



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:22 PM UTC

PDB ID : 6E5P / pdb_00006e5p
EMDB ID : EMD-8981
Title : Backbone model based on cryo-EM map at 8.5 Å of domain-swapped, glycan-reactive, neutralizing antibody 2G12 bound to HIV-1 Env BG505 DS-SOSIP, which was also bound to CD4-binding site antibody VRC03
Authors : Acharya, P.; Kwong, P.D.
Deposited on : 2018-07-21
Resolution : 8.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

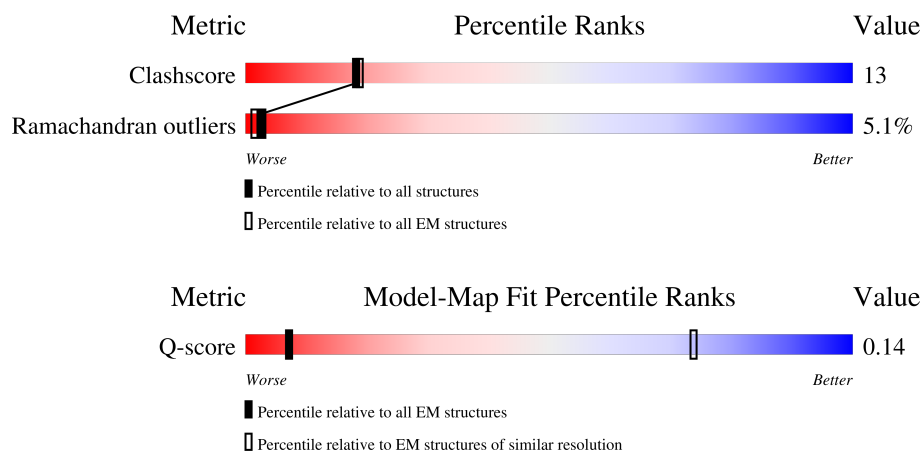
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 8.80 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	-
Q-score	-	25397	265 (8.30 - 9.30)

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	1	212	
1	4	212	
1	K	212	
1	L	212	
1	Q	212	

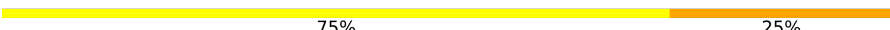
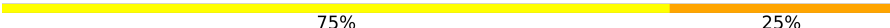
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Mol	Chain	Length	Quality of chain
1	T	212	
2	2	225	
2	3	225	
2	H	225	
2	M	225	
2	R	225	
2	S	225	
3	A	474	
3	C	474	
3	E	474	
4	B	170	
4	D	170	
4	F	170	
5	I	227	
5	O	227	
5	V	227	
6	J	208	
6	P	208	
6	W	208	
7	G	2	
7	N	2	
7	Y	2	
7	g	2	
7	h	2	
7	i	2	

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Mol	Chain	Length	Quality of chain
7	k	2	
7	l	2	
7	o	2	
8	U	6	
8	j	6	
8	m	6	
9	X	7	
9	Z	7	
9	b	7	
9	d	7	
9	f	7	
9	n	7	
10	a	4	
10	c	4	
10	e	4	

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
7	MAN	G	1	-	-	X	-
7	MAN	N	1	-	-	X	-
7	MAN	N	2	X	-	-	-
7	MAN	Y	1	-	-	X	-
7	MAN	Y	2	X	-	-	-
7	MAN	g	1	-	-	X	-
7	MAN	g	2	X	-	-	-
7	MAN	h	1	-	-	X	-
7	MAN	i	1	-	-	X	-
7	MAN	i	2	X	-	-	-
7	MAN	k	1	-	-	X	-
7	MAN	l	1	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	l	2	X	-	-	-
7	MAN	o	1	-	-	X	-
7	MAN	o	2	X	-	-	-
9	MAN	X	7	-	-	X	-
9	MAN	Z	4	-	-	X	-
9	MAN	Z	5	-	-	X	-
9	MAN	Z	7	-	-	X	-
9	MAN	b	4	-	-	X	-
9	MAN	b	5	-	-	X	-
9	MAN	b	7	-	-	X	-
9	MAN	d	5	-	-	X	-
9	MAN	d	7	-	-	X	-
9	MAN	f	7	-	-	X	-
9	MAN	n	7	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21252 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 2G12 Light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	212	Total	C	N	O	0	0
			848	424	212	212		
1	4	212	Total	C	N	O	0	0
			848	424	212	212		
1	K	212	Total	C	N	O	0	0
			848	424	212	212		
1	L	212	Total	C	N	O	0	0
			848	424	212	212		
1	Q	212	Total	C	N	O	0	0
			848	424	212	212		
1	T	212	Total	C	N	O	0	0
			848	424	212	212		

- Molecule 2 is a protein called 2G12 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	225	Total	C	N	O	0	0
			900	450	225	225		
2	3	225	Total	C	N	O	0	0
			900	450	225	225		
2	H	225	Total	C	N	O	0	0
			900	450	225	225		
2	M	225	Total	C	N	O	0	0
			900	450	225	225		
2	R	225	Total	C	N	O	0	0
			900	450	225	225		
2	S	225	Total	C	N	O	0	0
			900	450	225	225		

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	453	Total	C	N	O	0	0
			1812	906	453	453		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	453	Total	C	N	O	0	0
			1812	906	453	453		
3	E	453	Total	C	N	O	0	0
			1812	906	453	453		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	CYS	ILE	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	433	CYS	ALA	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
E	201	CYS	ILE	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	433	CYS	ALA	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	126	Total	C	N	O	0	0
			504	252	126	126		
4	D	126	Total	C	N	O	0	0
			504	252	126	126		
4	F	126	Total	C	N	O	0	0
			504	252	126	126		

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S9
B	605	CYS	THR	conflict	UNP Q2N0S9
B	665	GLY	-	expression tag	UNP Q2N0S9
B	666	SER	-	expression tag	UNP Q2N0S9
B	667	ALA	-	expression tag	UNP Q2N0S9
B	668	PRO	-	expression tag	UNP Q2N0S9
B	669	THR	-	expression tag	UNP Q2N0S9
B	670	LYS	-	expression tag	UNP Q2N0S9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	671	ALA	-	expression tag	UNP Q2N0S9
B	672	LYS	-	expression tag	UNP Q2N0S9
B	673	ARG	-	expression tag	UNP Q2N0S9
B	674	ARG	-	expression tag	UNP Q2N0S9
B	675	VAL	-	expression tag	UNP Q2N0S9
B	676	VAL	-	expression tag	UNP Q2N0S9
B	677	GLN	-	expression tag	UNP Q2N0S9
B	678	ARG	-	expression tag	UNP Q2N0S9
B	679	GLU	-	expression tag	UNP Q2N0S9
B	680	LYS	-	expression tag	UNP Q2N0S9
B	681	ARG	-	expression tag	UNP Q2N0S9
D	559	PRO	ILE	conflict	UNP Q2N0S9
D	605	CYS	THR	conflict	UNP Q2N0S9
D	665	GLY	-	expression tag	UNP Q2N0S9
D	666	SER	-	expression tag	UNP Q2N0S9
D	667	ALA	-	expression tag	UNP Q2N0S9
D	668	PRO	-	expression tag	UNP Q2N0S9
D	669	THR	-	expression tag	UNP Q2N0S9
D	670	LYS	-	expression tag	UNP Q2N0S9
D	671	ALA	-	expression tag	UNP Q2N0S9
D	672	LYS	-	expression tag	UNP Q2N0S9
D	673	ARG	-	expression tag	UNP Q2N0S9
D	674	ARG	-	expression tag	UNP Q2N0S9
D	675	VAL	-	expression tag	UNP Q2N0S9
D	676	VAL	-	expression tag	UNP Q2N0S9
D	677	GLN	-	expression tag	UNP Q2N0S9
D	678	ARG	-	expression tag	UNP Q2N0S9
D	679	GLU	-	expression tag	UNP Q2N0S9
D	680	LYS	-	expression tag	UNP Q2N0S9
D	681	ARG	-	expression tag	UNP Q2N0S9
F	559	PRO	ILE	conflict	UNP Q2N0S9
F	605	CYS	THR	conflict	UNP Q2N0S9
F	665	GLY	-	expression tag	UNP Q2N0S9
F	666	SER	-	expression tag	UNP Q2N0S9
F	667	ALA	-	expression tag	UNP Q2N0S9
F	668	PRO	-	expression tag	UNP Q2N0S9
F	669	THR	-	expression tag	UNP Q2N0S9
F	670	LYS	-	expression tag	UNP Q2N0S9
F	671	ALA	-	expression tag	UNP Q2N0S9
F	672	LYS	-	expression tag	UNP Q2N0S9
F	673	ARG	-	expression tag	UNP Q2N0S9
F	674	ARG	-	expression tag	UNP Q2N0S9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	675	VAL	-	expression tag	UNP Q2N0S9
F	676	VAL	-	expression tag	UNP Q2N0S9
F	677	GLN	-	expression tag	UNP Q2N0S9
F	678	ARG	-	expression tag	UNP Q2N0S9
F	679	GLU	-	expression tag	UNP Q2N0S9
F	680	LYS	-	expression tag	UNP Q2N0S9
F	681	ARG	-	expression tag	UNP Q2N0S9

- Molecule 5 is a protein called VRC03 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	128	Total	C	N	O	0	0
			512	256	128	128		
5	O	128	Total	C	N	O	0	0
			512	256	128	128		
5	V	128	Total	C	N	O	0	0
			512	256	128	128		

- Molecule 6 is a protein called VRC03 Light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	101	Total	C	N	O	0	0
			404	202	101	101		
6	P	101	Total	C	N	O	0	0
			404	202	101	101		
6	W	101	Total	C	N	O	0	0
			404	202	101	101		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



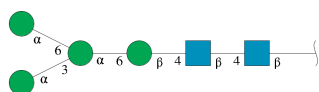
Mol	Chain	Residues	Atoms			AltConf	Trace
7	G	2	Total	C	O	0	0
			22	12	10		
7	N	2	Total	C	O	0	0
			22	12	10		
7	Y	2	Total	C	O	0	0
			22	12	10		

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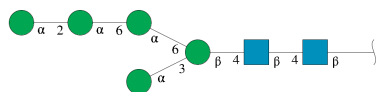
Mol	Chain	Residues	Atoms			AltConf	Trace
7	g	2	Total	C	O	0	0
			22	12	10		
7	h	2	Total	C	O	0	0
			22	12	10		
7	i	2	Total	C	O	0	0
			22	12	10		
7	k	2	Total	C	O	0	0
			22	12	10		
7	l	2	Total	C	O	0	0
			22	12	10		
7	o	2	Total	C	O	0	0
			22	12	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
8	U	6	Total	C	N	O	0	0
			72	40	2	30		
8	j	6	Total	C	N	O	0	0
			72	40	2	30		
8	m	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
9	X	7	Total	C	N	O	0	0
			84	46	2	36		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	7	Total	C	N	O	0	0
			84	46	2	36		
9	b	7	Total	C	N	O	0	0
			84	46	2	36		
9	d	7	Total	C	N	O	0	0
			84	46	2	36		
9	f	7	Total	C	N	O	0	0
			84	46	2	36		
9	n	7	Total	C	N	O	0	0
			84	46	2	36		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

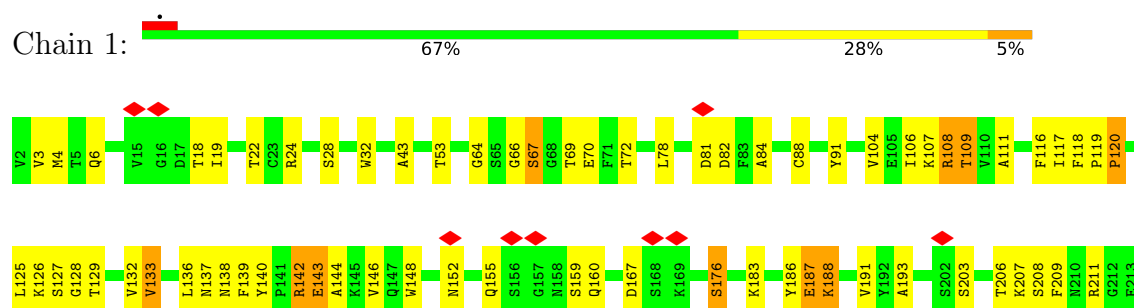


Mol	Chain	Residues	Atoms				AltConf	Trace
10	a	4	Total	C	N	O	0	0
			50	28	2	20		
10	c	4	Total	C	N	O	0	0
			50	28	2	20		
10	e	4	Total	C	N	O	0	0
			50	28	2	20		

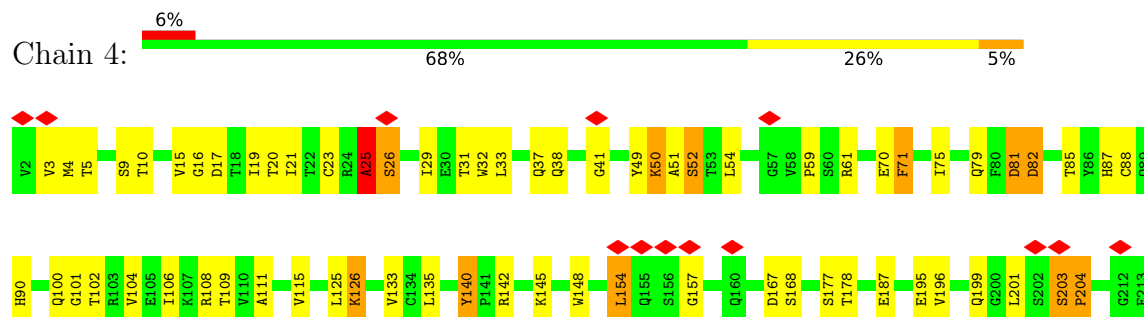
3 Residue-property plots

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.

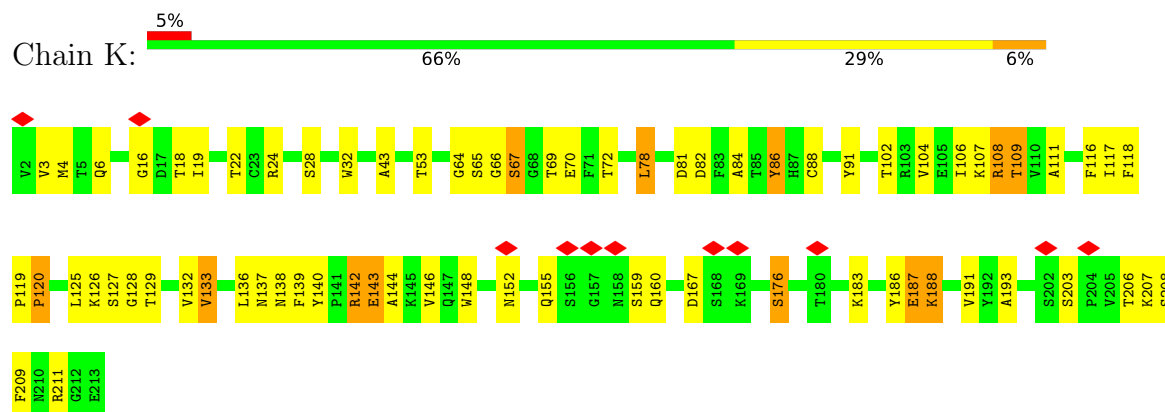
- Molecule 1: 2G12 Light chain



- Molecule 1: 2G12 Light chain

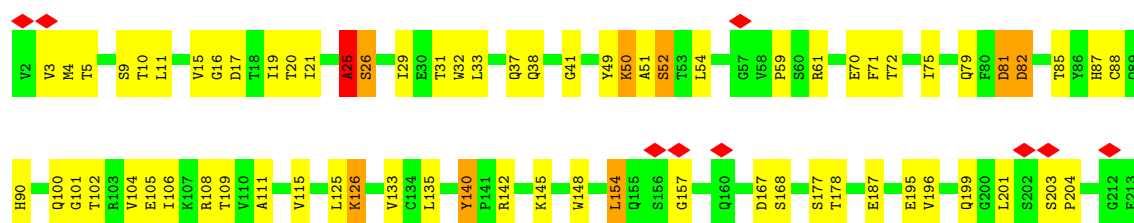


- Molecule 1: 2G12 Light chain



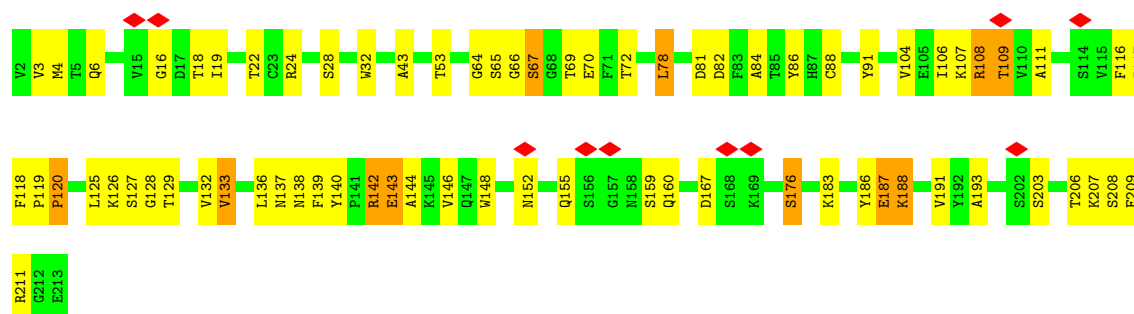
- Molecule 1: 2G12 Light chain

Chain L:  67% 29%



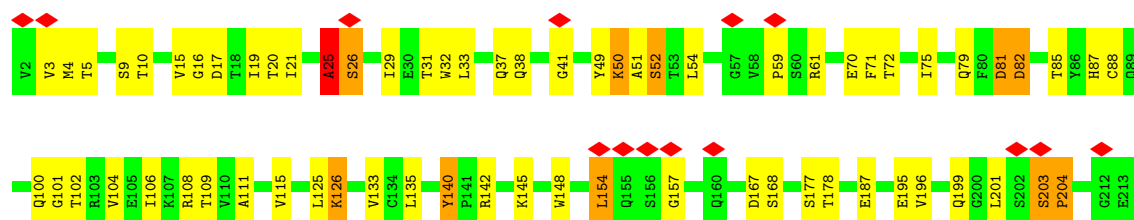
• Molecule 1: 2G12 Light chain

Chain Q:  5% 66% 29% 5%



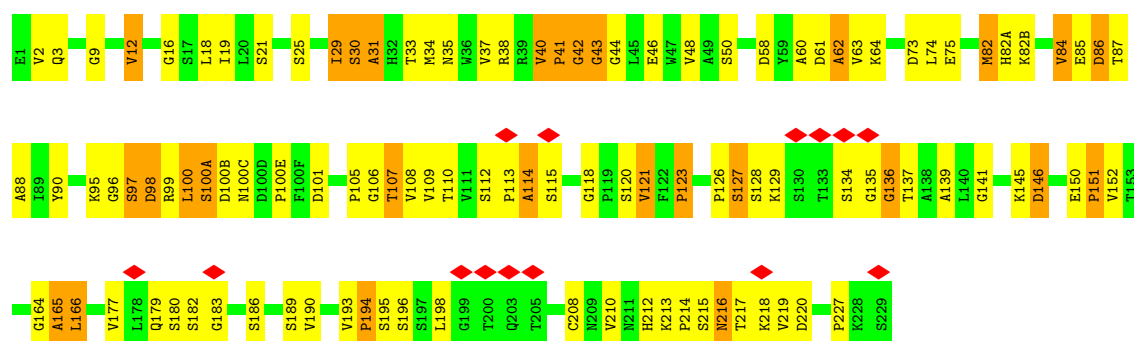
• Molecule 1: 2G12 Light chain

Chain T:  7% 68% 27% 5%

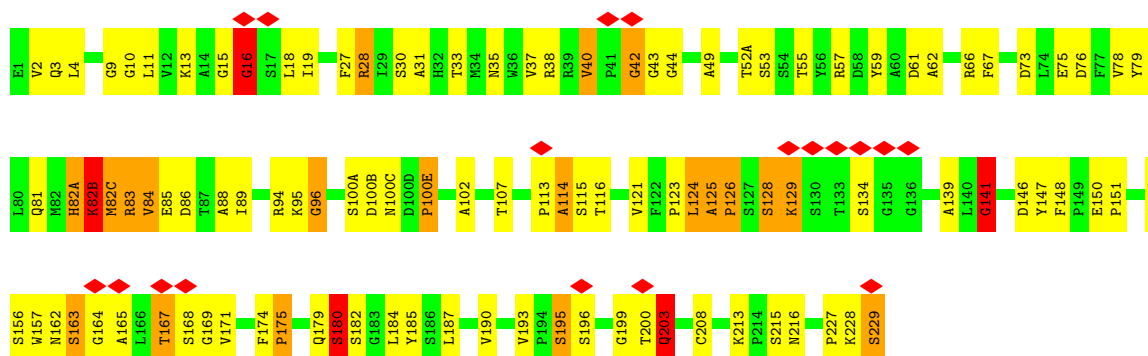


• Molecule 2: 2G12 heavy chain

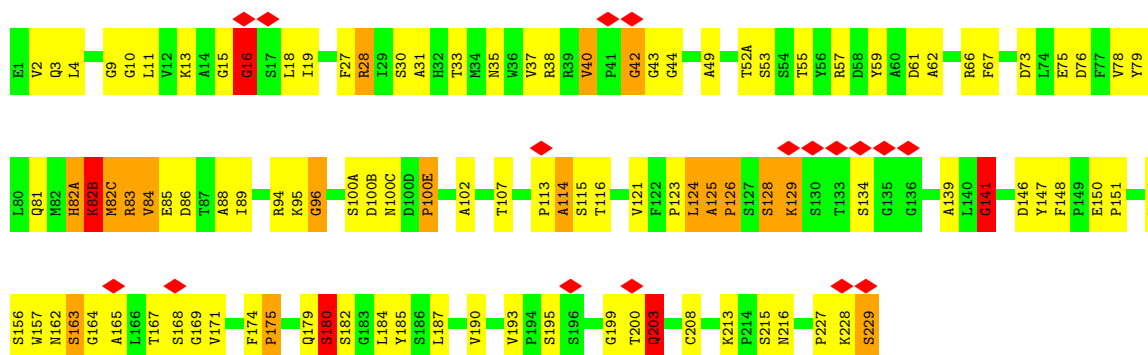
Chain 2:  7% 51% 37% 12%



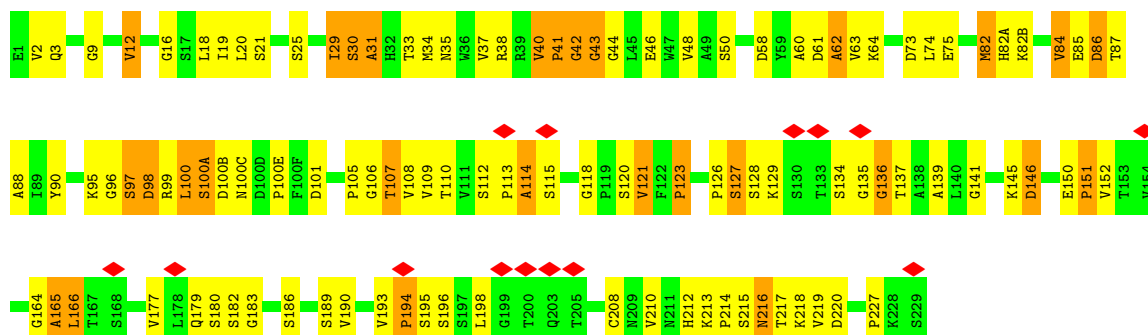
• Molecule 2: 2G12 heavy chain



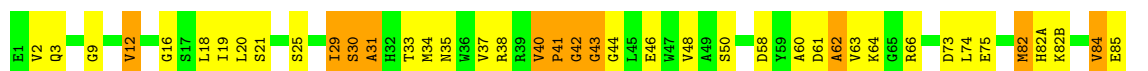
• Molecule 2: 2G12 heavy chain



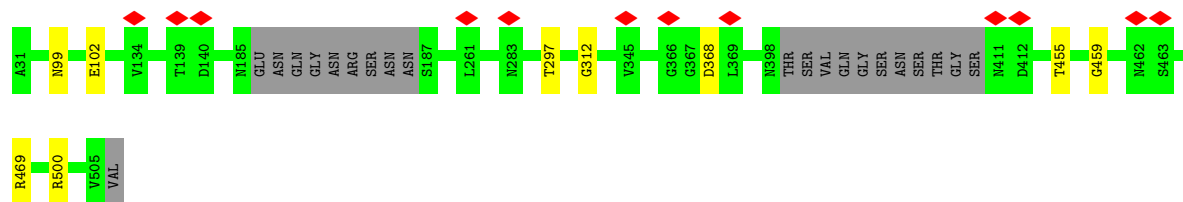
• Molecule 2: 2G12 heavy chain



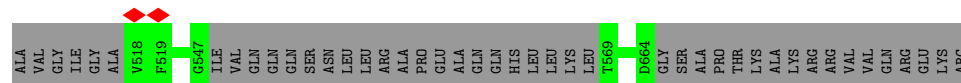
• Molecule 2: 2G12 heavy chain



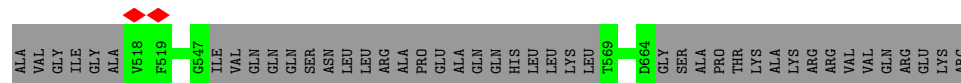
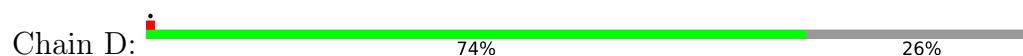




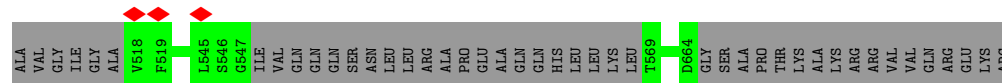
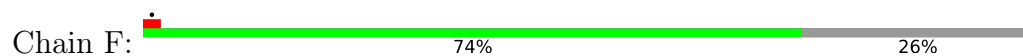
- Molecule 4: Envelope glycoprotein gp160



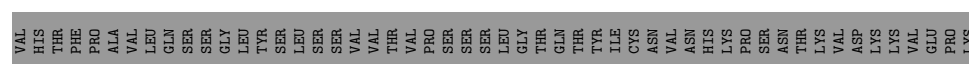
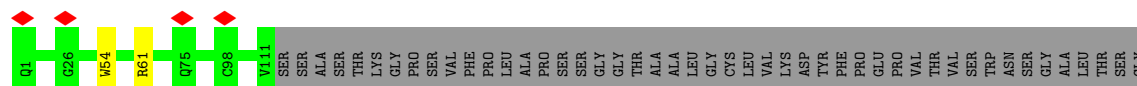
- Molecule 4: Envelope glycoprotein gp160



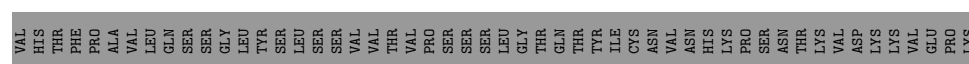
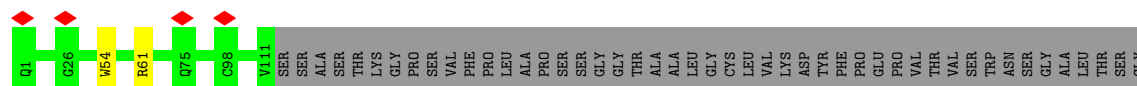
- Molecule 4: Envelope glycoprotein gp160



- Molecule 5: VRC03 heavy chain



- Molecule 5: VRC03 heavy chain



- Molecule 5: VRC03 heavy chain



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain N:



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain Y:



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain g:



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain h:



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain i:



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain k:



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain l:



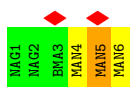
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain o:  100%



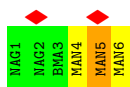
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  33% 50% 33% 17%



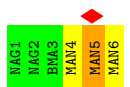
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  33% 50% 33% 17%



- Molecule 8: alpha-D-mannopyranose-(1-3)-[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

Chain m:  17% 50% 33% 17%



- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  29% 29% 71%



- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  29% 71%



- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  29% 71%



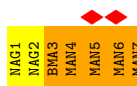
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  29% 71%



- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  29% 71%



- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  29% 71%



- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  75% 25%



- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	5245	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 ($e^-/\text{\AA}^2$)	63.84	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.203	Depositor
Minimum map value	-0.294	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.734	Depositor
Map size (Å)	420.9024, 420.9024, 420.9024	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0961, 1.0961, 1.0961	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	1	1.95	25/847 (3.0%)	2.23	38/1057 (3.6%)
1	4	2.18	27/847 (3.2%)	2.42	45/1057 (4.3%)
1	K	1.95	26/847 (3.1%)	2.23	38/1057 (3.6%)
1	L	2.18	28/847 (3.3%)	2.42	45/1057 (4.3%)
1	Q	1.95	26/847 (3.1%)	2.23	38/1057 (3.6%)
1	T	2.18	28/847 (3.3%)	2.42	45/1057 (4.3%)
2	2	1.92	19/899 (2.1%)	2.44	58/1122 (5.2%)
2	3	2.17	33/899 (3.7%)	2.42	71/1122 (6.3%)
2	H	2.16	32/899 (3.6%)	2.42	69/1122 (6.1%)
2	M	1.92	20/899 (2.2%)	2.44	58/1122 (5.2%)
2	R	1.93	20/899 (2.2%)	2.44	59/1122 (5.3%)
2	S	2.17	34/899 (3.8%)	2.42	69/1122 (6.1%)
3	A	0.39	0/1809	1.03	1/2256 (0.0%)
3	C	0.39	0/1809	1.03	1/2256 (0.0%)
3	E	0.39	0/1809	1.03	1/2256 (0.0%)
4	B	0.38	0/502	1.00	0/624
4	D	0.38	0/502	1.00	0/624
4	F	0.38	0/502	1.00	0/624
5	I	0.46	0/511	0.86	0/637
5	O	0.46	0/511	0.86	0/637
5	V	0.46	0/511	0.86	0/637
6	J	0.51	0/403	0.88	0/502
6	P	0.52	0/403	0.88	0/502
6	W	0.51	0/403	0.87	0/502
All	All	1.51	318/20151 (1.6%)	1.85	636/25131 (2.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	4	0	1
1	K	0	1
1	L	0	1
1	Q	0	1
1	T	0	1
2	2	0	9
2	3	0	4
2	H	0	4
2	M	0	9
2	R	0	9
2	S	0	4
All	All	0	45

All (318) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	123	PRO	C-O	14.11	1.42	1.24
2	H	123	PRO	C-O	14.11	1.42	1.24
2	3	123	PRO	C-O	14.06	1.42	1.24
2	2	44	GLY	N-CA	10.54	1.58	1.45
2	M	44	GLY	N-CA	10.49	1.58	1.45
2	R	44	GLY	N-CA	10.49	1.58	1.45
1	Q	67	SER	N-CA	8.75	1.57	1.46
1	K	67	SER	N-CA	8.73	1.57	1.46
1	1	67	SER	N-CA	8.69	1.57	1.46
2	S	18	LEU	CA-C	-8.63	1.41	1.52
2	H	18	LEU	CA-C	-8.62	1.41	1.52
1	4	19	ILE	CA-C	-8.61	1.42	1.52
2	3	18	LEU	CA-C	-8.57	1.41	1.52
1	L	19	ILE	CA-C	-8.55	1.42	1.52
1	T	19	ILE	CA-C	-8.52	1.42	1.52
1	L	9	SER	C-O	8.42	1.33	1.24
1	T	9	SER	C-O	8.39	1.33	1.24
1	4	9	SER	C-O	8.36	1.33	1.24
1	1	66	GLY	C-N	8.13	1.45	1.33
1	K	66	GLY	C-N	8.08	1.45	1.33
1	Q	66	GLY	C-N	8.06	1.45	1.33
2	R	109	VAL	C-O	7.97	1.32	1.24
2	M	109	VAL	C-O	7.92	1.32	1.24
2	2	109	VAL	C-O	7.90	1.32	1.24
2	3	124	LEU	CA-C	7.83	1.62	1.53
2	H	124	LEU	CA-C	7.75	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	124	LEU	CA-C	7.71	1.62	1.53
2	H	28	ARG	CA-C	7.68	1.63	1.52
2	3	28	ARG	CA-C	7.67	1.63	1.52
2	S	28	ARG	CA-C	7.66	1.63	1.52
1	4	54	LEU	CA-C	7.56	1.62	1.52
1	4	90	HIS	N-CA	-7.54	1.37	1.46
1	L	54	LEU	CA-C	7.53	1.62	1.52
1	T	54	LEU	CA-C	7.53	1.62	1.52
1	Q	203	SER	CA-C	7.50	1.59	1.52
1	1	203	SER	CA-C	7.49	1.59	1.52
1	K	203	SER	CA-C	7.49	1.59	1.52
1	L	90	HIS	N-CA	-7.47	1.37	1.46
1	T	90	HIS	N-CA	-7.47	1.37	1.46
2	S	2	VAL	CA-C	7.39	1.61	1.52
2	3	2	VAL	CA-C	7.38	1.61	1.52
2	H	2	VAL	CA-C	7.36	1.61	1.52
2	S	229	SER	C-O	7.27	1.38	1.23
2	H	229	SER	C-O	7.25	1.38	1.23
2	3	44	GLY	C-O	7.24	1.31	1.23
2	H	44	GLY	C-O	7.24	1.31	1.23
2	3	229	SER	C-O	7.23	1.38	1.23
1	K	119	PRO	CA-C	7.21	1.58	1.52
1	L	4	MET	CA-C	-7.21	1.43	1.52
2	S	44	GLY	C-O	7.21	1.31	1.23
2	3	38	ARG	CA-C	-7.19	1.43	1.52
1	Q	119	PRO	CA-C	7.17	1.58	1.52
1	1	119	PRO	CA-C	7.17	1.58	1.52
1	4	4	MET	CA-C	-7.15	1.44	1.52
1	T	4	MET	CA-C	-7.15	1.44	1.52
1	4	21	ILE	CA-C	7.14	1.61	1.52
2	S	38	ARG	CA-C	-7.13	1.43	1.52
2	H	38	ARG	CA-C	-7.12	1.44	1.52
1	L	21	ILE	CA-C	7.10	1.61	1.52
1	T	21	ILE	CA-C	7.10	1.61	1.52
1	L	145	LYS	CA-C	-7.08	1.44	1.52
2	S	35	ASN	CA-C	-7.08	1.43	1.52
2	3	35	ASN	CA-C	-7.06	1.43	1.52
1	T	145	LYS	CA-C	-7.05	1.44	1.52
2	H	35	ASN	CA-C	-7.05	1.44	1.52
1	4	145	LYS	CA-C	-7.05	1.44	1.52
2	S	4	LEU	CA-C	6.97	1.61	1.52
2	H	4	LEU	CA-C	6.96	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	100(C)	ASN	CA-C	6.92	1.60	1.53
2	R	100(C)	ASN	CA-C	6.92	1.60	1.53
2	3	4	LEU	CA-C	6.91	1.60	1.52
2	M	100(C)	ASN	CA-C	6.89	1.60	1.53
2	3	82(B)	LYS	C-O	-6.88	1.15	1.24
2	S	82(B)	LYS	C-O	-6.85	1.15	1.24
2	H	82(B)	LYS	C-O	-6.84	1.15	1.24
2	2	121	VAL	CA-C	6.82	1.61	1.52
1	T	104	VAL	C-O	6.79	1.31	1.24
1	4	104	VAL	C-O	6.78	1.31	1.24
1	K	116	PHE	CA-C	6.78	1.61	1.52
1	L	104	VAL	C-O	6.76	1.31	1.24
1	1	116	PHE	CA-C	6.76	1.61	1.52
2	M	121	VAL	CA-C	6.75	1.61	1.52
1	Q	116	PHE	CA-C	6.74	1.61	1.52
2	M	43	GLY	N-CA	6.73	1.54	1.45
2	R	43	GLY	N-CA	6.71	1.54	1.45
2	2	43	GLY	N-CA	6.70	1.54	1.45
2	R	121	VAL	CA-C	6.68	1.61	1.52
2	R	35	ASN	CA-C	-6.64	1.44	1.52
2	2	35	ASN	CA-C	-6.64	1.44	1.52
2	M	35	ASN	CA-C	-6.59	1.44	1.52
2	3	100(E)	PRO	C-O	-6.56	1.15	1.24
2	3	213	LYS	CA-C	6.54	1.61	1.52
2	H	100(E)	PRO	C-O	-6.54	1.15	1.24
2	H	83	ARG	N-CA	6.53	1.53	1.45
1	4	37	GLN	CA-C	-6.52	1.44	1.52
2	S	100(E)	PRO	C-O	-6.50	1.15	1.24
2	3	83	ARG	N-CA	6.50	1.53	1.45
2	H	213	LYS	CA-C	6.50	1.61	1.52
2	S	213	LYS	CA-C	6.50	1.61	1.52
1	L	37	GLN	CA-C	-6.48	1.45	1.52
2	S	83	ARG	N-CA	6.48	1.53	1.45
1	T	37	GLN	CA-C	-6.47	1.45	1.52
1	1	209	PHE	CA-C	6.46	1.60	1.52
2	R	121	VAL	N-CA	6.45	1.54	1.46
2	M	121	VAL	N-CA	6.43	1.54	1.46
2	2	121	VAL	N-CA	6.41	1.54	1.46
1	K	209	PHE	CA-C	6.40	1.60	1.52
1	4	33	LEU	CA-C	-6.39	1.44	1.52
1	L	50	LYS	C-O	-6.39	1.16	1.23
1	Q	209	PHE	CA-C	6.38	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	50	LYS	C-O	-6.38	1.16	1.23
1	L	33	LEU	CA-C	-6.37	1.44	1.52
1	4	50	LYS	C-O	-6.37	1.16	1.23
1	1	193	ALA	CA-C	6.36	1.60	1.52
1	T	33	LEU	CA-C	-6.35	1.44	1.52
1	K	193	ALA	CA-C	6.35	1.60	1.52
1	1	106	ILE	CA-C	6.34	1.59	1.53
2	H	95	LYS	N-CA	-6.33	1.37	1.45
2	S	95	LYS	N-CA	-6.32	1.37	1.45
1	K	67	SER	CA-C	6.32	1.61	1.52
2	3	95	LYS	N-CA	-6.32	1.37	1.45
1	Q	67	SER	CA-C	6.31	1.61	1.52
1	1	67	SER	CA-C	6.30	1.61	1.52
1	Q	106	ILE	CA-C	6.30	1.59	1.53
1	K	106	ILE	CA-C	6.30	1.59	1.53
1	Q	193	ALA	CA-C	6.30	1.60	1.52
2	S	67	PHE	N-CA	6.28	1.54	1.46
2	H	67	PHE	N-CA	6.28	1.54	1.46
1	K	136	LEU	CA-C	-6.26	1.44	1.52
2	3	67	PHE	N-CA	6.23	1.53	1.46
1	Q	136	LEU	CA-C	-6.22	1.44	1.52
2	H	84	VAL	CA-C	-6.21	1.45	1.52
1	1	136	LEU	CA-C	-6.20	1.44	1.52
2	S	84	VAL	CA-C	-6.19	1.45	1.52
1	T	154	LEU	CA-C	6.18	1.61	1.52
1	4	154	LEU	CA-C	6.16	1.61	1.52
1	L	154	LEU	CA-C	6.16	1.61	1.52
2	3	84	VAL	CA-C	-6.13	1.45	1.52
2	H	180	SER	CA-C	6.13	1.60	1.52
2	3	180	SER	CA-C	6.13	1.60	1.52
2	S	180	SER	CA-C	6.12	1.60	1.52
2	H	10	GLY	C-O	6.11	1.30	1.23
2	S	10	GLY	C-O	6.09	1.30	1.23
1	T	201	LEU	CA-C	-6.09	1.45	1.52
1	1	78	LEU	CA-C	-6.08	1.45	1.52
1	K	78	LEU	CA-C	-6.07	1.45	1.52
1	4	201	LEU	CA-C	-6.06	1.45	1.52
2	3	10	GLY	C-O	6.06	1.30	1.23
1	1	88	CYS	CA-C	-6.05	1.45	1.52
1	1	24	ARG	CA-C	6.05	1.59	1.53
1	L	201	LEU	CA-C	-6.04	1.45	1.52
1	Q	78	LEU	CA-C	-6.03	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	88	CYS	CA-C	-6.03	1.45	1.52
1	Q	24	ARG	CA-C	6.02	1.59	1.53
1	Q	88	CYS	CA-C	-6.00	1.45	1.52
1	T	203	SER	CA-C	5.99	1.59	1.52
1	L	203	SER	CA-C	5.95	1.59	1.52
1	4	203	SER	CA-C	5.95	1.59	1.52
1	K	24	ARG	CA-C	5.93	1.59	1.53
1	1	3	VAL	CA-C	5.92	1.59	1.52
1	Q	3	VAL	CA-C	5.92	1.59	1.52
1	L	142	ARG	C-O	-5.91	1.17	1.24
1	T	142	ARG	C-O	-5.89	1.17	1.24
1	K	3	VAL	CA-C	5.88	1.59	1.52
2	R	34	MET	CA-C	-5.87	1.45	1.52
1	Q	108	ARG	CA-C	-5.86	1.45	1.52
2	2	34	MET	CA-C	-5.86	1.45	1.52
2	M	34	MET	CA-C	-5.86	1.45	1.52
1	4	142	ARG	C-O	-5.86	1.17	1.24
2	S	123	PRO	C-N	5.86	1.43	1.33
1	K	108	ARG	CA-C	-5.85	1.45	1.52
2	3	123	PRO	C-N	5.84	1.43	1.33
2	H	123	PRO	C-N	5.84	1.43	1.33
1	T	106	ILE	C-O	-5.83	1.17	1.24
1	1	108	ARG	CA-C	-5.83	1.45	1.52
1	T	29	ILE	C-O	5.83	1.31	1.24
1	L	106	ILE	C-O	-5.82	1.17	1.24
1	4	187	GLU	CA-C	5.81	1.60	1.52
1	4	106	ILE	C-O	-5.81	1.17	1.24
1	L	187	GLU	CA-C	5.80	1.60	1.52
1	L	29	ILE	C-O	5.79	1.30	1.24
1	4	29	ILE	C-O	5.78	1.30	1.24
1	T	187	GLU	CA-C	5.76	1.60	1.52
1	Q	32	TRP	CA-C	5.68	1.60	1.52
1	K	32	TRP	CA-C	5.67	1.60	1.52
2	H	61	ASP	N-CA	-5.67	1.39	1.46
1	1	32	TRP	CA-C	5.67	1.60	1.52
2	3	61	ASP	N-CA	-5.65	1.39	1.46
2	S	61	ASP	N-CA	-5.65	1.39	1.46
2	S	49	ALA	C-O	5.64	1.30	1.23
2	3	49	ALA	C-O	5.62	1.30	1.23
2	3	33	THR	C-O	-5.61	1.17	1.23
2	H	49	ALA	C-O	5.61	1.30	1.23
2	H	33	THR	C-O	-5.59	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	11	LEU	N-CA	5.58	1.52	1.46
2	S	33	THR	C-O	-5.57	1.17	1.23
2	S	11	LEU	N-CA	5.56	1.52	1.46
2	3	11	LEU	N-CA	5.55	1.52	1.46
1	Q	117	ILE	CA-C	5.53	1.59	1.52
1	K	117	ILE	CA-C	5.53	1.59	1.52
2	R	120	SER	CA-C	5.51	1.60	1.53
2	2	120	SER	CA-C	5.51	1.60	1.53
2	M	120	SER	CA-C	5.51	1.60	1.53
2	2	101	ASP	CA-C	5.50	1.60	1.52
1	K	125	LEU	CA-C	5.49	1.60	1.52
2	3	96	GLY	CA-C	5.48	1.59	1.51
2	S	96	GLY	CA-C	5.48	1.59	1.51
2	M	101	ASP	CA-C	5.48	1.60	1.52
2	M	38	ARG	CA-C	-5.48	1.45	1.52
1	T	85	THR	C-O	5.48	1.30	1.23
1	L	90	HIS	C-O	-5.47	1.16	1.23
2	H	96	GLY	CA-C	5.47	1.59	1.51
2	R	129	LYS	CA-C	5.46	1.58	1.52
1	T	90	HIS	C-O	-5.46	1.17	1.23
1	Q	125	LEU	CA-C	5.46	1.60	1.52
1	Q	129	THR	CA-C	5.46	1.59	1.52
1	1	125	LEU	CA-C	5.45	1.60	1.52
2	R	58	ASP	C-O	5.45	1.30	1.23
1	1	117	ILE	CA-C	5.45	1.58	1.52
2	2	58	ASP	C-O	5.44	1.30	1.23
1	4	90	HIS	C-O	-5.44	1.17	1.23
2	M	58	ASP	C-O	5.44	1.30	1.23
2	R	101	ASP	CA-C	5.44	1.60	1.52
1	Q	176	SER	C-O	5.44	1.30	1.24
1	L	85	THR	C-O	5.43	1.30	1.23
2	R	38	ARG	CA-C	-5.43	1.45	1.52
1	K	129	THR	CA-C	5.43	1.59	1.52
1	K	176	SER	C-O	5.42	1.30	1.24
1	1	129	THR	CA-C	5.42	1.58	1.52
1	4	32	TRP	CA-C	-5.42	1.47	1.53
2	2	38	ARG	CA-C	-5.42	1.45	1.52
1	1	176	SER	C-O	5.42	1.30	1.24
1	L	32	TRP	CA-C	-5.42	1.47	1.53
2	2	129	LYS	CA-C	5.41	1.57	1.52
2	M	129	LYS	CA-C	5.41	1.57	1.52
2	3	203	GLN	C-O	5.41	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	85	THR	C-O	5.41	1.30	1.23
2	2	218	LYS	CA-C	-5.41	1.46	1.52
2	3	190	VAL	CA-C	-5.41	1.46	1.52
1	T	32	TRP	CA-C	-5.40	1.47	1.53
2	H	203	GLN	C-O	5.38	1.30	1.24
2	S	190	VAL	CA-C	-5.38	1.46	1.52
2	S	203	GLN	C-O	5.38	1.30	1.24
2	H	190	VAL	CA-C	-5.37	1.46	1.52
2	M	218	LYS	CA-C	-5.37	1.46	1.52
1	1	107	LYS	C-O	5.35	1.30	1.23
2	R	218	LYS	CA-C	-5.34	1.46	1.52
2	M	46	GLU	CA-C	5.33	1.58	1.52
1	1	146	VAL	CA-C	-5.33	1.45	1.52
1	K	146	VAL	CA-C	-5.33	1.45	1.52
1	Q	107	LYS	C-O	5.33	1.30	1.23
2	R	46	GLU	CA-C	5.33	1.58	1.52
1	Q	146	VAL	CA-C	-5.32	1.45	1.52
1	K	107	LYS	C-O	5.31	1.30	1.23
2	S	208	CYS	CA-C	-5.31	1.46	1.52
2	2	46	GLU	CA-C	5.30	1.58	1.52
2	2	62	ALA	CA-C	5.30	1.59	1.52
2	3	40	VAL	CA-C	5.30	1.58	1.52
2	R	62	ALA	CA-C	5.29	1.59	1.52
2	M	62	ALA	CA-C	5.26	1.59	1.52
2	3	208	CYS	CA-C	-5.25	1.46	1.52
2	H	208	CYS	CA-C	-5.24	1.46	1.52
2	2	46	GLU	C-O	5.24	1.30	1.24
1	4	15	VAL	C-O	-5.23	1.18	1.24
1	L	135	LEU	C-O	-5.23	1.17	1.24
2	3	75	GLU	CA-C	-5.23	1.45	1.52
2	H	40	VAL	CA-C	5.23	1.58	1.52
1	L	15	VAL	C-O	-5.22	1.18	1.24
1	4	115	VAL	C-O	5.21	1.29	1.24
2	M	152	VAL	C-O	5.21	1.29	1.24
2	3	193	VAL	CA-C	5.20	1.58	1.52
1	L	115	VAL	C-O	5.20	1.29	1.24
1	T	15	VAL	C-O	-5.19	1.19	1.24
1	T	135	LEU	C-O	-5.19	1.17	1.24
2	H	193	VAL	CA-C	5.18	1.58	1.52
1	4	20	THR	CA-C	5.18	1.58	1.52
1	Q	70	GLU	N-CA	5.18	1.52	1.45
2	2	152	VAL	C-O	5.18	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	135	LEU	C-O	-5.17	1.17	1.24
1	1	43	ALA	CA-C	-5.17	1.46	1.53
2	R	152	VAL	C-O	5.17	1.29	1.24
2	S	193	VAL	CA-C	5.16	1.58	1.52
2	S	40	VAL	CA-C	5.16	1.58	1.52
1	K	70	GLU	N-CA	5.16	1.51	1.45
2	R	46	GLU	C-O	5.16	1.30	1.24
2	H	75	GLU	CA-C	-5.16	1.45	1.52
1	T	20	THR	CA-C	5.16	1.58	1.52
1	L	20	THR	CA-C	5.15	1.58	1.52
2	M	46	GLU	C-O	5.15	1.30	1.24
2	S	75	GLU	CA-C	-5.14	1.45	1.52
1	T	115	VAL	C-O	5.14	1.29	1.24
2	R	100(C)	ASN	C-N	5.14	1.45	1.34
1	1	70	GLU	N-CA	5.13	1.51	1.45
1	Q	43	ALA	CA-C	-5.13	1.46	1.53
1	K	43	ALA	CA-C	-5.13	1.46	1.53
1	L	52	SER	CA-C	-5.13	1.45	1.52
2	H	89	ILE	C-O	5.13	1.30	1.24
2	2	100(C)	ASN	C-N	5.12	1.45	1.34
2	M	100(C)	ASN	C-N	5.12	1.45	1.34
2	3	89	ILE	C-O	5.10	1.30	1.24
1	T	52	SER	CA-C	-5.10	1.45	1.52
2	S	89	ILE	C-O	5.10	1.30	1.24
1	4	52	SER	CA-C	-5.08	1.45	1.52
2	R	20	LEU	CA-C	-5.08	1.46	1.53
1	1	18	THR	CA-C	-5.07	1.46	1.53
1	T	167	ASP	CA-C	-5.07	1.45	1.52
1	T	72	THR	CA-C	-5.06	1.46	1.52
2	S	82	MET	C-O	-5.06	1.17	1.24
1	L	167	ASP	CA-C	-5.05	1.45	1.52
1	4	167	ASP	CA-C	-5.04	1.45	1.52
1	K	18	THR	CA-C	-5.04	1.46	1.53
1	L	72	THR	CA-C	-5.03	1.46	1.52
1	Q	18	THR	CA-C	-5.03	1.46	1.53
2	M	20	LEU	CA-C	-5.03	1.46	1.53
1	K	86	TYR	CA-C	-5.03	1.46	1.53
1	Q	86	TYR	CA-C	-5.03	1.46	1.53
2	3	94	ARG	N-CA	-5.01	1.39	1.45
2	S	32	HIS	CA-C	-5.00	1.46	1.52

All (636) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	96	GLY	N-CA-C	16.34	138.55	111.27
2	M	96	GLY	N-CA-C	16.33	138.54	111.27
2	R	96	GLY	N-CA-C	16.32	138.52	111.27
1	Q	133	VAL	N-CA-C	12.66	127.60	108.23
1	1	133	VAL	N-CA-C	12.65	127.58	108.23
1	K	133	VAL	N-CA-C	12.64	127.57	108.23
1	4	140	TYR	N-CA-C	-11.94	97.48	108.22
1	T	140	TYR	N-CA-C	-11.94	97.48	108.22
1	L	140	TYR	N-CA-C	-11.92	97.49	108.22
2	H	66	ARG	N-CA-C	-10.77	98.77	114.39
2	3	66	ARG	N-CA-C	-10.76	98.79	114.39
2	S	66	ARG	N-CA-C	-10.76	98.79	114.39
1	1	148	TRP	N-CA-C	-10.12	93.53	109.72
1	K	148	TRP	N-CA-C	-10.08	93.59	109.72
1	Q	148	TRP	N-CA-C	-10.08	93.59	109.72
2	R	121	VAL	N-CA-C	9.71	129.53	109.34
2	M	121	VAL	N-CA-C	9.68	129.48	109.34
2	2	121	VAL	N-CA-C	9.68	129.47	109.34
1	1	160	GLN	N-CA-C	9.53	123.94	108.41
1	Q	160	GLN	N-CA-C	9.53	123.94	108.41
1	K	160	GLN	N-CA-C	9.52	123.93	108.41
2	3	2	VAL	N-CA-C	9.27	121.54	109.58
2	H	2	VAL	N-CA-C	9.27	121.53	109.58
2	S	2	VAL	N-CA-C	9.25	121.51	109.58
1	K	3	VAL	N-CA-C	9.10	120.91	108.17
1	1	3	VAL	N-CA-C	9.07	120.87	108.17
1	Q	3	VAL	N-CA-C	9.07	120.87	108.17
1	L	59	PRO	CA-C-N	-9.03	109.72	123.17
1	L	59	PRO	C-N-CA	-9.03	109.72	123.17
1	4	59	PRO	CA-C-N	-9.02	109.73	123.17
1	4	59	PRO	C-N-CA	-9.02	109.73	123.17
1	T	59	PRO	CA-C-N	-9.02	109.74	123.17
1	T	59	PRO	C-N-CA	-9.02	109.74	123.17
2	S	3	GLN	N-CA-C	8.97	123.42	109.52
2	3	3	GLN	N-CA-C	8.97	123.42	109.52
2	H	3	GLN	N-CA-C	8.97	123.42	109.52
2	3	78	VAL	N-CA-C	-8.92	96.58	108.35
2	S	78	VAL	N-CA-C	-8.87	96.64	108.35
2	H	78	VAL	N-CA-C	-8.87	96.65	108.35
2	S	114	ALA	N-CA-C	-8.75	97.17	110.30
2	H	114	ALA	N-CA-C	-8.74	97.19	110.30
2	3	114	ALA	N-CA-C	-8.72	97.22	110.30
2	R	95	LYS	N-CA-C	8.68	125.00	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	95	LYS	N-CA-C	8.67	124.99	113.72
2	2	95	LYS	N-CA-C	8.65	124.97	113.72
1	1	137	ASN	N-CA-C	8.30	121.03	110.24
1	K	137	ASN	N-CA-C	8.30	121.03	110.24
1	Q	137	ASN	N-CA-C	8.30	121.03	110.24
2	S	19	ILE	N-CA-C	-8.23	98.20	109.55
2	3	19	ILE	N-CA-C	-8.22	98.21	109.55
2	H	19	ILE	N-CA-C	-8.20	98.24	109.55
1	L	102	THR	CA-C-N	-8.16	111.63	123.05
1	L	102	THR	C-N-CA	-8.16	111.63	123.05
1	T	102	THR	CA-C-N	-8.15	111.64	123.05
1	T	102	THR	C-N-CA	-8.15	111.64	123.05
1	4	102	THR	CA-C-N	-8.14	111.65	123.05
1	4	102	THR	C-N-CA	-8.14	111.65	123.05
2	H	11	LEU	N-CA-C	8.09	123.02	109.76
2	S	11	LEU	N-CA-C	8.08	123.01	109.76
2	3	11	LEU	N-CA-C	8.06	122.98	109.76
2	2	183	GLY	N-CA-C	-8.02	103.45	115.00
2	M	183	GLY	N-CA-C	-8.01	103.46	115.00
2	R	183	GLY	N-CA-C	-8.00	103.48	115.00
1	L	203	SER	N-CA-C	7.97	121.15	108.23
1	T	203	SER	N-CA-C	7.97	121.14	108.23
1	4	203	SER	N-CA-C	7.96	121.12	108.23
2	M	21	SER	N-CA-C	7.94	121.79	108.13
2	R	21	SER	N-CA-C	7.94	121.78	108.13
2	2	21	SER	N-CA-C	7.93	121.77	108.13
2	3	86	ASP	N-CA-C	-7.90	103.54	113.02
2	S	86	ASP	N-CA-C	-7.90	103.54	113.02
2	H	86	ASP	N-CA-C	-7.90	103.54	113.02
1	4	199	GLN	N-CA-C	-7.87	103.47	113.23
1	L	199	GLN	N-CA-C	-7.85	103.50	113.23
1	T	199	GLN	N-CA-C	-7.84	103.51	113.23
1	T	41	GLY	CA-C-N	-7.82	107.25	122.02
1	T	41	GLY	C-N-CA	-7.82	107.25	122.02
2	R	150	GLU	N-CA-C	-7.79	99.92	110.36
1	4	41	GLY	CA-C-N	-7.79	107.30	122.02
1	4	41	GLY	C-N-CA	-7.79	107.30	122.02
1	L	41	GLY	CA-C-N	-7.78	107.31	122.02
1	L	41	GLY	C-N-CA	-7.78	107.31	122.02
2	M	150	GLU	N-CA-C	-7.77	99.94	110.36
2	2	150	GLU	N-CA-C	-7.77	99.95	110.36
2	3	62	ALA	CA-C-N	-7.74	111.96	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	62	ALA	C-N-CA	-7.74	111.96	122.72
1	K	70	GLU	N-CA-C	7.74	122.26	109.95
2	M	42	GLY	N-CA-C	-7.74	103.75	114.67
1	Q	70	GLU	N-CA-C	7.73	122.25	109.95
2	R	42	GLY	N-CA-C	-7.73	103.78	114.67
1	1	70	GLU	N-CA-C	7.72	122.22	109.95
2	2	42	GLY	N-CA-C	-7.71	103.79	114.67
2	H	62	ALA	CA-C-N	-7.70	112.02	122.72
2	H	62	ALA	C-N-CA	-7.70	112.02	122.72
2	S	62	ALA	CA-C-N	-7.67	112.06	122.72
2	S	62	ALA	C-N-CA	-7.67	112.06	122.72
2	3	150	GLU	N-CA-C	-7.67	100.35	110.40
2	H	150	GLU	N-CA-C	-7.67	100.36	110.40
1	L	102	THR	N-CA-C	7.67	121.02	108.52
1	T	102	THR	N-CA-C	7.65	120.99	108.52
1	4	115	VAL	N-CA-C	7.65	119.33	108.17
1	4	102	THR	N-CA-C	7.65	120.98	108.52
1	T	115	VAL	N-CA-C	7.64	119.33	108.17
1	L	115	VAL	N-CA-C	7.64	119.33	108.17
2	S	150	GLU	N-CA-C	-7.64	100.39	110.40
1	1	119	PRO	CA-C-N	7.61	129.35	119.84
1	1	119	PRO	C-N-CA	7.61	129.35	119.84
1	Q	119	PRO	CA-C-N	7.59	129.33	119.84
1	Q	119	PRO	C-N-CA	7.59	129.33	119.84
1	K	119	PRO	CA-C-N	7.59	129.33	119.84
1	K	119	PRO	C-N-CA	7.59	129.33	119.84
2	3	94	ARG	CA-C-N	-7.25	110.73	122.26
2	3	94	ARG	C-N-CA	-7.25	110.73	122.26
1	T	70	GLU	CA-C-N	-7.25	110.64	122.82
1	T	70	GLU	C-N-CA	-7.25	110.64	122.82
2	2	120	SER	N-CA-C	7.25	121.82	112.26
2	H	94	ARG	CA-C-N	-7.24	110.75	122.26
2	H	94	ARG	C-N-CA	-7.24	110.75	122.26
2	S	94	ARG	CA-C-N	-7.24	110.75	122.26
2	S	94	ARG	C-N-CA	-7.24	110.75	122.26
1	L	70	GLU	CA-C-N	-7.23	110.67	122.82
1	L	70	GLU	C-N-CA	-7.23	110.67	122.82
2	R	120	SER	N-CA-C	7.23	121.81	112.26
1	4	70	GLU	CA-C-N	-7.23	110.68	122.82
1	4	70	GLU	C-N-CA	-7.23	110.68	122.82
2	M	120	SER	N-CA-C	7.21	121.78	112.26
1	L	178	THR	N-CA-C	7.17	120.56	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	13	LYS	N-CA-C	-7.16	98.94	110.32
2	S	13	LYS	N-CA-C	-7.16	98.94	110.32
1	4	178	THR	N-CA-C	7.15	120.53	108.02
2	3	13	LYS	N-CA-C	-7.15	98.96	110.32
1	T	178	THR	N-CA-C	7.14	120.52	108.02
1	T	177	SER	N-CA-C	7.14	120.54	108.90
2	3	82(A)	HIS	N-CA-C	7.13	119.31	109.18
2	H	82(A)	HIS	N-CA-C	7.12	119.29	109.18
1	L	177	SER	N-CA-C	7.12	120.50	108.90
2	S	82(A)	HIS	N-CA-C	7.11	119.28	109.18
1	4	177	SER	N-CA-C	7.10	120.48	108.90
2	M	214	PRO	N-CA-C	-6.97	105.46	114.03
2	2	214	PRO	N-CA-C	-6.96	105.46	114.03
1	T	100	GLN	N-CA-C	-6.96	104.26	112.89
2	R	214	PRO	N-CA-C	-6.96	105.47	114.03
1	4	100	GLN	N-CA-C	-6.95	104.27	112.89
1	T	5	THR	N-CA-C	6.95	121.66	107.69
1	L	5	THR	N-CA-C	6.95	121.66	107.69
1	L	100	GLN	N-CA-C	-6.93	104.29	112.89
2	H	52(A)	THR	N-CA-C	-6.93	101.59	110.53
1	4	5	THR	N-CA-C	6.93	121.62	107.69
2	3	52(A)	THR	N-CA-C	-6.92	101.61	110.53
2	3	102	ALA	CA-C-N	-6.91	109.62	121.85
2	3	102	ALA	C-N-CA	-6.91	109.62	121.85
2	S	52(A)	THR	N-CA-C	-6.90	101.62	110.53
2	S	102	ALA	CA-C-N	-6.90	109.63	121.85
2	S	102	ALA	C-N-CA	-6.90	109.63	121.85
2	H	102	ALA	CA-C-N	-6.90	109.64	121.85
2	H	102	ALA	C-N-CA	-6.90	109.64	121.85
2	2	44	GLY	N-CA-C	-6.90	101.75	112.85
2	M	44	GLY	N-CA-C	-6.88	101.77	112.85
2	R	44	GLY	N-CA-C	-6.88	101.78	112.85
2	S	215	SER	N-CA-C	-6.87	104.71	113.23
2	H	215	SER	N-CA-C	-6.85	104.74	113.23
1	1	4	MET	N-CA-C	6.84	120.09	107.99
2	S	44	GLY	CA-C-N	-6.83	113.02	122.93
2	S	44	GLY	C-N-CA	-6.83	113.02	122.93
1	1	159	SER	N-CA-C	6.83	119.62	108.55
1	K	4	MET	N-CA-C	6.83	120.07	107.99
1	K	159	SER	N-CA-C	6.83	119.61	108.55
2	H	44	GLY	CA-C-N	-6.82	113.04	122.93
2	H	44	GLY	C-N-CA	-6.82	113.04	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	44	GLY	CA-C-N	-6.82	113.05	122.93
2	3	44	GLY	C-N-CA	-6.82	113.05	122.93
1	Q	4	MET	N-CA-C	6.82	120.06	107.99
2	3	215	SER	N-CA-C	-6.81	104.78	113.23
2	S	121	VAL	N-CA-C	6.80	118.09	107.28
2	3	121	VAL	N-CA-C	6.80	118.09	107.28
1	T	133	VAL	N-CA-C	6.80	118.58	108.46
1	Q	159	SER	N-CA-C	6.79	119.55	108.55
2	H	121	VAL	N-CA-C	6.79	118.07	107.28
1	L	133	VAL	N-CA-C	6.78	118.57	108.46
1	4	133	VAL	N-CA-C	6.78	118.56	108.46
2	M	82(A)	HIS	N-CA-C	6.77	120.72	109.95
2	R	82(A)	HIS	N-CA-C	6.77	120.72	109.95
2	2	82(A)	HIS	N-CA-C	6.76	120.71	109.95
1	L	82	ASP	N-CA-C	6.76	121.28	112.89
1	Q	28	SER	N-CA-C	6.76	120.51	109.76
1	T	3	VAL	N-CA-C	6.75	118.01	107.28
1	4	3	VAL	N-CA-C	6.75	118.01	107.28
1	K	28	SER	N-CA-C	6.75	120.49	109.76
1	L	3	VAL	N-CA-C	6.74	118.00	107.28
1	1	28	SER	N-CA-C	6.74	120.47	109.76
1	4	82	ASP	N-CA-C	6.74	121.25	112.89
1	T	82	ASP	N-CA-C	6.74	121.25	112.89
2	M	50	SER	N-CA-C	6.73	119.45	108.55
2	2	50	SER	N-CA-C	6.72	119.43	108.55
2	R	50	SER	N-CA-C	6.70	119.40	108.55
1	Q	146	VAL	N-CA-C	-6.69	97.99	107.75
1	1	146	VAL	N-CA-C	-6.68	98.00	107.75
2	R	82	MET	N-CA-C	6.67	119.70	108.02
1	K	146	VAL	N-CA-C	-6.67	98.01	107.75
1	4	61	ARG	N-CA-C	-6.66	105.19	113.38
2	2	82	MET	N-CA-C	6.65	119.66	108.02
2	M	82	MET	N-CA-C	6.65	119.66	108.02
1	L	61	ARG	N-CA-C	-6.65	105.20	113.38
2	M	118	GLY	CA-C-N	6.64	126.59	120.21
2	M	118	GLY	C-N-CA	6.64	126.59	120.21
2	2	118	GLY	CA-C-N	6.64	126.59	120.21
2	2	118	GLY	C-N-CA	6.64	126.59	120.21
1	T	61	ARG	N-CA-C	-6.64	105.22	113.38
1	Q	32	TRP	N-CA-C	6.63	121.22	113.20
2	R	118	GLY	CA-C-N	6.62	126.57	120.21
2	R	118	GLY	C-N-CA	6.62	126.57	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	59	TYR	N-CA-C	-6.60	99.30	109.14
1	1	207	LYS	N-CA-C	6.60	120.28	109.72
1	K	207	LYS	N-CA-C	6.60	120.28	109.72
1	Q	207	LYS	N-CA-C	6.60	120.28	109.72
1	K	32	TRP	N-CA-C	6.59	121.18	113.20
2	H	59	TYR	N-CA-C	-6.59	99.32	109.14
2	S	59	TYR	N-CA-C	-6.59	99.33	109.14
1	1	32	TRP	N-CA-C	6.57	121.15	113.20
2	H	73	ASP	CA-C-N	-6.57	109.51	120.68
2	H	73	ASP	C-N-CA	-6.57	109.51	120.68
2	S	73	ASP	CA-C-N	-6.57	109.52	120.68
2	S	73	ASP	C-N-CA	-6.57	109.52	120.68
2	2	110	THR	N-CA-C	6.57	120.11	107.44
2	R	107	THR	CA-C-N	6.56	131.53	122.93
2	R	107	THR	C-N-CA	6.56	131.53	122.93
2	M	107	THR	CA-C-N	6.56	131.52	122.93
2	M	107	THR	C-N-CA	6.56	131.52	122.93
2	M	110	THR	N-CA-C	6.55	120.09	107.44
2	3	73	ASP	CA-C-N	-6.55	109.55	120.68
2	3	73	ASP	C-N-CA	-6.55	109.55	120.68
2	2	107	THR	CA-C-N	6.54	131.50	122.93
2	2	107	THR	C-N-CA	6.54	131.50	122.93
2	R	110	THR	N-CA-C	6.53	120.04	107.44
2	S	2	VAL	CA-C-N	-6.51	112.37	122.59
2	S	2	VAL	C-N-CA	-6.51	112.37	122.59
2	3	95	LYS	CA-C-N	-6.51	108.66	121.41
2	3	95	LYS	C-N-CA	-6.51	108.66	121.41
2	3	2	VAL	CA-C-N	-6.50	112.39	122.59
2	3	2	VAL	C-N-CA	-6.50	112.39	122.59
2	H	2	VAL	CA-C-N	-6.49	112.39	122.59
2	H	2	VAL	C-N-CA	-6.49	112.39	122.59
2	H	95	LYS	CA-C-N	-6.49	108.68	121.41
2	H	95	LYS	C-N-CA	-6.49	108.68	121.41
2	S	95	LYS	CA-C-N	-6.48	108.70	121.41
2	S	95	LYS	C-N-CA	-6.48	108.70	121.41
2	M	107	THR	N-CA-C	6.47	120.17	110.14
2	R	107	THR	N-CA-C	6.46	120.16	110.14
2	2	107	THR	N-CA-C	6.45	120.13	110.14
1	4	10	THR	N-CA-C	6.43	119.49	109.52
2	H	37	VAL	CA-C-N	-6.43	112.49	122.59
2	H	37	VAL	C-N-CA	-6.43	112.49	122.59
2	S	37	VAL	CA-C-N	-6.42	112.50	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	37	VAL	C-N-CA	-6.42	112.50	122.59
2	3	37	VAL	CA-C-N	-6.42	112.52	122.59
2	3	37	VAL	C-N-CA	-6.42	112.52	122.59
1	1	127	SER	N-CA-C	-6.41	104.01	112.34
1	T	10	THR	N-CA-C	6.41	119.45	109.52
1	K	127	SER	N-CA-C	-6.40	104.02	112.34
1	L	10	THR	N-CA-C	6.40	119.44	109.52
2	2	38	ARG	CA-C-N	-6.39	113.90	122.72
2	2	38	ARG	C-N-CA	-6.39	113.90	122.72
1	1	206	THR	CA-C-N	-6.39	112.78	122.81
1	1	206	THR	C-N-CA	-6.39	112.78	122.81
1	K	206	THR	CA-C-N	-6.39	112.78	122.81
1	K	206	THR	C-N-CA	-6.39	112.78	122.81
2	R	38	ARG	CA-C-N	-6.38	113.91	122.72
2	R	38	ARG	C-N-CA	-6.38	113.91	122.72
1	T	142	ARG	N-CA-C	6.38	118.32	111.36
2	M	38	ARG	CA-C-N	-6.38	113.91	122.72
2	M	38	ARG	C-N-CA	-6.38	113.91	122.72
1	Q	127	SER	N-CA-C	-6.37	104.06	112.34
1	Q	206	THR	CA-C-N	-6.37	112.81	122.81
1	Q	206	THR	C-N-CA	-6.37	112.81	122.81
1	4	142	ARG	N-CA-C	6.37	118.30	111.36
1	L	142	ARG	N-CA-C	6.37	118.30	111.36
2	3	18	LEU	N-CA-C	-6.35	97.27	110.80
2	H	18	LEU	N-CA-C	-6.33	97.33	110.80
2	S	18	LEU	N-CA-C	-6.32	97.34	110.80
2	3	156	SER	N-CA-C	-6.31	99.74	109.52
2	H	156	SER	N-CA-C	-6.31	99.74	109.52
2	S	156	SER	N-CA-C	-6.30	99.75	109.52
2	2	129	LYS	N-CA-C	6.23	119.07	108.67
2	M	129	LYS	N-CA-C	6.22	119.06	108.67
2	R	129	LYS	N-CA-C	6.22	119.06	108.67
2	2	219	VAL	N-CA-C	6.20	116.80	108.11
2	M	219	VAL	N-CA-C	6.20	116.79	108.11
2	R	29	ILE	N-CA-C	6.19	116.31	110.30
2	M	29	ILE	N-CA-C	6.19	116.31	110.30
2	R	219	VAL	N-CA-C	6.17	116.74	108.11
2	2	110	THR	CA-C-N	6.14	130.04	122.37
2	2	110	THR	C-N-CA	6.14	130.04	122.37
2	3	57	ARG	N-CA-C	-6.14	100.63	110.14
2	2	29	ILE	N-CA-C	6.13	116.25	110.30
2	H	57	ARG	N-CA-C	-6.13	100.64	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	57	ARG	N-CA-C	-6.12	100.66	110.14
2	M	110	THR	CA-C-N	6.10	130.00	122.37
2	M	110	THR	C-N-CA	6.10	130.00	122.37
1	1	81	ASP	N-CA-C	6.10	118.43	111.11
1	K	167	ASP	N-CA-C	6.10	118.64	110.35
1	K	81	ASP	N-CA-C	6.09	118.42	111.11
1	Q	81	ASP	N-CA-C	6.09	118.42	111.11
1	1	167	ASP	N-CA-C	6.08	118.61	110.35
2	R	110	THR	CA-C-N	6.06	129.95	122.37
2	R	110	THR	C-N-CA	6.06	129.95	122.37
1	Q	167	ASP	N-CA-C	6.06	118.59	110.35
2	R	137	THR	N-CA-C	6.05	118.91	109.52
2	2	137	THR	N-CA-C	6.05	118.90	109.52
2	M	137	THR	N-CA-C	6.04	118.88	109.52
2	M	164	GLY	N-CA-C	6.02	121.95	114.37
1	K	132	VAL	N-CA-C	6.00	121.81	109.34
2	R	164	GLY	N-CA-C	5.99	121.92	114.37
1	Q	132	VAL	N-CA-C	5.99	121.80	109.34
2	2	164	GLY	N-CA-C	5.99	121.92	114.37
1	1	132	VAL	N-CA-C	5.98	121.79	109.34
2	S	195	SER	N-CA-C	5.97	117.59	111.14
2	H	195	SER	N-CA-C	5.96	117.58	111.14
1	Q	6	GLN	N-CA-C	5.95	119.64	110.42
1	K	6	GLN	N-CA-C	5.95	119.64	110.42
2	2	75	GLU	CA-C-N	5.95	132.90	121.54
2	2	75	GLU	C-N-CA	5.95	132.90	121.54
2	R	75	GLU	CA-C-N	5.94	132.89	121.54
2	R	75	GLU	C-N-CA	5.94	132.89	121.54
2	R	95	LYS	CA-C-O	-5.94	112.51	119.05
2	M	75	GLU	CA-C-N	5.94	132.88	121.54
2	M	75	GLU	C-N-CA	5.94	132.88	121.54
2	R	19	ILE	N-CA-C	5.93	116.55	107.77
2	2	19	ILE	N-CA-C	5.93	116.55	107.77
2	3	195	SER	N-CA-C	5.93	117.55	111.14
2	M	19	ILE	N-CA-C	5.93	116.55	107.77
1	1	6	GLN	N-CA-C	5.93	119.61	110.42
2	M	95	LYS	CA-C-O	-5.92	112.53	119.05
2	2	95	LYS	CA-C-O	-5.92	112.54	119.05
2	2	190	VAL	N-CA-C	-5.91	101.61	108.82
2	M	190	VAL	N-CA-C	-5.91	101.61	108.82
2	R	190	VAL	N-CA-C	-5.90	101.62	108.82
1	L	177	SER	CA-C-N	-5.90	114.46	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	177	SER	C-N-CA	-5.90	114.46	123.07
1	T	177	SER	CA-C-N	-5.89	114.46	123.07
1	T	177	SER	C-N-CA	-5.89	114.46	123.07
1	4	177	SER	CA-C-N	-5.86	114.52	123.07
1	4	177	SER	C-N-CA	-5.86	114.52	123.07
1	L	31	THR	N-CA-C	-5.84	104.82	112.41
2	H	19	ILE	CA-C-O	-5.83	114.42	121.54
1	T	31	THR	N-CA-C	-5.83	104.83	112.41
1	4	31	THR	N-CA-C	-5.83	104.83	112.41
2	S	19	ILE	CA-C-O	-5.81	114.45	121.54
2	3	19	ILE	CA-C-O	-5.80	114.47	121.54
1	Q	155	GLN	N-CA-C	5.79	118.81	107.57
1	1	155	GLN	N-CA-C	5.79	118.80	107.57
1	K	155	GLN	N-CA-C	5.79	118.80	107.57
1	4	16	GLY	N-CA-C	-5.76	108.22	115.08
1	1	138	ASN	N-CA-C	5.75	123.05	110.80
1	L	16	GLY	N-CA-C	-5.75	108.24	115.08
1	K	138	ASN	N-CA-C	5.74	123.02	110.80
1	1	193	ALA	N-CA-C	5.73	119.03	110.14
1	Q	138	ASN	N-CA-C	5.73	123.01	110.80
2	S	139	ALA	N-CA-C	-5.73	98.60	110.80
2	H	139	ALA	N-CA-C	-5.73	98.60	110.80
2	3	139	ALA	N-CA-C	-5.72	98.61	110.80
1	Q	193	ALA	N-CA-C	5.72	119.01	110.14
2	H	30	SER	CA-C-N	-5.72	113.34	122.66
2	H	30	SER	C-N-CA	-5.72	113.34	122.66
2	S	30	SER	CA-C-N	-5.72	113.34	122.66
2	S	30	SER	C-N-CA	-5.72	113.34	122.66
1	K	193	ALA	N-CA-C	5.71	118.99	110.14
1	T	16	GLY	N-CA-C	-5.70	108.29	115.08
2	S	83	ARG	CA-C-N	-5.70	113.30	120.77
2	S	83	ARG	C-N-CA	-5.70	113.30	120.77
2	3	30	SER	CA-C-N	-5.69	113.38	122.66
2	3	30	SER	C-N-CA	-5.69	113.38	122.66
2	H	123	PRO	O-C-N	5.69	130.32	122.64
2	R	105	PRO	CA-C-O	5.69	126.20	118.81
2	S	123	PRO	O-C-N	5.69	130.32	122.64
2	2	105	PRO	CA-C-O	5.68	126.20	118.81
2	H	83	ARG	CA-C-N	-5.68	113.33	120.77
2	H	83	ARG	C-N-CA	-5.68	113.33	120.77
2	M	105	PRO	CA-C-O	5.67	126.19	118.81
2	3	123	PRO	O-C-N	5.67	130.30	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	84	ALA	CA-C-N	-5.67	113.39	121.50
1	K	84	ALA	C-N-CA	-5.67	113.39	121.50
2	R	86	ASP	N-CA-C	-5.67	106.03	113.17
1	1	84	ALA	CA-C-N	-5.67	113.40	121.50
1	1	84	ALA	C-N-CA	-5.67	113.40	121.50
2	3	83	ARG	CA-C-N	-5.67	113.35	120.77
2	3	83	ARG	C-N-CA	-5.67	113.35	120.77
1	Q	84	ALA	CA-C-N	-5.67	113.40	121.50
1	Q	84	ALA	C-N-CA	-5.67	113.40	121.50
2	2	86	ASP	N-CA-C	-5.66	106.04	113.17
2	M	86	ASP	N-CA-C	-5.65	106.05	113.17
1	4	9	SER	O-C-N	5.63	128.09	122.12
2	R	108	VAL	N-CA-C	5.63	115.90	107.51
1	4	88	CYS	CA-C-N	-5.62	113.62	122.73
1	4	88	CYS	C-N-CA	-5.62	113.62	122.73
1	T	9	SER	O-C-N	5.62	128.08	122.12
2	M	108	VAL	N-CA-C	5.62	115.88	107.51
1	L	9	SER	O-C-N	5.62	128.07	122.12
2	2	108	VAL	N-CA-C	5.62	115.88	107.51
1	4	167	ASP	N-CA-C	5.61	118.72	110.30
1	T	167	ASP	N-CA-C	5.61	118.72	110.30
1	4	195	GLU	N-CA-C	5.61	119.61	107.49
1	T	195	GLU	N-CA-C	5.61	119.60	107.49
1	L	195	GLU	N-CA-C	5.60	119.59	107.49
2	H	76	ASP	N-CA-C	5.60	117.46	110.91
1	T	88	CYS	CA-C-N	-5.59	113.68	122.73
1	T	88	CYS	C-N-CA	-5.59	113.68	122.73
1	L	167	ASP	N-CA-C	5.59	118.68	110.30
2	3	76	ASP	N-CA-C	5.59	117.45	110.91
1	L	88	CYS	CA-C-N	-5.58	113.69	122.73
1	L	88	CYS	C-N-CA	-5.58	113.69	122.73
2	S	76	ASP	N-CA-C	5.58	117.44	110.91
2	3	79	TYR	CA-C-N	-5.58	114.94	122.86
2	3	79	TYR	C-N-CA	-5.58	114.94	122.86
1	L	25	ALA	N-CA-C	5.58	117.39	108.41
2	S	79	TYR	CA-C-N	-5.58	114.94	122.86
2	S	79	TYR	C-N-CA	-5.58	114.94	122.86
2	H	79	TYR	CA-C-N	-5.57	114.95	122.86
2	H	79	TYR	C-N-CA	-5.57	114.95	122.86
1	4	25	ALA	N-CA-C	5.57	117.37	108.41
1	T	25	ALA	N-CA-C	5.56	117.36	108.41
2	S	200	THR	N-CA-C	-5.53	105.74	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	200	THR	N-CA-C	-5.53	105.74	113.37
1	L	9	SER	N-CA-C	-5.53	105.26	111.28
2	H	154	VAL	N-CA-C	5.52	116.42	108.48
1	1	208	SER	N-CA-C	5.52	115.84	108.23
2	3	107	THR	CA-C-N	-5.51	115.27	122.37
2	3	107	THR	C-N-CA	-5.51	115.27	122.37
1	K	208	SER	N-CA-C	5.51	115.83	108.23
1	4	9	SER	N-CA-C	-5.50	105.28	111.28
2	S	154	VAL	N-CA-C	5.50	116.40	108.48
2	3	200	THR	N-CA-C	-5.50	105.79	113.37
2	3	154	VAL	N-CA-C	5.49	116.39	108.48
2	H	107	THR	CA-C-N	-5.48	115.30	122.37
2	H	107	THR	C-N-CA	-5.48	115.30	122.37
1	4	71	PHE	N-CA-C	-5.47	101.09	109.41
1	Q	208	SER	N-CA-C	5.47	115.78	108.23
1	L	71	PHE	N-CA-C	-5.47	101.10	109.41
2	S	107	THR	CA-C-N	-5.46	115.32	122.37
2	S	107	THR	C-N-CA	-5.46	115.32	122.37
2	M	19	ILE	CA-C-N	-5.46	112.97	122.64
2	M	19	ILE	C-N-CA	-5.46	112.97	122.64
2	R	19	ILE	CA-C-N	-5.46	112.97	122.64
2	R	19	ILE	C-N-CA	-5.46	112.97	122.64
1	T	71	PHE	N-CA-C	-5.46	101.11	109.41
1	T	9	SER	N-CA-C	-5.46	105.33	111.28
2	H	187	LEU	N-CA-C	5.46	116.57	108.60
2	R	97	SER	N-CA-C	5.45	117.80	109.62
2	S	141	GLY	N-CA-C	5.45	126.10	113.18
2	3	187	LEU	N-CA-C	5.45	116.56	108.60
2	H	141	GLY	N-CA-C	5.45	126.09	113.18
2	2	19	ILE	CA-C-N	-5.44	113.00	122.64
2	2	19	ILE	C-N-CA	-5.44	113.00	122.64
2	3	141	GLY	N-CA-C	5.44	126.08	113.18
2	2	97	SER	N-CA-C	5.44	117.77	109.62
2	M	97	SER	N-CA-C	5.43	117.77	109.62
2	S	187	LEU	N-CA-C	5.42	116.52	108.60
2	M	123	PRO	N-CA-C	5.42	119.10	110.21
2	2	123	PRO	N-CA-C	5.42	119.09	110.21
2	R	123	PRO	N-CA-C	5.41	119.08	110.21
1	L	148	TRP	CA-C-N	-5.41	115.26	122.72
1	L	148	TRP	C-N-CA	-5.41	115.26	122.72
1	T	148	TRP	CA-C-N	-5.40	115.26	122.72
1	T	148	TRP	C-N-CA	-5.40	115.26	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	88	ALA	N-CA-C	5.40	116.19	108.74
1	4	148	TRP	CA-C-N	-5.39	115.27	122.72
1	4	148	TRP	C-N-CA	-5.39	115.27	122.72
1	Q	66	GLY	CA-C-N	5.39	131.84	121.54
1	Q	66	GLY	C-N-CA	5.39	131.84	121.54
2	H	88	ALA	N-CA-C	5.39	116.18	108.74
2	3	171	VAL	N-CA-C	-5.38	101.97	109.45
2	S	88	ALA	N-CA-C	5.38	116.17	108.74
1	1	66	GLY	CA-C-N	5.37	131.80	121.54
1	1	66	GLY	C-N-CA	5.37	131.80	121.54
2	2	146	ASP	N-CA-C	5.37	122.24	110.80
1	K	66	GLY	CA-C-N	5.37	131.80	121.54
1	K	66	GLY	C-N-CA	5.37	131.80	121.54
2	M	146	ASP	N-CA-C	5.37	122.24	110.80
2	S	18	LEU	O-C-N	5.37	129.73	122.59
2	3	18	LEU	O-C-N	5.37	129.72	122.59
2	S	129	LYS	N-CA-C	-5.36	99.38	110.80
2	3	129	LYS	N-CA-C	-5.36	99.39	110.80
2	H	171	VAL	N-CA-C	-5.36	102.00	109.45
1	Q	139	PHE	N-CA-C	5.36	118.42	109.96
2	S	61	ASP	N-CA-C	5.36	118.61	111.75
2	H	129	LYS	N-CA-C	-5.35	99.39	110.80
2	S	171	VAL	N-CA-C	-5.35	102.01	109.45
2	H	18	LEU	O-C-N	5.35	129.70	122.59
2	R	146	ASP	N-CA-C	5.35	122.19	110.80
1	1	104	VAL	N-CA-C	-5.34	99.95	107.75
1	T	81	ASP	N-CA-C	5.33	122.16	110.80
2	2	19	ILE	CA-C-O	-5.33	114.89	120.27
1	4	81	ASP	N-CA-C	5.33	122.14	110.80
1	L	81	ASP	N-CA-C	5.33	122.14	110.80
2	R	19	ILE	CA-C-O	-5.33	114.89	120.27
1	K	104	VAL	N-CA-C	-5.32	99.98	107.75
2	M	19	ILE	CA-C-O	-5.32	114.90	120.27
1	Q	104	VAL	N-CA-C	-5.32	99.98	107.75
1	K	139	PHE	N-CA-C	5.32	118.36	109.96
2	R	100	LEU	N-CA-C	5.32	122.12	110.80
2	H	61	ASP	N-CA-C	5.31	118.55	111.75
2	M	100	LEU	N-CA-C	5.31	122.10	110.80
2	2	100	LEU	N-CA-C	5.30	122.10	110.80
2	3	61	ASP	N-CA-C	5.30	118.54	111.75
1	Q	91	TYR	N-CA-C	5.30	116.95	108.41
1	1	139	PHE	N-CA-C	5.30	118.33	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	91	TYR	N-CA-C	5.29	116.93	108.41
1	K	91	TYR	N-CA-C	5.29	116.93	108.41
1	1	69	THR	N-CA-C	5.29	118.52	111.75
1	1	120	PRO	N-CA-C	5.29	123.36	112.47
1	K	120	PRO	N-CA-C	5.29	123.36	112.47
1	Q	120	PRO	N-CA-C	5.29	123.36	112.47
1	1	22	THR	N-CA-C	5.28	117.26	107.60
2	H	96	GLY	N-CA-C	5.28	125.69	113.18
1	K	69	THR	N-CA-C	5.28	118.51	111.75
2	3	96	GLY	N-CA-C	5.28	125.68	113.18
2	R	210	VAL	CA-C-N	-5.27	115.17	123.13
2	R	210	VAL	C-N-CA	-5.27	115.17	123.13
2	S	96	GLY	N-CA-C	5.27	125.67	113.18
1	T	38	GLN	N-CA-C	5.27	117.96	108.48
2	3	81	GLN	CA-C-O	-5.26	114.38	120.49
1	L	38	GLN	N-CA-C	5.26	117.95	108.48
2	2	12	VAL	N-CA-C	5.26	116.95	108.85
2	M	210	VAL	CA-C-N	-5.26	115.19	123.13
2	M	210	VAL	C-N-CA	-5.26	115.19	123.13
1	K	22	THR	N-CA-C	5.26	117.22	107.60
1	Q	69	THR	N-CA-C	5.25	118.48	111.75
2	2	210	VAL	CA-C-N	-5.25	115.20	123.13
2	2	210	VAL	C-N-CA	-5.25	115.20	123.13
1	4	38	GLN	N-CA-C	5.25	117.93	108.48
2	H	81	GLN	CA-C-O	-5.25	114.40	120.49
1	Q	22	THR	N-CA-C	5.25	117.20	107.60
2	R	12	VAL	N-CA-C	5.24	116.92	108.85
1	Q	43	ALA	N-CA-C	-5.24	102.66	110.20
2	S	81	GLN	CA-C-O	-5.24	114.42	120.49
1	K	43	ALA	N-CA-C	-5.23	102.67	110.20
2	M	12	VAL	N-CA-C	5.23	116.90	108.85
1	1	43	ALA	N-CA-C	-5.22	102.69	110.20
2	S	10	GLY	CA-C-O	-5.22	116.30	120.79
1	4	87	HIS	CA-C-N	-5.21	114.88	122.65
1	4	87	HIS	C-N-CA	-5.21	114.88	122.65
1	L	87	HIS	CA-C-N	-5.21	114.88	122.65
1	L	87	HIS	C-N-CA	-5.21	114.88	122.65
2	3	10	GLY	CA-C-O	-5.21	116.31	120.79
2	2	82(B)	LYS	N-CA-C	-5.21	104.94	111.92
2	M	82(B)	LYS	N-CA-C	-5.20	104.95	111.92
2	H	10	GLY	CA-C-O	-5.20	116.32	120.79
1	T	87	HIS	CA-C-N	-5.20	114.90	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	87	HIS	C-N-CA	-5.20	114.90	122.65
2	R	82(B)	LYS	N-CA-C	-5.19	104.97	111.92
3	C	297	THR	N-CA-C	5.18	116.94	108.76
3	A	297	THR	N-CA-C	5.18	116.94	108.76
2	H	86	ASP	CA-C-N	-5.18	114.28	121.99
2	H	86	ASP	C-N-CA	-5.18	114.28	121.99
2	3	86	ASP	CA-C-N	-5.17	114.29	121.99
2	3	86	ASP	C-N-CA	-5.17	114.29	121.99
1	L	101	GLY	CA-C-N	-5.17	115.82	123.05
1	L	101	GLY	C-N-CA	-5.17	115.82	123.05
1	T	101	GLY	CA-C-N	-5.16	115.82	123.05
1	T	101	GLY	C-N-CA	-5.16	115.82	123.05
2	R	217	THR	CA-C-N	-5.16	115.82	123.05
2	R	217	THR	C-N-CA	-5.16	115.82	123.05
2	S	125	ALA	N-CA-C	5.16	121.21	109.81
3	E	297	THR	N-CA-C	5.15	116.90	108.76
2	M	33	THR	N-CA-C	-5.15	101.30	109.59
2	3	125	ALA	N-CA-C	5.15	121.19	109.81
2	R	33	THR	N-CA-C	-5.15	101.30	109.59
2	S	86	ASP	CA-C-N	-5.15	114.32	121.99
2	S	86	ASP	C-N-CA	-5.15	114.32	121.99
1	4	101	GLY	CA-C-N	-5.15	115.85	123.05
1	4	101	GLY	C-N-CA	-5.15	115.85	123.05
2	H	125	ALA	N-CA-C	5.14	121.18	109.81
2	2	217	THR	CA-C-N	-5.14	115.85	123.05
2	2	217	THR	C-N-CA	-5.14	115.85	123.05
2	2	227	PRO	CA-C-O	-5.14	114.91	122.31
2	R	212	HIS	N-CA-C	5.14	117.54	107.57
2	M	212	HIS	N-CA-C	5.13	117.53	107.57
2	M	227	PRO	CA-C-O	-5.13	114.92	122.31
2	2	212	HIS	N-CA-C	5.13	117.53	107.57
2	2	33	THR	N-CA-C	-5.13	101.33	109.59
2	3	141	GLY	CA-C-N	5.13	128.61	121.02
2	3	141	GLY	C-N-CA	5.13	128.61	121.02
2	M	217	THR	CA-C-N	-5.13	115.87	123.05
2	M	217	THR	C-N-CA	-5.13	115.87	123.05
2	R	227	PRO	CA-C-O	-5.13	114.93	122.31
2	H	141	GLY	CA-C-N	5.12	128.60	121.02
2	H	141	GLY	C-N-CA	5.12	128.60	121.02
2	S	141	GLY	CA-C-N	5.12	128.59	121.02
2	S	141	GLY	C-N-CA	5.12	128.59	121.02
2	H	82(C)	MET	N-CA-C	5.11	117.12	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	37	VAL	N-CA-C	5.11	116.26	108.80
1	4	75	ILE	N-CA-C	5.11	115.70	107.73
2	R	37	VAL	N-CA-C	5.11	116.26	108.80
1	1	111	ALA	N-CA-C	5.11	116.71	108.34
1	L	75	ILE	N-CA-C	5.11	115.69	107.73
2	S	82(C)	MET	N-CA-C	5.10	117.11	110.43
2	2	37	VAL	N-CA-C	5.10	116.24	108.80
1	T	75	ILE	N-CA-C	5.10	115.68	107.73
1	K	111	ALA	N-CA-C	5.09	116.69	108.34
2	M	198	LEU	N-CA-C	5.09	117.27	109.07
2	R	64	LYS	N-CA-C	-5.09	102.38	109.96
2	R	198	LEU	N-CA-C	5.09	117.26	109.07
2	3	82(C)	MET	N-CA-C	5.09	117.09	110.43
2	M	42	GLY	O-C-N	5.08	127.91	122.52
2	S	16	GLY	N-CA-C	5.08	125.22	113.18
2	2	198	LEU	N-CA-C	5.08	117.24	109.07
2	H	16	GLY	N-CA-C	5.08	125.21	113.18
2	2	64	LYS	N-CA-C	-5.07	102.40	109.96
2	M	177	VAL	CA-C-N	-5.07	115.95	123.05
2	M	177	VAL	C-N-CA	-5.07	115.95	123.05
2	2	42	GLY	O-C-N	5.07	127.89	122.52
2	M	64	LYS	N-CA-C	-5.07	102.41	109.96
2	3	16	GLY	N-CA-C	5.07	125.18	113.18
1	4	196	VAL	N-CA-C	5.07	116.57	108.87
2	R	42	GLY	O-C-N	5.06	127.89	122.52
1	Q	111	ALA	N-CA-C	5.06	116.64	108.34
1	L	196	VAL	N-CA-C	5.05	116.55	108.87
2	S	187	LEU	CA-C-N	-5.05	113.95	122.29
2	S	187	LEU	C-N-CA	-5.05	113.95	122.29
1	T	196	VAL	N-CA-C	5.05	116.55	108.87
2	H	184	LEU	N-CA-C	5.05	117.66	110.24
2	H	187	LEU	CA-C-N	-5.05	113.96	122.29
2	H	187	LEU	C-N-CA	-5.05	113.96	122.29
2	2	177	VAL	CA-C-N	-5.04	115.99	123.05
2	2	177	VAL	C-N-CA	-5.04	115.99	123.05
1	1	53	THR	N-CA-C	5.04	117.83	109.46
2	3	184	LEU	N-CA-C	5.04	117.65	110.24
2	3	187	LEU	CA-C-N	-5.04	113.97	122.29
2	3	187	LEU	C-N-CA	-5.04	113.97	122.29
2	R	177	VAL	CA-C-N	-5.04	116.00	123.05
2	R	177	VAL	C-N-CA	-5.04	116.00	123.05
2	S	184	LEU	N-CA-C	5.03	117.64	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	53	THR	N-CA-C	5.02	117.79	109.46
2	R	66	ARG	N-CA-C	-5.02	107.70	113.88
1	Q	53	THR	N-CA-C	5.02	117.79	109.46
2	3	167	THR	CA-C-N	-5.01	111.97	121.54
2	3	167	THR	C-N-CA	-5.01	111.97	121.54

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	19	ILE	Peptide
2	2	100(A)	SER	Peptide
2	2	123	PRO	Peptide
2	2	145	LYS	Peptide
2	2	151	PRO	Peptide
2	2	215	SER	Peptide
2	2	40	VAL	Peptide
2	2	42	GLY	Peptide
2	2	88	ALA	Peptide
2	2	97	SER	Peptide
2	3	128	SER	Peptide
2	3	141	GLY	Peptide
2	3	42	GLY	Peptide
2	3	96	GLY	Peptide
1	4	25	ALA	Peptide
2	H	128	SER	Peptide
2	H	141	GLY	Peptide
2	H	42	GLY	Peptide
2	H	96	GLY	Peptide
1	K	19	ILE	Peptide
1	L	25	ALA	Peptide
2	M	100(A)	SER	Peptide
2	M	123	PRO	Peptide
2	M	145	LYS	Peptide
2	M	151	PRO	Peptide
2	M	215	SER	Peptide
2	M	40	VAL	Peptide
2	M	42	GLY	Peptide
2	M	88	ALA	Peptide
2	M	97	SER	Peptide
1	Q	19	ILE	Peptide
2	R	100(A)	SER	Peptide

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Mol	Chain	Res	Type	Group
2	R	123	PRO	Peptide
2	R	145	LYS	Peptide
2	R	151	PRO	Peptide
2	R	215	SER	Peptide
2	R	40	VAL	Peptide
2	R	42	GLY	Peptide
2	R	88	ALA	Peptide
2	R	97	SER	Peptide
2	S	128	SER	Peptide
2	S	141	GLY	Peptide
2	S	42	GLY	Peptide
2	S	96	GLY	Peptide
1	T	25	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	848	0	230	9	0
1	4	848	0	230	9	0
1	K	848	0	230	11	0
1	L	848	0	230	8	0
1	Q	848	0	230	11	0
1	T	848	0	230	8	0
2	2	900	0	256	25	0
2	3	900	0	256	32	0
2	H	900	0	256	31	0
2	M	900	0	256	24	0
2	R	900	0	256	25	0
2	S	900	0	256	32	0
3	A	1812	0	482	12	0
3	C	1812	0	482	13	0
3	E	1812	0	482	11	0
4	B	504	0	143	0	0
4	D	504	0	143	0	0
4	F	504	0	143	0	0
5	I	512	0	147	9	0
5	O	512	0	147	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	512	0	147	10	0
6	J	404	0	121	0	0
6	P	404	0	121	0	0
6	W	404	0	121	0	0
7	G	22	0	19	8	0
7	N	22	0	17	7	0
7	Y	22	0	17	8	0
7	g	22	0	17	8	0
7	h	22	0	19	8	0
7	i	22	0	17	8	0
7	k	22	0	19	8	0
7	l	22	0	17	7	0
7	o	22	0	17	8	0
8	U	72	0	61	1	0
8	j	72	0	61	1	0
8	m	72	0	61	1	0
9	X	84	0	72	13	0
9	Z	84	0	72	19	0
9	b	84	0	72	20	0
9	d	84	0	72	18	0
9	f	84	0	72	13	0
9	n	84	0	72	14	0
10	a	50	0	43	4	0
10	c	50	0	43	4	0
10	e	50	0	43	4	0
All	All	21252	0	6498	367	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 13.

All (367) 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)
3:C:459:GLY:CA	5:O:61:ARG:H	1.25	1.50
3:A:459:GLY:HA3	5:V:61:ARG:CA	1.44	1.47
3:C:459:GLY:HA3	5:O:61:ARG:CA	1.44	1.47
3:A:459:GLY:CA	5:V:61:ARG:H	1.25	1.46
3:E:459:GLY:CA	5:I:61:ARG:H	1.25	1.46
3:E:459:GLY:HA3	5:I:61:ARG:CA	1.44	1.45
3:E:459:GLY:CA	5:I:61:ARG:N	1.90	1.35
3:A:459:GLY:CA	5:V:61:ARG:N	1.89	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:459:GLY:CA	5:O:61:ARG:N	1.90	1.32
3:E:459:GLY:HA2	5:I:61:ARG:H	1.09	1.10
7:N:1:MAN:C1	9:Z:7:MAN:O2	2.00	1.10
9:X:7:MAN:O2	7:Y:1:MAN:C1	2.00	1.10
9:b:7:MAN:O2	7:i:1:MAN:C1	2.00	1.10
9:n:7:MAN:O2	7:o:1:MAN:C1	2.00	1.10
9:f:7:MAN:O2	7:g:1:MAN:C1	2.00	1.09
3:C:459:GLY:HA2	5:O:61:ARG:H	1.09	1.08
9:d:7:MAN:O2	7:l:1:MAN:C1	2.00	1.08
3:A:459:GLY:HA2	5:V:61:ARG:N	1.66	1.06
3:A:459:GLY:HA2	5:V:61:ARG:H	1.09	1.04
3:E:459:GLY:CA	5:I:61:ARG:CA	2.32	1.03
3:A:459:GLY:CA	5:V:61:ARG:CA	2.32	1.01
9:f:3:BMA:H62	9:f:4:MAN:H3	1.43	1.00
3:E:459:GLY:HA2	5:I:61:ARG:N	1.66	1.00
9:n:3:BMA:H62	9:n:4:MAN:H3	1.43	1.00
9:Z:3:BMA:H62	9:Z:4:MAN:H3	1.43	1.00
3:C:459:GLY:HA3	5:O:61:ARG:N	1.60	0.99
9:X:3:BMA:H62	9:X:4:MAN:H3	1.43	0.99
3:C:459:GLY:HA2	5:O:61:ARG:N	1.66	0.98
9:d:3:BMA:H62	9:d:4:MAN:H3	1.43	0.98
3:A:459:GLY:HA3	5:V:61:ARG:N	1.60	0.97
3:C:459:GLY:CA	5:O:61:ARG:CA	2.32	0.97
9:b:3:BMA:H62	9:b:4:MAN:H3	1.43	0.97
9:b:7:MAN:HO2	7:i:1:MAN:C1	1.77	0.96
7:G:1:MAN:C1	10:e:4:MAN:O2	2.14	0.96
10:c:4:MAN:O2	7:k:1:MAN:C1	2.14	0.95
2:R:194:PRO:O	2:R:196:SER:N	1.99	0.95
9:d:7:MAN:HO2	7:l:1:MAN:C1	1.80	0.94
2:M:194:PRO:O	2:M:196:SER:N	1.99	0.94
9:X:7:MAN:HO2	7:Y:1:MAN:C1	1.78	0.94
10:a:4:MAN:O2	7:h:1:MAN:C1	2.14	0.94
3:E:459:GLY:HA3	5:I:61:ARG:N	1.60	0.94
9:n:7:MAN:O2	7:o:1:MAN:C2	2.16	0.94
2:2:194:PRO:O	2:2:196:SER:N	1.99	0.94
9:b:7:MAN:O2	7:i:1:MAN:C2	2.16	0.94
9:d:7:MAN:O2	7:l:1:MAN:C2	2.16	0.93
7:N:1:MAN:C2	9:Z:7:MAN:O2	2.16	0.93
9:f:7:MAN:O2	7:g:1:MAN:C2	2.16	0.93
9:X:7:MAN:O2	7:Y:1:MAN:C2	2.16	0.92
3:A:459:GLY:N	5:V:61:ARG:H	1.68	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100(A):SER:O	2:H:100(C):ASN:N	2.05	0.90
2:2:84:VAL:O	2:2:86:ASP:N	2.05	0.89
3:E:459:GLY:N	5:I:61:ARG:H	1.68	0.89
2:R:84:VAL:O	2:R:86:ASP:N	2.05	0.89
2:S:100(A):SER:O	2:S:100(C):ASN:N	2.05	0.89
9:f:7:MAN:HO2	7:g:1:MAN:C1	1.83	0.89
3:C:459:GLY:N	5:O:61:ARG:H	1.68	0.89
2:M:84:VAL:O	2:M:86:ASP:N	2.05	0.89
2:3:100(A):SER:O	2:3:100(C):ASN:N	2.05	0.89
2:M:90:TYR:N	2:M:107:THR:O	2.06	0.88
9:f:7:MAN:HO2	7:g:1:MAN:C2	1.87	0.88
2:R:90:TYR:N	2:R:107:THR:O	2.06	0.87
7:N:1:MAN:C1	9:Z:7:MAN:HO2	1.86	0.87
9:n:7:MAN:HO2	7:o:1:MAN:C2	1.86	0.87
7:N:1:MAN:C2	9:Z:7:MAN:HO2	1.86	0.86
2:2:90:TYR:N	2:2:107:THR:O	2.06	0.86
9:b:7:MAN:HO2	7:i:1:MAN:C2	1.89	0.86
9:X:7:MAN:HO2	7:Y:1:MAN:C2	1.89	0.85
9:d:7:MAN:HO2	7:l:1:MAN:C2	1.88	0.85
9:n:7:MAN:HO2	7:o:1:MAN:C1	1.86	0.83
9:n:7:MAN:HO2	7:o:1:MAN:H2	1.44	0.83
7:N:1:MAN:H2	9:Z:7:MAN:HO2	1.44	0.81
2:S:28:ARG:H	9:d:5:MAN:C6	1.94	0.81
9:X:3:BMA:C6	9:X:4:MAN:H3	2.12	0.80
9:f:7:MAN:HO2	7:g:1:MAN:H2	1.45	0.80
9:Z:3:BMA:C6	9:Z:4:MAN:H3	2.12	0.80
9:b:3:BMA:C6	9:b:4:MAN:H3	2.12	0.79
2:H:28:ARG:H	9:b:5:MAN:C6	1.94	0.79
9:n:3:BMA:C6	9:n:4:MAN:H3	2.12	0.79
2:3:28:ARG:H	9:Z:5:MAN:C6	1.94	0.79
7:G:1:MAN:C2	10:e:4:MAN:O2	2.31	0.79
10:c:4:MAN:O2	7:k:1:MAN:C2	2.31	0.79
9:f:3:BMA:C6	9:f:4:MAN:H3	2.12	0.79
10:a:4:MAN:O2	7:h:1:MAN:C2	2.31	0.78
9:d:3:BMA:C6	9:d:4:MAN:H3	2.12	0.78
9:d:7:MAN:HO2	7:l:1:MAN:H2	1.48	0.76
2:M:31:ALA:O	7:h:1:MAN:O3	2.04	0.76
9:X:7:MAN:HO2	7:Y:1:MAN:H2	1.49	0.76
2:2:31:ALA:O	7:G:1:MAN:O3	2.04	0.75
2:H:124:LEU:N	2:H:141:GLY:O	2.20	0.75
2:S:124:LEU:N	2:S:141:GLY:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:7:MAN:HO2	7:i:1:MAN:H2	1.50	0.75
2:R:31:ALA:O	7:k:1:MAN:O3	2.04	0.74
9:d:3:BMA:C6	9:d:4:MAN:C3	2.63	0.74
2:3:124:LEU:N	2:3:141:GLY:O	2.20	0.74
7:G:1:MAN:H2	10:e:4:MAN:O2	1.88	0.74
10:a:4:MAN:O2	7:h:1:MAN:H2	1.88	0.74
7:h:1:MAN:O3	7:h:2:MAN:C1	2.36	0.73
10:c:4:MAN:O2	7:k:1:MAN:H2	1.88	0.72
7:G:1:MAN:O3	7:G:2:MAN:C1	2.36	0.71
1:Q:186:TYR:O	1:Q:188:LYS:N	2.22	0.71
1:Q:142:ARG:O	1:Q:143:GLU:C	2.34	0.70
9:Z:3:BMA:C6	9:Z:4:MAN:C3	2.63	0.70
1:1:142:ARG:O	1:1:143:GLU:C	2.34	0.70
7:k:1:MAN:O3	7:k:2:MAN:C1	2.36	0.70
1:1:186:TYR:O	1:1:188:LYS:N	2.22	0.70
9:b:7:MAN:O2	7:i:1:MAN:C3	2.40	0.69
9:X:7:MAN:O2	7:Y:1:MAN:C3	2.40	0.69
9:f:7:MAN:O2	7:g:1:MAN:C3	2.40	0.69
1:K:142:ARG:O	1:K:143:GLU:C	2.34	0.69
1:K:186:TYR:O	1:K:188:LYS:N	2.22	0.69
7:N:1:MAN:C3	9:Z:7:MAN:O2	2.40	0.69
9:d:7:MAN:O2	7:l:1:MAN:C3	2.40	0.69
9:n:7:MAN:O2	7:o:1:MAN:C3	2.40	0.69
2:H:179:GLN:O	2:H:180:SER:C	2.36	0.69
9:X:3:BMA:C6	9:X:4:MAN:C3	2.63	0.68
2:3:179:GLN:O	2:3:180:SER:C	2.36	0.68
2:S:179:GLN:O	2:S:180:SER:C	2.36	0.68
2:H:83:ARG:O	2:H:84:VAL:C	2.37	0.67
1:L:50:LYS:O	1:L:52:SER:N	2.29	0.66
2:R:84:VAL:C	2:R:86:ASP:H	2.04	0.66
2:S:83:ARG:O	2:S:84:VAL:C	2.37	0.66
1:T:50:LYS:O	1:T:52:SER:N	2.29	0.66
9:b:5:MAN:C1	9:b:6:MAN:O5	2.44	0.65
2:2:84:VAL:C	2:2:86:ASP:H	2.04	0.65
9:d:5:MAN:C1	9:d:6:MAN:O5	2.44	0.65
9:Z:5:MAN:C1	9:Z:6:MAN:O5	2.44	0.65
2:S:15:GLY:O	2:S:16:GLY:O	2.15	0.65
9:X:5:MAN:C1	9:X:6:MAN:O5	2.44	0.65
2:M:84:VAL:C	2:M:86:ASP:H	2.04	0.65
9:n:5:MAN:C1	9:n:6:MAN:O5	2.44	0.65
2:3:15:GLY:O	2:3:16:GLY:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:25:ALA:O	1:4:26:SER:C	2.41	0.64
9:f:5:MAN:C1	9:f:6:MAN:O5	2.44	0.64
2:H:15:GLY:O	2:H:16:GLY:O	2.15	0.64
2:3:83:ARG:O	2:3:84:VAL:C	2.37	0.63
2:M:165:ALA:O	2:M:166:LEU:C	2.42	0.63
2:2:165:ALA:O	2:2:166:LEU:C	2.42	0.63
2:3:31:ALA:O	7:Y:2:MAN:O2	2.09	0.63
9:b:3:BMA:C6	9:b:4:MAN:C3	2.63	0.63
1:L:25:ALA:O	1:L:26:SER:C	2.41	0.63
2:3:113:PRO:O	2:3:114:ALA:C	2.41	0.63
1:T:25:ALA:O	1:T:26:SER:C	2.41	0.63
2:R:165:ALA:O	2:R:166:LEU:C	2.42	0.62
2:S:113:PRO:O	2:S:114:ALA:C	2.41	0.62
2:S:31:ALA:O	7:o:2:MAN:O2	2.09	0.61
1:4:50:LYS:O	1:4:52:SER:N	2.29	0.61
1:K:183:LYS:O	1:K:187:GLU:N	2.34	0.61
1:1:183:LYS:O	1:1:187:GLU:N	2.34	0.61
2:H:31:ALA:O	7:g:2:MAN:O2	2.09	0.60
2:R:126:PRO:O	2:R:127:SER:O	2.19	0.60
2:2:113:PRO:C	2:2:114:ALA:O	2.43	0.60
2:M:113:PRO:C	2:M:114:ALA:O	2.43	0.60
2:M:126:PRO:O	2:M:127:SER:O	2.20	0.60
9:b:7:MAN:O2	7:i:1:MAN:H3	2.02	0.60
1:L:79:GLN:O	1:L:82:ASP:N	2.31	0.60
9:f:7:MAN:O2	7:g:1:MAN:H3	2.02	0.59
7:N:1:MAN:H3	9:Z:7:MAN:O2	2.02	0.59
2:2:126:PRO:O	2:2:127:SER:O	2.20	0.59
9:X:7:MAN:O2	7:Y:1:MAN:H3	2.02	0.59
2:H:167:THR:O	2:H:168:SER:C	2.42	0.59
2:R:113:PRO:C	2:R:114:ALA:O	2.43	0.59
9:d:7:MAN:O2	7:l:1:MAN:H3	2.02	0.59
1:4:79:GLN:O	1:4:82:ASP:N	2.31	0.59
2:S:167:THR:O	2:S:168:SER:C	2.42	0.59
1:1:118:PHE:N	1:1:133:VAL:O	2.36	0.58
2:M:141:GLY:HA3	2:M:189:SER:O	2.03	0.58
1:T:79:GLN:O	1:T:82:ASP:N	2.31	0.58
9:n:7:MAN:O2	7:o:1:MAN:H3	2.02	0.58
1:Q:183:LYS:O	1:Q:187:GLU:N	2.34	0.58
2:R:141:GLY:HA3	2:R:189:SER:O	2.04	0.58
1:Q:118:PHE:N	1:Q:133:VAL:O	2.36	0.57
2:S:27:PHE:O	2:S:28:ARG:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:141:GLY:HA3	2:2:189:SER:O	2.04	0.57
1:K:118:PHE:N	1:K:133:VAL:O	2.36	0.57
2:3:28:ARG:H	9:Z:5:MAN:H61	1.68	0.57
2:H:113:PRO:O	2:H:114:ALA:C	2.48	0.57
2:S:28:ARG:H	9:d:5:MAN:H61	1.69	0.57
2:3:167:THR:O	2:3:168:SER:C	2.42	0.57
2:3:27:PHE:O	2:3:28:ARG:C	2.47	0.56
2:S:199:GLY:C	2:S:203:GLN:H	2.14	0.56
2:3:199:GLY:C	2:3:203:GLN:H	2.14	0.56
2:H:27:PHE:O	2:H:28:ARG:C	2.47	0.55
2:M:98:ASP:C	2:M:100:LEU:H	2.15	0.55
2:2:98:ASP:C	2:2:100:LEU:H	2.15	0.55
2:R:98:ASP:C	2:R:100:LEU:H	2.15	0.55
1:K:126:LYS:C	1:K:128:GLY:N	2.62	0.54
2:H:28:ARG:H	9:b:5:MAN:H61	1.68	0.54
1:Q:126:LYS:C	1:Q:128:GLY:N	2.62	0.54
2:H:55:THR:O	8:j:5:MAN:H3	2.08	0.54
2:S:55:THR:O	8:m:5:MAN:H3	2.08	0.54
2:3:55:THR:O	8:U:5:MAN:H3	2.08	0.53
2:3:199:GLY:C	2:3:203:GLN:N	2.66	0.53
2:H:199:GLY:C	2:H:203:GLN:H	2.14	0.53
2:R:113:PRO:O	2:R:114:ALA:O	2.27	0.53
1:1:126:LYS:C	1:1:128:GLY:N	2.62	0.53
2:2:113:PRO:O	2:2:114:ALA:O	2.26	0.53
2:2:12:VAL:O	2:2:112:SER:N	2.39	0.53
2:R:134:SER:O	2:R:136:GLY:N	2.41	0.53
2:3:179:GLN:O	2:3:182:SER:N	2.42	0.53
2:H:199:GLY:C	2:H:203:GLN:N	2.66	0.53
2:2:134:SER:O	2:2:136:GLY:N	2.41	0.52
2:3:82(A):HIS:O	2:3:82(B):LYS:C	2.52	0.52
2:S:179:GLN:O	2:S:182:SER:N	2.42	0.52
2:S:199:GLY:C	2:S:203:GLN:N	2.66	0.52
2:M:113:PRO:O	2:M:114:ALA:O	2.27	0.52
2:H:179:GLN:O	2:H:182:SER:N	2.42	0.52
2:H:174:PHE:O	2:H:175:PRO:C	2.53	0.51
2:3:174:PHE:O	2:3:175:PRO:C	2.53	0.51
2:M:12:VAL:O	2:M:112:SER:N	2.39	0.51
2:H:82(A):HIS:O	2:H:82(B):LYS:C	2.52	0.51
2:3:125:ALA:O	2:3:126:PRO:C	2.54	0.51
2:R:60:ALA:O	2:R:63:VAL:N	2.40	0.51
2:2:60:ALA:O	2:2:63:VAL:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:ALA:O	2:H:126:PRO:C	2.54	0.51
2:M:134:SER:O	2:M:136:GLY:N	2.41	0.50
1:T:125:LEU:O	1:T:126:LYS:C	2.54	0.50
9:Z:3:BMA:H62	9:Z:4:MAN:C3	2.21	0.50
2:S:174:PHE:O	2:S:175:PRO:C	2.53	0.50
2:M:60:ALA:O	2:M:63:VAL:N	2.40	0.50
2:S:125:ALA:O	2:S:126:PRO:C	2.54	0.50
1:L:125:LEU:O	1:L:126:LYS:C	2.54	0.49
1:4:125:LEU:O	1:4:126:LYS:C	2.54	0.49
2:R:12:VAL:O	2:R:112:SER:N	2.40	0.49
2:S:82(A):HIS:O	2:S:82(B):LYS:C	2.52	0.49
1:K:108:ARG:O	1:K:109:THR:C	2.56	0.49
2:M:213:LYS:O	2:M:216:ASN:N	2.38	0.49
2:H:163:SER:O	2:H:165:ALA:N	2.41	0.49
1:Q:108:ARG:O	1:Q:109:THR:C	2.56	0.49
2:R:98:ASP:C	2:R:100:LEU:N	2.71	0.49
1:1:142:ARG:O	1:1:144:ALA:N	2.46	0.49
2:2:98:ASP:C	2:2:100:LEU:N	2.71	0.49
1:Q:142:ARG:O	1:Q:144:ALA:N	2.46	0.49
1:1:108:ARG:O	1:1:109:THR:C	2.56	0.48
1:L:49:TYR:O	1:L:50:LYS:C	2.56	0.48
2:M:98:ASP:C	2:M:100:LEU:N	2.71	0.48
2:2:213:LYS:O	2:2:216:ASN:N	2.38	0.48
1:4:49:TYR:O	1:4:50:LYS:C	2.56	0.48
1:K:142:ARG:O	1:K:144:ALA:N	2.46	0.48
1:T:49:TYR:O	1:T:50:LYS:C	2.56	0.48
7:h:1:MAN:C2	7:h:2:MAN:C5	2.92	0.48
7:k:1:MAN:C2	7:k:2:MAN:C5	2.92	0.48
7:G:1:MAN:C2	7:G:2:MAN:C5	2.92	0.48
3:E:368:ASP:N	5:I:54:TRP:O	2.46	0.47
2:S:163:SER:O	2:S:165:ALA:N	2.41	0.47
2:R:208:CYS:O	2:R:220:ASP:CA	2.63	0.47
2:3:113:PRO:O	2:3:115:SER:N	2.48	0.47
2:R:41:PRO:C	2:R:43:GLY:N	2.72	0.47
2:M:208:CYS:O	2:M:220:ASP:CA	2.63	0.47
2:2:208:CYS:O	2:2:220:ASP:CA	2.63	0.47
2:3:163:SER:O	2:3:165:ALA:N	2.41	0.47
1:4:111:ALA:O	1:4:140:TYR:O	2.33	0.47
2:M:3:GLN:O	2:M:25:SER:N	2.47	0.47
9:X:5:MAN:C1	9:X:6:MAN:C5	2.93	0.47
9:b:3:BMA:H61	9:b:4:MAN:H2	1.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:5:MAN:C1	9:b:6:MAN:C5	2.93	0.46
3:A:455:THR:N	3:A:469:ARG:O	2.48	0.46
2:S:113:PRO:O	2:S:115:SER:N	2.48	0.46
9:Z:5:MAN:C1	9:Z:6:MAN:C5	2.93	0.46
9:n:5:MAN:C1	9:n:6:MAN:C5	2.93	0.46
10:c:4:MAN:HO2	7:k:1:MAN:H2	1.79	0.46
2:M:41:PRO:C	2:M:43:GLY:N	2.72	0.46
2:R:3:GLN:O	2:R:25:SER:N	2.47	0.46
2:R:213:LYS:O	2:R:216:ASN:N	2.38	0.46
2:H:163:SER:C	2:H:165:ALA:H	2.22	0.46
2:S:228:LYS:O	2:S:229:SER:O	2.34	0.46
9:d:3:BMA:H61	9:d:4:MAN:H2	1.41	0.46
9:d:5:MAN:C1	9:d:6:MAN:C5	2.93	0.46
2:H:228:LYS:O	2:H:229:SER:O	2.34	0.46
9:f:5:MAN:C1	9:f:6:MAN:C5	2.93	0.46
1:L:111:ALA:O	1:L:140:TYR:O	2.33	0.46
2:S:163:SER:C	2:S:165:ALA:H	2.22	0.46
3:C:368:ASP:N	5:O:54:TRP:O	2.46	0.45
3:C:455:THR:N	3:C:469:ARG:O	2.48	0.45
1:T:111:ALA:O	1:T:140:TYR:O	2.33	0.45
1:Q:64:GLY:HA2	1:Q:72:THR:O	2.17	0.45
2:3:40:VAL:O	2:3:43:GLY:HA2	2.17	0.45
2:H:40:VAL:O	2:H:43:GLY:HA2	2.17	0.45
2:M:29:ILE:O	2:M:30:SER:C	2.60	0.45
2:S:100(A):SER:C	2:S:100(C):ASN:H	2.25	0.45
2:H:167:THR:O	2:H:169:GLY:N	2.51	0.44
1:K:64:GLY:HA2	1:K:72:THR:O	2.17	0.44
1:1:64:GLY:HA2	1:1:72:THR:O	2.17	0.44
2:2:29:ILE:O	2:2:30:SER:C	2.60	0.44
2:3:228:LYS:O	2:3:229:SER:O	2.34	0.44
9:Z:3:BMA:H61	9:Z:4:MAN:H2	1.41	0.44
10:a:4:MAN:HO2	7:h:1:MAN:H2	1.81	0.44
2:3:100(A):SER:C	2:3:100(C):ASN:H	2.25	0.44
9:f:3:BMA:H61	9:f:4:MAN:H2	1.41	0.44
9:b:7:MAN:O2	7:i:1:MAN:H2	2.02	0.44
2:2:3:GLN:O	2:2:25:SER:N	2.47	0.44
2:2:179:GLN:O	2:2:182:SER:N	2.51	0.44
2:3:163:SER:C	2:3:165:ALA:H	2.22	0.44
2:3:167:THR:O	2:3:169:GLY:N	2.51	0.44
2:R:179:GLN:O	2:R:182:SER:N	2.51	0.44
3:E:455:THR:N	3:E:469:ARG:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:179:GLN:O	2:M:182:SER:N	2.51	0.44
2:R:29:ILE:O	2:R:30:SER:C	2.60	0.44
7:h:1:MAN:C2	7:h:2:MAN:H5	2.48	0.44
1:Q:186:TYR:C	1:Q:188:LYS:H	2.22	0.44
2:2:41:PRO:C	2:2:43:GLY:N	2.72	0.43
2:3:82(A):HIS:C	2:3:82(C):MET:N	2.75	0.43
2:S:40:VAL:O	2:S:43:GLY:HA2	2.17	0.43
2:H:100(A):SER:C	2:H:100(C):ASN:H	2.25	0.43
2:S:147:TYR:O	2:S:185:TYR:N	2.51	0.43
9:n:3:BMA:C6	9:n:4:MAN:C3	2.63	0.43
1:1:186:TYR:C	1:1:188:LYS:H	2.22	0.43
3:A:368:ASP:N	5:V:54:TRP:O	2.46	0.43
2:M:194:PRO:C	2:M:196:SER:N	2.75	0.43
2:R:194:PRO:C	2:R:196:SER:N	2.75	0.43
2:H:147:TYR:O	2:H:185:TYR:N	2.51	0.43
7:G:1:MAN:C2	7:G:2:MAN:H5	2.48	0.43
1:4:23:CYS:O	1:4:71:PHE:N	2.49	0.43
2:R:18:LEU:N	2:R:82:MET:O	2.49	0.43
2:3:28:ARG:N	9:Z:5:MAN:C6	2.74	0.43
2:3:147:TYR:O	2:3:185:TYR:N	2.51	0.43
2:S:167:THR:O	2:S:169:GLY:N	2.51	0.43
9:X:3:BMA:H61	9:X:4:MAN:H2	1.41	0.43
9:n:3:BMA:H61	9:n:4:MAN:H2	1.41	0.43
1:4:108:ARG:O	1:4:109:THR:C	2.62	0.43
7:k:1:MAN:C2	7:k:2:MAN:H5	2.48	0.43
2:3:28:ARG:N	9:Z:5:MAN:O6	2.52	0.42
1:K:86:TYR:N	1:K:102:THR:O	2.39	0.42
2:2:18:LEU:N	2:2:82:MET:O	2.49	0.42
3:C:459:GLY:N	5:O:61:ARG:N	2.46	0.42
2:M:18:LEU:N	2:M:82:MET:O	2.49	0.42
2:S:82(A):HIS:C	2:S:82(C):MET:N	2.75	0.42
1:T:108:ARG:O	1:T:109:THR:C	2.62	0.42
3:A:99:ASN:O	3:A:102:GLU:N	2.53	0.42
3:C:99:ASN:O	3:C:102:GLU:N	2.53	0.42
1:L:108:ARG:O	1:L:109:THR:C	2.62	0.42
3:A:459:GLY:N	5:V:61:ARG:N	2.46	0.42
2:H:82(A):HIS:C	2:H:82(C):MET:N	2.75	0.42
2:H:113:PRO:O	2:H:115:SER:N	2.53	0.42
1:Q:16:GLY:N	1:Q:78:LEU:O	2.52	0.42
2:S:28:ARG:N	9:d:5:MAN:C6	2.74	0.41
2:2:30:SER:O	2:2:31:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:ARG:N	9:b:5:MAN:O6	2.52	0.41
2:3:199:GLY:N	2:3:203:GLN:H	2.19	0.41
2:R:84:VAL:O	2:R:87:THR:N	2.53	0.41
3:E:99:ASN:O	3:E:102:GLU:N	2.53	0.41
2:M:84:VAL:O	2:M:87:THR:N	2.53	0.41
9:b:3:BMA:H62	9:b:4:MAN:C3	2.21	0.41
9:b:4:MAN:H61	9:b:5:MAN:C5	2.51	0.41
2:2:84:VAL:O	2:2:87:THR:N	2.53	0.41
2:H:199:GLY:N	2:H:203:GLN:H	2.19	0.41
1:K:65:SER:N	1:K:72:THR:O	2.54	0.41
7:G:1:MAN:H2	10:e:4:MAN:HO2	1.80	0.41
2:2:84:VAL:C	2:2:86:ASP:N	2.67	0.41
1:Q:65:SER:N	1:Q:72:THR:O	2.54	0.41
9:Z:4:MAN:H61	9:Z:5:MAN:C5	2.51	0.41
9:f:4:MAN:H61	9:f:5:MAN:C5	2.51	0.41
3:C:303:THR:O	3:C:321:GLY:N	2.49	0.41
2:3:157:TRP:O	2:3:162:ASN:C	2.63	0.41
2:3:195:SER:O	2:3:196:SER:C	2.63	0.41
2:H:157:TRP:O	2:H:162:ASN:C	2.63	0.41
1:K:16:GLY:N	1:K:78:LEU:O	2.52	0.41
1:L:11:LEU:O	1:L:105:GLU:N	2.39	0.41
9:n:4:MAN:H61	9:n:5:MAN:C5	2.51	0.41
2:S:195:SER:O	2:S:196:SER:C	2.63	0.40
2:S:199:GLY:N	2:S:203:GLN:H	2.19	0.40
9:d:4:MAN:H61	9:d:5:MAN:C5	2.51	0.40
2:S:157:TRP:O	2:S:162:ASN:C	2.63	0.40
1:4:203:SER:O	1:4:204:PRO:C	2.64	0.40
2:H:28:ARG:N	9:b:5:MAN:C6	2.74	0.40
2:R:30:SER:O	2:R:31:ALA:C	2.63	0.40
2:S:28:ARG:N	9:d:5:MAN:O6	2.52	0.40
1:T:203:SER:O	1:T:204:PRO:C	2.64	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	1	210/212 (99%)	158 (75%)	39 (19%)	13 (6%)	1	13
1	4	210/212 (99%)	177 (84%)	24 (11%)	9 (4%)	2	17
1	K	210/212 (99%)	158 (75%)	39 (19%)	13 (6%)	1	13
1	L	210/212 (99%)	177 (84%)	24 (11%)	9 (4%)	2	17
1	Q	210/212 (99%)	158 (75%)	39 (19%)	13 (6%)	1	13
1	T	210/212 (99%)	177 (84%)	24 (11%)	9 (4%)	2	17
2	2	223/225 (99%)	157 (70%)	28 (13%)	38 (17%)	0	2
2	3	223/225 (99%)	160 (72%)	40 (18%)	23 (10%)	0	6
2	H	223/225 (99%)	159 (71%)	41 (18%)	23 (10%)	0	6
2	M	223/225 (99%)	157 (70%)	28 (13%)	38 (17%)	0	2
2	R	223/225 (99%)	157 (70%)	28 (13%)	38 (17%)	0	2
2	S	223/225 (99%)	159 (71%)	41 (18%)	23 (10%)	0	6
3	A	447/474 (94%)	406 (91%)	39 (9%)	2 (0%)	30	67
3	C	447/474 (94%)	406 (91%)	39 (9%)	2 (0%)	30	67
3	E	447/474 (94%)	406 (91%)	39 (9%)	2 (0%)	30	67
4	B	122/170 (72%)	109 (89%)	13 (11%)	0	100	100
4	D	122/170 (72%)	109 (89%)	13 (11%)	0	100	100
4	F	122/170 (72%)	109 (89%)	13 (11%)	0	100	100
5	I	126/227 (56%)	124 (98%)	2 (2%)	0	100	100
5	O	126/227 (56%)	125 (99%)	1 (1%)	0	100	100
5	V	126/227 (56%)	123 (98%)	3 (2%)	0	100	100
6	J	99/208 (48%)	96 (97%)	3 (3%)	0	100	100
6	P	99/208 (48%)	96 (97%)	3 (3%)	0	100	100
6	W	99/208 (48%)	96 (97%)	3 (3%)	0	100	100
All	All	4980/5859 (85%)	4159 (84%)	566 (11%)	255 (5%)	3	15

All (255) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	152	ASN
1	1	176	SER
1	1	187	GLU

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Mol	Chain	Res	Type
2	2	16	GLY
2	2	30	SER
2	2	48	VAL
2	2	74	LEU
2	2	85	GLU
2	2	98	ASP
2	2	100(A)	SER
2	2	114	ALA
2	2	115	SER
2	2	121	VAL
2	2	127	SER
2	2	139	ALA
2	2	146	ASP
2	2	165	ALA
2	2	166	LEU
2	2	180	SER
2	2	195	SER
2	3	16	GLY
2	3	53	SER
2	3	100(B)	ASP
2	3	129	LYS
2	3	180	SER
2	3	227	PRO
1	4	26	SER
1	4	51	ALA
1	4	168	SER
2	H	16	GLY
2	H	53	SER
2	H	100(B)	ASP
2	H	129	LYS
2	H	180	SER
2	H	227	PRO
1	K	152	ASN
1	K	176	SER
1	K	187	GLU
1	L	26	SER
1	L	51	ALA
1	L	168	SER
2	M	16	GLY
2	M	30	SER
2	M	48	VAL
2	M	74	LEU

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Mol	Chain	Res	Type
2	M	85	GLU
2	M	98	ASP
2	M	100(A)	SER
2	M	114	ALA
2	M	115	SER
2	M	121	VAL
2	M	127	SER
2	M	139	ALA
2	M	146	ASP
2	M	165	ALA
2	M	166	LEU
2	M	180	SER
2	M	195	SER
1	Q	152	ASN
1	Q	176	SER
1	Q	187	GLU
2	R	16	GLY
2	R	30	SER
2	R	48	VAL
2	R	74	LEU
2	R	85	GLU
2	R	98	ASP
2	R	100(A)	SER
2	R	114	ALA
2	R	115	SER
2	R	121	VAL
2	R	127	SER
2	R	139	ALA
2	R	146	ASP
2	R	165	ALA
2	R	166	LEU
2	R	180	SER
2	R	195	SER
2	S	16	GLY
2	S	53	SER
2	S	100(B)	ASP
2	S	129	LYS
2	S	180	SER
2	S	227	PRO
1	T	26	SER
1	T	51	ALA
1	T	168	SER

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Mol	Chain	Res	Type
1	1	82	ASP
1	1	109	THR
1	1	143	GLU
1	1	191	VAL
1	1	211	ARG
2	2	2	VAL
2	2	9	GLY
2	2	61	ASP
2	2	100(B)	ASP
2	2	106	GLY
2	2	135	GLY
2	2	136	GLY
2	2	186	SER
2	2	216	ASN
2	3	9	GLY
2	3	134	SER
2	3	163	SER
2	3	164	GLY
1	4	154	LEU
2	H	9	GLY
2	H	134	SER
2	H	163	SER
2	H	164	GLY
1	K	82	ASP
1	K	109	THR
1	K	143	GLU
1	K	188	LYS
1	K	191	VAL
1	K	211	ARG
1	L	154	LEU
2	M	2	VAL
2	M	9	GLY
2	M	61	ASP
2	M	100(B)	ASP
2	M	106	GLY
2	M	135	GLY
2	M	136	GLY
2	M	186	SER
2	M	216	ASN
1	Q	82	ASP
1	Q	109	THR
1	Q	143	GLU

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Mol	Chain	Res	Type
1	Q	188	LYS
1	Q	191	VAL
1	Q	211	ARG
2	R	2	VAL
2	R	9	GLY
2	R	61	ASP
2	R	100(B)	ASP
2	R	106	GLY
2	R	135	GLY
2	R	136	GLY
2	R	186	SER
2	R	216	ASN
2	S	9	GLY
2	S	134	SER
2	S	163	SER
2	S	164	GLY
1	T	154	LEU
1	1	67	SER
1	1	188	LYS
2	2	31	ALA
2	2	73	ASP
2	3	42	GLY
2	3	85	GLU
2	3	116	THR
1	4	126	LYS
2	H	42	GLY
2	H	85	GLU
2	H	116	THR
1	K	67	SER
1	L	126	LYS
2	M	31	ALA
2	M	73	ASP
1	Q	67	SER
2	R	31	ALA
2	R	73	ASP
2	S	42	GLY
2	S	85	GLU
2	S	116	THR
1	T	126	LYS
1	1	120	PRO
2	2	40	VAL
2	2	99	ARG

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Mol	Chain	Res	Type
2	2	128	SER
2	2	151	PRO
2	2	193	VAL
2	3	146	ASP
2	3	175	PRO
1	4	17	ASP
1	4	157	GLY
3	A	500	ARG
3	C	500	ARG
3	E	500	ARG
2	H	146	ASP
2	H	175	PRO
1	K	120	PRO
1	L	17	ASP
1	L	157	GLY
2	M	40	VAL
2	M	99	ARG
2	M	128	SER
2	M	151	PRO
2	M	193	VAL
1	Q	120	PRO
1	Q	142	ARG
2	R	40	VAL
2	R	99	ARG
2	R	128	SER
2	R	151	PRO
2	R	193	VAL
2	S	146	ASP
2	S	175	PRO
1	T	17	ASP
1	T	157	GLY
1	1	142	ARG
2	2	62	ALA
2	3	82(B)	LYS
2	3	100(E)	PRO
2	3	128	SER
2	3	148	PHE
2	3	203	GLN
2	3	216	ASN
1	4	204	PRO
2	H	82(B)	LYS
2	H	100(E)	PRO

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Mol	Chain	Res	Type
2	H	128	SER
2	H	148	PHE
2	H	203	GLN
2	H	216	ASN
1	K	142	ARG
1	L	204	PRO
2	M	62	ALA
2	R	62	ALA
2	S	82(B)	LYS
2	S	100(E)	PRO
2	S	128	SER
2	S	148	PHE
2	S	203	GLN
2	S	216	ASN
1	T	204	PRO
1	1	140	TYR
2	2	100(E)	PRO
1	4	81	ASP
1	K	140	TYR
1	L	81	ASP
2	M	100(E)	PRO
1	Q	140	TYR
2	R	100(E)	PRO
1	T	81	ASP
2	2	41	PRO
3	A	312	GLY
3	C	312	GLY
3	E	312	GLY
2	M	41	PRO
2	R	41	PRO
2	2	194	PRO
2	M	194	PRO
2	R	194	PRO
2	3	126	PRO
2	H	126	PRO
2	S	126	PRO
2	2	84	VAL
2	M	84	VAL
2	R	84	VAL
2	3	151	PRO
2	H	151	PRO
2	S	151	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

90 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	MAN	G	1	7	11,11,12	1.57	3 (27%)	15,15,17	3.27	9 (60%)
7	MAN	G	2	7	11,11,12	1.20	1 (9%)	15,15,17	3.14	6 (40%)
7	MAN	N	1	7	11,11,12	1.27	2 (18%)	15,15,17	3.88	10 (66%)
7	MAN	N	2	7	11,11,12	1.33	2 (18%)	15,15,17	3.00	7 (46%)
8	NAG	U	1	8	14,14,15	0.31	0	17,19,21	0.46	0
8	NAG	U	2	8	14,14,15	0.36	0	17,19,21	0.67	0
8	BMA	U	3	8	11,11,12	0.63	0	15,15,17	0.82	0
8	MAN	U	4	8	11,11,12	0.73	0	15,15,17	1.00	2 (13%)
8	MAN	U	5	8	11,11,12	0.75	1 (9%)	15,15,17	1.04	2 (13%)
8	MAN	U	6	8	11,11,12	0.66	0	15,15,17	1.00	2 (13%)
9	NAG	X	1	9	15,15,15	1.22	1 (6%)	21,21,21	2.66	9 (42%)
9	NAG	X	2	9	14,14,15	0.92	0	17,19,21	2.21	5 (29%)
9	BMA	X	3	9	11,11,12	1.18	0	15,15,17	2.84	8 (53%)
9	MAN	X	4	9	11,11,12	0.92	0	15,15,17	2.28	5 (33%)
9	MAN	X	5	9	11,11,12	1.80	2 (18%)	15,15,17	3.39	10 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	X	6	9	11,11,12	2.12	5 (45%)	15,15,17	2.61	4 (26%)
9	MAN	X	7	9	11,11,12	1.47	2 (18%)	15,15,17	2.01	5 (33%)
7	MAN	Y	1	7	11,11,12	1.27	2 (18%)	15,15,17	3.88	10 (66%)
7	MAN	Y	2	7	11,11,12	1.32	2 (18%)	15,15,17	3.01	7 (46%)
9	NAG	Z	1	9	15,15,15	1.22	1 (6%)	21,21,21	2.67	9 (42%)
9	NAG	Z	2	9	14,14,15	0.92	0	17,19,21	2.22	5 (29%)
9	BMA	Z	3	9	11,11,12	1.19	0	15,15,17	2.84	8 (53%)
9	MAN	Z	4	9	11,11,12	0.93	0	15,15,17	2.27	5 (33%)
9	MAN	Z	5	9	11,11,12	1.81	3 (27%)	15,15,17	3.40	10 (66%)
9	MAN	Z	6	9	11,11,12	2.12	5 (45%)	15,15,17	2.60	4 (26%)
9	MAN	Z	7	9	11,11,12	1.47	2 (18%)	15,15,17	1.99	5 (33%)
10	NAG	a	1	10	14,14,15	1.65	4 (28%)	17,19,21	2.94	8 (47%)
10	NAG	a	2	10	14,14,15	1.00	1 (7%)	17,19,21	2.70	8 (47%)
10	BMA	a	3	10	11,11,12	1.33	2 (18%)	15,15,17	2.60	7 (46%)
10	MAN	a	4	10	11,11,12	1.08	1 (9%)	15,15,17	2.40	6 (40%)
9	NAG	b	1	9	15,15,15	1.23	1 (6%)	21,21,21	2.66	9 (42%)
9	NAG	b	2	9	14,14,15	0.92	0	17,19,21	2.21	5 (29%)
9	BMA	b	3	9	11,11,12	1.19	0	15,15,17	2.84	8 (53%)
9	MAN	b	4	9	11,11,12	0.93	0	15,15,17	2.28	5 (33%)
9	MAN	b	5	9	11,11,12	1.81	3 (27%)	15,15,17	3.40	10 (66%)
9	MAN	b	6	9	11,11,12	2.12	5 (45%)	15,15,17	2.60	4 (26%)
9	MAN	b	7	9	11,11,12	1.47	2 (18%)	15,15,17	1.99	5 (33%)
10	NAG	c	1	10	14,14,15	1.65	4 (28%)	17,19,21	2.94	8 (47%)
10	NAG	c	2	10	14,14,15	1.01	1 (7%)	17,19,21	2.70	8 (47%)
10	BMA	c	3	10	11,11,12	1.33	2 (18%)	15,15,17	2.59	7 (46%)
10	MAN	c	4	10	11,11,12	1.08	1 (9%)	15,15,17	2.39	6 (40%)
9	NAG	d	1	9	15,15,15	1.22	1 (6%)	21,21,21	2.66	9 (42%)
9	NAG	d	2	9	14,14,15	0.92	0	17,19,21	2.21	5 (29%)
9	BMA	d	3	9	11,11,12	1.19	0	15,15,17	2.84	7 (46%)
9	MAN	d	4	9	11,11,12	0.92	0	15,15,17	2.28	5 (33%)
9	MAN	d	5	9	11,11,12	1.81	3 (27%)	15,15,17	3.40	10 (66%)
9	MAN	d	6	9	11,11,12	2.12	5 (45%)	15,15,17	2.60	4 (26%)
9	MAN	d	7	9	11,11,12	1.47	2 (18%)	15,15,17	1.99	5 (33%)
10	NAG	e	1	10	14,14,15	1.65	4 (28%)	17,19,21	2.94	8 (47%)
10	NAG	e	2	10	14,14,15	1.01	1 (7%)	17,19,21	2.71	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	e	3	10	11,11,12	1.33	2 (18%)	15,15,17	2.60	7 (46%)
10	MAN	e	4	10	11,11,12	1.08	1 (9%)	15,15,17	2.39	6 (40%)
9	NAG	f	1	9	15,15,15	1.22	1 (6%)	21,21,21	2.66	9 (42%)
9	NAG	f	2	9	14,14,15	0.92	0	17,19,21	2.21	5 (29%)
9	BMA	f	3	9	11,11,12	1.18	0	15,15,17	2.84	7 (46%)
9	MAN	f	4	9	11,11,12	0.92	0	15,15,17	2.27	5 (33%)
9	MAN	f	5	9	11,11,12	1.80	3 (27%)	15,15,17	3.39	10 (66%)
9	MAN	f	6	9	11,11,12	2.13	5 (45%)	15,15,17	2.61	4 (26%)
9	MAN	f	7	9	11,11,12	1.47	2 (18%)	15,15,17	2.00	5 (33%)
7	MAN	g	1	7	11,11,12	1.28	2 (18%)	15,15,17	3.87	10 (66%)
7	MAN	g	2	7	11,11,12	1.32	2 (18%)	15,15,17	3.00	7 (46%)
7	MAN	h	1	7	11,11,12	1.57	3 (27%)	15,15,17	3.27	9 (60%)
7	MAN	h	2	7	11,11,12	1.21	1 (9%)	15,15,17	3.14	6 (40%)
7	MAN	i	1	7	11,11,12	1.28	2 (18%)	15,15,17	3.88	10 (66%)
7	MAN	i	2	7	11,11,12	1.32	2 (18%)	15,15,17	3.00	7 (46%)
8	NAG	j	1	8	14,14,15	0.31	0	17,19,21	0.47	0
8	NAG	j	2	8	14,14,15	0.37	0	17,19,21	0.66	0
8	BMA	j	3	8	11,11,12	0.63	0	15,15,17	0.83	0
8	MAN	j	4	8	11,11,12	0.72	0	15,15,17	0.99	2 (13%)
8	MAN	j	5	8	11,11,12	0.76	1 (9%)	15,15,17	1.04	1 (6%)
8	MAN	j	6	8	11,11,12	0.66	0	15,15,17	1.01	2 (13%)
7	MAN	k	1	7	11,11,12	1.57	3 (27%)	15,15,17	3.27	9 (60%)
7	MAN	k	2	7	11,11,12	1.21	1 (9%)	15,15,17	3.15	6 (40%)
7	MAN	l	1	7	11,11,12	1.28	2 (18%)	15,15,17	3.87	10 (66%)
7	MAN	l	2	7	11,11,12	1.30	2 (18%)	15,15,17	3.01	7 (46%)
8	NAG	m	1	8	14,14,15	0.31	0	17,19,21	0.47	0
8	NAG	m	2	8	14,14,15	0.38	0	17,19,21	0.67	0
8	BMA	m	3	8	11,11,12	0.63	0	15,15,17	0.83	0
8	MAN	m	4	8	11,11,12	0.72	0	15,15,17	1.00	2 (13%)
8	MAN	m	5	8	11,11,12	0.77	1 (9%)	15,15,17	1.04	1 (6%)
8	MAN	m	6	8	11,11,12	0.66	0	15,15,17	1.01	2 (13%)
9	NAG	n	1	9	15,15,15	1.22	1 (6%)	21,21,21	2.66	9 (42%)
9	NAG	n	2	9	14,14,15	0.92	0	17,19,21	2.21	5 (29%)
9	BMA	n	3	9	11,11,12	1.19	0	15,15,17	2.85	7 (46%)
9	MAN	n	4	9	11,11,12	0.92	0	15,15,17	2.27	5 (33%)
9	MAN	n	5	9	11,11,12	1.79	3 (27%)	15,15,17	3.40	10 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	n	6	9	11,11,12	2.13	5 (45%)	15,15,17	2.60	4 (26%)
9	MAN	n	7	9	11,11,12	1.46	2 (18%)	15,15,17	2.01	5 (33%)
7	MAN	o	1	7	11,11,12	1.27	2 (18%)	15,15,17	3.87	10 (66%)
7	MAN	o	2	7	11,11,12	1.32	2 (18%)	15,15,17	3.00	7 (46%)

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	MAN	G	1	7	-	1/2/19/22	0/1/1/1
7	MAN	G	2	7	-	1/2/19/22	0/1/1/1
7	MAN	N	1	7	-	1/2/19/22	0/1/1/1
7	MAN	N	2	7	1/1/4/5	2/2/19/22	0/1/1/1
8	NAG	U	1	8	-	2/6/23/26	0/1/1/1
8	NAG	U	2	8	-	4/6/23/26	0/1/1/1
8	BMA	U	3	8	-	0/2/19/22	0/1/1/1
8	MAN	U	4	8	-	2/2/19/22	0/1/1/1
8	MAN	U	5	8	-	1/2/19/22	0/1/1/1
8	MAN	U	6	8	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9	-	4/6/26/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
9	BMA	X	3	9	-	2/2/19/22	0/1/1/1
9	MAN	X	4	9	-	2/2/19/22	0/1/1/1
9	MAN	X	5	9	-	2/2/19/22	0/1/1/1
9	MAN	X	6	9	-	0/2/19/22	0/1/1/1
9	MAN	X	7	9	-	2/2/19/22	0/1/1/1
7	MAN	Y	1	7	-	1/2/19/22	0/1/1/1
7	MAN	Y	2	7	1/1/4/5	2/2/19/22	0/1/1/1
9	NAG	Z	1	9	-	4/6/26/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	2/2/19/22	0/1/1/1
9	MAN	Z	4	9	-	2/2/19/22	0/1/1/1
9	MAN	Z	5	9	-	2/2/19/22	0/1/1/1
9	MAN	Z	6	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	7	9	-	2/2/19/22	0/1/1/1
10	NAG	a	1	10	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	a	2	10	-	4/6/23/26	0/1/1/1
10	BMA	a	3	10	-	2/2/19/22	0/1/1/1
10	MAN	a	4	10	-	0/2/19/22	0/1/1/1
9	NAG	b	1	9	-	4/6/26/26	0/1/1/1
9	NAG	b	2	9	-	2/6/23/26	0/1/1/1
9	BMA	b	3	9	-	2/2/19/22	0/1/1/1
9	MAN	b	4	9	-	2/2/19/22	0/1/1/1
9	MAN	b	5	9	-	2/2/19/22	0/1/1/1
9	MAN	b	6	9	-	0/2/19/22	0/1/1/1
9	MAN	b	7	9	-	2/2/19/22	0/1/1/1
10	NAG	c	1	10	-	1/6/23/26	0/1/1/1
10	NAG	c	2	10	-	4/6/23/26	0/1/1/1
10	BMA	c	3	10	-	2/2/19/22	0/1/1/1
10	MAN	c	4	10	-	0/2/19/22	0/1/1/1
9	NAG	d	1	9	-	4/6/26/26	0/1/1/1
9	NAG	d	2	9	-	2/6/23/26	0/1/1/1
9	BMA	d	3	9	-	2/2/19/22	0/1/1/1
9	MAN	d	4	9	-	2/2/19/22	0/1/1/1
9	MAN	d	5	9	-	2/2/19/22	0/1/1/1
9	MAN	d	6	9	-	0/2/19/22	0/1/1/1
9	MAN	d	7	9	-	2/2/19/22	0/1/1/1
10	NAG	e	1	10	-	1/6/23/26	0/1/1/1
10	NAG	e	2	10	-	4/6/23/26	0/1/1/1
10	BMA	e	3	10	-	2/2/19/22	0/1/1/1
10	MAN	e	4	10	-	0/2/19/22	0/1/1/1
9	NAG	f	1	9	-	4/6/26/26	0/1/1/1
9	NAG	f	2	9	-	2/6/23/26	0/1/1/1
9	BMA	f	3	9	-	2/2/19/22	0/1/1/1
9	MAN	f	4	9	-	2/2/19/22	0/1/1/1
9	MAN	f	5	9	-	2/2/19/22	0/1/1/1
9	MAN	f	6	9	-	0/2/19/22	0/1/1/1
9	MAN	f	7	9	-	2/2/19/22	0/1/1/1
7	MAN	g	1	7	-	1/2/19/22	0/1/1/1
7	MAN	g	2	7	1/1/4/5	2/2/19/22	0/1/1/1
7	MAN	h	1	7	-	1/2/19/22	0/1/1/1
7	MAN	h	2	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	i	1	7	-	1/2/19/22	0/1/1/1
7	MAN	i	2	7	1/1/4/5	2/2/19/22	0/1/1/1
8	NAG	j	1	8	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	4/6/23/26	0/1/1/1
8	BMA	j	3	8	-	0/2/19/22	0/1/1/1
8	MAN	j	4	8	-	2/2/19/22	0/1/1/1
8	MAN	j	5	8	-	1/2/19/22	0/1/1/1
8	MAN	j	6	8	-	0/2/19/22	0/1/1/1
7	MAN	k	1	7	-	1/2/19/22	0/1/1/1
7	MAN	k	2	7	-	1/2/19/22	0/1/1/1
7	MAN	l	1	7	-	1/2/19/22	0/1/1/1
7	MAN	l	2	7	1/1/4/5	2/2/19/22	0/1/1/1
8	NAG	m	1	8	-	2/6/23/26	0/1/1/1
8	NAG	m	2	8	-	4/6/23/26	0/1/1/1
8	BMA	m	3	8	-	0/2/19/22	0/1/1/1
8	MAN	m	4	8	-	2/2/19/22	0/1/1/1
8	MAN	m	5	8	-	1/2/19/22	0/1/1/1
8	MAN	m	6	8	-	0/2/19/22	0/1/1/1
9	NAG	n	1	9	-	4/6/26/26	0/1/1/1
9	NAG	n	2	9	-	2/6/23/26	0/1/1/1
9	BMA	n	3	9	-	2/2/19/22	0/1/1/1
9	MAN	n	4	9	-	2/2/19/22	0/1/1/1
9	MAN	n	5	9	-	2/2/19/22	0/1/1/1
9	MAN	n	6	9	-	0/2/19/22	0/1/1/1
9	MAN	n	7	9	-	2/2/19/22	0/1/1/1
7	MAN	o	1	7	-	1/2/19/22	0/1/1/1
7	MAN	o	2	7	1/1/4/5	2/2/19/22	0/1/1/1

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	c	1	NAG	C1-C2	4.01	1.57	1.52
10	e	1	NAG	C1-C2	3.97	1.57	1.52
10	a	1	NAG	C1-C2	3.97	1.57	1.52
9	f	5	MAN	C4-C5	3.66	1.60	1.53
9	X	5	MAN	C4-C5	3.66	1.60	1.53
9	b	5	MAN	C4-C5	3.65	1.60	1.53
9	d	5	MAN	C4-C5	3.65	1.60	1.53
9	Z	5	MAN	C4-C5	3.64	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	n	5	MAN	C4-C5	3.62	1.60	1.53
9	Z	6	MAN	C4-C5	3.61	1.60	1.53
9	b	6	MAN	C4-C5	3.59	1.60	1.53
9	f	6	MAN	C4-C5	3.59	1.60	1.53
9	n	6	MAN	C4-C5	3.58	1.60	1.53
9	d	6	MAN	C4-C5	3.57	1.60	1.53
9	X	6	MAN	C4-C5	3.56	1.60	1.53
9	n	6	MAN	O5-C1	3.35	1.49	1.43
9	f	6	MAN	O5-C1	3.32	1.49	1.43
9	X	6	MAN	O5-C1	3.30	1.49	1.43
9	d	6	MAN	O5-C1	3.29	1.49	1.43
9	b	6	MAN	O5-C1	3.29	1.49	1.43
9	b	1	NAG	C1-C2	3.28	1.56	1.52
9	Z	6	MAN	O5-C1	3.27	1.49	1.43
9	f	1	NAG	C1-C2	3.25	1.56	1.52
9	X	1	NAG	C1-C2	3.24	1.56	1.52
9	d	1	NAG	C1-C2	3.24	1.56	1.52
9	n	1	NAG	C1-C2	3.23	1.56	1.52
9	Z	1	NAG	C1-C2	3.21	1.56	1.52
9	f	6	MAN	C1-C2	3.13	1.59	1.52
9	n	6	MAN	C1-C2	3.13	1.59	1.52
9	X	6	MAN	C1-C2	3.12	1.59	1.52
9	Z	6	MAN	C1-C2	3.11	1.59	1.52
9	d	6	MAN	C1-C2	3.11	1.59	1.52
9	b	6	MAN	C1-C2	3.10	1.59	1.52
9	X	5	MAN	C1-C2	3.06	1.59	1.52
9	n	5	MAN	C1-C2	3.03	1.59	1.52
9	f	5	MAN	C1-C2	3.03	1.59	1.52
9	Z	5	MAN	C1-C2	3.02	1.59	1.52
9	b	5	MAN	C1-C2	3.01	1.59	1.52
9	d	5	MAN	C1-C2	2.99	1.59	1.52
7	k	1	MAN	O5-C1	-2.89	1.38	1.43
7	N	2	MAN	O4-C4	-2.88	1.35	1.43
7	o	2	MAN	O4-C4	-2.87	1.35	1.43
7	h	1	MAN	O5-C1	-2.86	1.38	1.43
7	i	2	MAN	O4-C4	-2.85	1.35	1.43
7	g	2	MAN	O4-C4	-2.84	1.35	1.43
7	l	2	MAN	O4-C4	-2.84	1.35	1.43
7	Y	2	MAN	O4-C4	-2.83	1.35	1.43
7	k	2	MAN	O5-C5	-2.83	1.37	1.43
7	G	1	MAN	O5-C1	-2.83	1.38	1.43
9	d	7	MAN	C4-C5	-2.79	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	e	2	NAG	C1-C2	2.79	1.56	1.52
7	h	2	MAN	O5-C5	-2.79	1.38	1.43
9	b	7	MAN	C4-C5	-2.78	1.47	1.53
9	Z	7	MAN	C4-C5	-2.78	1.47	1.53
7	G	2	MAN	O5-C5	-2.77	1.38	1.43
10	a	2	NAG	C1-C2	2.77	1.56	1.52
10	c	2	NAG	C1-C2	2.75	1.56	1.52
9	f	7	MAN	C4-C5	-2.74	1.47	1.53
9	X	7	MAN	C4-C5	-2.73	1.47	1.53
7	G	1	MAN	C2-C3	-2.73	1.48	1.52
7	h	1	MAN	C2-C3	-2.71	1.48	1.52
9	n	7	MAN	C4-C5	-2.70	1.47	1.53
7	k	1	MAN	C2-C3	-2.70	1.48	1.52
9	n	7	MAN	O5-C5	-2.51	1.38	1.43
10	c	3	BMA	O5-C5	-2.51	1.38	1.43
10	e	3	BMA	O5-C5	-2.50	1.38	1.43
9	b	7	MAN	O5-C5	-2.50	1.38	1.43
9	Z	6	MAN	C2-C3	2.49	1.56	1.52
9	X	6	MAN	C2-C3	2.49	1.56	1.52
9	d	7	MAN	O5-C5	-2.49	1.38	1.43
9	b	6	MAN	C2-C3	2.49	1.56	1.52
9	Z	7	MAN	O5-C5	-2.48	1.38	1.43
9	f	7	MAN	O5-C5	-2.48	1.38	1.43
10	a	3	BMA	O5-C5	-2.48	1.38	1.43
10	a	1	NAG	C2-N2	2.47	1.50	1.46
10	e	1	NAG	C2-N2	2.47	1.50	1.46
7	l	1	MAN	C1-C2	2.46	1.58	1.52
9	X	7	MAN	O5-C5	-2.46	1.38	1.43
10	c	1	NAG	C2-N2	2.46	1.50	1.46
9	n	6	MAN	C2-C3	2.45	1.56	1.52
9	f	6	MAN	C2-C3	2.45	1.56	1.52
9	d	6	MAN	C2-C3	2.44	1.56	1.52
7	i	1	MAN	C1-C2	2.44	1.58	1.52
7	Y	2	MAN	C2-C3	2.42	1.56	1.52
7	N	1	MAN	C1-C2	2.42	1.58	1.52
10	a	1	NAG	C3-C2	2.42	1.57	1.52
7	o	1	MAN	C1-C2	2.41	1.58	1.52
7	Y	1	MAN	C1-C2	2.41	1.57	1.52
7	N	2	MAN	C2-C3	2.40	1.56	1.52
7	g	1	MAN	C1-C2	2.39	1.57	1.52
10	e	1	NAG	C3-C2	2.39	1.57	1.52
7	g	2	MAN	C2-C3	2.39	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	i	2	MAN	C2-C3	2.39	1.56	1.52
10	c	1	NAG	C3-C2	2.39	1.57	1.52
7	o	2	MAN	C2-C3	2.37	1.56	1.52
7	l	2	MAN	C2-C3	2.34	1.56	1.52
10	a	4	MAN	C1-C2	2.33	1.57	1.52
10	c	4	MAN	C1-C2	2.32	1.57	1.52
10	e	4	MAN	C1-C2	2.31	1.57	1.52
7	g	1	MAN	O5-C5	-2.30	1.39	1.43
7	Y	1	MAN	O5-C5	-2.30	1.39	1.43
7	o	1	MAN	O5-C5	-2.28	1.39	1.43
10	a	3	BMA	C2-C3	-2.28	1.49	1.52
10	e	3	BMA	C2-C3	-2.27	1.49	1.52
7	i	1	MAN	O5-C5	-2.27	1.39	1.43
7	N	1	MAN	O5-C5	-2.27	1.39	1.43
10	c	3	BMA	C2-C3	-2.26	1.49	1.52
7	l	1	MAN	O5-C5	-2.26	1.39	1.43
9	X	6	MAN	O5-C5	2.21	1.47	1.43
9	n	6	MAN	O5-C5	2.21	1.47	1.43
7	k	1	MAN	O5-C5	-2.20	1.39	1.43
9	d	6	MAN	O5-C5	2.19	1.47	1.43
7	G	1	MAN	O5-C5	-2.19	1.39	1.43
9	f	6	MAN	O5-C5	2.18	1.47	1.43
7	h	1	MAN	O5-C5	-2.18	1.39	1.43
9	b	6	MAN	O5-C5	2.16	1.47	1.43
9	Z	6	MAN	O5-C5	2.15	1.47	1.43
10	e	1	NAG	C4-C5	2.13	1.57	1.53
10	a	1	NAG	C4-C5	2.11	1.57	1.53
9	d	5	MAN	C2-C3	2.10	1.55	1.52
10	c	1	NAG	C4-C5	2.08	1.57	1.53
9	b	5	MAN	C2-C3	2.06	1.55	1.52
9	Z	5	MAN	C2-C3	2.05	1.55	1.52
8	m	5	MAN	C1-C2	2.03	1.57	1.52
8	j	5	MAN	C1-C2	2.02	1.57	1.52
9	n	5	MAN	C2-C3	2.02	1.55	1.52
9	f	5	MAN	C2-C3	2.01	1.55	1.52
8	U	5	MAN	C1-C2	2.00	1.57	1.52

All (523) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1	MAN	O2-C2-C3	-7.76	94.07	110.15
7	h	1	MAN	O2-C2-C3	-7.76	94.07	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	k	1	MAN	O2-C2-C3	-7.75	94.10	110.15
7	Y	2	MAN	C1-C2-C3	-7.66	98.49	109.64
7	N	2	MAN	C1-C2-C3	-7.64	98.52	109.64
7	i	2	MAN	C1-C2-C3	-7.64	98.52	109.64
7	l	2	MAN	C1-C2-C3	-7.64	98.52	109.64
7	g	2	MAN	C1-C2-C3	-7.64	98.52	109.64
7	o	2	MAN	C1-C2-C3	-7.62	98.55	109.64
10	e	1	NAG	C2-N2-C7	7.61	133.10	122.90
10	a	1	NAG	C2-N2-C7	7.59	133.07	122.90
10	c	1	NAG	C2-N2-C7	7.55	133.02	122.90
7	Y	1	MAN	O4-C4-C5	7.05	126.69	109.32
7	g	1	MAN	O4-C4-C5	7.04	126.67	109.32
7	o	1	MAN	O4-C4-C5	7.04	126.65	109.32
7	N	1	MAN	O4-C4-C5	7.03	126.64	109.32
7	i	1	MAN	O4-C4-C5	7.03	126.63	109.32
7	l	1	MAN	O4-C4-C5	7.01	126.60	109.32
9	n	3	BMA	C1-O5-C5	6.87	121.40	112.19
9	f	3	BMA	C1-O5-C5	6.84	121.36	112.19
9	Z	3	BMA	C1-O5-C5	6.83	121.35	112.19
9	X	3	BMA	C1-O5-C5	6.83	121.34	112.19
9	b	3	BMA	C1-O5-C5	6.82	121.33	112.19
9	d	3	BMA	C1-O5-C5	6.81	121.31	112.19
7	h	2	MAN	O5-C5-C6	-6.48	95.04	107.66
7	k	2	MAN	O5-C5-C6	-6.48	95.06	107.66
7	G	2	MAN	O5-C5-C6	-6.47	95.06	107.66
7	l	1	MAN	O3-C3-C4	-6.44	95.19	110.38
7	i	1	MAN	O3-C3-C4	-6.44	95.19	110.38
7	N	1	MAN	O3-C3-C4	-6.44	95.21	110.38
7	o	1	MAN	O3-C3-C4	-6.43	95.21	110.38
7	Y	1	MAN	O3-C3-C4	-6.43	95.22	110.38
7	g	1	MAN	O3-C3-C4	-6.43	95.23	110.38
7	k	2	MAN	C1-C2-C3	-6.42	100.29	109.64
7	G	2	MAN	C1-C2-C3	-6.41	100.31	109.64
7	h	2	MAN	C1-C2-C3	-6.40	100.32	109.64
9	Z	6	MAN	C1-O5-C5	6.13	120.40	112.19
9	f	6	MAN	C1-O5-C5	6.11	120.37	112.19
9	X	6	MAN	C1-O5-C5	6.10	120.36	112.19
9	b	6	MAN	C1-O5-C5	6.10	120.36	112.19
9	X	5	MAN	C6-C5-C4	6.08	127.95	113.02
9	n	6	MAN	C1-O5-C5	6.08	120.33	112.19
9	d	6	MAN	C1-O5-C5	6.07	120.33	112.19
9	n	5	MAN	C6-C5-C4	6.07	127.92	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	f	5	MAN	C6-C5-C4	6.07	127.92	113.02
9	Z	5	MAN	C6-C5-C4	6.06	127.90	113.02
9	b	5	MAN	C6-C5-C4	6.05	127.87	113.02
9	d	5	MAN	C6-C5-C4	6.05	127.87	113.02
10	e	2	NAG	C1-O5-C5	-5.81	104.40	112.19
10	a	2	NAG	C1-O5-C5	-5.78	104.44	112.19
10	c	2	NAG	C1-O5-C5	-5.76	104.47	112.19
9	Z	1	NAG	C1-C2-N2	5.66	117.28	110.73
9	X	1	NAG	C1-C2-N2	5.65	117.28	110.73
9	b	1	NAG	C1-C2-N2	5.65	117.27	110.73
9	n	1	NAG	C1-C2-N2	5.64	117.26	110.73
9	f	1	NAG	C1-C2-N2	5.64	117.26	110.73
9	d	1	NAG	C1-C2-N2	5.62	117.24	110.73
9	Z	2	NAG	C1-C2-N2	-5.62	101.58	110.43
9	b	2	NAG	C1-C2-N2	-5.62	101.58	110.43
9	d	2	NAG	C1-C2-N2	-5.61	101.59	110.43
10	c	4	MAN	C1-O5-C5	-5.60	104.67	112.19
9	f	2	NAG	C1-C2-N2	-5.60	101.61	110.43
9	X	2	NAG	C1-C2-N2	-5.60	101.61	110.43
9	n	2	NAG	C1-C2-N2	-5.60	101.61	110.43
10	a	4	MAN	C1-O5-C5	-5.59	104.70	112.19
10	e	4	MAN	C1-O5-C5	-5.56	104.73	112.19
7	N	1	MAN	O4-C4-C3	-5.54	97.31	110.38
7	i	1	MAN	O4-C4-C3	-5.53	97.34	110.38
7	Y	1	MAN	O4-C4-C3	-5.53	97.34	110.38
7	l	1	MAN	O4-C4-C3	-5.53	97.35	110.38
7	o	1	MAN	O4-C4-C3	-5.52	97.37	110.38
7	g	1	MAN	O4-C4-C3	-5.51	97.38	110.38
7	h	1	MAN	C1-O5-C5	-5.44	104.90	112.19
7	G	1	MAN	C1-O5-C5	-5.43	104.90	112.19
7	k	1	MAN	C1-O5-C5	-5.43	104.91	112.19
9	b	4	MAN	C1-O5-C5	-5.38	104.98	112.19
9	Z	4	MAN	C1-O5-C5	-5.37	104.99	112.19
9	d	4	MAN	C1-O5-C5	-5.36	105.00	112.19
9	X	4	MAN	C1-O5-C5	-5.35	105.02	112.19
9	f	4	MAN	C1-O5-C5	-5.32	105.05	112.19
9	n	4	MAN	C1-O5-C5	-5.30	105.08	112.19
9	Z	5	MAN	C1-C2-C3	5.18	117.19	109.64
9	b	5	MAN	C1-C2-C3	5.16	117.16	109.64
9	d	5	MAN	C1-C2-C3	5.16	117.16	109.64
9	n	5	MAN	C1-C2-C3	5.15	117.15	109.64
9	f	5	MAN	C1-C2-C3	5.15	117.14	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	X	5	MAN	C1-C2-C3	5.14	117.13	109.64
9	n	1	NAG	C3-C2-N2	-5.07	101.27	110.62
9	X	1	NAG	C3-C2-N2	-5.06	101.29	110.62
9	f	1	NAG	C3-C2-N2	-5.06	101.29	110.62
9	Z	1	NAG	C3-C2-N2	-5.06	101.30	110.62
9	d	1	NAG	C3-C2-N2	-5.05	101.31	110.62
9	b	1	NAG	C3-C2-N2	-5.03	101.35	110.62
10	e	3	BMA	C2-C3-C4	-4.99	102.08	110.86
10	c	3	BMA	C2-C3-C4	-4.98	102.10	110.86
10	a	3	BMA	C2-C3-C4	-4.98	102.10	110.86
9	n	5	MAN	O4-C4-C3	-4.81	99.04	110.38
9	d	5	MAN	O4-C4-C3	-4.81	99.04	110.38
9	Z	5	MAN	O4-C4-C3	-4.80	99.05	110.38
9	b	5	MAN	O4-C4-C3	-4.80	99.06	110.38
9	f	5	MAN	O4-C4-C3	-4.78	99.11	110.38
9	X	5	MAN	O4-C4-C3	-4.77	99.13	110.38
10	a	4	MAN	O2-C2-C1	4.75	120.09	109.22
10	e	4	MAN	O2-C2-C1	4.74	120.08	109.22
10	c	4	MAN	O2-C2-C1	4.74	120.08	109.22
7	l	2	MAN	O2-C2-C3	4.69	119.87	110.15
7	o	2	MAN	O2-C2-C3	4.69	119.86	110.15
9	d	2	NAG	O5-C1-C2	4.69	118.54	111.29
9	b	2	NAG	O5-C1-C2	4.68	118.53	111.29
7	i	2	MAN	O2-C2-C3	4.67	119.83	110.15
7	Y	2	MAN	O2-C2-C3	4.67	119.82	110.15
7	g	2	MAN	O2-C2-C3	4.67	119.82	110.15
9	n	2	NAG	O5-C1-C2	4.67	118.51	111.29
9	n	6	MAN	C1-C2-C3	4.66	116.43	109.64
9	Z	2	NAG	O5-C1-C2	4.66	118.50	111.29
9	f	2	NAG	O5-C1-C2	4.66	118.50	111.29
9	f	6	MAN	C1-C2-C3	4.66	116.43	109.64
7	l	1	MAN	O5-C5-C6	-4.66	98.60	107.66
9	Z	5	MAN	O5-C5-C6	-4.65	98.62	107.66
9	b	5	MAN	O5-C5-C6	-4.65	98.62	107.66
9	X	6	MAN	C1-C2-C3	4.65	116.41	109.64
9	X	5	MAN	O5-C5-C6	-4.65	98.62	107.66
7	N	2	MAN	O2-C2-C3	4.64	119.77	110.15
7	o	1	MAN	O5-C5-C6	-4.64	98.62	107.66
9	X	2	NAG	O5-C1-C2	4.64	118.47	111.29
9	n	5	MAN	O5-C5-C6	-4.64	98.63	107.66
9	d	6	MAN	C1-C2-C3	4.64	116.40	109.64
7	i	1	MAN	O5-C5-C6	-4.64	98.63	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	d	5	MAN	O5-C5-C6	-4.64	98.63	107.66
9	f	5	MAN	O5-C5-C6	-4.64	98.64	107.66
7	g	1	MAN	O5-C5-C6	-4.63	98.64	107.66
7	N	1	MAN	O5-C5-C6	-4.63	98.64	107.66
7	Y	1	MAN	O5-C5-C6	-4.62	98.67	107.66
9	b	6	MAN	C1-C2-C3	4.62	116.37	109.64
9	Z	6	MAN	C1-C2-C3	4.60	116.34	109.64
10	e	2	NAG	C4-C3-C2	-4.56	104.34	111.02
10	a	2	NAG	C4-C3-C2	-4.53	104.38	111.02
10	c	2	NAG	C4-C3-C2	-4.50	104.43	111.02
7	k	1	MAN	O3-C3-C4	-4.43	99.94	110.38
7	h	1	MAN	O3-C3-C4	-4.42	99.96	110.38
7	G	1	MAN	O3-C3-C4	-4.41	99.98	110.38
9	d	3	BMA	C6-C5-C4	-4.35	102.33	113.02
9	b	3	BMA	C6-C5-C4	-4.34	102.36	113.02
9	n	3	BMA	C6-C5-C4	-4.34	102.37	113.02
9	f	3	BMA	C6-C5-C4	-4.34	102.37	113.02
9	Z	3	BMA	C6-C5-C4	-4.34	102.38	113.02
9	X	3	BMA	C6-C5-C4	-4.33	102.38	113.02
10	c	1	NAG	C1-O5-C5	4.33	117.99	112.19
10	a	1	NAG	C1-O5-C5	4.32	117.97	112.19
10	e	1	NAG	C1-O5-C5	4.31	117.97	112.19
7	o	1	MAN	O5-C1-C2	4.30	121.04	110.79
7	N	1	MAN	O5-C1-C2	4.29	121.03	110.79
7	i	1	MAN	O5-C1-C2	4.29	121.02	110.79
7	Y	1	MAN	O5-C1-C2	4.29	121.02	110.79
7	l	1	MAN	O5-C1-C2	4.29	121.02	110.79
7	g	1	MAN	O5-C1-C2	4.29	121.01	110.79
9	n	1	NAG	C3-C4-C5	4.25	117.94	110.23
7	h	2	MAN	O2-C2-C1	4.24	118.94	109.22
7	G	2	MAN	O2-C2-C1	4.24	118.94	109.22
10	e	3	BMA	O3-C3-C2	-4.24	101.40	110.05
7	k	2	MAN	O2-C2-C1	4.24	118.93	109.22
9	X	1	NAG	C3-C4-C5	4.24	117.92	110.23
10	c	3	BMA	O3-C3-C2	-4.24	101.40	110.05
9	b	1	NAG	C3-C4-C5	4.24	117.92	110.23
9	f	1	NAG	C3-C4-C5	4.24	117.92	110.23
9	d	1	NAG	C3-C4-C5	4.24	117.92	110.23
9	Z	1	NAG	C3-C4-C5	4.23	117.91	110.23
10	a	3	BMA	O3-C3-C2	-4.23	101.42	110.05
10	a	2	NAG	C6-C5-C4	4.22	123.39	113.02
10	e	2	NAG	C6-C5-C4	4.22	123.38	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	c	2	NAG	C6-C5-C4	4.22	123.38	113.02
10	a	3	BMA	O5-C5-C6	-4.21	99.46	107.66
10	e	3	BMA	O5-C5-C6	-4.21	99.47	107.66
9	d	6	MAN	O4-C4-C5	4.20	119.66	109.32
10	c	3	BMA	O5-C5-C6	-4.19	99.51	107.66
9	X	6	MAN	O4-C4-C5	4.19	119.64	109.32
9	b	6	MAN	O4-C4-C5	4.19	119.64	109.32
9	f	6	MAN	O4-C4-C5	4.19	119.64	109.32
9	Z	6	MAN	O4-C4-C5	4.18	119.63	109.32
9	n	6	MAN	O4-C4-C5	4.18	119.63	109.32
9	Z	1	NAG	O5-C5-C4	4.13	117.13	109.70
9	d	1	NAG	O5-C5-C4	4.13	117.13	109.70
9	b	1	NAG	O5-C5-C4	4.12	117.11	109.70
9	f	1	NAG	O5-C5-C4	4.11	117.10	109.70
9	X	1	NAG	O5-C5-C4	4.10	117.09	109.70
9	d	5	MAN	O4-C4-C5	4.08	119.38	109.32
9	n	1	NAG	O5-C5-C4	4.08	117.04	109.70
9	n	5	MAN	O4-C4-C5	4.07	119.36	109.32
9	b	5	MAN	O4-C4-C5	4.07	119.36	109.32
10	c	1	NAG	C4-C3-C2	4.07	116.98	111.02
9	f	5	MAN	O4-C4-C5	4.07	119.34	109.32
10	a	1	NAG	C4-C3-C2	4.06	116.97	111.02
9	X	5	MAN	O4-C4-C5	4.06	119.32	109.32
10	e	1	NAG	C4-C3-C2	4.06	116.97	111.02
9	Z	5	MAN	O4-C4-C5	4.05	119.31	109.32
9	X	7	MAN	C1-O5-C5	4.05	117.61	112.19
9	n	7	MAN	C1-O5-C5	4.03	117.59	112.19
9	f	7	MAN	C1-O5-C5	4.02	117.57	112.19
7	l	2	MAN	C1-O5-C5	4.01	117.56	112.19
9	Z	7	MAN	C1-O5-C5	3.99	117.54	112.19
9	n	6	MAN	C6-C5-C4	3.99	122.82	113.02
7	i	2	MAN	C1-O5-C5	3.99	117.53	112.19
7	N	2	MAN	C1-O5-C5	3.99	117.53	112.19
7	Y	2	MAN	C1-O5-C5	3.99	117.53	112.19
9	X	6	MAN	C6-C5-C4	3.98	122.80	113.02
9	b	1	NAG	C4-C3-C2	3.98	116.20	110.40
9	b	7	MAN	C1-O5-C5	3.98	117.52	112.19
7	g	2	MAN	C1-O5-C5	3.98	117.52	112.19
9	f	6	MAN	C6-C5-C4	3.98	122.79	113.02
9	d	7	MAN	C1-O5-C5	3.98	117.52	112.19
9	X	1	NAG	C4-C3-C2	3.97	116.19	110.40
9	f	1	NAG	C4-C3-C2	3.97	116.19	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	n	1	NAG	C4-C3-C2	3.97	116.18	110.40
7	o	2	MAN	C1-O5-C5	3.97	117.50	112.19
9	Z	6	MAN	C6-C5-C4	3.97	122.76	113.02
9	d	1	NAG	C4-C3-C2	3.96	116.17	110.40
9	d	6	MAN	C6-C5-C4	3.96	122.74	113.02
9	b	6	MAN	C6-C5-C4	3.96	122.74	113.02
9	Z	1	NAG	C4-C3-C2	3.95	116.16	110.40
7	l	1	MAN	C6-C5-C4	-3.92	103.41	113.02
7	o	1	MAN	C6-C5-C4	-3.91	103.42	113.02
7	N	1	MAN	C6-C5-C4	-3.91	103.42	113.02
7	g	1	MAN	C6-C5-C4	-3.91	103.43	113.02
7	Y	1	MAN	C6-C5-C4	-3.90	103.44	113.02
7	i	1	MAN	C6-C5-C4	-3.90	103.44	113.02
9	n	4	MAN	C3-C4-C5	3.72	116.98	110.23
9	X	4	MAN	C3-C4-C5	3.72	116.97	110.23
7	k	2	MAN	C2-C3-C4	3.71	117.39	110.86
9	b	4	MAN	C3-C4-C5	3.71	116.96	110.23
9	f	4	MAN	C3-C4-C5	3.71	116.96	110.23
9	d	4	MAN	C3-C4-C5	3.71	116.96	110.23
7	h	2	MAN	C2-C3-C4	3.70	117.37	110.86
7	G	2	MAN	C2-C3-C4	3.69	117.35	110.86
7	N	1	MAN	C2-C3-C4	-3.69	104.38	110.86
9	Z	4	MAN	C3-C4-C5	3.69	116.92	110.23
7	g	1	MAN	C2-C3-C4	-3.67	104.40	110.86
7	i	1	MAN	C2-C3-C4	-3.67	104.40	110.86
7	Y	1	MAN	C2-C3-C4	-3.67	104.40	110.86
7	l	1	MAN	C2-C3-C4	-3.66	104.42	110.86
7	o	1	MAN	C2-C3-C4	-3.66	104.42	110.86
7	Y	2	MAN	O5-C5-C4	-3.55	102.19	110.83
7	g	2	MAN	O5-C5-C4	-3.54	102.21	110.83
7	l	2	MAN	O5-C5-C4	-3.53	102.23	110.83
7	o	2	MAN	O5-C5-C4	-3.53	102.23	110.83
7	i	2	MAN	O5-C5-C4	-3.53	102.24	110.83
7	N	2	MAN	O5-C5-C4	-3.52	102.27	110.83
9	X	5	MAN	C1-O5-C5	3.52	116.90	112.19
9	Z	5	MAN	C1-O5-C5	3.51	116.89	112.19
9	Z	3	BMA	O5-C5-C6	-3.51	100.84	107.66
9	n	5	MAN	C1-O5-C5	3.50	116.88	112.19
9	d	5	MAN	C1-O5-C5	3.50	116.87	112.19
9	f	5	MAN	C1-O5-C5	3.50	116.87	112.19
9	b	3	BMA	O5-C5-C6	-3.49	100.86	107.66
9	b	5	MAN	C1-O5-C5	3.49	116.86	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	d	3	BMA	O5-C5-C6	-3.48	100.89	107.66
10	a	4	MAN	O6-C6-C5	-3.48	99.48	111.33
10	e	4	MAN	O6-C6-C5	-3.48	99.50	111.33
9	f	3	BMA	O5-C5-C6	-3.47	100.90	107.66
9	n	3	BMA	O5-C5-C6	-3.47	100.91	107.66
7	k	1	MAN	O3-C3-C2	-3.47	102.98	110.05
9	X	3	BMA	O5-C5-C6	-3.46	100.92	107.66
10	c	4	MAN	O6-C6-C5	-3.46	99.55	111.33
7	G	1	MAN	O3-C3-C2	-3.45	103.01	110.05
7	h	1	MAN	O3-C3-C2	-3.45	103.01	110.05
9	n	3	BMA	C3-C4-C5	3.45	116.49	110.23
9	Z	1	NAG	O1-C1-C2	3.45	116.38	109.22
9	f	1	NAG	O1-C1-C2	3.44	116.36	109.22
9	d	1	NAG	O1-C1-C2	3.43	116.35	109.22
9	X	1	NAG	O1-C1-C2	3.43	116.35	109.22
9	f	3	BMA	C3-C4-C5	3.43	116.45	110.23
9	b	1	NAG	O1-C1-C2	3.43	116.34	109.22
9	n	1	NAG	O1-C1-C2	3.42	116.33	109.22
9	Z	3	BMA	C3-C4-C5	3.42	116.43	110.23
9	X	3	BMA	C3-C4-C5	3.41	116.42	110.23
9	b	3	BMA	C3-C4-C5	3.41	116.41	110.23
9	d	3	BMA	C3-C4-C5	3.40	116.40	110.23
10	c	2	NAG	O5-C1-C2	-3.32	106.15	111.29
10	c	1	NAG	O5-C1-C2	3.32	116.42	111.29
10	a	1	NAG	O5-C1-C2	3.32	116.42	111.29
7	G	2	MAN	O5-C5-C4	-3.32	102.76	110.83
10	e	2	NAG	O5-C1-C2	-3.31	106.16	111.29
10	a	2	NAG	O5-C1-C2	-3.31	106.17	111.29
7	h	2	MAN	O5-C5-C4	-3.30	102.80	110.83
10	a	1	NAG	O7-C7-N2	3.30	127.81	121.98
10	e	1	NAG	O5-C1-C2	3.30	116.39	111.29
9	X	7	MAN	C2-C3-C4	3.29	116.65	110.86
10	c	1	NAG	O7-C7-N2	3.29	127.80	121.98
10	e	1	NAG	O7-C7-N2	3.29	127.80	121.98
7	k	2	MAN	O5-C5-C4	-3.29	102.82	110.83
9	f	7	MAN	C2-C3-C4	3.29	116.64	110.86
7	Y	1	MAN	O2-C2-C3	-3.29	103.35	110.15
9	n	7	MAN	C2-C3-C4	3.29	116.64	110.86
10	a	2	NAG	O3-C3-C2	3.28	116.22	109.40
9	b	7	MAN	C2-C3-C4	3.28	116.63	110.86
10	e	2	NAG	O3-C3-C2	3.28	116.21	109.40
9	Z	7	MAN	C2-C3-C4	3.28	116.63	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	1	MAN	O2-C2-C3	-3.27	103.37	110.15
7	i	1	MAN	O2-C2-C3	-3.27	103.37	110.15
7	N	1	MAN	O2-C2-C3	-3.27	103.38	110.15
7	o	1	MAN	O2-C2-C3	-3.27	103.38	110.15
10	c	2	NAG	O3-C3-C2	3.27	116.19	109.40
7	l	1	MAN	O2-C2-C3	-3.26	103.39	110.15
9	d	7	MAN	C2-C3-C4	3.26	116.59	110.86
9	d	5	MAN	C3-C4-C5	3.22	116.06	110.23
7	N	1	MAN	C1-C2-C3	3.21	114.33	109.64
9	n	5	MAN	C3-C4-C5	3.21	116.06	110.23
9	Z	5	MAN	C3-C4-C5	3.21	116.05	110.23
7	i	1	MAN	C1-C2-C3	3.21	114.31	109.64
9	f	5	MAN	C3-C4-C5	3.20	116.04	110.23
9	b	5	MAN	C3-C4-C5	3.20	116.04	110.23
7	Y	1	MAN	C1-C2-C3	3.20	114.31	109.64
7	g	1	MAN	C1-C2-C3	3.20	114.31	109.64
9	X	5	MAN	C3-C4-C5	3.19	116.02	110.23
7	G	1	MAN	O4-C4-C5	3.19	117.19	109.32
7	l	1	MAN	C1-C2-C3	3.18	114.28	109.64
7	h	1	MAN	O4-C4-C5	3.18	117.16	109.32
7	k	1	MAN	O4-C4-C5	3.18	117.16	109.32
7	o	1	MAN	C1-C2-C3	3.16	114.24	109.64
9	Z	2	NAG	O3-C3-C4	3.15	117.80	110.38
10	c	2	NAG	O5-C5-C6	3.15	113.79	107.66
10	e	3	BMA	O2-C2-C3	-3.15	103.64	110.15
10	a	3	BMA	O2-C2-C3	-3.14	103.65	110.15
10	c	3	BMA	O2-C2-C3	-3.14	103.66	110.15
10	a	2	NAG	O5-C5-C6	3.13	113.75	107.66
9	d	3	BMA	O3-C3-C4	-3.13	103.00	110.38
9	b	2	NAG	O3-C3-C4	3.12	117.74	110.38
9	b	3	BMA	O3-C3-C4	-3.12	103.02	110.38
10	e	2	NAG	O5-C5-C6	3.12	113.73	107.66
9	f	3	BMA	O3-C3-C4	-3.12	103.03	110.38
9	Z	3	BMA	O3-C3-C4	-3.11	103.04	110.38
9	n	3	BMA	O3-C3-C4	-3.11	103.04	110.38
9	X	3	BMA	O3-C3-C4	-3.11	103.04	110.38
9	d	2	NAG	O3-C3-C4	3.11	117.70	110.38
9	X	2	NAG	O3-C3-C4	3.10	117.69	110.38
9	f	2	NAG	O3-C3-C4	3.10	117.68	110.38
9	n	2	NAG	O3-C3-C4	3.10	117.67	110.38
9	d	5	MAN	O2-C2-C1	3.08	116.28	109.22
9	b	5	MAN	O2-C2-C1	3.08	116.28	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	n	5	MAN	O2-C2-C1	3.08	116.28	109.22
9	f	5	MAN	O2-C2-C1	3.08	116.27	109.22
9	Z	5	MAN	O2-C2-C1	3.07	116.24	109.22
9	X	5	MAN	O2-C2-C1	3.05	116.21	109.22
10	c	1	NAG	C8-C7-N2	-3.01	111.12	116.12
10	a	1	NAG	C8-C7-N2	-2.98	111.17	116.12
10	c	1	NAG	C1-C2-N2	2.98	115.13	110.43
10	a	1	NAG	C1-C2-N2	2.97	115.12	110.43
9	X	7	MAN	O5-C5-C4	-2.96	103.62	110.83
9	n	7	MAN	O5-C5-C4	-2.96	103.63	110.83
10	e	1	NAG	C1-C2-N2	2.96	115.10	110.43
10	e	1	NAG	C8-C7-N2	-2.96	111.22	116.12
9	f	7	MAN	O5-C5-C4	-2.96	103.64	110.83
9	d	7	MAN	O5-C5-C4	-2.95	103.66	110.83
9	Z	7	MAN	O5-C5-C4	-2.94	103.67	110.83
9	b	7	MAN	O5-C5-C4	-2.94	103.69	110.83
9	Z	1	NAG	C2-N2-C7	2.91	129.93	123.11
9	f	1	NAG	C2-N2-C7	2.91	129.92	123.11
9	b	1	NAG	C2-N2-C7	2.91	129.92	123.11
9	n	1	NAG	C2-N2-C7	2.90	129.90	123.11
9	d	1	NAG	C2-N2-C7	2.90	129.90	123.11
9	X	1	NAG	C2-N2-C7	2.89	129.88	123.11
7	k	1	MAN	C3-C4-C5	-2.81	105.14	110.23
10	c	3	BMA	O3-C3-C4	-2.79	103.80	110.38
10	a	3	BMA	O3-C3-C4	-2.79	103.80	110.38
7	h	1	MAN	C3-C4-C5	-2.79	105.18	110.23
10	e	3	BMA	O3-C3-C4	-2.77	103.83	110.38
7	G	1	MAN	C3-C4-C5	-2.77	105.20	110.23
9	X	7	MAN	O4-C4-C5	-2.76	102.52	109.32
9	n	2	NAG	O4-C4-C5	-2.76	102.52	109.32
9	X	2	NAG	O4-C4-C5	-2.76	102.53	109.32
9	f	2	NAG	O4-C4-C5	-2.75	102.54	109.32
9	f	7	MAN	O4-C4-C5	-2.75	102.56	109.32
7	k	1	MAN	O5-C5-C4	-2.74	104.15	110.83
9	d	7	MAN	O4-C4-C5	-2.74	102.57	109.32
9	Z	7	MAN	O4-C4-C5	-2.74	102.57	109.32
7	G	1	MAN	O5-C5-C4	-2.74	104.16	110.83
7	h	1	MAN	O5-C5-C4	-2.74	104.16	110.83
9	Z	2	NAG	O4-C4-C5	-2.74	102.58	109.32
9	n	7	MAN	O4-C4-C5	-2.74	102.58	109.32
9	b	2	NAG	O4-C4-C5	-2.74	102.58	109.32
9	d	2	NAG	O4-C4-C5	-2.73	102.61	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	7	MAN	O4-C4-C5	-2.73	102.61	109.32
7	h	1	MAN	C1-C2-C3	2.68	113.54	109.64
7	G	1	MAN	C1-C2-C3	2.67	113.54	109.64
9	X	5	MAN	C2-C3-C4	2.67	115.56	110.86
7	k	1	MAN	C1-C2-C3	2.65	113.51	109.64
9	f	5	MAN	C2-C3-C4	2.65	115.51	110.86
9	n	5	MAN	C2-C3-C4	2.63	115.48	110.86
10	c	3	BMA	C6-C5-C4	-2.62	106.57	113.02
10	e	3	BMA	C6-C5-C4	-2.62	106.58	113.02
9	b	5	MAN	C2-C3-C4	2.62	115.46	110.86
10	a	3	BMA	C6-C5-C4	-2.61	106.60	113.02
9	d	5	MAN	C2-C3-C4	2.61	115.45	110.86
9	Z	5	MAN	C2-C3-C4	2.60	115.43	110.86
8	m	4	MAN	C1-O5-C5	2.59	115.66	112.19
9	Z	4	MAN	O2-C2-C1	-2.57	103.34	109.22
9	f	4	MAN	O2-C2-C1	-2.56	103.37	109.22
8	U	4	MAN	C1-O5-C5	2.55	115.61	112.19
8	j	4	MAN	C1-O5-C5	2.55	115.61	112.19
9	n	4	MAN	O2-C2-C1	-2.55	103.38	109.22
9	X	4	MAN	O2-C2-C1	-2.55	103.38	109.22
9	d	4	MAN	O2-C2-C1	-2.54	103.40	109.22
9	b	4	MAN	O2-C2-C1	-2.54	103.41	109.22
10	c	2	NAG	C3-C4-C5	-2.53	105.64	110.23
10	e	1	NAG	O5-C5-C6	-2.52	102.76	107.66
10	e	2	NAG	C3-C4-C5	-2.52	105.67	110.23
9	X	3	BMA	O2-C2-C3	2.51	115.35	110.15
10	a	2	NAG	C3-C4-C5	-2.51	105.68	110.23
9	d	3	BMA	O2-C2-C3	2.51	115.34	110.15
10	a	1	NAG	O5-C5-C6	-2.51	102.79	107.66
10	c	1	NAG	O5-C5-C6	-2.50	102.79	107.66
9	d	5	MAN	O5-C1-C2	2.50	116.76	110.79
9	f	7	MAN	C6-C5-C4	-2.50	106.89	113.02
9	n	7	MAN	C6-C5-C4	-2.50	106.89	113.02
9	b	3	BMA	O2-C2-C3	2.50	115.32	110.15
9	f	5	MAN	O5-C1-C2	2.49	116.74	110.79
9	b	5	MAN	O5-C1-C2	2.49	116.74	110.79
9	X	5	MAN	O5-C1-C2	2.49	116.73	110.79
9	n	5	MAN	O5-C1-C2	2.49	116.72	110.79
9	f	3	BMA	O2-C2-C3	2.48	115.30	110.15
7	k	2	MAN	O6-C6-C5	-2.48	102.88	111.33
9	n	3	BMA	O2-C2-C3	2.48	115.30	110.15
9	X	7	MAN	C6-C5-C4	-2.48	106.92	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Z	3	BMA	O2-C2-C3	2.48	115.29	110.15
9	Z	5	MAN	O5-C1-C2	2.48	116.71	110.79
7	h	2	MAN	O6-C6-C5	-2.48	102.89	111.33
7	G	2	MAN	O6-C6-C5	-2.48	102.90	111.33
8	m	6	MAN	C1-O5-C5	2.47	115.50	112.19
10	e	4	MAN	O5-C5-C6	2.47	112.47	107.66
8	j	6	MAN	C1-O5-C5	2.46	115.49	112.19
7	Y	2	MAN	C3-C4-C5	2.46	114.70	110.23
9	b	7	MAN	C6-C5-C4	-2.46	106.97	113.02
10	a	4	MAN	O5-C5-C6	2.46	112.44	107.66
9	Z	7	MAN	C6-C5-C4	-2.45	107.00	113.02
7	g	2	MAN	C3-C4-C5	2.45	114.67	110.23
9	d	7	MAN	C6-C5-C4	-2.45	107.02	113.02
10	c	4	MAN	O5-C5-C6	2.43	112.40	107.66
7	l	1	MAN	O6-C6-C5	-2.43	103.07	111.33
7	o	2	MAN	C3-C4-C5	2.43	114.63	110.23
7	N	1	MAN	O6-C6-C5	-2.42	103.08	111.33
7	i	1	MAN	O6-C6-C5	-2.42	103.08	111.33
7	l	2	MAN	C3-C4-C5	2.42	114.62	110.23
7	o	1	MAN	O6-C6-C5	-2.42	103.09	111.33
7	Y	2	MAN	O2-C2-C1	2.42	114.76	109.22
8	U	6	MAN	C1-O5-C5	2.42	115.43	112.19
7	g	1	MAN	O6-C6-C5	-2.42	103.10	111.33
7	Y	1	MAN	O6-C6-C5	-2.41	103.11	111.33
7	i	2	MAN	C3-C4-C5	2.41	114.60	110.23
7	o	2	MAN	O2-C2-C1	2.41	114.74	109.22
9	n	4	MAN	O5-C5-C6	2.41	112.35	107.66
9	f	4	MAN	O5-C5-C6	2.41	112.35	107.66
7	g	2	MAN	O2-C2-C1	2.40	114.72	109.22
9	X	3	BMA	O2-C2-C1	-2.40	103.73	109.22
9	d	4	MAN	O5-C5-C6	2.40	112.33	107.66
7	N	2	MAN	C3-C4-C5	2.40	114.58	110.23
9	X	4	MAN	O5-C5-C6	2.39	112.32	107.66
7	N	2	MAN	O2-C2-C1	2.39	114.70	109.22
10	a	4	MAN	O4-C4-C3	-2.39	104.73	110.38
9	b	3	BMA	O2-C2-C1	-2.39	103.75	109.22
9	Z	3	BMA	O2-C2-C1	-2.39	103.75	109.22
10	e	4	MAN	O4-C4-C3	-2.39	104.74	110.38
9	b	4	MAN	O5-C5-C6	2.39	112.31	107.66
9	f	3	BMA	O2-C2-C1	-2.39	103.76	109.22
10	c	4	MAN	O4-C4-C3	-2.39	104.75	110.38
9	Z	4	MAN	O5-C5-C6	2.38	112.30	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	n	3	BMA	O2-C2-C1	-2.38	103.78	109.22
7	i	2	MAN	O2-C2-C1	2.38	114.66	109.22
7	l	2	MAN	O2-C2-C1	2.37	114.65	109.22
7	N	2	MAN	O5-C1-C2	2.37	116.45	110.79
9	d	3	BMA	O2-C2-C1	-2.37	103.81	109.22
7	i	2	MAN	O5-C1-C2	2.36	116.43	110.79
7	l	2	MAN	O5-C1-C2	2.36	116.42	110.79
7	g	2	MAN	O5-C1-C2	2.36	116.42	110.79
7	Y	2	MAN	O5-C1-C2	2.35	116.39	110.79
7	o	2	MAN	O5-C1-C2	2.34	116.37	110.79
10	c	4	MAN	O5-C1-C2	2.33	116.35	110.79
9	X	2	NAG	C1-O5-C5	2.31	115.29	112.19
10	a	4	MAN	O5-C1-C2	2.31	116.31	110.79
9	f	2	NAG	C1-O5-C5	2.31	115.28	112.19
9	n	2	NAG	C1-O5-C5	2.31	115.28	112.19
9	Z	2	NAG	C1-O5-C5	2.31	115.28	112.19
10	e	4	MAN	O5-C1-C2	2.30	116.29	110.79
9	b	2	NAG	C1-O5-C5	2.29	115.25	112.19
9	d	2	NAG	C1-O5-C5	2.28	115.24	112.19
10	e	2	NAG	O3-C3-C4	2.25	115.67	110.38
10	a	2	NAG	O3-C3-C4	2.24	115.67	110.38
10	c	2	NAG	O3-C3-C4	2.23	115.64	110.38
8	j	6	MAN	O2-C2-C3	-2.23	105.53	110.15
8	m	6	MAN	O2-C2-C3	-2.22	105.55	110.15
8	U	6	MAN	O2-C2-C3	-2.22	105.56	110.15
9	Z	1	NAG	O3-C3-C4	2.21	115.59	110.38
8	U	4	MAN	O2-C2-C3	-2.21	105.57	110.15
9	b	1	NAG	O3-C3-C4	2.21	115.59	110.38
8	j	4	MAN	O2-C2-C3	-2.20	105.60	110.15
9	d	1	NAG	O3-C3-C4	2.19	115.53	110.38
8	m	4	MAN	O2-C2-C3	-2.18	105.63	110.15
9	f	1	NAG	O3-C3-C4	2.18	115.52	110.38
9	X	1	NAG	O3-C3-C4	2.18	115.51	110.38
9	n	1	NAG	O3-C3-C4	2.17	115.50	110.38
9	d	4	MAN	O6-C6-C5	-2.14	104.06	111.33
9	f	4	MAN	O6-C6-C5	-2.14	104.06	111.33
9	b	4	MAN	O6-C6-C5	-2.13	104.07	111.33
9	X	4	MAN	O6-C6-C5	-2.13	104.08	111.33
9	Z	4	MAN	O6-C6-C5	-2.12	104.10	111.33
9	n	4	MAN	O6-C6-C5	-2.12	104.10	111.33
9	n	1	NAG	C1-O5-C5	2.11	117.74	113.65
10	e	3	BMA	O6-C6-C5	-2.10	104.18	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	f	1	NAG	C1-O5-C5	2.10	117.71	113.65
10	a	3	BMA	O6-C6-C5	-2.09	104.21	111.33
10	c	3	BMA	O6-C6-C5	-2.09	104.21	111.33
9	X	1	NAG	C1-O5-C5	2.09	117.69	113.65
9	b	1	NAG	C1-O5-C5	2.07	117.65	113.65
9	Z	1	NAG	C1-O5-C5	2.06	117.64	113.65
9	d	1	NAG	C1-O5-C5	2.06	117.64	113.65
7	G	1	MAN	O5-C5-C6	2.06	111.68	107.66
7	h	1	MAN	O5-C5-C6	2.06	111.66	107.66
7	k	1	MAN	O5-C5-C6	2.05	111.65	107.66
8	m	5	MAN	C1-O5-C5	2.03	114.91	112.19
9	X	3	BMA	C2-C3-C4	2.01	114.40	110.86
8	U	5	MAN	C1-O5-C5	2.01	114.88	112.19
8	j	5	MAN	C1-O5-C5	2.01	114.88	112.19
9	Z	3	BMA	C2-C3-C4	2.01	114.39	110.86
9	b	3	BMA	C2-C3-C4	2.00	114.38	110.86
8	U	5	MAN	O2-C2-C3	-2.00	106.01	110.15

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	N	2	MAN	C1
7	Y	2	MAN	C1
7	g	2	MAN	C1
7	i	2	MAN	C1
7	l	2	MAN	C1
7	o	2	MAN	C1

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	X	1	NAG	C8-C7-N2-C2
9	X	1	NAG	O7-C7-N2-C2
9	Z	1	NAG	C8-C7-N2-C2
9	Z	1	NAG	O7-C7-N2-C2
9	b	1	NAG	C8-C7-N2-C2
9	b	1	NAG	O7-C7-N2-C2
9	d	1	NAG	C8-C7-N2-C2
9	d	1	NAG	O7-C7-N2-C2
9	f	1	NAG	C8-C7-N2-C2
9	f	1	NAG	O7-C7-N2-C2
9	n	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	n	1	NAG	O7-C7-N2-C2
10	a	2	NAG	C8-C7-N2-C2
10	a	2	NAG	O7-C7-N2-C2
10	c	2	NAG	C8-C7-N2-C2
10	c	2	NAG	O7-C7-N2-C2
10	e	2	NAG	C8-C7-N2-C2
10	e	2	NAG	O7-C7-N2-C2
7	N	2	MAN	C4-C5-C6-O6
7	Y	2	MAN	C4-C5-C6-O6
7	g	2	MAN	C4-C5-C6-O6
7	i	2	MAN	C4-C5-C6-O6
7	l	2	MAN	C4-C5-C6-O6
7	o	2	MAN	C4-C5-C6-O6
10	a	3	BMA	O5-C5-C6-O6
10	c	3	BMA	O5-C5-C6-O6
10	e	3	BMA	O5-C5-C6-O6
10	a	2	NAG	C4-C5-C6-O6
10	c	2	NAG	C4-C5-C6-O6
10	e	2	NAG	C4-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6
8	m	2	NAG	O5-C5-C6-O6
8	j	2	NAG	O5-C5-C6-O6
9	X	1	NAG	O5-C5-C6-O6
9	Z	1	NAG	O5-C5-C6-O6
9	b	1	NAG	O5-C5-C6-O6
9	d	1	NAG	O5-C5-C6-O6
9	f	1	NAG	O5-C5-C6-O6
9	n	1	NAG	O5-C5-C6-O6
9	Z	4	MAN	C4-C5-C6-O6
9	X	3	BMA	O5-C5-C6-O6
9	Z	3	BMA	O5-C5-C6-O6
9	b	3	BMA	O5-C5-C6-O6
9	d	3	BMA	O5-C5-C6-O6
9	f	3	BMA	O5-C5-C6-O6
9	n	3	BMA	O5-C5-C6-O6
9	X	4	MAN	C4-C5-C6-O6
9	b	4	MAN	C4-C5-C6-O6
9	d	4	MAN	C4-C5-C6-O6
9	f	4	MAN	C4-C5-C6-O6
9	n	4	MAN	C4-C5-C6-O6
10	a	2	NAG	O5-C5-C6-O6
10	c	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	e	2	NAG	O5-C5-C6-O6
10	a	3	BMA	C4-C5-C6-O6
10	c	3	BMA	C4-C5-C6-O6
10	e	3	BMA	C4-C5-C6-O6
9	X	4	MAN	O5-C5-C6-O6
9	Z	4	MAN	O5-C5-C6-O6
9	b	4	MAN	O5-C5-C6-O6
9	d	4	MAN	O5-C5-C6-O6
9	f	4	MAN	O5-C5-C6-O6
9	n	4	MAN	O5-C5-C6-O6
8	U	2	NAG	C4-C5-C6-O6
8	j	2	NAG	C4-C5-C6-O6
8	m	2	NAG	C4-C5-C6-O6
7	N	2	MAN	O5-C5-C6-O6
7	Y	2	MAN	O5-C5-C6-O6
7	g	2	MAN	O5-C5-C6-O6
7	i	2	MAN	O5-C5-C6-O6
7	l	2	MAN	O5-C5-C6-O6
7	o	2	MAN	O5-C5-C6-O6
9	X	7	MAN	C4-C5-C6-O6
9	Z	7	MAN	C4-C5-C6-O6
9	b	7	MAN	C4-C5-C6-O6
9	d	7	MAN	C4-C5-C6-O6
9	f	7	MAN	C4-C5-C6-O6
9	n	7	MAN	C4-C5-C6-O6
9	X	1	NAG	C4-C5-C6-O6
9	Z	1	NAG	C4-C5-C6-O6
9	b	1	NAG	C4-C5-C6-O6
9	d	1	NAG	C4-C5-C6-O6
9	f	1	NAG	C4-C5-C6-O6
9	n	1	NAG	C4-C5-C6-O6
9	X	7	MAN	O5-C5-C6-O6
9	Z	7	MAN	O5-C5-C6-O6
9	b	7	MAN	O5-C5-C6-O6
9	d	7	MAN	O5-C5-C6-O6
9	f	7	MAN	O5-C5-C6-O6
9	n	7	MAN	O5-C5-C6-O6
7	G	1	MAN	O5-C5-C6-O6
7	h	1	MAN	O5-C5-C6-O6
7	k	1	MAN	O5-C5-C6-O6
9	X	3	BMA	C4-C5-C6-O6
9	Z	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	b	3	BMA	C4-C5-C6-O6
9	d	3	BMA	C4-C5-C6-O6
9	f	3	BMA	C4-C5-C6-O6
9	n	3	BMA	C4-C5-C6-O6
7	G	2	MAN	C4-C5-C6-O6
7	h	2	MAN	C4-C5-C6-O6
7	k	2	MAN	C4-C5-C6-O6
9	Z	2	NAG	C4-C5-C6-O6
9	X	2	NAG	C4-C5-C6-O6
9	b	2	NAG	C4-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
9	f	2	NAG	C4-C5-C6-O6
9	n	2	NAG	C4-C5-C6-O6
10	a	1	NAG	O5-C5-C6-O6
10	c	1	NAG	O5-C5-C6-O6
10	e	1	NAG	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
9	Z	2	NAG	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
9	b	2	NAG	O5-C5-C6-O6
9	f	2	NAG	O5-C5-C6-O6
9	n	2	NAG	O5-C5-C6-O6
7	N	1	MAN	O5-C5-C6-O6
7	Y	1	MAN	O5-C5-C6-O6
7	g	1	MAN	O5-C5-C6-O6
7	i	1	MAN	O5-C5-C6-O6
7	l	1	MAN	O5-C5-C6-O6
7	o	1	MAN	O5-C5-C6-O6
8	U	5	MAN	O5-C5-C6-O6
8	j	5	MAN	O5-C5-C6-O6
8	m	5	MAN	O5-C5-C6-O6
9	Z	5	MAN	O5-C5-C6-O6
9	b	5	MAN	O5-C5-C6-O6
9	d	5	MAN	O5-C5-C6-O6
9	f	5	MAN	O5-C5-C6-O6
9	n	5	MAN	O5-C5-C6-O6
9	X	5	MAN	O5-C5-C6-O6
9	X	5	MAN	C4-C5-C6-O6
9	Z	5	MAN	C4-C5-C6-O6
9	b	5	MAN	C4-C5-C6-O6
9	d	5	MAN	C4-C5-C6-O6
9	f	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	n	5	MAN	C4-C5-C6-O6
8	U	2	NAG	C3-C2-N2-C7
8	j	2	NAG	C3-C2-N2-C7
8	m	2	NAG	C3-C2-N2-C7
8	j	4	MAN	C4-C5-C6-O6
8	U	4	MAN	C4-C5-C6-O6
8	m	4	MAN	C4-C5-C6-O6
8	U	1	NAG	C4-C5-C6-O6
8	j	1	NAG	C4-C5-C6-O6
8	m	1	NAG	C4-C5-C6-O6
8	U	2	NAG	C1-C2-N2-C7
8	j	2	NAG	C1-C2-N2-C7
8	m	2	NAG	C1-C2-N2-C7
8	m	1	NAG	O5-C5-C6-O6
8	j	1	NAG	O5-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
8	U	4	MAN	O5-C5-C6-O6
8	m	4	MAN	O5-C5-C6-O6
8	j	4	MAN	O5-C5-C6-O6

There are no ring outliers.

51 monomers are involved in 127 short contacts:

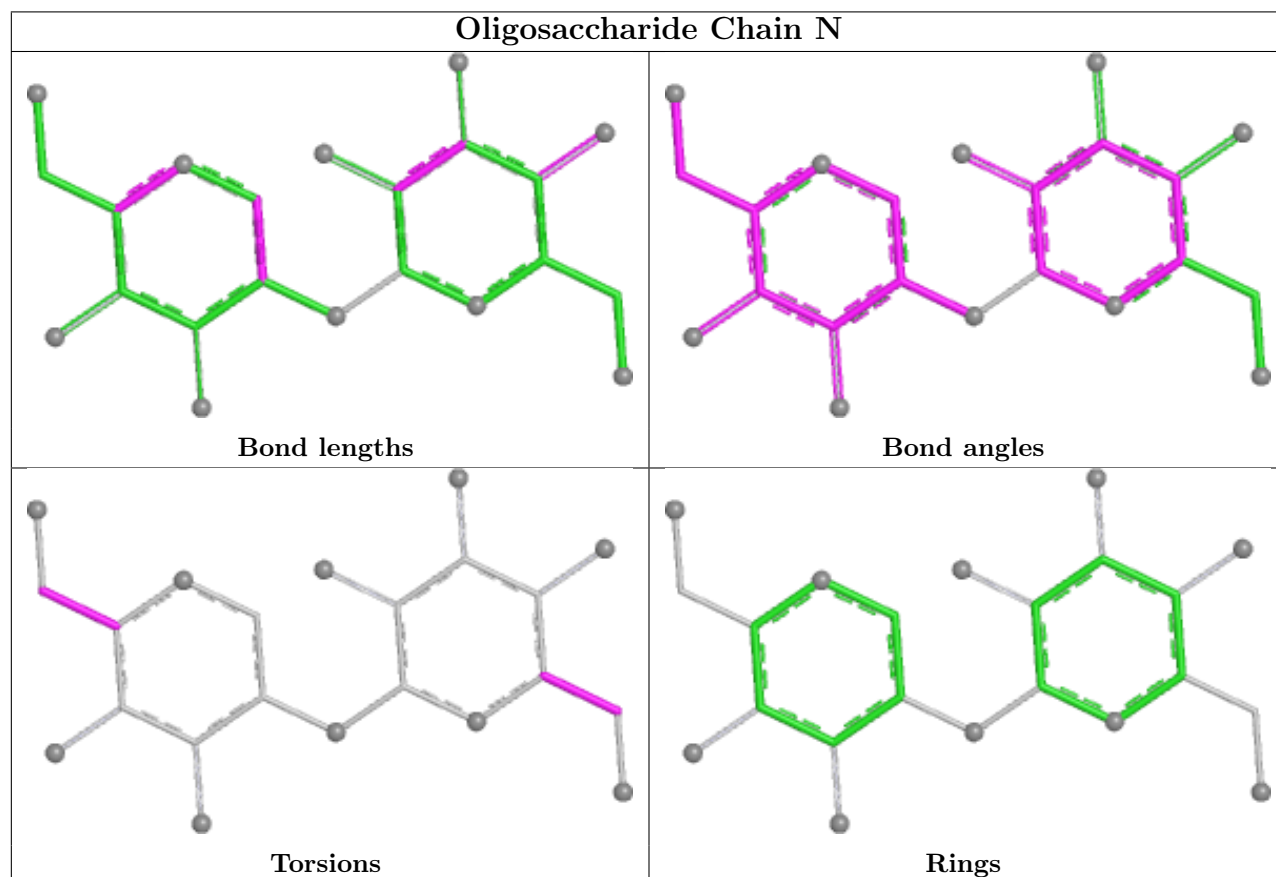
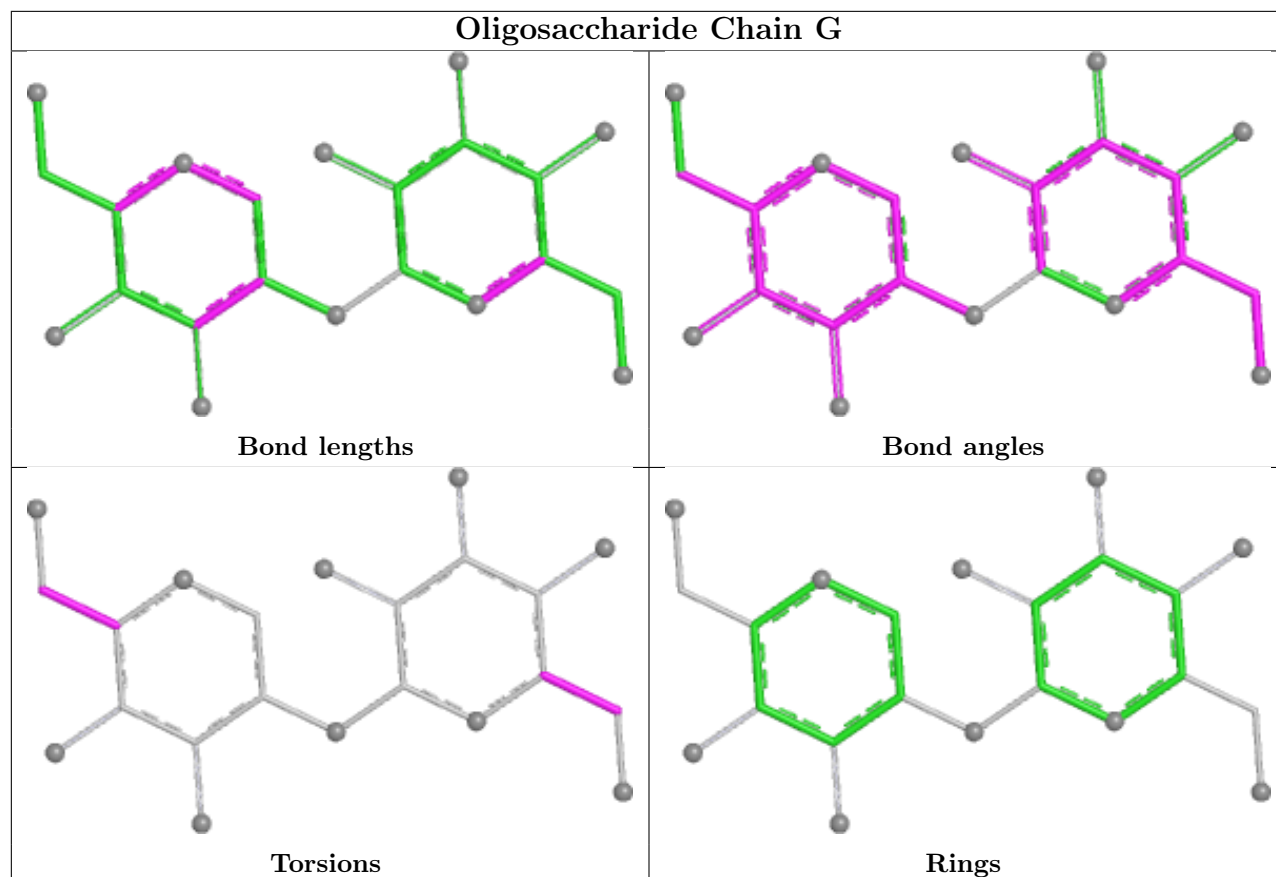
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Z	5	MAN	7	0
9	X	3	BMA	4	0
7	i	1	MAN	8	0
7	k	2	MAN	3	0
9	b	3	BMA	5	0
9	n	4	MAN	5	0
7	Y	1	MAN	7	0
7	o	2	MAN	1	0
7	o	1	MAN	7	0
9	Z	3	BMA	5	0
9	b	5	MAN	7	0
9	n	5	MAN	3	0
9	f	7	MAN	7	0
9	f	4	MAN	4	0
10	a	4	MAN	4	0
9	f	6	MAN	2	0
7	G	2	MAN	3	0
7	h	1	MAN	8	0

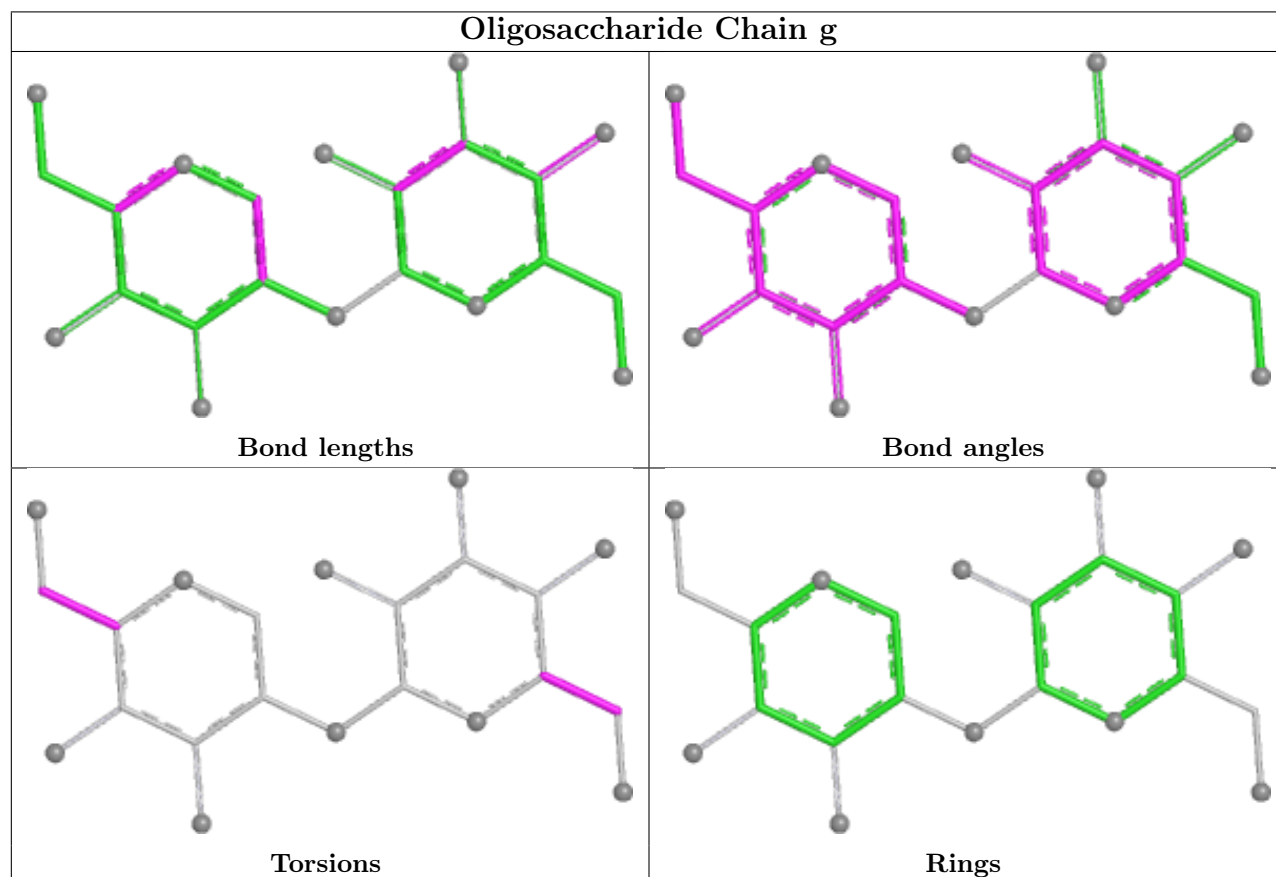
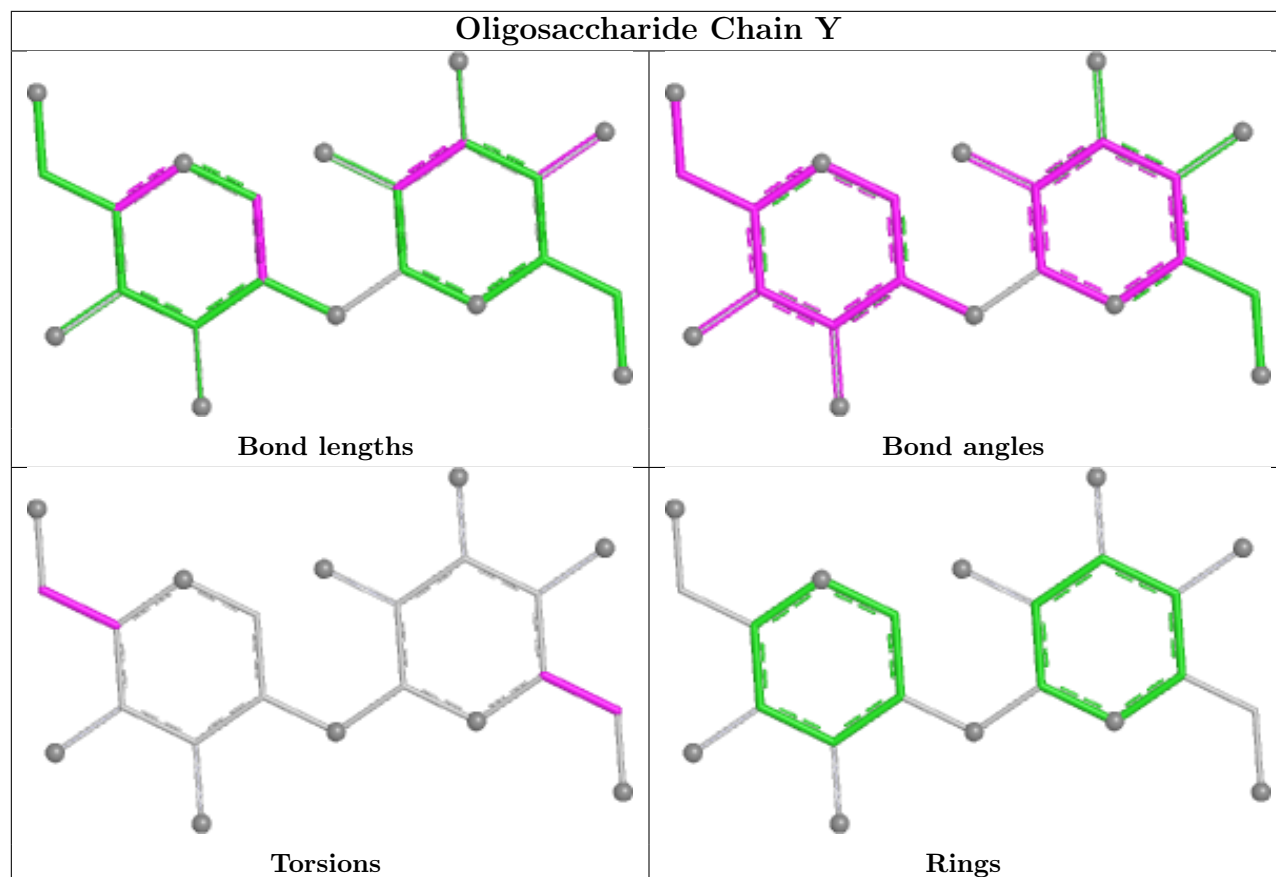
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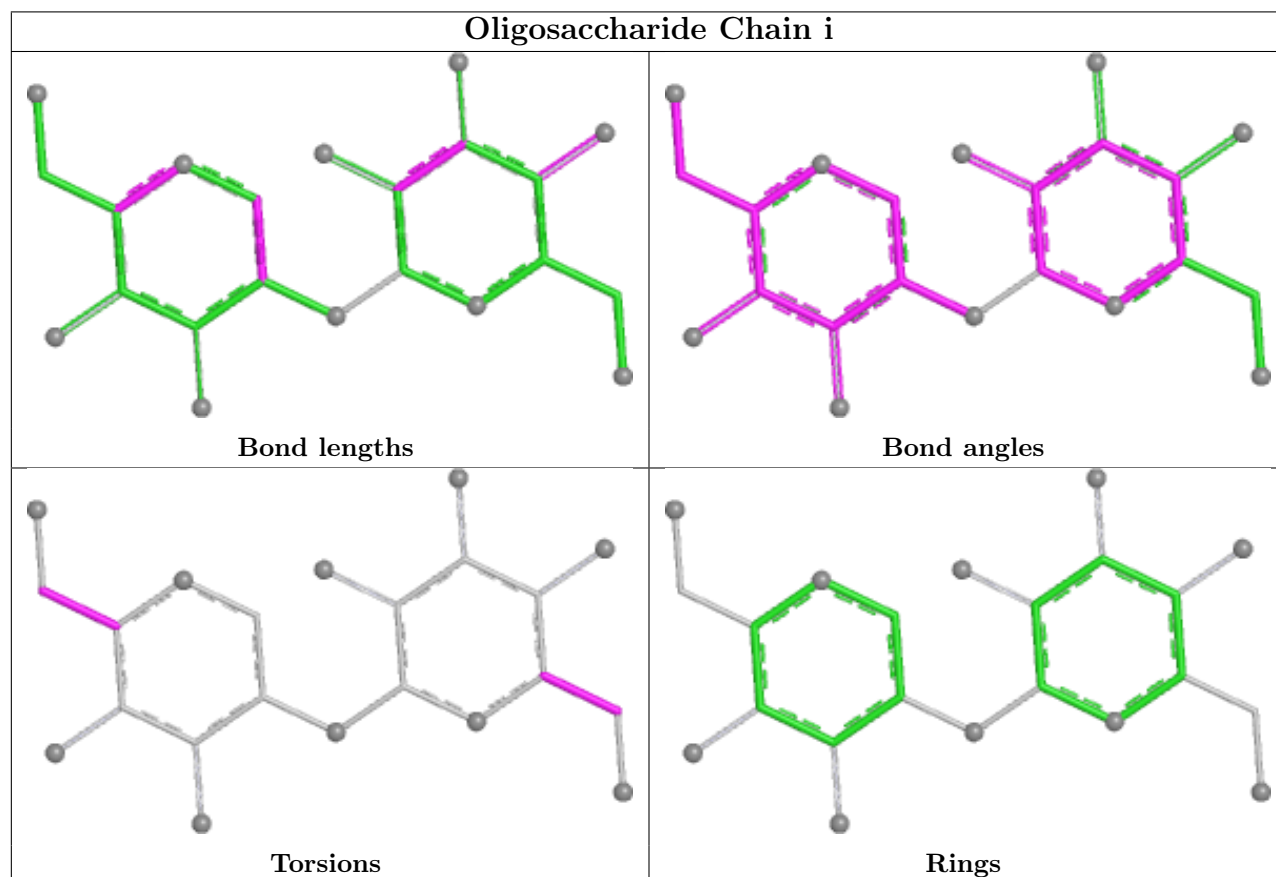
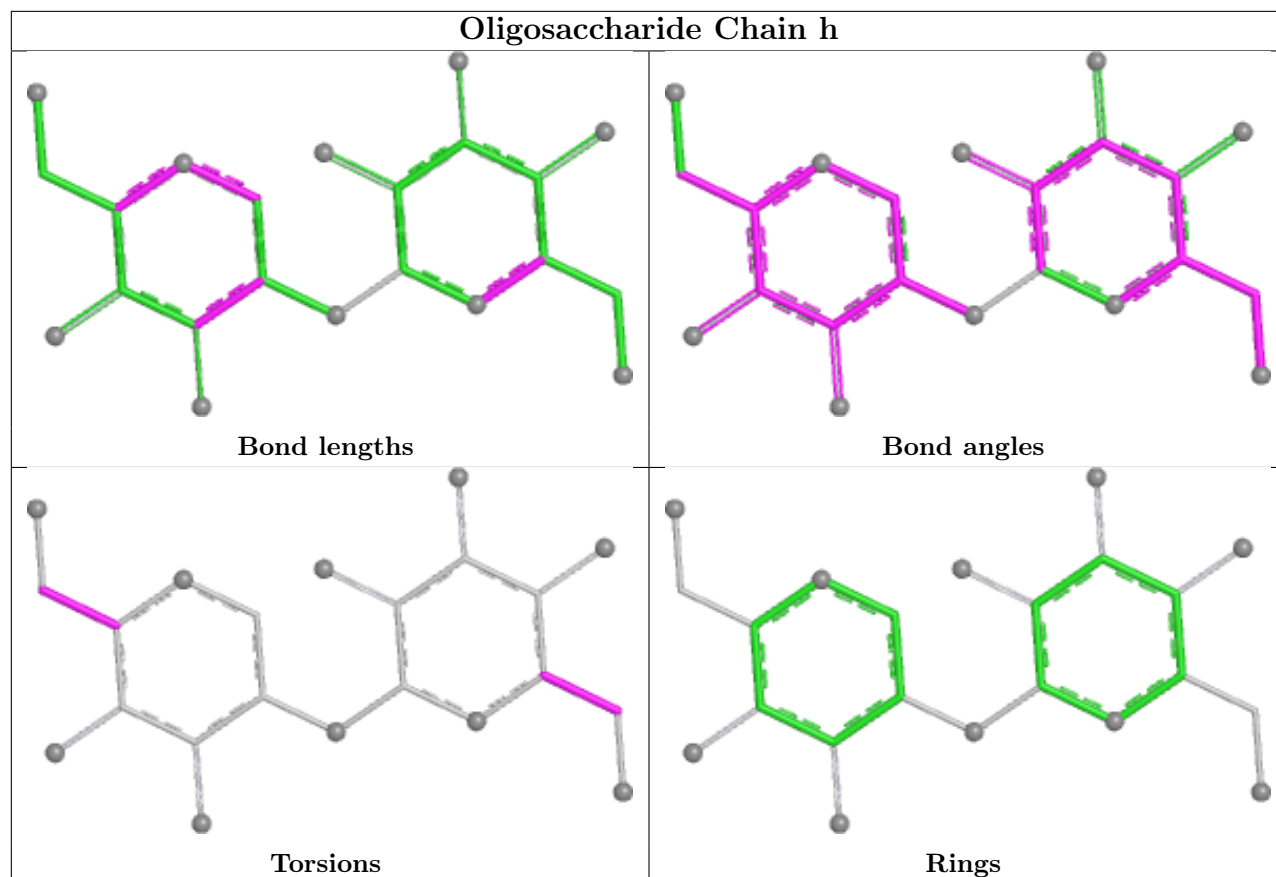
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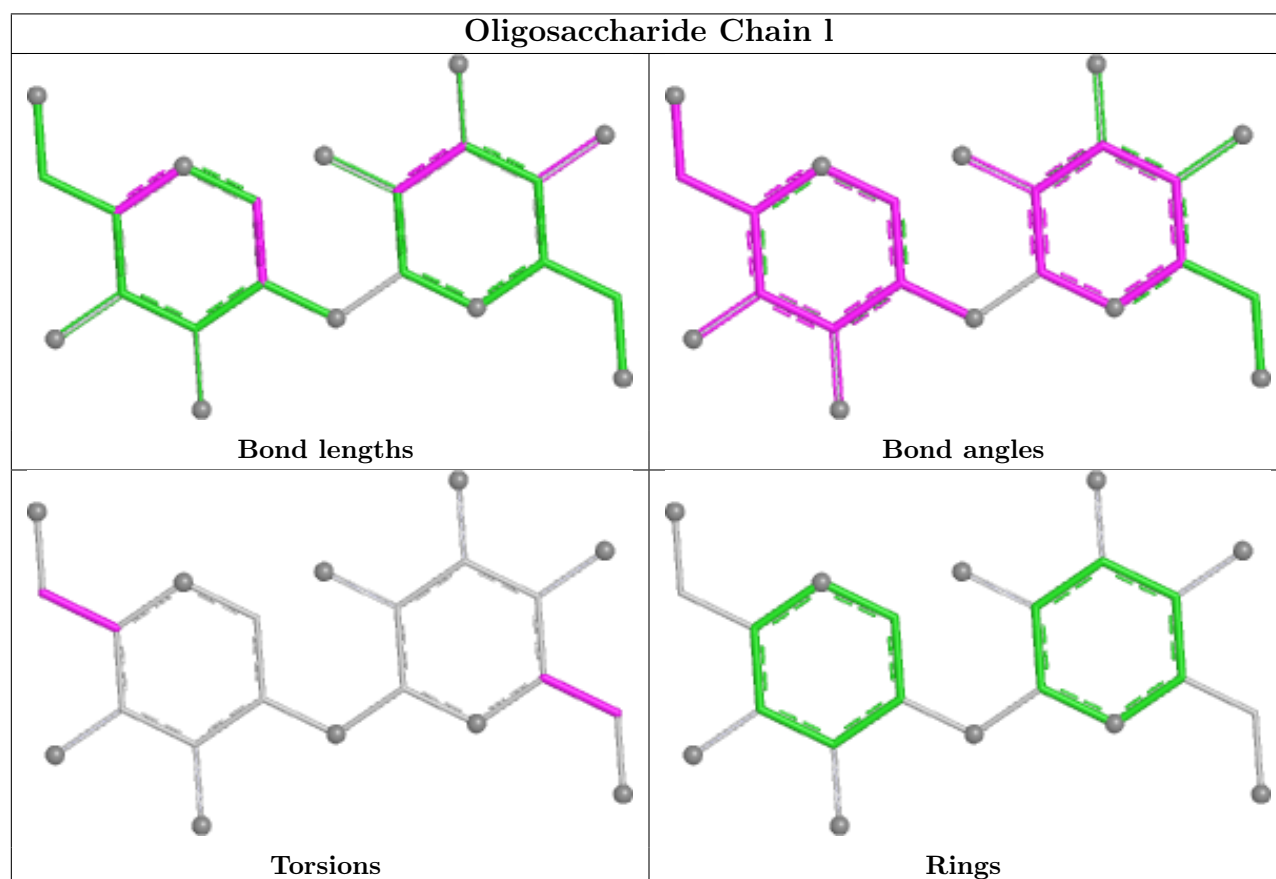
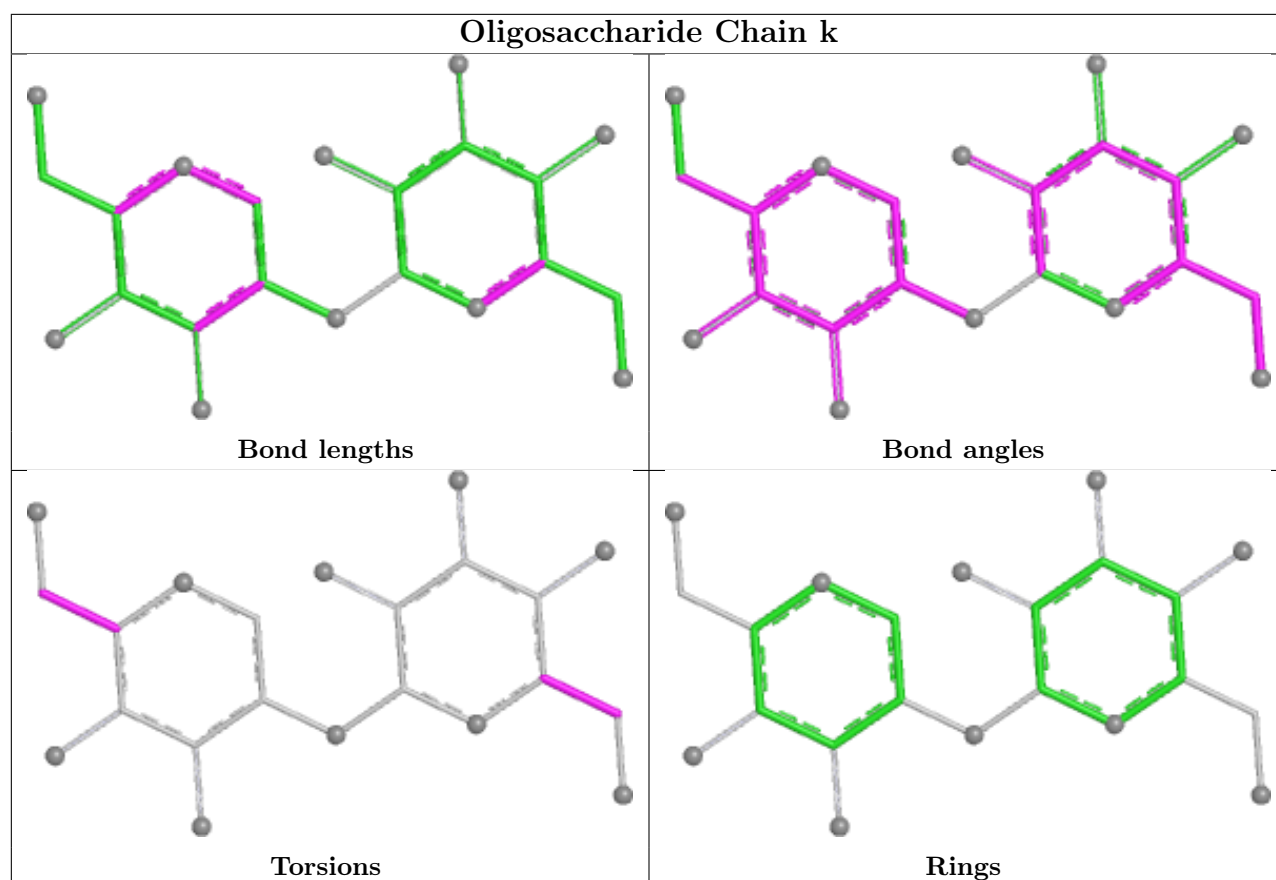
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	b	7	MAN	8	0
9	d	3	BMA	4	0
7	k	1	MAN	8	0
7	g	2	MAN	1	0
9	X	5	MAN	2	0
7	N	1	MAN	7	0
7	g	1	MAN	7	0
9	Z	4	MAN	6	0
8	U	5	MAN	1	0
9	f	5	MAN	3	0
10	e	4	MAN	4	0
7	h	2	MAN	3	0
8	j	5	MAN	1	0
9	X	7	MAN	7	0
9	n	3	BMA	4	0
9	f	3	BMA	3	0
9	d	4	MAN	5	0
9	Z	6	MAN	2	0
7	l	1	MAN	7	0
9	d	6	MAN	2	0
9	d	7	MAN	7	0
9	X	6	MAN	2	0
10	c	4	MAN	4	0
8	m	5	MAN	1	0
9	d	5	MAN	7	0
7	Y	2	MAN	1	0
9	Z	7	MAN	7	0
9	b	4	MAN	6	0
9	n	6	MAN	2	0
9	n	7	MAN	7	0
7	G	1	MAN	8	0
9	X	4	MAN	4	0
9	b	6	MAN	2	0

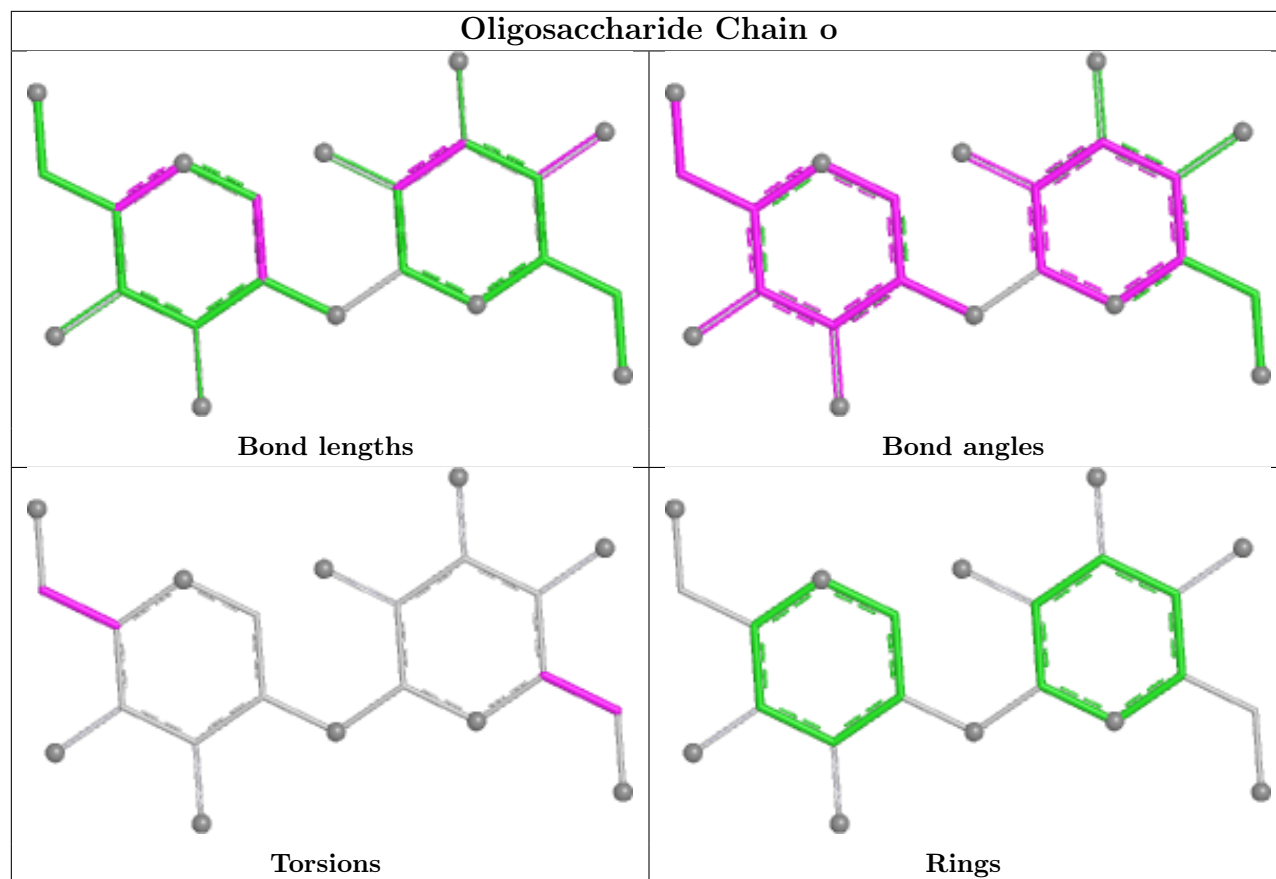
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

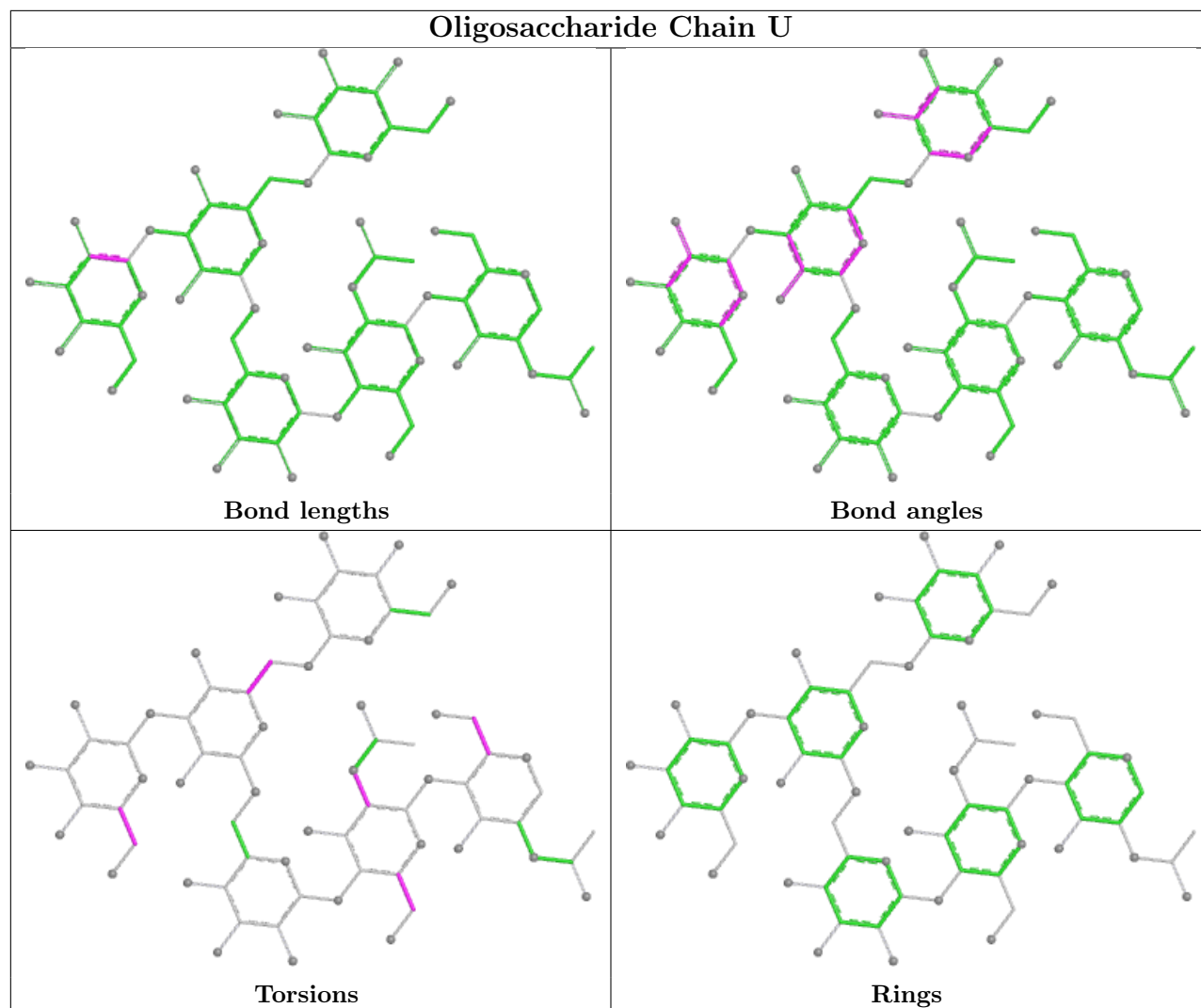


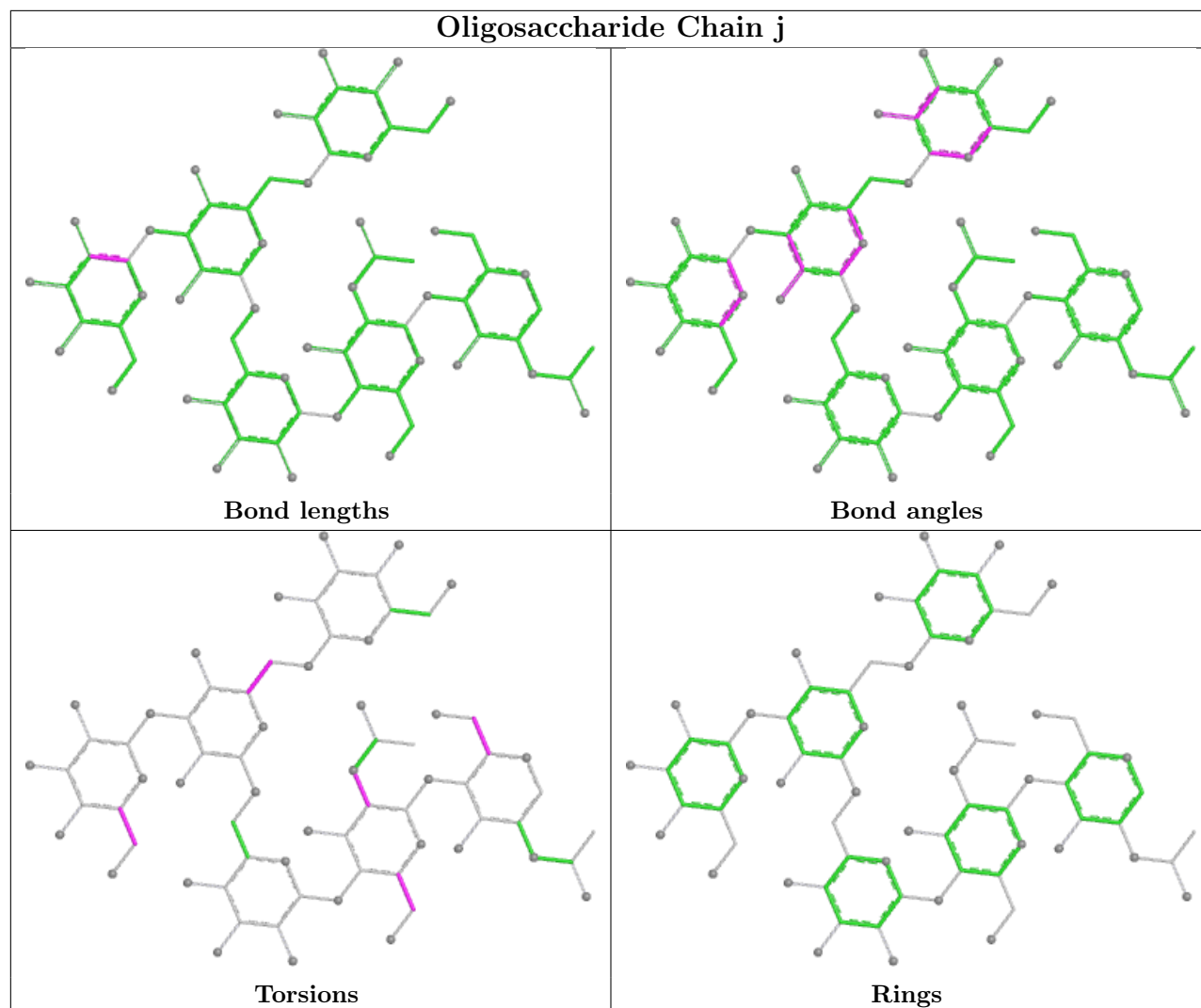


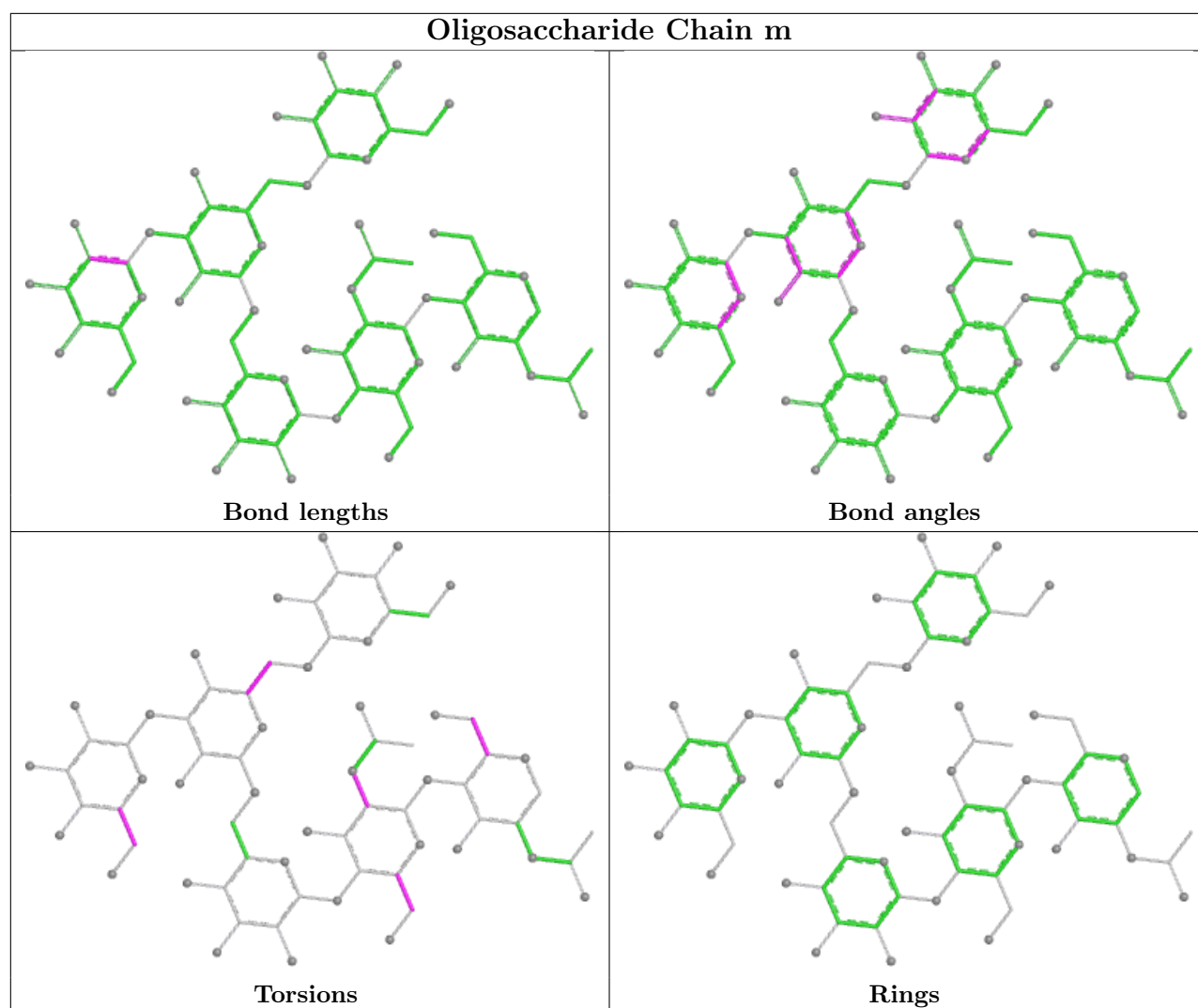


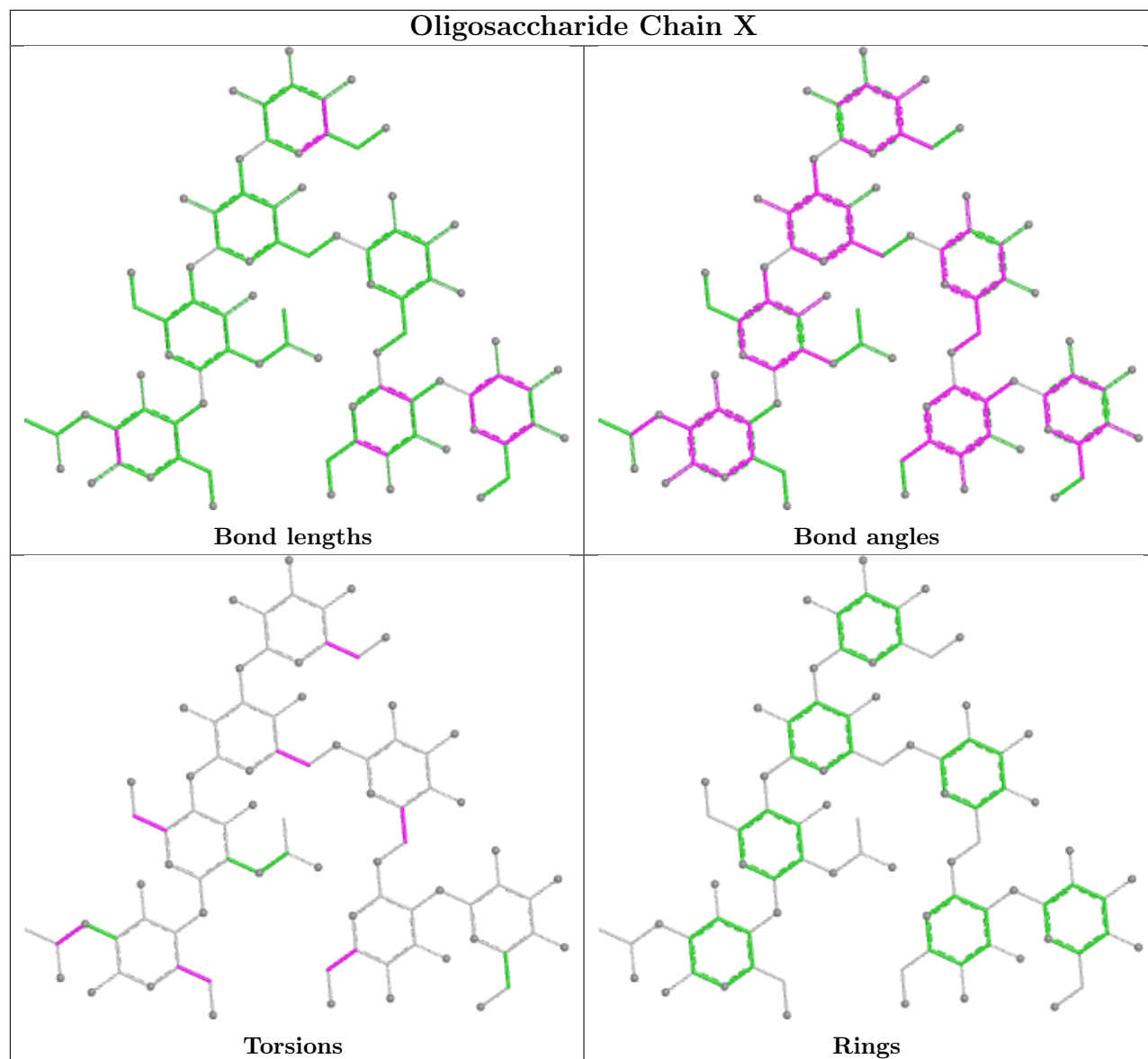


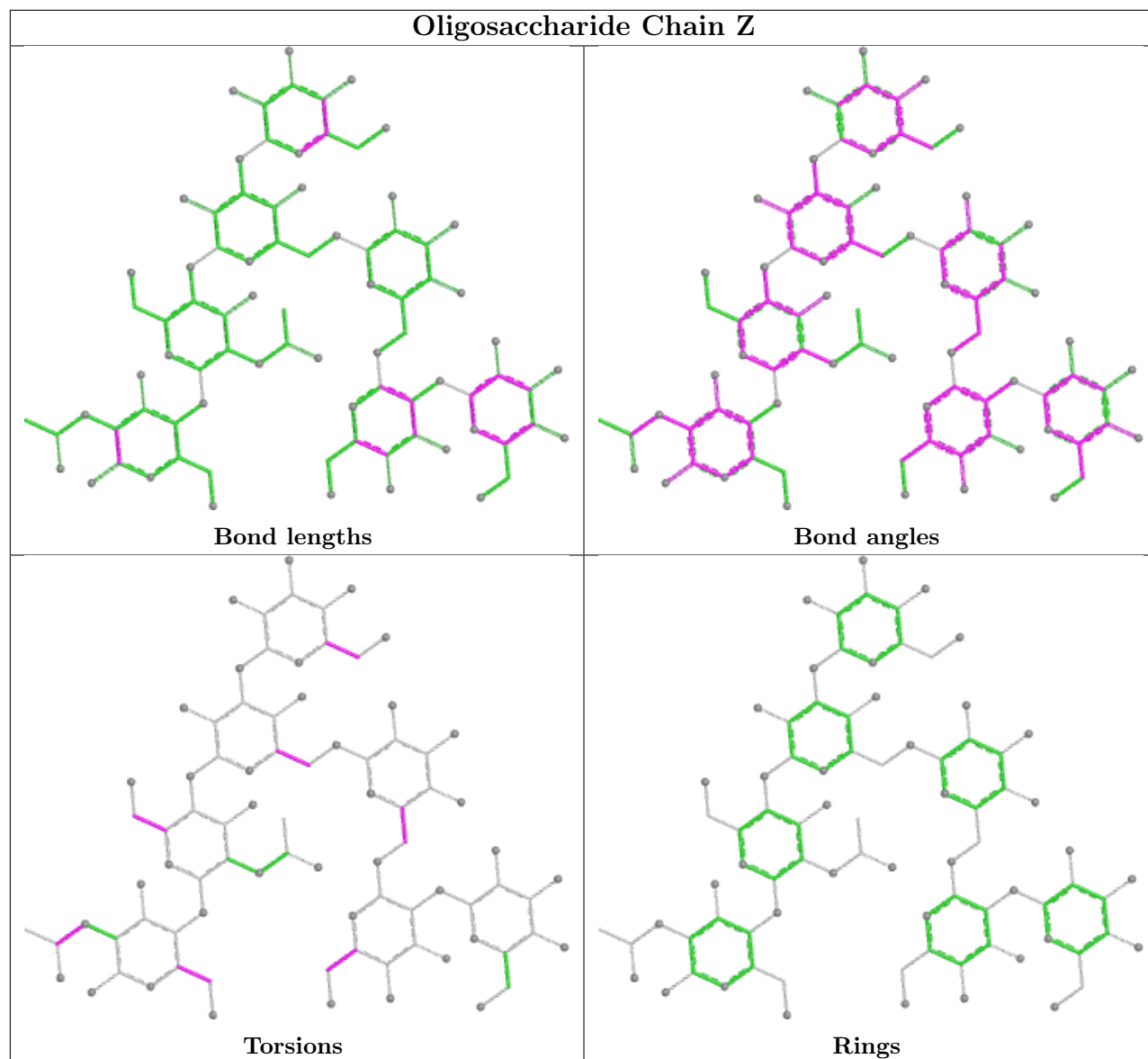


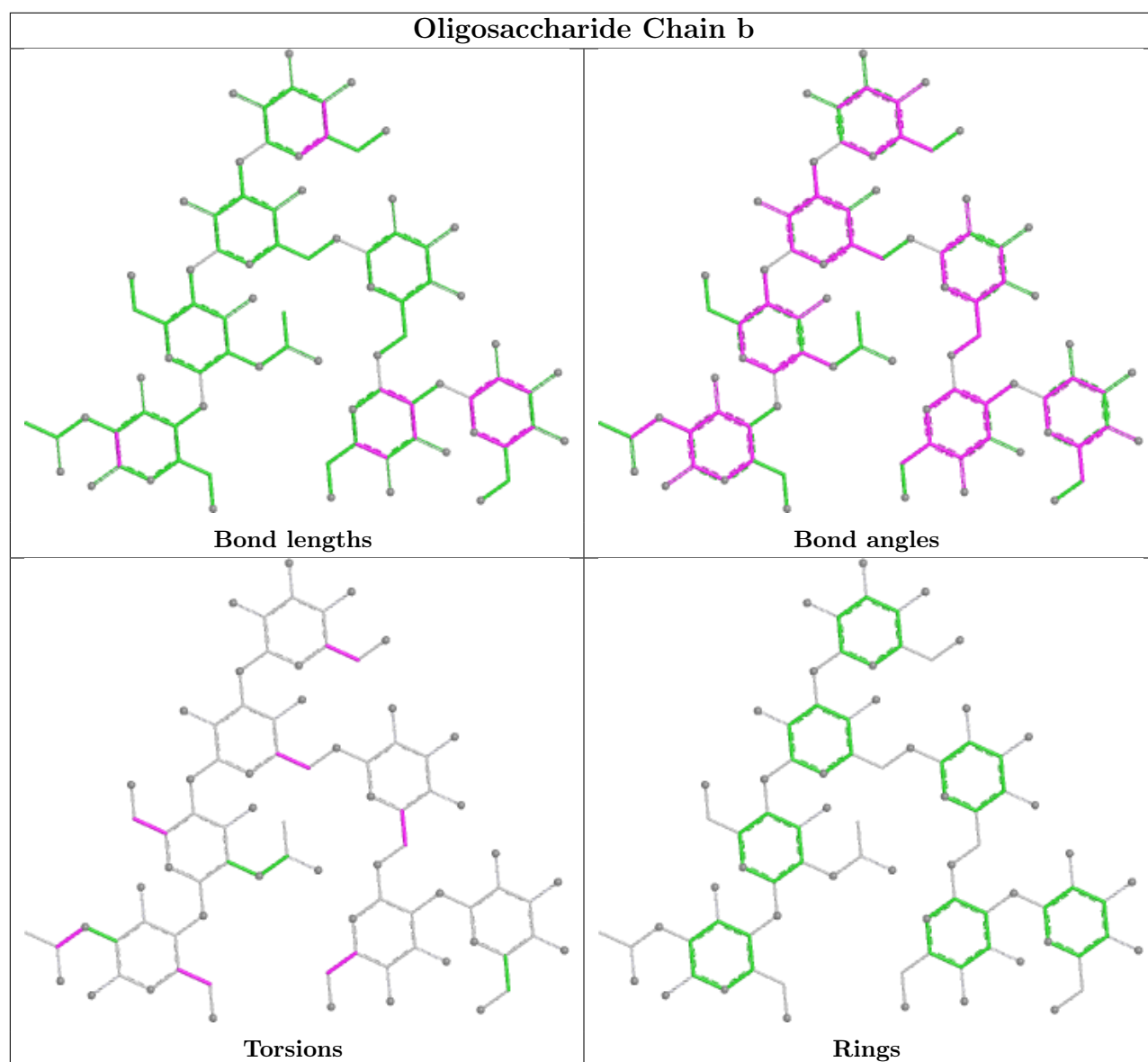


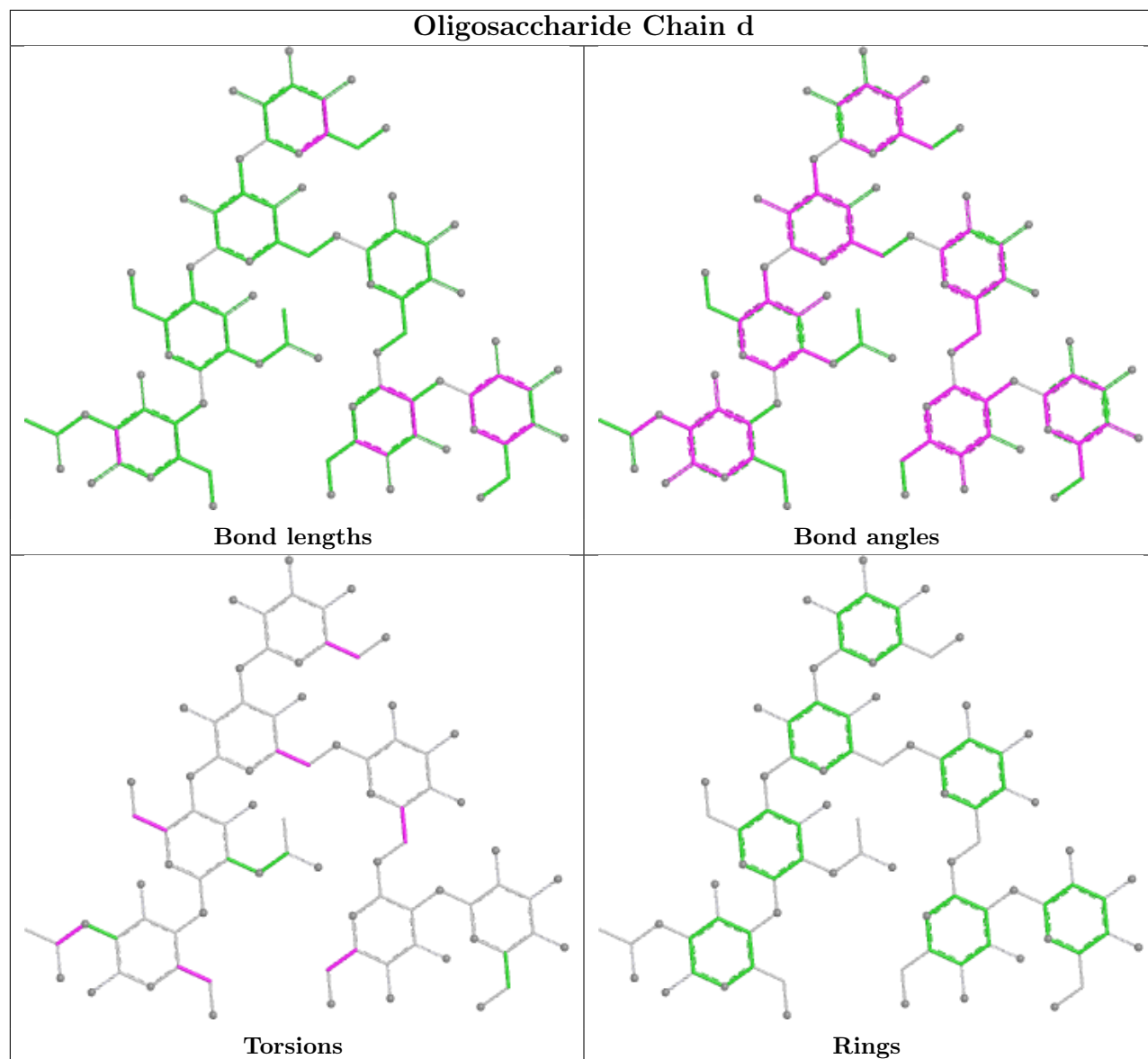


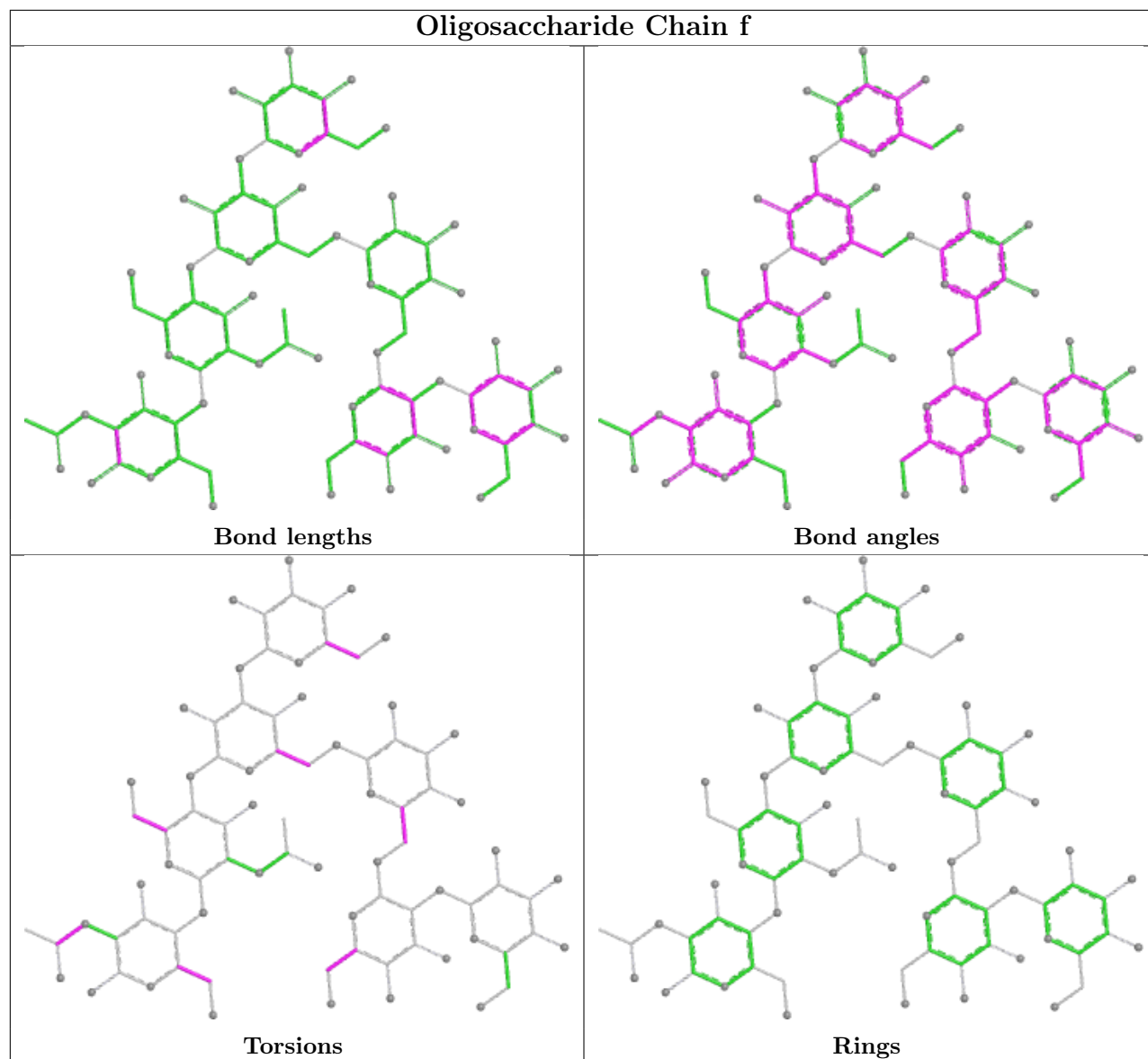


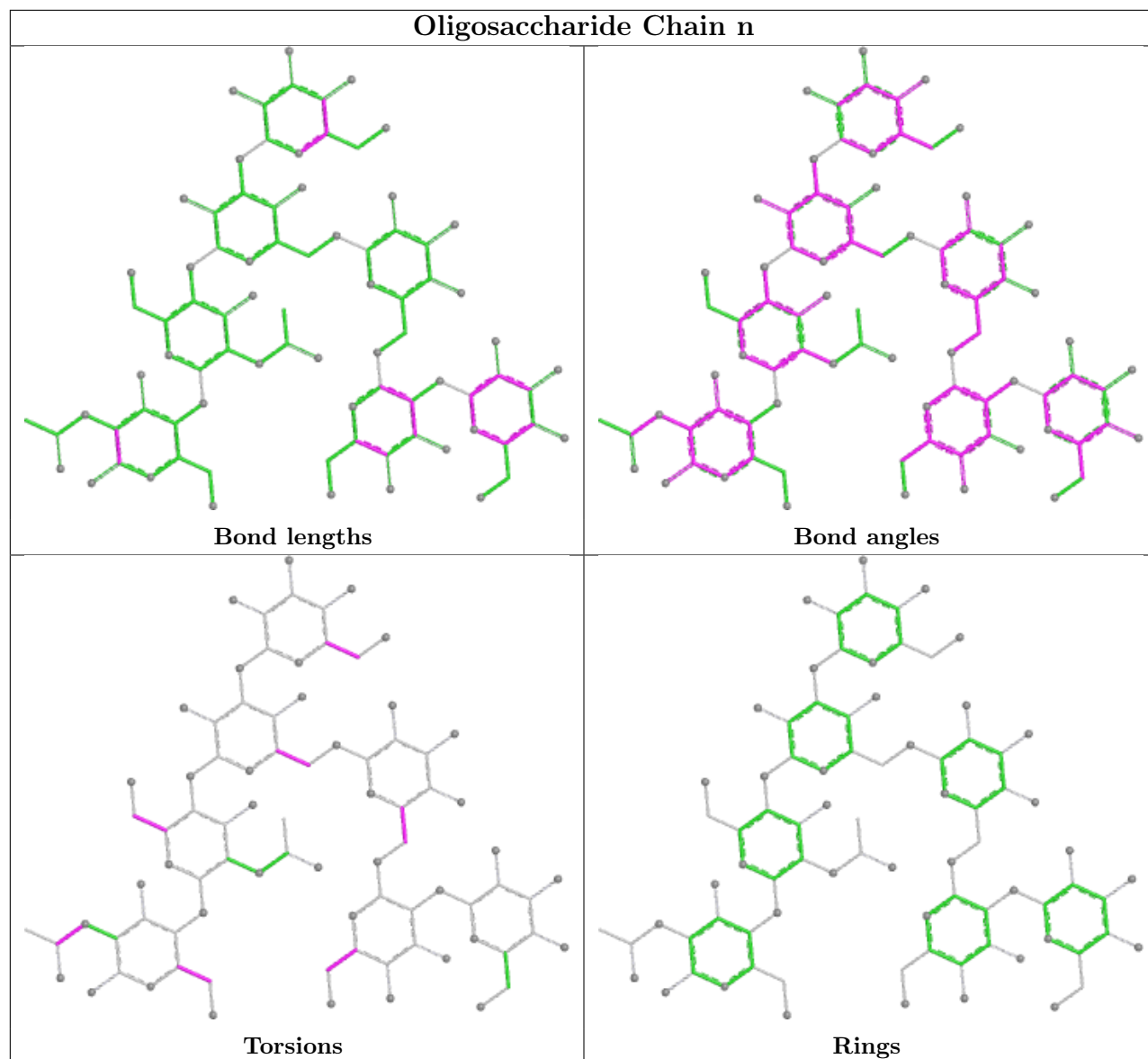


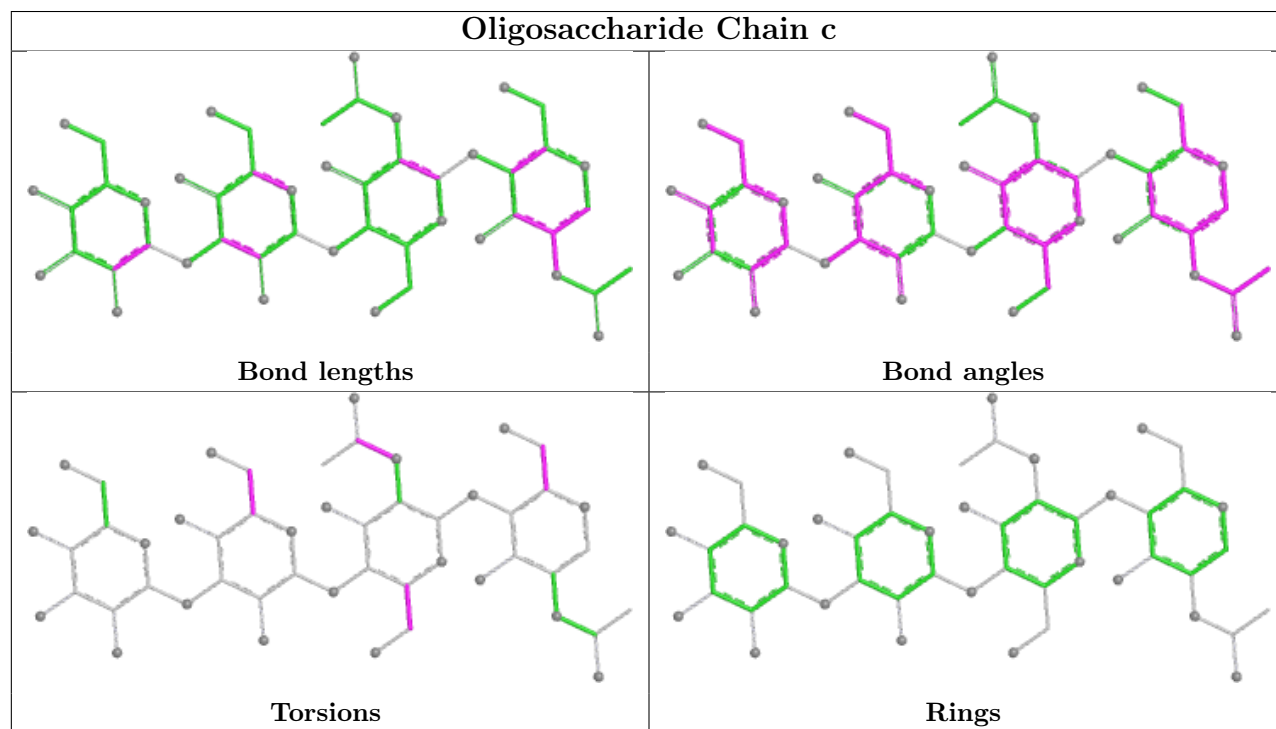
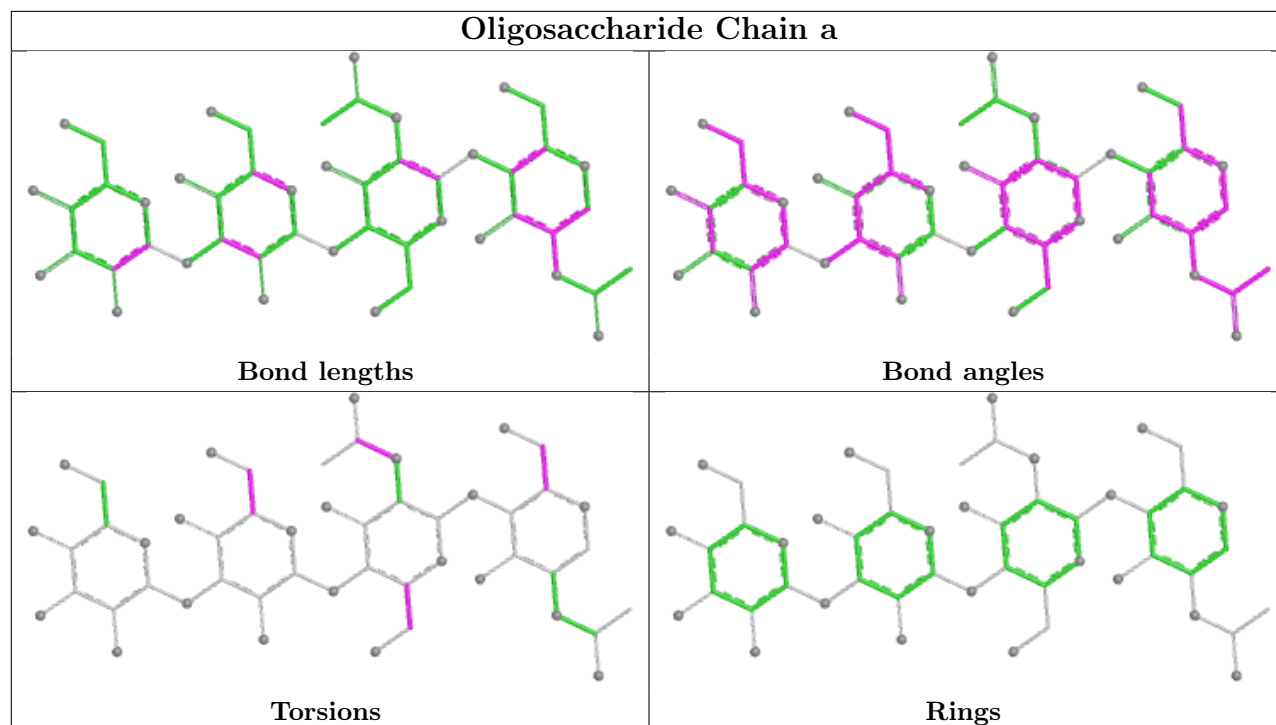


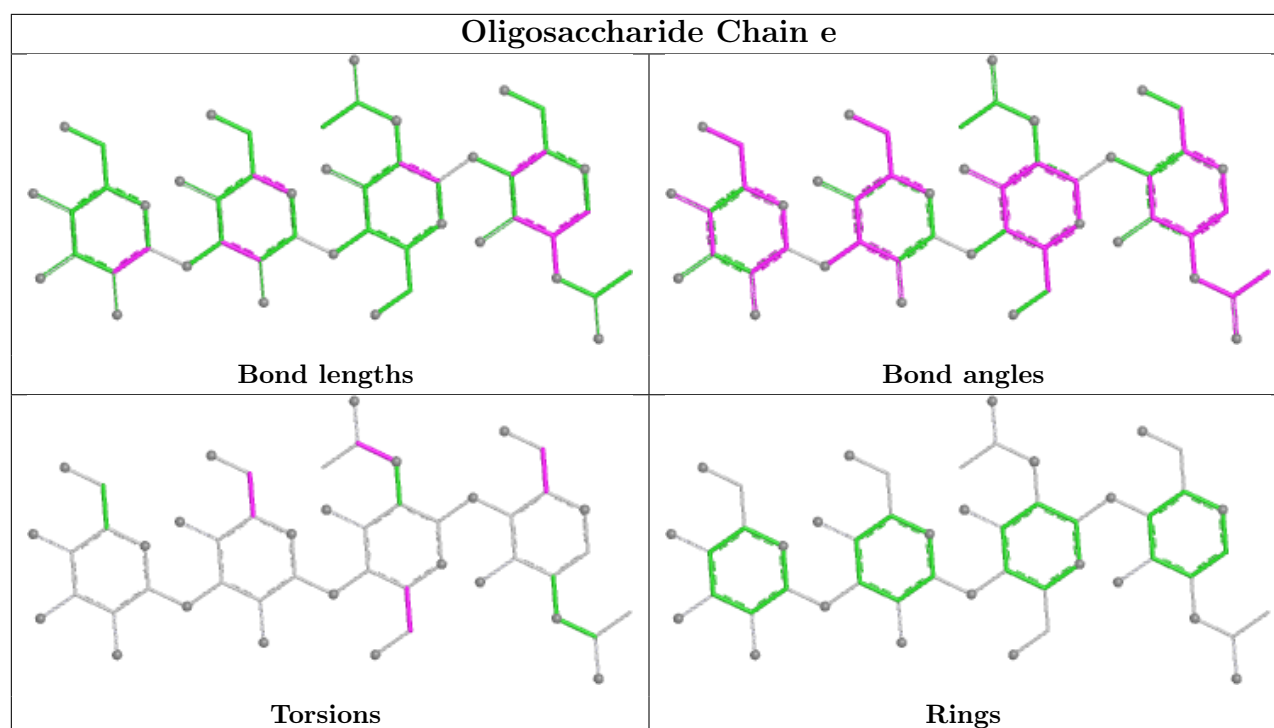












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

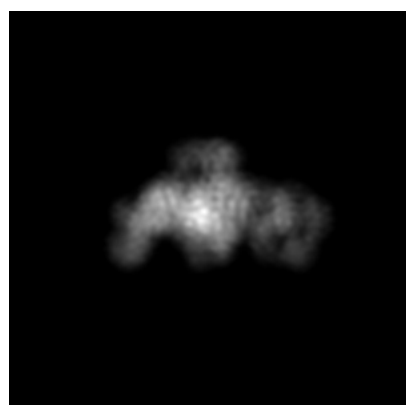
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8981. These allow visual inspection of the internal detail of the map and identification of artifacts.

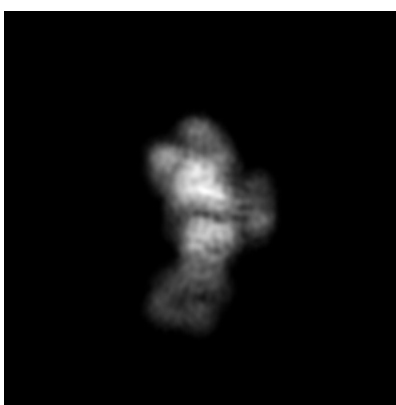
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

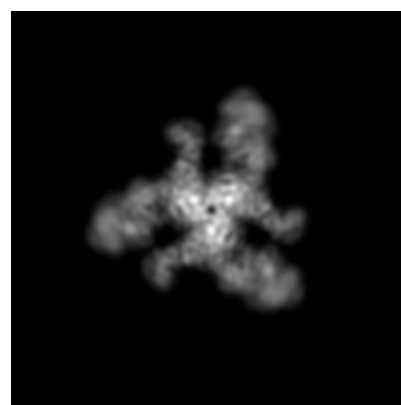
6.1.1 Primary map



X



Y

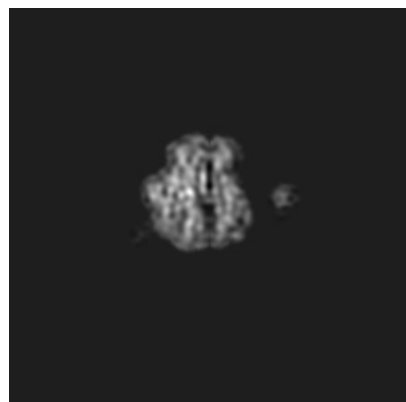


Z

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

6.2 Central slices [i](#)

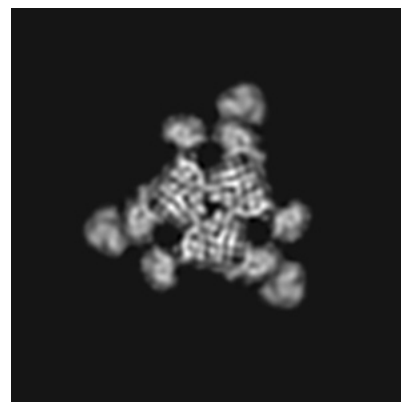
6.2.1 Primary map



X Index: 192



Y Index: 192

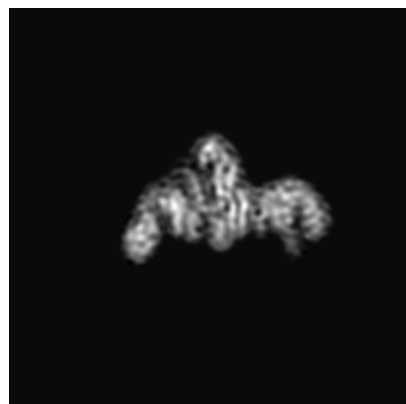


Z Index: 192

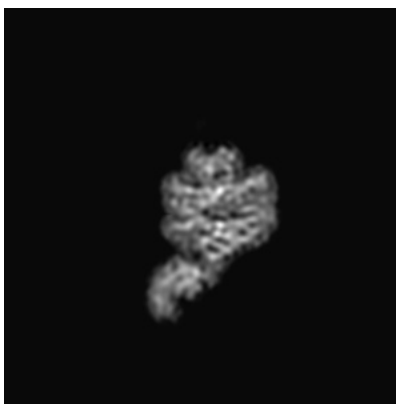
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 211



Y Index: 202

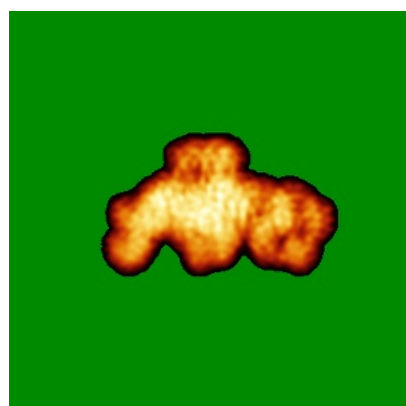


Z Index: 188

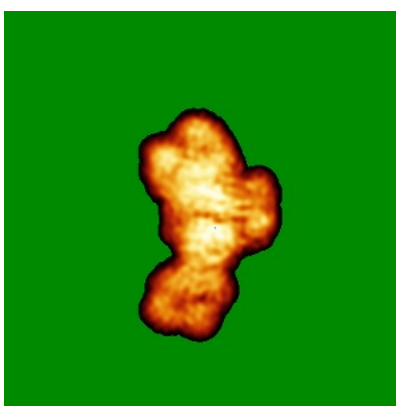
The images above show the largest variance slices of the map in three orthogonal directions.

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

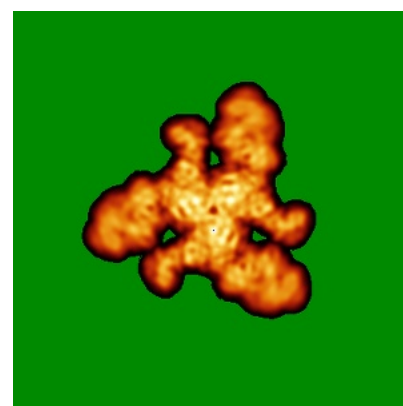
6.4.1 Primary map



X



Y

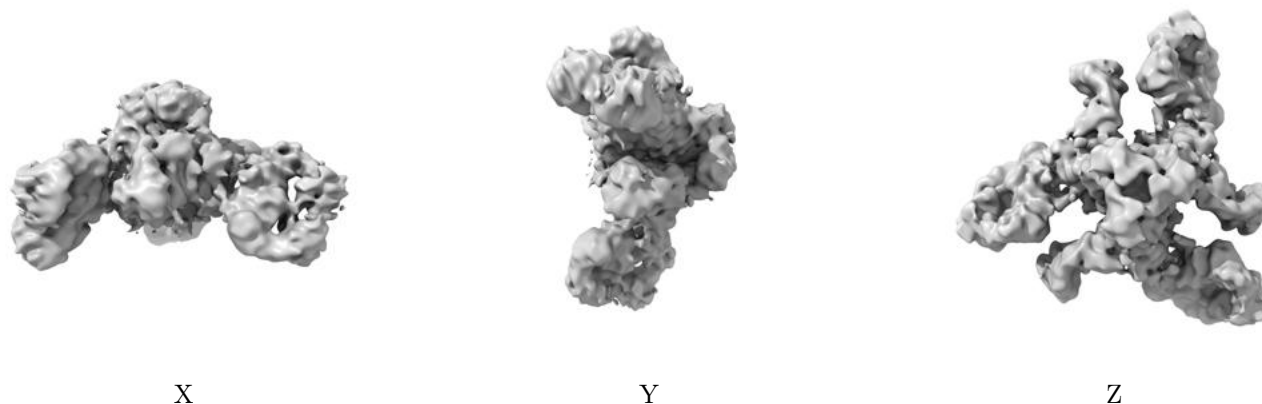


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.734. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

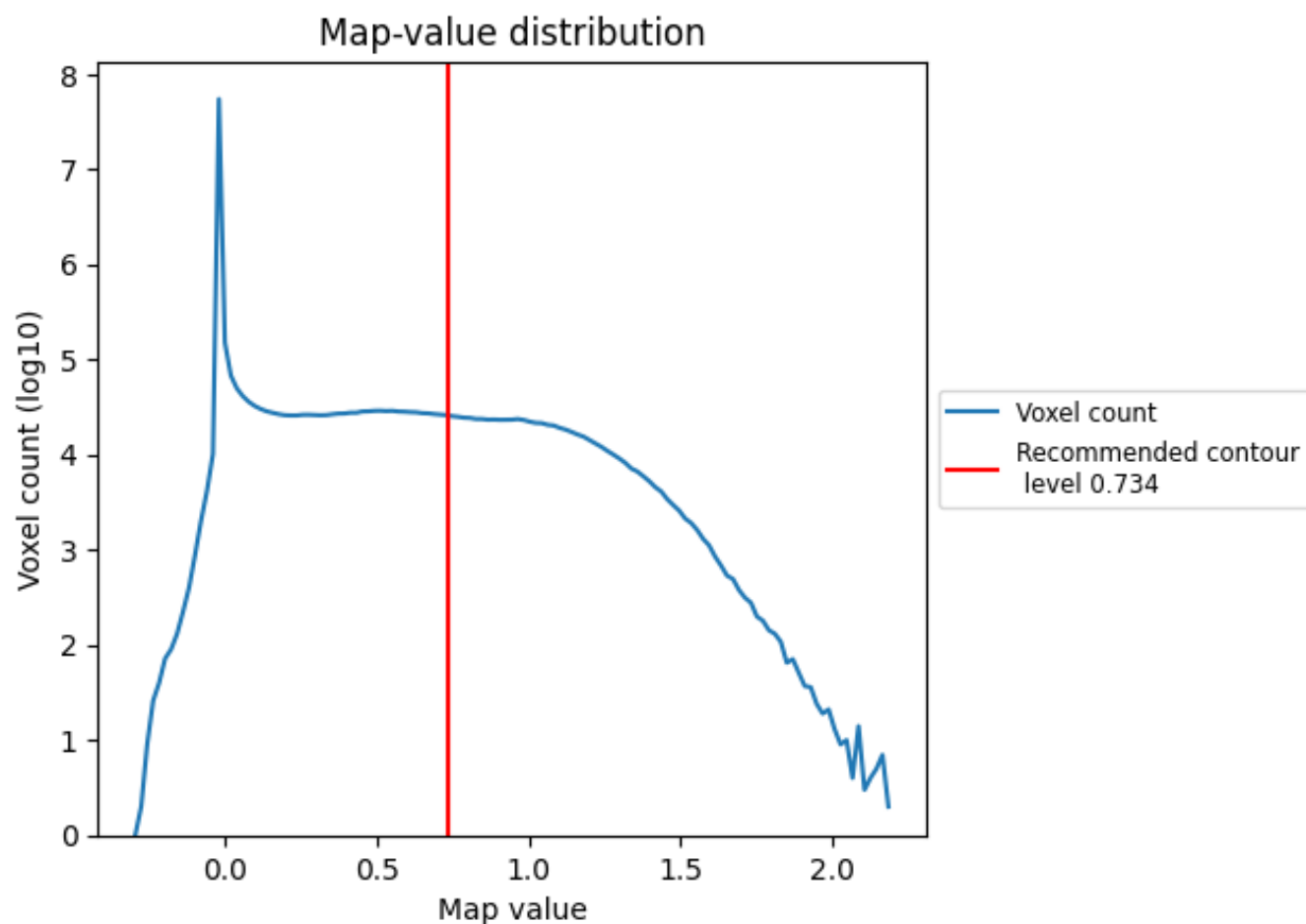
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

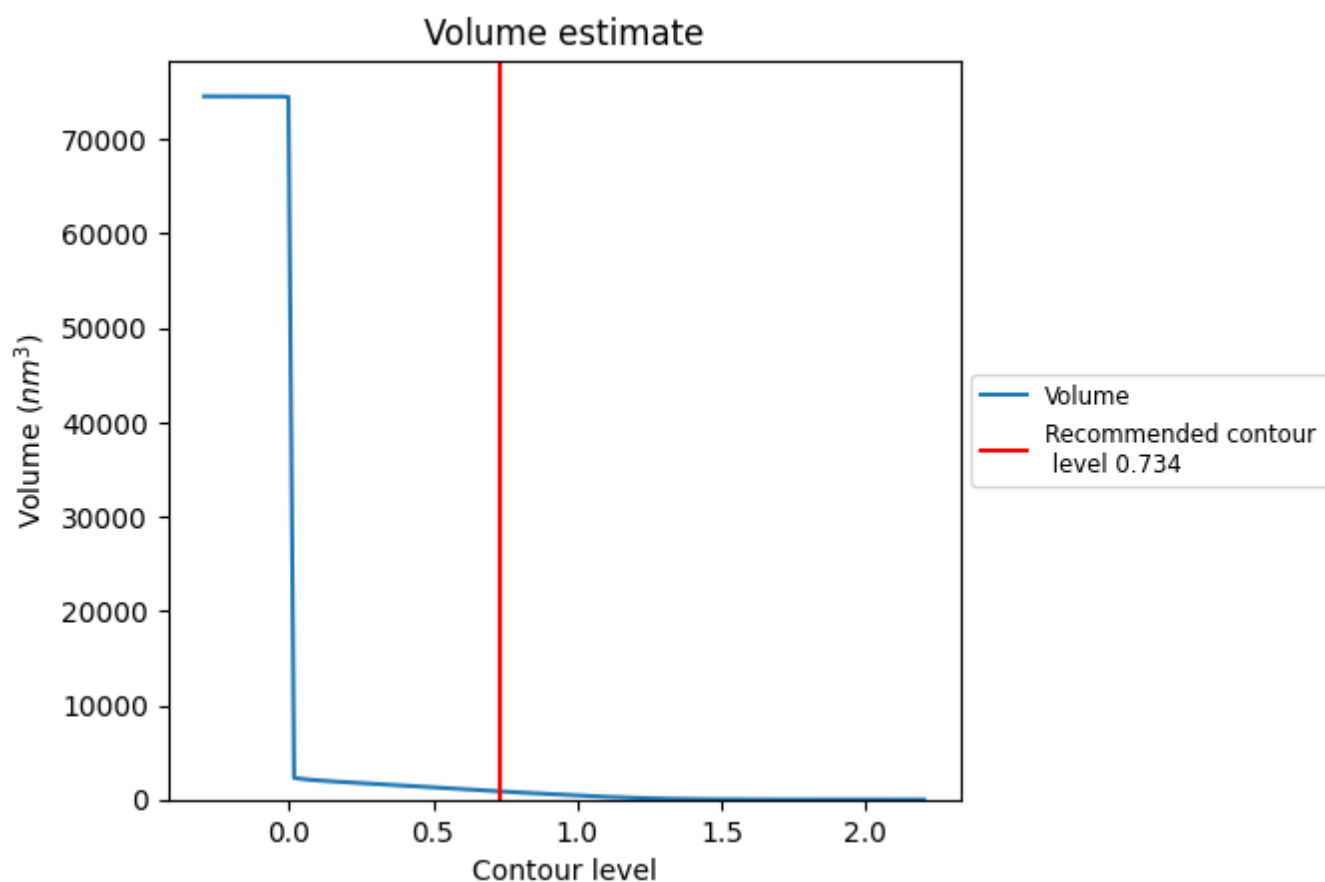
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

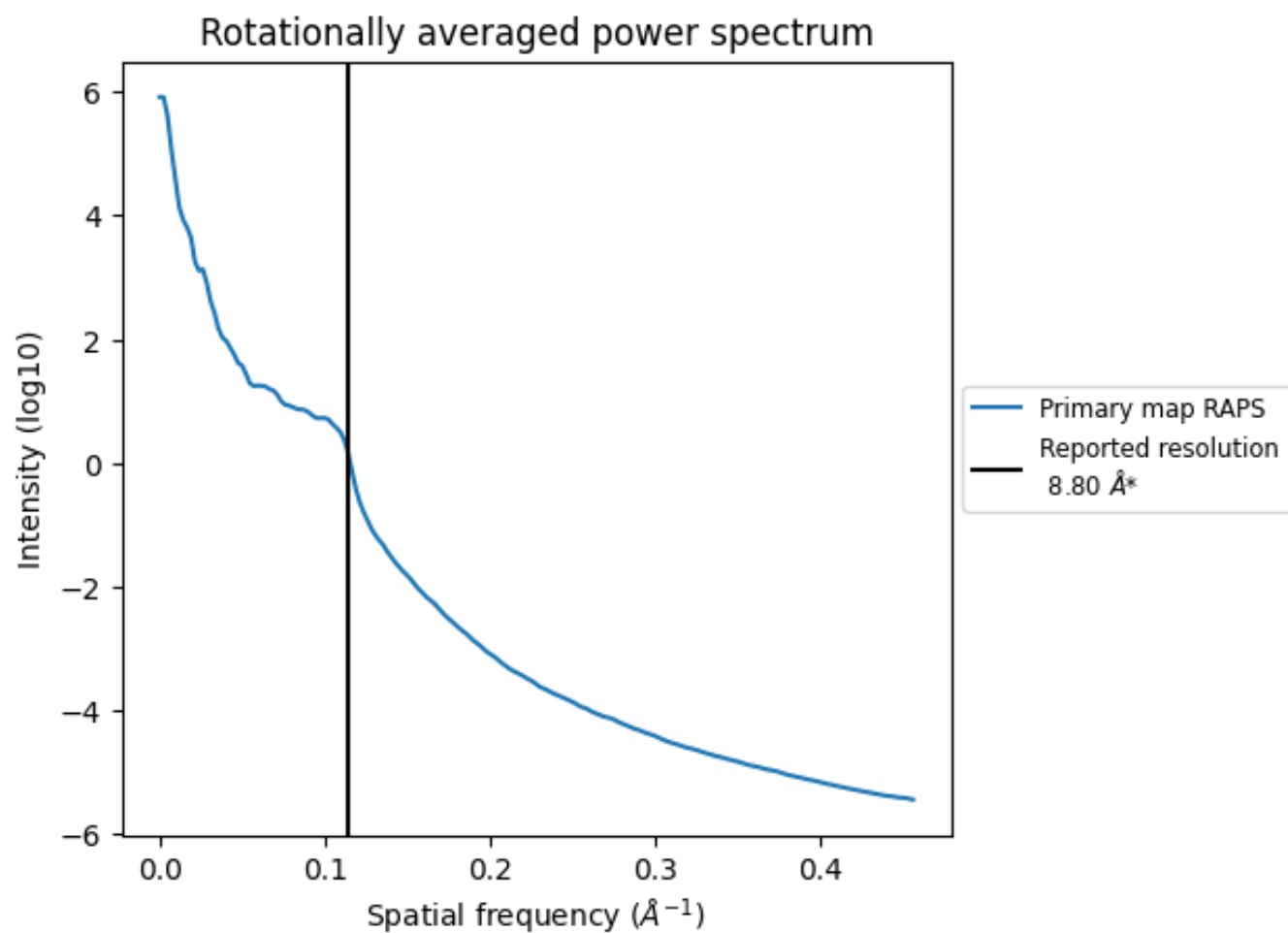
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 861 nm^3 ; this corresponds to an approximate mass of 778 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 ⓘ

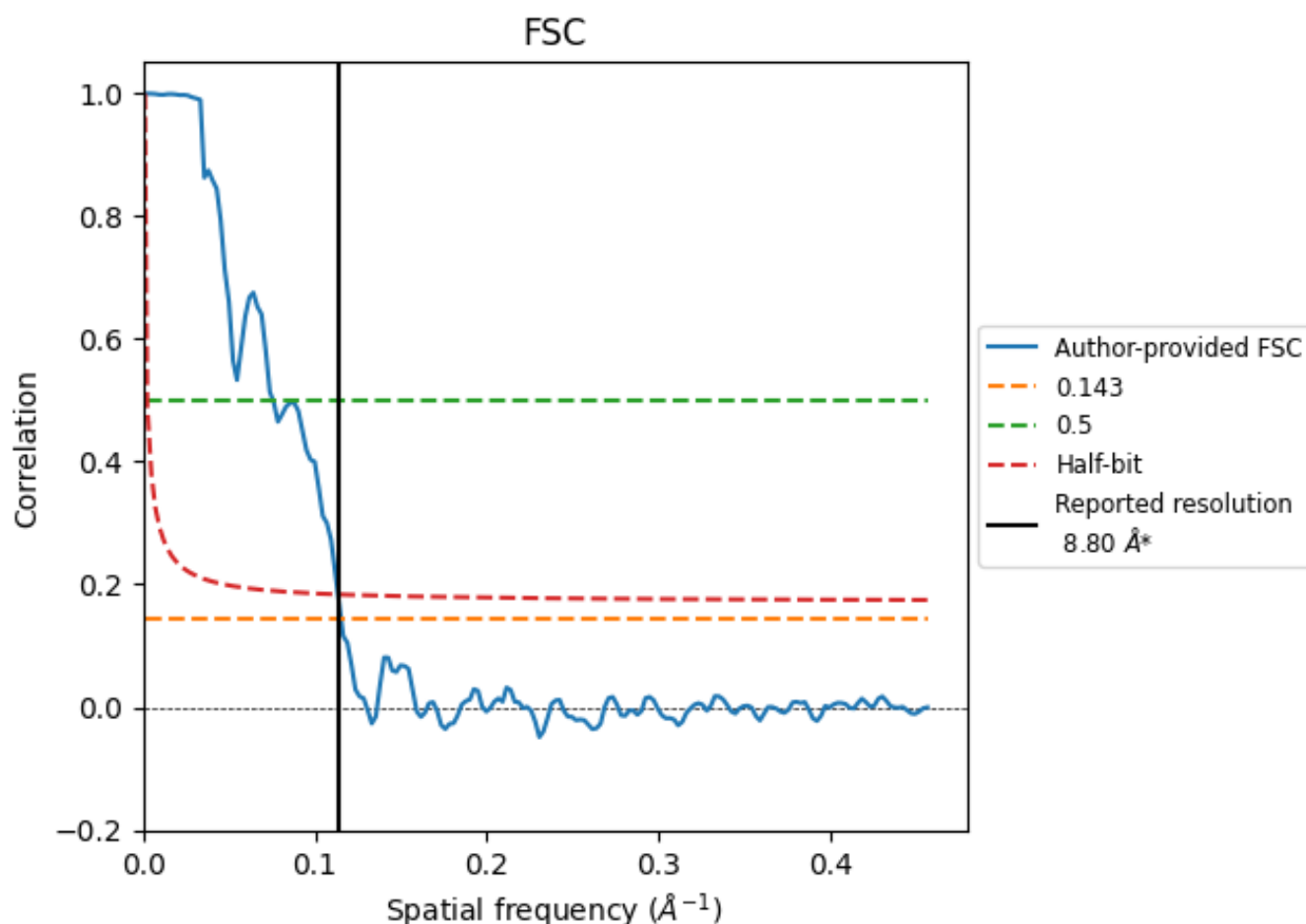


*Reported resolution corresponds to spatial frequency of 0.114 Å⁻¹

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 0.114 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.80	-	-
Author-provided FSC curve	8.68	13.23	8.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-8981 and PDB model 6E5P. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay ⓘ

This section was not generated.

9.2 Q-score mapped to coordinate model ⓘ

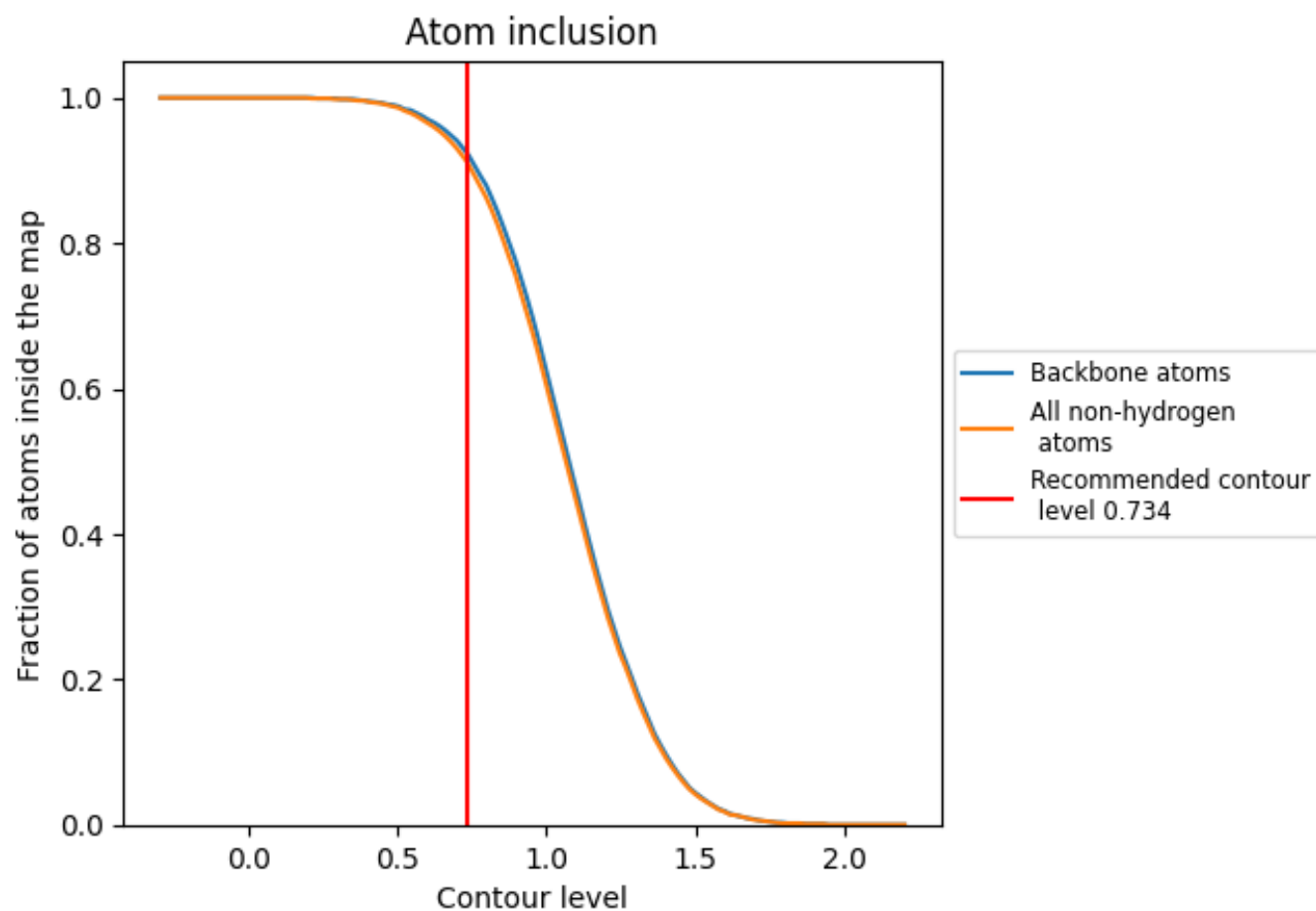


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.734) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9120	 0.1400
1	 0.9280	 0.1350
2	 0.8900	 0.1290
3	 0.8910	 0.1210
4	 0.9120	 0.1170
A	 0.9650	 0.1770
B	 0.9540	 0.1830
C	 0.9650	 0.1730
D	 0.9520	 0.1920
E	 0.9600	 0.1690
F	 0.9480	 0.1790
G	 0.9090	 0.0740
H	 0.9010	 0.1270
I	 0.9280	 0.1320
J	 0.8440	 0.0520
K	 0.9300	 0.1350
L	 0.9240	 0.1230
M	 0.8930	 0.1400
N	 0.7730	 0.1640
O	 0.9380	 0.1360
P	 0.8610	 0.0750
Q	 0.9240	 0.1430
R	 0.8920	 0.1310
S	 0.8830	 0.1200
T	 0.9120	 0.1060
U	 0.5420	 0.0340
V	 0.9380	 0.1380
W	 0.8640	 0.0690
X	 0.5480	 0.2050
Y	 0.9550	 0.2170
Z	 0.7140	 0.0910
a	 0.8000	 0.1850
b	 0.6790	 0.0940
c	 0.8000	 0.1990
d	 0.7020	 0.0960



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Chain	Atom inclusion	Q-score
e	 0.8000	 0.1750
f	 0.5710	 0.1800
g	 0.9550	 0.1940
h	 0.9090	 0.0520
i	 0.5910	 0.2480
j	 0.5560	 0.0460
k	 0.9090	 0.1050
l	 0.6360	 0.1800
m	 0.5690	 0.0470
n	 0.5590	 0.1810
o	 0.9090	 0.2140