0/1/1/1
14	NAG	I	604	1	-	3/6/23/26	0/1/1/1
14	NAG	A	1005	1	-	1/6/23/26	0/1/1/1
14	NAG	E	612	1	-	1/6/23/26	0/1/1/1
14	NAG	I	607	1	-	4/6/23/26	0/1/1/1
14	NAG	F	703	2	-	2/6/23/26	0/1/1/1
14	NAG	E	601	1	-	2/6/23/26	0/1/1/1
14	NAG	E	608	1	-	1/6/23/26	0/1/1/1
14	NAG	I	602	1	-	2/6/23/26	0/1/1/1
14	NAG	J	701	2	-	0/6/23/26	0/1/1/1
14	NAG	B	701	2	-	2/6/23/26	0/1/1/1
14	NAG	E	610	1	-	4/6/23/26	0/1/1/1
14	NAG	E	603	1	-	2/6/23/26	0/1/1/1
14	NAG	F	701	2	-	2/6/23/26	0/1/1/1
14	NAG	A	1002	1	-	3/6/23/26	0/1/1/1
14	NAG	I	601	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
14	NAG	E	605	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
14	NAG	B	702	2	-	3/6/23/26	0/1/1/1
14	NAG	C	301	3	-	2/6/23/26	0/1/1/1
14	NAG	F	702	2	-	2/6/23/26	0/1/1/1
14	NAG	E	609	1	-	4/6/23/26	0/1/1/1
14	NAG	I	603	1	-	2/6/23/26	0/1/1/1
14	NAG	I	605	1	-	2/6/23/26	0/1/1/1
14	NAG	J	703	2	-	1/6/23/26	0/1/1/1
14	NAG	A	1008	1	-	4/6/23/26	0/1/1/1
14	NAG	E	611	1	-	2/6/23/26	0/1/1/1
14	NAG	A	1010	1	-	2/6/23/26	0/1/1/1
14	NAG	I	609	1	-	0/6/23/26	0/1/1/1
14	NAG	A	1009	1	-	1/6/23/26	0/1/1/1
14	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
14	NAG	E	606	1	-	2/6/23/26	0/1/1/1
14	NAG	E	604	1	-	2/6/23/26	0/1/1/1
14	NAG	K	301	3	-	2/6/23/26	0/1/1/1
14	NAG	A	1003	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
14	NAG	J	702	2	-	2/6/23/26	0/1/1/1
14	NAG	I	608	1	-	4/6/23/26	0/1/1/1
14	NAG	I	606	1	-	2/6/23/26	0/1/1/1
14	NAG	G	301	3	-	2/6/23/26	0/1/1/1
14	NAG	E	602	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	E	608	NAG	O5-C1	3.31	1.49	1.43
14	I	609	NAG	O5-C1	2.37	1.47	1.43
14	I	609	NAG	C1-C2	2.10	1.55	1.52
14	B	702	NAG	C1-C2	2.05	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	608	NAG	C1-O5-C5	5.26	119.23	112.19
14	I	609	NAG	C1-O5-C5	3.90	117.42	112.19
14	A	1007	NAG	C1-O5-C5	3.44	116.79	112.19
14	E	602	NAG	C1-O5-C5	2.81	115.95	112.19
14	A	1007	NAG	O5-C1-C2	2.44	115.06	111.29
14	A	1007	NAG	C4-C3-C2	-2.43	107.45	111.02
14	A	1002	NAG	C1-O5-C5	2.23	115.17	112.19

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	1007	NAG	C8-C7-N2-C2
14	A	1007	NAG	O7-C7-N2-C2
14	E	603	NAG	O5-C5-C6-O6
14	E	605	NAG	O5-C5-C6-O6
14	I	603	NAG	O5-C5-C6-O6
14	E	604	NAG	C4-C5-C6-O6
14	A	1003	NAG	O5-C5-C6-O6
14	G	301	NAG	O5-C5-C6-O6
14	I	604	NAG	O5-C5-C6-O6
14	A	1004	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	A	1010	NAG	O5-C5-C6-O6
14	A	1008	NAG	C4-C5-C6-O6
14	A	1002	NAG	O5-C5-C6-O6
14	E	611	NAG	O5-C5-C6-O6
14	I	602	NAG	O5-C5-C6-O6
14	I	605	NAG	O5-C5-C6-O6
14	E	605	NAG	C4-C5-C6-O6
14	A	1006	NAG	O5-C5-C6-O6
14	I	607	NAG	O5-C5-C6-O6
14	I	605	NAG	C4-C5-C6-O6
14	G	301	NAG	C4-C5-C6-O6
14	E	604	NAG	O5-C5-C6-O6
14	E	603	NAG	C4-C5-C6-O6
14	I	602	NAG	C4-C5-C6-O6
14	F	701	NAG	O5-C5-C6-O6
14	A	1002	NAG	C4-C5-C6-O6
14	I	603	NAG	C4-C5-C6-O6
14	E	606	NAG	O5-C5-C6-O6
14	A	1003	NAG	C4-C5-C6-O6
14	A	1004	NAG	O5-C5-C6-O6
14	B	702	NAG	O5-C5-C6-O6
14	F	702	NAG	O5-C5-C6-O6
14	I	604	NAG	C4-C5-C6-O6
14	A	1008	NAG	O5-C5-C6-O6
14	I	606	NAG	O5-C5-C6-O6
14	F	703	NAG	O5-C5-C6-O6
14	E	607	NAG	O5-C5-C6-O6
14	J	702	NAG	O5-C5-C6-O6
14	A	1010	NAG	C4-C5-C6-O6
14	E	611	NAG	C4-C5-C6-O6
14	I	607	NAG	C4-C5-C6-O6
14	A	1006	NAG	C4-C5-C6-O6
14	E	606	NAG	C4-C5-C6-O6
14	F	703	NAG	C4-C5-C6-O6
14	B	702	NAG	C4-C5-C6-O6
14	E	607	NAG	C4-C5-C6-O6
14	I	606	NAG	C4-C5-C6-O6
14	E	609	NAG	O5-C5-C6-O6
14	K	301	NAG	O5-C5-C6-O6
14	F	701	NAG	C4-C5-C6-O6
14	K	301	NAG	C4-C5-C6-O6
14	A	1008	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
14	A	1008	NAG	O7-C7-N2-C2
14	E	610	NAG	C8-C7-N2-C2
14	E	610	NAG	O7-C7-N2-C2
14	I	607	NAG	C8-C7-N2-C2
14	I	607	NAG	O7-C7-N2-C2
14	F	702	NAG	C4-C5-C6-O6
14	B	701	NAG	C4-C5-C6-O6
14	I	608	NAG	O5-C5-C6-O6
14	A	1001	NAG	C4-C5-C6-O6
14	E	609	NAG	C4-C5-C6-O6
14	J	703	NAG	O5-C5-C6-O6
14	J	702	NAG	C4-C5-C6-O6
14	A	1005	NAG	O5-C5-C6-O6
14	B	701	NAG	O5-C5-C6-O6
14	C	301	NAG	C4-C5-C6-O6
14	I	601	NAG	C4-C5-C6-O6
14	E	608	NAG	C4-C5-C6-O6
14	A	1001	NAG	O5-C5-C6-O6
14	E	609	NAG	C1-C2-N2-C7
14	B	702	NAG	C3-C2-N2-C7
14	E	601	NAG	C3-C2-N2-C7
14	E	609	NAG	C3-C2-N2-C7
14	E	612	NAG	C3-C2-N2-C7
14	I	608	NAG	C3-C2-N2-C7
14	I	601	NAG	O5-C5-C6-O6
14	C	301	NAG	O5-C5-C6-O6
14	E	610	NAG	C4-C5-C6-O6
14	I	608	NAG	C1-C2-N2-C7
14	A	1002	NAG	C3-C2-N2-C7
14	A	1009	NAG	C3-C2-N2-C7
14	I	604	NAG	C3-C2-N2-C7
14	I	608	NAG	C4-C5-C6-O6
14	E	610	NAG	O5-C5-C6-O6
14	E	601	NAG	O5-C5-C6-O6

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	E	607	NAG	1	0
14	E	601	NAG	2	0
14	E	608	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	702	NAG	1	0
14	F	702	NAG	1	0
14	E	609	NAG	1	0
14	J	703	NAG	2	0
14	I	609	NAG	1	0
14	A	1009	NAG	7	0
14	A	1004	NAG	1	0
14	E	604	NAG	1	0
14	A	1003	NAG	1	0
14	A	1006	NAG	1	0
14	I	608	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

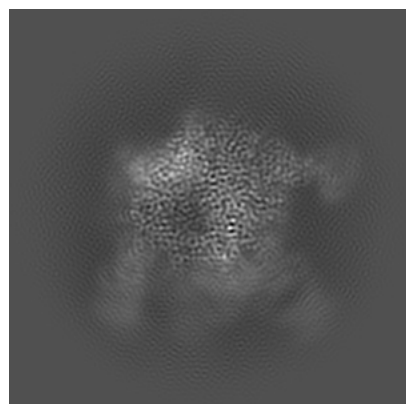
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27596. These allow visual inspection of the internal detail of the map and identification of artifacts.

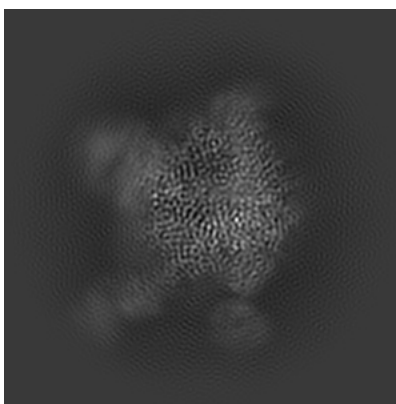
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

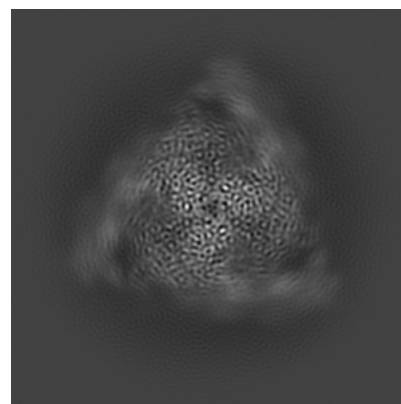
6.1.1 Primary map



X

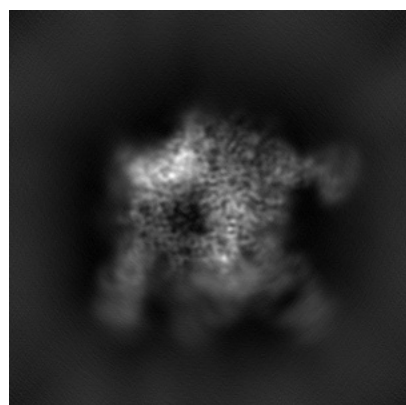


Y

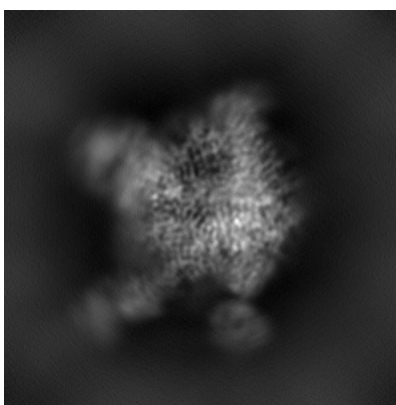


Z

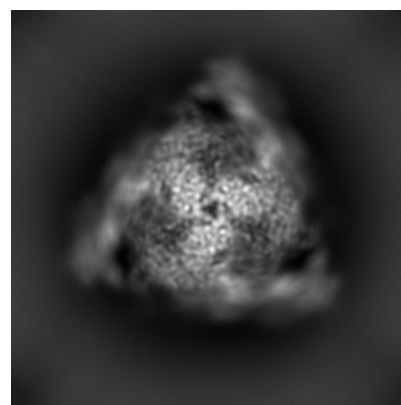
6.1.2 Raw map



X



Y

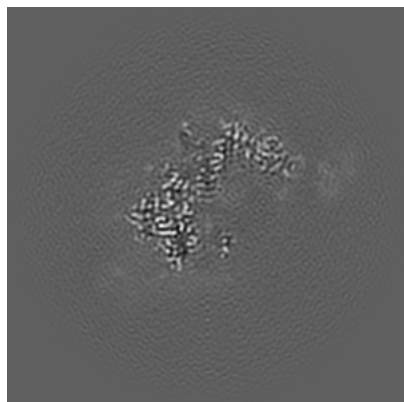


Z

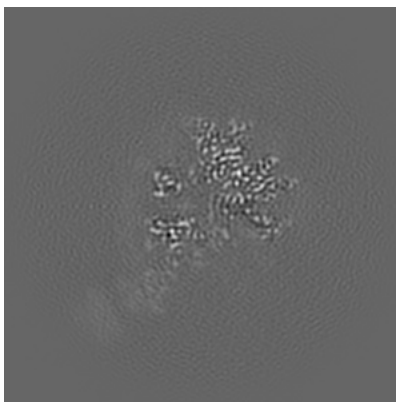
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

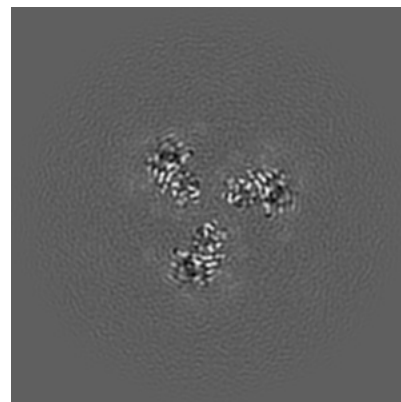
6.2.1 Primary map



X Index: 162

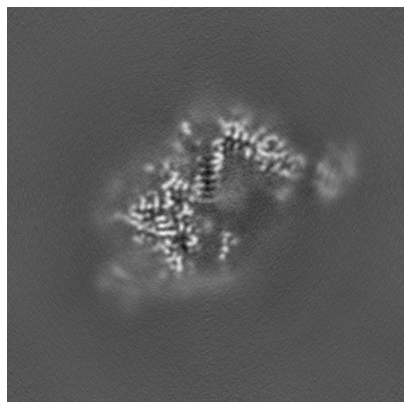


Y Index: 162

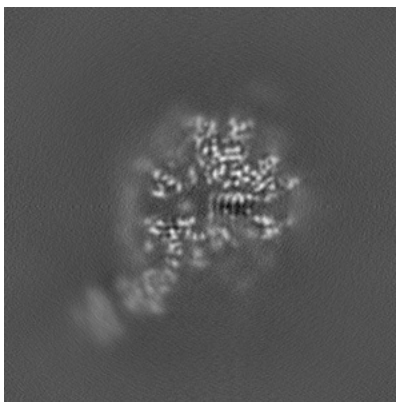


Z Index: 162

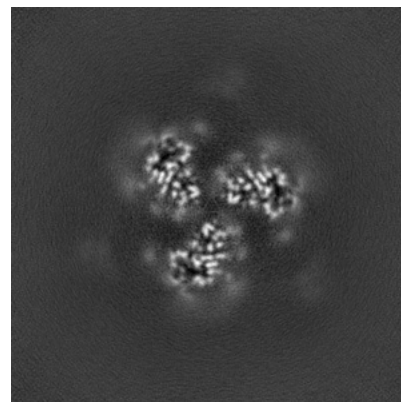
6.2.2 Raw map



X Index: 162



Y Index: 162

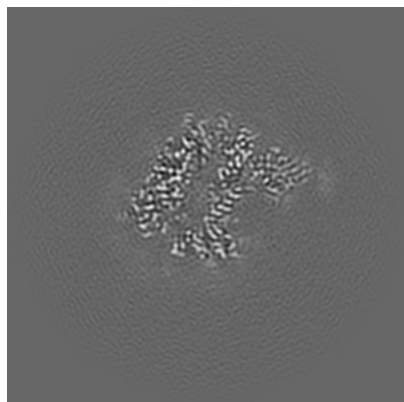


Z Index: 162

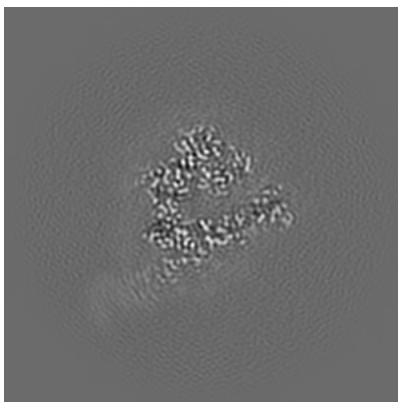
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

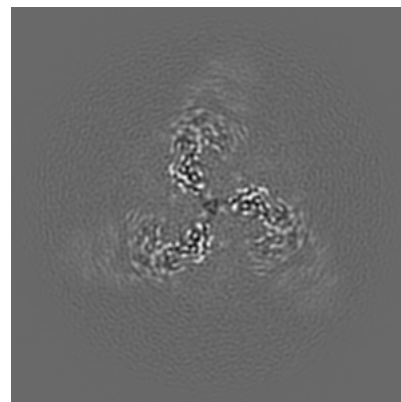
6.3.1 Primary map



X Index: 150

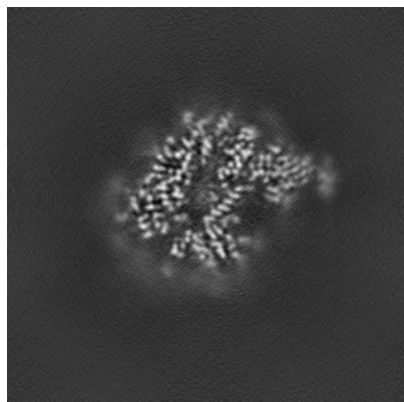


Y Index: 177

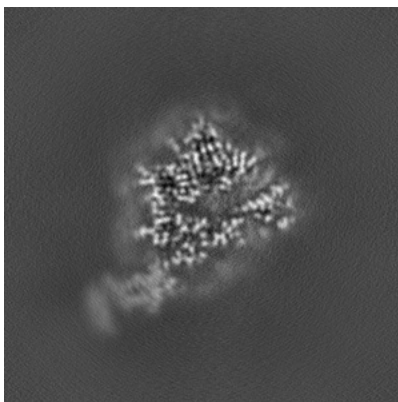


Z Index: 188

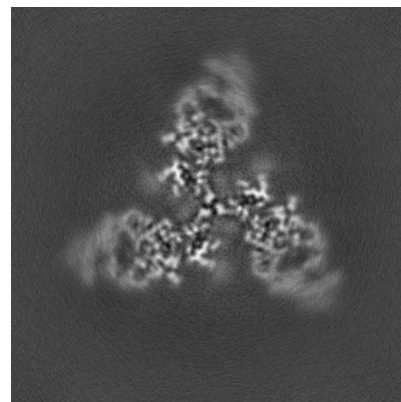
6.3.2 Raw map



X Index: 150



Y Index: 173

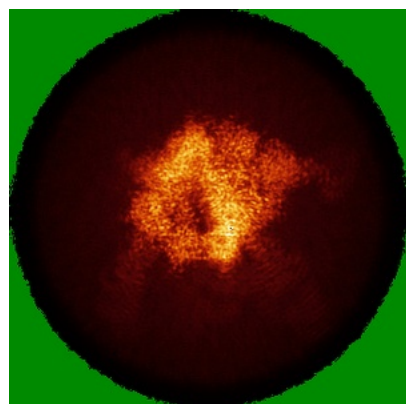


Z Index: 193

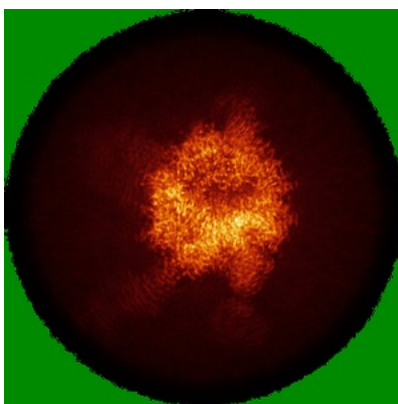
The images above show the largest variance slices of the map in three orthogonal directions.

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

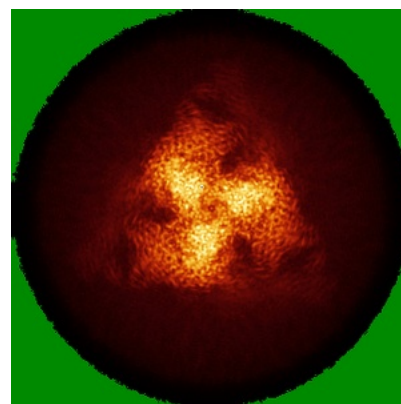
6.4.1 Primary map



X

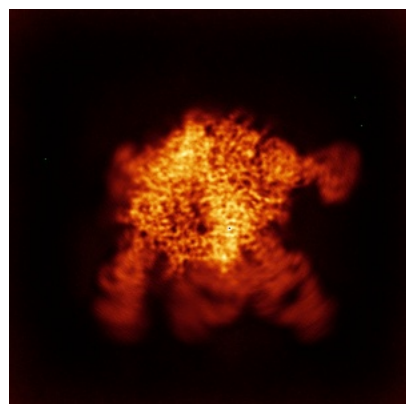


Y

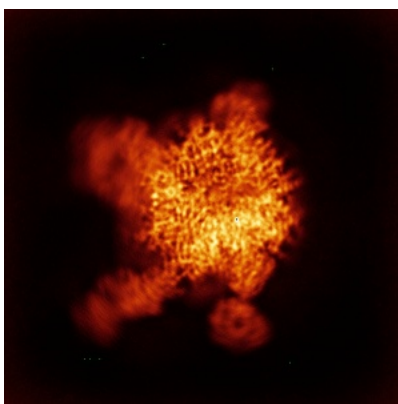


Z

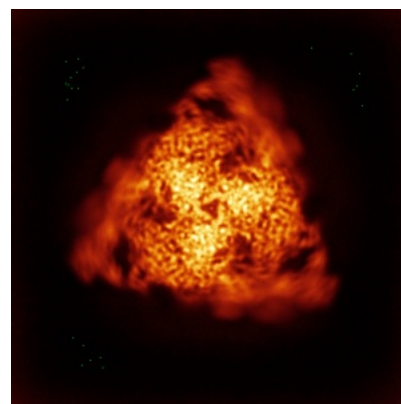
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



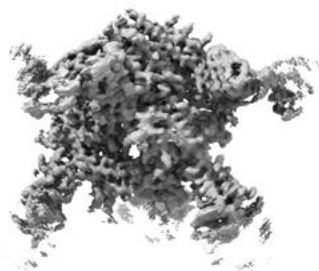
Y



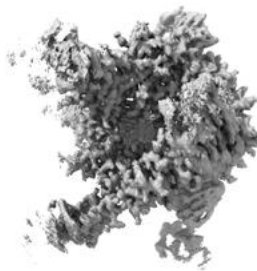
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

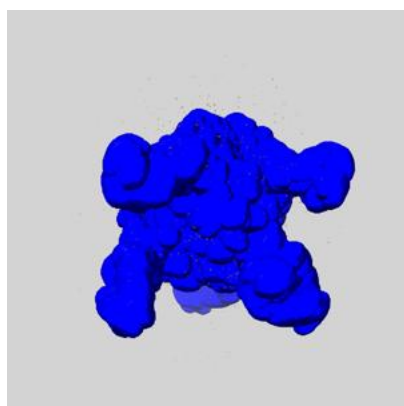
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

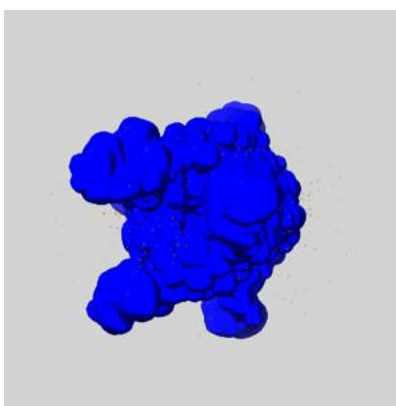
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

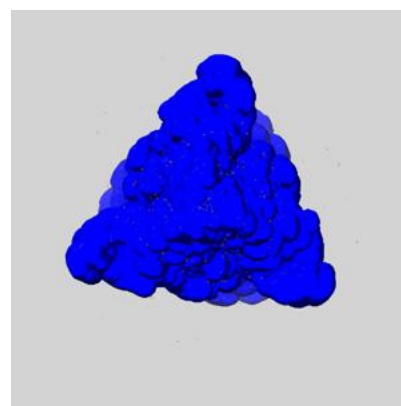
6.6.1 emd_27596_msk_1.map [i](#)



X



Y

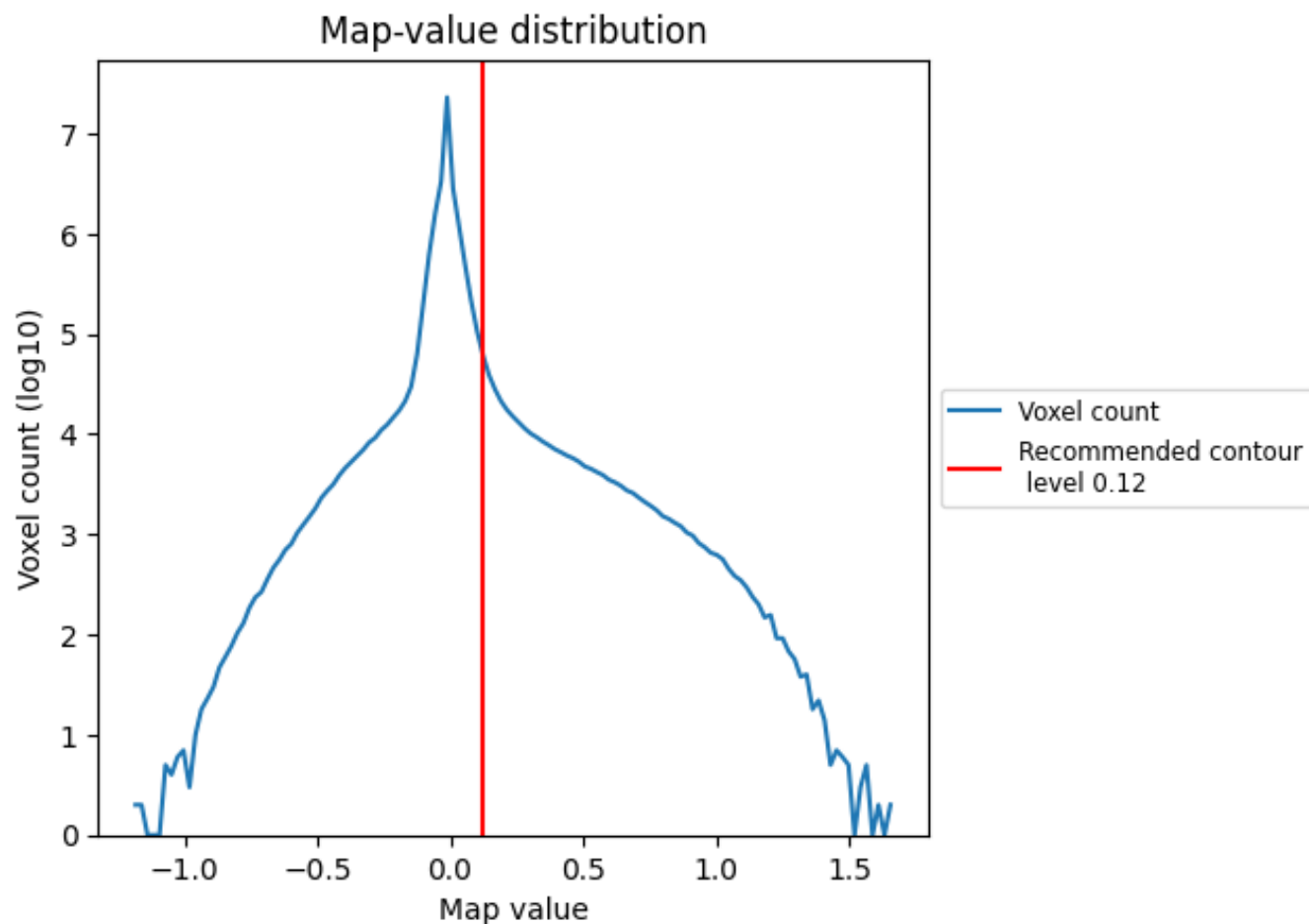


Z

7 Map analysis [i](#)

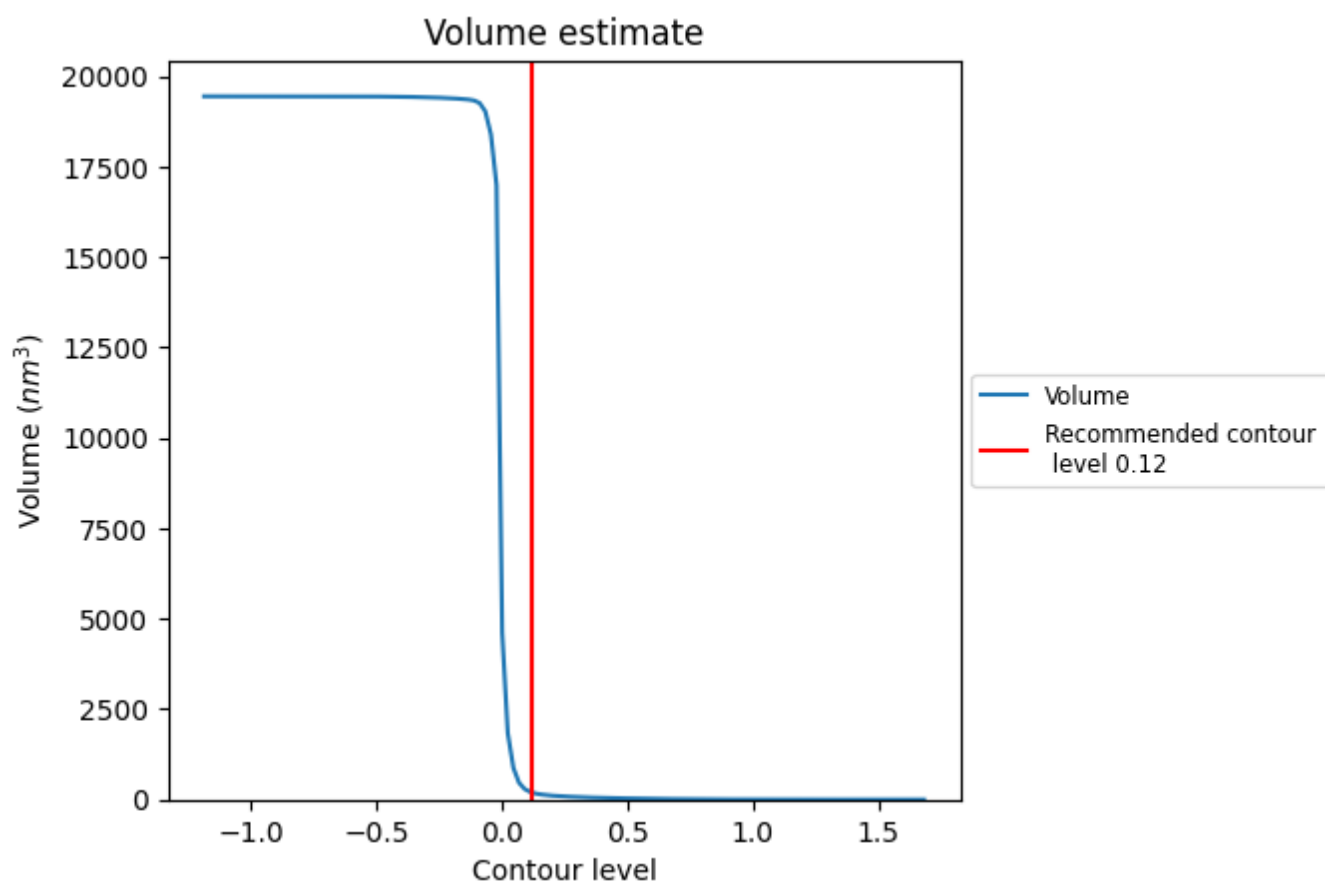
This section contains the results of statistical analysis of the map.

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.

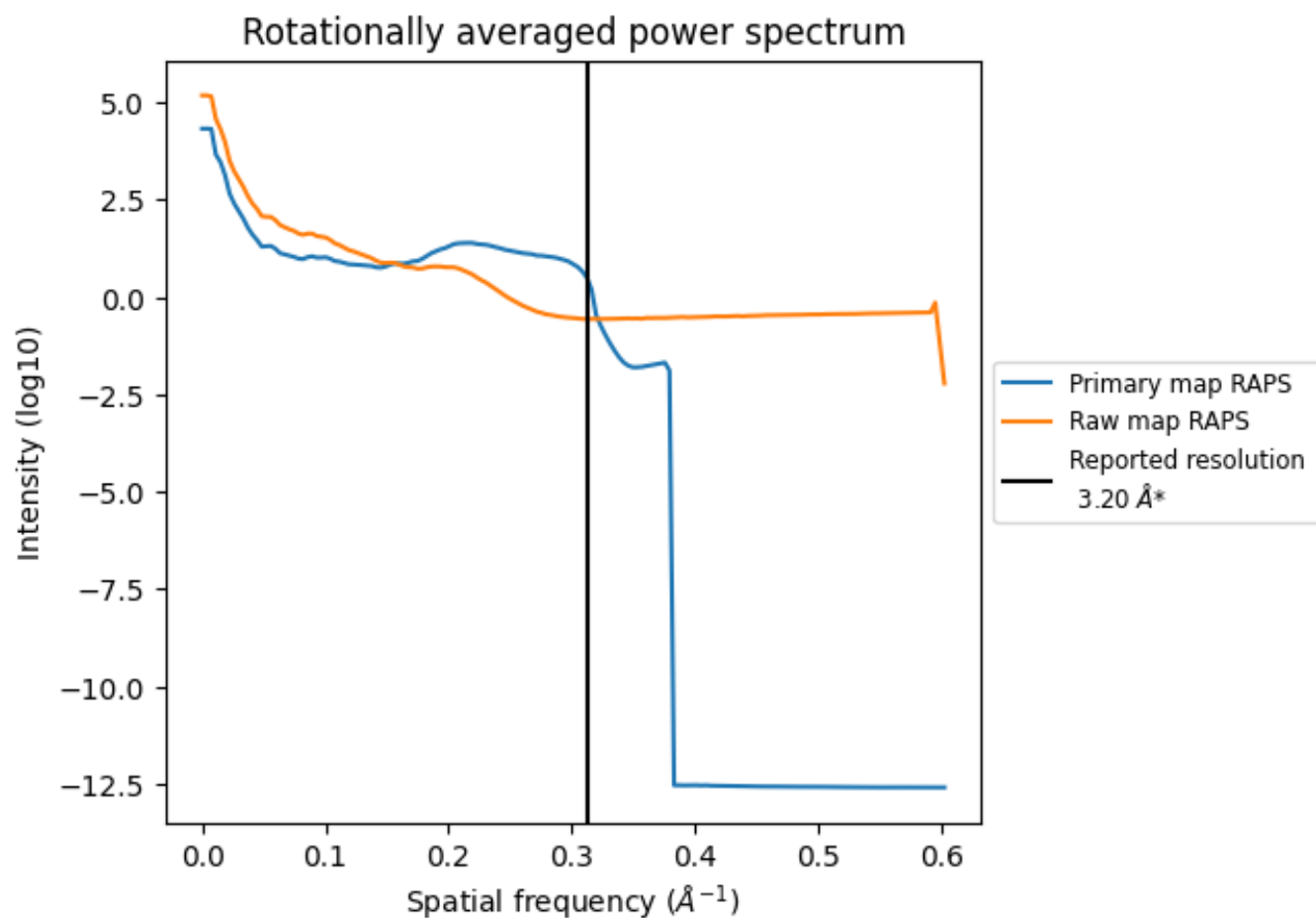
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm³; this corresponds to an approximate mass of 178 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 ⓘ

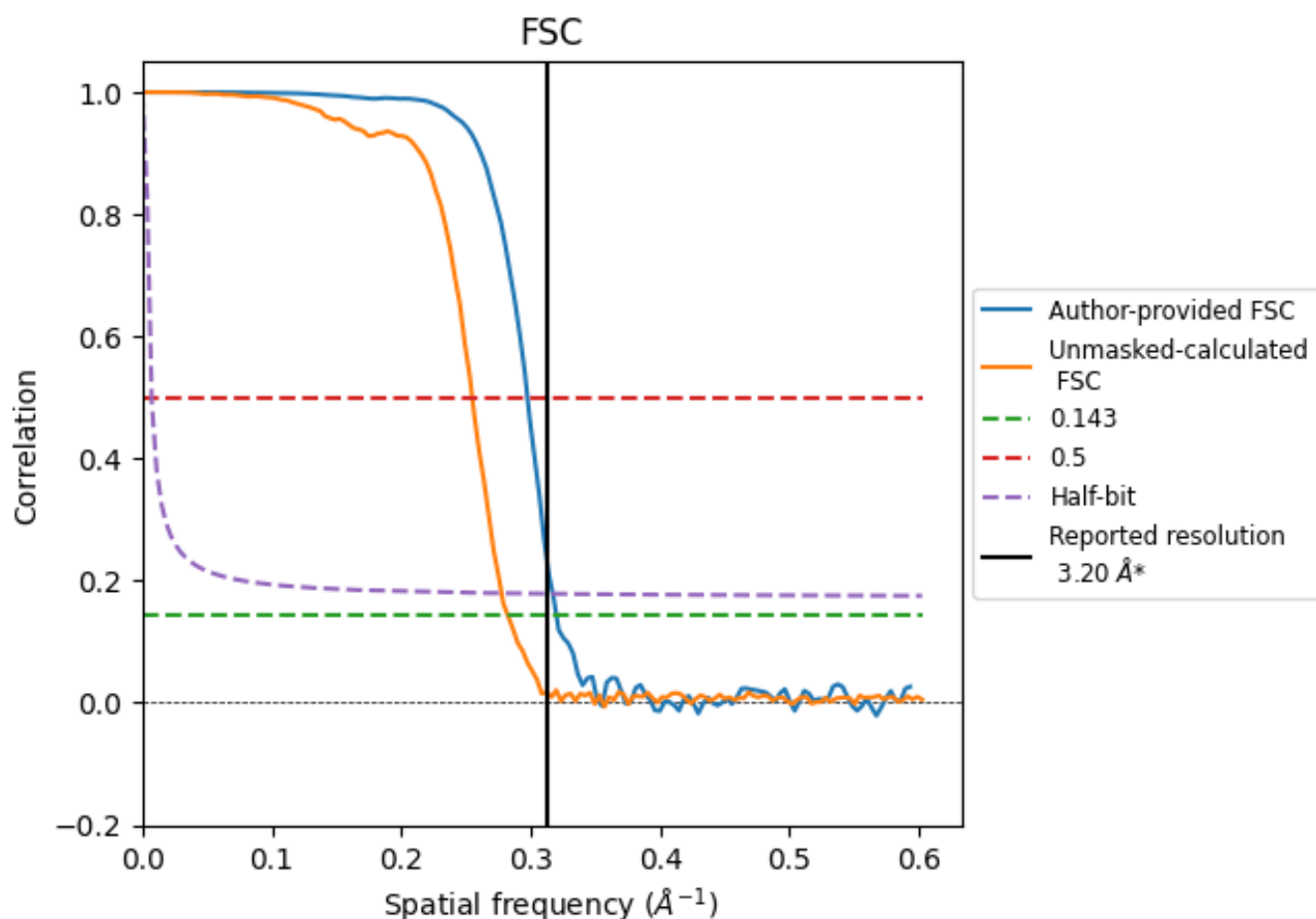


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates

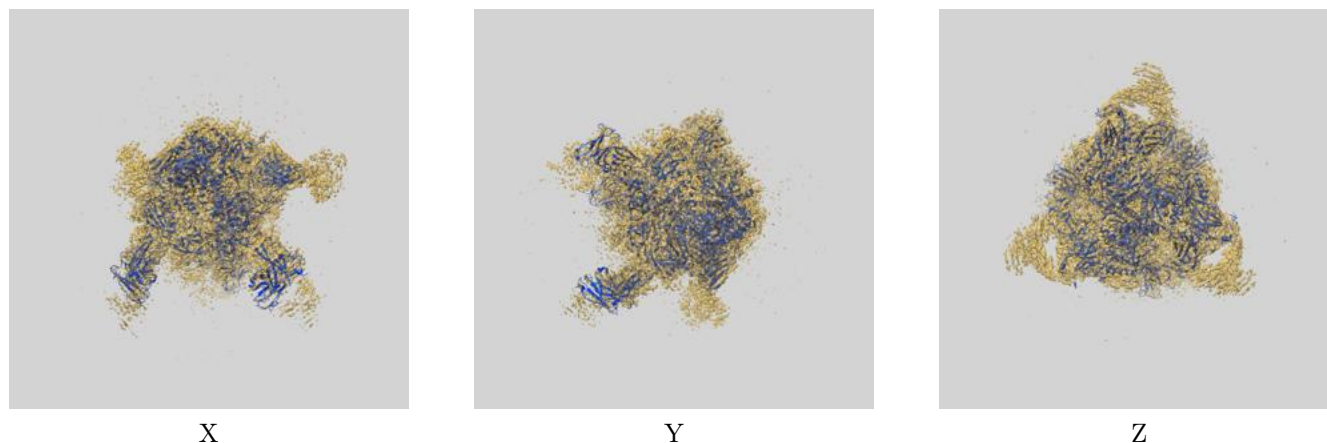
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.13	3.36	3.15
Unmasked-calculated*	3.54	3.92	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

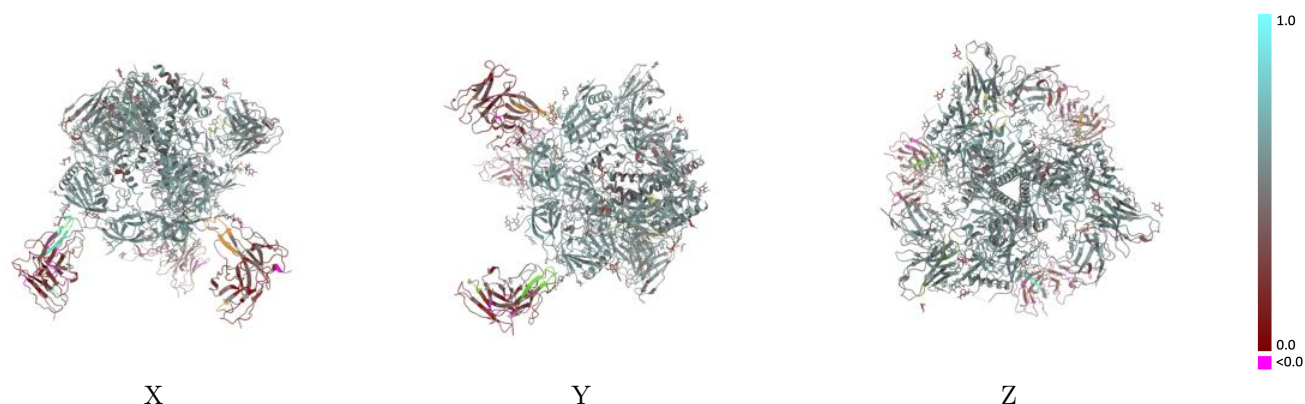
This section contains information regarding the fit between EMDB map EMD-27596 and PDB model 8DOK. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



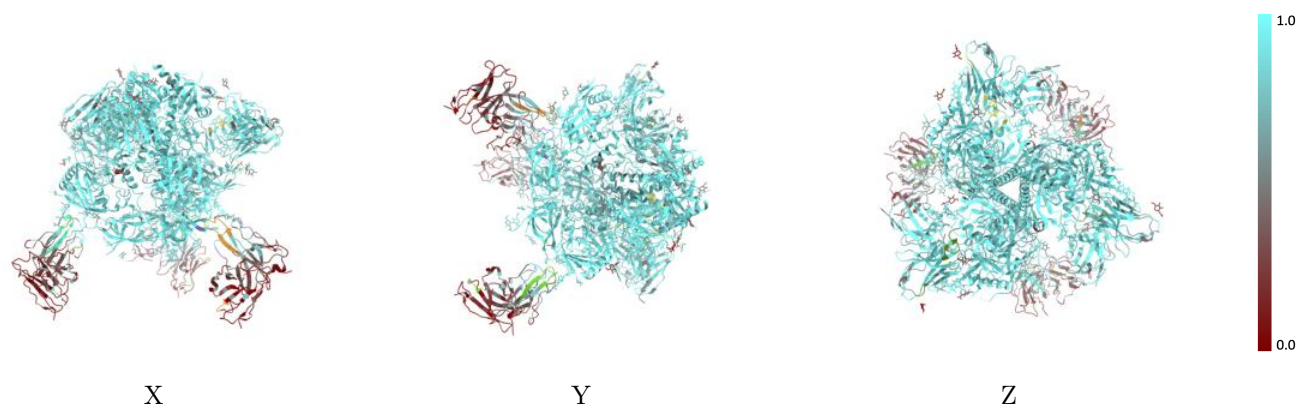
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



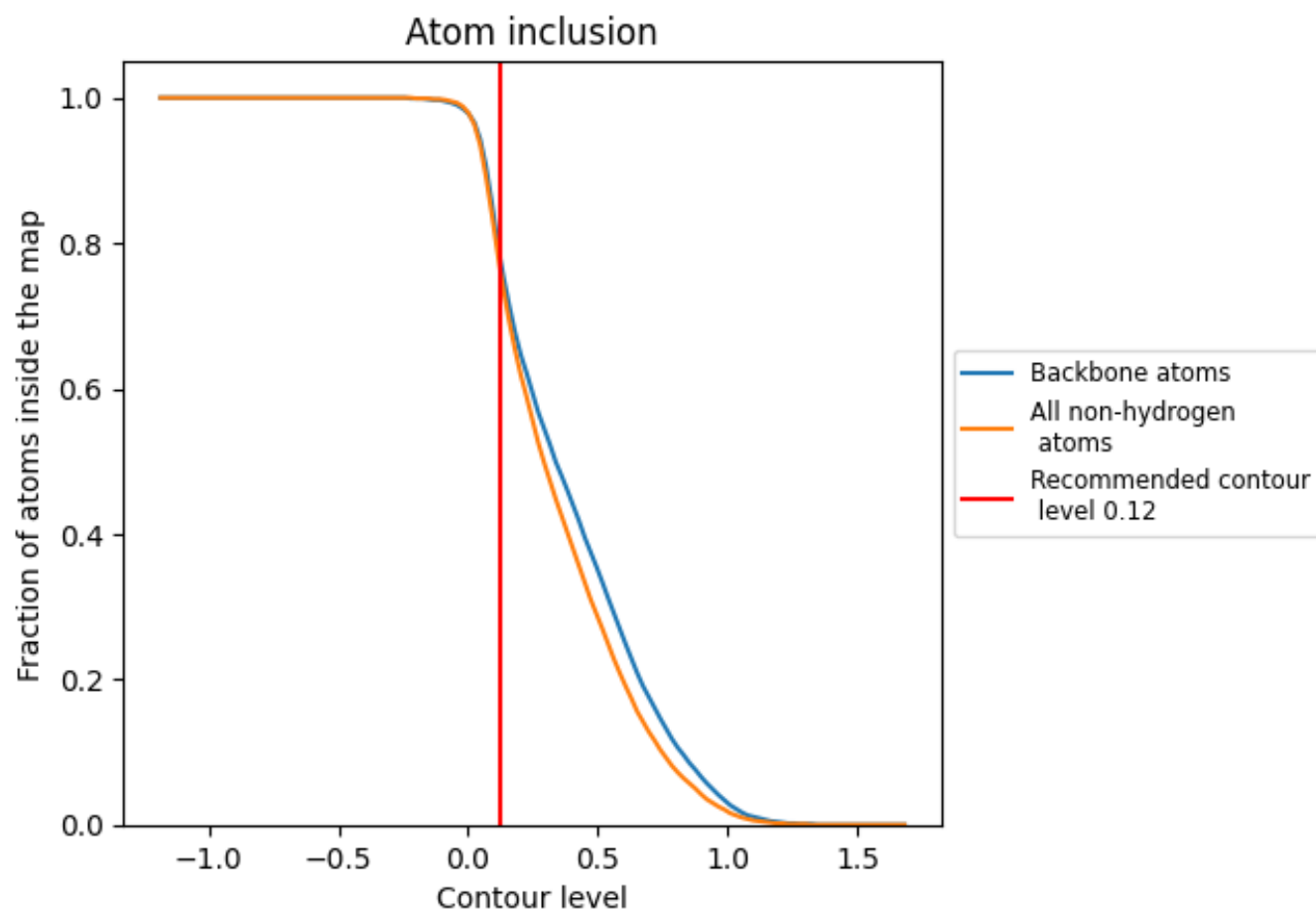
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7700	 0.4840
A	 0.8950	 0.5470
B	 0.8690	 0.5240
C	 0.8670	 0.5220
D	 0.8360	 0.5120
E	 0.8920	 0.5480
F	 0.8530	 0.5180
G	 0.8720	 0.5290
H	 0.8340	 0.5040
I	 0.8910	 0.5420
J	 0.8570	 0.5140
K	 0.8570	 0.5270
L	 0.8350	 0.5080
M	 0.3250	 0.3050
N	 0.4610	 0.3350
O	 0.3390	 0.2950
P	 0.4200	 0.3050
Q	 0.3390	 0.2970
R	 0.4500	 0.3270
S	 0.9140	 0.5360
T	 0.9490	 0.5410
U	 0.8040	 0.4310
V	 0.7500	 0.4680
W	 0.9230	 0.5560
X	 0.9230	 0.5220
Y	 0.8880	 0.5260
Z	 0.7220	 0.4570
b	 0.8040	 0.4420
g	 0.8970	 0.5470
h	 0.8970	 0.5290
i	 0.9330	 0.5370
j	 0.7380	 0.4390
l	 0.7860	 0.4830
m	 0.8040	 0.4180
p	 0.8210	 0.4590



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Chain	Atom inclusion	Q-score
q	 0.7860	 0.4680
r	 0.9230	 0.5600
s	 0.9230	 0.5380