



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:06 AM UTC

PDB ID : 8YW2 / pdb_00008yw2
EMDB ID : EMD-39620
Title : Semliki Forest virus viron in complex with VLDLR
Authors : Wang, J.; Zheng, T.; Yang, D.
Deposited on : 2024-03-29
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

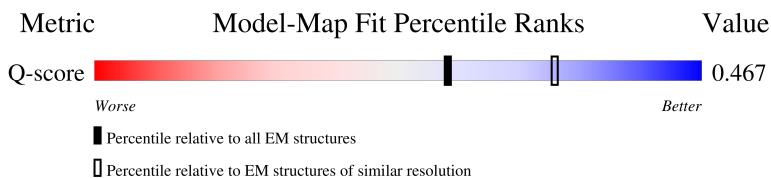
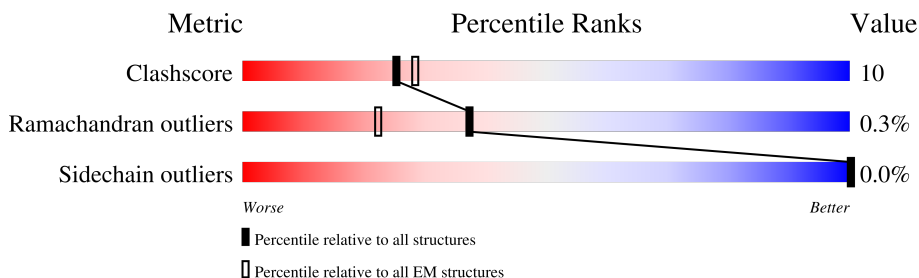
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



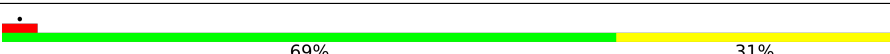
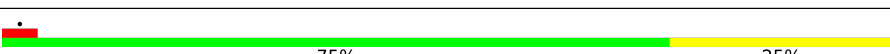
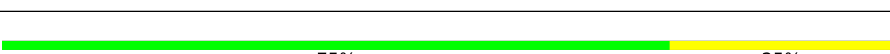
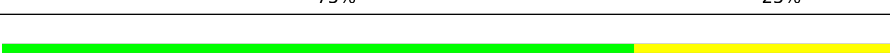
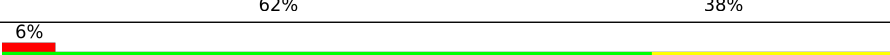
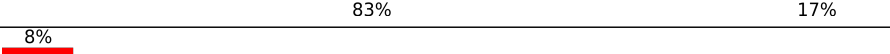
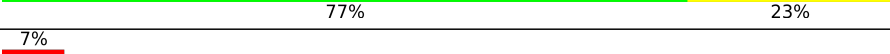
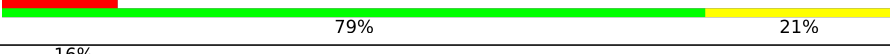
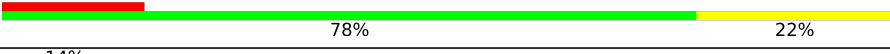
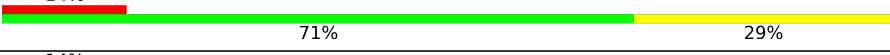
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	0	52	
1	2	52	
1	AA	52	
1	AB	52	

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Mol	Chain	Length	Quality of chain
1	L	52	
1	M	52	
1	N	52	
1	S	52	
1	a	52	
1	b	52	
1	c	52	
1	g	52	
1	l	52	
1	u	52	
1	v	52	
1	w	52	
2	1	161	
2	3	161	
2	AC	161	
2	AD	161	
2	AE	161	
2	D	161	
2	O	161	
2	P	161	
2	Q	161	
2	T	161	
2	d	161	
2	e	161	
2	f	161	

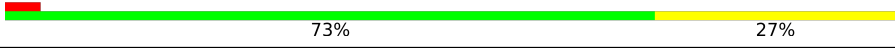
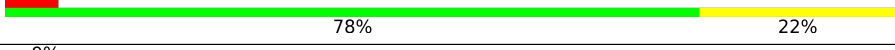
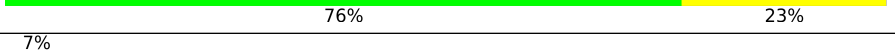
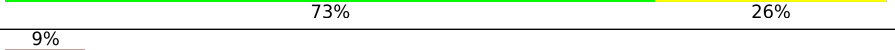
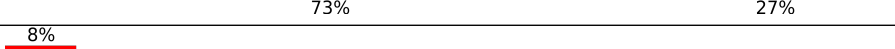
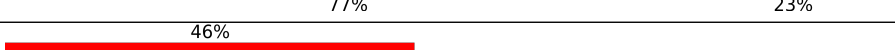
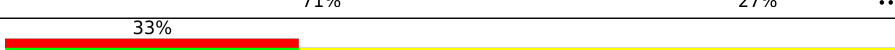
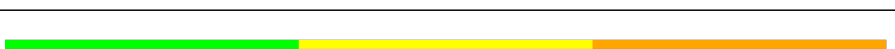
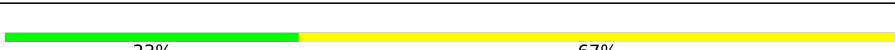
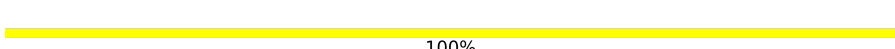
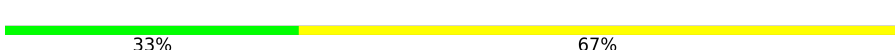
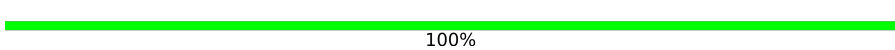
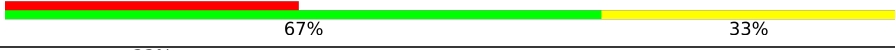
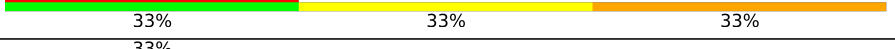
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Mol	Chain	Length	Quality of chain
2	n	161	
2	x	161	
2	y	161	
3	4	438	
3	5	438	
3	6	438	
3	E	438	
3	F	438	
3	G	438	
3	H	438	
3	U	438	
3	V	438	
3	W	438	
3	h	438	
3	i	438	
3	m	438	
3	o	438	
3	p	438	
3	q	438	
4	7	418	
4	8	418	
4	9	418	
4	B	418	
4	I	418	
4	J	418	

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Mol	Chain	Length	Quality of chain
4	K	418	
4	R	418	
4	X	418	
4	Y	418	
4	Z	418	
4	j	418	
4	r	418	
4	s	418	
4	t	418	
4	z	418	
5	A	162	
6	BA	3	
6	C	3	
6	CA	3	
6	DA	3	
6	EA	3	
6	FA	3	
6	GA	3	
6	HA	3	
6	IA	3	
6	JA	3	
6	KA	3	
6	LA	3	
6	MA	3	
6	NA	3	

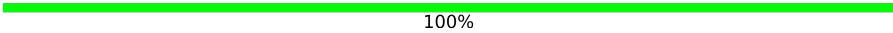
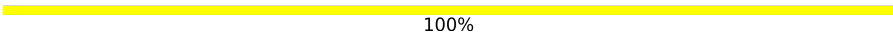
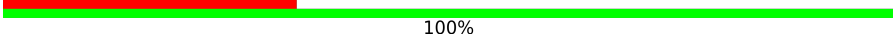
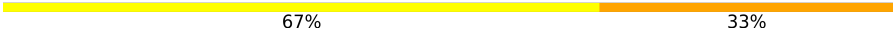
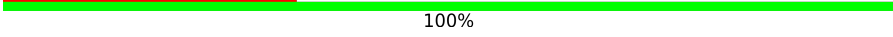
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Mol	Chain	Length	Quality of chain
6	OA	3	100%
6	PA	3	67% 33%
6	QA	3	33% 67%
6	RA	3	67% 33%
6	SA	3	33% 67%
6	TA	3	67% 33%
6	UA	3	67% 33%
6	VA	3	33% 67%
6	WA	3	33% 67% 33%
6	XA	3	33% 67% 33%
6	YA	3	33% 67% 33%
6	ZA	3	33% 33% 33%
6	aA	3	100%
6	bA	3	33% 67%
6	cA	3	33% 100%
6	dA	3	100%
6	eA	3	33% 100%
6	fA	3	67% 33%
6	gA	3	33% 33% 33%
6	hA	3	67% 33%
6	iA	3	33% 67%
6	jA	3	100%
6	k	3	33% 67%
6	kA	3	67% 33%
6	lA	3	33% 33% 33%

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Mol	Chain	Length	Quality of chain
6	mA	3	
6	nA	3	
6	oA	3	
6	pA	3	
6	qA	3	
6	rA	3	
6	sA	3	
6	tA	3	
6	uA	3	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 134901 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein E3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	2	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	AA	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	AB	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	L	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	M	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	N	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	S	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	a	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	b	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	c	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	g	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	l	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	u	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	v	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
1	w	52	Total	C	N	O	S	0	0
			404	252	67	77	8		

- Molecule 2 is a protein called capsid protein, partial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	3	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	AC	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	AD	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	AE	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	D	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	O	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	P	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	Q	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	T	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	d	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	e	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	f	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	n	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	x	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	y	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		

- Molecule 3 is a protein called Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	5	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	6	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	E	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	G	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	H	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	U	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	V	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	W	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	h	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	i	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	m	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	o	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	p	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	q	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		

- Molecule 4 is a protein called Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	8	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	9	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	B	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	I	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	J	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	K	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		

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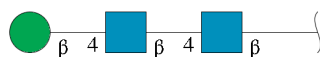
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	X	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	Y	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	Z	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	j	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	r	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	s	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	t	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	z	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		

- Molecule 5 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	162	Total	C	N	O	S	0	0
			1205	694	210	276	25		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	C	3	Total	C	N	O	0	0
			39	22	2	15		
6	k	3	Total	C	N	O	0	0
			39	22	2	15		
6	BA	3	Total	C	N	O	0	0
			39	22	2	15		
6	CA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	DA	3	Total	C	N	O	0	0
			39	22	2	15		
6	EA	3	Total	C	N	O	0	0
			39	22	2	15		
6	FA	3	Total	C	N	O	0	0
			39	22	2	15		
6	GA	3	Total	C	N	O	0	0
			39	22	2	15		
6	HA	3	Total	C	N	O	0	0
			39	22	2	15		
6	IA	3	Total	C	N	O	0	0
			39	22	2	15		
6	JA	3	Total	C	N	O	0	0
			39	22	2	15		
6	KA	3	Total	C	N	O	0	0
			39	22	2	15		
6	LA	3	Total	C	N	O	0	0
			39	22	2	15		
6	MA	3	Total	C	N	O	0	0
			39	22	2	15		
6	NA	3	Total	C	N	O	0	0
			39	22	2	15		
6	OA	3	Total	C	N	O	0	0
			39	22	2	15		
6	PA	3	Total	C	N	O	0	0
			39	22	2	15		
6	QA	3	Total	C	N	O	0	0
			39	22	2	15		
6	RA	3	Total	C	N	O	0	0
			39	22	2	15		
6	SA	3	Total	C	N	O	0	0
			39	22	2	15		
6	TA	3	Total	C	N	O	0	0
			39	22	2	15		
6	UA	3	Total	C	N	O	0	0
			39	22	2	15		
6	VA	3	Total	C	N	O	0	0
			39	22	2	15		
6	WA	3	Total	C	N	O	0	0
			39	22	2	15		
6	XA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	YA	3	Total	C	N	O	0	0
			39	22	2	15		
6	ZA	3	Total	C	N	O	0	0
			39	22	2	15		
6	aA	3	Total	C	N	O	0	0
			39	22	2	15		
6	bA	3	Total	C	N	O	0	0
			39	22	2	15		
6	cA	3	Total	C	N	O	0	0
			39	22	2	15		
6	dA	3	Total	C	N	O	0	0
			39	22	2	15		
6	eA	3	Total	C	N	O	0	0
			39	22	2	15		
6	fA	3	Total	C	N	O	0	0
			39	22	2	15		
6	gA	3	Total	C	N	O	0	0
			39	22	2	15		
6	hA	3	Total	C	N	O	0	0
			39	22	2	15		
6	iA	3	Total	C	N	O	0	0
			39	22	2	15		
6	jA	3	Total	C	N	O	0	0
			39	22	2	15		
6	kA	3	Total	C	N	O	0	0
			39	22	2	15		
6	lA	3	Total	C	N	O	0	0
			39	22	2	15		
6	mA	3	Total	C	N	O	0	0
			39	22	2	15		
6	nA	3	Total	C	N	O	0	0
			39	22	2	15		
6	oA	3	Total	C	N	O	0	0
			39	22	2	15		
6	pA	3	Total	C	N	O	0	0
			39	22	2	15		
6	qA	3	Total	C	N	O	0	0
			39	22	2	15		
6	rA	3	Total	C	N	O	0	0
			39	22	2	15		
6	sA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	tA	3	Total	C	N	O	0	0
			39	22	2	15		
6	uA	3	Total	C	N	O	0	0
			39	22	2	15		

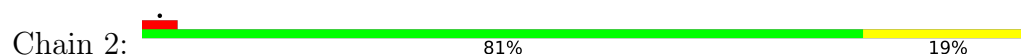
3 Residue-property plots

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.

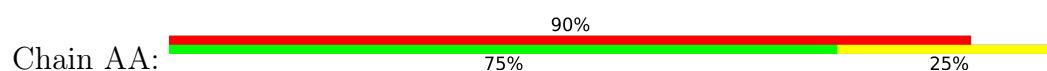
- Molecule 1: Spike glycoprotein E3



- Molecule 1: Spike glycoprotein E3



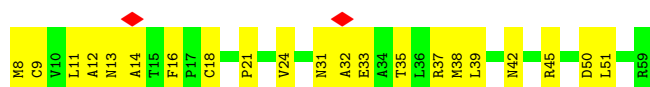
- Molecule 1: Spike glycoprotein E3



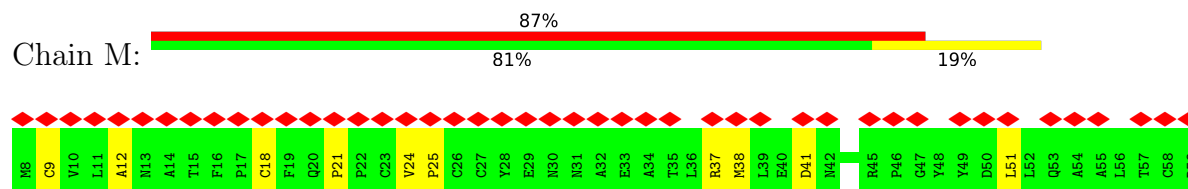
- Molecule 1: Spike glycoprotein E3



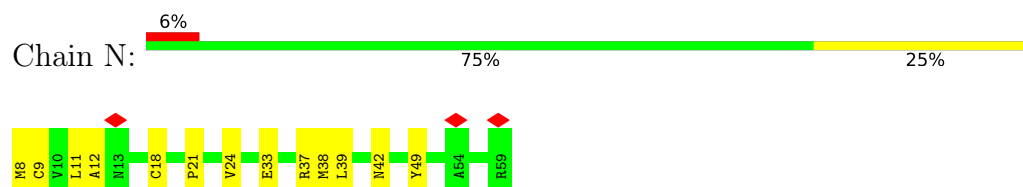
- Molecule 1: Spike glycoprotein E3



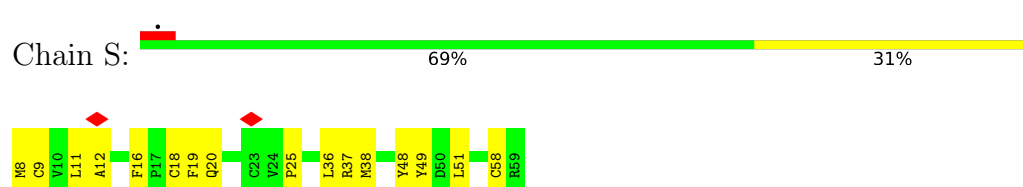
- Molecule 1: Spike glycoprotein E3



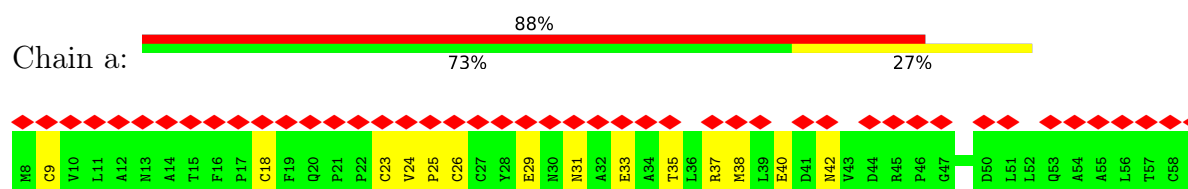
- Molecule 1: Spike glycoprotein E3



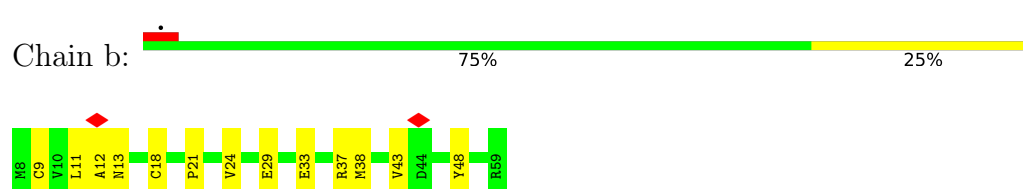
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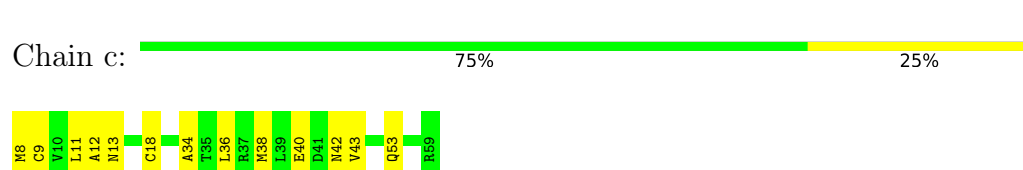
- Molecule 1: Spike glycoprotein E3



- Molecule 1: Spike glycoprotein E3



- Molecule 1: Spike glycoprotein E3



- Molecule 1: Spike glycoprotein E3

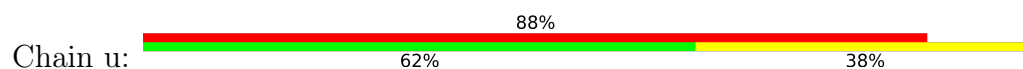




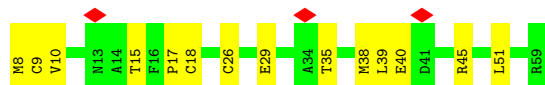
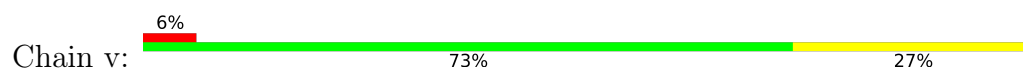
- Molecule 1: Spike glycoprotein E3



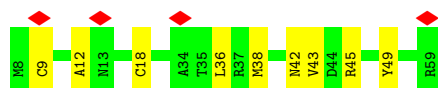
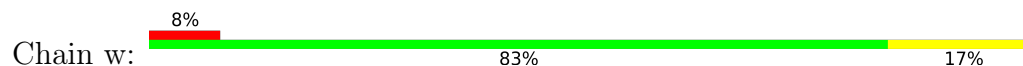
- Molecule 1: Spike glycoprotein E3



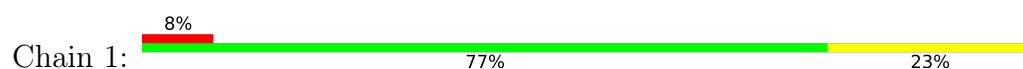
- Molecule 1: Spike glycoprotein E3



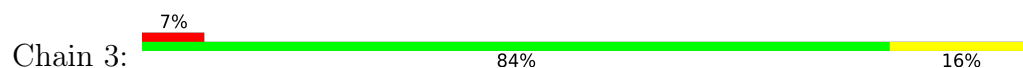
- Molecule 1: Spike glycoprotein E3



- Molecule 2: capsid protein, partial

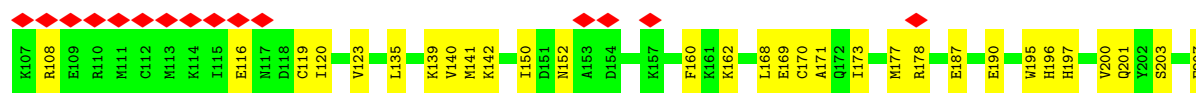


- Molecule 2: capsid protein, partial

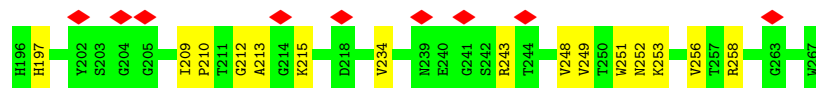
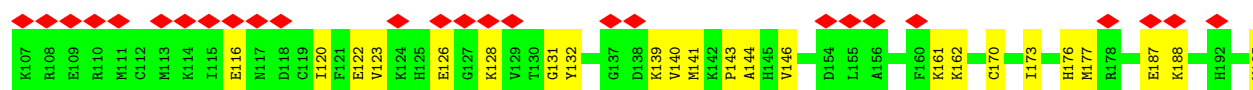
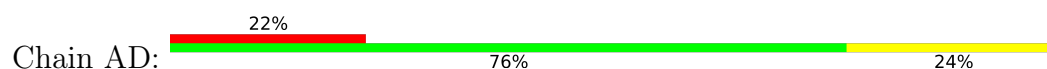




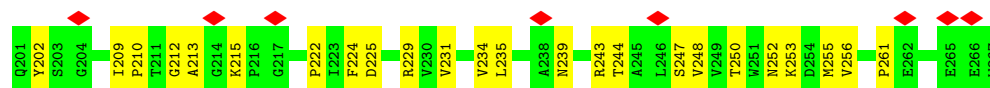
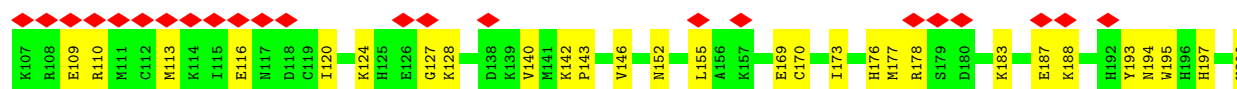
- Molecule 2: capsid protein, partial



- Molecule 2: capsid protein, partial



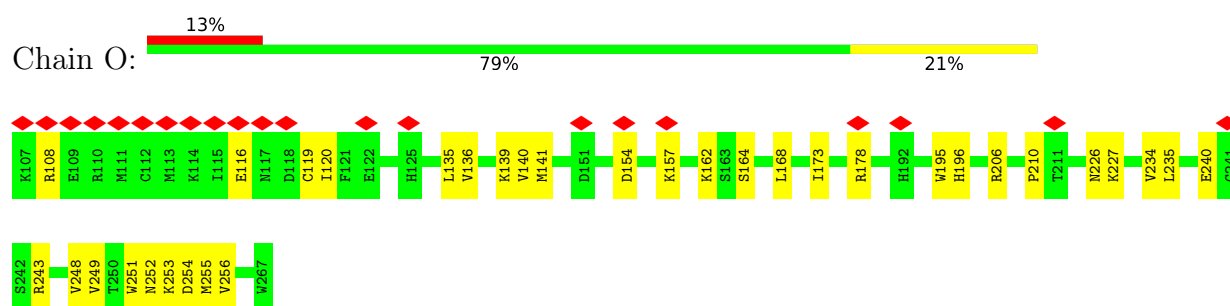
- Molecule 2: capsid protein, partial



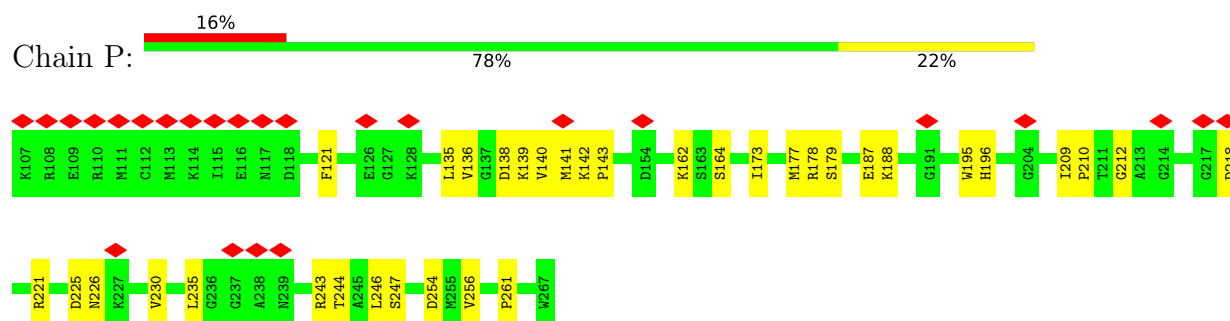
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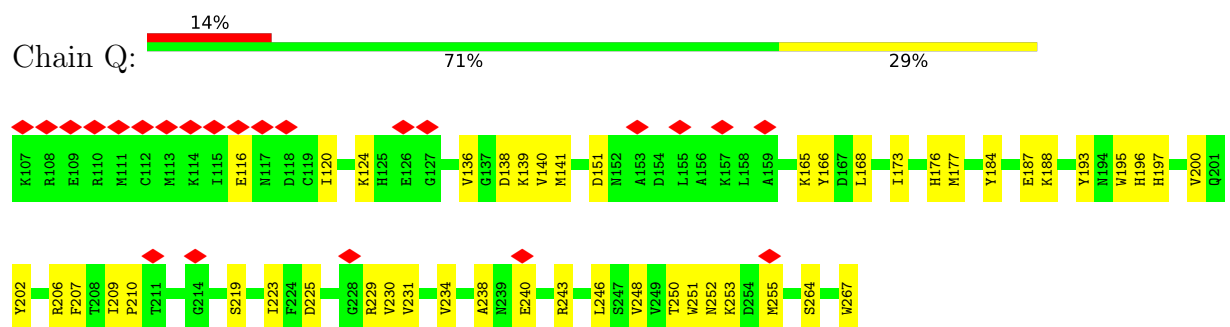
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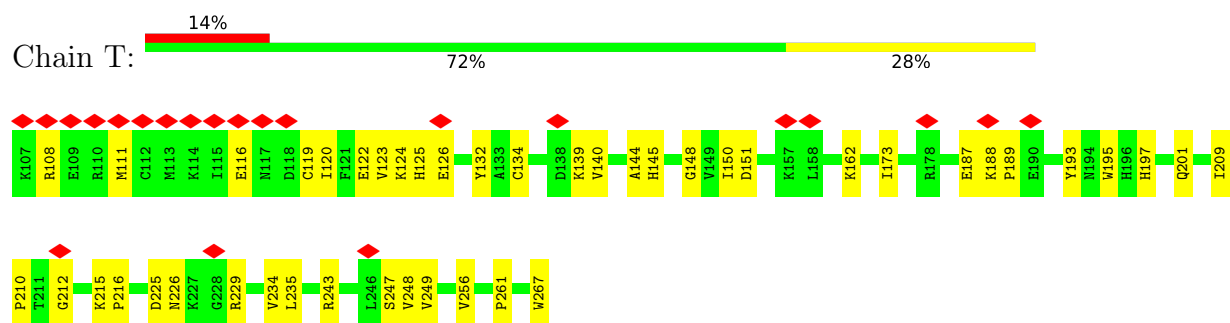
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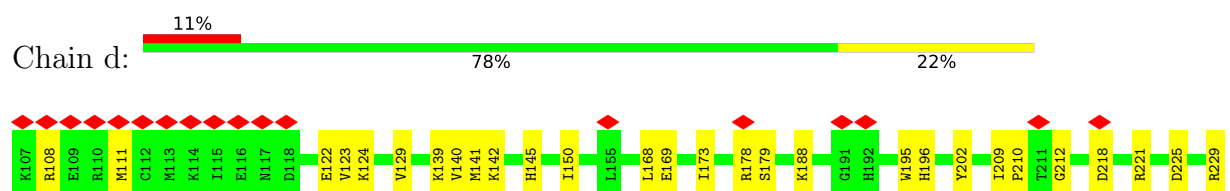
- Molecule 2: capsid protein, partial



- Molecule 2: capsid protein, partial



- Molecule 2: capsid protein, partial

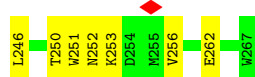
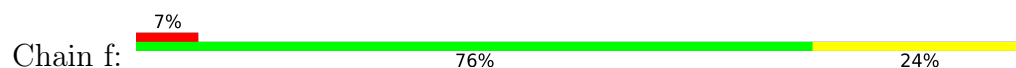




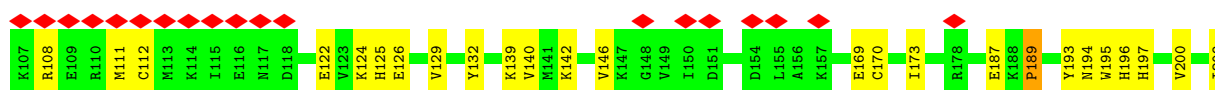
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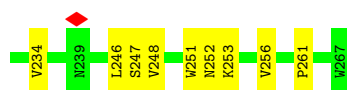
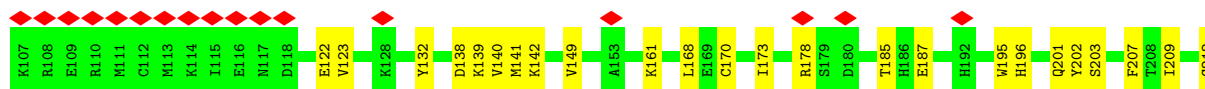
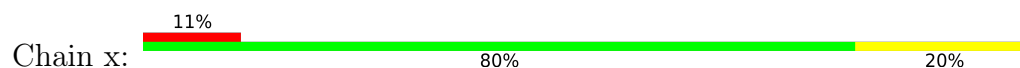
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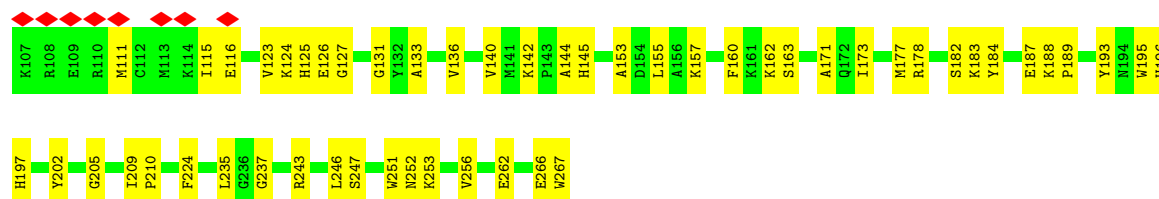
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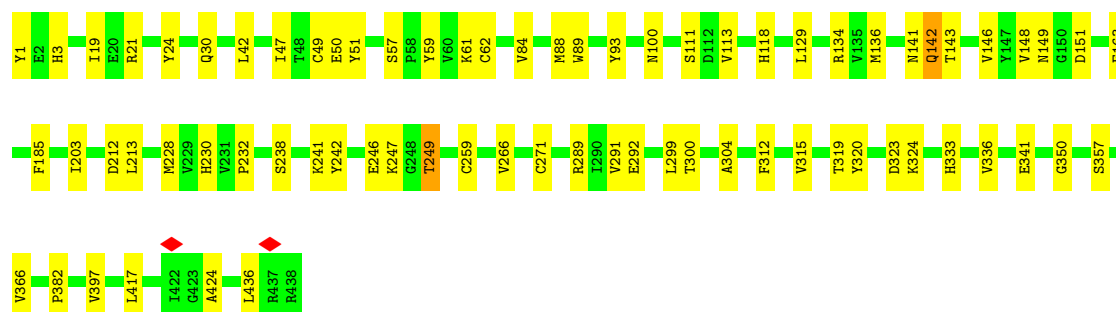
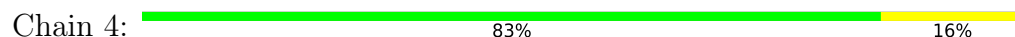
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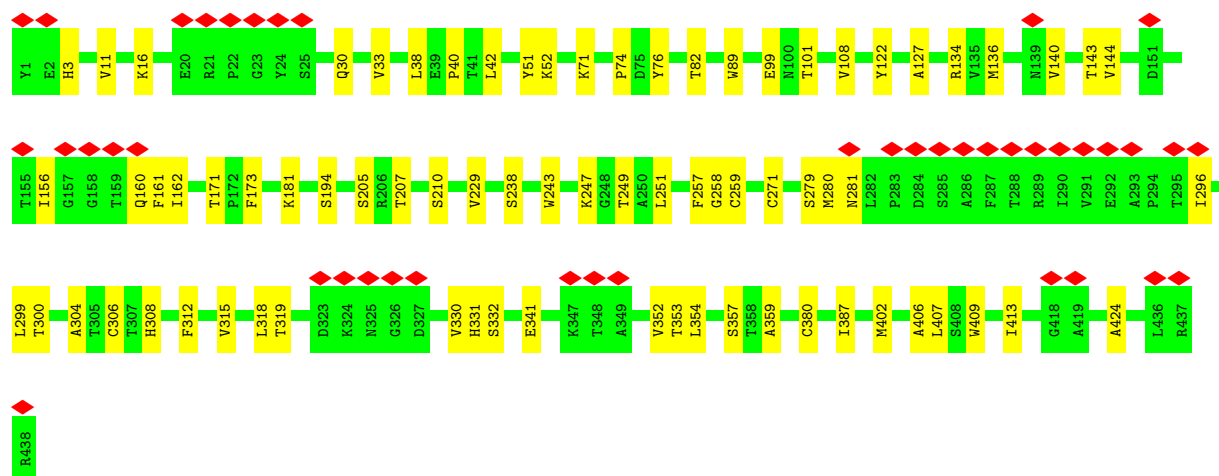
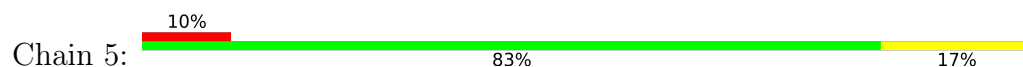
- Molecule 2: capsid protein, partial



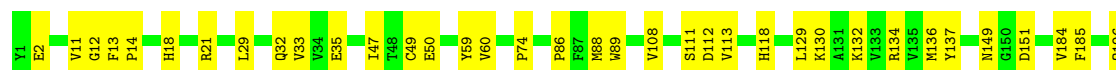
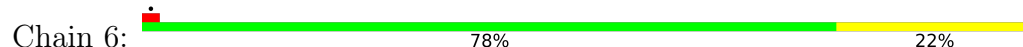
• Molecule 3: Spike glycoprotein E1

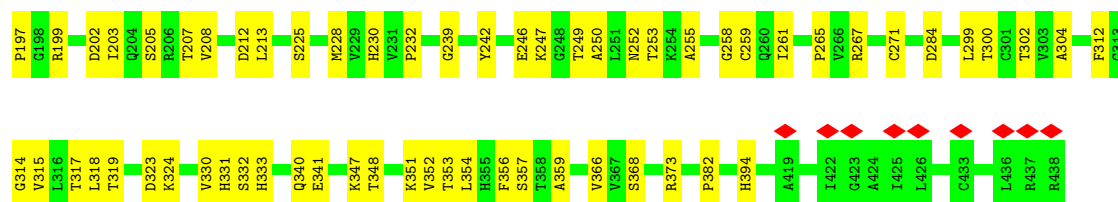


• Molecule 3: Spike glycoprotein E1

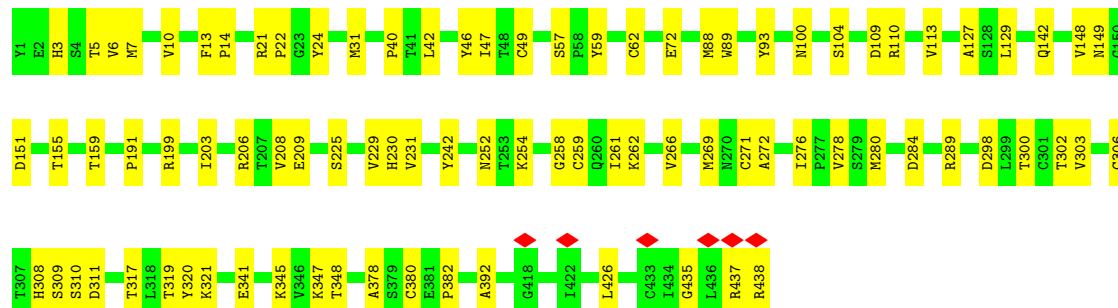
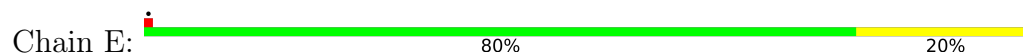


• Molecule 3: Spike glycoprotein E1

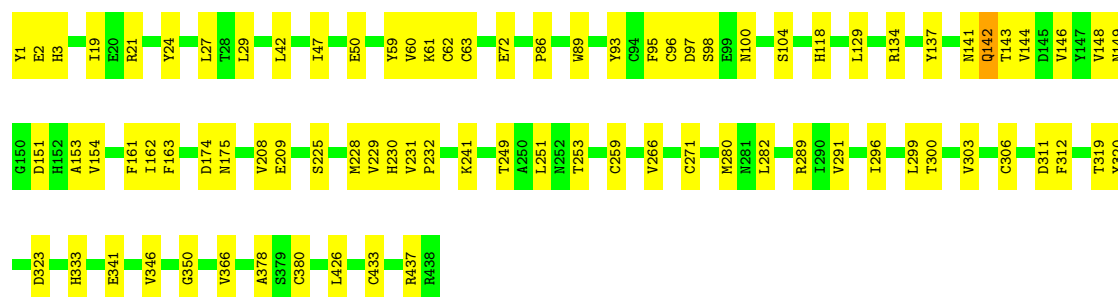
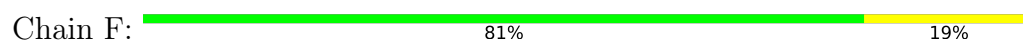




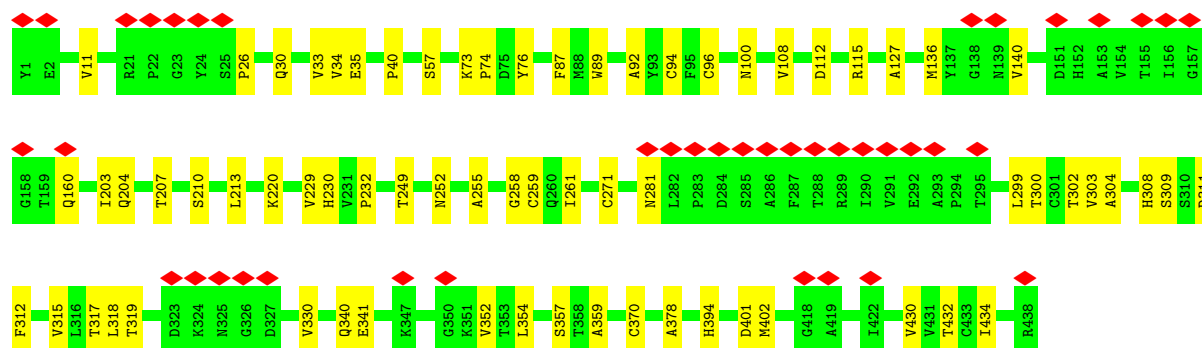
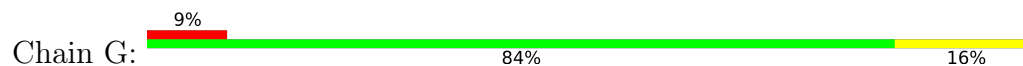
• Molecule 3: Spike glycoprotein E1



• Molecule 3: Spike glycoprotein E1

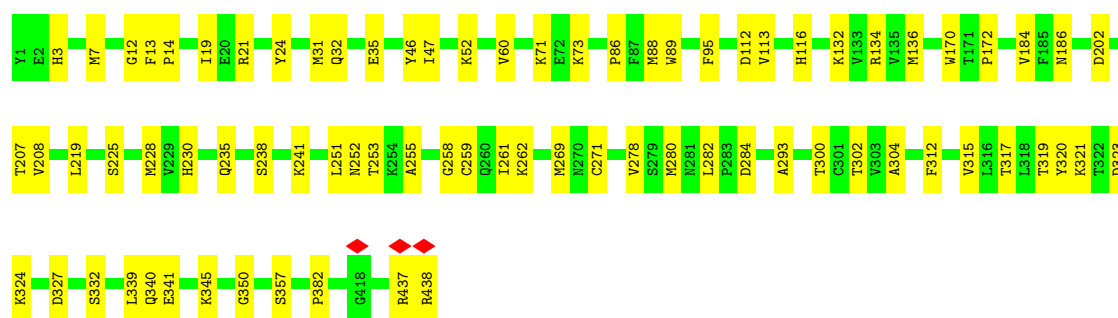


• Molecule 3: Spike glycoprotein E1



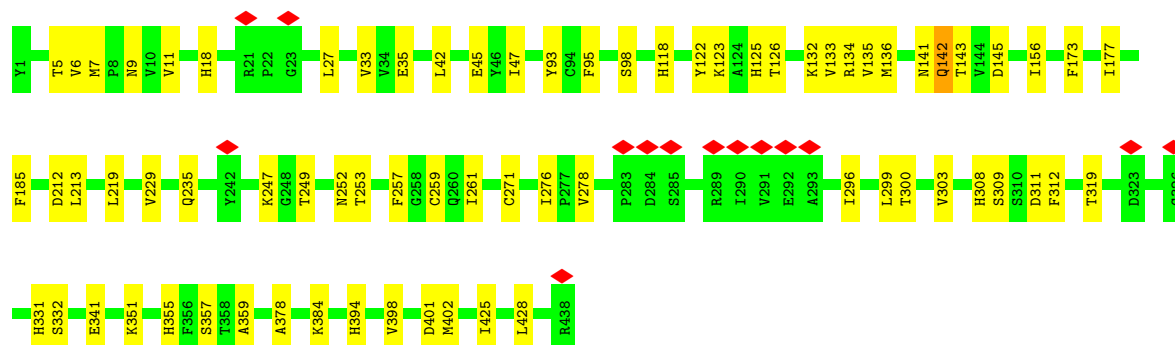
• Molecule 3: Spike glycoprotein E1

Chain H:  82% 18%



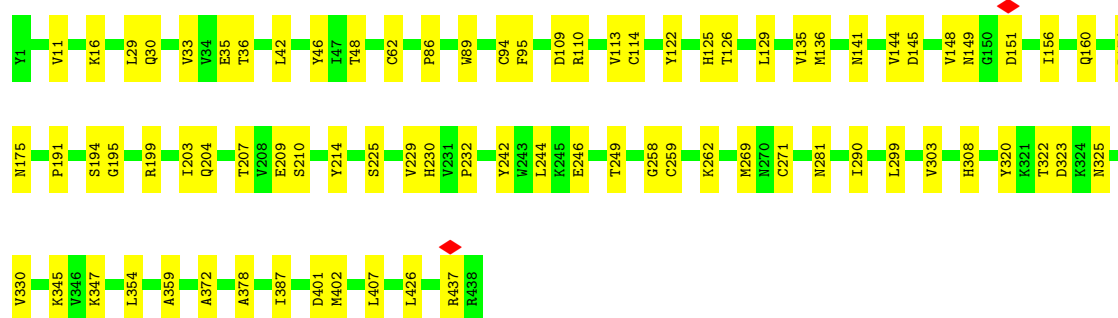
• Molecule 3: Spike glycoprotein E1

Chain U:  84% 16%



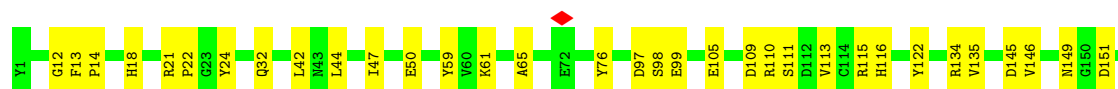
• Molecule 3: Spike glycoprotein E1

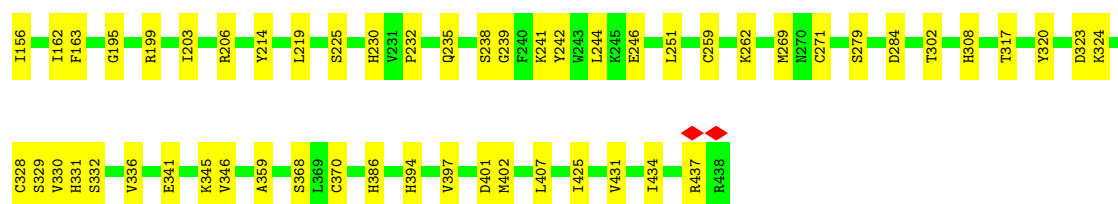
Chain V:  82% 18%



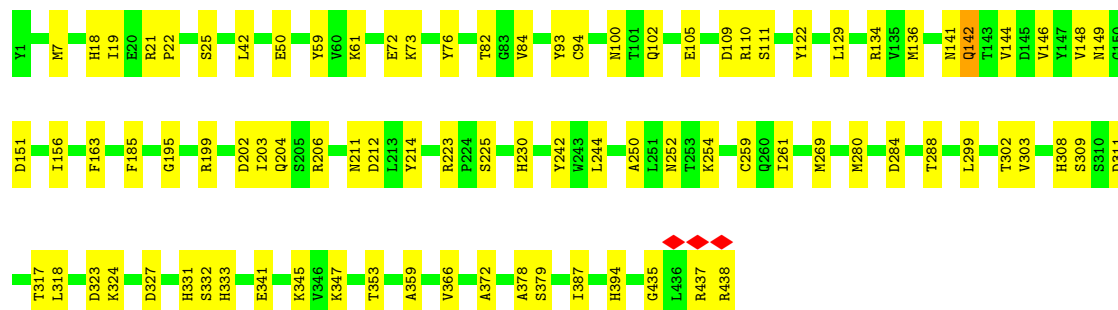
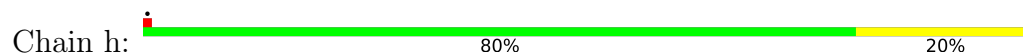
• Molecule 3: Spike glycoprotein E1

Chain W:  80% 20%

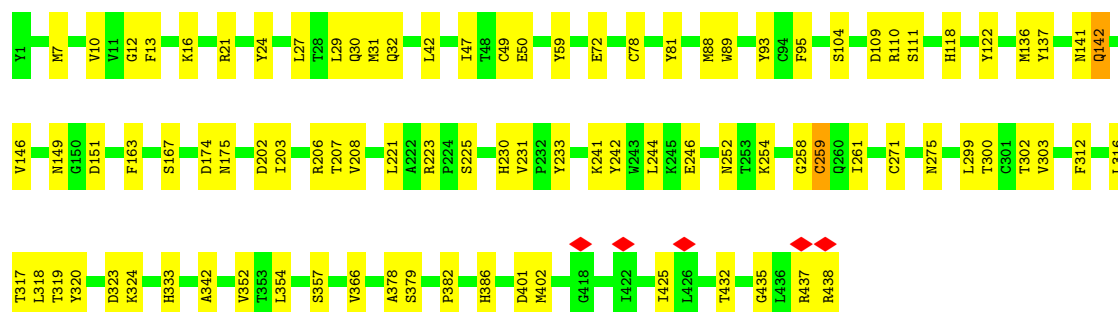




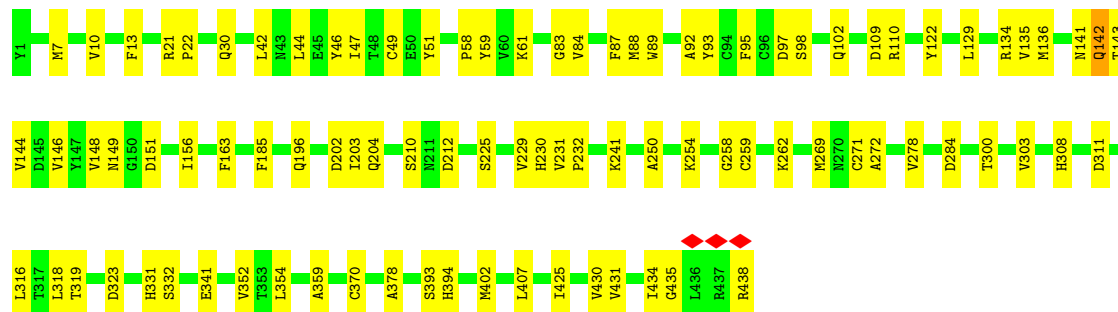
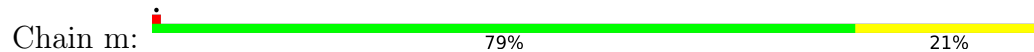
• Molecule 3: Spike glycoprotein E1



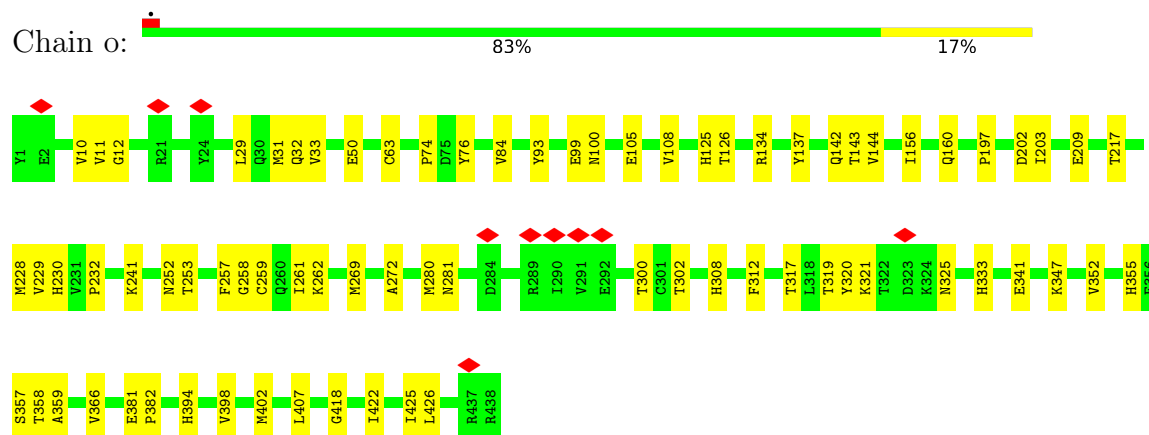
• Molecule 3: Spike glycoprotein E1



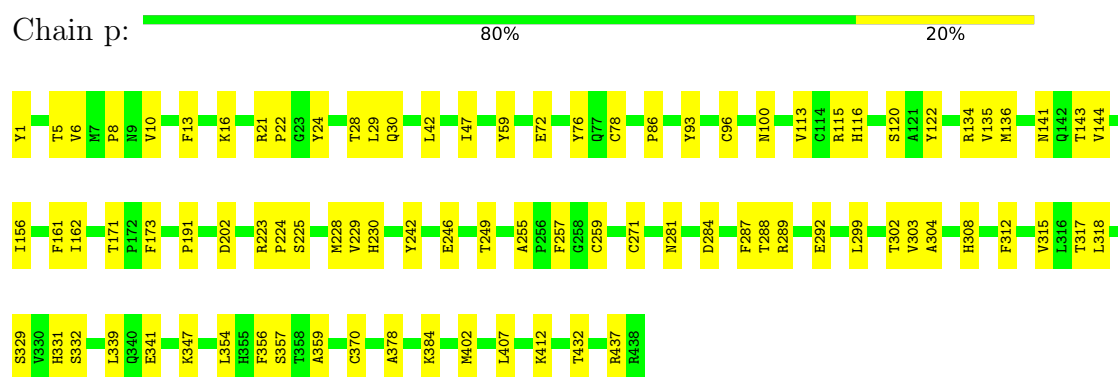
• Molecule 3: Spike glycoprotein E1



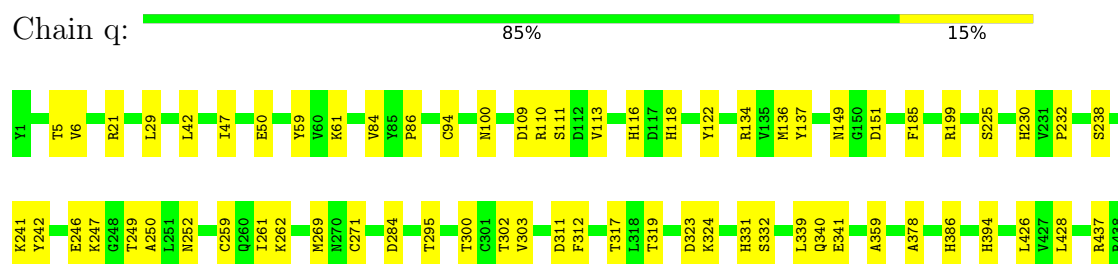
• Molecule 3: Spike glycoprotein E1



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• Molecule 3: Spike glycoprotein E1

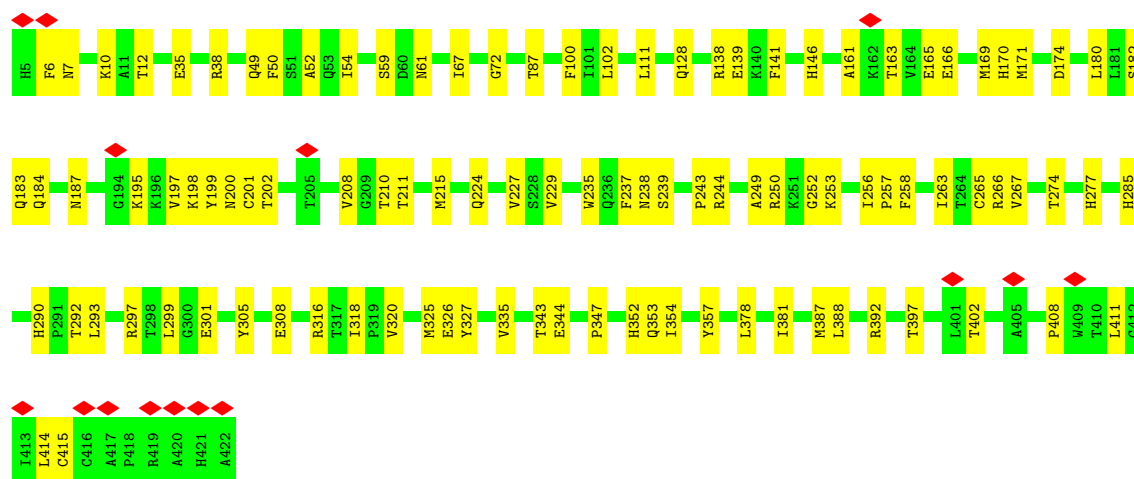
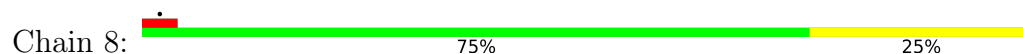


• Molecule 4: Spike glycoprotein E2





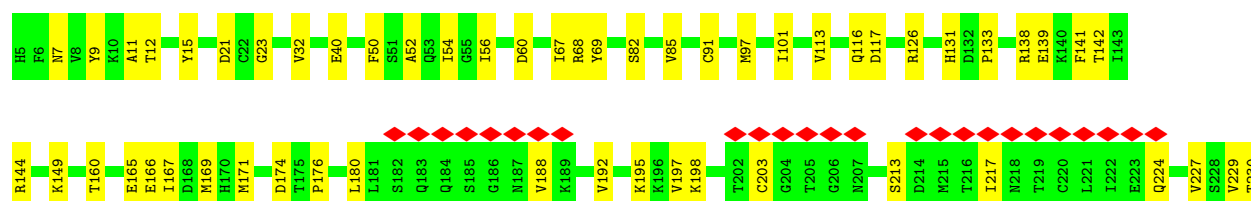
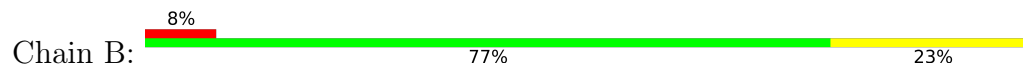
• Molecule 4: Spike glycoprotein E2

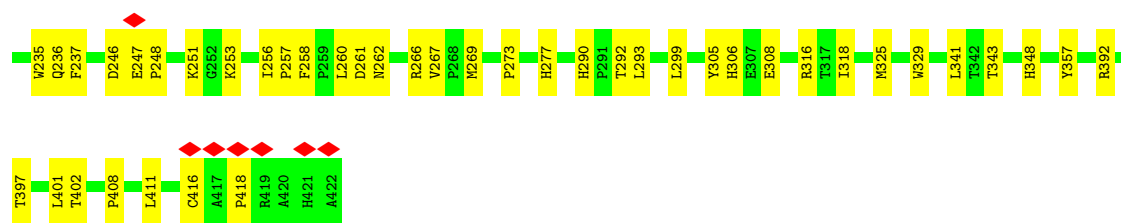


• Molecule 4: Spike glycoprotein E2



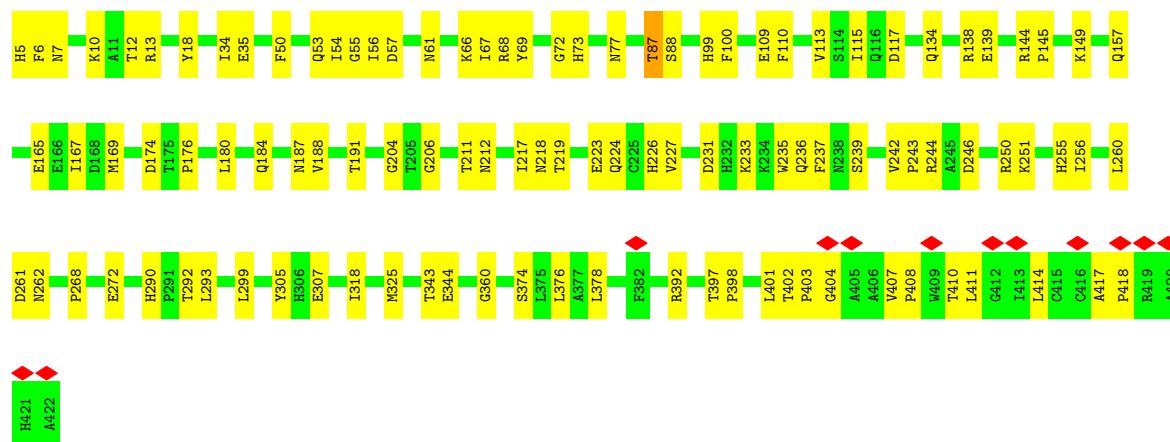
• Molecule 4: Spike glycoprotein E2





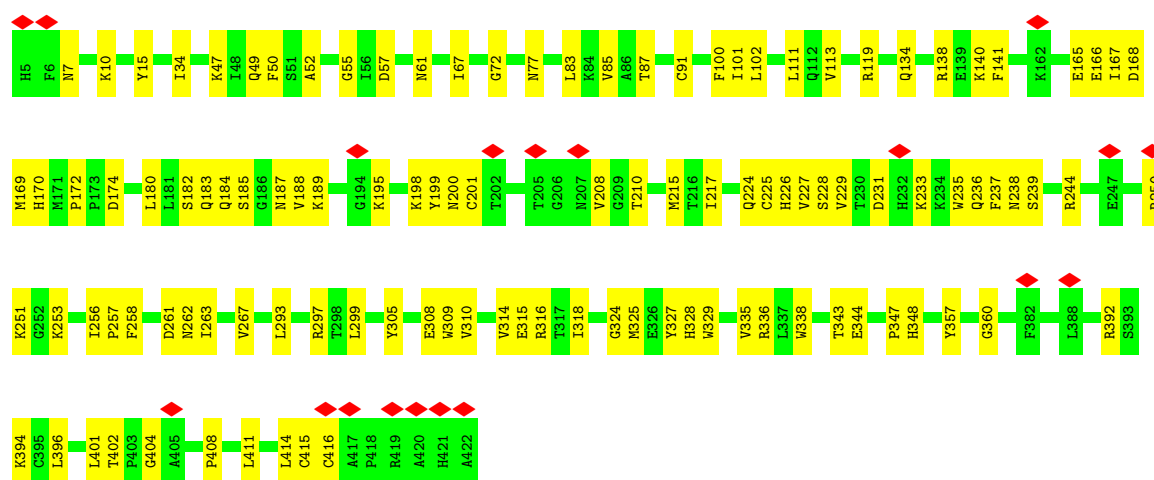
• Molecule 4: Spike glycoprotein E2

Chain I: 74% 25%



• Molecule 4: Spike glycoprotein E2

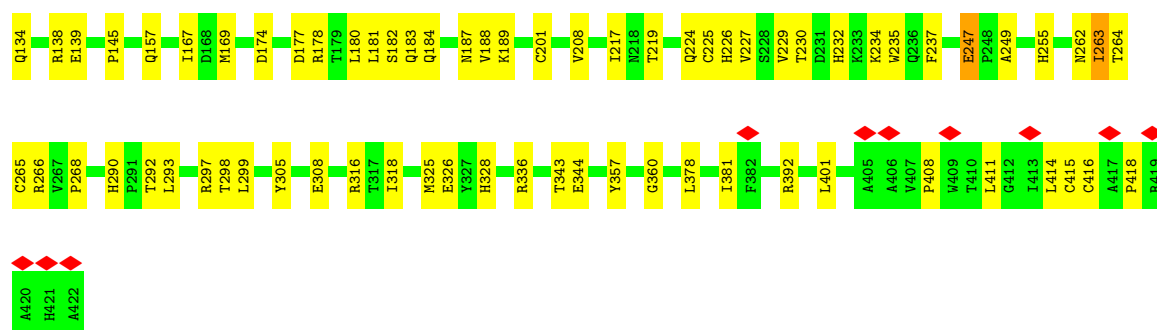
Chain J: 5% 73% 27%



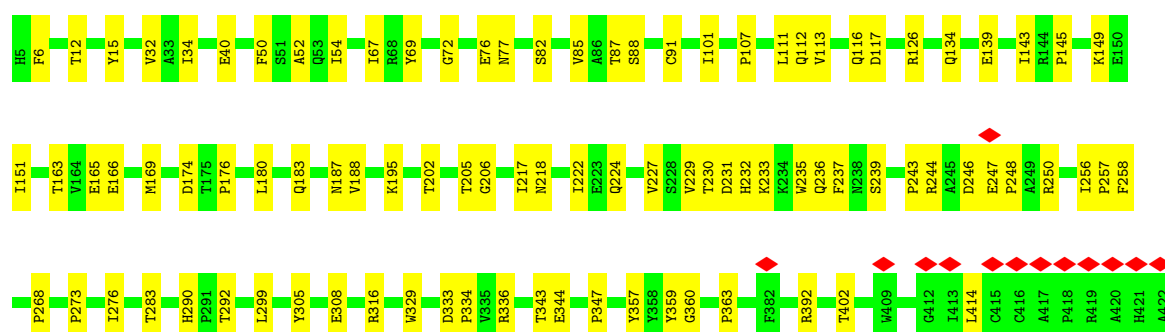
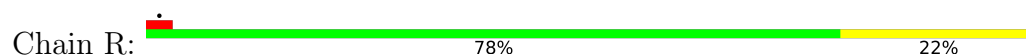
• Molecule 4: Spike glycoprotein E2

Chain K: 75% 24%

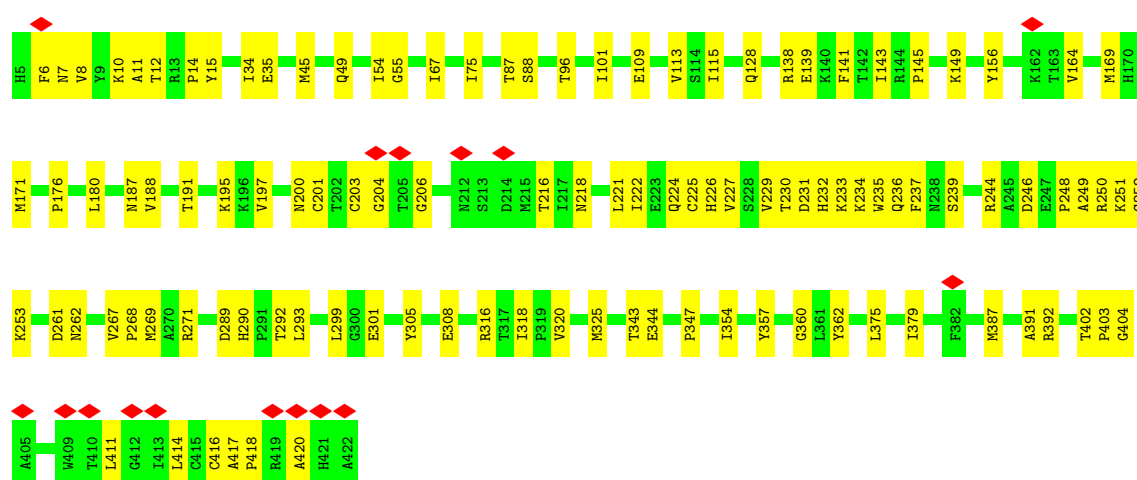




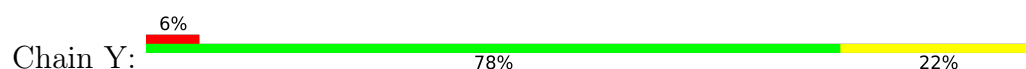
• Molecule 4: Spike glycoprotein E2

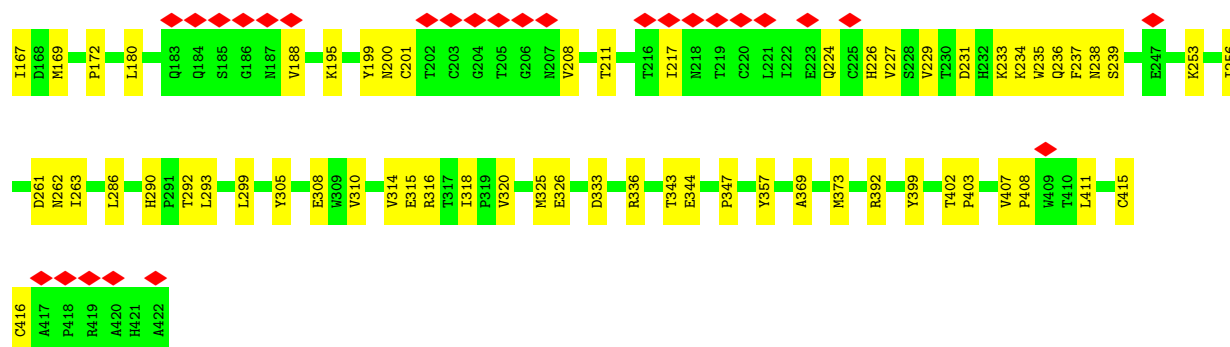


• Molecule 4: Spike glycoprotein E2

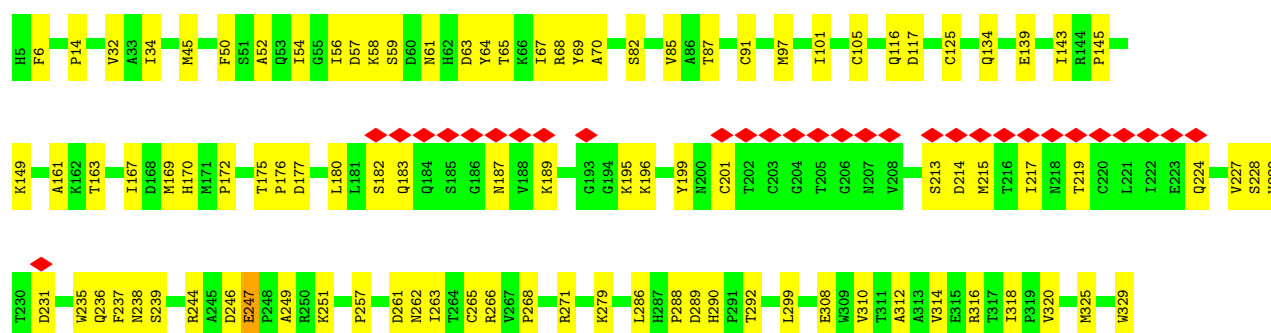
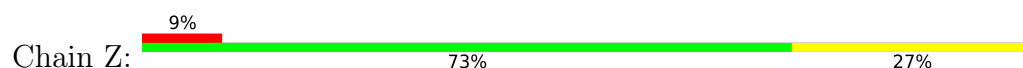


• Molecule 4: Spike glycoprotein E2

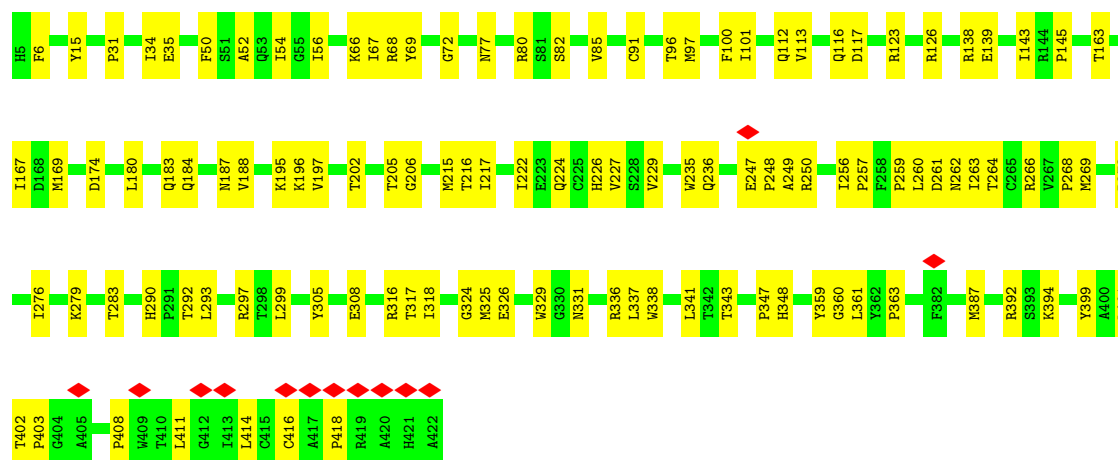




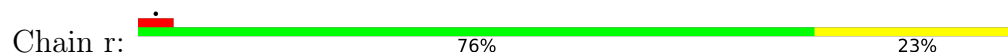
• Molecule 4: Spike glycoprotein E2

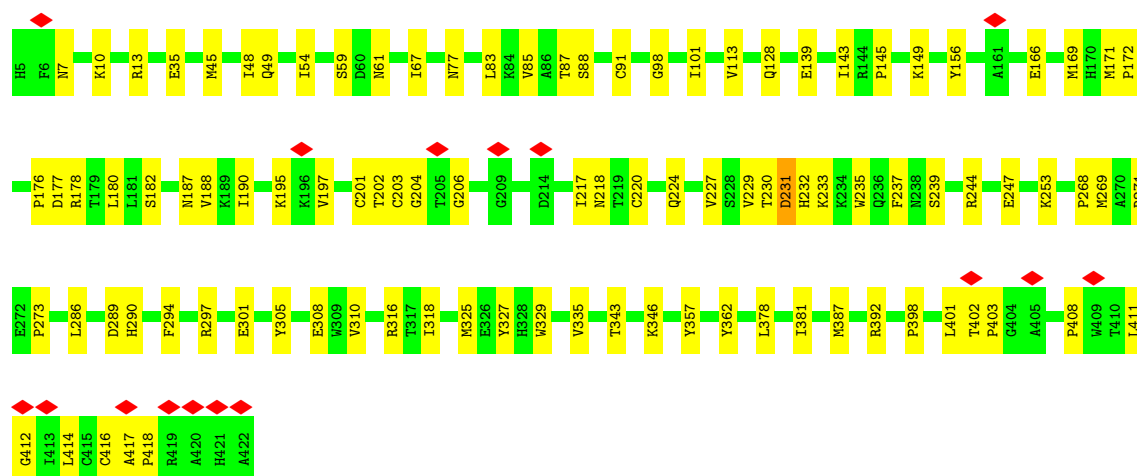


• Molecule 4: Spike glycoprotein E2

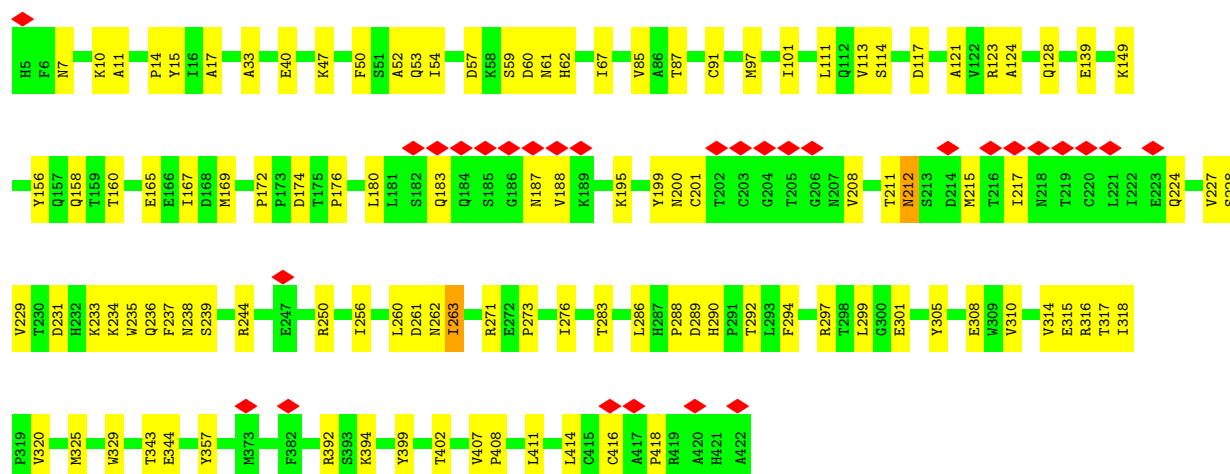


• Molecule 4: Spike glycoprotein E2

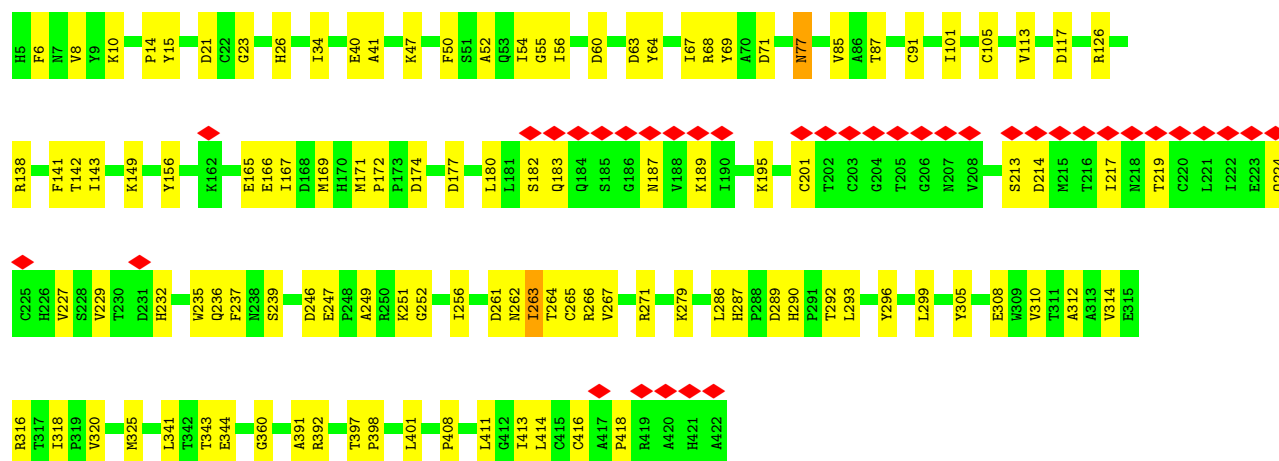




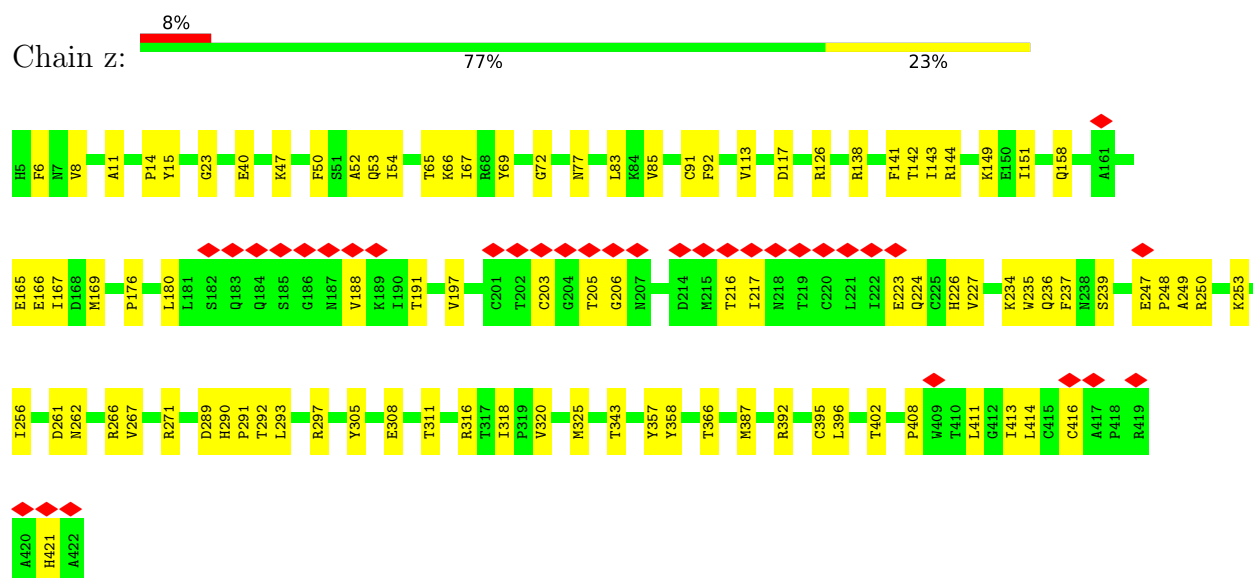
• Molecule 4: Spike glycoprotein E2



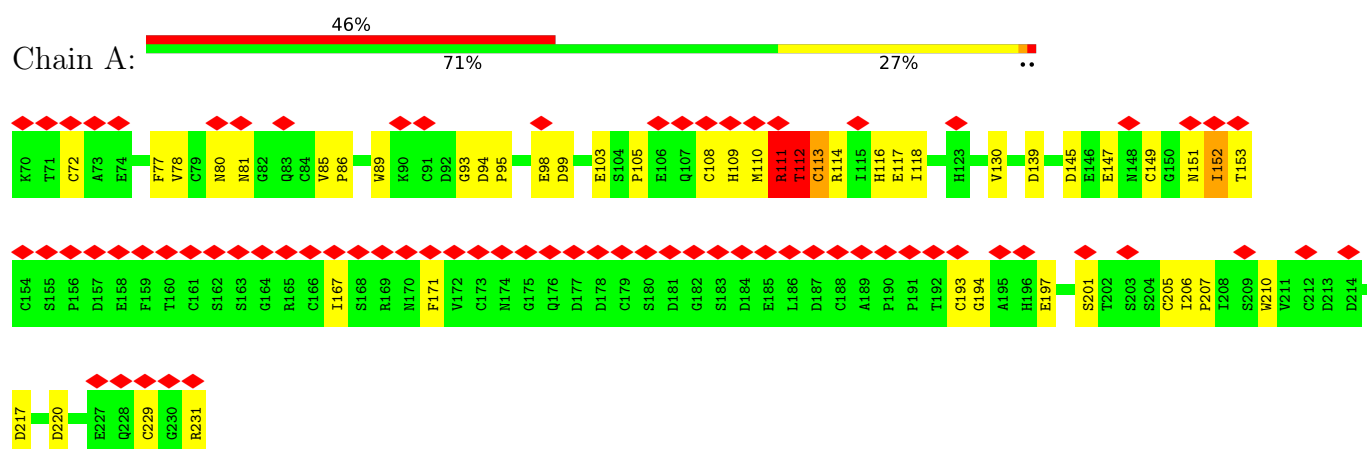
• Molecule 4: Spike glycoprotein E2



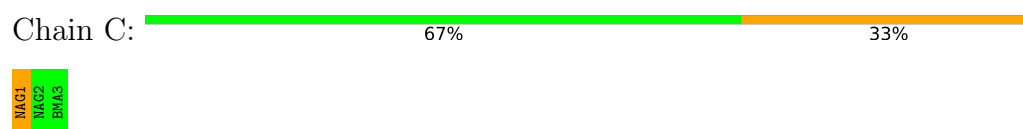
- Molecule 4: Spike glycoprotein E2



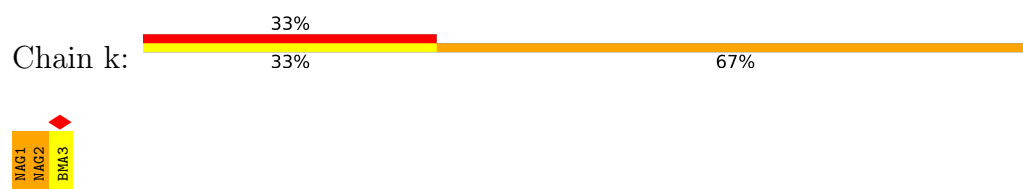
- Molecule 5: Very low-density lipoprotein receptor



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

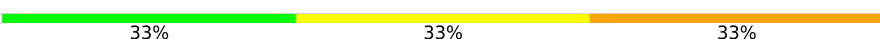


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:  33% 33% 67%

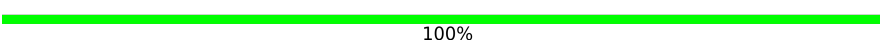


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA:  33% 33% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:  100%

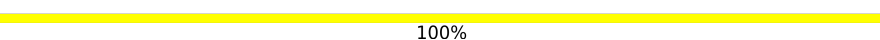


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:  33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:  100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:  33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:  100%

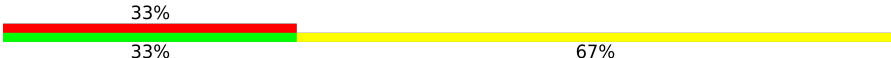


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:  67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA:  33% 33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KA:  33% 67% 33%

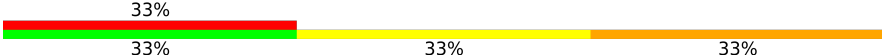


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LA:  33% 67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MA:  33% 33% 33% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aA: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain bA: 33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain cA: 33% 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain dA: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain eA: 33% 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fA: 67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

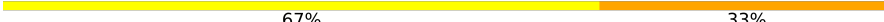


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain tA:  67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain uA:  33% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.827	Depositor
Minimum map value	-1.282	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, 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	0	0.19	0/413	0.37	0/563
1	2	0.17	0/413	0.38	0/563
1	AA	0.10	0/413	0.29	0/563
1	AB	0.21	0/413	0.42	0/563
1	L	0.21	0/413	0.40	0/563
1	M	0.10	0/413	0.28	0/563
1	N	0.18	0/413	0.43	0/563
1	S	0.17	0/413	0.38	0/563
1	a	0.12	0/413	0.31	0/563
1	b	0.16	0/413	0.32	0/563
1	c	0.17	0/413	0.38	0/563
1	g	0.17	0/413	0.41	0/563
1	l	0.21	0/413	0.41	0/563
1	u	0.11	0/413	0.30	0/563
1	v	0.21	0/413	0.42	0/563
1	w	0.17	0/413	0.40	0/563
2	1	0.25	0/1273	0.42	0/1714
2	3	0.25	0/1273	0.42	0/1714
2	AC	0.21	0/1273	0.38	0/1714
2	AD	0.18	0/1273	0.36	0/1714
2	AE	0.20	0/1273	0.43	0/1714
2	D	0.25	0/1273	0.42	0/1714
2	O	0.21	0/1273	0.38	0/1714
2	P	0.20	0/1273	0.40	0/1714
2	Q	0.19	0/1273	0.41	0/1714
2	T	0.19	0/1273	0.42	0/1714
2	d	0.20	0/1273	0.40	0/1714
2	e	0.26	0/1273	0.40	0/1714
2	f	0.25	0/1273	0.43	0/1714
2	n	0.26	0/1273	0.54	2/1714 (0.1%)
2	x	0.20	0/1273	0.38	0/1714
2	y	0.26	0/1273	0.39	0/1714

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	4	0.35	0/3416	0.46	1/4660 (0.0%)
3	5	0.27	0/3416	0.41	0/4660
3	6	0.35	0/3416	0.48	0/4660
3	E	0.35	0/3416	0.48	0/4660
3	F	0.36	0/3416	0.49	0/4660
3	G	0.26	0/3416	0.41	0/4660
3	H	0.35	0/3416	0.46	0/4660
3	U	0.28	0/3416	0.43	0/4660
3	V	0.33	0/3416	0.45	2/4660 (0.0%)
3	W	0.36	0/3416	0.47	0/4660
3	h	0.35	0/3416	0.49	0/4660
3	i	0.35	0/3416	0.49	1/4660 (0.0%)
3	m	0.35	0/3416	0.47	0/4660
3	o	0.28	0/3416	0.44	0/4660
3	p	0.33	0/3416	0.47	0/4660
3	q	0.36	0/3416	0.44	0/4660
4	7	0.32	0/3354	0.49	0/4574
4	8	0.30	0/3354	0.47	0/4574
4	9	0.32	0/3354	0.49	0/4574
4	B	0.32	0/3354	0.47	0/4574
4	I	0.31	0/3354	0.49	1/4574 (0.0%)
4	J	0.30	0/3354	0.47	0/4574
4	K	0.32	0/3354	0.51	0/4574
4	R	0.33	0/3354	0.51	0/4574
4	X	0.31	0/3354	0.48	0/4574
4	Y	0.32	0/3354	0.47	0/4574
4	Z	0.32	0/3354	0.49	0/4574
4	j	0.34	0/3354	0.49	1/4574 (0.0%)
4	r	0.30	0/3354	0.46	1/4574 (0.0%)
4	s	0.32	0/3354	0.48	0/4574
4	t	0.33	0/3354	0.49	0/4574
4	z	0.33	0/3354	0.48	0/4574
5	A	0.26	0/1226	0.48	0/1661
All	All	0.31	0/136522	0.46	9/185837 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	9	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	K	0	1
4	Z	0	1
4	t	0	1
5	A	0	1
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	189	PRO	CA-N-CD	-12.38	94.66	112.00
2	n	189	PRO	N-CD-CG	-6.63	93.26	103.20
3	4	249	THR	CB-CA-C	-6.48	108.08	115.79
4	r	398	PRO	CA-N-CD	-6.27	103.22	112.00
4	j	248	PRO	N-CD-CG	-5.65	94.72	103.20
3	i	259	CYS	CA-CB-SG	5.28	126.54	114.40
3	V	141	ASN	CA-C-N	-5.20	112.76	121.75
3	V	141	ASN	C-N-CA	-5.20	112.76	121.75
4	I	87	THR	N-CA-C	-5.01	101.78	108.34

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	9	247	GLU	Peptide
5	A	111	ARG	Sidechain
4	K	247	GLU	Peptide
4	Z	247	GLU	Peptide
4	t	247	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	404	0	377	14	0
1	2	404	0	377	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	404	0	377	10	0
1	AB	404	0	377	11	0
1	L	404	0	377	16	0
1	M	404	0	377	8	0
1	N	404	0	377	8	0
1	S	404	0	377	10	0
1	a	404	0	377	12	0
1	b	404	0	377	8	0
1	c	404	0	377	8	0
1	g	404	0	377	14	0
1	l	404	0	377	14	0
1	u	404	0	377	16	0
1	v	404	0	377	9	0
1	w	404	0	377	7	0
2	1	1245	0	1229	23	0
2	3	1245	0	1229	21	0
2	AC	1245	0	1229	40	0
2	AD	1245	0	1229	23	0
2	AE	1245	0	1229	40	0
2	D	1245	0	1229	33	0
2	O	1245	0	1229	30	0
2	P	1245	0	1229	30	0
2	Q	1245	0	1229	35	0
2	T	1245	0	1229	29	0
2	d	1245	0	1229	33	0
2	e	1245	0	1229	43	0
2	f	1245	0	1229	34	0
2	n	1245	0	1229	31	0
2	x	1245	0	1229	26	0
2	y	1245	0	1229	38	0
3	4	3330	0	3247	58	0
3	5	3330	0	3247	52	0
3	6	3330	0	3247	68	0
3	E	3330	0	3247	59	0
3	F	3330	0	3247	68	0
3	G	3330	0	3247	46	0
3	H	3330	0	3247	62	0
3	U	3330	0	3247	52	0
3	V	3330	0	3247	58	0
3	W	3330	0	3247	63	0
3	h	3330	0	3247	59	0
3	i	3330	0	3247	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	m	3330	0	3247	69	0
3	o	3330	0	3247	51	0
3	p	3330	0	3247	62	0
3	q	3330	0	3247	46	0
4	7	3260	0	3172	94	0
4	8	3260	0	3172	82	0
4	9	3260	0	3172	91	0
4	B	3260	0	3172	75	0
4	I	3260	0	3172	87	0
4	J	3260	0	3172	85	0
4	K	3260	0	3172	81	0
4	R	3260	0	3172	74	0
4	X	3260	0	3172	89	0
4	Y	3260	0	3172	77	0
4	Z	3260	0	3172	79	0
4	j	3260	0	3172	92	0
4	r	3260	0	3172	81	0
4	s	3260	0	3172	92	0
4	t	3260	0	3172	93	0
4	z	3260	0	3172	78	0
5	A	1205	0	1000	52	0
6	BA	39	0	34	6	0
6	C	39	0	34	1	0
6	CA	39	0	34	1	0
6	DA	39	0	34	0	0
6	EA	39	0	34	0	0
6	FA	39	0	34	2	0
6	GA	39	0	34	1	0
6	HA	39	0	34	0	0
6	IA	39	0	34	1	0
6	JA	39	0	34	1	0
6	KA	39	0	34	0	0
6	LA	39	0	34	0	0
6	MA	39	0	34	2	0
6	NA	39	0	34	3	0
6	OA	39	0	34	0	0
6	PA	39	0	34	2	0
6	QA	39	0	34	1	0
6	RA	39	0	34	1	0
6	SA	39	0	34	1	0
6	TA	39	0	34	3	0
6	UA	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	VA	39	0	34	1	0
6	WA	39	0	34	0	0
6	XA	39	0	34	1	0
6	YA	39	0	34	2	0
6	ZA	39	0	34	2	0
6	aA	39	0	34	0	0
6	bA	39	0	34	0	0
6	cA	39	0	34	0	0
6	dA	39	0	34	0	0
6	eA	39	0	34	0	0
6	fA	39	0	34	1	0
6	gA	39	0	34	1	0
6	hA	39	0	34	1	0
6	iA	39	0	34	3	0
6	jA	39	0	34	0	0
6	k	39	0	34	3	0
6	kA	39	0	34	2	0
6	lA	39	0	34	1	0
6	mA	39	0	34	3	0
6	nA	39	0	34	1	0
6	oA	39	0	34	0	0
6	pA	39	0	34	1	0
6	qA	39	0	34	0	0
6	rA	39	0	34	0	0
6	sA	39	0	34	0	0
6	tA	39	0	34	2	0
6	uA	39	0	34	0	0
All	All	134901	0	131032	2759	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 10.

All (2759) 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)
5:A:105:PRO:HB3	5:A:110:MET:HA	1.30	1.13
5:A:95:PRO:HA	5:A:111:ARG:HG3	1.35	1.06
4:t:177:ASP:O	4:t:227:VAL:HB	1.65	0.97
4:r:392:ARG:HG3	4:r:414:LEU:HD21	1.54	0.90
2:AE:140:VAL:HG23	2:AE:173:ILE:HG22	1.55	0.88
3:m:258:GLY:HA2	4:z:297:ARG:HH12	1.38	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:157:GLN:HE22	4:7:261:ASP:HB2	1.42	0.85
2:d:140:VAL:HG23	2:d:173:ILE:HG22	1.58	0.85
4:Z:180:LEU:HD12	4:Z:227:VAL:HG11	1.59	0.84
3:q:84:VAL:HG12	3:q:86:PRO:HD3	1.59	0.84
4:R:180:LEU:HD12	4:R:227:VAL:HG11	1.60	0.83
5:A:94:ASP:OD2	3:V:345:LYS:NZ	2.12	0.82
3:F:311:ASP:OD1	3:F:312:PHE:N	2.13	0.82
4:K:177:ASP:O	4:K:227:VAL:HB	1.79	0.82
2:3:140:VAL:HG23	2:3:173:ILE:HG22	1.61	0.82
4:z:85:VAL:HG12	4:z:113:VAL:HG12	1.63	0.81
4:Z:261:ASP:OD1	4:Z:262:ASN:N	2.14	0.81
2:AE:252:ASN:OD1	2:AE:253:LYS:N	2.12	0.81
3:F:1:TYR:HB2	3:F:21:ARG:HH11	1.45	0.80
5:A:105:PRO:CB	5:A:110:MET:HA	2.09	0.80
4:J:169:MET:HB3	4:J:235:TRP:HB3	1.62	0.80
4:I:246:ASP:OD2	4:I:250:ARG:NH1	2.14	0.80
2:x:252:ASN:OD1	2:x:253:LYS:N	2.14	0.80
2:3:255:MET:HE1	3:m:438:ARG:HD3	1.64	0.79
3:E:21:ARG:NH1	3:E:284:ASP:OD1	2.14	0.79
3:H:134:ARG:HH22	6:NA:1:NAG:H5	1.48	0.79
4:9:69:TYR:OH	4:9:117:ASP:OD1	2.00	0.79
5:A:95:PRO:CA	5:A:111:ARG:HG3	2.13	0.79
4:Y:308:GLU:OE1	4:Y:316:ARG:NH1	2.16	0.79
4:Z:180:LEU:HB2	4:Z:227:VAL:HG21	1.65	0.79
4:Z:57:ASP:OD1	4:Z:58:LYS:N	2.14	0.78
4:j:283:THR:HG22	4:j:317:THR:HG22	1.66	0.78
4:J:392:ARG:HG2	4:J:414:LEU:HD12	1.63	0.78
5:A:103:GLU:HB2	5:A:111:ARG:HG2	1.65	0.78
3:U:45:GLU:OE2	3:U:123:LYS:NZ	2.17	0.78
2:f:212:GLY:HA2	2:f:244:THR:HG23	1.66	0.78
4:I:87:THR:HG22	4:I:88:SER:H	1.48	0.78
2:y:210:PRO:HA	2:y:243:ARG:HE	1.48	0.78
2:y:209:ILE:HG12	2:y:246:LEU:HD11	1.64	0.78
2:AD:210:PRO:HA	2:AD:243:ARG:HE	1.46	0.78
2:O:140:VAL:HG23	2:O:173:ILE:HG22	1.66	0.78
2:O:210:PRO:HA	2:O:243:ARG:HE	1.49	0.78
4:8:318:ILE:HD12	4:8:325:MET:HE1	1.66	0.78
2:f:140:VAL:HG23	2:f:173:ILE:HG22	1.64	0.78
4:s:283:THR:HG22	4:s:317:THR:HG22	1.65	0.78
2:e:136:VAL:HG11	2:e:251:TRP:HH2	1.47	0.77
4:s:7:ASN:HB2	4:s:10:LYS:HE2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:140:VAL:HG23	2:Q:173:ILE:HG22	1.66	0.77
4:X:87:THR:HG22	4:X:88:SER:H	1.49	0.77
3:i:259:CYS:HB3	3:i:271:CYS:HA	1.67	0.77
4:9:109:GLU:HG2	4:t:142:THR:HG21	1.65	0.77
4:R:392:ARG:HG3	4:R:414:LEU:HD21	1.67	0.77
3:V:113:VAL:HG21	4:Y:40:GLU:HG3	1.67	0.77
3:H:21:ARG:NH2	3:H:284:ASP:OD1	2.18	0.77
3:H:136:MET:HE1	6:NA:1:NAG:H82	1.65	0.76
2:1:140:VAL:HG23	2:1:173:ILE:HG22	1.66	0.76
2:n:189:PRO:O	2:n:189:PRO:HD2	1.85	0.76
5:A:112:THR:O	5:A:113:CYS:HB2	1.85	0.76
5:A:139:ASP:N	5:A:145:ASP:OD2	2.19	0.76
2:P:210:PRO:HA	2:P:243:ARG:HE	1.49	0.76
4:9:177:ASP:O	4:9:227:VAL:HB	1.86	0.76
2:AD:140:VAL:HG23	2:AD:173:ILE:HG22	1.67	0.76
4:K:87:THR:HG22	4:K:88:SER:H	1.51	0.75
4:K:145:PRO:HG3	4:K:268:PRO:HB3	1.68	0.75
1:b:11:LEU:HD12	1:b:38:MET:HG3	1.66	0.75
3:F:29:LEU:HD11	3:F:280:MET:HE1	1.68	0.75
3:5:330:VAL:HG21	3:5:354:LEU:HD21	1.68	0.75
4:B:85:VAL:HG12	4:B:113:VAL:HG12	1.68	0.75
4:R:54:ILE:HG22	4:R:67:ILE:HG23	1.68	0.75
3:m:435:GLY:HA2	3:m:438:ARG:HD2	1.67	0.75
2:AC:210:PRO:HA	2:AC:243:ARG:HE	1.52	0.74
1:AB:38:MET:O	1:AB:42:ASN:ND2	2.21	0.74
2:n:235:LEU:HD11	2:n:249:VAL:HG13	1.69	0.74
5:A:93:GLY:HA2	5:A:109:HIS:CG	2.23	0.74
4:Y:97:MET:HE1	4:Y:160:THR:HG21	1.68	0.74
3:m:259:CYS:HB3	3:m:271:CYS:HA	1.69	0.74
2:P:135:LEU:HD21	2:P:177:MET:HE2	1.70	0.74
2:d:218:ASP:HA	2:d:221:ARG:HH12	1.51	0.74
4:r:85:VAL:HG12	4:r:113:VAL:HG12	1.69	0.73
4:B:50:PHE:HB3	4:B:52:ALA:H	1.53	0.73
4:B:180:LEU:HD12	4:B:227:VAL:HG11	1.69	0.73
3:F:174:ASP:OD1	3:F:175:ASN:N	2.19	0.73
4:K:263:ILE:HG13	4:K:264:THR:H	1.53	0.73
3:E:300:THR:OG1	3:E:319:THR:OG1	2.06	0.73
2:AE:239:ASN:HA	2:AE:244:THR:HG22	1.71	0.73
4:s:308:GLU:OE1	4:s:316:ARG:NH1	2.22	0.73
4:z:15:TYR:HB2	4:z:236:GLN:HE21	1.54	0.73
4:r:235:TRP:NE1	1:u:40:GLU:OE2	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:97:MET:HE3	4:Z:257:PRO:HB3	1.71	0.72
2:e:162:LYS:NZ	2:e:169:GLU:OE2	2.18	0.72
4:j:318:ILE:HD12	4:j:325:MET:HE1	1.70	0.72
2:P:209:ILE:HB	2:P:244:THR:HB	1.70	0.72
2:AC:140:VAL:HG23	2:AC:173:ILE:HG22	1.69	0.72
4:K:180:LEU:HB2	4:K:227:VAL:HG21	1.71	0.72
4:Z:408:PRO:HA	4:Z:411:LEU:HB3	1.71	0.72
2:x:201:GLN:HE22	2:x:203:SER:HB2	1.55	0.72
4:z:50:PHE:HB3	4:z:52:ALA:H	1.54	0.72
4:Z:50:PHE:CZ	4:Z:101:ILE:HD11	2.25	0.72
3:p:259:CYS:HB3	3:p:271:CYS:HA	1.72	0.72
4:j:85:VAL:HG12	4:j:113:VAL:HG12	1.71	0.72
4:8:139:GLU:HG2	4:8:292:THR:HG22	1.71	0.72
1:c:38:MET:O	1:c:42:ASN:ND2	2.22	0.72
3:m:254:LYS:HG3	4:z:305:TYR:CE1	2.25	0.72
4:9:392:ARG:NH1	4:9:415:CYS:O	2.23	0.71
1:0:9:CYS:N	1:0:18:CYS:SG	2.62	0.71
3:6:89:TRP:CH2	4:9:72:GLY:HA2	2.24	0.71
3:q:199:ARG:NH1	3:q:246:GLU:OE2	2.22	0.71
4:r:180:LEU:HD13	4:r:227:VAL:HG11	1.71	0.71
4:K:180:LEU:HD12	4:K:227:VAL:HG11	1.71	0.71
4:j:180:LEU:HD12	4:j:227:VAL:HG11	1.71	0.71
4:s:180:LEU:HD11	4:s:227:VAL:HG11	1.72	0.71
4:s:392:ARG:HH21	4:s:416:CYS:HA	1.55	0.71
3:W:21:ARG:HG3	3:W:22:PRO:HD2	1.72	0.71
3:H:300:THR:OG1	3:H:319:THR:OG1	2.08	0.71
2:AC:139:LYS:HG3	2:AC:141:MET:HE3	1.73	0.71
4:j:6:PHE:CE1	1:l:53:GLN:HA	2.25	0.71
3:p:135:VAL:HG11	3:p:156:ILE:HD13	1.71	0.71
4:I:392:ARG:HG3	4:I:414:LEU:HD21	1.73	0.71
2:n:140:VAL:HG23	2:n:173:ILE:HG22	1.72	0.71
3:5:300:THR:OG1	3:5:319:THR:OG1	2.09	0.71
3:F:259:CYS:HB3	3:F:271:CYS:HA	1.72	0.71
4:I:55:GLY:H	4:I:67:ILE:HG22	1.55	0.71
4:R:230:THR:HG22	4:R:232:HIS:HE1	1.56	0.70
2:T:235:LEU:HD11	2:T:249:VAL:HG23	1.73	0.70
4:7:187:ASN:HB3	4:7:218:ASN:HA	1.73	0.70
4:J:318:ILE:HD12	4:J:325:MET:HE1	1.72	0.70
4:B:50:PHE:CZ	4:B:101:ILE:HD11	2.26	0.70
4:B:308:GLU:OE2	4:B:316:ARG:NH1	2.25	0.70
3:H:259:CYS:HB3	3:H:271:CYS:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:392:ARG:NH1	4:J:415:CYS:O	2.24	0.70
3:m:95:PHE:HD1	4:z:226:HIS:HE2	1.39	0.70
2:AE:116:GLU:O	2:AE:120:ILE:HB	1.91	0.70
3:G:304:ALA:HB3	3:G:315:VAL:HG13	1.73	0.70
3:G:302:THR:HG1	3:G:317:THR:HG1	1.38	0.70
4:s:212:ASN:O	4:s:212:ASN:ND2	2.23	0.70
3:E:435:GLY:HA2	3:E:438:ARG:HD2	1.74	0.70
4:I:401:LEU:O	2:O:139:LYS:NZ	2.24	0.70
3:q:136:MET:HE1	6:mA:1:NAG:H82	1.71	0.70
1:u:38:MET:O	1:u:42:ASN:ND2	2.25	0.70
3:6:304:ALA:HB3	3:6:315:VAL:HG23	1.74	0.69
4:B:54:ILE:HG22	4:B:67:ILE:HG23	1.72	0.69
3:m:93:TYR:HB3	4:z:176:PRO:HG3	1.73	0.69
2:n:234:VAL:HA	2:n:248:VAL:HG12	1.73	0.69
2:e:196:HIS:CG	2:e:221:ARG:HH21	2.10	0.69
4:r:233:LYS:HZ1	1:u:32:ALA:HB3	1.57	0.69
1:w:38:MET:O	1:w:42:ASN:ND2	2.25	0.69
3:i:254:LYS:HG3	4:j:305:TYR:CZ	2.28	0.69
4:7:54:ILE:HG23	4:7:67:ILE:HG21	1.75	0.69
4:9:308:GLU:OE1	4:9:316:ARG:NH1	2.26	0.69
4:9:263:ILE:HG13	4:9:264:THR:H	1.58	0.69
3:q:300:THR:OG1	3:q:319:THR:OG1	2.10	0.69
3:4:259:CYS:HB3	3:4:271:CYS:HA	1.73	0.69
4:7:408:PRO:HA	4:7:411:LEU:HB3	1.74	0.69
2:P:140:VAL:HG23	2:P:173:ILE:HG22	1.75	0.69
3:i:47:ILE:HD11	3:i:118:HIS:CG	2.28	0.69
3:i:95:PHE:HD1	4:j:226:HIS:HE2	1.40	0.69
3:m:300:THR:OG1	3:m:319:THR:OG1	2.11	0.69
3:o:381:GLU:OE1	4:r:346:LYS:NZ	2.26	0.68
4:7:139:GLU:OE2	4:7:290:HIS:NE2	2.26	0.68
4:R:195:LYS:HB3	4:R:229:VAL:HG13	1.76	0.68
4:Y:392:ARG:NH2	4:Y:416:CYS:HA	2.08	0.68
4:9:183:GLN:NE2	4:9:187:ASN:O	2.27	0.68
1:L:38:MET:O	1:L:42:ASN:ND2	2.26	0.68
4:X:54:ILE:HG22	4:X:67:ILE:HD12	1.76	0.68
2:e:141:MET:HE1	2:e:168:LEU:HD21	1.75	0.68
2:y:140:VAL:HG23	2:y:173:ILE:HG22	1.76	0.68
4:z:85:VAL:HG23	4:z:91:CYS:HB2	1.75	0.68
3:p:59:TYR:HB2	4:s:244:ARG:HH21	1.58	0.68
3:5:304:ALA:HB3	3:5:315:VAL:HG13	1.75	0.68
4:R:85:VAL:HG12	4:R:113:VAL:HG12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:40:GLU:HG3	4:7:235:TRP:HZ2	1.59	0.68
4:t:320:VAL:HG12	4:t:325:MET:HG2	1.75	0.68
4:9:180:LEU:HB2	4:9:227:VAL:HG21	1.75	0.67
4:j:139:GLU:HG3	4:j:292:THR:HG22	1.77	0.67
3:6:259:CYS:HB3	3:6:271:CYS:HA	1.74	0.67
4:J:180:LEU:HD12	4:J:227:VAL:HG11	1.74	0.67
2:AD:126:GLU:O	2:AD:128:LYS:NZ	2.27	0.67
4:Y:172:PRO:HB3	4:Y:236:GLN:HE21	1.58	0.67
1:v:26:CYS:HB3	1:v:29:GLU:HB2	1.76	0.67
2:y:124:LYS:HE3	2:y:127:GLY:HA2	1.75	0.67
4:I:188:VAL:HG22	4:I:217:ILE:HG22	1.76	0.67
4:K:308:GLU:OE1	4:K:316:ARG:NH1	2.27	0.67
4:z:308:GLU:OE2	4:z:316:ARG:NH1	2.27	0.67
4:z:318:ILE:HD12	4:z:325:MET:HE1	1.76	0.67
5:A:201:SER:OG	5:A:220:ASP:OD2	2.13	0.67
2:AE:213:ALA:O	2:AE:215:LYS:NZ	2.28	0.67
4:8:392:ARG:HG2	4:8:414:LEU:HD12	1.76	0.67
1:AB:9:CYS:N	1:AB:18:CYS:SG	2.68	0.67
3:E:302:THR:HG1	3:E:317:THR:HG1	1.41	0.67
4:R:202:THR:O	4:R:224:GLN:NE2	2.27	0.67
2:D:255:MET:HE1	3:h:438:ARG:HD3	1.77	0.67
3:5:259:CYS:HB3	3:5:271:CYS:HA	1.75	0.67
4:K:183:GLN:NE2	4:K:187:ASN:O	2.28	0.67
3:p:304:ALA:HB3	3:p:315:VAL:HG13	1.76	0.67
4:t:169:MET:HE2	4:t:235:TRP:HB3	1.75	0.67
3:F:59:TYR:CE1	3:F:61:LYS:HB2	2.30	0.66
3:6:136:MET:HE1	6:BA:1:NAG:H82	1.77	0.66
4:R:188:VAL:HG22	4:R:217:ILE:HG12	1.76	0.66
3:o:312:PHE:HA	3:o:357:SER:HB2	1.78	0.66
3:4:304:ALA:HB3	3:4:315:VAL:HG13	1.76	0.66
2:f:210:PRO:HA	2:f:243:ARG:HE	1.61	0.66
4:t:263:ILE:HG13	4:t:264:THR:H	1.59	0.66
2:D:259:VAL:HG12	2:D:261:PRO:HD3	1.75	0.66
4:I:53:GLN:OE1	4:I:99:HIS:NE2	2.27	0.66
4:I:233:LYS:HE3	1:L:32:ALA:HB3	1.76	0.66
4:t:50:PHE:CZ	4:t:101:ILE:HD11	2.30	0.66
4:B:69:TYR:OH	4:B:117:ASP:OD1	2.10	0.66
2:f:173:ILE:HD11	2:f:178:ARG:HH11	1.58	0.66
4:s:50:PHE:HB3	4:s:52:ALA:H	1.60	0.66
4:7:349:GLY:H	4:7:354:ILE:HD11	1.59	0.66
2:T:247:SER:HB2	2:T:261:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:300:THR:OG1	3:F:319:THR:OG1	2.12	0.66
3:W:259:CYS:HB3	3:W:271:CYS:HA	1.77	0.66
2:n:189:PRO:O	2:n:193:TYR:OH	2.11	0.66
4:7:34:ILE:HD11	4:7:113:VAL:HG22	1.77	0.66
4:j:69:TYR:OH	4:j:117:ASP:OD1	2.04	0.66
4:Z:392:ARG:NH1	4:Z:415:CYS:O	2.29	0.66
4:R:235:TRP:NE1	1:g:40:GLU:OE2	2.26	0.65
3:o:300:THR:OG1	3:o:319:THR:OG1	2.14	0.65
4:s:7:ASN:OD1	4:s:62:HIS:NE2	2.28	0.65
2:x:247:SER:HB2	2:x:261:PRO:HD2	1.78	0.65
2:3:210:PRO:HA	2:3:243:ARG:HE	1.60	0.65
2:AE:188:LYS:HE3	2:AE:231:VAL:HG13	1.78	0.65
3:o:50:GLU:OE2	3:o:241:LYS:HE2	1.97	0.65
5:A:105:PRO:HG3	5:A:111:ARG:H	1.62	0.65
4:7:403:PRO:HD3	2:AC:139:LYS:NZ	2.11	0.65
4:8:195:LYS:HB3	4:8:229:VAL:HG13	1.77	0.65
4:8:297:ARG:NH1	4:8:326:GLU:OE2	2.29	0.65
2:AE:252:ASN:HB3	2:AE:255:MET:HB3	1.79	0.65
3:E:254:LYS:HG3	4:R:305:TYR:CE1	2.31	0.65
3:E:320:TYR:OH	3:E:347:LYS:O	2.11	0.65
2:x:234:VAL:HA	2:x:248:VAL:HG12	1.79	0.65
4:8:139:GLU:OE1	4:8:290:HIS:NE2	2.29	0.65
4:K:34:ILE:HD11	4:K:113:VAL:HG22	1.79	0.65
2:e:140:VAL:HG23	2:e:173:ILE:HG22	1.77	0.65
4:9:14:PRO:HD3	4:9:68:ARG:HH21	1.61	0.65
3:p:21:ARG:HE	3:p:287:PHE:HE2	1.44	0.65
2:AD:252:ASN:OD1	2:AD:253:LYS:HD2	1.97	0.65
4:K:255:HIS:CE1	1:N:49:TYR:HE2	2.15	0.65
4:z:392:ARG:HH21	4:z:416:CYS:HA	1.62	0.65
5:A:95:PRO:HB3	5:A:111:ARG:HH11	1.62	0.65
4:R:183:GLN:HB2	4:R:222:ILE:HG23	1.78	0.65
3:U:141:ASN:O	3:U:142:GLN:HB3	1.97	0.65
4:Z:271:ARG:NH2	4:Z:289:ASP:OD1	2.29	0.65
4:t:180:LEU:HB2	4:t:227:VAL:HG21	1.79	0.65
6:CA:1:NAG:H3	6:CA:1:NAG:H83	1.78	0.65
4:j:85:VAL:HG23	4:j:91:CYS:HB2	1.79	0.65
2:AE:116:GLU:HG3	2:AE:224:PHE:HE2	1.61	0.64
4:J:199:TYR:CD1	4:J:215:MET:HE1	2.32	0.64
4:r:87:THR:HG22	4:r:88:SER:H	1.62	0.64
4:t:229:VAL:HG12	4:t:232:HIS:HE1	1.62	0.64
1:AB:11:LEU:HD12	1:AB:38:MET:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:407:VAL:HB	4:I:410:THR:HG22	1.77	0.64
4:r:169:MET:HB3	4:r:235:TRP:HB3	1.78	0.64
1:l:26:CYS:HB3	1:l:29:GLU:HB2	1.79	0.64
4:X:230:THR:HB	4:X:232:HIS:HE1	1.61	0.64
3:h:435:GLY:HA2	3:h:438:ARG:HD2	1.78	0.64
3:p:21:ARG:HG3	3:p:22:PRO:HD2	1.77	0.64
4:7:12:THR:O	4:7:68:ARG:NH2	2.30	0.64
4:K:138:ARG:HH21	4:K:293:LEU:HD23	1.62	0.64
4:R:12:THR:HG22	4:R:169:MET:HE2	1.79	0.64
3:V:149:ASN:ND2	3:V:151:ASP:OD1	2.30	0.64
4:7:67:ILE:HD11	4:7:115:ILE:HD13	1.80	0.64
2:AE:183:LYS:HE2	2:AE:229:ARG:HG2	1.78	0.64
3:E:7:MET:HE3	3:E:31:MET:HE3	1.78	0.64
3:E:104:SER:HB2	3:E:231:VAL:HG23	1.80	0.64
3:H:304:ALA:HB3	3:H:315:VAL:HG23	1.79	0.64
4:X:12:THR:HG22	4:X:169:MET:HE2	1.80	0.64
4:Y:392:ARG:HH21	4:Y:416:CYS:HA	1.61	0.64
2:D:219:SER:OG	2:D:267:TRP:O	2.14	0.64
2:d:210:PRO:HA	2:d:243:ARG:HE	1.62	0.64
2:3:256:VAL:HG23	4:z:402:THR:HG23	1.80	0.64
3:4:300:THR:HG1	3:4:319:THR:HG1	1.45	0.64
4:R:112:GLN:HB3	4:R:126:ARG:HB3	1.80	0.64
3:4:436:LEU:HD22	4:X:420:ALA:HB2	1.80	0.64
2:d:209:ILE:HB	2:d:244:THR:HB	1.80	0.64
6:lA:2:NAG:H83	6:lA:2:NAG:H3	1.80	0.64
2:D:140:VAL:HG23	2:D:173:ILE:HG22	1.79	0.64
3:E:259:CYS:HB3	3:E:271:CYS:HA	1.80	0.64
4:J:200:ASN:HA	4:J:208:VAL:HG12	1.80	0.64
4:z:203:CYS:SG	4:z:224:GLN:NE2	2.71	0.64
4:B:203:CYS:SG	4:B:224:GLN:NE2	2.70	0.63
3:V:259:CYS:HB3	3:V:271:CYS:HA	1.80	0.63
4:j:180:LEU:HB2	4:j:227:VAL:HG21	1.79	0.63
3:5:424:ALA:HB1	4:8:387:MET:SD	2.38	0.63
4:I:54:ILE:HG23	4:I:67:ILE:HG21	1.80	0.63
4:I:69:TYR:OH	4:I:117:ASP:OD1	2.13	0.63
4:K:392:ARG:NH1	4:K:415:CYS:O	2.31	0.63
2:AD:195:TRP:CZ3	2:AD:197:HIS:HB2	2.33	0.63
4:J:408:PRO:HA	4:J:411:LEU:HB3	1.79	0.63
4:j:6:PHE:HE1	1:l:53:GLN:HA	1.62	0.63
4:s:50:PHE:CZ	4:s:101:ILE:HD11	2.34	0.63
4:t:271:ARG:NH2	4:t:289:ASP:OD1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:9:CYS:N	1:b:18:CYS:SG	2.72	0.63
2:d:218:ASP:OD1	2:d:221:ARG:NH2	2.31	0.63
4:8:169:MET:HB3	4:8:235:TRP:HB3	1.79	0.63
3:W:44:LEU:HD11	3:W:47:ILE:HD11	1.80	0.63
3:i:21:ARG:HG2	3:i:24:TYR:HD2	1.64	0.63
4:t:308:GLU:OE1	4:t:316:ARG:NH1	2.30	0.63
2:1:179:SER:OG	2:3:240:GLU:O	2.17	0.63
1:N:38:MET:O	1:N:42:ASN:ND2	2.31	0.63
4:X:235:TRP:NE1	1:a:40:GLU:OE2	2.22	0.63
4:X:261:ASP:OD1	4:X:262:ASN:N	2.32	0.63
3:q:295:THR:OG1	3:q:323:ASP:OD2	2.17	0.63
4:8:392:ARG:NH1	4:8:415:CYS:O	2.30	0.63
4:B:257:PRO:HB2	4:B:258:PHE:CD2	2.34	0.63
3:o:29:LEU:HD13	3:o:137:TYR:HB3	1.81	0.63
4:z:180:LEU:HD12	4:z:227:VAL:HG11	1.79	0.63
3:6:319:THR:HG22	3:6:351:LYS:HE2	1.81	0.63
2:AD:116:GLU:HA	2:AD:120:ILE:HD13	1.81	0.63
4:K:69:TYR:OH	4:K:117:ASP:OD1	2.08	0.63
3:W:135:VAL:HG11	3:W:156:ILE:HD13	1.81	0.63
4:Y:308:GLU:CD	4:Y:316:ARG:HH12	2.07	0.63
3:F:144:VAL:HG21	3:F:154:VAL:HG21	1.81	0.62
3:W:21:ARG:NH1	3:W:284:ASP:OD1	2.23	0.62
2:d:188:LYS:NZ	2:d:250:THR:OG1	2.27	0.62
3:p:299:LEU:HD21	3:p:318:LEU:HD11	1.80	0.62
5:A:103:GLU:CB	5:A:111:ARG:HG2	2.29	0.62
4:B:197:VAL:HG12	4:B:229:VAL:HA	1.82	0.62
3:G:220:LYS:NZ	4:I:272:GLU:OE1	2.31	0.62
2:T:108:ARG:HA	2:T:111:MET:SD	2.39	0.62
3:U:132:LYS:NZ	3:U:145:ASP:OD1	2.26	0.62
2:e:111:MET:HE3	2:e:115:ILE:HD11	1.80	0.62
2:n:200:VAL:HG12	2:n:209:ILE:HG22	1.80	0.62
2:D:125:HIS:ND1	2:D:126:GLU:OE1	2.30	0.62
4:X:145:PRO:HG3	4:X:268:PRO:HB3	1.82	0.62
4:j:50:PHE:HB3	4:j:52:ALA:H	1.63	0.62
3:p:28:THR:HG23	3:p:329:SER:HB2	1.80	0.62
1:w:9:CYS:N	1:w:18:CYS:SG	2.72	0.62
2:1:182:SER:OG	2:1:183:LYS:N	2.29	0.62
4:B:85:VAL:HG23	4:B:91:CYS:HB2	1.81	0.62
3:G:259:CYS:HB3	3:G:271:CYS:HA	1.80	0.62
2:e:138:ASP:OD2	2:f:206:ARG:NH2	2.33	0.62
4:9:165:GLU:HB2	4:9:256:ILE:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:24:TYR:HE1	3:E:289:ARG:HE	1.48	0.62
3:F:280:MET:HE2	3:F:282:LEU:HD11	1.81	0.62
4:J:238:ASN:HD22	4:J:251:LYS:HD2	1.65	0.62
4:X:55:GLY:H	4:X:67:ILE:HG22	1.65	0.62
4:Z:59:SER:OG	4:Z:61:ASN:OD1	2.16	0.62
2:f:116:GLU:OE1	2:f:196:HIS:ND1	2.32	0.62
3:V:109:ASP:OD1	3:V:110:ARG:N	2.33	0.62
1:a:38:MET:O	1:a:42:ASN:ND2	2.33	0.62
3:q:302:THR:HG1	3:q:317:THR:HG1	1.47	0.62
4:s:47:LYS:HG3	4:s:156:TYR:CE2	2.34	0.62
4:7:87:THR:HG22	4:7:88:SER:H	1.63	0.62
2:O:255:MET:HA	2:O:255:MET:HE2	1.82	0.62
4:Z:251:LYS:HA	4:Z:251:LYS:HE3	1.82	0.62
3:q:259:CYS:HB3	3:q:271:CYS:HA	1.80	0.62
2:3:251:TRP:HD1	4:z:402:THR:HG22	1.64	0.62
5:A:86:PRO:HG2	5:A:89:TRP:CD1	2.34	0.62
5:A:197:GLU:HA	5:A:207:PRO:HA	1.82	0.62
3:W:323:ASP:OD1	3:W:324:LYS:N	2.32	0.62
4:B:142:THR:HG21	4:I:109:GLU:HG2	1.81	0.62
4:X:54:ILE:HA	4:X:67:ILE:HB	1.82	0.62
3:i:300:THR:OG1	3:i:319:THR:OG1	2.16	0.62
4:s:318:ILE:HG21	4:s:325:MET:HE3	1.82	0.62
4:t:261:ASP:OD1	4:t:262:ASN:N	2.31	0.62
1:2:48:TYR:CE2	4:z:253:LYS:HB2	2.34	0.61
4:t:183:GLN:NE2	4:t:187:ASN:O	2.33	0.61
4:9:195:LYS:HB3	4:9:229:VAL:HG13	1.82	0.61
4:j:308:GLU:OE1	4:j:316:ARG:NH1	2.33	0.61
1:l:8:MET:O	1:l:45:ARG:NH2	2.33	0.61
4:t:54:ILE:HG22	4:t:67:ILE:HB	1.81	0.61
4:8:102:LEU:HD13	4:8:258:PHE:CD2	2.36	0.61
3:H:60:VAL:HG11	3:H:86:PRO:HG2	1.82	0.61
3:U:259:CYS:HB3	3:U:271:CYS:HA	1.82	0.61
4:t:77:ASN:HD22	4:t:77:ASN:C	2.09	0.61
3:G:300:THR:HG1	3:G:319:THR:HG1	1.43	0.61
3:V:330:VAL:HG11	3:V:354:LEU:HD11	1.82	0.61
4:X:230:THR:HB	4:X:232:HIS:CE1	2.36	0.61
3:6:89:TRP:HH2	4:9:72:GLY:HA2	1.64	0.61
4:j:163:THR:HG23	4:j:259:PRO:HB3	1.83	0.61
4:j:408:PRO:HA	4:j:411:LEU:HB3	1.82	0.61
4:Y:200:ASN:HA	4:Y:208:VAL:HG12	1.81	0.61
2:T:140:VAL:HG23	2:T:173:ILE:HG22	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:8:165:GLU:HB2	4:8:256:ILE:HG12	1.80	0.61
1:S:9:CYS:N	1:S:18:CYS:SG	2.73	0.61
3:p:136:MET:HE3	3:p:141:ASN:OD1	2.01	0.61
3:6:242:TYR:HE2	4:t:287:HIS:HD1	1.48	0.61
4:8:146:HIS:HA	4:8:266:ARG:HH22	1.65	0.61
4:Z:286:LEU:HD23	4:Z:310:VAL:HG21	1.82	0.61
4:j:145:PRO:HG3	4:j:268:PRO:HB3	1.82	0.61
4:t:85:VAL:HG13	4:t:91:CYS:HB2	1.81	0.61
4:9:145:PRO:HG3	4:9:268:PRO:HB3	1.81	0.61
2:AD:188:LYS:NZ	2:AD:251:TRP:O	2.32	0.61
1:N:11:LEU:HD12	1:N:38:MET:HB3	1.82	0.61
3:p:402:MET:HA	3:p:407:LEU:HD12	1.83	0.61
4:r:244:ARG:HH21	4:r:247:GLU:HA	1.65	0.61
4:9:180:LEU:HD12	4:9:227:VAL:HG11	1.82	0.60
4:j:235:TRP:NE1	1:l:40:GLU:OE2	2.32	0.60
4:z:54:ILE:HG22	4:z:67:ILE:HG23	1.83	0.60
3:4:212:ASP:OD1	3:4:213:LEU:N	2.33	0.60
4:B:166:GLU:OE2	1:S:49:TYR:OH	2.19	0.60
4:X:195:LYS:HB3	4:X:229:VAL:HG13	1.83	0.60
4:s:85:VAL:HG23	4:s:91:CYS:HB2	1.83	0.60
4:s:139:GLU:OE1	4:s:290:HIS:NE2	2.34	0.60
2:3:178:ARG:HB2	2:e:240:GLU:OE1	2.02	0.60
2:Q:196:HIS:HD2	2:Q:197:HIS:CE1	2.19	0.60
4:X:402:THR:HA	2:d:139:LYS:HZ3	1.66	0.60
4:Z:63:ASP:OD1	4:Z:64:TYR:N	2.34	0.60
4:j:54:ILE:HG22	4:j:67:ILE:HG23	1.83	0.60
4:r:13:ARG:NH1	4:r:231:ASP:OD2	2.34	0.60
4:t:408:PRO:HA	4:t:411:LEU:HB3	1.82	0.60
2:y:210:PRO:HA	2:y:243:ARG:NE	2.15	0.60
3:H:255:ALA:O	4:K:297:ARG:NH1	2.34	0.60
2:P:187:GLU:C	2:P:188:LYS:HD3	2.26	0.60
4:Y:326:GLU:OE2	4:Y:336:ARG:NH2	2.33	0.60
2:e:184:TYR:HB2	2:e:251:TRP:HZ3	1.67	0.60
3:m:87:PHE:CE1	3:m:92:ALA:HB2	2.35	0.60
3:5:38:LEU:HD21	3:5:171:THR:HG22	1.83	0.60
5:A:105:PRO:HG3	5:A:111:ARG:N	2.16	0.60
6:XA:2:NAG:H3	6:XA:2:NAG:H83	1.83	0.60
4:B:401:LEU:HD12	2:D:168:LEU:HD23	1.82	0.60
4:J:100:PHE:HE2	4:J:256:ILE:HB	1.66	0.60
2:Q:116:GLU:HA	2:Q:120:ILE:HD13	1.84	0.60
3:U:303:VAL:HG11	3:U:378:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:242:TYR:O	3:q:246:GLU:HG2	2.01	0.60
4:z:14:PRO:HD3	4:z:53:GLN:HG2	1.83	0.60
2:AE:247:SER:HB3	2:AE:261:PRO:HD2	1.82	0.60
4:I:408:PRO:HA	4:I:411:LEU:HB3	1.84	0.60
4:X:180:LEU:HD22	4:X:191:THR:HB	1.83	0.60
4:Y:54:ILE:HG22	4:Y:67:ILE:HB	1.84	0.60
2:e:158:LEU:HD11	2:e:174:PRO:HD3	1.84	0.60
2:e:226:ASN:HB2	2:e:227:LYS:NZ	2.17	0.60
3:m:21:ARG:NH1	3:m:284:ASP:OD1	2.28	0.60
4:r:318:ILE:HD12	4:r:325:MET:HE1	1.84	0.60
1:u:9:CYS:N	1:u:18:CYS:SG	2.74	0.60
2:Q:238:ALA:HB2	2:Q:264:SER:HA	1.83	0.60
4:X:14:PRO:HD2	4:X:75:ILE:HD12	1.82	0.60
2:f:201:GLN:OE1	2:f:243:ARG:NH2	2.34	0.60
4:z:69:TYR:OH	4:z:117:ASP:OD1	2.16	0.60
3:4:146:VAL:HG11	3:4:163:PHE:CD1	2.37	0.60
4:7:271:ARG:NH1	4:7:289:ASP:OD1	2.34	0.60
4:8:235:TRP:NE1	1:AA:36:LEU:HG	2.17	0.60
1:M:9:CYS:N	1:M:18:CYS:SG	2.75	0.60
2:e:152:ASN:HB3	2:e:155:LEU:HB2	1.83	0.60
4:j:67:ILE:O	4:j:77:ASN:HA	2.02	0.60
4:j:263:ILE:HG13	4:j:264:THR:H	1.67	0.60
2:n:142:LYS:NZ	2:n:146:VAL:O	2.35	0.60
4:s:261:ASP:OD1	4:s:262:ASN:N	2.32	0.60
5:A:105:PRO:HB3	5:A:110:MET:CA	2.20	0.60
2:O:210:PRO:HA	2:O:243:ARG:NE	2.17	0.60
4:Z:183:GLN:NE2	4:Z:187:ASN:O	2.35	0.60
4:t:87:THR:HG21	4:t:105:CYS:HB3	1.84	0.60
3:H:438:ARG:HB3	2:Q:255:MET:HE1	1.84	0.59
4:I:187:ASN:HB3	4:I:218:ASN:HA	1.84	0.59
3:V:249:THR:HG22	4:Y:305:TYR:CZ	2.37	0.59
4:t:34:ILE:HD11	4:t:113:VAL:HG22	1.84	0.59
4:8:250:ARG:NH2	1:AA:41:ASP:OD1	2.36	0.59
4:J:49:GLN:HE21	4:J:100:PHE:HE1	1.49	0.59
4:R:308:GLU:OE1	4:R:316:ARG:NH1	2.31	0.59
3:i:7:MET:HE1	3:i:31:MET:HE3	1.84	0.59
3:p:242:TYR:O	3:p:246:GLU:HG2	2.02	0.59
3:q:109:ASP:OD1	3:q:110:ARG:N	2.35	0.59
4:s:15:TYR:HB2	4:s:236:GLN:HE21	1.67	0.59
4:s:392:ARG:HG3	4:s:414:LEU:HD23	1.84	0.59
2:y:187:GLU:HG3	2:y:189:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AE:120:ILE:HD11	2:AE:222:PRO:HD2	1.82	0.59
3:U:42:LEU:HD12	3:U:122:TYR:HB3	1.83	0.59
3:U:212:ASP:OD1	3:U:213:LEU:N	2.35	0.59
3:V:303:VAL:HG11	3:V:378:ALA:HB2	1.84	0.59
4:Y:180:LEU:HD21	4:Y:227:VAL:HG11	1.83	0.59
4:t:180:LEU:HD12	4:t:227:VAL:HG11	1.83	0.59
4:8:235:TRP:HE1	1:AA:36:LEU:HG	1.67	0.59
3:H:228:MET:HE1	4:K:18:TYR:CE2	2.37	0.59
4:Y:261:ASP:OD1	4:Y:262:ASN:N	2.32	0.59
1:a:33:GLU:O	1:a:37:ARG:HG2	2.02	0.59
3:o:252:ASN:HA	3:o:261:ILE:HD12	1.84	0.59
4:I:50:PHE:CE2	4:I:54:ILE:HD11	2.38	0.59
4:Z:54:ILE:HG22	4:Z:67:ILE:HB	1.84	0.59
4:r:202:THR:HB	4:r:224:GLN:HG2	1.82	0.59
4:s:165:GLU:HB2	4:s:256:ILE:HG12	1.83	0.59
6:MA:2:NAG:H3	6:MA:2:NAG:H83	1.84	0.59
3:F:19:ILE:HD11	3:F:27:LEU:HD23	1.84	0.59
4:J:318:ILE:HD12	4:J:325:MET:CE	2.32	0.59
2:O:108:ARG:NH2	2:O:226:ASN:OD1	2.35	0.59
3:U:300:THR:OG1	3:U:319:THR:OG1	2.21	0.59
2:d:173:ILE:HD11	2:d:178:ARG:HG2	1.84	0.59
4:r:308:GLU:OE2	4:r:316:ARG:NH2	2.35	0.59
4:J:308:GLU:CD	4:J:316:ARG:HH12	2.11	0.59
4:X:246:ASP:OD2	4:X:250:ARG:NH1	2.35	0.59
3:6:134:ARG:HH22	6:BA:1:NAG:H5	1.67	0.59
4:Y:188:VAL:HG22	4:Y:217:ILE:H	1.68	0.59
1:c:9:CYS:N	1:c:18:CYS:SG	2.76	0.59
6:k:2:NAG:H3	6:k:2:NAG:H83	1.85	0.59
6:iA:1:NAG:O6	6:iA:2:NAG:N2	2.35	0.59
5:A:95:PRO:HD3	5:A:111:ARG:HE	1.67	0.59
4:B:195:LYS:HB3	4:B:229:VAL:HG13	1.84	0.59
4:X:318:ILE:HD12	4:X:325:MET:HE1	1.84	0.59
4:t:50:PHE:HB3	4:t:52:ALA:H	1.68	0.59
3:6:225:SER:H	3:6:230:HIS:CE1	2.21	0.59
4:8:171:MET:HE1	4:8:235:TRP:CD1	2.38	0.59
5:A:105:PRO:HA	5:A:110:MET:HE3	1.83	0.59
4:X:6:PHE:HD2	4:X:8:VAL:HG23	1.68	0.59
2:n:108:ARG:HH21	2:n:226:ASN:HA	1.68	0.59
2:y:111:MET:HE3	2:y:115:ILE:HG13	1.84	0.59
3:p:21:ARG:NH2	3:p:284:ASP:OD1	2.36	0.58
4:t:169:MET:HE1	4:t:236:GLN:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:55:GLY:H	4:7:67:ILE:HG22	1.67	0.58
1:N:9:CYS:N	1:N:18:CYS:SG	2.76	0.58
4:Y:180:LEU:HD23	4:Y:180:LEU:H	1.68	0.58
4:Y:408:PRO:HA	4:Y:411:LEU:HB3	1.86	0.58
2:e:188:LYS:HB3	2:e:202:TYR:HE2	1.68	0.58
4:s:14:PRO:HB3	4:s:52:ALA:HA	1.84	0.58
4:s:14:PRO:HG3	4:s:53:GLN:HG2	1.84	0.58
3:F:93:TYR:HB3	4:I:176:PRO:HG3	1.85	0.58
4:K:117:ASP:OD1	4:K:118:THR:N	2.35	0.58
3:G:308:HIS:HB2	3:G:359:ALA:HA	1.85	0.58
3:i:323:ASP:OD1	3:i:324:LYS:N	2.37	0.58
4:s:85:VAL:HG12	4:s:113:VAL:HG22	1.86	0.58
4:8:102:LEU:HD13	4:8:258:PHE:HD2	1.68	0.58
2:AE:109:GLU:HG2	2:AE:113:MET:HE1	1.84	0.58
4:Y:318:ILE:HD12	4:Y:325:MET:HE1	1.84	0.58
2:n:210:PRO:HA	2:n:243:ARG:HG2	1.85	0.58
3:6:196:GLN:HG3	3:6:197:PRO:HD2	1.86	0.58
5:A:193:CYS:HB2	5:A:197:GLU:CD	2.28	0.58
2:Q:225:ASP:OD2	2:Q:229:ARG:NH2	2.36	0.58
3:i:425:ILE:HG12	4:j:387:MET:HE1	1.86	0.58
4:8:308:GLU:CD	4:8:316:ARG:HH12	2.12	0.58
4:B:408:PRO:HA	4:B:411:LEU:HB3	1.86	0.58
1:N:21:PRO:HG2	1:N:24:VAL:HG23	1.86	0.58
4:Y:22:CYS:SG	4:Y:30:SER:OG	2.61	0.58
4:Z:308:GLU:OE1	4:Z:316:ARG:NH1	2.36	0.58
5:A:105:PRO:HA	5:A:109:HIS:O	2.03	0.58
1:l:9:CYS:N	1:l:18:CYS:SG	2.77	0.58
4:t:10:LYS:HG2	4:t:60:ASP:HB3	1.86	0.58
4:t:229:VAL:HG12	4:t:232:HIS:CE1	2.39	0.58
1:v:10:VAL:HG23	1:v:15:THR:H	1.67	0.58
4:B:176:PRO:HG3	3:h:93:TYR:HB3	1.84	0.58
2:T:225:ASP:N	2:T:229:ARG:O	2.36	0.58
3:4:149:ASN:O	3:4:151:ASP:N	2.35	0.57
3:H:225:SER:H	3:H:230:HIS:CE1	2.21	0.57
1:N:8:MET:N	1:N:8:MET:SD	2.77	0.57
4:R:230:THR:HG22	4:R:232:HIS:CE1	2.36	0.57
2:AE:210:PRO:HA	2:AE:243:ARG:NE	2.19	0.57
3:q:21:ARG:NH2	3:q:284:ASP:OD1	2.31	0.57
4:s:200:ASN:HA	4:s:208:VAL:HG12	1.86	0.57
3:6:134:ARG:HH21	6:BA:1:NAG:H3	1.69	0.57
4:R:169:MET:HE3	4:R:235:TRP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:139:GLU:OE2	4:r:290:HIS:NE2	2.37	0.57
4:B:348:HIS:ND1	3:h:379:SER:OG	2.34	0.57
4:I:139:GLU:OE1	4:I:290:HIS:NE2	2.38	0.57
4:I:402:THR:HG23	2:O:256:VAL:HG23	1.86	0.57
4:J:87:THR:HG22	4:J:111:LEU:HB3	1.86	0.57
2:Q:176:HIS:CE1	2:Q:177:MET:HE2	2.39	0.57
2:T:145:HIS:NE2	2:T:267:TRP:O	2.28	0.57
3:U:93:TYR:HB3	4:X:176:PRO:HG3	1.86	0.57
3:W:12:GLY:HA2	3:W:32:GLN:HE21	1.70	0.57
6:tA:2:NAG:H83	6:tA:2:NAG:H3	1.86	0.57
4:8:180:LEU:HD23	4:8:180:LEU:H	1.69	0.57
4:9:343:THR:OG1	4:9:344:GLU:OE1	2.20	0.57
4:B:54:ILE:HB	4:B:67:ILE:HG12	1.86	0.57
4:Z:145:PRO:HG3	4:Z:268:PRO:HB3	1.87	0.57
4:r:145:PRO:HG3	4:r:268:PRO:HB3	1.85	0.57
2:1:168:LEU:HD23	4:t:401:LEU:HD13	1.86	0.57
3:4:134:ARG:HB2	3:4:143:THR:HG22	1.85	0.57
3:4:228:MET:HE1	4:7:18:TYR:CE2	2.40	0.57
5:A:114:ARG:HD2	5:A:116:HIS:H	1.70	0.57
1:L:11:LEU:HB2	1:L:16:PHE:HE1	1.70	0.57
1:b:21:PRO:HG2	1:b:24:VAL:HG23	1.86	0.57
2:1:256:VAL:HG21	4:t:401:LEU:HB2	1.87	0.57
4:8:100:PHE:HD2	4:8:257:PRO:HD2	1.70	0.57
4:9:117:ASP:OD1	4:9:118:THR:N	2.37	0.57
4:R:257:PRO:HB2	4:R:258:PHE:CD2	2.40	0.57
3:U:135:VAL:HG11	3:U:156:ILE:HD13	1.86	0.57
4:X:403:PRO:HD3	2:d:139:LYS:HZ3	1.69	0.57
4:Y:34:ILE:HD11	4:Y:113:VAL:HG22	1.87	0.57
3:h:84:VAL:HG21	3:h:102:GLN:HB2	1.86	0.57
4:s:50:PHE:CE1	4:s:113:VAL:HG11	2.39	0.57
4:s:271:ARG:NH1	4:s:289:ASP:OD1	2.37	0.57
4:t:262:ASN:O	4:t:263:ILE:HG22	2.03	0.57
6:BA:1:NAG:H62	6:BA:2:NAG:C7	2.35	0.57
4:7:308:GLU:OE2	4:7:316:ARG:NH2	2.36	0.57
4:J:50:PHE:CZ	4:J:101:ILE:HD11	2.40	0.57
4:8:402:THR:C	2:AD:139:LYS:HZ1	2.12	0.57
4:9:341:LEU:HD22	4:9:361:LEU:HD22	1.86	0.57
4:I:34:ILE:HD11	4:I:113:VAL:HG22	1.87	0.57
4:J:170:HIS:NE2	4:J:237:PHE:O	2.38	0.57
4:J:184:GLN:HG2	4:J:185:SER:H	1.70	0.57
4:R:50:PHE:HB3	4:R:52:ALA:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:87:THR:HG21	4:Z:105:CYS:HB3	1.87	0.57
1:2:9:CYS:N	1:2:18:CYS:SG	2.78	0.57
4:9:50:PHE:CE2	4:9:101:ILE:HD11	2.40	0.57
3:5:299:LEU:HD21	3:5:318:LEU:HD12	1.85	0.56
4:9:166:GLU:OE2	1:AB:49:TYR:OH	2.23	0.56
4:9:263:ILE:HG13	4:9:264:THR:N	2.19	0.56
1:AA:9:CYS:N	1:AA:18:CYS:SG	2.77	0.56
3:E:229:VAL:HG11	4:R:243:PRO:HG3	1.87	0.56
4:K:263:ILE:HG13	4:K:264:THR:N	2.19	0.56
4:R:85:VAL:HG23	4:R:91:CYS:HB2	1.86	0.56
4:X:67:ILE:HD11	4:X:115:ILE:CD1	2.35	0.56
4:j:34:ILE:HD11	4:j:113:VAL:HG22	1.86	0.56
3:4:323:ASP:OD1	3:4:324:LYS:N	2.38	0.56
4:Y:169:MET:HG3	4:Y:235:TRP:HB3	1.88	0.56
4:Y:369:ALA:O	4:Y:373:MET:HG3	2.05	0.56
1:c:8:MET:N	1:c:8:MET:SD	2.77	0.56
3:h:21:ARG:HG3	3:h:22:PRO:HD2	1.87	0.56
3:i:401:ASP:OD1	3:i:402:MET:N	2.37	0.56
3:5:207:THR:HG22	3:5:210:SER:HB2	1.88	0.56
5:A:93:GLY:HA2	5:A:109:HIS:CD2	2.40	0.56
3:W:242:TYR:HB3	3:W:246:GLU:OE2	2.04	0.56
4:Y:11:ALA:O	4:Y:235:TRP:N	2.38	0.56
4:Z:14:PRO:HB2	4:Z:70:ALA:HB2	1.87	0.56
2:e:262:GLU:OE2	4:z:421:HIS:NE2	2.36	0.56
2:n:111:MET:HE1	2:n:228:GLY:HA3	1.85	0.56
4:z:23:GLY:HA2	4:z:126:ARG:HE	1.70	0.56
5:A:147:GLU:O	5:A:149:CYS:N	2.39	0.56
4:J:165:GLU:HB2	4:J:256:ILE:HG12	1.87	0.56
1:L:11:LEU:HB3	1:L:14:ALA:HB3	1.87	0.56
4:X:244:ARG:HH11	4:X:249:ALA:HB2	1.68	0.56
4:t:413:ILE:HG22	4:t:414:LEU:HD12	1.87	0.56
1:AB:36:LEU:O	1:AB:40:GLU:HG2	2.06	0.56
2:f:209:ILE:HD11	2:f:246:LEU:HD11	1.88	0.56
3:m:149:ASN:O	3:m:151:ASP:N	2.38	0.56
4:s:308:GLU:CD	4:s:316:ARG:HH12	2.13	0.56
4:s:402:THR:HG22	2:y:256:VAL:HG23	1.86	0.56
4:t:201:CYS:HA	4:t:224:GLN:HG3	1.87	0.56
3:F:228:MET:HE1	4:I:18:TYR:CE2	2.41	0.56
2:P:179:SER:OG	2:Q:240:GLU:O	2.23	0.56
4:Y:14:PRO:HG3	4:Y:53:GLN:HG2	1.86	0.56
2:e:189:PRO:O	2:e:193:TYR:OH	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:226:ASN:OD1	2:f:227:LYS:N	2.38	0.56
3:q:252:ASN:ND2	3:q:261:ILE:HB	2.21	0.56
4:t:392:ARG:HG2	4:t:414:LEU:HD23	1.88	0.56
6:UA:2:NAG:H3	6:UA:2:NAG:H83	1.87	0.56
3:5:308:HIS:HB2	3:5:359:ALA:HA	1.86	0.56
4:7:95:GLY:H	4:7:102:LEU:HB2	1.70	0.56
4:K:50:PHE:CZ	4:K:101:ILE:HD11	2.41	0.56
4:7:69:TYR:OH	4:7:117:ASP:OD1	2.19	0.56
2:AC:240:GLU:O	2:d:179:SER:OG	2.15	0.56
3:E:208:VAL:HG23	3:E:209:GLU:HG3	1.88	0.56
4:J:166:GLU:OE1	4:J:253:LYS:HE3	2.05	0.56
2:T:189:PRO:O	2:T:193:TYR:OH	2.17	0.56
3:V:195:GLY:H	3:V:214:TYR:HE2	1.54	0.56
4:Z:69:TYR:OH	4:Z:117:ASP:OD1	2.18	0.56
4:s:97:MET:HE1	4:s:160:THR:HG22	1.87	0.56
3:4:242:TYR:O	3:4:246:GLU:HG2	2.06	0.56
3:4:259:CYS:HB3	3:4:271:CYS:CA	2.32	0.56
4:9:95:GLY:H	4:9:102:LEU:HB2	1.71	0.56
3:G:255:ALA:O	4:J:297:ARG:NH1	2.39	0.56
4:Z:85:VAL:HG13	4:Z:91:CYS:HB2	1.88	0.56
4:B:247:GLU:HG3	4:B:248:PRO:HD3	1.88	0.56
3:F:230:HIS:CD2	3:F:232:PRO:HG3	2.41	0.56
4:K:139:GLU:OE1	4:K:290:HIS:NE2	2.38	0.56
2:P:195:TRP:CD1	2:P:196:HIS:N	2.75	0.56
3:W:425:ILE:HG12	4:Z:387:MET:HE1	1.87	0.56
4:s:174:ASP:HB3	4:s:228:SER:HB3	1.87	0.56
1:v:8:MET:O	1:v:45:ARG:NH1	2.39	0.56
3:E:10:VAL:HG12	3:E:272:ALA:HB1	1.86	0.55
2:Q:195:TRP:CZ3	2:Q:197:HIS:HB2	2.41	0.55
3:U:9:ASN:HD22	3:U:276:ILE:HD11	1.70	0.55
2:f:252:ASN:OD1	2:f:253:LYS:N	2.35	0.55
1:g:31:ASN:O	1:g:35:THR:OG1	2.22	0.55
4:j:392:ARG:HG3	4:j:414:LEU:HD21	1.88	0.55
4:r:403:PRO:HD3	2:x:139:LYS:NZ	2.20	0.55
4:s:54:ILE:HG22	4:s:67:ILE:HB	1.87	0.55
4:8:50:PHE:HB3	4:8:52:ALA:H	1.71	0.55
4:Z:177:ASP:O	4:Z:227:VAL:HB	2.05	0.55
2:e:209:ILE:HB	2:e:244:THR:HB	1.86	0.55
4:z:166:GLU:O	4:z:167:ILE:HD13	2.07	0.55
6:IA:2:NAG:H83	6:IA:2:NAG:H3	1.89	0.55
1:2:11:LEU:HB2	1:2:16:PHE:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:271:ARG:NH1	4:X:289:ASP:OD1	2.36	0.55
3:H:21:ARG:HG2	3:H:24:TYR:CD1	2.42	0.55
3:U:173:PHE:HB3	3:U:177:ILE:HD11	1.87	0.55
3:V:42:LEU:HD23	3:V:122:TYR:CG	2.42	0.55
3:m:129:LEU:HD22	3:m:148:VAL:HB	1.89	0.55
3:o:93:TYR:HB3	4:r:176:PRO:HG3	1.87	0.55
4:r:187:ASN:HB3	4:r:218:ASN:HA	1.87	0.55
4:s:10:LYS:O	4:s:234:LYS:NZ	2.38	0.55
3:4:382:PRO:HG3	4:7:357:TYR:HE1	1.72	0.55
3:G:312:PHE:HA	3:G:357:SER:HB2	1.89	0.55
3:U:401:ASP:OD1	3:U:402:MET:N	2.39	0.55
4:X:252:GLY:O	4:X:253:LYS:HD3	2.06	0.55
4:Y:57:ASP:OD1	4:Y:77:ASN:ND2	2.24	0.55
4:j:269:MET:HE2	4:j:269:MET:HA	1.88	0.55
3:o:202:ASP:OD1	3:o:203:ILE:N	2.39	0.55
3:p:432:THR:HG22	4:s:394:LYS:NZ	2.21	0.55
4:z:261:ASP:OD1	4:z:262:ASN:N	2.37	0.55
4:8:408:PRO:HA	4:8:411:LEU:HB3	1.88	0.55
4:9:261:ASP:OD1	4:9:262:ASN:N	2.37	0.55
4:K:87:THR:HG23	4:K:110:PHE:O	2.06	0.55
4:K:298:THR:HA	4:K:325:MET:HB3	1.89	0.55
2:Q:184:TYR:HA	2:Q:230:VAL:HG22	1.88	0.55
2:Q:210:PRO:HA	2:Q:243:ARG:NE	2.21	0.55
4:X:318:ILE:HD12	4:X:325:MET:CE	2.37	0.55
4:X:343:THR:OG1	4:X:344:GLU:N	2.40	0.55
4:r:402:THR:HG22	2:x:251:TRP:HD1	1.72	0.55
4:K:247:GLU:HG3	4:K:247:GLU:O	2.07	0.55
4:R:145:PRO:HG3	4:R:268:PRO:HB3	1.88	0.55
1:S:11:LEU:HB2	1:S:16:PHE:HE1	1.72	0.55
2:e:221:ARG:HG2	2:e:221:ARG:HH11	1.70	0.55
4:t:344:GLU:N	4:t:344:GLU:OE2	2.40	0.55
2:y:136:VAL:HG11	2:y:251:TRP:HH2	1.70	0.55
6:hA:2:NAG:H3	6:hA:2:NAG:H83	1.88	0.55
3:F:253:THR:HG23	4:I:305:TYR:HE1	1.72	0.55
2:O:173:ILE:HD11	2:O:178:ARG:HG2	1.87	0.55
4:X:139:GLU:OE1	4:X:290:HIS:NE2	2.40	0.55
4:X:143:ILE:HD11	4:Y:128:GLN:N	2.21	0.55
3:h:195:GLY:N	3:h:214:TYR:OH	2.40	0.55
3:o:12:GLY:HA2	3:o:32:GLN:HE21	1.71	0.55
3:4:84:VAL:O	3:4:100:ASN:ND2	2.34	0.55
4:7:11:ALA:O	4:7:235:TRP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:262:ASN:O	4:9:263:ILE:HG22	2.07	0.55
4:J:201:CYS:HA	4:J:224:GLN:HG3	1.88	0.55
4:X:169:MET:HB3	4:X:235:TRP:HB3	1.89	0.55
3:h:252:ASN:ND2	3:h:261:ILE:HB	2.22	0.55
3:m:10:VAL:HG23	3:m:13:PHE:HB2	1.88	0.55
1:u:33:GLU:O	1:u:37:ARG:HG2	2.07	0.55
1:S:19:PHE:HB3	1:S:20:GLN:NE2	2.21	0.55
2:D:206:ARG:NH1	2:f:178:ARG:HH21	2.05	0.54
3:E:129:LEU:HD22	3:E:148:VAL:HB	1.89	0.54
4:I:72:GLY:O	4:I:73:HIS:ND1	2.40	0.54
3:U:95:PHE:CZ	4:X:226:HIS:HB2	2.43	0.54
3:p:255:ALA:O	4:s:297:ARG:NH1	2.40	0.54
4:t:167:ILE:HG12	4:t:256:ILE:HG22	1.89	0.54
3:6:47:ILE:HD11	3:6:118:HIS:CG	2.42	0.54
5:A:217:ASP:OD2	3:p:347:LYS:NZ	2.40	0.54
3:V:225:SER:H	3:V:230:HIS:CE1	2.25	0.54
3:W:42:LEU:HD13	3:W:122:TYR:CD2	2.42	0.54
4:X:67:ILE:HD11	4:X:115:ILE:HD11	1.90	0.54
4:Z:201:CYS:HA	4:Z:224:GLN:HG3	1.89	0.54
2:d:124:LYS:HG2	2:d:129:VAL:HA	1.89	0.54
4:8:180:LEU:HD21	4:8:227:VAL:HG11	1.89	0.54
2:AC:116:GLU:OE1	2:AC:196:HIS:ND1	2.33	0.54
3:H:320:TYR:CE1	3:H:350:GLY:HA2	2.43	0.54
4:Y:85:VAL:HG13	4:Y:91:CYS:HB2	1.89	0.54
2:f:173:ILE:HD11	2:f:178:ARG:HD2	1.89	0.54
4:j:183:GLN:HB2	4:j:222:ILE:HG23	1.89	0.54
2:x:140:VAL:HG23	2:x:173:ILE:HG22	1.89	0.54
3:h:42:LEU:HD12	3:h:122:TYR:HB3	1.90	0.54
4:z:343:THR:HG21	4:z:357:TYR:CD1	2.42	0.54
4:7:85:VAL:HG22	4:7:113:VAL:HG12	1.90	0.54
2:AC:173:ILE:HD11	2:AC:178:ARG:HG2	1.88	0.54
4:B:171:MET:HE2	4:B:235:TRP:CD1	2.42	0.54
3:E:258:GLY:O	4:R:336:ARG:NH2	2.36	0.54
4:I:223:GLU:O	4:I:224:GLN:NE2	2.41	0.54
2:T:108:ARG:HH21	2:T:226:ASN:HA	1.73	0.54
4:j:143:ILE:HD11	4:r:128:GLN:N	2.23	0.54
2:n:125:HIS:CE1	2:n:126:GLU:OE2	2.61	0.54
3:4:93:TYR:HB3	4:7:176:PRO:HG3	1.88	0.54
3:5:42:LEU:HD12	3:5:122:TYR:HB3	1.89	0.54
3:5:249:THR:HA	4:8:305:TYR:OH	2.08	0.54
4:8:166:GLU:OE2	1:AA:49:TYR:OH	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:184:GLN:HG2	4:9:185:SER:H	1.72	0.54
2:AC:160:PHE:HD1	2:AC:171:ALA:HB2	1.73	0.54
4:J:401:LEU:C	2:P:139:LYS:HE3	2.33	0.54
4:X:7:ASN:HB3	4:X:10:LYS:HE2	1.89	0.54
4:Y:69:TYR:OH	4:Y:117:ASP:OD1	2.21	0.54
4:Y:286:LEU:HD23	4:Y:310:VAL:HG21	1.89	0.54
3:o:230:HIS:CD2	3:o:232:PRO:HG3	2.43	0.54
6:PA:1:NAG:H3	6:PA:1:NAG:H83	1.90	0.54
2:1:252:ASN:CG	2:1:253:LYS:H	2.15	0.54
4:8:180:LEU:HD11	4:8:227:VAL:HG11	1.88	0.54
2:AC:116:GLU:O	2:AC:120:ILE:HG12	2.08	0.54
3:E:62:CYS:HB2	3:E:100:ASN:OD1	2.07	0.54
1:L:9:CYS:N	1:L:18:CYS:SG	2.81	0.54
3:V:401:ASP:OD1	3:V:402:MET:N	2.40	0.54
3:W:341:GLU:N	3:W:341:GLU:OE2	2.40	0.54
4:X:187:ASN:HB3	4:X:218:ASN:HA	1.90	0.54
2:d:169:GLU:OE2	2:d:169:GLU:N	2.40	0.54
2:e:173:ILE:HD12	2:e:178:ARG:HA	1.89	0.54
3:i:89:TRP:CH2	4:j:72:GLY:HA2	2.42	0.54
3:q:262:LYS:HD2	3:q:269:MET:HE2	1.88	0.54
4:t:172:PRO:HG2	4:t:232:HIS:HD2	1.73	0.54
1:w:9:CYS:HA	1:w:45:ARG:HD2	1.89	0.54
3:5:258:GLY:HA3	4:8:299:LEU:HB2	1.89	0.54
3:F:146:VAL:HG11	3:F:163:PHE:CD1	2.43	0.54
3:G:11:VAL:HA	3:G:33:VAL:HG23	1.89	0.54
4:R:34:ILE:HD11	4:R:113:VAL:HG22	1.90	0.54
3:U:331:HIS:CD2	3:U:332:SER:H	2.26	0.54
4:Z:50:PHE:HB3	4:Z:52:ALA:H	1.73	0.54
2:d:195:TRP:CD1	2:d:196:HIS:H	2.25	0.54
4:j:15:TYR:HB3	4:j:236:GLN:HG3	1.90	0.54
4:r:85:VAL:HG23	4:r:91:CYS:HB2	1.90	0.54
2:1:212:GLY:HA2	2:1:244:THR:HG23	1.90	0.54
2:AE:176:HIS:CD2	2:AE:177:MET:HE2	2.43	0.54
2:Q:188:LYS:HZ2	2:Q:231:VAL:HG13	1.71	0.54
3:U:257:PHE:CE1	4:X:301:GLU:HA	2.43	0.54
3:V:144:VAL:HG21	3:V:156:ILE:HD11	1.89	0.54
1:0:21:PRO:HG2	1:0:24:VAL:HG13	1.90	0.54
4:9:128:GLN:N	4:t:143:ILE:HD11	2.23	0.54
4:9:416:CYS:SG	4:9:418:PRO:HD2	2.48	0.54
4:I:169:MET:HE1	4:I:236:GLN:C	2.33	0.54
3:U:35:GLU:HB3	3:U:132:LYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:218:ASP:CG	2:d:221:ARG:HH22	2.16	0.54
2:e:178:ARG:HH22	2:f:262:GLU:HB3	1.72	0.54
4:r:48:ILE:HB	4:r:101:ILE:HG23	1.89	0.54
4:s:15:TYR:CB	4:s:236:GLN:HE21	2.19	0.54
4:I:237:PHE:HD2	4:I:239:SER:HB2	1.73	0.53
4:K:174:ASP:HB2	4:K:230:THR:HG22	1.90	0.53
4:R:244:ARG:HH21	4:R:247:GLU:HA	1.73	0.53
2:T:195:TRP:CZ3	2:T:197:HIS:HB2	2.43	0.53
4:Y:347:PRO:HG3	4:Y:357:TYR:CG	2.43	0.53
4:7:184:GLN:HG3	4:7:189:LYS:HD3	1.90	0.53
4:8:244:ARG:NH1	4:8:249:ALA:HB2	2.24	0.53
2:AC:169:GLU:OE1	2:AC:169:GLU:N	2.41	0.53
3:E:341:GLU:N	3:E:341:GLU:OE2	2.41	0.53
3:F:149:ASN:O	3:F:151:ASP:N	2.33	0.53
3:G:299:LEU:HD21	3:G:318:LEU:HD22	1.90	0.53
4:K:109:GLU:OE2	4:K:109:GLU:N	2.42	0.53
4:X:15:TYR:HB3	4:X:236:GLN:HG3	1.91	0.53
6:kA:1:NAG:H61	6:kA:2:NAG:HN2	1.73	0.53
6:nA:1:NAG:H3	6:nA:1:NAG:H83	1.88	0.53
1:AB:10:VAL:HG11	1:AB:45:ARG:HH21	1.73	0.53
2:AC:195:TRP:CD1	2:AC:196:HIS:H	2.26	0.53
4:K:343:THR:OG1	4:K:360:GLY:HA3	2.09	0.53
3:m:87:PHE:HE1	3:m:92:ALA:HB2	1.72	0.53
4:s:286:LEU:HD23	4:s:310:VAL:HG21	1.91	0.53
4:7:7:ASN:HB3	4:7:10:LYS:HE2	1.89	0.53
5:A:111:ARG:NH1	5:A:111:ARG:HA	2.24	0.53
2:D:225:ASP:N	2:D:229:ARG:O	2.38	0.53
4:R:139:GLU:OE1	4:R:290:HIS:NE2	2.41	0.53
3:V:207:THR:HG22	3:V:210:SER:HB2	1.91	0.53
3:W:331:HIS:CD2	3:W:332:SER:H	2.26	0.53
4:X:403:PRO:HD3	2:d:139:LYS:NZ	2.22	0.53
4:Y:10:LYS:HA	4:Y:60:ASP:OD2	2.09	0.53
3:h:204:GLN:HB2	3:h:214:TYR:HD2	1.73	0.53
4:s:59:SER:OG	4:s:61:ASN:OD1	2.19	0.53
4:9:50:PHE:HB3	4:9:52:ALA:H	1.72	0.53
2:AE:173:ILE:HD11	2:AE:178:ARG:HG2	1.91	0.53
2:D:125:HIS:HD1	2:D:126:GLU:CD	2.17	0.53
2:D:131:GLY:HA3	2:D:146:VAL:HG21	1.91	0.53
2:D:178:ARG:NH2	2:y:262:GLU:OE1	2.41	0.53
3:E:109:ASP:OD1	3:E:110:ARG:N	2.42	0.53
3:U:341:GLU:N	3:U:341:GLU:OE1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:s:188:VAL:HG22	4:s:217:ILE:H	1.74	0.53
3:6:199:ARG:NH1	3:6:246:GLU:OE1	2.40	0.53
5:A:111:ARG:HA	5:A:111:ARG:CZ	2.39	0.53
4:I:305:TYR:OH	4:I:307:GLU:OE1	2.22	0.53
4:J:250:ARG:HH22	1:M:37:ARG:HE	1.56	0.53
3:W:401:ASP:OD1	3:W:402:MET:N	2.41	0.53
3:m:402:MET:HA	3:m:407:LEU:HD12	1.91	0.53
3:6:225:SER:H	3:6:230:HIS:HE1	1.56	0.53
2:AE:209:ILE:HG23	2:AE:212:GLY:H	1.74	0.53
3:E:21:ARG:HG3	3:E:22:PRO:HD2	1.91	0.53
2:O:206:ARG:NH2	2:x:138:ASP:OD2	2.42	0.53
3:W:109:ASP:OD1	3:W:110:ARG:N	2.40	0.53
4:Y:160:THR:HG22	4:Y:160:THR:O	2.08	0.53
3:m:21:ARG:HG3	3:m:22:PRO:HD2	1.91	0.53
3:o:252:ASN:ND2	3:o:261:ILE:HB	2.24	0.53
6:ZA:1:NAG:H3	6:ZA:1:NAG:H83	1.91	0.53
3:6:12:GLY:HA2	3:6:32:GLN:HE21	1.73	0.53
2:AD:213:ALA:O	2:AD:215:LYS:NZ	2.42	0.53
4:Y:10:LYS:O	4:Y:234:LYS:NZ	2.40	0.53
4:Z:56:ILE:HG21	4:Z:68:ARG:HH21	1.73	0.53
3:p:202:ASP:OD1	3:p:202:ASP:N	2.38	0.53
4:s:212:ASN:HD22	4:s:212:ASN:C	2.15	0.53
4:t:171:MET:HG3	4:t:172:PRO:HD2	1.91	0.53
4:7:247:GLU:HB3	4:7:248:PRO:HD3	1.91	0.53
4:7:318:ILE:HD12	4:7:325:MET:CE	2.39	0.53
4:I:318:ILE:HD12	4:I:325:MET:CE	2.38	0.53
2:T:144:ALA:HB1	2:T:162:LYS:HE3	1.90	0.53
3:V:16:LYS:HA	3:V:29:LEU:O	2.09	0.53
3:W:134:ARG:NH1	6:YA:1:NAG:H5	2.24	0.53
4:Y:165:GLU:HB2	4:Y:256:ILE:HG12	1.90	0.53
3:4:51:TYR:HE2	3:4:238:SER:HA	1.74	0.53
4:8:397:THR:HA	2:AD:161:LYS:NZ	2.24	0.53
2:AC:152:ASN:HD21	2:AC:177:MET:HE1	1.74	0.53
4:R:343:THR:OG1	4:R:360:GLY:HA3	2.09	0.53
3:o:308:HIS:HB2	3:o:359:ALA:HA	1.90	0.53
3:q:134:ARG:HH12	6:mA:1:NAG:H5	1.73	0.53
4:s:47:LYS:HA	4:s:101:ILE:O	2.09	0.53
4:s:343:THR:HG21	4:s:357:TYR:CD1	2.44	0.53
6:JA:1:NAG:O6	6:JA:2:NAG:N2	2.42	0.53
3:4:51:TYR:HB3	3:4:203:ILE:HD13	1.92	0.52
5:A:77:PHE:N	5:A:85:VAL:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:LYS:NZ	2:D:151:ASP:OD1	2.38	0.52
4:K:134:GLN:OE1	4:K:134:GLN:HA	2.08	0.52
3:h:333:HIS:HB2	3:h:366:VAL:HG13	1.91	0.52
4:r:149:LYS:HG3	4:r:269:MET:SD	2.48	0.52
4:s:231:ASP:O	4:s:233:LYS:N	2.42	0.52
4:t:263:ILE:HG13	4:t:264:THR:N	2.23	0.52
3:4:341:GLU:OE1	3:4:341:GLU:N	2.42	0.52
3:6:302:THR:OG1	3:6:317:THR:OG1	2.27	0.52
4:7:100:PHE:HZ	4:7:167:ILE:HD11	1.72	0.52
5:A:197:GLU:HG2	5:A:206:ILE:O	2.09	0.52
3:E:303:VAL:HG11	3:E:378:ALA:HB2	1.91	0.52
4:I:403:PRO:HD3	2:O:139:LYS:HZ3	1.74	0.52
4:K:50:PHE:HB3	4:K:52:ALA:H	1.73	0.52
2:Q:202:TYR:HD2	2:Q:207:PHE:CE1	2.28	0.52
2:T:209:ILE:HG23	2:T:212:GLY:H	1.75	0.52
4:Y:402:THR:HG22	2:e:256:VAL:HG23	1.91	0.52
4:Z:169:MET:HB3	4:Z:235:TRP:HB3	1.91	0.52
4:Z:308:GLU:CD	4:Z:316:ARG:HH12	2.18	0.52
3:q:230:HIS:CD2	3:q:232:PRO:HG3	2.44	0.52
4:r:401:LEU:O	2:x:139:LYS:NZ	2.42	0.52
2:y:160:PHE:HD1	2:y:171:ALA:HB2	1.73	0.52
1:0:31:ASN:O	1:0:35:THR:OG1	2.19	0.52
3:G:57:SER:HB2	4:J:244:ARG:HG3	1.90	0.52
3:H:112:ASP:N	3:H:112:ASP:OD1	2.42	0.52
3:H:312:PHE:HD2	3:H:340:GLN:HE21	1.56	0.52
4:I:67:ILE:HD11	4:I:115:ILE:CD1	2.39	0.52
4:J:324:GLY:HA3	4:J:338:TRP:CD1	2.43	0.52
4:Z:343:THR:HG21	4:Z:357:TYR:CD1	2.44	0.52
1:g:9:CYS:N	1:g:18:CYS:SG	2.83	0.52
3:h:72:GLU:O	3:h:73:LYS:HD2	2.09	0.52
2:n:142:LYS:HE3	2:n:169:GLU:OE2	2.09	0.52
4:r:318:ILE:HD12	4:r:325:MET:CE	2.39	0.52
2:3:209:ILE:HD11	2:3:246:LEU:HD11	1.91	0.52
3:4:228:MET:HE1	4:7:18:TYR:CZ	2.44	0.52
3:5:161:PHE:HE1	3:5:280:MET:HE2	1.74	0.52
4:9:201:CYS:HA	4:9:224:GLN:HG3	1.91	0.52
3:H:253:THR:HG23	4:K:305:TYR:HE1	1.75	0.52
2:Q:210:PRO:HA	2:Q:243:ARG:HE	1.73	0.52
3:m:51:TYR:HB3	3:m:203:ILE:HD13	1.90	0.52
3:m:259:CYS:HB3	3:m:271:CYS:CA	2.34	0.52
4:z:40:GLU:OE2	4:z:40:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:54:ILE:HG23	4:7:67:ILE:CG2	2.39	0.52
4:8:12:THR:HA	4:8:235:TRP:O	2.10	0.52
5:A:114:ARG:HE	5:A:117:GLU:HB2	1.75	0.52
4:B:305:TYR:O	4:B:306:HIS:HB2	2.09	0.52
3:G:203:ILE:HD11	3:G:213:LEU:HD21	1.91	0.52
4:J:49:GLN:NE2	4:J:100:PHE:HE1	2.06	0.52
2:P:162:LYS:NZ	2:P:164:SER:HB3	2.24	0.52
2:T:187:GLU:C	2:T:188:LYS:HD3	2.34	0.52
3:W:98:SER:OG	3:W:99:GLU:OE2	2.23	0.52
4:X:402:THR:HA	2:d:139:LYS:NZ	2.25	0.52
4:Y:139:GLU:OE1	4:Y:290:HIS:NE2	2.43	0.52
1:a:26:CYS:HB3	1:a:29:GLU:HB2	1.92	0.52
2:f:207:PHE:HB3	2:f:246:LEU:HD12	1.90	0.52
3:i:146:VAL:HG11	3:i:163:PHE:CD1	2.45	0.52
4:j:195:LYS:HB3	4:j:229:VAL:HG13	1.90	0.52
3:o:262:LYS:HD2	3:o:269:MET:HE2	1.90	0.52
3:5:229:VAL:HG11	4:8:243:PRO:HG3	1.91	0.52
3:6:21:ARG:NH1	3:6:284:ASP:OD1	2.41	0.52
4:9:343:THR:OG1	4:9:360:GLY:HA3	2.08	0.52
5:A:147:GLU:OE1	5:A:153:THR:OG1	2.27	0.52
4:J:299:LEU:HD22	4:J:336:ARG:NH1	2.24	0.52
4:K:112:GLN:HB3	4:K:126:ARG:HB3	1.92	0.52
4:R:166:GLU:OE1	1:g:49:TYR:OH	2.27	0.52
1:a:9:CYS:N	1:a:18:CYS:SG	2.83	0.52
2:f:182:SER:OG	2:f:183:LYS:N	2.39	0.52
4:j:266:ARG:HH12	3:o:228:MET:HE1	1.75	0.52
3:p:303:VAL:HG11	3:p:378:ALA:HB2	1.92	0.52
3:p:312:PHE:HD1	3:p:357:SER:HB2	1.74	0.52
2:AC:210:PRO:HA	2:AC:243:ARG:NE	2.21	0.52
2:AD:144:ALA:HB1	2:AD:162:LYS:HZ3	1.73	0.52
3:G:249:THR:HG22	4:J:305:TYR:CZ	2.45	0.52
4:R:50:PHE:CZ	4:R:101:ILE:HD11	2.44	0.52
2:d:210:PRO:HA	2:d:243:ARG:NE	2.23	0.52
3:i:16:LYS:NZ	3:i:342:ALA:HB2	2.24	0.52
3:q:262:LYS:HD2	3:q:269:MET:CE	2.40	0.52
4:9:34:ILE:HD11	4:9:113:VAL:HG22	1.92	0.52
2:AE:110:ARG:HA	2:AE:113:MET:SD	2.50	0.52
2:AE:142:LYS:NZ	2:AE:146:VAL:O	2.43	0.52
4:B:253:LYS:HB2	1:S:48:TYR:CE2	2.44	0.52
3:F:1:TYR:HB2	3:F:21:ARG:NH1	2.21	0.52
4:R:82:SER:CB	4:R:116:GLN:HG3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:343:THR:HG21	4:r:357:TYR:CD1	2.45	0.52
4:B:50:PHE:CE2	4:B:101:ILE:HD11	2.44	0.52
2:P:139:LYS:HG3	2:P:141:MET:HE1	1.92	0.52
2:P:247:SER:HB2	2:P:261:PRO:HD2	1.92	0.52
2:d:139:LYS:HG3	2:d:141:MET:SD	2.50	0.52
3:h:21:ARG:NH1	3:h:284:ASP:OD1	2.37	0.52
4:j:100:PHE:HZ	4:j:167:ILE:HD11	1.74	0.52
4:j:276:ILE:HB	4:j:283:THR:OG1	2.10	0.52
4:r:171:MET:HG3	4:r:172:PRO:HD2	1.92	0.52
4:s:262:ASN:O	4:s:263:ILE:HG12	2.10	0.52
2:x:122:GLU:HG2	2:x:132:TYR:HE1	1.75	0.52
4:z:413:ILE:HG22	4:z:414:LEU:HD12	1.91	0.52
3:4:47:ILE:HD11	3:4:118:HIS:CG	2.44	0.52
3:E:302:THR:OG1	3:E:317:THR:OG1	2.18	0.52
2:O:154:ASP:HA	2:O:157:LYS:HE3	1.91	0.52
2:e:196:HIS:CD2	2:e:221:ARG:HH21	2.28	0.52
4:j:169:MET:HB3	4:j:235:TRP:HB3	1.92	0.52
4:r:59:SER:OG	4:r:61:ASN:OD1	2.26	0.52
4:9:100:PHE:CD2	4:9:257:PRO:HD2	2.45	0.51
4:B:165:GLU:HB2	4:B:256:ILE:HG12	1.93	0.51
3:H:258:GLY:O	4:K:336:ARG:NH2	2.41	0.51
3:V:129:LEU:HD22	3:V:148:VAL:HB	1.91	0.51
2:f:210:PRO:HA	2:f:243:ARG:NE	2.24	0.51
1:v:9:CYS:N	1:v:18:CYS:SG	2.84	0.51
3:6:212:ASP:OD1	3:6:213:LEU:N	2.43	0.51
4:B:97:MET:HE1	4:B:160:THR:HG21	1.92	0.51
3:F:291:VAL:HG12	3:o:355:HIS:CD2	2.45	0.51
3:G:230:HIS:CD2	3:G:232:PRO:HG3	2.45	0.51
3:H:202:ASP:N	3:H:202:ASP:OD1	2.40	0.51
4:I:318:ILE:HD12	4:I:325:MET:HE3	1.92	0.51
3:W:302:THR:HG1	3:W:317:THR:HG1	1.57	0.51
4:Z:199:TYR:CE2	4:Z:215:MET:HE1	2.45	0.51
3:p:30:GLN:HB2	3:p:136:MET:CG	2.40	0.51
4:t:166:GLU:OE1	1:w:49:TYR:OH	2.29	0.51
4:8:200:ASN:HA	4:8:208:VAL:HG12	1.90	0.51
4:8:343:THR:OG1	4:8:344:GLU:N	2.44	0.51
3:H:95:PHE:CD1	4:K:226:HIS:HE1	2.29	0.51
4:K:169:MET:HB3	4:K:235:TRP:HB3	1.92	0.51
4:X:411:LEU:HD11	4:X:416:CYS:HB3	1.91	0.51
4:Z:170:HIS:HE1	4:Z:238:ASN:HA	1.76	0.51
1:a:35:THR:HA	1:a:38:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:316:LEU:HD22	3:m:354:LEU:HD12	1.92	0.51
4:r:190:ILE:HG21	4:r:197:VAL:HG11	1.92	0.51
4:z:158:GLN:OE1	4:z:158:GLN:N	2.43	0.51
4:z:408:PRO:HA	4:z:411:LEU:HB3	1.92	0.51
2:1:196:HIS:CD2	2:1:221:ARG:HH22	2.28	0.51
3:4:230:HIS:CD2	3:4:232:PRO:HG3	2.45	0.51
3:5:341:GLU:OE1	3:5:341:GLU:N	2.43	0.51
3:6:29:LEU:HD23	3:6:137:TYR:HB3	1.91	0.51
4:7:163:THR:HG22	4:7:259:PRO:HG3	1.91	0.51
4:7:322:VAL:HA	4:7:339:SER:HB3	1.91	0.51
4:8:6:PHE:CE1	1:AA:53:GLN:HA	2.46	0.51
3:U:253:THR:HG23	4:X:305:TYR:HE1	1.74	0.51
2:f:202:TYR:HD1	2:f:207:PHE:CE1	2.29	0.51
4:j:56:ILE:HG21	4:j:68:ARG:HH21	1.75	0.51
4:s:57:ASP:OD1	4:s:61:ASN:N	2.29	0.51
4:t:235:TRP:NE1	1:w:36:LEU:HD22	2.25	0.51
4:z:167:ILE:HD11	4:z:256:ILE:HG22	1.91	0.51
6:VA:1:NAG:O6	6:VA:2:NAG:N2	2.39	0.51
3:6:242:TYR:HE2	4:t:287:HIS:ND1	2.08	0.51
3:V:125:HIS:ND1	3:V:126:THR:HG22	2.26	0.51
4:Y:314:VAL:HG22	4:Y:315:GLU:H	1.76	0.51
4:Z:6:PHE:CE1	1:c:53:GLN:HA	2.46	0.51
3:h:309:SER:OG	3:h:311:ASP:OD1	2.24	0.51
4:j:50:PHE:CZ	4:j:101:ILE:HD11	2.45	0.51
2:3:251:TRP:CD1	4:z:402:THR:HG22	2.44	0.51
4:B:408:PRO:HB3	3:p:437:ARG:NH1	2.25	0.51
4:I:417:ALA:HB3	4:I:418:PRO:HD3	1.92	0.51
2:P:121:PHE:HE1	2:P:135:LEU:HD13	1.74	0.51
4:X:87:THR:HG22	4:X:88:SER:N	2.23	0.51
4:t:41:ALA:HB2	4:t:156:TYR:CE1	2.46	0.51
2:x:141:MET:HE1	2:x:251:TRP:CZ2	2.45	0.51
4:B:343:THR:HG21	4:B:357:TYR:CD1	2.46	0.51
2:D:210:PRO:HA	2:D:243:ARG:NE	2.26	0.51
3:H:95:PHE:HE2	6:TA:1:NAG:H61	1.76	0.51
2:P:139:LYS:HG3	2:P:141:MET:CE	2.41	0.51
4:Y:85:VAL:HG23	4:Y:113:VAL:HG12	1.92	0.51
3:o:160:GLN:HB3	3:o:281:ASN:HB3	1.92	0.51
3:o:425:ILE:HD13	4:r:387:MET:SD	2.51	0.51
3:p:171:THR:HG22	3:p:173:PHE:H	1.75	0.51
4:r:166:GLU:OE2	4:r:253:LYS:HD3	2.09	0.51
4:s:11:ALA:O	4:s:235:TRP:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:195:LYS:HB3	4:t:229:VAL:HG13	1.93	0.51
2:y:189:PRO:O	2:y:193:TYR:OH	2.22	0.51
3:4:50:GLU:OE1	3:4:241:LYS:HE2	2.11	0.51
3:5:312:PHE:HA	3:5:357:SER:HB2	1.92	0.51
4:9:100:PHE:HD2	4:9:257:PRO:HD2	1.75	0.51
4:9:151:ILE:HD12	4:9:267:VAL:HG21	1.93	0.51
4:B:348:HIS:CE1	3:h:379:SER:HG	2.27	0.51
3:G:34:VAL:HG12	3:G:35:GLU:HG2	1.92	0.51
3:H:225:SER:H	3:H:230:HIS:HE1	1.57	0.51
3:V:199:ARG:NH1	3:V:246:GLU:OE2	2.43	0.51
4:X:290:HIS:O	4:X:292:THR:HG23	2.11	0.51
4:X:392:ARG:HG3	4:X:414:LEU:HD21	1.92	0.51
3:i:12:GLY:HA2	3:i:32:GLN:HE21	1.76	0.51
1:l:9:CYS:HB3	1:l:42:ASN:HD22	1.75	0.51
3:m:323:ASP:OD1	3:m:323:ASP:N	2.43	0.51
3:o:259:CYS:HB2	3:o:269:MET:O	2.11	0.51
3:q:225:SER:H	3:q:230:HIS:CE1	2.29	0.51
2:y:125:HIS:NE2	2:y:126:GLU:OE2	2.42	0.51
3:4:249:THR:HG22	4:7:305:TYR:OH	2.11	0.51
3:4:300:THR:OG1	3:4:319:THR:OG1	2.18	0.51
4:9:246:ASP:OD1	4:9:246:ASP:N	2.43	0.51
4:9:344:GLU:OE1	4:9:344:GLU:N	2.44	0.51
2:AC:141:MET:HB2	2:AC:168:LEU:HD11	1.92	0.51
3:E:347:LYS:NZ	3:E:348:THR:HG22	2.26	0.51
4:J:188:VAL:HG22	4:J:217:ILE:H	1.76	0.51
4:J:344:GLU:OE1	4:J:344:GLU:N	2.43	0.51
1:L:21:PRO:HG2	1:L:24:VAL:HG23	1.91	0.51
4:R:82:SER:HB2	4:R:116:GLN:HG3	1.91	0.51
1:b:11:LEU:O	1:b:13:ASN:N	2.44	0.51
3:p:30:GLN:HB2	3:p:136:MET:HG3	1.91	0.51
3:p:96:CYS:O	3:p:100:ASN:ND2	2.43	0.51
4:7:404:GLY:HA3	2:AC:254:ASP:OD1	2.11	0.51
4:8:35:GLU:HB2	4:8:49:GLN:HG2	1.92	0.51
4:K:188:VAL:HG22	4:K:217:ILE:H	1.75	0.51
3:W:134:ARG:HH12	6:YA:1:NAG:H5	1.76	0.51
3:W:230:HIS:CD2	3:W:232:PRO:HG3	2.46	0.51
4:X:347:PRO:HG3	4:X:357:TYR:CG	2.46	0.51
4:Z:246:ASP:N	4:Z:246:ASP:OD1	2.43	0.51
2:e:201:GLN:HB3	2:e:208:THR:OG1	2.11	0.51
3:h:299:LEU:HD13	3:h:372:ALA:HB3	1.93	0.51
3:o:257:PHE:CE1	4:r:301:GLU:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:1:TYR:CE2	3:4:21:ARG:HG3	2.45	0.50
3:5:406:ALA:HB2	4:8:354:ILE:HG21	1.93	0.50
4:7:145:PRO:HG3	4:7:268:PRO:HB3	1.93	0.50
4:B:56:ILE:HB	4:B:68:ARG:HD2	1.93	0.50
4:I:87:THR:HG22	4:I:88:SER:N	2.22	0.50
2:P:173:ILE:HD12	2:P:178:ARG:HA	1.93	0.50
4:R:165:GLU:HB3	4:R:256:ILE:HD12	1.93	0.50
3:p:432:THR:HG22	4:s:394:LYS:HZ2	1.76	0.50
3:q:29:LEU:HD23	3:q:137:TYR:HB3	1.93	0.50
4:t:165:GLU:HB2	4:t:256:ILE:HG12	1.93	0.50
1:0:40:GLU:HG3	4:7:235:TRP:CZ2	2.43	0.50
3:6:250:ALA:HB3	3:6:253:THR:HG22	1.93	0.50
4:I:261:ASP:OD1	4:I:262:ASN:N	2.45	0.50
4:R:276:ILE:HB	4:R:283:THR:HB	1.93	0.50
4:Y:172:PRO:HB3	4:Y:236:GLN:NE2	2.25	0.50
3:i:50:GLU:OE1	3:i:241:LYS:HE2	2.10	0.50
3:o:257:PHE:HE1	4:r:301:GLU:HA	1.76	0.50
1:2:41:ASP:OD1	4:z:250:ARG:NH2	2.45	0.50
3:G:73:LYS:HB2	3:G:76:TYR:HB2	1.93	0.50
4:Y:347:PRO:HG3	4:Y:357:TYR:CD2	2.47	0.50
4:7:180:LEU:HD22	4:7:191:THR:HB	1.93	0.50
4:7:407:VAL:O	4:7:410:THR:N	2.45	0.50
5:A:105:PRO:CA	5:A:110:MET:HE3	2.41	0.50
3:G:89:TRP:CH2	4:J:72:GLY:HA2	2.47	0.50
4:K:262:ASN:O	4:K:263:ILE:HG22	2.10	0.50
2:P:136:VAL:HG13	2:P:230:VAL:HG21	1.93	0.50
2:T:122:GLU:HG2	2:T:132:TYR:CE1	2.47	0.50
3:h:76:TYR:OH	3:h:105:GLU:OE2	2.24	0.50
2:y:193:TYR:HB3	2:y:224:PHE:O	2.11	0.50
4:z:392:ARG:HG3	4:z:414:LEU:HD23	1.92	0.50
4:8:146:HIS:HA	4:8:266:ARG:NH2	2.27	0.50
4:8:274:THR:HB	4:8:285:HIS:HB2	1.94	0.50
4:I:12:THR:HA	4:I:235:TRP:O	2.12	0.50
4:J:57:ASP:OD1	4:J:61:ASN:N	2.34	0.50
4:K:297:ARG:NE	4:K:326:GLU:OE1	2.34	0.50
3:U:252:ASN:ND2	3:U:261:ILE:HB	2.27	0.50
2:d:195:TRP:CD1	2:d:196:HIS:N	2.80	0.50
2:f:123:VAL:HG22	2:f:150:ILE:HA	1.92	0.50
4:r:253:LYS:HB2	1:u:48:TYR:CE2	2.47	0.50
4:z:247:GLU:HG3	4:z:248:PRO:HD3	1.94	0.50
3:6:228:MET:HE1	4:9:18:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:298:ASP:OD2	3:E:321:LYS:NZ	2.41	0.50
3:E:309:SER:OG	3:E:311:ASP:OD1	2.28	0.50
3:F:320:TYR:CZ	3:F:346:VAL:HG13	2.47	0.50
3:H:312:PHE:HD2	3:H:340:GLN:NE2	2.10	0.50
4:J:250:ARG:NH2	1:M:41:ASP:OD1	2.43	0.50
2:P:210:PRO:HA	2:P:243:ARG:NE	2.22	0.50
4:Z:196:LYS:HD2	4:Z:231:ASP:HB2	1.93	0.50
3:q:332:SER:HB2	3:q:339:LEU:HD13	1.93	0.50
6:NA:1:NAG:H61	6:NA:2:NAG:C7	2.41	0.50
4:B:401:LEU:HD13	2:D:170:CYS:HB3	1.94	0.50
2:D:218:ASP:O	2:D:221:ARG:HG3	2.12	0.50
4:J:167:ILE:HG12	4:J:256:ILE:HG22	1.93	0.50
2:e:141:MET:HE3	2:e:168:LEU:HD11	1.93	0.50
3:h:144:VAL:HG21	3:h:156:ILE:HD11	1.94	0.50
2:1:209:ILE:HD11	2:1:246:LEU:HD11	1.94	0.50
3:5:160:GLN:HB2	3:5:281:ASN:HB3	1.94	0.50
1:g:37:ARG:HA	1:g:37:ARG:HE	1.77	0.50
4:r:143:ILE:HD11	4:s:128:GLN:N	2.27	0.50
2:3:250:THR:OG1	2:3:251:TRP:N	2.45	0.50
3:4:129:LEU:HD22	3:4:148:VAL:HB	1.94	0.50
3:6:300:THR:OG1	3:6:319:THR:OG1	2.15	0.50
4:8:174:ASP:N	4:8:174:ASP:OD1	2.43	0.50
4:9:119:ARG:HB2	4:9:119:ARG:NH1	2.27	0.50
4:J:310:VAL:HG11	4:J:329:TRP:HZ3	1.77	0.50
4:K:318:ILE:HD12	4:K:325:MET:CE	2.42	0.50
2:O:226:ASN:HB2	2:O:227:LYS:NZ	2.27	0.50
3:U:249:THR:HG22	4:X:305:TYR:CE2	2.47	0.50
2:f:202:TYR:CD1	2:f:207:PHE:HE1	2.29	0.50
4:t:343:THR:OG1	4:t:344:GLU:N	2.45	0.50
4:z:165:GLU:HB2	4:z:256:ILE:HG12	1.94	0.50
3:5:40:PRO:HA	3:5:127:ALA:HA	1.93	0.49
4:7:100:PHE:CZ	4:7:167:ILE:HD11	2.47	0.49
4:9:359:TYR:HA	4:9:366:THR:HG21	1.92	0.49
2:AC:247:SER:HB2	2:AC:261:PRO:HD2	1.94	0.49
3:F:303:VAL:HG21	3:F:378:ALA:HB2	1.94	0.49
4:Y:318:ILE:HD12	4:Y:325:MET:CE	2.41	0.49
3:i:312:PHE:HA	3:i:357:SER:HB3	1.93	0.49
3:m:135:VAL:HG11	3:m:156:ILE:HD13	1.94	0.49
4:s:167:ILE:HG23	4:s:237:PHE:HE1	1.77	0.49
4:t:235:TRP:CE2	1:w:36:LEU:HD22	2.47	0.49
3:G:136:MET:HA	3:G:140:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:403:PRO:HD3	2:O:139:LYS:NZ	2.27	0.49
4:K:290:HIS:O	4:K:292:THR:HG23	2.11	0.49
4:Z:57:ASP:HB3	4:Z:61:ASN:HB2	1.94	0.49
2:e:226:ASN:HB2	2:e:227:LYS:HZ2	1.76	0.49
2:f:202:TYR:HD1	2:f:207:PHE:HE1	1.60	0.49
4:j:297:ARG:NE	4:j:326:GLU:OE2	2.34	0.49
3:p:136:MET:HB3	3:p:141:ASN:OD1	2.12	0.49
2:3:252:ASN:CG	2:3:253:LYS:H	2.20	0.49
4:9:413:ILE:HG22	4:9:414:LEU:HD12	1.93	0.49
4:B:198:LYS:HE3	4:B:230:THR:HG21	1.94	0.49
2:D:108:ARG:NH2	2:D:226:ASN:OD1	2.45	0.49
3:E:42:LEU:HD21	3:E:266:VAL:HG11	1.94	0.49
4:K:105:CYS:SG	4:K:106:PRO:HD2	2.52	0.49
4:K:265:CYS:SG	4:K:266:ARG:N	2.85	0.49
2:Q:250:THR:OG1	2:Q:251:TRP:N	2.41	0.49
4:Z:290:HIS:O	4:Z:292:THR:HG23	2.12	0.49
4:r:195:LYS:HB3	4:r:229:VAL:HG13	1.93	0.49
4:7:197:VAL:HG21	4:7:227:VAL:HG13	1.93	0.49
5:A:194:GLY:O	5:A:197:GLU:HB3	2.13	0.49
3:E:59:TYR:CZ	4:R:247:GLU:HB3	2.47	0.49
3:G:160:GLN:HB2	3:G:281:ASN:HB3	1.93	0.49
4:K:169:MET:SD	4:K:237:PHE:HA	2.53	0.49
4:R:69:TYR:OH	4:R:117:ASP:OD1	2.15	0.49
3:U:312:PHE:HD1	3:U:357:SER:HB2	1.77	0.49
1:a:23:CYS:SG	1:a:38:MET:HE1	2.53	0.49
1:c:34:ALA:O	1:c:38:MET:HG2	2.11	0.49
3:m:58:PRO:HG3	3:m:231:VAL:CG2	2.42	0.49
3:m:109:ASP:OD1	3:m:110:ARG:N	2.42	0.49
2:n:124:LYS:HA	2:n:129:VAL:HA	1.95	0.49
4:7:12:THR:HG22	4:7:169:MET:HE2	1.94	0.49
4:7:273:PRO:HD3	4:7:329:TRP:CD1	2.47	0.49
4:9:57:ASP:O	4:9:68:ARG:HD2	2.12	0.49
3:F:341:GLU:OE1	3:F:341:GLU:N	2.45	0.49
4:K:174:ASP:OD1	4:K:174:ASP:O	2.31	0.49
2:O:116:GLU:O	2:O:120:ILE:HG12	2.13	0.49
4:R:250:ARG:HH11	1:g:37:ARG:HH22	1.60	0.49
4:X:34:ILE:HD11	4:X:113:VAL:HG22	1.94	0.49
4:X:417:ALA:HB3	4:X:418:PRO:HD3	1.94	0.49
3:i:149:ASN:O	3:i:151:ASP:N	2.45	0.49
3:o:10:VAL:HG22	3:o:272:ALA:HB1	1.94	0.49
4:s:50:PHE:HE1	4:s:113:VAL:HG11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:185:THR:HG22	2:x:187:GLU:H	1.77	0.49
4:z:188:VAL:HG22	4:z:217:ILE:HG22	1.94	0.49
4:7:13:ARG:HA	4:7:68:ARG:HH21	1.76	0.49
4:7:195:LYS:HB3	4:7:229:VAL:HG13	1.95	0.49
4:8:347:PRO:HG3	4:8:357:TYR:CG	2.47	0.49
4:9:63:ASP:OD1	4:9:64:TYR:N	2.40	0.49
3:F:62:CYS:HB2	3:F:100:ASN:OD1	2.12	0.49
4:J:134:GLN:OE1	4:J:140:LYS:HD2	2.13	0.49
3:p:228:MET:HE2	3:p:230:HIS:CG	2.47	0.49
3:q:47:ILE:HD11	3:q:118:HIS:CG	2.48	0.49
3:6:47:ILE:HG22	3:6:205:SER:O	2.13	0.49
2:AE:142:LYS:HD3	2:AE:143:PRO:O	2.13	0.49
2:D:190:GLU:OE1	2:D:191:GLY:N	2.45	0.49
3:H:312:PHE:HA	3:H:357:SER:HB2	1.93	0.49
4:K:416:CYS:SG	4:K:418:PRO:HD2	2.52	0.49
2:O:141:MET:HB3	2:O:168:LEU:HD11	1.95	0.49
4:R:143:ILE:HG12	4:X:128:GLN:HB2	1.94	0.49
4:R:402:THR:HG23	2:T:256:VAL:HG23	1.94	0.49
3:U:257:PHE:HE1	4:X:301:GLU:HA	1.76	0.49
4:Y:169:MET:HE3	4:Y:235:TRP:C	2.37	0.49
4:Z:170:HIS:CE1	4:Z:238:ASN:HA	2.48	0.49
3:i:299:LEU:HD12	3:i:320:TYR:HB3	1.94	0.49
3:i:316:LEU:HD22	3:i:354:LEU:HD12	1.95	0.49
4:z:65:THR:HB	4:z:66:LYS:HE2	1.94	0.49
4:z:138:ARG:NH2	4:z:293:LEU:HD23	2.28	0.49
2:3:125:HIS:ND1	2:3:126:GLU:OE1	2.46	0.49
4:8:183:GLN:NE2	4:8:187:ASN:O	2.45	0.49
4:9:378:LEU:HA	4:9:381:ILE:HG22	1.95	0.49
4:B:138:ARG:NH2	4:B:293:LEU:HD23	2.28	0.49
4:B:171:MET:HG3	1:S:37:ARG:HH12	1.77	0.49
4:B:261:ASP:OD1	4:B:262:ASN:N	2.42	0.49
1:M:38:MET:HE2	1:M:51:LEU:HD21	1.95	0.49
2:Q:165:LYS:HE3	2:Q:166:TYR:CE1	2.48	0.49
4:R:347:PRO:HG3	4:R:357:TYR:CD1	2.48	0.49
3:W:328:CYS:HB3	3:W:370:CYS:H	1.77	0.49
4:Y:138:ARG:NH2	4:Y:293:LEU:HD23	2.28	0.49
2:d:108:ARG:HA	2:d:111:MET:HE3	1.95	0.49
2:f:131:GLY:HA3	2:f:146:VAL:HG21	1.93	0.49
3:h:303:VAL:HG11	3:h:378:ALA:HB2	1.94	0.49
3:m:44:LEU:HD11	3:m:47:ILE:HD11	1.94	0.49
4:s:113:VAL:O	4:s:124:ALA:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:69:TYR:CE1	4:t:71:ASP:HB2	2.47	0.49
4:t:213:SER:OG	4:t:214:ASP:N	2.45	0.49
2:1:124:LYS:HA	2:1:129:VAL:HA	1.95	0.49
3:4:320:TYR:CE1	3:4:350:GLY:HA2	2.48	0.49
3:4:333:HIS:HB2	3:4:366:VAL:HG23	1.94	0.49
3:5:205:SER:OG	3:5:207:THR:O	2.29	0.49
4:B:141:PHE:CE1	4:B:267:VAL:HG23	2.47	0.49
3:H:12:GLY:HA2	3:H:32:GLN:HE21	1.78	0.49
4:J:198:LYS:HB3	4:J:210:THR:HG22	1.95	0.49
4:X:237:PHE:HD2	4:X:239:SER:HB2	1.78	0.49
4:j:66:LYS:HD3	4:j:77:ASN:HD22	1.78	0.49
4:r:403:PRO:HD3	2:x:139:LYS:HZ3	1.78	0.49
3:6:49:CYS:O	3:6:203:ILE:HD11	2.13	0.49
4:7:48:ILE:HB	4:7:101:ILE:HG23	1.95	0.49
4:7:139:GLU:OE1	4:7:270:ALA:HB2	2.13	0.49
4:8:59:SER:OG	4:8:61:ASN:OD1	2.30	0.49
4:8:100:PHE:CD2	4:8:257:PRO:HD2	2.48	0.49
3:F:3:HIS:CD2	3:F:19:ILE:HG22	2.48	0.49
4:I:344:GLU:N	4:I:344:GLU:OE2	2.46	0.49
4:R:32:VAL:O	4:R:32:VAL:HG12	2.13	0.49
3:W:42:LEU:HD13	3:W:122:TYR:HD2	1.78	0.49
2:e:195:TRP:CD1	2:e:196:HIS:H	2.30	0.49
1:0:38:MET:O	1:0:42:ASN:ND2	2.46	0.48
4:9:350:TRP:HB2	4:9:353:GLN:OE1	2.13	0.48
5:A:206:ILE:HB	5:A:210:TRP:CE3	2.48	0.48
4:Z:401:LEU:HD22	2:f:170:CYS:SG	2.53	0.48
4:j:174:ASP:OD1	4:j:174:ASP:N	2.44	0.48
4:j:263:ILE:HG13	4:j:264:THR:N	2.27	0.48
3:q:50:GLU:O	3:q:111:SER:HB3	2.13	0.48
2:x:195:TRP:CD1	2:x:196:HIS:H	2.31	0.48
2:y:133:ALA:HB2	2:y:142:LYS:HG3	1.94	0.48
4:9:139:GLU:OE2	4:9:290:HIS:NE2	2.45	0.48
4:9:290:HIS:O	4:9:292:THR:HG23	2.13	0.48
3:G:258:GLY:HA3	4:J:299:LEU:HB2	1.95	0.48
4:J:34:ILE:HD11	4:J:113:VAL:HG22	1.95	0.48
4:J:138:ARG:NH1	4:J:328:HIS:ND1	2.61	0.48
4:K:182:SER:HB3	4:K:189:LYS:HB2	1.95	0.48
2:T:125:HIS:HD1	2:T:126:GLU:CD	2.21	0.48
4:Y:50:PHE:HB3	4:Y:52:ALA:H	1.78	0.48
4:Y:201:CYS:HA	4:Y:224:GLN:HG3	1.95	0.48
3:o:258:GLY:HA2	4:r:297:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:333:HIS:HB2	3:6:366:VAL:HG23	1.96	0.48
4:7:199:TYR:HE1	4:7:207:ASN:HB3	1.78	0.48
2:AE:116:GLU:HG3	2:AE:224:PHE:CE2	2.46	0.48
2:D:210:PRO:HA	2:D:243:ARG:HE	1.78	0.48
3:F:320:TYR:CE1	3:F:350:GLY:HA2	2.49	0.48
4:I:180:LEU:HD22	4:I:191:THR:HB	1.94	0.48
4:K:10:LYS:HG2	4:K:60:ASP:HB3	1.94	0.48
3:W:59:TYR:CZ	3:W:61:LYS:HB2	2.47	0.48
2:e:162:LYS:HD3	2:e:169:GLU:HG2	1.94	0.48
2:e:174:PRO:HG2	2:e:177:MET:HE2	1.95	0.48
3:m:225:SER:H	3:m:230:HIS:CE1	2.31	0.48
3:o:358:THR:OG1	3:o:359:ALA:N	2.45	0.48
4:t:63:ASP:OD1	4:t:64:TYR:N	2.43	0.48
2:y:160:PHE:CD1	2:y:171:ALA:HB2	2.47	0.48
3:5:40:PRO:HG2	3:5:42:LEU:HD21	1.96	0.48
5:A:110:MET:N	5:A:110:MET:SD	2.86	0.48
4:B:7:ASN:ND2	4:B:60:ASP:O	2.46	0.48
3:F:1:TYR:CD2	3:F:21:ARG:HD2	2.47	0.48
3:H:3:HIS:CD2	3:H:19:ILE:HG12	2.48	0.48
1:l:11:LEU:HB2	1:l:16:PHE:HE1	1.77	0.48
3:m:262:LYS:HD2	3:m:269:MET:CE	2.43	0.48
3:q:323:ASP:OD1	3:q:324:LYS:N	2.46	0.48
4:t:265:CYS:SG	4:t:266:ARG:N	2.86	0.48
1:u:11:LEU:HD12	1:u:38:MET:HG3	1.96	0.48
2:y:196:HIS:CD2	2:y:197:HIS:CE1	3.02	0.48
2:1:250:THR:OG1	2:1:251:TRP:N	2.46	0.48
3:5:11:VAL:HA	3:5:33:VAL:HG23	1.95	0.48
4:8:163:THR:HG22	4:8:165:GLU:OE1	2.13	0.48
2:AE:200:VAL:HG12	2:AE:209:ILE:HD13	1.95	0.48
4:B:408:PRO:HB3	3:p:437:ARG:HH12	1.78	0.48
3:G:401:ASP:OD1	3:G:402:MET:N	2.46	0.48
3:H:21:ARG:HB3	3:H:24:TYR:HB2	1.95	0.48
4:K:54:ILE:HG22	4:K:67:ILE:HB	1.94	0.48
1:L:50:ASP:OD1	1:L:51:LEU:N	2.46	0.48
2:O:227:LYS:HD3	2:O:227:LYS:N	2.27	0.48
4:X:45:MET:HE3	4:X:156:TYR:HD2	1.78	0.48
4:X:171:MET:HE1	1:a:40:GLU:OE1	2.13	0.48
4:Z:213:SER:OG	4:Z:214:ASP:N	2.47	0.48
3:i:258:GLY:O	4:j:336:ARG:NH2	2.41	0.48
3:m:308:HIS:HB2	3:m:359:ALA:HA	1.95	0.48
3:o:320:TYR:HE2	3:o:352:VAL:HG23	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:89:TRP:CH2	4:8:72:GLY:HA2	2.48	0.48
5:A:95:PRO:CD	5:A:111:ARG:HE	2.26	0.48
1:AA:21:PRO:HG2	1:AA:24:VAL:HG23	1.94	0.48
3:F:47:ILE:HD11	3:F:118:HIS:CG	2.49	0.48
3:G:207:THR:HG22	3:G:210:SER:HB2	1.95	0.48
3:H:327:ASP:OD1	3:H:345:LYS:HD2	2.13	0.48
4:J:402:THR:HG22	2:P:256:VAL:HG23	1.96	0.48
2:O:195:TRP:CD1	2:O:196:HIS:H	2.32	0.48
3:U:312:PHE:HA	3:U:357:SER:HB2	1.96	0.48
3:V:160:GLN:HB2	3:V:281:ASN:HB3	1.95	0.48
4:j:139:GLU:OE1	4:j:331:ASN:HB2	2.14	0.48
2:1:226:ASN:HB2	2:1:227:LYS:NZ	2.29	0.48
3:F:333:HIS:HB2	3:F:366:VAL:HG23	1.95	0.48
4:I:66:LYS:HD3	4:I:77:ASN:ND2	2.29	0.48
4:J:308:GLU:OE1	4:J:316:ARG:NH1	2.47	0.48
4:R:231:ASP:OD1	4:R:232:HIS:N	2.46	0.48
1:g:37:ARG:HA	1:g:37:ARG:NE	2.28	0.48
4:j:260:LEU:HD12	4:j:261:ASP:H	1.77	0.48
3:6:230:HIS:CD2	3:6:232:PRO:HG3	2.48	0.48
2:AC:209:ILE:HB	2:AC:244:THR:HB	1.96	0.48
4:B:246:ASP:HB3	4:B:248:PRO:HD2	1.96	0.48
2:D:175:VAL:HA	2:D:178:ARG:HG3	1.95	0.48
4:K:201:CYS:HA	4:K:224:GLN:O	2.13	0.48
1:L:33:GLU:OE2	1:L:37:ARG:HG3	2.14	0.48
4:R:163:THR:HG21	4:R:256:ILE:O	2.13	0.48
4:R:359:TYR:O	4:R:363:PRO:HB3	2.13	0.48
3:V:308:HIS:HB2	3:V:359:ALA:HA	1.96	0.48
4:j:343:THR:OG1	4:j:360:GLY:HA3	2.14	0.48
3:m:59:TYR:CE2	3:m:61:LYS:HB2	2.48	0.48
1:v:8:MET:N	1:v:8:MET:SD	2.87	0.48
2:y:123:VAL:HG12	2:y:131:GLY:H	1.79	0.48
2:1:162:LYS:HD3	2:1:169:GLU:HG2	1.96	0.48
3:6:184:VAL:HG11	3:6:261:ILE:HG21	1.95	0.48
4:7:149:LYS:HB3	4:7:149:LYS:HE2	1.61	0.48
4:8:293:LEU:HD12	4:8:308:GLU:O	2.14	0.48
3:E:298:ASP:O	3:E:320:TYR:HA	2.14	0.48
4:I:169:MET:HE1	4:I:236:GLN:O	2.14	0.48
2:Q:202:TYR:HD2	2:Q:207:PHE:HE1	1.62	0.48
2:Q:207:PHE:HE2	2:Q:223:ILE:HG21	1.78	0.48
3:p:144:VAL:HG21	3:p:156:ILE:HD11	1.95	0.48
4:s:290:HIS:O	4:s:292:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:312:PHE:HA	3:4:357:SER:OG	2.14	0.48
4:J:195:LYS:HB3	4:J:229:VAL:HG13	1.95	0.48
4:J:396:LEU:O	4:J:396:LEU:HD23	2.14	0.48
4:K:100:PHE:HZ	4:K:167:ILE:HD11	1.79	0.48
2:P:218:ASP:O	2:P:221:ARG:HG2	2.14	0.48
3:W:219:LEU:HD12	3:W:235:GLN:HB2	1.94	0.48
4:Y:180:LEU:HD11	4:Y:227:VAL:HG11	1.96	0.48
4:Y:290:HIS:O	4:Y:292:THR:HG23	2.14	0.48
4:Z:343:THR:OG1	4:Z:344:GLU:N	2.46	0.48
2:d:225:ASP:N	2:d:229:ARG:O	2.43	0.48
3:h:317:THR:HG22	3:h:353:THR:HG22	1.96	0.48
2:y:195:TRP:CE3	2:y:197:HIS:HB2	2.49	0.48
4:z:290:HIS:O	4:z:292:THR:HG23	2.14	0.48
4:8:387:MET:SD	4:8:388:LEU:HD12	2.54	0.47
2:AD:122:GLU:HG2	2:AD:132:TYR:CE2	2.49	0.47
4:B:131:HIS:CE1	4:B:133:PRO:HD3	2.49	0.47
3:F:59:TYR:HE1	3:F:61:LYS:HB2	1.79	0.47
3:F:89:TRP:CZ2	4:I:72:GLY:HA2	2.49	0.47
4:J:250:ARG:NH2	1:M:37:ARG:HE	2.12	0.47
1:L:16:PHE:CE2	1:L:21:PRO:HA	2.49	0.47
3:U:308:HIS:HB2	3:U:359:ALA:HA	1.95	0.47
4:Z:217:ILE:HG23	4:Z:219:THR:H	1.79	0.47
4:j:197:VAL:HG11	4:j:227:VAL:HG22	1.96	0.47
3:p:257:PHE:HE1	4:s:301:GLU:HG3	1.79	0.47
1:v:38:MET:HE1	1:v:51:LEU:HD21	1.96	0.47
3:4:336:VAL:HG22	3:4:397:VAL:HG11	1.95	0.47
2:T:124:LYS:HZ1	2:T:151:ASP:HB2	1.78	0.47
3:V:249:THR:HA	4:Y:305:TYR:OH	2.13	0.47
3:W:149:ASN:O	3:W:151:ASP:N	2.46	0.47
4:X:204:GLY:C	4:X:206:GLY:H	2.21	0.47
3:i:303:VAL:HG11	3:i:378:ALA:HB2	1.96	0.47
3:i:432:THR:HG22	4:j:394:LYS:NZ	2.29	0.47
3:o:333:HIS:HB2	3:o:366:VAL:CG1	2.43	0.47
4:r:235:TRP:HZ2	1:u:40:GLU:HG3	1.78	0.47
4:s:237:PHE:HD2	4:s:239:SER:HB2	1.78	0.47
2:x:140:VAL:CG2	2:x:173:ILE:HG22	2.44	0.47
2:3:124:LYS:HA	2:3:129:VAL:HA	1.96	0.47
4:7:128:GLN:N	4:z:143:ILE:HD11	2.29	0.47
3:H:31:MET:HE1	3:H:278:VAL:HG11	1.95	0.47
3:H:184:VAL:HG12	3:H:261:ILE:HG21	1.95	0.47
4:I:100:PHE:HZ	4:I:167:ILE:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:55:GLY:H	4:J:67:ILE:HG22	1.78	0.47
4:R:180:LEU:HB2	4:R:227:VAL:HG21	1.96	0.47
4:R:231:ASP:OD1	4:R:233:LYS:N	2.34	0.47
4:X:404:GLY:HA3	2:d:254:ASP:OD1	2.14	0.47
1:g:10:VAL:HG13	1:g:45:ARG:HH12	1.77	0.47
3:h:136:MET:HE1	6:fA:1:NAG:H83	1.94	0.47
3:i:16:LYS:HZ1	3:i:342:ALA:HB2	1.80	0.47
4:j:188:VAL:HG22	4:j:217:ILE:HG22	1.95	0.47
1:AB:31:ASN:O	1:AB:35:THR:HG23	2.14	0.47
1:AB:35:THR:O	1:AB:39:LEU:HD23	2.15	0.47
2:AD:249:VAL:HG22	2:AD:258:ARG:HG3	1.95	0.47
4:B:169:MET:HB3	4:B:235:TRP:HB3	1.97	0.47
3:F:437:ARG:NE	4:r:412:GLY:HA2	2.29	0.47
3:U:95:PHE:CE2	4:X:226:HIS:HB2	2.48	0.47
3:V:230:HIS:CD2	3:V:232:PRO:HG3	2.49	0.47
4:X:35:GLU:HA	4:X:35:GLU:OE1	2.15	0.47
4:Y:199:TYR:HE1	4:Y:211:THR:HG23	1.77	0.47
2:e:188:LYS:HB3	2:e:202:TYR:CE2	2.49	0.47
1:g:9:CYS:SG	1:g:51:LEU:HD12	2.54	0.47
4:j:261:ASP:OD1	4:j:262:ASN:N	2.41	0.47
3:o:402:MET:HA	3:o:407:LEU:HD12	1.96	0.47
4:8:265:CYS:SG	4:8:266:ARG:N	2.87	0.47
4:9:54:ILE:HG22	4:9:67:ILE:HB	1.95	0.47
2:AD:210:PRO:HA	2:AD:243:ARG:NE	2.22	0.47
3:E:93:TYR:HB3	4:R:176:PRO:HG3	1.95	0.47
3:F:296:ILE:HD11	3:F:346:VAL:HG11	1.96	0.47
3:H:280:MET:HE3	3:H:282:LEU:HD11	1.96	0.47
4:I:204:GLY:C	4:I:206:GLY:H	2.20	0.47
2:O:235:LEU:HD11	2:O:249:VAL:HB	1.96	0.47
4:j:112:GLN:HB3	4:j:126:ARG:HB3	1.97	0.47
3:m:58:PRO:HG3	3:m:231:VAL:HG23	1.95	0.47
4:t:290:HIS:O	4:t:292:THR:HG23	2.14	0.47
3:4:62:CYS:HB2	3:4:100:ASN:OD1	2.15	0.47
3:6:60:VAL:HG11	3:6:86:PRO:HG2	1.96	0.47
2:AE:225:ASP:N	2:AE:229:ARG:O	2.34	0.47
2:AE:234:VAL:HA	2:AE:248:VAL:HG12	1.96	0.47
3:F:50:GLU:OE1	3:F:241:LYS:HE3	2.14	0.47
3:F:437:ARG:HH11	4:r:411:LEU:HG	1.79	0.47
4:J:15:TYR:HB2	4:J:236:GLN:HE21	1.79	0.47
3:U:398:VAL:HG21	4:X:362:TYR:OH	2.15	0.47
4:Z:320:VAL:HG12	4:Z:325:MET:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:88:MET:HE3	3:i:93:TYR:CE1	2.50	0.47
4:j:273:PRO:HD3	4:j:329:TRP:CD1	2.50	0.47
4:r:188:VAL:HG22	4:r:217:ILE:HG22	1.95	0.47
4:r:233:LYS:NZ	1:u:32:ALA:HB3	2.27	0.47
4:s:199:TYR:CZ	4:s:215:MET:HE1	2.50	0.47
2:y:202:TYR:CZ	2:y:205:GLY:HA2	2.50	0.47
3:4:50:GLU:O	3:4:111:SER:HB3	2.15	0.47
3:5:318:LEU:HB2	3:5:352:VAL:HG22	1.95	0.47
3:6:59:TYR:HB2	4:9:244:ARG:HD3	1.96	0.47
4:8:171:MET:N	4:8:171:MET:HE2	2.29	0.47
4:9:246:ASP:OD2	4:9:250:ARG:NE	2.48	0.47
4:9:299:LEU:HD12	4:9:299:LEU:O	2.14	0.47
5:A:103:GLU:OE1	5:A:111:ARG:HG2	2.15	0.47
2:AC:200:VAL:HG12	2:AC:209:ILE:HD13	1.96	0.47
4:B:174:ASP:OD1	4:B:174:ASP:N	2.46	0.47
4:B:188:VAL:HG22	4:B:217:ILE:HG22	1.97	0.47
2:D:176:HIS:ND1	2:D:177:MET:SD	2.87	0.47
2:D:195:TRP:CD1	2:D:196:HIS:H	2.33	0.47
2:D:238:ALA:O	2:D:244:THR:HA	2.15	0.47
3:E:46:TYR:O	3:E:47:ILE:HD13	2.14	0.47
4:I:138:ARG:CZ	4:I:293:LEU:HD23	2.44	0.47
2:P:195:TRP:HD1	2:P:196:HIS:H	1.62	0.47
3:V:209:GLU:OE1	3:V:209:GLU:N	2.48	0.47
4:X:149:LYS:HG3	4:X:269:MET:SD	2.54	0.47
4:Y:67:ILE:HD11	4:Y:115:ILE:HD13	1.96	0.47
4:Z:251:LYS:O	1:c:43:VAL:HG11	2.14	0.47
3:h:50:GLU:O	3:h:111:SER:HB3	2.14	0.47
3:h:149:ASN:O	3:h:151:ASP:N	2.47	0.47
3:i:167:SER:HB3	3:i:275:ASN:H	1.80	0.47
3:i:302:THR:OG1	3:i:317:THR:OG1	2.33	0.47
4:j:215:MET:SD	4:j:216:THR:N	2.88	0.47
3:m:84:VAL:HG21	3:m:102:GLN:HB2	1.97	0.47
3:o:359:ALA:HB2	3:o:394:HIS:CD2	2.50	0.47
3:p:42:LEU:HD23	3:p:122:TYR:CG	2.50	0.47
3:p:289:ARG:HB3	3:p:292:GLU:OE2	2.14	0.47
4:r:237:PHE:HD2	4:r:239:SER:HB2	1.80	0.47
4:r:310:VAL:HG11	4:r:329:TRP:HZ3	1.80	0.47
4:s:294:PHE:HZ	4:s:318:ILE:HD11	1.79	0.47
4:t:308:GLU:CD	4:t:316:ARG:HH12	2.21	0.47
4:z:169:MET:HA	4:z:169:MET:HE3	1.96	0.47
6:FA:2:NAG:O3	6:FA:3:BMA:O2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:134:ARG:NH2	6:BA:1:NAG:H3	2.30	0.47
3:6:149:ASN:O	3:6:151:ASP:N	2.47	0.47
1:AB:38:MET:SD	1:AB:51:LEU:HD11	2.55	0.47
2:AD:176:HIS:ND1	2:AD:177:MET:SD	2.88	0.47
3:F:42:LEU:HD11	3:F:266:VAL:HG22	1.97	0.47
4:K:208:VAL:HG11	6:TA:1:NAG:O7	2.15	0.47
3:V:322:THR:OG1	3:V:323:ASP:N	2.48	0.47
4:j:202:THR:OG1	4:j:224:GLN:OE1	2.25	0.47
1:l:31:ASN:O	1:l:35:THR:OG1	2.32	0.47
4:r:402:THR:HG23	2:x:256:VAL:HG23	1.96	0.47
4:t:77:ASN:C	4:t:77:ASN:ND2	2.73	0.47
4:t:169:MET:HA	4:t:169:MET:HE3	1.96	0.47
3:6:202:ASP:OD1	3:6:202:ASP:N	2.45	0.47
2:AC:162:LYS:HG2	2:AC:169:GLU:HB3	1.95	0.47
4:J:102:LEU:HD11	4:J:258:PHE:CD2	2.50	0.47
2:O:252:ASN:OD1	2:O:253:LYS:N	2.42	0.47
2:T:201:GLN:OE1	2:T:201:GLN:N	2.47	0.47
3:h:331:HIS:CD2	3:h:332:SER:H	2.33	0.47
3:m:46:TYR:O	3:m:47:ILE:HD13	2.15	0.47
3:m:341:GLU:N	3:m:341:GLU:OE1	2.48	0.47
3:o:382:PRO:HG3	4:r:357:TYR:HE1	1.79	0.47
4:s:169:MET:HB3	4:s:235:TRP:HB3	1.95	0.47
4:s:320:VAL:HG13	4:s:320:VAL:O	2.15	0.47
3:6:323:ASP:OD1	3:6:324:LYS:N	2.48	0.47
2:D:255:MET:CE	3:h:438:ARG:HD3	2.44	0.47
3:E:199:ARG:NH1	3:E:242:TYR:OH	2.49	0.47
4:I:211:THR:OG1	4:I:212:ASN:N	2.47	0.47
4:J:67:ILE:O	4:J:77:ASN:HA	2.15	0.47
2:Q:209:ILE:HD11	2:Q:246:LEU:HD11	1.97	0.47
3:V:437:ARG:NH1	4:z:408:PRO:HB3	2.29	0.47
2:e:227:LYS:HD3	2:e:227:LYS:N	2.29	0.47
2:f:201:GLN:HB2	2:f:208:THR:OG1	2.15	0.47
3:h:19:ILE:HD11	3:h:280:MET:HE1	1.96	0.47
3:h:225:SER:H	3:h:230:HIS:CE1	2.33	0.47
4:j:139:GLU:HB3	4:j:290:HIS:CD2	2.50	0.47
4:s:50:PHE:CE1	4:s:101:ILE:HD11	2.49	0.47
4:s:158:GLN:N	4:s:158:GLN:OE1	2.48	0.47
4:s:416:CYS:SG	4:s:418:PRO:HD2	2.55	0.47
4:t:69:TYR:OH	4:t:117:ASP:OD1	2.25	0.47
3:5:296:ILE:HG21	3:5:299:LEU:HD12	1.96	0.46
4:7:12:THR:HA	4:7:235:TRP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:180:LEU:HD12	4:7:227:VAL:HG11	1.95	0.46
5:A:151:ASN:O	5:A:152:ILE:HB	2.15	0.46
3:F:24:TYR:OH	3:F:289:ARG:NH2	2.48	0.46
3:F:306:CYS:HB3	3:F:380:CYS:HA	1.97	0.46
3:H:35:GLU:HB3	3:H:132:LYS:HG2	1.96	0.46
3:H:340:GLN:HB3	3:H:341:GLU:OE1	2.15	0.46
4:K:201:CYS:HA	4:K:224:GLN:HG3	1.97	0.46
3:V:30:GLN:HB2	3:V:136:MET:HG3	1.97	0.46
4:Z:237:PHE:HD2	4:Z:239:SER:HB2	1.80	0.46
4:j:67:ILE:HD11	4:j:80:ARG:HA	1.97	0.46
3:o:11:VAL:HA	3:o:33:VAL:HG23	1.97	0.46
2:y:144:ALA:HB1	2:y:162:LYS:HE2	1.97	0.46
3:5:99:GLU:N	3:5:99:GLU:OE2	2.49	0.46
5:A:111:ARG:N	5:A:111:ARG:HD2	2.30	0.46
4:R:76:GLU:N	4:R:76:GLU:OE2	2.48	0.46
3:V:11:VAL:HA	3:V:33:VAL:HG23	1.96	0.46
3:V:145:ASP:OD1	3:V:145:ASP:N	2.46	0.46
3:V:258:GLY:HA3	4:Y:299:LEU:HB2	1.97	0.46
4:Z:149:LYS:HB3	4:Z:149:LYS:HE2	1.68	0.46
2:d:123:VAL:HG22	2:d:150:ILE:HA	1.96	0.46
3:m:83:GLY:HA2	3:m:98:SER:O	2.16	0.46
3:p:384:LYS:HE2	3:p:384:LYS:HB2	1.73	0.46
3:q:341:GLU:OE1	3:q:341:GLU:N	2.49	0.46
4:s:50:PHE:HE2	4:s:54:ILE:HD13	1.80	0.46
4:t:246:ASP:OD1	4:t:246:ASP:N	2.47	0.46
3:4:49:CYS:O	3:4:203:ILE:HD11	2.15	0.46
3:6:330:VAL:HG21	3:6:354:LEU:HD21	1.96	0.46
4:B:11:ALA:O	4:B:235:TRP:N	2.48	0.46
4:B:260:LEU:HD23	4:B:260:LEU:H	1.80	0.46
3:G:30:GLN:HB2	3:G:136:MET:HG2	1.97	0.46
4:R:402:THR:O	2:T:139:LYS:NZ	2.48	0.46
4:Y:253:LYS:HE2	4:Y:253:LYS:HB3	1.74	0.46
2:d:108:ARG:HA	2:d:111:MET:CE	2.46	0.46
3:i:379:SER:HG	4:j:348:HIS:CE1	2.32	0.46
3:m:30:GLN:HB2	3:m:136:MET:HG2	1.98	0.46
4:s:211:THR:HG21	4:s:215:MET:SD	2.55	0.46
4:s:250:ARG:HG2	1:v:40:GLU:HB3	1.96	0.46
4:t:174:ASP:N	4:t:174:ASP:OD1	2.49	0.46
2:3:210:PRO:HA	2:3:243:ARG:NE	2.28	0.46
3:4:249:THR:HG22	4:7:305:TYR:CZ	2.50	0.46
4:7:288:PRO:HG3	4:7:310:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:8:402:THR:HG22	2:AD:256:VAL:HG23	1.97	0.46
2:AC:141:MET:HE2	2:AC:141:MET:HB3	1.88	0.46
2:AD:143:PRO:HB2	2:AD:146:VAL:HG12	1.97	0.46
3:E:306:CYS:HB3	3:E:380:CYS:HA	1.97	0.46
3:H:323:ASP:OD1	3:H:324:LYS:N	2.47	0.46
4:K:138:ARG:NH2	4:K:293:LEU:HD23	2.27	0.46
4:K:408:PRO:HA	4:K:411:LEU:HB3	1.97	0.46
1:L:8:MET:O	1:L:45:ARG:NH2	2.49	0.46
3:U:7:MET:HE3	3:U:278:VAL:HG21	1.96	0.46
3:U:33:VAL:HA	3:U:133:VAL:HG12	1.97	0.46
3:m:202:ASP:N	3:m:202:ASP:OD1	2.47	0.46
4:r:204:GLY:C	4:r:206:GLY:H	2.22	0.46
4:s:314:VAL:HG22	4:s:315:GLU:H	1.80	0.46
4:s:343:THR:OG1	4:s:344:GLU:N	2.49	0.46
4:t:182:SER:HB2	4:t:189:LYS:HB2	1.96	0.46
4:9:56:ILE:O	4:9:68:ARG:HG3	2.15	0.46
4:9:203:CYS:SG	4:9:224:GLN:HG2	2.55	0.46
5:A:197:GLU:OE2	5:A:205:CYS:HA	2.15	0.46
2:D:174:PRO:HG2	2:D:177:MET:HE2	1.97	0.46
3:E:149:ASN:O	3:E:151:ASP:N	2.48	0.46
3:F:59:TYR:HB2	4:I:244:ARG:NE	2.30	0.46
4:I:34:ILE:HG22	4:I:35:GLU:O	2.15	0.46
4:J:316:ARG:HD3	4:J:316:ARG:HA	1.71	0.46
4:K:87:THR:HG22	4:K:88:SER:N	2.26	0.46
4:Z:271:ARG:O	4:Z:329:TRP:NE1	2.40	0.46
4:Z:346:LYS:HB2	4:Z:346:LYS:HE2	1.72	0.46
4:j:138:ARG:CZ	4:j:293:LEU:HD23	2.46	0.46
3:o:144:VAL:HG21	3:o:156:ILE:HD11	1.97	0.46
2:x:209:ILE:HG22	2:x:212:GLY:H	1.81	0.46
4:8:54:ILE:HG22	4:8:67:ILE:HB	1.95	0.46
3:H:437:ARG:HH12	4:J:411:LEU:HG	1.80	0.46
4:K:401:LEU:HD22	2:Q:168:LEU:HD23	1.97	0.46
2:T:122:GLU:HG2	2:T:132:TYR:HE1	1.81	0.46
2:d:141:MET:SD	2:d:141:MET:N	2.89	0.46
2:e:218:ASP:OD1	2:e:221:ARG:HD3	2.15	0.46
4:j:54:ILE:HG22	4:j:67:ILE:CG2	2.45	0.46
3:m:146:VAL:HG11	3:m:163:PHE:CD1	2.51	0.46
3:p:161:PHE:O	3:p:162:ILE:HD13	2.15	0.46
3:q:59:TYR:CE2	3:q:61:LYS:HB2	2.50	0.46
3:q:94:CYS:HB3	3:q:100:ASN:OD1	2.16	0.46
4:r:201:CYS:HA	4:r:224:GLN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:271:ARG:NH2	4:r:289:ASP:OD1	2.46	0.46
2:y:173:ILE:HD12	2:y:178:ARG:HA	1.97	0.46
4:7:188:VAL:HG22	4:7:217:ILE:HG22	1.96	0.46
4:7:298:THR:HA	4:7:325:MET:HB3	1.97	0.46
2:AC:142:LYS:HE3	2:AC:169:GLU:OE2	2.15	0.46
3:F:153:ALA:HB2	3:F:162:ILE:HG12	1.98	0.46
3:H:71:LYS:HE2	3:H:73:LYS:HZ2	1.81	0.46
3:U:428:LEU:HD13	4:X:391:ALA:HB2	1.97	0.46
4:X:138:ARG:CZ	4:X:293:LEU:HD23	2.45	0.46
4:X:235:TRP:HZ2	1:a:40:GLU:HG3	1.80	0.46
4:Z:195:LYS:HD2	4:Z:229:VAL:HG11	1.97	0.46
3:i:42:LEU:HD23	3:i:122:TYR:CG	2.50	0.46
4:s:288:PRO:HG3	4:s:310:VAL:HG12	1.98	0.46
4:z:237:PHE:HD2	4:z:239:SER:HB2	1.81	0.46
1:0:37:ARG:HH12	4:7:171:MET:HG3	1.80	0.46
1:0:40:GLU:OE2	4:7:235:TRP:NE1	2.34	0.46
3:6:50:GLU:O	3:6:111:SER:HB3	2.16	0.46
3:6:252:ASN:HB3	3:6:261:ILE:HB	1.98	0.46
3:6:318:LEU:HB2	3:6:352:VAL:CG1	2.45	0.46
4:7:204:GLY:C	4:7:206:GLY:H	2.23	0.46
4:9:158:GLN:OE1	4:9:158:GLN:N	2.48	0.46
3:F:129:LEU:HD22	3:F:148:VAL:HB	1.98	0.46
4:J:15:TYR:CB	4:J:236:GLN:HE21	2.29	0.46
4:J:168:ASP:O	4:J:169:MET:HE2	2.16	0.46
3:U:125:HIS:ND1	3:U:126:THR:HG22	2.31	0.46
4:X:411:LEU:HD11	4:X:416:CYS:SG	2.55	0.46
4:Y:320:VAL:O	4:Y:320:VAL:HG13	2.16	0.46
2:e:221:ARG:HG2	2:e:221:ARG:NH1	2.31	0.46
2:f:250:THR:OG1	2:f:251:TRP:N	2.49	0.46
1:l:11:LEU:O	1:l:13:ASN:N	2.48	0.46
3:o:253:THR:HG23	4:r:305:TYR:HE1	1.80	0.46
3:o:333:HIS:HB2	3:o:366:VAL:HG13	1.97	0.46
4:z:141:PHE:CE2	4:z:267:VAL:HG12	2.51	0.46
4:z:396:LEU:HD12	4:z:396:LEU:HA	1.80	0.46
4:7:402:THR:HG23	2:AC:256:VAL:HG23	1.98	0.46
4:8:182:SER:OG	4:8:184:GLN:OE1	2.32	0.46
5:A:118:ILE:HB	5:A:130:VAL:HG22	1.98	0.46
4:K:13:ARG:HB3	4:K:234:LYS:HD3	1.98	0.46
2:O:226:ASN:C	2:O:227:LYS:HD3	2.41	0.46
2:T:215:LYS:HE3	2:T:216:PRO:HD2	1.97	0.46
3:W:225:SER:H	3:W:230:HIS:CE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:316:ARG:HD3	4:Y:316:ARG:HA	1.72	0.46
3:h:82:THR:O	3:h:223:ARG:NH2	2.49	0.46
3:h:109:ASP:OD1	3:h:110:ARG:N	2.45	0.46
3:p:93:TYR:HD1	4:s:176:PRO:HG3	1.81	0.46
3:p:113:VAL:HG22	3:p:116:HIS:HB2	1.98	0.46
3:p:308:HIS:HB2	3:p:359:ALA:HA	1.98	0.46
4:s:408:PRO:HA	4:s:411:LEU:HB3	1.98	0.46
3:4:289:ARG:N	3:4:292:GLU:OE2	2.47	0.46
3:4:299:LEU:HD12	3:4:320:TYR:HB3	1.98	0.46
3:6:228:MET:HE1	4:9:18:TYR:CE2	2.51	0.46
4:7:73:HIS:CD2	4:7:195:LYS:HD3	2.51	0.46
2:AD:234:VAL:HA	2:AD:248:VAL:HG23	1.98	0.46
4:B:144:ARG:NH2	4:B:266:ARG:HD3	2.31	0.46
3:H:382:PRO:HG3	4:K:357:TYR:HE1	1.80	0.46
4:I:144:ARG:HA	4:I:145:PRO:HD3	1.82	0.46
4:J:50:PHE:HB3	4:J:52:ALA:H	1.80	0.46
4:J:327:TYR:CE1	4:J:335:VAL:HB	2.51	0.46
4:K:299:LEU:HD12	4:K:299:LEU:O	2.16	0.46
4:K:378:LEU:O	4:K:381:ILE:HG22	2.16	0.46
3:V:225:SER:H	3:V:230:HIS:HE1	1.64	0.46
4:X:54:ILE:HD11	4:X:101:ILE:HG22	1.98	0.46
4:X:246:ASP:OD1	4:X:248:PRO:HD2	2.16	0.46
2:e:175:VAL:HA	2:e:178:ARG:HG3	1.98	0.46
3:h:146:VAL:HG11	3:h:163:PHE:HD1	1.81	0.46
3:i:437:ARG:HD3	3:i:437:ARG:HA	1.76	0.46
3:p:341:GLU:OE1	3:p:354:LEU:HA	2.16	0.46
4:t:397:THR:N	4:t:398:PRO:HD2	2.31	0.46
2:y:145:HIS:NE2	2:y:266:GLU:HB3	2.30	0.46
6:PA:1:NAG:H61	6:PA:2:NAG:HN2	1.81	0.46
4:7:376:LEU:HD23	4:7:376:LEU:HA	1.75	0.45
4:B:402:THR:HG23	2:D:256:VAL:HG23	1.97	0.45
3:E:252:ASN:ND2	3:E:261:ILE:HB	2.31	0.45
3:H:258:GLY:HA3	4:K:299:LEU:HB2	1.98	0.45
4:I:54:ILE:HG23	4:I:67:ILE:CG2	2.45	0.45
4:J:172:PRO:HB3	4:J:236:GLN:OE1	2.16	0.45
4:K:181:LEU:HD12	4:K:227:VAL:HG23	1.98	0.45
2:T:125:HIS:HD2	2:T:148:GLY:HA2	1.80	0.45
4:X:10:LYS:O	4:X:234:LYS:NZ	2.48	0.45
2:f:141:MET:HE1	2:f:251:TRP:HZ2	1.81	0.45
3:m:430:VAL:O	3:m:434:ILE:HG12	2.15	0.45
4:r:182:SER:O	4:r:188:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:203:CYS:HB3	4:r:220:CYS:HB3	1.53	0.45
1:u:38:MET:SD	1:u:51:LEU:HD21	2.56	0.45
2:y:184:TYR:HB2	2:y:251:TRP:HZ3	1.81	0.45
6:tA:3:BMA:O4	6:tA:3:BMA:O6	2.29	0.45
3:5:407:LEU:HD23	3:5:407:LEU:HA	1.71	0.45
4:9:308:GLU:CD	4:9:316:ARG:HH12	2.22	0.45
3:H:95:PHE:CE2	6:TA:1:NAG:H61	2.51	0.45
4:R:134:GLN:OE1	4:R:134:GLN:HA	2.16	0.45
3:U:18:HIS:HD2	3:U:27:LEU:O	1.98	0.45
4:Y:195:LYS:HB3	4:Y:229:VAL:HG13	1.97	0.45
4:Y:343:THR:OG1	4:Y:344:GLU:N	2.44	0.45
4:Y:403:PRO:HG3	2:e:139:LYS:NZ	2.31	0.45
4:Z:299:LEU:HD12	4:Z:299:LEU:O	2.16	0.45
4:Z:411:LEU:HG	3:h:437:ARG:HH12	1.80	0.45
1:b:33:GLU:O	1:b:37:ARG:HG2	2.15	0.45
4:j:403:PRO:N	2:n:139:LYS:HZ1	2.13	0.45
3:o:134:ARG:HG3	3:o:143:THR:HG22	1.98	0.45
3:o:321:LYS:HD3	3:o:321:LYS:HA	1.74	0.45
4:r:327:TYR:CE1	4:r:335:VAL:HB	2.51	0.45
4:r:411:LEU:HD11	4:r:416:CYS:SG	2.55	0.45
2:y:252:ASN:OD1	2:y:253:LYS:N	2.45	0.45
4:z:271:ARG:NH2	4:z:289:ASP:OD1	2.44	0.45
3:6:112:ASP:OD1	3:6:113:VAL:N	2.49	0.45
4:7:83:LEU:HB2	4:7:115:ILE:HD12	1.97	0.45
4:8:237:PHE:HD2	4:8:239:SER:HB2	1.82	0.45
4:9:50:PHE:CZ	4:9:101:ILE:HD11	2.52	0.45
5:A:72:CYS:SG	5:A:78:VAL:HG22	2.56	0.45
2:AC:119:CYS:O	2:AC:120:ILE:HD13	2.16	0.45
4:B:167:ILE:HG23	4:B:237:PHE:HE1	1.81	0.45
3:H:89:TRP:CZ2	4:K:72:GLY:HA2	2.52	0.45
4:I:237:PHE:CD2	4:I:239:SER:HB2	2.51	0.45
4:I:290:HIS:O	4:I:292:THR:HG23	2.15	0.45
4:K:138:ARG:HH12	4:K:328:HIS:CG	2.34	0.45
2:P:138:ASP:OD2	2:Q:206:ARG:NH2	2.49	0.45
2:Q:200:VAL:HG12	2:Q:209:ILE:HD13	1.99	0.45
3:V:62:CYS:HB3	3:V:94:CYS:HA	1.97	0.45
3:V:290:ILE:H	3:V:290:ILE:HD12	1.81	0.45
3:W:259:CYS:HB3	3:W:271:CYS:CA	2.37	0.45
4:Y:166:GLU:OE1	4:Y:253:LYS:HD3	2.16	0.45
4:j:249:ALA:O	4:j:250:ARG:HD2	2.17	0.45
3:o:341:GLU:OE1	3:o:341:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:134:ARG:NH1	6:mA:1:NAG:H5	2.32	0.45
4:t:237:PHE:HD2	4:t:239:SER:HB2	1.80	0.45
2:3:173:ILE:HD11	2:3:178:ARG:HG2	1.98	0.45
3:6:207:THR:HG22	3:6:208:VAL:N	2.31	0.45
4:7:403:PRO:HD3	2:AC:139:LYS:HZ2	1.81	0.45
4:I:246:ASP:CG	4:I:250:ARG:HH11	2.20	0.45
4:J:183:GLN:NE2	4:J:187:ASN:O	2.49	0.45
2:Q:195:TRP:CD1	2:Q:196:HIS:H	2.35	0.45
4:R:67:ILE:O	4:R:77:ASN:HA	2.16	0.45
3:U:296:ILE:HG21	3:U:299:LEU:HD12	1.99	0.45
3:V:89:TRP:CH2	4:Y:72:GLY:HA2	2.51	0.45
3:W:262:LYS:HD2	3:W:269:MET:CE	2.47	0.45
3:W:330:VAL:HA	3:W:368:SER:O	2.17	0.45
2:d:188:LYS:HB3	2:d:202:TYR:HE2	1.81	0.45
3:h:341:GLU:N	3:h:341:GLU:OE2	2.49	0.45
4:j:167:ILE:HG13	4:j:256:ILE:HG12	1.98	0.45
1:l:38:MET:HE2	1:l:38:MET:HB3	1.80	0.45
3:o:197:PRO:HB3	3:o:217:THR:HA	1.98	0.45
4:t:416:CYS:SG	4:t:418:PRO:HD2	2.56	0.45
2:1:131:GLY:O	2:1:132:TYR:HD1	1.99	0.45
3:4:113:VAL:HG21	4:7:40:GLU:HG2	1.98	0.45
3:6:299:LEU:HD23	3:6:373:ARG:C	2.42	0.45
4:8:352:HIS:CE1	4:8:353:GLN:HG3	2.51	0.45
2:AE:195:TRP:CZ3	2:AE:197:HIS:HB2	2.52	0.45
3:H:332:SER:HB2	3:H:339:LEU:HD13	1.99	0.45
4:J:237:PHE:HD2	4:J:239:SER:HB2	1.81	0.45
4:J:404:GLY:HA3	2:P:254:ASP:OD1	2.15	0.45
4:X:141:PHE:CE1	4:X:267:VAL:HG23	2.51	0.45
4:Z:401:LEU:HD12	2:f:166:TYR:HD2	1.81	0.45
3:h:129:LEU:HD22	3:h:148:VAL:HB	1.99	0.45
4:j:416:CYS:SG	4:j:418:PRO:HD2	2.56	0.45
3:m:331:HIS:CD2	3:m:332:SER:H	2.35	0.45
3:o:31:MET:HE1	3:o:280:MET:HE2	1.97	0.45
3:o:84:VAL:O	3:o:100:ASN:ND2	2.47	0.45
3:o:325:ASN:HB3	3:o:347:LYS:HA	1.99	0.45
3:q:42:LEU:HD23	3:q:122:TYR:CD2	2.52	0.45
3:q:113:VAL:HG22	3:q:116:HIS:HB2	1.98	0.45
4:s:402:THR:CG2	2:y:256:VAL:HG23	2.46	0.45
1:u:8:MET:O	1:u:45:ARG:NH2	2.50	0.45
2:y:196:HIS:CD2	2:y:197:HIS:HD1	2.34	0.45
4:z:15:TYR:CB	4:z:236:GLN:HE21	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:120:ILE:HG23	2:3:132:TYR:HB3	1.97	0.45
5:A:229:CYS:HB3	5:A:231:ARG:HG3	1.98	0.45
2:AC:201:GLN:HB3	2:AC:208:THR:OG1	2.17	0.45
4:B:139:GLU:OE1	4:B:290:HIS:NE2	2.50	0.45
3:H:184:VAL:CG1	3:H:261:ILE:HG21	2.47	0.45
4:R:15:TYR:HB3	4:R:236:GLN:HG3	1.97	0.45
3:V:242:TYR:O	3:V:246:GLU:HG2	2.17	0.45
3:W:431:VAL:O	3:W:434:ILE:HG22	2.17	0.45
3:h:327:ASP:N	3:h:327:ASP:OD1	2.50	0.45
4:j:235:TRP:HZ2	1:l:40:GLU:HG3	1.80	0.45
3:m:318:LEU:HB2	3:m:352:VAL:CG2	2.46	0.45
3:q:185:PHE:CD1	3:q:250:ALA:HA	2.51	0.45
4:r:171:MET:HE3	4:r:171:MET:HB2	1.85	0.45
4:s:172:PRO:HB3	4:s:236:GLN:OE1	2.16	0.45
4:z:66:LYS:HD2	4:z:77:ASN:ND2	2.31	0.45
3:5:243:TRP:O	3:5:247:LYS:HB3	2.17	0.45
4:8:197:VAL:HG13	4:8:227:VAL:HG13	1.98	0.45
4:9:13:ARG:HA	4:9:68:ARG:NH2	2.32	0.45
4:9:347:PRO:HG3	4:9:357:TYR:CG	2.52	0.45
2:AE:124:LYS:HD3	2:AE:127:GLY:C	2.42	0.45
2:D:209:ILE:HG22	2:D:211:THR:H	1.81	0.45
3:E:5:THR:HG22	3:E:6:VAL:N	2.32	0.45
3:F:151:ASP:HA	3:p:191:PRO:HB3	1.99	0.45
3:G:318:LEU:HB2	3:G:352:VAL:HG12	1.99	0.45
4:I:157:GLN:NE2	4:I:261:ASP:HB3	2.32	0.45
3:W:50:GLU:O	3:W:111:SER:HB3	2.16	0.45
4:X:201:CYS:HA	4:X:224:GLN:O	2.17	0.45
4:r:149:LYS:HE2	4:r:149:LYS:HB3	1.68	0.45
4:t:21:ASP:HA	4:t:26:HIS:O	2.17	0.45
1:u:38:MET:HE1	1:u:51:LEU:HD11	1.99	0.45
1:0:10:VAL:HG13	1:0:45:ARG:HH12	1.81	0.45
3:5:3:HIS:HB3	3:5:280:MET:HG3	1.99	0.45
3:6:331:HIS:CD2	3:6:332:SER:H	2.34	0.45
4:7:417:ALA:HB3	4:7:418:PRO:HD3	1.99	0.45
4:B:23:GLY:HA2	4:B:126:ARG:HD2	1.97	0.45
3:E:40:PRO:HA	3:E:127:ALA:HA	1.98	0.45
3:F:2:GLU:HG3	3:F:3:HIS:N	2.32	0.45
3:F:323:ASP:OD1	3:F:323:ASP:N	2.48	0.45
3:W:113:VAL:HG22	3:W:116:HIS:HB2	1.98	0.45
4:X:203:CYS:HB3	4:X:224:GLN:OE1	2.16	0.45
4:Y:57:ASP:OD1	4:Y:58:LYS:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:172:PRO:HG3	4:Z:236:GLN:HB2	1.99	0.45
4:Z:244:ARG:NH2	4:Z:247:GLU:OE1	2.49	0.45
3:i:27:LEU:HD12	3:i:27:LEU:HA	1.80	0.45
3:m:141:ASN:O	3:m:142:GLN:CB	2.64	0.45
4:r:235:TRP:CD1	1:u:36:LEU:HD23	2.52	0.45
2:1:252:ASN:CG	2:1:253:LYS:N	2.74	0.45
4:7:195:LYS:HD2	4:7:229:VAL:HG21	1.99	0.45
4:8:166:GLU:OE1	4:8:253:LYS:HB3	2.16	0.45
4:8:347:PRO:HG3	4:8:357:TYR:CD1	2.52	0.45
4:9:401:LEU:HB2	2:AE:256:VAL:HG21	1.97	0.45
2:AC:123:VAL:HG22	2:AC:150:ILE:HA	1.98	0.45
2:AE:124:LYS:HG2	2:AE:128:LYS:C	2.42	0.45
4:B:21:ASP:OD2	4:B:126:ARG:HD3	2.17	0.45
3:F:29:LEU:HD23	3:F:137:TYR:HB3	1.99	0.45
3:G:330:VAL:HG11	3:G:354:LEU:HD11	1.98	0.45
3:H:302:THR:OG1	3:H:317:THR:OG1	2.35	0.45
3:H:437:ARG:HA	3:H:437:ARG:HD3	1.83	0.45
2:Q:138:ASP:C	2:Q:139:LYS:HD3	2.42	0.45
4:j:399:TYR:CE1	2:n:255:MET:HE1	2.52	0.45
4:t:235:TRP:CH2	4:t:252:GLY:HA3	2.52	0.45
4:t:320:VAL:HG12	4:t:325:MET:CG	2.44	0.45
1:v:8:MET:N	1:v:17:PRO:HA	2.32	0.45
3:6:347:LYS:HE3	3:6:348:THR:HG22	1.99	0.45
3:E:149:ASN:C	3:E:151:ASP:H	2.25	0.45
3:F:104:SER:HB3	3:F:231:VAL:HG23	1.99	0.45
3:G:94:CYS:HB3	3:G:100:ASN:ND2	2.31	0.45
3:G:340:GLN:HB3	3:G:341:GLU:OE1	2.17	0.45
4:I:145:PRO:HG2	4:I:268:PRO:HB3	1.98	0.45
4:J:225:CYS:O	4:J:226:HIS:ND1	2.50	0.45
4:R:88:SER:OG	4:R:107:PRO:O	2.29	0.45
2:d:218:ASP:HA	2:d:221:ARG:NH1	2.27	0.45
3:h:94:CYS:HB3	3:h:100:ASN:HD21	1.81	0.45
3:m:311:ASP:N	3:m:311:ASP:OD1	2.50	0.45
2:n:111:MET:SD	2:n:112:CYS:N	2.90	0.45
4:r:230:THR:O	4:r:232:HIS:N	2.50	0.45
1:2:8:MET:O	1:2:45:ARG:NH2	2.49	0.44
3:4:289:ARG:HB2	3:4:292:GLU:OE1	2.17	0.44
3:5:136:MET:HA	3:5:140:VAL:O	2.17	0.44
4:8:67:ILE:O	4:8:67:ILE:HG13	2.16	0.44
2:AE:215:LYS:HE2	2:AE:215:LYS:HB2	1.79	0.44
4:B:318:ILE:HD12	4:B:325:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:341:LEU:HD23	4:B:341:LEU:HA	1.87	0.44
3:E:225:SER:H	3:E:230:HIS:CE1	2.35	0.44
2:Q:136:VAL:HB	2:Q:141:MET:HE3	1.99	0.44
3:V:320:TYR:OH	3:V:347:LYS:N	2.47	0.44
4:Z:32:VAL:O	4:Z:32:VAL:HG12	2.18	0.44
4:Z:34:ILE:HG22	4:Z:125:CYS:SG	2.58	0.44
4:Z:82:SER:HB2	4:Z:116:GLN:HG3	1.98	0.44
4:Z:170:HIS:CE1	4:Z:237:PHE:O	2.70	0.44
4:Z:279:LYS:NZ	4:Z:344:GLU:OE2	2.46	0.44
1:a:31:ASN:O	1:a:35:THR:OG1	2.23	0.44
3:h:359:ALA:HB2	3:h:394:HIS:CD2	2.53	0.44
3:i:435:GLY:HA2	3:i:438:ARG:HD2	1.98	0.44
3:m:42:LEU:HD23	3:m:122:TYR:CD1	2.52	0.44
3:m:49:CYS:O	3:m:203:ILE:HD11	2.17	0.44
3:p:115:ARG:NH1	6:pA:2:NAG:H83	2.32	0.44
4:s:50:PHE:CE2	4:s:54:ILE:HD13	2.52	0.44
3:E:10:VAL:HG23	3:E:13:PHE:HB2	2.00	0.44
3:F:60:VAL:HG13	3:F:60:VAL:O	2.17	0.44
3:F:437:ARG:HB3	4:r:408:PRO:HB3	1.99	0.44
3:H:228:MET:HE1	4:K:18:TYR:CZ	2.52	0.44
3:H:252:ASN:ND2	3:H:261:ILE:HB	2.31	0.44
4:I:5:HIS:ND1	4:I:6:PHE:O	2.51	0.44
4:J:85:VAL:HG13	4:J:91:CYS:HB2	1.99	0.44
2:Q:219:SER:OG	2:Q:267:TRP:O	2.28	0.44
3:V:174:ASP:CG	3:V:175:ASN:H	2.25	0.44
4:Y:167:ILE:HG23	4:Y:237:PHE:HE1	1.81	0.44
3:i:88:MET:HE3	3:i:93:TYR:HE1	1.83	0.44
4:j:34:ILE:HG22	4:j:35:GLU:O	2.18	0.44
4:j:100:PHE:CZ	4:j:167:ILE:HD11	2.52	0.44
3:m:149:ASN:C	3:m:151:ASP:H	2.25	0.44
3:m:196:GLN:OE1	3:m:196:GLN:HA	2.18	0.44
3:p:8:PRO:HB2	3:p:10:VAL:HG12	1.99	0.44
3:p:47:ILE:HD13	3:p:120:SER:HA	1.99	0.44
2:y:173:ILE:HD11	2:y:178:ARG:HG2	2.00	0.44
2:y:237:GLY:HA3	2:y:267:TRP:CH2	2.52	0.44
3:4:141:ASN:O	3:4:142:GLN:HB3	2.18	0.44
3:5:331:HIS:CD2	3:5:332:SER:H	2.35	0.44
3:5:331:HIS:CD2	3:5:332:SER:N	2.86	0.44
4:8:161:ALA:O	4:8:163:THR:OG1	2.34	0.44
2:AD:123:VAL:HG22	2:AD:131:GLY:O	2.17	0.44
2:D:145:HIS:CE1	2:D:266:GLU:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:219:LEU:HD13	3:H:235:GLN:HG3	1.99	0.44
4:J:182:SER:OG	4:J:189:LYS:HB3	2.18	0.44
4:K:392:ARG:HG2	4:K:414:LEU:HD22	2.00	0.44
1:L:9:CYS:HB3	1:L:42:ASN:OD1	2.16	0.44
2:Q:252:ASN:OD1	2:Q:253:LYS:N	2.45	0.44
2:d:247:SER:HB2	2:d:261:PRO:HD2	1.98	0.44
3:i:29:LEU:HG	3:i:137:TYR:HB3	1.99	0.44
3:i:30:GLN:HB2	3:i:136:MET:HG2	1.98	0.44
4:s:399:TYR:HE2	4:s:407:VAL:HG23	1.81	0.44
6:k:1:NAG:H4	6:k:2:NAG:H2	1.75	0.44
6:GA:1:NAG:O6	6:GA:2:NAG:N2	2.50	0.44
3:6:134:ARG:NH2	6:BA:1:NAG:H5	2.33	0.44
4:7:24:ALA:HB2	4:z:92:PHE:HE2	1.83	0.44
4:7:320:VAL:HG12	4:7:325:MET:CG	2.47	0.44
4:9:184:GLN:HG2	4:9:185:SER:N	2.31	0.44
4:9:217:ILE:HG23	4:9:219:THR:H	1.82	0.44
2:D:157:LYS:HE2	2:D:157:LYS:HB3	1.85	0.44
2:D:240:GLU:OE1	2:f:178:ARG:HG3	2.18	0.44
4:I:87:THR:CG2	4:I:88:SER:H	2.25	0.44
4:R:299:LEU:HD12	4:R:299:LEU:O	2.17	0.44
3:V:35:GLU:HG2	3:V:36:THR:N	2.32	0.44
3:W:238:SER:OG	3:W:241:LYS:HB2	2.17	0.44
4:Y:138:ARG:CZ	4:Y:293:LEU:HD23	2.47	0.44
3:h:345:LYS:HE3	3:h:347:LYS:NZ	2.33	0.44
4:j:341:LEU:HD22	4:j:361:LEU:HD22	2.00	0.44
3:m:393:SER:O	3:m:393:SER:OG	2.32	0.44
3:p:16:LYS:HA	3:p:29:LEU:O	2.18	0.44
3:p:437:ARG:HA	3:p:437:ARG:HD3	1.68	0.44
3:q:359:ALA:HB2	3:q:394:HIS:CG	2.52	0.44
4:s:10:LYS:HA	4:s:60:ASP:OD2	2.17	0.44
4:z:141:PHE:HE2	4:z:267:VAL:HG12	1.83	0.44
6:k:1:NAG:H61	6:k:2:NAG:O5	2.17	0.44
4:7:290:HIS:O	4:7:292:THR:HG23	2.17	0.44
4:8:320:VAL:HG13	4:8:320:VAL:O	2.17	0.44
4:B:12:THR:HA	4:B:235:TRP:O	2.17	0.44
3:F:299:LEU:HD12	3:F:320:TYR:HB3	1.99	0.44
4:J:347:PRO:HG3	4:J:357:TYR:CG	2.53	0.44
2:Q:234:VAL:HA	2:Q:248:VAL:HG12	1.99	0.44
2:T:234:VAL:HA	2:T:248:VAL:HG12	2.00	0.44
3:W:76:TYR:OH	3:W:105:GLU:OE1	2.27	0.44
2:f:125:HIS:CE1	2:f:126:GLU:OE2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:259:CYS:HB2	3:h:269:MET:O	2.17	0.44
3:i:141:ASN:O	3:i:142:GLN:CB	2.65	0.44
3:i:244:LEU:HD12	3:i:244:LEU:HA	1.78	0.44
3:i:382:PRO:HD3	4:j:347:PRO:HG3	1.99	0.44
4:j:139:GLU:HB3	4:j:290:HIS:HD2	1.82	0.44
3:m:262:LYS:HD2	3:m:269:MET:HE2	2.00	0.44
3:m:359:ALA:HB2	3:m:394:HIS:CD2	2.53	0.44
2:n:250:THR:OG1	2:n:251:TRP:N	2.50	0.44
3:p:72:GLU:O	3:p:72:GLU:HG2	2.18	0.44
4:t:23:GLY:HA2	4:t:126:ARG:HD2	2.00	0.44
1:v:35:THR:O	1:v:39:LEU:HD23	2.17	0.44
2:1:225:ASP:OD2	2:1:229:ARG:NH2	2.39	0.44
3:4:151:ASP:HA	3:V:191:PRO:HB3	1.99	0.44
4:8:402:THR:CG2	2:AD:256:VAL:HG23	2.48	0.44
4:9:181:LEU:HD11	4:9:225:CYS:HB2	2.00	0.44
4:9:297:ARG:NE	4:9:326:GLU:OE2	2.37	0.44
4:B:32:VAL:O	4:B:32:VAL:HG12	2.17	0.44
2:O:135:LEU:HD23	2:O:140:VAL:HG22	1.98	0.44
2:P:142:LYS:NZ	2:P:143:PRO:O	2.50	0.44
2:P:235:LEU:HB2	2:P:247:SER:O	2.18	0.44
3:U:331:HIS:CD2	3:U:332:SER:N	2.86	0.44
4:Z:169:MET:HE1	4:Z:236:GLN:O	2.18	0.44
3:h:323:ASP:OD1	3:h:324:LYS:N	2.50	0.44
3:i:95:PHE:CD2	6:iA:1:NAG:H62	2.52	0.44
3:i:318:LEU:HB2	3:i:352:VAL:CG2	2.48	0.44
4:j:80:ARG:NH2	4:j:96:THR:OG1	2.51	0.44
3:p:225:SER:H	3:p:230:HIS:CE1	2.36	0.44
3:q:259:CYS:HB3	3:q:271:CYS:CA	2.40	0.44
3:q:303:VAL:HG11	3:q:378:ALA:HB2	2.00	0.44
4:t:138:ARG:CZ	4:t:293:LEU:HD23	2.47	0.44
4:z:320:VAL:O	4:z:320:VAL:HG13	2.17	0.44
1:2:36:LEU:HD22	4:z:235:TRP:CE2	2.53	0.44
3:4:291:VAL:HG23	3:U:355:HIS:NE2	2.33	0.44
3:5:402:MET:HA	3:5:407:LEU:HD13	1.99	0.44
3:E:3:HIS:HB3	3:E:280:MET:HE3	1.98	0.44
4:I:165:GLU:CB	4:I:256:ILE:HG12	2.48	0.44
4:R:246:ASP:OD2	4:R:248:PRO:HG2	2.18	0.44
1:S:38:MET:SD	1:S:51:LEU:HD21	2.58	0.44
4:X:411:LEU:HA	4:X:411:LEU:HD12	1.70	0.44
4:j:299:LEU:HD12	4:j:299:LEU:O	2.18	0.44
3:m:10:VAL:HG12	3:m:272:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:97:ASP:N	3:m:97:ASP:OD1	2.49	0.44
4:t:320:VAL:O	4:t:320:VAL:HG23	2.18	0.44
2:y:187:GLU:OE2	2:y:188:LYS:N	2.51	0.44
1:0:16:PHE:CE2	1:0:21:PRO:HA	2.53	0.44
3:4:21:ARG:HH11	3:4:24:TYR:HE2	1.65	0.44
4:7:35:GLU:HB2	4:7:49:GLN:HG2	1.98	0.44
4:7:318:ILE:HD12	4:7:325:MET:HE1	1.99	0.44
4:B:251:LYS:HE2	4:B:251:LYS:HB3	1.83	0.44
3:E:49:CYS:O	3:E:203:ILE:HD11	2.18	0.44
3:F:97:ASP:OD1	3:F:98:SER:N	2.51	0.44
3:F:146:VAL:HG11	3:F:163:PHE:HD1	1.83	0.44
4:J:293:LEU:HD13	4:J:309:TRP:CE2	2.52	0.44
4:J:392:ARG:NH1	4:J:416:CYS:HA	2.33	0.44
1:S:8:MET:N	1:S:18:CYS:SG	2.91	0.44
4:X:169:MET:HE1	4:X:236:GLN:O	2.18	0.44
1:b:29:GLU:OE2	1:b:29:GLU:N	2.48	0.44
3:i:318:LEU:HB2	3:i:352:VAL:HG22	2.00	0.44
4:j:67:ILE:CD1	4:j:80:ARG:HA	2.48	0.44
3:o:398:VAL:HG21	4:r:362:TYR:OH	2.18	0.44
4:r:54:ILE:HG22	4:r:98:GLY:O	2.18	0.44
4:s:276:ILE:HB	4:s:283:THR:OG1	2.18	0.44
4:t:316:ARG:HD3	4:t:316:ARG:HA	1.69	0.44
3:6:359:ALA:HB2	3:6:394:HIS:CD2	2.52	0.44
4:7:181:LEU:HD23	4:7:181:LEU:HA	1.84	0.44
4:8:199:TYR:CE1	4:8:215:MET:HE1	2.53	0.44
2:AC:196:HIS:HD2	2:AC:197:HIS:CD2	2.35	0.44
4:B:299:LEU:HD12	4:B:299:LEU:O	2.17	0.44
3:F:72:GLU:HA	3:F:72:GLU:OE1	2.18	0.44
3:F:95:PHE:CZ	4:I:226:HIS:HB3	2.53	0.44
3:G:26:PRO:HG2	3:G:370:CYS:O	2.18	0.44
3:G:304:ALA:HB3	3:G:315:VAL:CG1	2.46	0.44
2:O:234:VAL:HA	2:O:248:VAL:HG12	1.99	0.44
2:P:138:ASP:CG	2:Q:206:ARG:HH22	2.26	0.44
3:W:146:VAL:HG11	3:W:163:PHE:CD1	2.52	0.44
3:W:437:ARG:HH12	4:Y:411:LEU:HG	1.83	0.44
3:m:89:TRP:CH2	4:z:72:GLY:HA2	2.53	0.44
3:m:425:ILE:HD13	4:z:387:MET:SD	2.58	0.44
3:o:76:TYR:OH	3:o:105:GLU:OE2	2.25	0.44
4:r:197:VAL:HG21	4:r:227:VAL:HG13	2.00	0.44
2:y:153:ALA:O	2:y:157:LYS:HE3	2.17	0.44
3:6:74:PRO:HG2	3:6:108:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:177:ASP:OD1	4:7:178:ARG:N	2.48	0.43
4:9:87:THR:HG21	4:9:105:CYS:HB3	2.00	0.43
5:A:89:TRP:CZ3	3:V:347:LYS:HD3	2.53	0.43
4:B:15:TYR:CB	4:B:236:GLN:HE21	2.31	0.43
3:G:303:VAL:HG21	3:G:378:ALA:HB2	2.00	0.43
3:G:359:ALA:HB2	3:G:394:HIS:CD2	2.53	0.43
4:I:149:LYS:HB3	4:I:149:LYS:HE2	1.60	0.43
4:I:402:THR:HG22	2:O:251:TRP:HD1	1.83	0.43
4:Z:288:PRO:HG3	4:Z:310:VAL:HG12	1.99	0.43
2:e:138:ASP:O	2:e:173:ILE:HG12	2.18	0.43
3:h:302:THR:OG1	3:h:317:THR:OG1	2.30	0.43
3:m:134:ARG:HB2	3:m:143:THR:HG22	2.00	0.43
3:m:144:VAL:HG21	3:m:156:ILE:HD11	1.99	0.43
3:q:185:PHE:CZ	3:q:247:LYS:HD2	2.53	0.43
3:q:238:SER:OG	3:q:241:LYS:HB2	2.18	0.43
4:t:172:PRO:HG2	4:t:232:HIS:CD2	2.51	0.43
4:t:341:LEU:HD23	4:t:341:LEU:HA	1.86	0.43
2:y:182:SER:OG	2:y:183:LYS:N	2.50	0.43
4:8:87:THR:HG22	4:8:111:LEU:HB3	2.01	0.43
4:8:170:HIS:NE2	4:8:238:ASN:HA	2.34	0.43
4:9:32:VAL:HG12	4:9:32:VAL:O	2.18	0.43
5:A:145:ASP:OD1	5:A:145:ASP:N	2.50	0.43
3:G:115:ARG:HD2	6:RA:2:NAG:H83	2.00	0.43
3:G:203:ILE:CG1	3:G:213:LEU:HD11	2.49	0.43
4:R:6:PHE:CZ	1:g:53:GLN:HA	2.53	0.43
4:R:149:LYS:HB3	4:R:149:LYS:HE2	1.59	0.43
3:i:50:GLU:O	3:i:111:SER:HB3	2.18	0.43
3:p:134:ARG:HB2	3:p:143:THR:HG22	2.01	0.43
1:u:21:PRO:HG2	1:u:24:VAL:HG23	1.99	0.43
1:u:24:VAL:HA	1:u:25:PRO:HA	1.82	0.43
4:z:358:TYR:O	4:z:366:THR:OG1	2.32	0.43
2:1:216:PRO:HA	2:1:267:TRP:HB3	2.00	0.43
3:5:40:PRO:HG3	3:5:173:PHE:CD2	2.53	0.43
3:5:162:ILE:HB	3:5:279:SER:OG	2.19	0.43
4:8:198:LYS:HB3	4:8:210:THR:HG22	2.00	0.43
2:AC:108:ARG:HH21	2:AC:226:ASN:HA	1.82	0.43
2:AD:141:MET:HE1	2:AD:170:CYS:SG	2.59	0.43
3:E:155:THR:HA	3:E:159:THR:O	2.19	0.43
3:F:437:ARG:HD2	4:r:411:LEU:HG	2.01	0.43
3:G:229:VAL:HG23	3:G:229:VAL:O	2.19	0.43
3:G:430:VAL:O	3:G:434:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:432:THR:HG22	4:J:394:LYS:HZ1	1.82	0.43
4:I:180:LEU:HB2	4:I:227:VAL:HG21	2.00	0.43
4:K:308:GLU:CD	4:K:316:ARG:HH12	2.25	0.43
3:W:331:HIS:CD2	3:W:332:SER:N	2.87	0.43
3:W:359:ALA:HB2	3:W:394:HIS:CD2	2.54	0.43
4:Y:7:ASN:O	4:Y:10:LYS:HG3	2.17	0.43
4:Y:237:PHE:CG	4:Y:238:ASN:N	2.86	0.43
1:l:9:CYS:HB3	1:l:42:ASN:ND2	2.33	0.43
3:p:1:TYR:O	3:p:281:ASN:HA	2.19	0.43
4:r:7:ASN:HB3	4:r:10:LYS:HE2	2.00	0.43
4:r:67:ILE:O	4:r:77:ASN:HA	2.18	0.43
4:r:402:THR:HG22	2:x:251:TRP:CD1	2.52	0.43
4:t:251:LYS:O	1:w:43:VAL:HG11	2.17	0.43
3:6:382:PRO:HG3	4:9:357:TYR:CE1	2.54	0.43
4:7:299:LEU:HD12	4:7:299:LEU:O	2.19	0.43
4:8:378:LEU:HA	4:8:381:ILE:HG22	2.00	0.43
4:9:212:ASN:O	4:9:212:ASN:ND2	2.43	0.43
4:9:251:LYS:O	1:AB:43:VAL:HG11	2.18	0.43
5:A:81:ASN:ND2	5:A:98:GLU:HB2	2.33	0.43
1:AB:16:PHE:CE2	1:AB:21:PRO:HA	2.54	0.43
2:AD:209:ILE:HG22	2:AD:212:GLY:H	1.82	0.43
4:I:299:LEU:O	4:I:299:LEU:HD12	2.18	0.43
4:I:343:THR:OG1	4:I:344:GLU:N	2.51	0.43
4:R:333:ASP:OD1	4:R:334:PRO:HD2	2.19	0.43
3:U:134:ARG:HB2	3:U:143:THR:HG22	2.00	0.43
3:V:262:LYS:HD2	3:V:269:MET:CE	2.48	0.43
3:W:59:TYR:CE2	3:W:61:LYS:HB2	2.53	0.43
3:W:206:ARG:HD3	3:W:206:ARG:HA	1.85	0.43
3:W:329:SER:O	3:W:329:SER:OG	2.35	0.43
4:Z:318:ILE:HD12	4:Z:325:MET:CE	2.48	0.43
4:Z:341:LEU:HD22	4:Z:361:LEU:HD22	2.00	0.43
2:e:265:GLU:N	2:e:265:GLU:OE1	2.51	0.43
2:f:108:ARG:O	2:f:111:MET:HG2	2.17	0.43
2:f:240:GLU:HB3	2:f:243:ARG:C	2.43	0.43
3:i:174:ASP:CG	3:i:175:ASN:H	2.27	0.43
4:j:318:ILE:HD12	4:j:325:MET:CE	2.43	0.43
6:MA:1:NAG:H4	6:MA:2:NAG:H2	1.66	0.43
1:0:11:LEU:HD12	1:0:38:MET:HG3	2.01	0.43
1:0:33:GLU:OE2	1:0:37:ARG:NH2	2.45	0.43
2:1:234:VAL:HA	2:1:248:VAL:HG12	1.99	0.43
3:F:161:PHE:CE1	3:F:280:MET:HE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:231:ASP:O	4:J:233:LYS:N	2.49	0.43
4:J:343:THR:OG1	4:J:344:GLU:OE1	2.33	0.43
4:K:85:VAL:HG13	4:K:91:CYS:HB2	2.00	0.43
1:L:11:LEU:O	1:L:13:ASN:N	2.50	0.43
4:R:205:THR:OG1	4:R:206:GLY:N	2.52	0.43
3:U:98:SER:O	3:U:98:SER:OG	2.36	0.43
3:V:437:ARG:HD3	3:V:437:ARG:HA	1.60	0.43
4:Z:101:ILE:HG21	4:Z:101:ILE:HD13	1.79	0.43
4:Z:312:ALA:O	4:Z:314:VAL:HG13	2.19	0.43
1:a:35:THR:HG23	1:a:38:MET:HE2	2.00	0.43
3:m:146:VAL:HG11	3:m:163:PHE:HD1	1.83	0.43
3:q:113:VAL:HG11	4:t:40:GLU:HG2	2.00	0.43
4:r:45:MET:HE3	4:r:156:TYR:HB2	2.00	0.43
2:1:210:PRO:HA	2:1:243:ARG:NE	2.33	0.43
2:3:225:ASP:OD2	2:3:229:ARG:NH2	2.47	0.43
3:4:382:PRO:HG3	4:7:357:TYR:CE1	2.52	0.43
4:9:375:LEU:HA	4:9:375:LEU:HD12	1.80	0.43
3:F:86:PRO:HB3	3:F:229:VAL:HG13	2.00	0.43
4:J:261:ASP:OD1	4:J:262:ASN:N	2.45	0.43
4:K:128:GLN:N	4:Z:143:ILE:HD11	2.34	0.43
1:L:31:ASN:O	1:L:35:THR:OG1	2.19	0.43
4:X:35:GLU:HB2	4:X:49:GLN:HG2	2.01	0.43
4:X:375:LEU:O	4:X:379:ILE:HG12	2.18	0.43
4:Y:133:PRO:O	4:Y:134:GLN:NE2	2.52	0.43
3:m:7:MET:HE3	3:m:7:MET:HB2	1.77	0.43
2:n:187:GLU:OE2	2:n:229:ARG:NH2	2.51	0.43
4:r:273:PRO:HB3	4:r:286:LEU:HD23	2.01	0.43
4:s:40:GLU:OE2	4:s:156:TYR:OH	2.37	0.43
4:s:97:MET:HE1	4:s:160:THR:CG2	2.49	0.43
1:u:26:CYS:HB3	1:u:29:GLU:HB2	2.01	0.43
3:4:185:PHE:CZ	3:4:247:LYS:HD2	2.53	0.43
3:6:199:ARG:O	3:6:239:GLY:HA3	2.19	0.43
4:B:176:PRO:CG	3:h:93:TYR:HB3	2.48	0.43
3:F:19:ILE:HG13	3:F:27:LEU:HB3	2.00	0.43
4:I:180:LEU:HD12	4:I:227:VAL:HG11	1.99	0.43
4:I:260:LEU:HD23	4:I:260:LEU:H	1.83	0.43
4:J:347:PRO:HG3	4:J:357:TYR:CD1	2.54	0.43
4:K:177:ASP:OD1	4:K:178:ARG:N	2.52	0.43
2:T:119:CYS:O	2:T:134:CYS:HA	2.18	0.43
2:d:209:ILE:HG22	2:d:212:GLY:H	1.84	0.43
3:i:221:LEU:HD23	3:i:233:TYR:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:231:VAL:HG13	3:i:231:VAL:O	2.18	0.43
4:j:123:ARG:HA	4:j:123:ARG:HD2	1.90	0.43
2:n:249:VAL:HG12	2:n:258:ARG:HG3	2.01	0.43
3:p:21:ARG:NE	3:p:287:PHE:HE2	2.14	0.43
3:p:223:ARG:HG2	3:p:224:PRO:HD2	2.00	0.43
2:y:116:GLU:OE2	2:y:196:HIS:HB2	2.19	0.43
3:4:141:ASN:O	3:4:142:GLN:CB	2.67	0.43
4:8:327:TYR:CE1	4:8:335:VAL:HB	2.53	0.43
3:E:31:MET:HE1	3:E:278:VAL:HG11	2.00	0.43
3:H:13:PHE:HA	3:H:14:PRO:HD3	1.86	0.43
3:H:52:LYS:HE2	3:H:52:LYS:HB3	1.91	0.43
3:V:325:ASN:HB3	3:V:347:LYS:HD2	2.01	0.43
3:V:426:LEU:HD23	3:V:426:LEU:HA	1.86	0.43
4:X:138:ARG:NH2	4:X:293:LEU:HD23	2.33	0.43
4:Y:314:VAL:HG22	4:Y:315:GLU:N	2.34	0.43
2:f:136:VAL:HG11	2:f:251:TRP:HH2	1.84	0.43
3:p:10:VAL:HG13	3:p:13:PHE:HB2	2.00	0.43
4:r:35:GLU:HB2	4:r:49:GLN:HG2	2.01	0.43
4:r:169:MET:SD	4:r:237:PHE:HA	2.59	0.43
4:t:299:LEU:O	4:t:299:LEU:HD12	2.18	0.43
2:y:155:LEU:HD21	2:y:177:MET:SD	2.59	0.43
6:FA:1:NAG:H62	6:FA:2:NAG:C7	2.48	0.43
4:7:402:THR:HG22	2:AC:251:TRP:HD1	1.84	0.43
4:8:235:TRP:CD1	4:8:235:TRP:N	2.87	0.43
4:9:230:THR:OG1	4:9:231:ASP:N	2.52	0.43
4:9:347:PRO:HG3	4:9:357:TYR:CD2	2.53	0.43
3:G:40:PRO:HA	3:G:127:ALA:HA	1.99	0.43
4:J:50:PHE:HZ	4:J:83:LEU:HD11	1.84	0.43
4:K:46:LEU:O	4:K:102:LEU:HA	2.19	0.43
1:M:24:VAL:HA	1:M:25:PRO:HA	1.87	0.43
2:Q:252:ASN:CG	2:Q:253:LYS:H	2.26	0.43
4:R:50:PHE:CE2	4:R:101:ILE:HD11	2.54	0.43
3:V:407:LEU:HD23	3:V:407:LEU:HA	1.84	0.43
3:W:308:HIS:HB2	3:W:359:ALA:HA	2.01	0.43
4:X:299:LEU:HD12	4:X:299:LEU:O	2.19	0.43
4:X:343:THR:OG1	4:X:360:GLY:HA3	2.19	0.43
4:Y:253:LYS:HG2	1:b:48:TYR:CE2	2.53	0.43
4:Z:134:GLN:OE1	4:Z:134:GLN:HA	2.18	0.43
2:d:122:GLU:OE1	2:d:124:LYS:NZ	2.48	0.43
3:i:242:TYR:OH	3:i:246:GLU:OE1	2.32	0.43
3:i:333:HIS:HB2	3:i:366:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:j:324:GLY:HA3	4:j:338:TRP:CD1	2.54	0.43
4:j:402:THR:HG23	2:n:256:VAL:HG23	2.00	0.43
2:n:122:GLU:HG2	2:n:132:TYR:CE1	2.54	0.43
3:p:331:HIS:CD2	3:p:332:SER:H	2.37	0.43
3:q:386:HIS:ND1	4:t:279:LYS:HA	2.33	0.43
4:s:195:LYS:HB3	4:s:229:VAL:HG13	2.00	0.43
4:s:299:LEU:HD12	4:s:299:LEU:O	2.19	0.43
4:t:6:PHE:CE2	4:t:8:VAL:HB	2.54	0.43
3:4:3:HIS:CD2	3:4:19:ILE:HG22	2.54	0.43
4:8:197:VAL:CG1	4:8:227:VAL:HG13	2.49	0.43
5:A:139:ASP:OD1	3:W:345:LYS:NZ	2.44	0.43
4:B:397:THR:O	4:B:401:LEU:HD23	2.19	0.43
3:E:72:GLU:OE1	3:E:72:GLU:N	2.47	0.43
3:F:21:ARG:HE	3:F:24:TYR:HE2	1.64	0.43
4:I:56:ILE:HG21	4:I:68:ARG:HH21	1.83	0.43
4:I:184:GLN:HB2	4:I:187:ASN:OD1	2.19	0.43
4:K:229:VAL:HG12	4:K:232:HIS:CE1	2.54	0.43
1:M:21:PRO:HG2	1:M:24:VAL:HG23	2.01	0.43
2:Q:187:GLU:O	2:Q:188:LYS:HD3	2.19	0.43
2:Q:207:PHE:HB3	2:Q:246:LEU:HD12	2.00	0.43
3:U:229:VAL:HG23	3:U:229:VAL:O	2.19	0.43
3:U:428:LEU:HD22	4:X:387:MET:HG3	1.99	0.43
3:W:195:GLY:N	3:W:214:TYR:OH	2.52	0.43
4:Y:167:ILE:O	4:Y:253:LYS:HA	2.19	0.43
3:i:379:SER:OG	4:j:348:HIS:ND1	2.42	0.43
4:j:196:LYS:HG3	4:j:196:LYS:O	2.18	0.43
2:n:218:ASP:HB3	2:n:221:ARG:HD2	2.01	0.43
3:o:74:PRO:HG2	3:o:108:VAL:O	2.19	0.43
4:t:47:LYS:HD2	4:t:156:TYR:CE2	2.54	0.43
2:x:246:LEU:HD23	2:x:246:LEU:HA	1.86	0.43
3:6:35:GLU:HB3	3:6:132:LYS:HG2	2.01	0.42
4:8:38:ARG:HH11	4:8:38:ARG:HG3	1.84	0.42
5:A:109:HIS:CE1	5:A:111:ARG:HH21	2.37	0.42
3:E:89:TRP:CH2	4:R:72:GLY:HA2	2.53	0.42
3:F:208:VAL:HG13	3:F:209:GLU:HG2	2.01	0.42
3:G:309:SER:OG	3:G:311:ASP:OD1	2.36	0.42
3:G:432:THR:CG2	4:J:394:LYS:HZ1	2.32	0.42
1:L:39:LEU:HD23	1:L:51:LEU:CD2	2.48	0.42
1:N:33:GLU:OE2	1:N:37:ARG:NH2	2.30	0.42
4:R:233:LYS:HD3	4:R:233:LYS:HA	1.88	0.42
3:U:384:LYS:HD3	3:U:384:LYS:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:194:SER:O	3:V:194:SER:OG	2.35	0.42
3:V:242:TYR:HB3	3:V:246:GLU:OE1	2.19	0.42
3:W:244:LEU:HD12	3:W:244:LEU:HA	1.88	0.42
3:i:206:ARG:HD3	3:i:206:ARG:HA	1.86	0.42
3:p:412:LYS:HE3	3:p:412:LYS:HB2	1.60	0.42
2:y:162:LYS:HD3	2:y:163:SER:N	2.34	0.42
4:7:143:ILE:HG12	4:8:128:GLN:HB2	2.00	0.42
4:7:174:ASP:OD1	4:7:174:ASP:N	2.42	0.42
4:7:192:VAL:HG11	4:7:213:SER:HA	2.01	0.42
4:8:235:TRP:CZ3	4:8:252:GLY:HA3	2.53	0.42
3:F:251:LEU:HD12	3:F:251:LEU:HA	1.78	0.42
3:H:88:MET:HE2	3:H:88:MET:HB3	1.82	0.42
4:I:134:GLN:OE1	4:I:134:GLN:HA	2.19	0.42
3:V:135:VAL:HG11	3:V:156:ILE:HD13	2.02	0.42
3:V:244:LEU:HD23	3:V:244:LEU:HA	1.90	0.42
4:X:237:PHE:CD2	4:X:239:SER:HB2	2.54	0.42
4:X:320:VAL:HG13	4:X:320:VAL:O	2.19	0.42
4:Y:333:ASP:OD1	4:Y:333:ASP:N	2.51	0.42
4:Z:416:CYS:SG	4:Z:418:PRO:HD2	2.58	0.42
3:h:7:MET:HE3	3:h:7:MET:HB2	1.80	0.42
3:h:244:LEU:HD12	3:h:244:LEU:HA	1.76	0.42
3:h:308:HIS:HB2	3:h:359:ALA:HA	2.01	0.42
3:i:320:TYR:HE2	3:i:352:VAL:HG13	1.85	0.42
3:o:125:HIS:ND1	3:o:126:THR:HG22	2.34	0.42
3:p:347:LYS:HE2	3:p:347:LYS:HB2	1.80	0.42
4:7:392:ARG:HG2	4:7:414:LEU:HD21	2.00	0.42
4:9:213:SER:OG	4:9:214:ASP:N	2.53	0.42
4:9:242:VAL:HA	4:9:243:PRO:HD3	1.90	0.42
2:AE:187:GLU:C	2:AE:188:LYS:HD2	2.44	0.42
3:E:88:MET:HE2	3:E:88:MET:HB3	1.94	0.42
3:E:206:ARG:HA	3:E:206:ARG:HD3	1.81	0.42
3:F:249:THR:HA	4:I:305:TYR:OH	2.19	0.42
3:H:321:LYS:HE3	3:H:321:LYS:HB3	1.81	0.42
4:R:236:GLN:O	4:R:237:PHE:HB2	2.20	0.42
2:T:116:GLU:HA	2:T:120:ILE:CD1	2.49	0.42
3:V:149:ASN:O	3:V:151:ASP:N	2.46	0.42
4:X:200:ASN:O	4:X:225:CYS:HA	2.19	0.42
4:X:232:HIS:O	4:X:233:LYS:HG2	2.19	0.42
1:g:39:LEU:HD23	1:g:51:LEU:HD22	2.01	0.42
3:i:72:GLU:HA	3:i:72:GLU:OE2	2.20	0.42
4:j:290:HIS:O	4:j:292:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:j:359:TYR:O	4:j:363:PRO:HB3	2.19	0.42
3:m:185:PHE:CE1	3:m:250:ALA:HA	2.54	0.42
3:p:249:THR:HG22	4:s:305:TYR:OH	2.19	0.42
4:r:83:LEU:HD21	4:r:101:ILE:HD12	2.00	0.42
4:r:378:LEU:HA	4:r:381:ILE:HG22	2.01	0.42
2:3:173:ILE:CD1	2:3:178:ARG:HG2	2.49	0.42
3:5:251:LEU:HD12	3:5:251:LEU:HA	1.89	0.42
4:B:318:ILE:HD12	4:B:325:MET:CE	2.50	0.42
4:K:316:ARG:HA	4:K:316:ARG:HD3	1.80	0.42
1:N:39:LEU:HD23	1:N:39:LEU:HA	1.80	0.42
2:P:246:LEU:HD23	2:P:246:LEU:HA	1.90	0.42
4:R:87:THR:HG22	4:R:111:LEU:HB3	2.01	0.42
4:X:11:ALA:O	4:X:235:TRP:N	2.50	0.42
4:Z:176:PRO:HA	4:Z:227:VAL:O	2.19	0.42
4:Z:316:ARG:HD3	4:Z:316:ARG:HA	1.72	0.42
2:e:209:ILE:HG12	2:e:246:LEU:HD21	2.00	0.42
3:h:141:ASN:O	3:h:142:GLN:HB2	2.19	0.42
3:i:252:ASN:ND2	3:i:261:ILE:HB	2.34	0.42
3:p:76:TYR:CE2	3:p:78:CYS:HB2	2.55	0.42
4:s:316:ARG:HA	4:s:316:ARG:HD3	1.81	0.42
2:x:123:VAL:HG23	2:x:149:VAL:C	2.44	0.42
3:4:59:TYR:CZ	3:4:61:LYS:HB2	2.55	0.42
3:5:16:LYS:NZ	3:5:30:GLN:OE1	2.52	0.42
3:6:11:VAL:HA	3:6:33:VAL:HG23	2.02	0.42
4:8:138:ARG:CZ	4:8:293:LEU:HD23	2.50	0.42
5:A:193:CYS:HB2	5:A:197:GLU:OE1	2.19	0.42
2:AC:140:VAL:O	2:AC:170:CYS:HA	2.20	0.42
2:AC:187:GLU:OE2	2:AC:187:GLU:N	2.51	0.42
2:AE:142:LYS:HD2	2:AE:169:GLU:OE2	2.18	0.42
3:E:345:LYS:HE3	3:E:345:LYS:HB3	1.85	0.42
3:H:7:MET:HE2	3:H:7:MET:HB3	1.78	0.42
4:I:376:LEU:HD23	4:I:376:LEU:HA	1.74	0.42
4:J:100:PHE:CD2	4:J:257:PRO:HD2	2.55	0.42
2:O:162:LYS:NZ	2:O:164:SER:OG	2.52	0.42
3:V:95:PHE:CZ	4:Y:226:HIS:HB2	2.55	0.42
4:Z:402:THR:HG23	2:f:256:VAL:HG23	2.02	0.42
1:a:24:VAL:HA	1:a:25:PRO:HA	1.83	0.42
3:h:134:ARG:HH11	3:h:134:ARG:HG3	1.85	0.42
2:n:232:ALA:HA	2:n:251:TRP:HZ3	1.85	0.42
3:p:24:TYR:HB3	3:p:288:THR:O	2.20	0.42
4:s:183:GLN:NE2	4:s:187:ASN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:z:223:GLU:HG2	4:z:224:GLN:HG3	2.02	0.42
3:6:314:GLY:HA3	3:6:356:PHE:CE1	2.55	0.42
3:6:330:VAL:HA	3:6:368:SER:O	2.19	0.42
3:6:347:LYS:HA	3:6:347:LYS:HD2	1.79	0.42
4:8:211:THR:HG21	4:8:215:MET:SD	2.59	0.42
3:G:87:PHE:CD1	3:G:92:ALA:HB2	2.55	0.42
3:H:95:PHE:CD1	4:K:226:HIS:CE1	3.08	0.42
4:I:217:ILE:HG23	4:I:219:THR:H	1.85	0.42
4:I:242:VAL:HA	4:I:243:PRO:HD3	1.90	0.42
4:J:343:THR:OG1	4:J:360:GLY:HA3	2.19	0.42
2:Q:124:LYS:NZ	2:Q:151:ASP:HB2	2.35	0.42
2:T:124:LYS:NZ	2:T:151:ASP:HB2	2.34	0.42
2:T:210:PRO:HA	2:T:243:ARG:HE	1.83	0.42
3:V:48:THR:HG23	3:V:203:ILE:O	2.20	0.42
3:V:110:ARG:HD3	3:V:114:CYS:HB3	2.00	0.42
2:f:111:MET:HE2	2:f:111:MET:HB3	1.86	0.42
3:h:59:TYR:CE2	3:h:61:LYS:HB2	2.54	0.42
3:h:146:VAL:HG11	3:h:163:PHE:CD1	2.54	0.42
3:i:95:PHE:HD2	6:iA:1:NAG:H62	1.84	0.42
3:i:259:CYS:HB3	3:i:271:CYS:CA	2.43	0.42
4:j:56:ILE:HG21	4:j:68:ARG:NH2	2.35	0.42
3:q:311:ASP:OD1	3:q:311:ASP:N	2.52	0.42
2:x:142:LYS:O	2:x:168:LEU:HD12	2.20	0.42
2:y:136:VAL:HG11	2:y:251:TRP:CH2	2.51	0.42
4:z:67:ILE:O	4:z:77:ASN:HA	2.19	0.42
3:5:259:CYS:HB3	3:5:271:CYS:CA	2.43	0.42
3:6:129:LEU:HD23	3:6:130:LYS:N	2.33	0.42
4:7:246:ASP:N	4:7:246:ASP:OD1	2.51	0.42
3:F:134:ARG:HB2	3:F:143:THR:HG22	2.02	0.42
3:F:433:CYS:O	3:F:437:ARG:HG2	2.20	0.42
3:H:238:SER:HB3	3:H:241:LYS:HB3	2.01	0.42
4:I:7:ASN:HB3	4:I:10:LYS:HE2	2.02	0.42
4:I:57:ASP:OD1	4:I:61:ASN:N	2.44	0.42
2:O:136:VAL:HB	2:O:141:MET:HE1	2.02	0.42
2:P:139:LYS:HA	2:P:173:ILE:HG23	2.01	0.42
3:U:259:CYS:HB2	3:U:271:CYS:HB2	1.91	0.42
3:W:21:ARG:HG2	3:W:24:TYR:HD1	1.85	0.42
4:X:308:GLU:CD	4:X:316:ARG:HH21	2.28	0.42
2:e:209:ILE:HG22	2:e:211:THR:H	1.85	0.42
3:i:59:TYR:CE2	4:j:247:GLU:HB3	2.55	0.42
3:p:86:PRO:HB3	3:p:229:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:331:HIS:CD2	3:q:332:SER:H	2.37	0.42
3:q:359:ALA:HB2	3:q:394:HIS:CD2	2.54	0.42
4:z:149:LYS:HE2	4:z:149:LYS:HB3	1.63	0.42
3:4:30:GLN:HB2	3:4:136:MET:HG3	2.02	0.42
3:4:42:LEU:HD11	3:4:266:VAL:HG22	2.01	0.42
3:4:336:VAL:HA	3:4:397:VAL:HG11	2.01	0.42
3:5:409:TRP:O	3:5:413:ILE:HG12	2.19	0.42
4:9:188:VAL:HG12	4:9:221:LEU:O	2.20	0.42
2:AE:143:PRO:HB2	2:AE:146:VAL:HG22	2.01	0.42
3:H:293:ALA:O	3:H:324:LYS:NZ	2.53	0.42
4:I:67:ILE:HD11	4:I:115:ILE:HD13	2.00	0.42
3:i:95:PHE:HD1	4:j:226:HIS:NE2	2.12	0.42
3:m:210:SER:OG	3:m:212:ASP:OD1	2.36	0.42
3:q:149:ASN:O	3:q:151:ASP:N	2.52	0.42
3:q:426:LEU:HD23	3:q:426:LEU:HA	1.85	0.42
4:s:156:TYR:HE1	4:s:260:LEU:HD12	1.83	0.42
4:t:15:TYR:HB3	4:t:236:GLN:HG3	2.02	0.42
4:t:141:PHE:CE1	4:t:267:VAL:HG23	2.54	0.42
4:t:286:LEU:HD23	4:t:310:VAL:HG21	2.02	0.42
4:t:312:ALA:O	4:t:314:VAL:HG13	2.20	0.42
2:3:157:LYS:HD3	2:3:157:LYS:C	2.45	0.42
3:4:417:LEU:HD23	3:4:417:LEU:HA	1.80	0.42
3:5:387:ILE:HB	4:8:277:HIS:ND1	2.35	0.42
3:6:88:MET:HE2	3:6:88:MET:HB3	1.94	0.42
3:G:74:PRO:HG2	3:G:108:VAL:O	2.20	0.42
4:I:404:GLY:HA3	2:O:254:ASP:OD1	2.19	0.42
4:J:47:LYS:HA	4:J:101:ILE:O	2.20	0.42
4:K:56:ILE:O	4:K:68:ARG:HG3	2.20	0.42
4:R:290:HIS:O	4:R:292:THR:HG23	2.20	0.42
3:U:47:ILE:HD11	3:U:118:HIS:CG	2.54	0.42
3:U:249:THR:HA	4:X:305:TYR:OH	2.19	0.42
3:W:437:ARG:HD3	3:W:437:ARG:HA	1.92	0.42
2:d:145:HIS:CD2	2:d:266:GLU:HB3	2.54	0.42
2:d:196:HIS:ND1	2:d:196:HIS:O	2.53	0.42
2:n:125:HIS:ND1	2:n:126:GLU:OE1	2.51	0.42
3:o:302:THR:OG1	3:o:317:THR:OG1	2.32	0.42
3:q:437:ARG:HA	3:q:437:ARG:HD3	1.87	0.42
4:z:54:ILE:HB	4:z:67:ILE:HG12	2.01	0.42
1:0:37:ARG:HD3	1:0:37:ARG:HA	1.87	0.42
4:9:222:ILE:HG13	4:9:223:GLU:CD	2.45	0.42
2:AC:235:LEU:HD11	2:AC:249:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:170:TRP:CH2	3:H:172:PRO:HG3	2.54	0.42
4:I:174:ASP:OD1	4:I:174:ASP:N	2.51	0.42
4:J:67:ILE:O	4:J:67:ILE:HG13	2.17	0.42
3:W:13:PHE:HA	3:W:14:PRO:HD3	1.85	0.42
4:Y:97:MET:HE1	4:Y:160:THR:CG2	2.45	0.42
2:e:183:LYS:NZ	2:e:229:ARG:HG2	2.35	0.42
2:e:235:LEU:HB2	2:e:247:SER:O	2.20	0.42
3:q:312:PHE:HE2	3:q:340:GLN:HA	1.85	0.42
4:z:11:ALA:HA	4:z:234:LYS:HG2	2.01	0.42
2:1:240:GLU:N	2:1:243:ARG:O	2.50	0.41
2:AC:190:GLU:OE2	2:AC:203:SER:HA	2.20	0.41
2:AC:207:PHE:CD2	2:AC:248:VAL:HG11	2.54	0.41
2:AC:226:ASN:OD1	2:AC:227:LYS:HG3	2.19	0.41
4:B:401:LEU:HB3	2:D:256:VAL:HG21	2.00	0.41
4:B:416:CYS:SG	4:B:418:PRO:HD2	2.60	0.41
3:E:310:SER:HB3	3:E:392:ALA:HA	2.01	0.41
3:F:93:TYR:CD1	4:I:176:PRO:HG3	2.55	0.41
3:G:112:ASP:OD1	3:G:112:ASP:N	2.53	0.41
3:H:113:VAL:O	3:H:113:VAL:HG12	2.20	0.41
2:P:162:LYS:HZ3	2:P:164:SER:HB3	1.84	0.41
4:R:231:ASP:OD1	4:R:231:ASP:C	2.63	0.41
3:W:320:TYR:CZ	3:W:346:VAL:HG23	2.55	0.41
4:Z:139:GLU:HG2	4:Z:292:THR:HG22	2.01	0.41
3:h:25:SER:HB3	3:h:288:THR:HG23	2.02	0.41
4:j:31:PRO:O	4:j:52:ALA:HB2	2.19	0.41
4:j:337:LEU:HD23	4:j:337:LEU:HA	1.70	0.41
3:m:88:MET:HE2	3:m:88:MET:HB3	1.81	0.41
3:m:225:SER:H	3:m:230:HIS:HE1	1.67	0.41
3:m:241:LYS:HA	3:m:241:LYS:HD2	1.86	0.41
4:r:417:ALA:HB3	4:r:418:PRO:HD3	2.02	0.41
4:t:47:LYS:HD2	4:t:156:TYR:CD2	2.55	0.41
4:z:166:GLU:HA	4:z:166:GLU:OE2	2.20	0.41
3:5:74:PRO:HG2	3:5:108:VAL:O	2.20	0.41
4:7:138:ARG:NH2	4:7:293:LEU:HD23	2.36	0.41
4:9:56:ILE:HB	4:9:68:ARG:HD3	2.02	0.41
4:9:341:LEU:HD23	4:9:341:LEU:HA	1.93	0.41
2:AE:124:LYS:HD3	2:AE:127:GLY:CA	2.50	0.41
4:B:15:TYR:HB3	4:B:236:GLN:HE21	1.84	0.41
3:H:46:TYR:O	3:H:47:ILE:HD13	2.19	0.41
3:H:116:HIS:CE1	6:SA:1:NAG:C7	3.03	0.41
4:I:343:THR:OG1	4:I:360:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:97:ASP:OD1	3:W:98:SER:N	2.53	0.41
3:W:149:ASN:C	3:W:151:ASP:H	2.27	0.41
4:X:188:VAL:O	4:X:216:THR:HA	2.20	0.41
1:g:26:CYS:HB3	1:g:29:GLU:HB2	2.02	0.41
3:o:209:GLU:OE1	3:o:209:GLU:HA	2.20	0.41
4:s:117:ASP:OD1	4:s:121:ALA:N	2.39	0.41
4:s:237:PHE:CG	4:s:238:ASN:N	2.88	0.41
4:z:66:LYS:HA	4:z:66:LYS:HD3	1.95	0.41
2:1:196:HIS:CG	2:1:221:ARG:HH12	2.39	0.41
3:5:194:SER:O	3:5:194:SER:OG	2.34	0.41
3:6:340:GLN:HB3	3:6:341:GLU:OE1	2.19	0.41
4:7:138:ARG:CZ	4:7:293:LEU:HD23	2.50	0.41
4:7:242:VAL:HA	4:7:243:PRO:HD3	1.95	0.41
2:AC:135:LEU:HG	2:AC:140:VAL:HG22	2.02	0.41
2:AE:152:ASN:HB3	2:AE:155:LEU:HB2	2.02	0.41
3:E:57:SER:OG	4:R:239:SER:O	2.38	0.41
3:E:426:LEU:HD23	3:E:426:LEU:HA	1.78	0.41
3:H:186:ASN:ND2	3:H:251:LEU:HD13	2.35	0.41
4:J:347:PRO:HB2	4:J:348:HIS:ND1	2.36	0.41
2:P:209:ILE:HG22	2:P:212:GLY:H	1.85	0.41
3:V:86:PRO:HB3	3:V:229:VAL:HG13	2.03	0.41
3:V:387:ILE:HD13	3:V:387:ILE:HA	1.87	0.41
4:Y:231:ASP:O	4:Y:233:LYS:N	2.52	0.41
3:i:49:CYS:O	3:i:203:ILE:HD11	2.21	0.41
4:r:166:GLU:OE1	4:r:166:GLU:HA	2.20	0.41
4:r:294:PHE:HB2	4:r:329:TRP:HE3	1.85	0.41
4:r:308:GLU:CD	4:r:316:ARG:HH21	2.28	0.41
2:y:235:LEU:HB2	2:y:247:SER:O	2.21	0.41
4:z:14:PRO:HB3	4:z:52:ALA:HA	2.02	0.41
4:z:54:ILE:HG22	4:z:67:ILE:CG2	2.48	0.41
2:3:166:TYR:OH	2:3:255:MET:HE3	2.20	0.41
5:A:109:HIS:HE1	5:A:111:ARG:HH21	1.66	0.41
2:AE:188:LYS:HE2	2:AE:250:THR:OG1	2.21	0.41
4:B:235:TRP:CD1	1:S:36:LEU:HD23	2.56	0.41
3:E:262:LYS:HD2	3:E:269:MET:SD	2.60	0.41
3:F:426:LEU:HD23	3:F:426:LEU:HA	1.80	0.41
4:I:138:ARG:NH2	4:I:293:LEU:HD23	2.35	0.41
4:R:250:ARG:HD3	1:g:37:ARG:NH2	2.36	0.41
3:U:134:ARG:NH1	3:U:136:MET:SD	2.93	0.41
3:W:145:ASP:C	3:W:145:ASP:OD1	2.63	0.41
3:W:199:ARG:O	3:W:239:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:386:HIS:ND1	4:Z:279:LYS:HA	2.36	0.41
4:X:197:VAL:HG21	4:X:227:VAL:HG13	2.01	0.41
2:e:162:LYS:HB2	2:e:162:LYS:HE2	1.73	0.41
3:h:149:ASN:C	3:h:151:ASP:H	2.28	0.41
3:i:207:THR:HG22	3:i:208:VAL:N	2.35	0.41
3:o:241:LYS:HD3	3:o:241:LYS:HA	1.88	0.41
4:s:149:LYS:HB3	4:s:149:LYS:HE2	1.66	0.41
4:t:14:PRO:HB3	4:t:52:ALA:HA	2.03	0.41
2:x:202:TYR:CG	2:x:207:PHE:HE1	2.39	0.41
4:z:142:THR:HG22	4:z:143:ILE:HG23	2.02	0.41
3:4:424:ALA:HB1	4:7:387:MET:HE2	2.02	0.41
3:5:257:PHE:CE1	4:8:301:GLU:HA	2.56	0.41
3:6:185:PHE:CZ	3:6:247:LYS:HD2	2.56	0.41
4:7:318:ILE:HD12	4:7:325:MET:HE3	2.01	0.41
4:8:201:CYS:HA	4:8:224:GLN:HG3	2.03	0.41
1:AA:32:ALA:O	1:AA:36:LEU:HD13	2.19	0.41
2:AC:209:ILE:HG22	2:AC:212:GLY:H	1.85	0.41
2:AE:188:LYS:HB3	2:AE:202:TYR:CE2	2.55	0.41
2:AE:235:LEU:HB2	2:AE:247:SER:O	2.20	0.41
3:E:191:PRO:HB3	3:W:151:ASP:HA	2.02	0.41
3:F:63:CYS:HB2	3:F:96:CYS:HB2	1.82	0.41
3:G:115:ARG:CZ	3:G:115:ARG:HB3	2.50	0.41
4:J:119:ARG:HB3	4:J:119:ARG:NH1	2.36	0.41
4:J:141:PHE:CE1	4:J:267:VAL:HG23	2.56	0.41
4:K:95:GLY:H	4:K:102:LEU:HB2	1.86	0.41
4:K:318:ILE:HD12	4:K:325:MET:HE1	2.02	0.41
1:L:11:LEU:HB2	1:L:16:PHE:CE1	2.52	0.41
1:M:38:MET:HB2	1:M:38:MET:HE3	1.87	0.41
4:R:235:TRP:HZ2	1:g:40:GLU:HG3	1.85	0.41
2:T:235:LEU:HB2	2:T:247:SER:O	2.20	0.41
3:U:425:ILE:HD13	4:X:387:MET:HE1	2.03	0.41
3:W:61:LYS:HZ3	3:W:65:ALA:N	2.17	0.41
3:h:18:HIS:HB2	3:h:331:HIS:CE1	2.55	0.41
3:m:431:VAL:HG11	4:z:395:CYS:HB2	2.03	0.41
2:n:194:ASN:OD1	2:n:195:TRP:N	2.53	0.41
3:p:228:MET:HG3	3:p:230:HIS:CE1	2.56	0.41
3:p:229:VAL:O	3:p:229:VAL:HG23	2.20	0.41
4:r:402:THR:HA	2:x:139:LYS:HZ3	1.86	0.41
4:t:296:TYR:CE2	4:t:318:ILE:HG23	2.55	0.41
4:z:249:ALA:O	4:z:250:ARG:HD2	2.21	0.41
3:4:241:LYS:HD3	3:4:241:LYS:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:82:THR:HG22	3:5:101:THR:HG22	2.01	0.41
3:5:306:CYS:HB2	3:5:380:CYS:HA	2.03	0.41
3:6:13:PHE:HA	3:6:14:PRO:HD3	1.86	0.41
3:6:312:PHE:CD1	3:6:357:SER:HB2	2.55	0.41
4:9:392:ARG:HG2	4:9:414:LEU:HD23	2.03	0.41
4:B:192:VAL:HG11	4:B:213:SER:HA	2.03	0.41
4:B:273:PRO:HD3	4:B:329:TRP:CD1	2.56	0.41
4:B:290:HIS:O	4:B:292:THR:HG23	2.21	0.41
3:E:113:VAL:HG21	4:R:40:GLU:HG3	2.03	0.41
3:H:382:PRO:HG3	4:K:357:TYR:CE1	2.56	0.41
4:I:397:THR:HG22	4:I:398:PRO:HD3	2.02	0.41
3:W:203:ILE:O	3:W:203:ILE:HG13	2.21	0.41
3:i:225:SER:H	3:i:230:HIS:CE1	2.38	0.41
4:j:138:ARG:NH2	4:j:293:LEU:HD23	2.35	0.41
4:j:184:GLN:HB2	4:j:187:ASN:OD1	2.20	0.41
1:l:10:VAL:H	1:l:42:ASN:HD21	1.69	0.41
3:m:303:VAL:HG11	3:m:378:ALA:HB2	2.03	0.41
3:p:5:THR:HG22	3:p:6:VAL:N	2.36	0.41
3:q:249:THR:HA	4:t:305:TYR:OH	2.20	0.41
4:s:57:ASP:OD1	4:s:60:ASP:N	2.54	0.41
2:x:161:LYS:HB2	2:x:170:CYS:SG	2.61	0.41
4:z:316:ARG:HD3	4:z:316:ARG:HA	1.82	0.41
3:4:89:TRP:CZ2	4:7:72:GLY:HA2	2.56	0.41
3:5:71:LYS:HD2	3:5:76:TYR:CZ	2.55	0.41
3:6:265:PRO:HD2	3:6:267:ARG:NH1	2.36	0.41
4:7:83:LEU:HD21	4:7:101:ILE:HD12	2.02	0.41
4:9:401:LEU:HD22	2:AE:170:CYS:SG	2.61	0.41
1:AA:24:VAL:HA	1:AA:25:PRO:HA	1.86	0.41
2:AD:187:GLU:C	2:AD:188:LYS:HD3	2.45	0.41
3:E:308:HIS:CE1	3:E:382:PRO:HA	2.56	0.41
4:I:87:THR:HG23	4:I:110:PHE:O	2.21	0.41
2:O:119:CYS:O	2:O:120:ILE:HD13	2.20	0.41
4:R:174:ASP:OD1	4:R:174:ASP:N	2.48	0.41
4:Y:392:ARG:NH2	4:Y:415:CYS:O	2.44	0.41
4:Z:63:ASP:OD1	4:Z:65:THR:N	2.53	0.41
2:e:226:ASN:HB2	2:e:227:LYS:HZ1	1.85	0.41
3:i:81:TYR:CD1	3:i:223:ARG:HG3	2.55	0.41
3:m:303:VAL:HG21	3:m:378:ALA:HB2	2.01	0.41
3:o:33:VAL:HG23	3:o:33:VAL:O	2.21	0.41
4:s:87:THR:HG22	4:s:111:LEU:HB3	2.02	0.41
4:t:56:ILE:O	4:t:68:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:z:6:PHE:HD2	4:z:8:VAL:H	1.68	0.41
3:4:88:MET:HE3	3:4:88:MET:HB3	2.00	0.41
3:6:255:ALA:O	4:9:297:ARG:NH1	2.54	0.41
4:8:49:GLN:OE1	4:8:100:PHE:HE1	2.04	0.41
2:AC:195:TRP:CZ3	2:AC:209:ILE:HD12	2.55	0.41
3:E:347:LYS:HG3	3:E:348:THR:N	2.35	0.41
3:H:207:THR:HG22	3:H:208:VAL:N	2.35	0.41
2:T:123:VAL:HG22	2:T:150:ILE:HA	2.03	0.41
4:X:54:ILE:CD1	4:X:96:THR:HG23	2.51	0.41
4:Z:167:ILE:HG23	4:Z:237:PHE:HE1	1.86	0.41
4:Z:175:THR:O	4:Z:228:SER:HA	2.21	0.41
1:c:11:LEU:O	1:c:13:ASN:N	2.54	0.41
3:h:206:ARG:HA	3:h:206:ARG:HD3	1.81	0.41
3:m:163:PHE:CD2	3:m:278:VAL:HG12	2.56	0.41
3:m:229:VAL:HG23	3:m:229:VAL:O	2.21	0.41
4:s:167:ILE:HG23	4:s:237:PHE:CE1	2.55	0.41
2:x:138:ASP:OD1	2:x:173:ILE:HD11	2.21	0.41
3:5:353:THR:O	3:5:354:LEU:HD12	2.21	0.41
3:6:249:THR:HA	4:9:305:TYR:OH	2.21	0.41
3:6:258:GLY:HA3	4:9:299:LEU:HB2	2.03	0.41
4:8:7:ASN:HB3	4:8:10:LYS:NZ	2.35	0.41
4:8:202:THR:OG1	4:8:224:GLN:OE1	2.16	0.41
4:9:127:ILE:C	4:t:143:ILE:HD11	2.46	0.41
4:B:9:TYR:CD2	4:B:56:ILE:HD11	2.56	0.41
4:B:40:GLU:OE1	4:B:40:GLU:N	2.46	0.41
2:D:144:ALA:HA	2:D:169:GLU:OE1	2.20	0.41
3:E:437:ARG:HA	3:E:437:ARG:HD3	1.78	0.41
3:G:96:CYS:O	3:G:100:ASN:ND2	2.51	0.41
4:J:402:THR:CG2	2:P:256:VAL:HG23	2.51	0.41
2:P:225:ASP:OD1	2:P:226:ASN:N	2.54	0.41
4:R:101:ILE:HG21	4:R:101:ILE:HD13	1.84	0.41
3:U:11:VAL:HG23	3:U:33:VAL:O	2.21	0.41
3:U:219:LEU:HD12	3:U:235:GLN:HB2	2.01	0.41
3:U:359:ALA:HB2	3:U:394:HIS:CD2	2.56	0.41
3:V:113:VAL:HG12	3:V:113:VAL:O	2.20	0.41
3:W:115:ARG:NH1	3:W:115:ARG:HB3	2.36	0.41
4:X:109:GLU:N	4:X:109:GLU:OE1	2.53	0.41
2:e:179:SER:HB2	2:f:240:GLU:HG3	2.03	0.41
3:h:185:PHE:CD1	3:h:250:ALA:HA	2.56	0.41
3:i:78:CYS:HA	3:i:104:SER:O	2.20	0.41
3:i:202:ASP:OD1	3:i:203:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:386:HIS:ND1	4:j:279:LYS:HA	2.36	0.41
3:m:230:HIS:NE2	3:m:232:PRO:HG3	2.35	0.41
2:n:239:ASN:HA	2:n:244:THR:HG22	2.03	0.41
3:o:229:VAL:HG23	3:o:229:VAL:O	2.20	0.41
3:o:426:LEU:HD23	3:o:426:LEU:HA	1.85	0.41
3:p:339:LEU:HD23	3:p:356:PHE:HB3	2.03	0.41
3:q:5:THR:HG22	3:q:6:VAL:N	2.36	0.41
3:q:42:LEU:HD23	3:q:122:TYR:CG	2.56	0.41
3:q:428:LEU:HD12	4:t:391:ALA:HB2	2.02	0.41
4:r:177:ASP:OD1	4:r:178:ARG:N	2.54	0.41
4:s:114:SER:HA	4:s:123:ARG:O	2.20	0.41
4:s:314:VAL:HG22	4:s:315:GLU:N	2.35	0.41
4:t:47:LYS:HA	4:t:101:ILE:O	2.21	0.41
4:t:52:ALA:O	4:t:54:ILE:HG23	2.21	0.41
4:t:217:ILE:HG23	4:t:219:THR:H	1.85	0.41
4:z:50:PHE:HZ	4:z:83:LEU:HD11	1.85	0.41
4:z:197:VAL:HB	4:z:227:VAL:HG13	2.02	0.41
4:z:291:PRO:HG3	4:z:311:THR:HG22	2.01	0.41
6:QA:1:NAG:H61	6:QA:2:NAG:N2	2.36	0.41
6:gA:1:NAG:H61	6:gA:2:NAG:N2	2.36	0.41
6:kA:3:BMA:O6	6:kA:3:BMA:O4	2.30	0.41
3:5:71:LYS:HD2	3:5:76:TYR:CE1	2.56	0.41
2:AE:194:ASN:HB2	2:AE:224:PHE:HB2	2.02	0.41
4:B:305:TYR:CZ	3:h:254:LYS:HG3	2.55	0.41
2:D:153:ALA:O	2:D:157:LYS:HG2	2.21	0.41
3:F:93:TYR:OH	4:I:243:PRO:HG2	2.21	0.41
3:G:252:ASN:HA	3:G:261:ILE:HD12	2.03	0.41
4:I:13:ARG:C	4:I:53:GLN:HE22	2.28	0.41
4:K:157:GLN:OE1	4:K:157:GLN:HA	2.20	0.41
4:K:181:LEU:HD21	4:K:225:CYS:HB2	2.03	0.41
4:R:273:PRO:HD3	4:R:329:TRP:CD1	2.56	0.41
4:R:344:GLU:N	4:R:344:GLU:OE1	2.54	0.41
3:U:5:THR:HG22	3:U:6:VAL:N	2.36	0.41
3:V:46:TYR:CD1	3:V:204:GLN:HG2	2.56	0.41
3:W:407:LEU:HD23	3:W:407:LEU:HA	1.78	0.41
4:Z:161:ALA:O	4:Z:163:THR:HG23	2.20	0.41
2:e:186:HIS:O	2:e:188:LYS:NZ	2.54	0.41
4:j:308:GLU:CD	4:j:316:ARG:HH12	2.29	0.41
2:n:195:TRP:CD1	2:n:196:HIS:H	2.38	0.41
4:r:411:LEU:HD12	4:r:414:LEU:O	2.22	0.41
4:s:17:ALA:HB3	4:s:33:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:s:180:LEU:H	4:s:180:LEU:HD23	1.85	0.41
4:t:149:LYS:HB3	4:t:149:LYS:HE2	1.58	0.41
6:ZA:1:NAG:H61	6:ZA:2:NAG:HN2	1.86	0.41
3:5:134:ARG:HB2	3:5:143:THR:HG22	2.02	0.40
3:6:2:GLU:OE1	3:6:2:GLU:HA	2.21	0.40
4:7:123:ARG:HA	4:7:123:ARG:HD2	1.96	0.40
4:7:347:PRO:HB3	4:7:357:TYR:CD2	2.56	0.40
4:9:31:PRO:HG2	4:9:32:VAL:HG23	2.01	0.40
4:9:346:LYS:HB2	4:9:346:LYS:HE3	1.80	0.40
2:AC:160:PHE:CD1	2:AC:171:ALA:HB2	2.52	0.40
2:AE:188:LYS:HB3	2:AE:202:TYR:HE2	1.86	0.40
2:D:142:LYS:HE2	2:D:142:LYS:HB3	1.87	0.40
3:H:262:LYS:HD2	3:H:269:MET:SD	2.61	0.40
4:J:343:THR:OG1	4:J:344:GLU:N	2.54	0.40
4:K:63:ASP:OD1	4:K:64:TYR:N	2.53	0.40
2:O:141:MET:SD	2:O:141:MET:N	2.95	0.40
3:W:241:LYS:HD3	3:W:241:LYS:HA	1.74	0.40
3:W:251:LEU:HA	3:W:251:LEU:HD12	1.81	0.40
4:X:221:LEU:HG	4:X:222:ILE:H	1.86	0.40
4:X:347:PRO:HA	4:X:354:ILE:HD13	2.04	0.40
4:Y:299:LEU:O	4:Y:299:LEU:HD12	2.20	0.40
4:Y:399:TYR:HE2	4:Y:407:VAL:HG23	1.86	0.40
4:Z:265:CYS:SG	4:Z:266:ARG:N	2.94	0.40
2:n:187:GLU:OE1	2:n:189:PRO:HG3	2.21	0.40
2:n:214:GLY:O	2:n:215:LYS:HD3	2.19	0.40
3:o:63:CYS:N	3:o:99:GLU:O	2.51	0.40
4:s:273:PRO:HD3	4:s:329:TRP:CD1	2.56	0.40
4:t:169:MET:HE1	4:t:236:GLN:O	2.21	0.40
4:z:144:ARG:HH21	4:z:266:ARG:HD3	1.86	0.40
3:4:146:VAL:HG11	3:4:163:PHE:HD1	1.84	0.40
4:7:73:HIS:HD2	4:7:195:LYS:HD3	1.86	0.40
4:7:189:LYS:HE3	4:7:216:THR:OG1	2.21	0.40
4:9:14:PRO:HD3	4:9:68:ARG:NH2	2.33	0.40
4:9:34:ILE:HG22	4:9:35:GLU:O	2.22	0.40
4:B:82:SER:HB2	4:B:116:GLN:HG3	2.02	0.40
3:F:141:ASN:O	3:F:142:GLN:CB	2.69	0.40
3:F:225:SER:H	3:F:230:HIS:CE1	2.40	0.40
3:G:204:GLN:O	3:G:213:LEU:HD12	2.21	0.40
4:K:217:ILE:HG23	4:K:219:THR:H	1.86	0.40
4:K:344:GLU:N	4:K:344:GLU:OE1	2.54	0.40
4:R:151:ILE:HD13	4:R:151:ILE:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:25:PRO:HB2	1:S:58:CYS:SG	2.61	0.40
3:V:299:LEU:HD13	3:V:372:ALA:HB3	2.02	0.40
2:d:142:LYS:O	2:d:168:LEU:HD12	2.21	0.40
4:j:97:MET:HE3	4:j:257:PRO:HB3	2.03	0.40
2:n:195:TRP:CZ3	2:n:197:HIS:HB2	2.56	0.40
4:r:416:CYS:SG	4:r:418:PRO:HD2	2.61	0.40
4:t:343:THR:HG1	4:t:360:GLY:HA3	1.87	0.40
2:3:138:ASP:O	2:3:173:ILE:HG12	2.21	0.40
3:6:184:VAL:CG1	3:6:261:ILE:HG21	2.52	0.40
3:6:353:THR:C	3:6:354:LEU:HD12	2.45	0.40
5:A:167:ILE:HD12	5:A:171:PHE:HB2	2.03	0.40
4:B:149:LYS:NZ	4:B:269:MET:SD	2.94	0.40
3:E:7:MET:HG3	3:E:276:ILE:HB	2.03	0.40
3:E:289:ARG:HG2	3:E:289:ARG:HH11	1.85	0.40
3:F:21:ARG:HH21	3:F:24:TYR:HE2	1.68	0.40
4:I:233:LYS:HD2	1:L:33:GLU:HB2	2.02	0.40
4:J:314:VAL:HG22	4:J:315:GLU:N	2.37	0.40
2:Q:193:TYR:HB2	2:Q:200:VAL:HG23	2.02	0.40
2:T:124:LYS:HE2	2:T:124:LYS:HB2	1.96	0.40
3:V:323:ASP:N	3:V:323:ASP:OD1	2.55	0.40
3:W:162:ILE:HG23	3:W:279:SER:HB2	2.03	0.40
4:Y:237:PHE:HD2	4:Y:239:SER:HB2	1.86	0.40
1:c:36:LEU:O	1:c:40:GLU:HG2	2.22	0.40
3:i:149:ASN:C	3:i:151:ASP:H	2.29	0.40
4:j:205:THR:OG1	4:j:206:GLY:N	2.54	0.40
4:j:401:LEU:HD23	2:n:170:CYS:SG	2.62	0.40
4:z:144:ARG:NH2	4:z:266:ARG:HD3	2.36	0.40
4:z:151:ILE:HD13	4:z:151:ILE:HA	1.96	0.40
4:z:180:LEU:HD22	4:z:191:THR:HB	2.02	0.40
4:z:188:VAL:O	4:z:216:THR:HA	2.22	0.40
1:0:50:ASP:N	1:0:50:ASP:OD1	2.54	0.40
2:1:255:MET:CE	4:t:398:PRO:HB2	2.52	0.40
3:4:57:SER:OG	4:7:239:SER:O	2.29	0.40
3:4:136:MET:HE1	6:C:1:NAG:HN2	1.86	0.40
3:5:52:LYS:HE2	3:5:52:LYS:HB3	1.77	0.40
4:7:397:THR:CG2	4:7:398:PRO:HD3	2.51	0.40
4:9:134:GLN:OE1	4:9:140:LYS:HE3	2.21	0.40
4:9:189:LYS:HE3	4:9:189:LYS:HB3	1.91	0.40
1:AA:11:LEU:HB2	1:AA:16:PHE:HE1	1.87	0.40
2:AC:246:LEU:HD23	2:AC:246:LEU:HA	1.87	0.40
3:E:13:PHE:HA	3:E:14:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:165:GLU:O	4:I:255:HIS:HA	2.22	0.40
4:I:374:SER:O	4:I:378:LEU:HD23	2.21	0.40
4:J:7:ASN:HD22	4:J:10:LYS:HD3	1.86	0.40
4:J:184:GLN:HG2	4:J:185:SER:N	2.34	0.40
4:K:343:THR:OG1	4:K:344:GLU:N	2.54	0.40
2:O:240:GLU:HG3	2:x:178:ARG:HB2	2.02	0.40
2:O:252:ASN:CG	2:O:253:LYS:H	2.26	0.40
2:Q:188:LYS:NZ	2:Q:231:VAL:HA	2.36	0.40
4:R:187:ASN:HB3	4:R:218:ASN:HA	2.03	0.40
3:W:18:HIS:HB2	3:W:331:HIS:CE1	2.56	0.40
4:Z:45:MET:HE2	4:Z:45:MET:HB3	1.89	0.40
3:h:202:ASP:OD1	3:h:203:ILE:N	2.55	0.40
3:i:109:ASP:OD1	3:i:110:ARG:N	2.55	0.40
3:m:46:TYR:CD2	3:m:204:GLN:HG2	2.56	0.40
4:s:201:CYS:HA	4:s:224:GLN:HG3	2.03	0.40
4:t:55:GLY:O	4:t:56:ILE:HD13	2.20	0.40
2:y:196:HIS:CD2	2:y:197:HIS:ND1	2.90	0.40
4:z:47:LYS:HE2	4:z:47:LYS:HB3	1.94	0.40
4:z:205:THR:OG1	4:z:206:GLY:N	2.54	0.40
2:1:188:LYS:HD2	2:1:231:VAL:HG13	2.04	0.40
3:5:51:TYR:HE2	3:5:238:SER:HA	1.86	0.40
3:5:144:VAL:HG21	3:5:156:ILE:HD11	2.02	0.40
3:6:18:HIS:HB2	3:6:331:HIS:CE1	2.57	0.40
4:7:237:PHE:HD2	4:7:239:SER:HB2	1.87	0.40
4:8:141:PHE:CE1	4:8:267:VAL:HG23	2.57	0.40
4:9:95:GLY:HA3	4:9:102:LEU:HD12	2.03	0.40
4:9:397:THR:N	4:9:398:PRO:HD2	2.37	0.40
5:A:80:ASN:HB2	5:A:99:ASP:OD2	2.21	0.40
2:AE:193:TYR:CE2	2:AE:231:VAL:HG21	2.57	0.40
4:B:277:HIS:CE1	3:h:387:ILE:HB	2.57	0.40
4:B:392:ARG:HH21	4:B:416:CYS:HA	1.87	0.40
4:J:174:ASP:HB3	4:J:228:SER:HB3	2.02	0.40
3:U:185:PHE:CZ	3:U:247:LYS:HD2	2.56	0.40
3:U:309:SER:OG	3:U:311:ASP:OD1	2.36	0.40
3:U:319:THR:HG22	3:U:351:LYS:HG2	2.04	0.40
3:W:336:VAL:HA	3:W:397:VAL:HG11	2.02	0.40
4:Y:344:GLU:N	4:Y:344:GLU:OE1	2.54	0.40
4:Z:182:SER:HB2	4:Z:189:LYS:HB2	2.03	0.40
1:b:43:VAL:HA	1:b:48:TYR:CD1	2.56	0.40
3:h:199:ARG:NH1	3:h:242:TYR:OH	2.55	0.40
3:h:211:ASN:OD1	3:h:212:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:299:LEU:HD21	3:h:318:LEU:HD22	2.04	0.40
3:i:10:VAL:HG23	3:i:13:PHE:HB2	2.02	0.40
4:j:82:SER:HB2	4:j:116:GLN:HG3	2.03	0.40
3:m:42:LEU:HD23	3:m:122:TYR:CG	2.56	0.40
3:o:418:GLY:O	3:o:422:ILE:HG12	2.22	0.40
3:p:302:THR:HG1	3:p:317:THR:HG1	1.68	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	0	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	32
1	2	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	32
1	AA	50/52 (96%)	49 (98%)	0	1 (2%)	6	32
1	AB	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	32
1	L	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	32
1	M	50/52 (96%)	49 (98%)	0	1 (2%)	6	32
1	N	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	32
1	S	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	32
1	a	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
1	b	50/52 (96%)	49 (98%)	0	1 (2%)	6	32
1	c	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	32
1	g	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	32
1	l	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	32
1	u	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	32
1	v	50/52 (96%)	48 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	50/52 (96%)	49 (98%)	0	1 (2%)	6	32
2	1	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
2	3	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	AC	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	AD	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	AE	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	D	159/161 (99%)	150 (94%)	9 (6%)	0	100	100
2	O	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	P	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	Q	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	T	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	d	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	e	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
2	f	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
2	n	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	x	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	y	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
3	4	436/438 (100%)	403 (92%)	32 (7%)	1 (0%)	43	72
3	5	436/438 (100%)	408 (94%)	27 (6%)	1 (0%)	43	72
3	6	436/438 (100%)	402 (92%)	34 (8%)	0	100	100
3	E	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	43	72
3	F	436/438 (100%)	399 (92%)	36 (8%)	1 (0%)	43	72
3	G	436/438 (100%)	411 (94%)	25 (6%)	0	100	100
3	H	436/438 (100%)	404 (93%)	32 (7%)	0	100	100
3	U	436/438 (100%)	404 (93%)	31 (7%)	1 (0%)	43	72
3	V	436/438 (100%)	407 (93%)	29 (7%)	0	100	100
3	W	436/438 (100%)	403 (92%)	33 (8%)	0	100	100
3	h	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	43	72
3	i	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	43	72
3	m	436/438 (100%)	410 (94%)	24 (6%)	2 (0%)	24	56
3	o	436/438 (100%)	406 (93%)	29 (7%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	p	436/438 (100%)	411 (94%)	24 (6%)	1 (0%)	43	72
3	q	436/438 (100%)	406 (93%)	30 (7%)	0	100	100
4	7	416/418 (100%)	363 (87%)	51 (12%)	2 (0%)	24	56
4	8	416/418 (100%)	371 (89%)	44 (11%)	1 (0%)	43	72
4	9	416/418 (100%)	359 (86%)	55 (13%)	2 (0%)	24	56
4	B	416/418 (100%)	373 (90%)	43 (10%)	0	100	100
4	I	416/418 (100%)	362 (87%)	52 (12%)	2 (0%)	24	56
4	J	416/418 (100%)	373 (90%)	42 (10%)	1 (0%)	43	72
4	K	416/418 (100%)	364 (88%)	50 (12%)	2 (0%)	24	56
4	R	416/418 (100%)	370 (89%)	46 (11%)	0	100	100
4	X	416/418 (100%)	365 (88%)	48 (12%)	3 (1%)	18	50
4	Y	416/418 (100%)	367 (88%)	48 (12%)	1 (0%)	43	72
4	Z	416/418 (100%)	364 (88%)	50 (12%)	2 (0%)	24	56
4	j	416/418 (100%)	371 (89%)	45 (11%)	0	100	100
4	r	416/418 (100%)	365 (88%)	50 (12%)	1 (0%)	43	72
4	s	416/418 (100%)	364 (88%)	51 (12%)	1 (0%)	43	72
4	t	416/418 (100%)	364 (88%)	50 (12%)	2 (0%)	24	56
4	z	416/418 (100%)	375 (90%)	41 (10%)	0	100	100
5	A	160/162 (99%)	145 (91%)	11 (7%)	4 (2%)	4	29
All	All	17136/17266 (99%)	15724 (92%)	1363 (8%)	49 (0%)	37	65

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	142	GLN
4	8	263	ILE
4	9	263	ILE
5	A	113	CYS
3	E	142	GLN
3	F	142	GLN
4	J	263	ILE
4	K	263	ILE
3	U	142	GLN
4	Y	263	ILE
4	Z	263	ILE

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Mol	Chain	Res	Type
3	h	142	GLN
3	i	142	GLN
3	m	142	GLN
3	o	142	GLN
4	s	263	ILE
4	t	263	ILE
1	2	12	ALA
5	A	112	THR
5	A	152	ILE
1	S	12	ALA
1	b	12	ALA
1	l	12	ALA
4	7	231	ASP
4	9	249	ALA
5	A	108	CYS
1	AA	12	ALA
1	AB	12	ALA
4	I	231	ASP
1	L	12	ALA
1	M	12	ALA
1	N	12	ALA
4	Z	249	ALA
1	c	12	ALA
1	g	12	ALA
4	r	231	ASP
4	t	249	ALA
4	I	251	LYS
4	K	249	ALA
4	X	231	ASP
4	7	251	LYS
3	m	370	CYS
1	0	12	ALA
3	5	181	LYS
4	X	251	LYS
3	p	370	CYS
1	u	12	ALA
1	w	12	ALA
4	X	164	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	45/45 (100%)	45 (100%)	0	100	100
1	2	45/45 (100%)	45 (100%)	0	100	100
1	AA	45/45 (100%)	45 (100%)	0	100	100
1	AB	45/45 (100%)	45 (100%)	0	100	100
1	L	45/45 (100%)	45 (100%)	0	100	100
1	M	45/45 (100%)	45 (100%)	0	100	100
1	N	45/45 (100%)	45 (100%)	0	100	100
1	S	45/45 (100%)	45 (100%)	0	100	100
1	a	45/45 (100%)	45 (100%)	0	100	100
1	b	45/45 (100%)	45 (100%)	0	100	100
1	c	45/45 (100%)	45 (100%)	0	100	100
1	g	45/45 (100%)	45 (100%)	0	100	100
1	l	45/45 (100%)	45 (100%)	0	100	100
1	u	45/45 (100%)	45 (100%)	0	100	100
1	v	45/45 (100%)	45 (100%)	0	100	100
1	w	45/45 (100%)	45 (100%)	0	100	100
2	1	132/132 (100%)	132 (100%)	0	100	100
2	3	132/132 (100%)	132 (100%)	0	100	100
2	AC	132/132 (100%)	132 (100%)	0	100	100
2	AD	132/132 (100%)	132 (100%)	0	100	100
2	AE	132/132 (100%)	132 (100%)	0	100	100
2	D	132/132 (100%)	132 (100%)	0	100	100
2	O	132/132 (100%)	132 (100%)	0	100	100
2	P	132/132 (100%)	132 (100%)	0	100	100
2	Q	132/132 (100%)	132 (100%)	0	100	100
2	T	132/132 (100%)	132 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d	132/132 (100%)	132 (100%)	0	100	100
2	e	132/132 (100%)	132 (100%)	0	100	100
2	f	132/132 (100%)	132 (100%)	0	100	100
2	n	132/132 (100%)	132 (100%)	0	100	100
2	x	132/132 (100%)	132 (100%)	0	100	100
2	y	132/132 (100%)	132 (100%)	0	100	100
3	4	372/372 (100%)	372 (100%)	0	100	100
3	5	372/372 (100%)	372 (100%)	0	100	100
3	6	372/372 (100%)	372 (100%)	0	100	100
3	E	372/372 (100%)	372 (100%)	0	100	100
3	F	372/372 (100%)	372 (100%)	0	100	100
3	G	372/372 (100%)	372 (100%)	0	100	100
3	H	372/372 (100%)	372 (100%)	0	100	100
3	U	372/372 (100%)	372 (100%)	0	100	100
3	V	372/372 (100%)	372 (100%)	0	100	100
3	W	372/372 (100%)	372 (100%)	0	100	100
3	h	372/372 (100%)	372 (100%)	0	100	100
3	i	372/372 (100%)	372 (100%)	0	100	100
3	m	372/372 (100%)	372 (100%)	0	100	100
3	o	372/372 (100%)	372 (100%)	0	100	100
3	p	372/372 (100%)	372 (100%)	0	100	100
3	q	372/372 (100%)	372 (100%)	0	100	100
4	7	356/356 (100%)	356 (100%)	0	100	100
4	8	356/356 (100%)	356 (100%)	0	100	100
4	9	356/356 (100%)	355 (100%)	1 (0%)	86	83
4	B	356/356 (100%)	356 (100%)	0	100	100
4	I	356/356 (100%)	356 (100%)	0	100	100
4	J	356/356 (100%)	356 (100%)	0	100	100
4	K	356/356 (100%)	355 (100%)	1 (0%)	86	83
4	R	356/356 (100%)	356 (100%)	0	100	100
4	X	356/356 (100%)	356 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Y	356/356 (100%)	356 (100%)	0	100	100
4	Z	356/356 (100%)	356 (100%)	0	100	100
4	j	356/356 (100%)	356 (100%)	0	100	100
4	r	356/356 (100%)	356 (100%)	0	100	100
4	s	356/356 (100%)	355 (100%)	1 (0%)	86	83
4	t	356/356 (100%)	355 (100%)	1 (0%)	86	83
4	z	356/356 (100%)	356 (100%)	0	100	100
5	A	145/145 (100%)	143 (99%)	2 (1%)	59	70
All	All	14625/14625 (100%)	14619 (100%)	6 (0%)	100	100

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	9	212	ASN
5	A	111	ARG
5	A	112	THR
4	K	184	GLN
4	s	212	ASN
4	t	77	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	13	ASN
2	1	125	HIS
2	1	172	GLN
2	1	194	ASN
2	1	196	HIS
3	4	18	HIS
3	4	43	ASN
3	4	152	HIS
3	5	196	GLN
3	6	18	HIS
3	6	32	GLN
3	6	230	HIS
3	6	235	GLN
3	6	270	ASN
3	6	340	GLN

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Mol	Chain	Res	Type
4	7	157	GLN
4	7	331	ASN
4	8	99	HIS
4	8	131	HIS
4	8	352	HIS
4	9	7	ASN
4	9	120	ASN
4	9	131	HIS
5	A	126	GLN
2	AC	145	HIS
2	AC	197	HIS
2	AD	192	HIS
2	AE	176	HIS
2	AE	197	HIS
2	AE	226	ASN
4	B	53	GLN
4	B	207	ASN
4	B	236	GLN
3	E	230	HIS
3	E	252	ASN
3	E	355	HIS
3	F	152	HIS
3	G	3	HIS
3	G	142	GLN
3	G	196	GLN
3	G	260	GLN
3	G	281	ASN
3	G	340	GLN
3	G	355	HIS
3	H	3	HIS
3	H	32	GLN
3	H	116	HIS
3	H	196	GLN
3	H	230	HIS
4	I	131	HIS
4	I	331	ASN
4	I	348	HIS
4	J	7	ASN
4	J	49	GLN
4	J	131	HIS
4	J	236	GLN
4	J	238	ASN

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Mol	Chain	Res	Type
4	J	277	HIS
4	K	183	GLN
4	K	238	ASN
4	K	331	ASN
4	K	332	ASN
4	K	348	HIS
1	M	13	ASN
1	M	53	GLN
2	O	194	ASN
2	P	172	GLN
2	P	194	ASN
4	R	53	GLN
4	R	131	HIS
4	R	170	HIS
1	S	42	ASN
1	S	53	GLN
3	U	3	HIS
3	W	32	GLN
3	W	152	HIS
3	W	230	HIS
3	W	355	HIS
4	X	61	ASN
4	X	232	HIS
4	X	304	GLN
4	Y	184	GLN
4	Y	236	GLN
4	Z	224	GLN
4	Z	232	HIS
4	Z	352	HIS
1	b	13	ASN
1	b	30	ASN
2	d	145	HIS
2	d	194	ASN
2	d	197	HIS
2	e	196	HIS
2	e	197	HIS
2	f	125	HIS
3	h	18	HIS
3	h	100	ASN
3	i	32	GLN
4	j	304	GLN
4	j	340	GLN

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Mol	Chain	Res	Type
3	m	355	HIS
3	o	32	GLN
3	o	230	HIS
3	o	331	HIS
3	p	102	GLN
3	p	116	HIS
3	q	3	HIS
3	q	204	GLN
3	q	230	HIS
3	q	340	GLN
3	q	355	HIS
4	r	26	HIS
4	r	53	GLN
4	r	62	HIS
4	s	5	HIS
4	s	26	HIS
4	s	53	GLN
4	s	99	HIS
4	s	184	GLN
4	s	236	GLN
4	t	53	GLN
4	t	116	GLN
4	t	224	GLN
4	t	232	HIS
4	t	340	GLN
4	t	348	HIS
4	t	352	HIS
1	v	13	ASN
1	w	13	ASN
2	x	194	ASN
2	x	201	GLN
2	y	176	HIS
2	y	194	ASN
2	y	196	HIS
4	z	207	ASN
4	z	236	GLN
4	z	340	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

144 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$
6	NAG	BA	1	6,3	14,14,15	0.43	0	17,19,21	0.62	0
6	NAG	BA	2	6	14,14,15	0.19	0	17,19,21	0.46	0
6	BMA	BA	3	6	11,11,12	0.53	0	15,15,17	0.65	0
6	NAG	C	1	6,3	14,14,15	0.19	0	17,19,21	0.63	1 (5%)
6	NAG	C	2	6	14,14,15	0.19	0	17,19,21	0.46	0
6	BMA	C	3	6	11,11,12	0.55	0	15,15,17	0.71	0
6	NAG	CA	1	6,4	14,14,15	0.49	0	17,19,21	1.36	2 (11%)
6	NAG	CA	2	6	14,14,15	0.21	0	17,19,21	0.45	0
6	BMA	CA	3	6	11,11,12	0.53	0	15,15,17	0.89	1 (6%)
6	NAG	DA	1	6,4	14,14,15	0.38	0	17,19,21	0.40	0
6	NAG	DA	2	6	14,14,15	0.28	0	17,19,21	0.51	0
6	BMA	DA	3	6	11,11,12	0.68	0	15,15,17	0.68	0
6	NAG	EA	1	6,4	14,14,15	0.59	1 (7%)	17,19,21	0.83	0
6	NAG	EA	2	6	14,14,15	0.31	0	17,19,21	0.81	0
6	BMA	EA	3	6	11,11,12	0.42	0	15,15,17	0.90	1 (6%)
6	NAG	FA	1	6,4	14,14,15	0.32	0	17,19,21	0.64	0
6	NAG	FA	2	6	14,14,15	0.20	0	17,19,21	0.61	0
6	BMA	FA	3	6	11,11,12	0.68	0	15,15,17	0.63	0
6	NAG	GA	1	6,4	14,14,15	0.19	0	17,19,21	0.54	0
6	NAG	GA	2	6	14,14,15	0.18	0	17,19,21	0.43	0
6	BMA	GA	3	6	11,11,12	0.51	0	15,15,17	0.82	0
6	NAG	HA	1	6,4	14,14,15	0.32	0	17,19,21	0.36	0
6	NAG	HA	2	6	14,14,15	0.23	0	17,19,21	0.53	0
6	BMA	HA	3	6	11,11,12	0.58	0	15,15,17	0.76	0
6	NAG	IA	1	6,4	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
6	NAG	IA	2	6	14,14,15	0.37	0	17,19,21	1.38	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	IA	3	6	11,11,12	0.86	1 (9%)	15,15,17	0.98	0
6	NAG	JA	1	6,4	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	JA	2	6	14,14,15	0.23	0	17,19,21	0.45	0
6	BMA	JA	3	6	11,11,12	0.55	0	15,15,17	0.69	0
6	NAG	KA	1	6,3	14,14,15	0.19	0	17,19,21	0.50	0
6	NAG	KA	2	6	14,14,15	0.20	0	17,19,21	0.44	0
6	BMA	KA	3	6	11,11,12	0.49	0	15,15,17	0.92	1 (6%)
6	NAG	LA	1	6,3	14,14,15	0.15	0	17,19,21	0.66	1 (5%)
6	NAG	LA	2	6	14,14,15	0.19	0	17,19,21	0.51	0
6	BMA	LA	3	6	11,11,12	0.56	0	15,15,17	0.71	0
6	NAG	MA	1	6,3	14,14,15	0.33	0	17,19,21	0.61	0
6	NAG	MA	2	6	14,14,15	0.75	1 (7%)	17,19,21	1.28	2 (11%)
6	BMA	MA	3	6	11,11,12	0.73	0	15,15,17	0.97	0
6	NAG	NA	1	6,3	14,14,15	0.20	0	17,19,21	0.56	0
6	NAG	NA	2	6	14,14,15	0.36	0	17,19,21	0.43	0
6	BMA	NA	3	6	11,11,12	0.56	0	15,15,17	0.71	0
6	NAG	OA	1	6,4	14,14,15	0.37	0	17,19,21	0.45	0
6	NAG	OA	2	6	14,14,15	0.26	0	17,19,21	0.49	0
6	BMA	OA	3	6	11,11,12	0.69	0	15,15,17	0.70	0
6	NAG	PA	1	6,4	14,14,15	0.26	0	17,19,21	1.36	2 (11%)
6	NAG	PA	2	6	14,14,15	0.21	0	17,19,21	0.42	0
6	BMA	PA	3	6	11,11,12	0.46	0	15,15,17	0.82	1 (6%)
6	NAG	QA	1	6,4	14,14,15	0.20	0	17,19,21	0.67	0
6	NAG	QA	2	6	14,14,15	0.22	0	17,19,21	0.48	0
6	BMA	QA	3	6	11,11,12	0.63	0	15,15,17	0.68	0
6	NAG	RA	1	6,4	14,14,15	0.55	0	17,19,21	0.72	0
6	NAG	RA	2	6	14,14,15	0.25	0	17,19,21	0.75	0
6	BMA	RA	3	6	11,11,12	0.48	0	15,15,17	0.82	0
6	NAG	SA	1	6,4	14,14,15	0.18	0	17,19,21	0.52	0
6	NAG	SA	2	6	14,14,15	0.21	0	17,19,21	0.38	0
6	BMA	SA	3	6	11,11,12	0.81	1 (9%)	15,15,17	1.06	0
6	NAG	TA	1	6,4	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	TA	2	6	14,14,15	0.17	0	17,19,21	0.49	0
6	BMA	TA	3	6	11,11,12	0.55	0	15,15,17	0.76	0
6	NAG	UA	1	6,4	14,14,15	0.37	0	17,19,21	0.51	0
6	NAG	UA	2	6	14,14,15	0.38	0	17,19,21	1.34	2 (11%)
6	BMA	UA	3	6	11,11,12	0.54	0	15,15,17	0.83	0
6	NAG	VA	1	6,4	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	VA	2	6	14,14,15	0.21	0	17,19,21	0.46	0
6	BMA	VA	3	6	11,11,12	0.45	0	15,15,17	0.73	0
6	NAG	WA	1	6,3	14,14,15	0.17	0	17,19,21	0.69	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	WA	2	6	14,14,15	0.19	0	17,19,21	0.37	0
6	BMA	WA	3	6	11,11,12	0.55	0	15,15,17	0.77	0
6	NAG	XA	1	6,3	14,14,15	0.49	0	17,19,21	0.77	0
6	NAG	XA	2	6	14,14,15	0.66	1 (7%)	17,19,21	1.31	2 (11%)
6	BMA	XA	3	6	11,11,12	0.86	0	15,15,17	0.73	0
6	NAG	YA	1	6,3	14,14,15	0.44	0	17,19,21	0.43	0
6	NAG	YA	2	6	14,14,15	0.29	0	17,19,21	0.47	0
6	BMA	YA	3	6	11,11,12	0.66	0	15,15,17	0.68	0
6	NAG	ZA	1	6,4	14,14,15	0.39	0	17,19,21	1.35	2 (11%)
6	NAG	ZA	2	6	14,14,15	0.23	0	17,19,21	0.60	0
6	BMA	ZA	3	6	11,11,12	0.53	0	15,15,17	0.70	0
6	NAG	aA	1	6,4	14,14,15	0.38	0	17,19,21	0.37	0
6	NAG	aA	2	6	14,14,15	0.19	0	17,19,21	0.45	0
6	BMA	aA	3	6	11,11,12	0.51	0	15,15,17	0.65	0
6	NAG	bA	1	6,4	14,14,15	0.66	1 (7%)	17,19,21	0.71	0
6	NAG	bA	2	6	14,14,15	0.33	0	17,19,21	0.60	0
6	BMA	bA	3	6	11,11,12	0.50	0	15,15,17	1.11	1 (6%)
6	NAG	cA	1	6,4	14,14,15	0.19	0	17,19,21	0.53	0
6	NAG	cA	2	6	14,14,15	0.23	0	17,19,21	0.48	0
6	BMA	cA	3	6	11,11,12	0.51	0	15,15,17	0.68	0
6	NAG	dA	1	6,4	14,14,15	0.19	0	17,19,21	0.57	0
6	NAG	dA	2	6	14,14,15	0.16	0	17,19,21	0.50	0
6	BMA	dA	3	6	11,11,12	0.62	0	15,15,17	0.82	0
6	NAG	eA	1	6,4	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	eA	2	6	14,14,15	0.20	0	17,19,21	0.45	0
6	BMA	eA	3	6	11,11,12	0.50	0	15,15,17	0.72	0
6	NAG	fA	1	6,3	14,14,15	0.18	0	17,19,21	0.68	1 (5%)
6	NAG	fA	2	6	14,14,15	0.29	0	17,19,21	0.48	0
6	BMA	fA	3	6	11,11,12	0.65	0	15,15,17	0.88	0
6	NAG	gA	1	6,3	14,14,15	0.19	0	17,19,21	0.67	1 (5%)
6	NAG	gA	2	6	14,14,15	0.21	0	17,19,21	0.47	0
6	BMA	gA	3	6	11,11,12	0.53	0	15,15,17	0.79	0
6	NAG	hA	1	6,4	14,14,15	0.36	0	17,19,21	0.59	0
6	NAG	hA	2	6	14,14,15	0.38	0	17,19,21	1.35	2 (11%)
6	BMA	hA	3	6	11,11,12	0.70	0	15,15,17	0.93	0
6	NAG	iA	1	6,4	14,14,15	0.50	0	17,19,21	0.39	0
6	NAG	iA	2	6	14,14,15	0.19	0	17,19,21	0.51	0
6	BMA	iA	3	6	11,11,12	0.67	0	15,15,17	0.70	0
6	NAG	jA	1	6,3	14,14,15	0.19	0	17,19,21	0.65	0
6	NAG	jA	2	6	14,14,15	0.21	0	17,19,21	0.47	0
6	BMA	jA	3	6	11,11,12	0.57	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	k	1	6,3	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
6	NAG	k	2	6	14,14,15	0.67	1 (7%)	17,19,21	1.34	2 (11%)
6	BMA	k	3	6	11,11,12	0.89	1 (9%)	15,15,17	0.89	0
6	NAG	kA	1	6,3	14,14,15	0.16	0	17,19,21	0.68	1 (5%)
6	NAG	kA	2	6	14,14,15	0.18	0	17,19,21	0.48	0
6	BMA	kA	3	6	11,11,12	0.56	0	15,15,17	0.80	0
6	NAG	lA	1	6,3	14,14,15	1.03	1 (7%)	17,19,21	1.03	1 (5%)
6	NAG	lA	2	6	14,14,15	1.12	1 (7%)	17,19,21	1.65	2 (11%)
6	BMA	lA	3	6	11,11,12	0.59	0	15,15,17	0.85	0
6	NAG	mA	1	6,3	14,14,15	0.30	0	17,19,21	0.75	0
6	NAG	mA	2	6	14,14,15	0.25	0	17,19,21	0.42	0
6	BMA	mA	3	6	11,11,12	0.59	0	15,15,17	0.66	0
6	NAG	nA	1	6,4	14,14,15	0.40	0	17,19,21	1.36	2 (11%)
6	NAG	nA	2	6	14,14,15	0.27	0	17,19,21	0.45	0
6	BMA	nA	3	6	11,11,12	0.51	0	15,15,17	0.73	0
6	NAG	oA	1	6,4	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	oA	2	6	14,14,15	0.18	0	17,19,21	0.52	0
6	BMA	oA	3	6	11,11,12	0.67	0	15,15,17	0.79	0
6	NAG	pA	1	6,4	14,14,15	0.89	1 (7%)	17,19,21	0.92	0
6	NAG	pA	2	6	14,14,15	0.29	0	17,19,21	0.73	0
6	BMA	pA	3	6	11,11,12	0.62	0	15,15,17	1.20	1 (6%)
6	NAG	qA	1	6,4	14,14,15	0.24	0	17,19,21	0.52	0
6	NAG	qA	2	6	14,14,15	0.19	0	17,19,21	0.46	0
6	BMA	qA	3	6	11,11,12	0.75	0	15,15,17	0.75	0
6	NAG	rA	1	6,4	14,14,15	0.21	0	17,19,21	0.58	0
6	NAG	rA	2	6	14,14,15	0.22	0	17,19,21	0.48	0
6	BMA	rA	3	6	11,11,12	0.60	0	15,15,17	0.77	1 (6%)
6	NAG	sA	1	6,4	14,14,15	0.17	0	17,19,21	0.45	0
6	NAG	sA	2	6	14,14,15	0.16	0	17,19,21	0.50	0
6	BMA	sA	3	6	11,11,12	0.59	0	15,15,17	0.86	0
6	NAG	tA	1	6,4	14,14,15	0.33	0	17,19,21	0.99	1 (5%)
6	NAG	tA	2	6	14,14,15	0.53	0	17,19,21	1.34	2 (11%)
6	BMA	tA	3	6	11,11,12	0.67	0	15,15,17	0.98	0
6	NAG	uA	1	6,4	14,14,15	0.22	0	17,19,21	0.48	0
6	NAG	uA	2	6	14,14,15	0.24	0	17,19,21	0.50	0
6	BMA	uA	3	6	11,11,12	0.61	0	15,15,17	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	BA	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	BA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	BA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	C	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	C	2	6	-	2/6/23/26	0/1/1/1
6	BMA	C	3	6	-	1/2/19/22	0/1/1/1
6	NAG	CA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	CA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	CA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	DA	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	DA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	DA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	EA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	EA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	EA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	FA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	FA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	FA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	GA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	GA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	GA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	HA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	HA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	HA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	IA	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	IA	2	6	-	5/6/23/26	0/1/1/1
6	BMA	IA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	JA	1	6,4	-	1/6/23/26	0/1/1/1
6	NAG	JA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	JA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	KA	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	KA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	KA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	LA	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	LA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	LA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	MA	1	6,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	MA	2	6	-	6/6/23/26	0/1/1/1
6	BMA	MA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	NA	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	NA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	NA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	OA	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	OA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	OA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	PA	1	6,4	-	6/6/23/26	0/1/1/1
6	NAG	PA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	PA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	QA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	QA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	QA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	RA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	RA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	RA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	SA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	SA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	SA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	TA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	TA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	TA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	UA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	UA	2	6	-	6/6/23/26	0/1/1/1
6	BMA	UA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	VA	1	6,4	-	1/6/23/26	0/1/1/1
6	NAG	VA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	VA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	WA	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	WA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	WA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	XA	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	XA	2	6	-	6/6/23/26	0/1/1/1
6	BMA	XA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	YA	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	YA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	YA	3	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	ZA	1	6,4	-	6/6/23/26	0/1/1/1
6	NAG	ZA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	ZA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	aA	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	aA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	aA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	bA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	bA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	bA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	cA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	cA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	cA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	dA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	dA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	dA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	eA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	eA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	eA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	fA	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	fA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	fA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	gA	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	gA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	gA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	hA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	hA	2	6	-	6/6/23/26	0/1/1/1
6	BMA	hA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	iA	1	6,4	-	1/6/23/26	0/1/1/1
6	NAG	iA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	iA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	jA	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	jA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	jA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	k	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	k	2	6	-	5/6/23/26	0/1/1/1
6	BMA	k	3	6	-	1/2/19/22	0/1/1/1
6	NAG	kA	1	6,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	kA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	kA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	lA	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	lA	2	6	-	6/6/23/26	0/1/1/1
6	BMA	lA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	mA	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	mA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	mA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	nA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	nA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	nA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	oA	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	oA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	oA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	pA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	pA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	pA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	qA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	qA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	qA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	rA	1	6,4	-	3/6/23/26	0/1/1/1
6	NAG	rA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	rA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	sA	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	sA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	sA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	tA	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	tA	2	6	-	5/6/23/26	0/1/1/1
6	BMA	tA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	uA	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	uA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	uA	3	6	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	lA	2	NAG	C1-C2	3.44	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	lA	1	NAG	O5-C1	-3.18	1.38	1.43
6	pA	1	NAG	O5-C1	-3.15	1.38	1.43
6	MA	2	NAG	C1-C2	2.46	1.55	1.52
6	IA	3	BMA	C1-C2	2.34	1.57	1.52
6	k	2	NAG	C1-C2	2.31	1.55	1.52
6	bA	1	NAG	O5-C1	-2.29	1.39	1.43
6	k	3	BMA	C1-C2	2.25	1.57	1.52
6	SA	3	BMA	C1-C2	2.24	1.57	1.52
6	XA	2	NAG	C1-C2	2.18	1.55	1.52
6	EA	1	NAG	O5-C1	-2.03	1.40	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	k	2	NAG	C2-N2-C7	4.57	129.02	122.90
6	IA	2	NAG	C2-N2-C7	4.54	128.99	122.90
6	UA	2	NAG	C2-N2-C7	4.52	128.96	122.90
6	nA	1	NAG	C2-N2-C7	4.49	128.92	122.90
6	PA	1	NAG	C2-N2-C7	4.49	128.91	122.90
6	CA	1	NAG	C2-N2-C7	4.48	128.90	122.90
6	tA	2	NAG	C2-N2-C7	4.47	128.89	122.90
6	hA	2	NAG	C2-N2-C7	4.46	128.88	122.90
6	ZA	1	NAG	C2-N2-C7	4.46	128.87	122.90
6	XA	2	NAG	C2-N2-C7	4.45	128.86	122.90
6	MA	2	NAG	C2-N2-C7	4.44	128.85	122.90
6	lA	2	NAG	C1-O5-C5	4.24	117.86	112.19
6	lA	2	NAG	C2-N2-C7	4.12	128.43	122.90
6	tA	1	NAG	C1-O5-C5	3.35	116.68	112.19
6	IA	1	NAG	C1-O5-C5	3.06	116.29	112.19
6	bA	3	BMA	C1-O5-C5	2.88	116.05	112.19
6	pA	3	BMA	C1-O5-C5	2.63	115.71	112.19
6	lA	1	NAG	C3-C4-C5	2.59	114.94	110.23
6	IA	2	NAG	C1-C2-N2	2.57	114.48	110.43
6	tA	2	NAG	C1-C2-N2	2.40	114.21	110.43
6	hA	2	NAG	C1-C2-N2	2.37	114.17	110.43
6	PA	1	NAG	C1-C2-N2	2.30	114.05	110.43
6	KA	3	BMA	C1-O5-C5	2.27	115.23	112.19
6	gA	1	NAG	C1-O5-C5	2.27	115.22	112.19
6	UA	2	NAG	C1-C2-N2	2.25	113.98	110.43
6	CA	3	BMA	O2-C2-C3	-2.23	105.54	110.15
6	nA	1	NAG	C1-C2-N2	2.20	113.90	110.43
6	WA	1	NAG	C1-O5-C5	2.18	115.11	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	rA	3	BMA	O2-C2-C3	-2.17	105.66	110.15
6	fA	1	NAG	C1-O5-C5	2.16	115.09	112.19
6	LA	1	NAG	C1-O5-C5	2.16	115.08	112.19
6	CA	1	NAG	C1-C2-N2	2.15	113.82	110.43
6	ZA	1	NAG	C1-C2-N2	2.15	113.81	110.43
6	kA	1	NAG	C1-O5-C5	2.14	115.06	112.19
6	EA	3	BMA	O2-C2-C3	-2.14	105.72	110.15
6	XA	2	NAG	C1-C2-N2	2.12	113.77	110.43
6	PA	3	BMA	O2-C2-C3	-2.09	105.83	110.15
6	C	1	NAG	C1-O5-C5	2.08	114.98	112.19
6	MA	2	NAG	C1-C2-N2	2.05	113.66	110.43
6	k	2	NAG	C1-C2-N2	2.02	113.62	110.43
6	k	1	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (285) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	mA	2	NAG	O5-C5-C6-O6
6	oA	2	NAG	O5-C5-C6-O6
6	NA	2	NAG	O5-C5-C6-O6
6	VA	2	NAG	O5-C5-C6-O6
6	aA	2	NAG	O5-C5-C6-O6
6	fA	2	NAG	O5-C5-C6-O6
6	DA	1	NAG	O5-C5-C6-O6
6	DA	2	NAG	O5-C5-C6-O6
6	NA	1	NAG	O5-C5-C6-O6
6	OA	1	NAG	O5-C5-C6-O6
6	TA	1	NAG	O5-C5-C6-O6
6	cA	1	NAG	O5-C5-C6-O6
6	gA	2	NAG	O5-C5-C6-O6
6	KA	2	NAG	O5-C5-C6-O6
6	eA	2	NAG	O5-C5-C6-O6
6	kA	3	BMA	O5-C5-C6-O6
6	NA	2	NAG	C4-C5-C6-O6
6	VA	2	NAG	C4-C5-C6-O6
6	gA	2	NAG	C4-C5-C6-O6
6	fA	2	NAG	C4-C5-C6-O6
6	tA	3	BMA	C4-C5-C6-O6
6	KA	3	BMA	O5-C5-C6-O6
6	lA	3	BMA	O5-C5-C6-O6
6	nA	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	aA	2	NAG	C4-C5-C6-O6
6	nA	2	NAG	C4-C5-C6-O6
6	oA	2	NAG	C4-C5-C6-O6
6	eA	1	NAG	O5-C5-C6-O6
6	jA	2	NAG	O5-C5-C6-O6
6	mA	2	NAG	C4-C5-C6-O6
6	FA	2	NAG	O5-C5-C6-O6
6	MA	3	BMA	O5-C5-C6-O6
6	lA	1	NAG	O5-C5-C6-O6
6	cA	1	NAG	C4-C5-C6-O6
6	hA	2	NAG	O5-C5-C6-O6
6	LA	1	NAG	O5-C5-C6-O6
6	PA	2	NAG	O5-C5-C6-O6
6	UA	2	NAG	O5-C5-C6-O6
6	ZA	2	NAG	O5-C5-C6-O6
6	sA	1	NAG	O5-C5-C6-O6
6	tA	3	BMA	O5-C5-C6-O6
6	WA	3	BMA	O5-C5-C6-O6
6	OA	1	NAG	C4-C5-C6-O6
6	DA	1	NAG	C4-C5-C6-O6
6	KA	2	NAG	C4-C5-C6-O6
6	NA	1	NAG	C4-C5-C6-O6
6	qA	2	NAG	C4-C5-C6-O6
6	sA	1	NAG	C4-C5-C6-O6
6	LA	1	NAG	C4-C5-C6-O6
6	PA	2	NAG	C4-C5-C6-O6
6	UA	2	NAG	C4-C5-C6-O6
6	eA	1	NAG	C4-C5-C6-O6
6	DA	2	NAG	C4-C5-C6-O6
6	uA	1	NAG	O5-C5-C6-O6
6	jA	3	BMA	O5-C5-C6-O6
6	ZA	2	NAG	C4-C5-C6-O6
6	hA	2	NAG	C4-C5-C6-O6
6	lA	1	NAG	C4-C5-C6-O6
6	k	2	NAG	C8-C7-N2-C2
6	k	2	NAG	O7-C7-N2-C2
6	BA	2	NAG	C8-C7-N2-C2
6	BA	2	NAG	O7-C7-N2-C2
6	CA	1	NAG	C8-C7-N2-C2
6	CA	1	NAG	O7-C7-N2-C2
6	DA	2	NAG	C8-C7-N2-C2
6	DA	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	GA	1	NAG	C8-C7-N2-C2
6	GA	1	NAG	O7-C7-N2-C2
6	HA	1	NAG	C8-C7-N2-C2
6	HA	1	NAG	O7-C7-N2-C2
6	HA	2	NAG	C8-C7-N2-C2
6	HA	2	NAG	O7-C7-N2-C2
6	IA	1	NAG	C8-C7-N2-C2
6	IA	1	NAG	O7-C7-N2-C2
6	IA	2	NAG	C8-C7-N2-C2
6	IA	2	NAG	O7-C7-N2-C2
6	MA	2	NAG	C8-C7-N2-C2
6	MA	2	NAG	O7-C7-N2-C2
6	NA	2	NAG	C8-C7-N2-C2
6	NA	2	NAG	O7-C7-N2-C2
6	OA	2	NAG	C8-C7-N2-C2
6	OA	2	NAG	O7-C7-N2-C2
6	PA	1	NAG	C8-C7-N2-C2
6	PA	1	NAG	O7-C7-N2-C2
6	SA	1	NAG	C8-C7-N2-C2
6	SA	1	NAG	O7-C7-N2-C2
6	TA	1	NAG	C8-C7-N2-C2
6	TA	1	NAG	O7-C7-N2-C2
6	TA	2	NAG	C8-C7-N2-C2
6	TA	2	NAG	O7-C7-N2-C2
6	UA	1	NAG	C8-C7-N2-C2
6	UA	1	NAG	O7-C7-N2-C2
6	UA	2	NAG	C8-C7-N2-C2
6	UA	2	NAG	O7-C7-N2-C2
6	XA	2	NAG	C8-C7-N2-C2
6	XA	2	NAG	O7-C7-N2-C2
6	YA	2	NAG	C8-C7-N2-C2
6	YA	2	NAG	O7-C7-N2-C2
6	ZA	1	NAG	C8-C7-N2-C2
6	ZA	1	NAG	O7-C7-N2-C2
6	aA	2	NAG	C8-C7-N2-C2
6	aA	2	NAG	O7-C7-N2-C2
6	dA	1	NAG	C8-C7-N2-C2
6	dA	1	NAG	O7-C7-N2-C2
6	eA	1	NAG	C8-C7-N2-C2
6	eA	1	NAG	O7-C7-N2-C2
6	eA	2	NAG	C8-C7-N2-C2
6	eA	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	hA	1	NAG	C8-C7-N2-C2
6	hA	1	NAG	O7-C7-N2-C2
6	hA	2	NAG	C8-C7-N2-C2
6	hA	2	NAG	O7-C7-N2-C2
6	lA	2	NAG	C8-C7-N2-C2
6	lA	2	NAG	O7-C7-N2-C2
6	mA	2	NAG	C8-C7-N2-C2
6	mA	2	NAG	O7-C7-N2-C2
6	nA	1	NAG	C8-C7-N2-C2
6	nA	1	NAG	O7-C7-N2-C2
6	oA	2	NAG	C8-C7-N2-C2
6	oA	2	NAG	O7-C7-N2-C2
6	rA	1	NAG	C8-C7-N2-C2
6	rA	1	NAG	O7-C7-N2-C2
6	sA	1	NAG	C8-C7-N2-C2
6	sA	1	NAG	O7-C7-N2-C2
6	sA	2	NAG	C8-C7-N2-C2
6	sA	2	NAG	O7-C7-N2-C2
6	tA	1	NAG	C8-C7-N2-C2
6	tA	1	NAG	O7-C7-N2-C2
6	tA	2	NAG	C8-C7-N2-C2
6	tA	2	NAG	O7-C7-N2-C2
6	C	1	NAG	O5-C5-C6-O6
6	UA	1	NAG	O5-C5-C6-O6
6	jA	2	NAG	C4-C5-C6-O6
6	UA	3	BMA	O5-C5-C6-O6
6	TA	1	NAG	C4-C5-C6-O6
6	BA	3	BMA	O5-C5-C6-O6
6	C	1	NAG	C4-C5-C6-O6
6	UA	1	NAG	C4-C5-C6-O6
6	qA	2	NAG	O5-C5-C6-O6
6	QA	1	NAG	C4-C5-C6-O6
6	kA	3	BMA	C4-C5-C6-O6
6	PA	1	NAG	O5-C5-C6-O6
6	oA	3	BMA	O5-C5-C6-O6
6	PA	1	NAG	C4-C5-C6-O6
6	eA	2	NAG	C4-C5-C6-O6
6	QA	1	NAG	O5-C5-C6-O6
6	RA	1	NAG	O5-C5-C6-O6
6	fA	1	NAG	O5-C5-C6-O6
6	fA	1	NAG	C4-C5-C6-O6
6	lA	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	hA	1	NAG	O5-C5-C6-O6
6	KA	1	NAG	O5-C5-C6-O6
6	NA	3	BMA	O5-C5-C6-O6
6	rA	2	NAG	O5-C5-C6-O6
6	jA	1	NAG	O5-C5-C6-O6
6	mA	3	BMA	O5-C5-C6-O6
6	hA	1	NAG	C4-C5-C6-O6
6	jA	1	NAG	C4-C5-C6-O6
6	rA	3	BMA	O5-C5-C6-O6
6	KA	1	NAG	C4-C5-C6-O6
6	FA	2	NAG	C4-C5-C6-O6
6	iA	2	NAG	C4-C5-C6-O6
6	oA	1	NAG	O5-C5-C6-O6
6	tA	2	NAG	O5-C5-C6-O6
6	gA	3	BMA	O5-C5-C6-O6
6	VA	1	NAG	O5-C5-C6-O6
6	rA	3	BMA	C4-C5-C6-O6
6	uA	2	NAG	C4-C5-C6-O6
6	HA	2	NAG	O5-C5-C6-O6
6	fA	3	BMA	O5-C5-C6-O6
6	rA	1	NAG	O5-C5-C6-O6
6	LA	3	BMA	O5-C5-C6-O6
6	SA	2	NAG	O5-C5-C6-O6
6	YA	3	BMA	O5-C5-C6-O6
6	aA	3	BMA	O5-C5-C6-O6
6	dA	1	NAG	O5-C5-C6-O6
6	C	3	BMA	O5-C5-C6-O6
6	TA	2	NAG	O5-C5-C6-O6
6	IA	3	BMA	O5-C5-C6-O6
6	bA	1	NAG	O5-C5-C6-O6
6	iA	1	NAG	O5-C5-C6-O6
6	XA	3	BMA	O5-C5-C6-O6
6	sA	2	NAG	O5-C5-C6-O6
6	GA	2	NAG	O5-C5-C6-O6
6	QA	2	NAG	O5-C5-C6-O6
6	YA	1	NAG	O5-C5-C6-O6
6	uA	2	NAG	O5-C5-C6-O6
6	IA	2	NAG	O5-C5-C6-O6
6	dA	2	NAG	O5-C5-C6-O6
6	HA	3	BMA	O5-C5-C6-O6
6	DA	3	BMA	O5-C5-C6-O6
6	EA	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	EA	3	BMA	O5-C5-C6-O6
6	RA	3	BMA	O5-C5-C6-O6
6	k	3	BMA	O5-C5-C6-O6
6	SA	1	NAG	O5-C5-C6-O6
6	cA	2	NAG	O5-C5-C6-O6
6	pA	1	NAG	O5-C5-C6-O6
6	OA	3	BMA	O5-C5-C6-O6
6	pA	3	BMA	O5-C5-C6-O6
6	JA	1	NAG	O5-C5-C6-O6
6	bA	3	BMA	O5-C5-C6-O6
6	hA	3	BMA	O5-C5-C6-O6
6	GA	1	NAG	O5-C5-C6-O6
6	HA	1	NAG	O5-C5-C6-O6
6	cA	3	BMA	O5-C5-C6-O6
6	uA	1	NAG	C4-C5-C6-O6
6	HA	3	BMA	C4-C5-C6-O6
6	ZA	1	NAG	C4-C5-C6-O6
6	cA	3	BMA	C4-C5-C6-O6
6	lA	2	NAG	O5-C5-C6-O6
6	RA	2	NAG	C4-C5-C6-O6
6	FA	1	NAG	C4-C5-C6-O6
6	ZA	1	NAG	O5-C5-C6-O6
6	iA	2	NAG	O5-C5-C6-O6
6	EA	1	NAG	C1-C2-N2-C7
6	PA	1	NAG	C1-C2-N2-C7
6	ZA	1	NAG	C1-C2-N2-C7
6	bA	1	NAG	C1-C2-N2-C7
6	nA	1	NAG	C1-C2-N2-C7
6	pA	1	NAG	C1-C2-N2-C7
6	C	2	NAG	C4-C5-C6-O6
6	OA	2	NAG	O5-C5-C6-O6
6	KA	3	BMA	C4-C5-C6-O6
6	CA	1	NAG	C3-C2-N2-C7
6	EA	1	NAG	C3-C2-N2-C7
6	FA	1	NAG	C3-C2-N2-C7
6	QA	1	NAG	C3-C2-N2-C7
6	RA	1	NAG	C3-C2-N2-C7
6	ZA	1	NAG	C3-C2-N2-C7
6	bA	1	NAG	C3-C2-N2-C7
6	cA	1	NAG	C3-C2-N2-C7
6	nA	1	NAG	C3-C2-N2-C7
6	pA	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	qA	1	NAG	C3-C2-N2-C7
6	lA	2	NAG	C4-C5-C6-O6
6	C	2	NAG	O5-C5-C6-O6
6	MA	2	NAG	C4-C5-C6-O6
6	gA	1	NAG	C4-C5-C6-O6
6	aA	1	NAG	O5-C5-C6-O6
6	MA	2	NAG	O5-C5-C6-O6
6	k	2	NAG	C4-C5-C6-O6
6	XA	2	NAG	C4-C5-C6-O6
6	jA	3	BMA	C4-C5-C6-O6
6	LA	2	NAG	C4-C5-C6-O6
6	XA	2	NAG	O5-C5-C6-O6
6	k	2	NAG	C1-C2-N2-C7
6	CA	1	NAG	C1-C2-N2-C7
6	FA	1	NAG	C1-C2-N2-C7
6	IA	2	NAG	C1-C2-N2-C7
6	MA	2	NAG	C1-C2-N2-C7
6	QA	1	NAG	C1-C2-N2-C7
6	RA	1	NAG	C1-C2-N2-C7
6	UA	2	NAG	C1-C2-N2-C7
6	XA	1	NAG	C1-C2-N2-C7
6	XA	2	NAG	C1-C2-N2-C7
6	cA	1	NAG	C1-C2-N2-C7
6	hA	2	NAG	C1-C2-N2-C7
6	lA	2	NAG	C1-C2-N2-C7
6	qA	1	NAG	C1-C2-N2-C7
6	tA	2	NAG	C1-C2-N2-C7
6	gA	1	NAG	O5-C5-C6-O6
6	k	2	NAG	C3-C2-N2-C7
6	IA	2	NAG	C3-C2-N2-C7
6	MA	2	NAG	C3-C2-N2-C7
6	PA	1	NAG	C3-C2-N2-C7
6	UA	2	NAG	C3-C2-N2-C7
6	XA	2	NAG	C3-C2-N2-C7
6	aA	1	NAG	C3-C2-N2-C7
6	fA	1	NAG	C3-C2-N2-C7
6	hA	2	NAG	C3-C2-N2-C7
6	jA	1	NAG	C3-C2-N2-C7
6	lA	2	NAG	C3-C2-N2-C7
6	tA	2	NAG	C3-C2-N2-C7
6	BA	2	NAG	C4-C5-C6-O6
6	MA	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	XA	1	NAG	C4-C5-C6-O6
6	WA	3	BMA	C4-C5-C6-O6
6	qA	1	NAG	O5-C5-C6-O6
6	FA	1	NAG	O5-C5-C6-O6
6	CA	2	NAG	C4-C5-C6-O6
6	k	1	NAG	C4-C5-C6-O6
6	BA	2	NAG	O5-C5-C6-O6
6	QA	3	BMA	O5-C5-C6-O6
6	oA	1	NAG	C4-C5-C6-O6

There are no ring outliers.

47 monomers are involved in 52 short contacts:

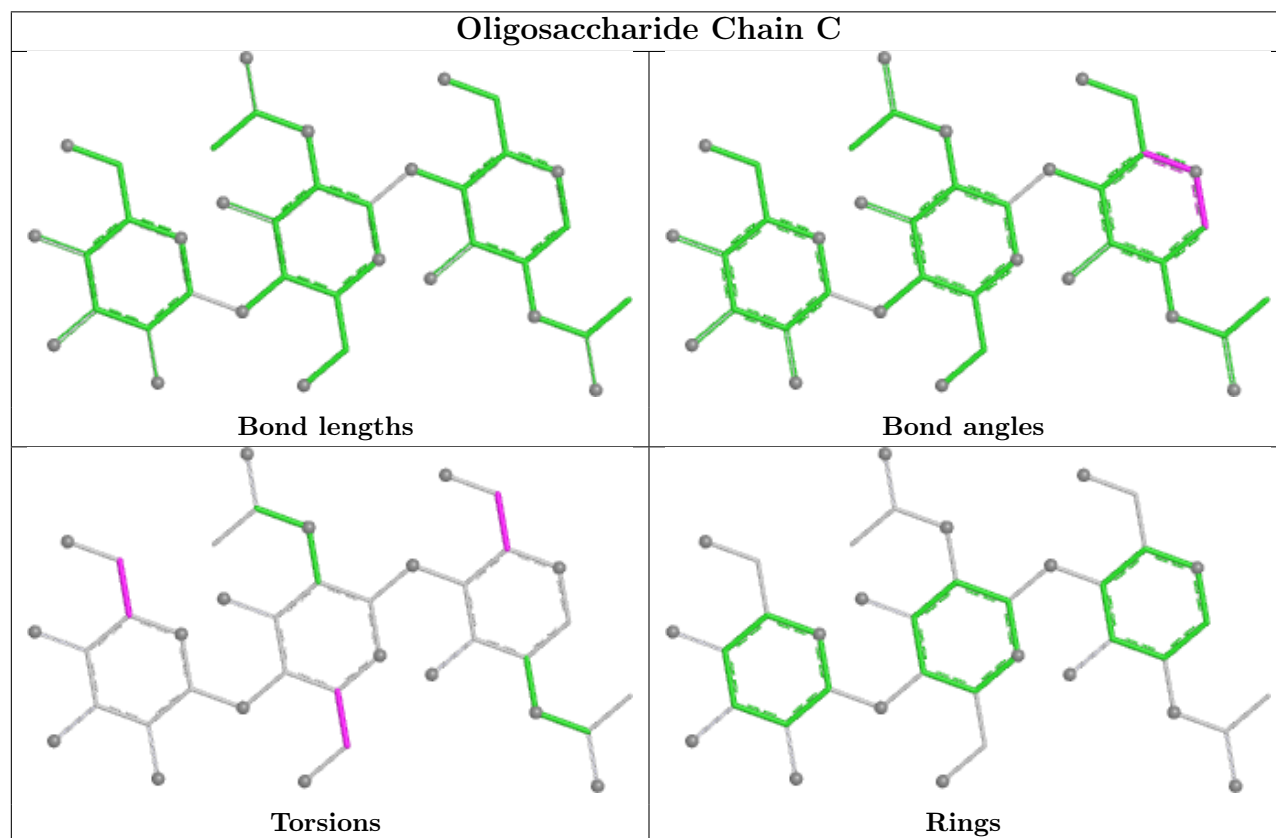
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	RA	2	NAG	1	0
6	IA	2	NAG	1	0
6	hA	2	NAG	1	0
6	ZA	2	NAG	1	0
6	XA	2	NAG	1	0
6	VA	2	NAG	1	0
6	GA	2	NAG	1	0
6	k	2	NAG	3	0
6	VA	1	NAG	1	0
6	gA	1	NAG	1	0
6	NA	2	NAG	1	0
6	GA	1	NAG	1	0
6	UA	2	NAG	1	0
6	FA	1	NAG	1	0
6	lA	2	NAG	1	0
6	PA	1	NAG	2	0
6	TA	1	NAG	3	0
6	FA	3	BMA	1	0
6	tA	2	NAG	1	0
6	MA	1	NAG	1	0
6	nA	1	NAG	1	0
6	JA	2	NAG	1	0
6	tA	3	BMA	1	0
6	gA	2	NAG	1	0
6	C	1	NAG	1	0
6	iA	2	NAG	1	0
6	YA	1	NAG	2	0
6	QA	2	NAG	1	0

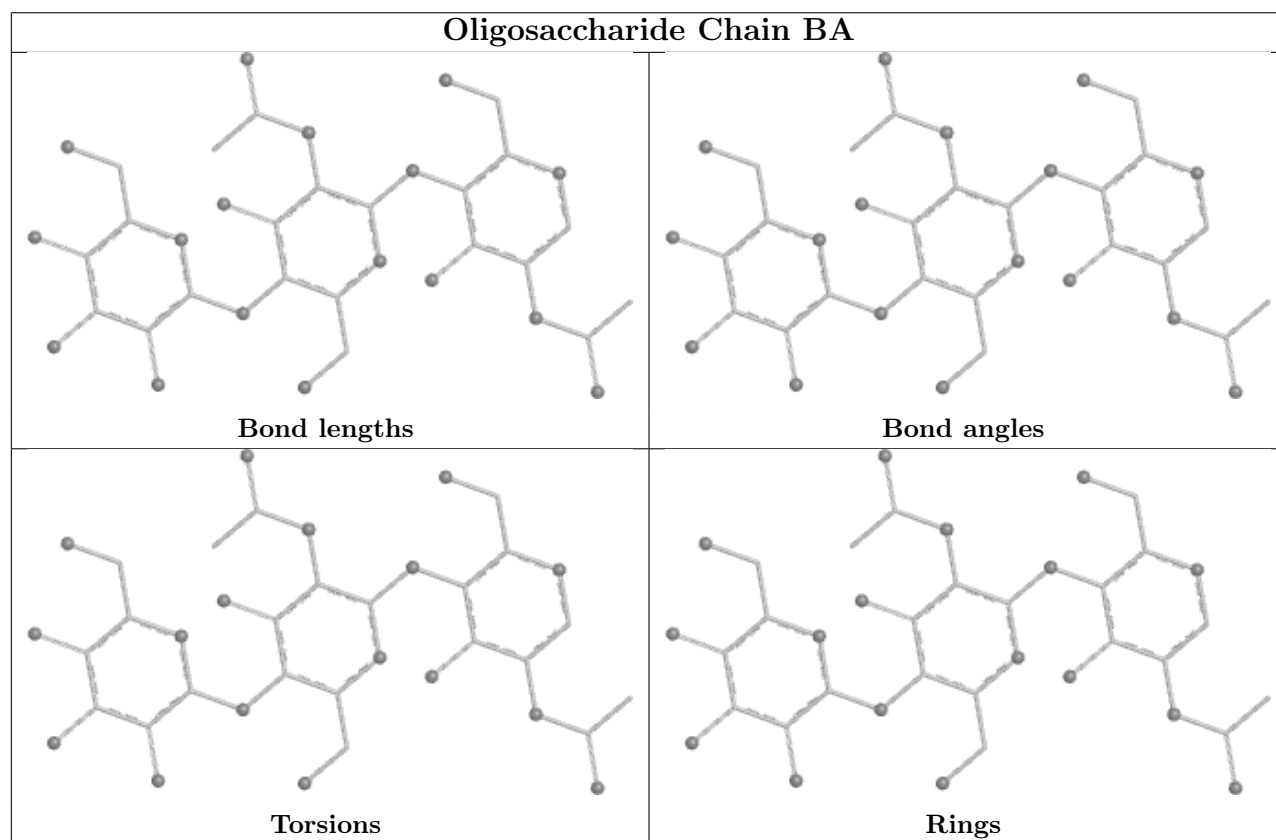
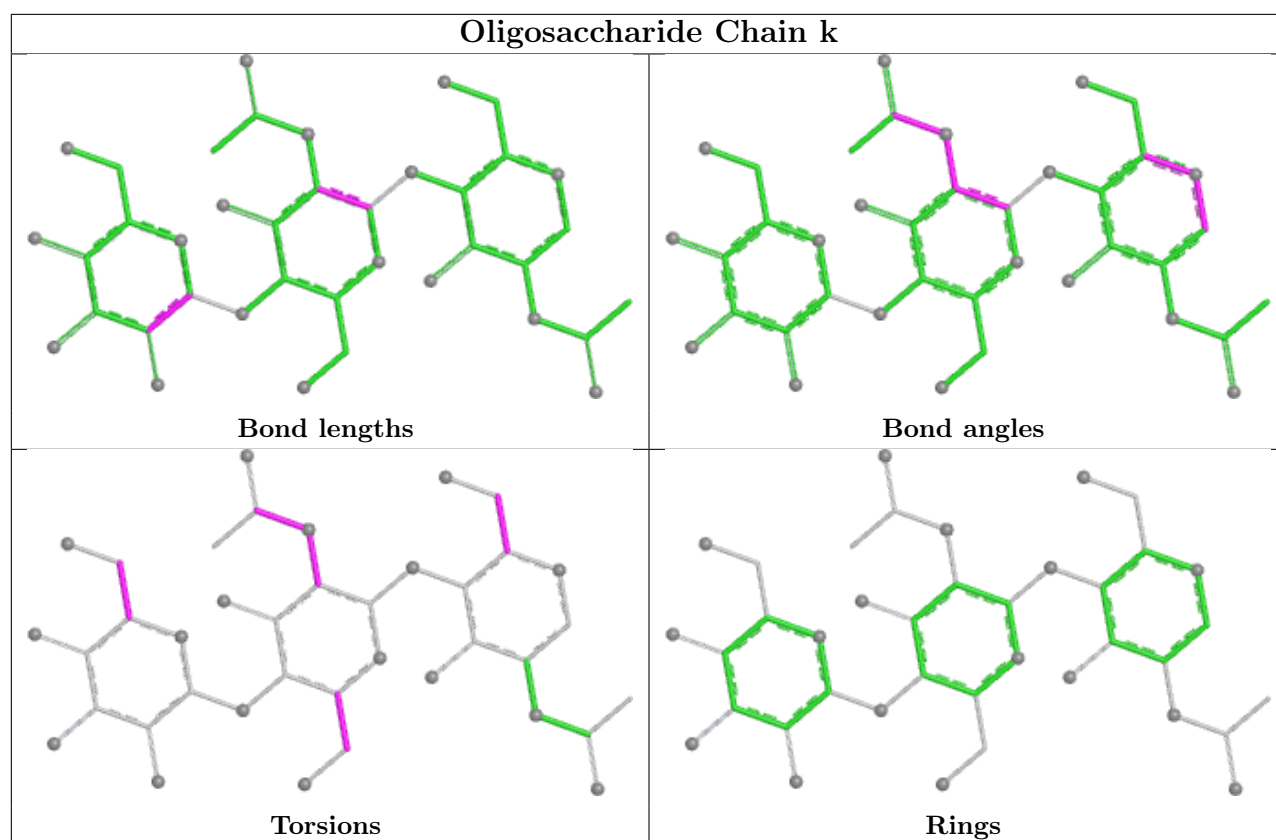
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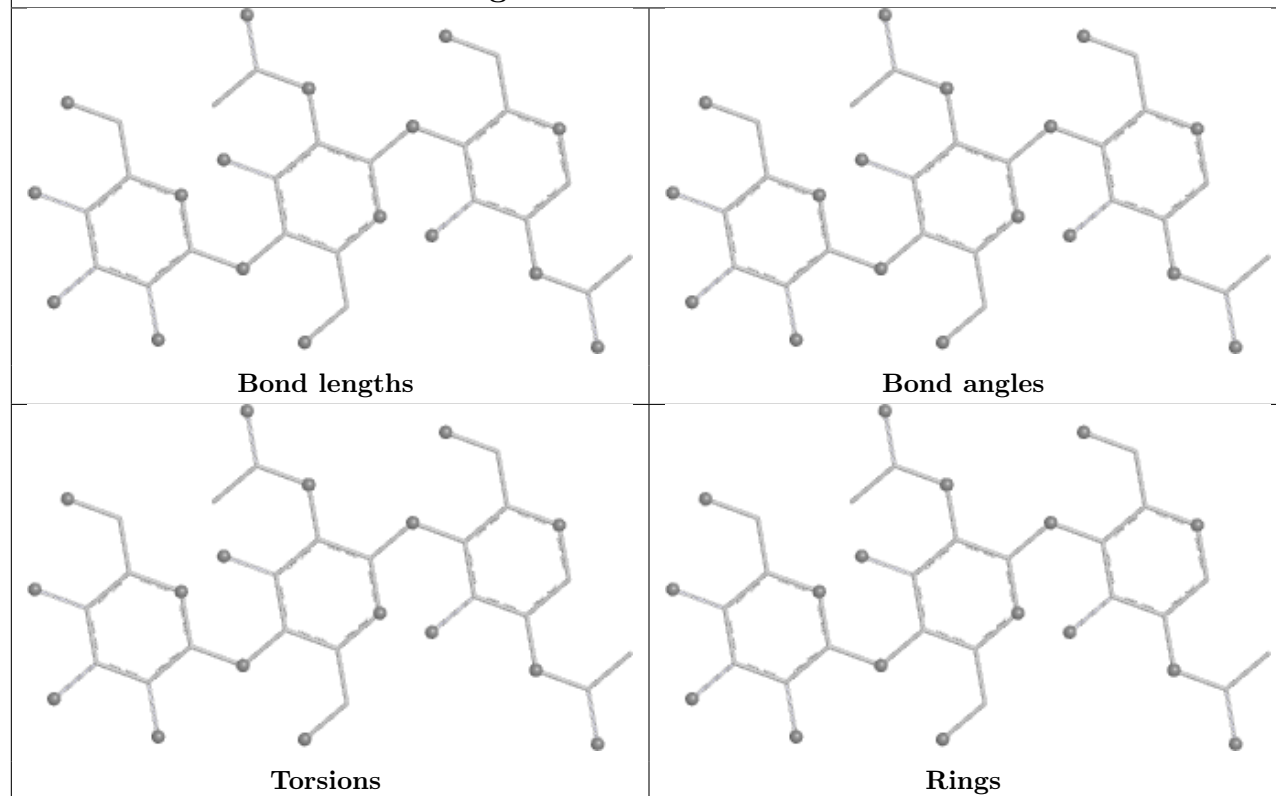
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	k	1	NAG	2	0
6	QA	1	NAG	1	0
6	BA	1	NAG	6	0
6	kA	1	NAG	1	0
6	iA	1	NAG	3	0
6	kA	2	NAG	1	0
6	PA	2	NAG	1	0
6	CA	1	NAG	1	0
6	SA	1	NAG	1	0
6	kA	3	BMA	1	0
6	mA	1	NAG	3	0
6	ZA	1	NAG	2	0
6	MA	2	NAG	2	0
6	NA	1	NAG	3	0
6	FA	2	NAG	2	0
6	BA	2	NAG	1	0
6	pA	2	NAG	1	0
6	JA	1	NAG	1	0
6	fA	1	NAG	1	0

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

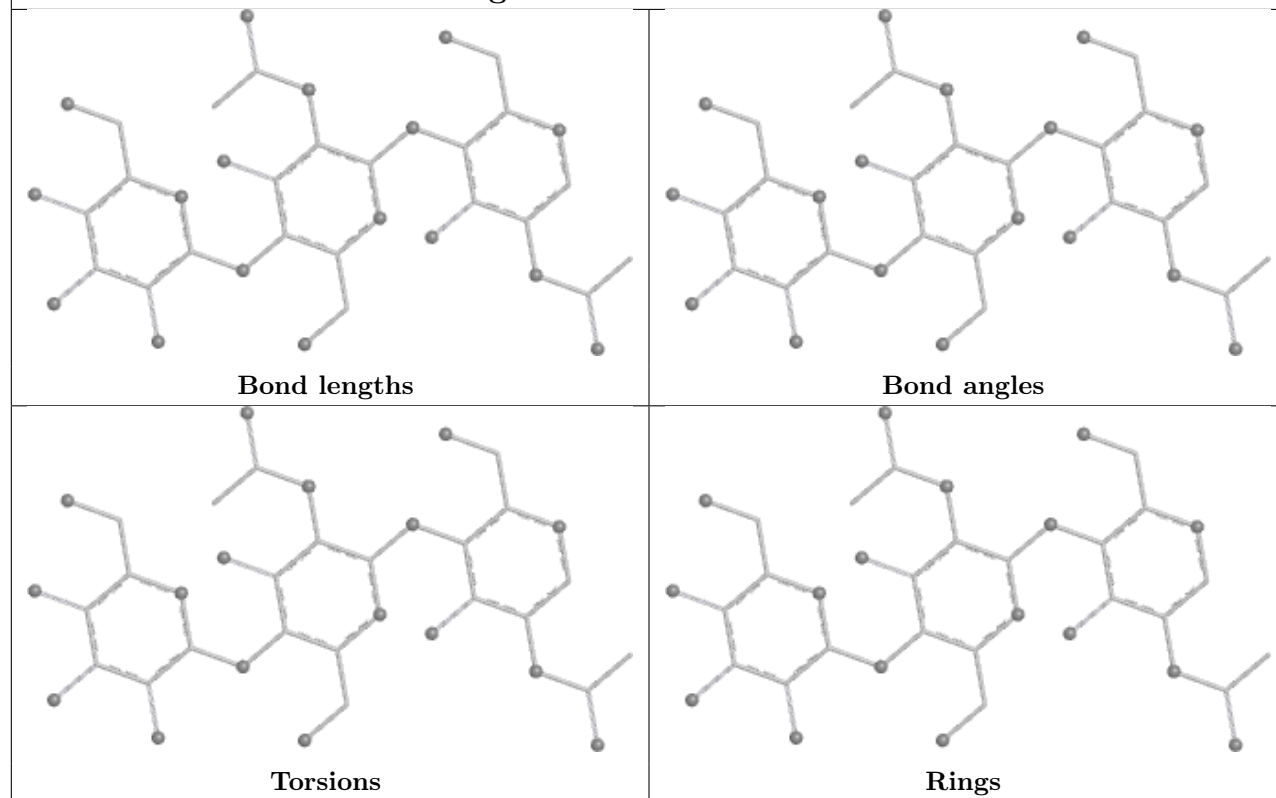




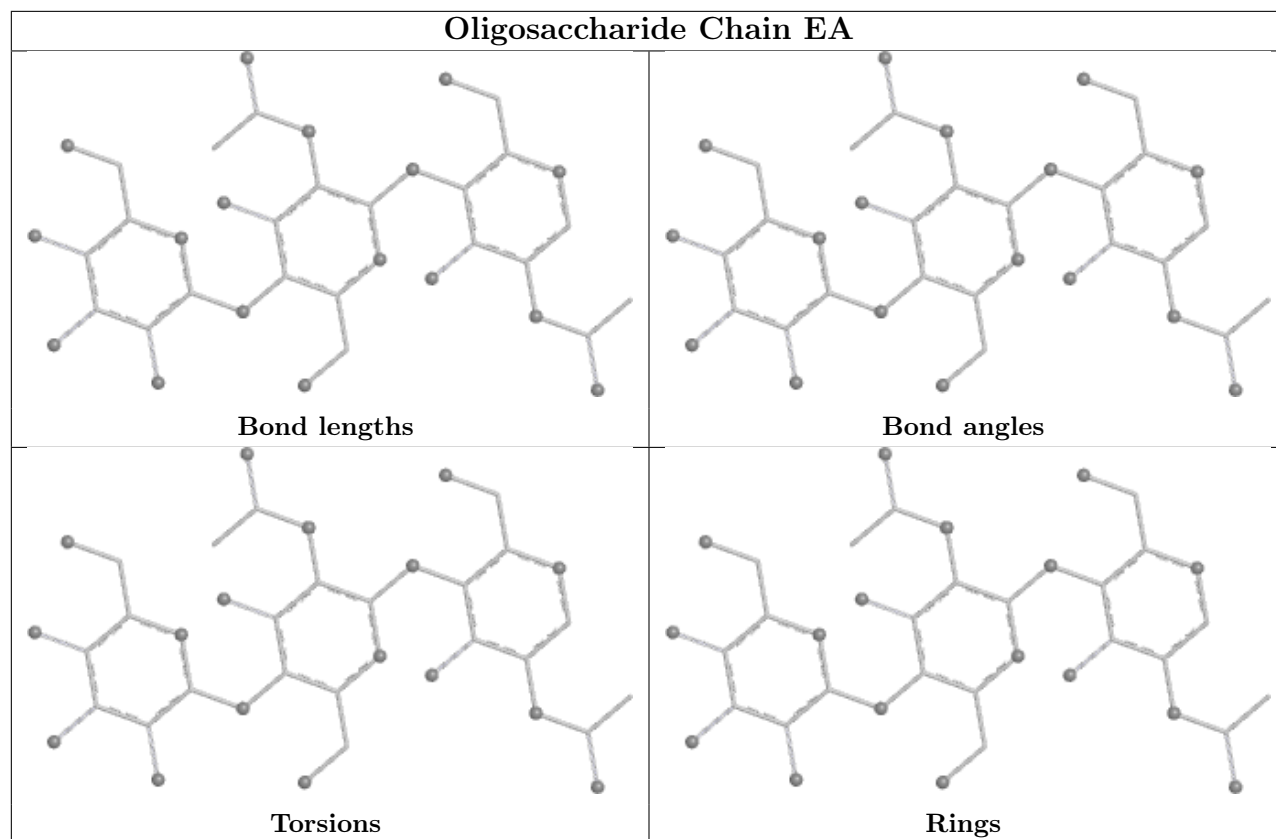
Oligosaccharide Chain CA



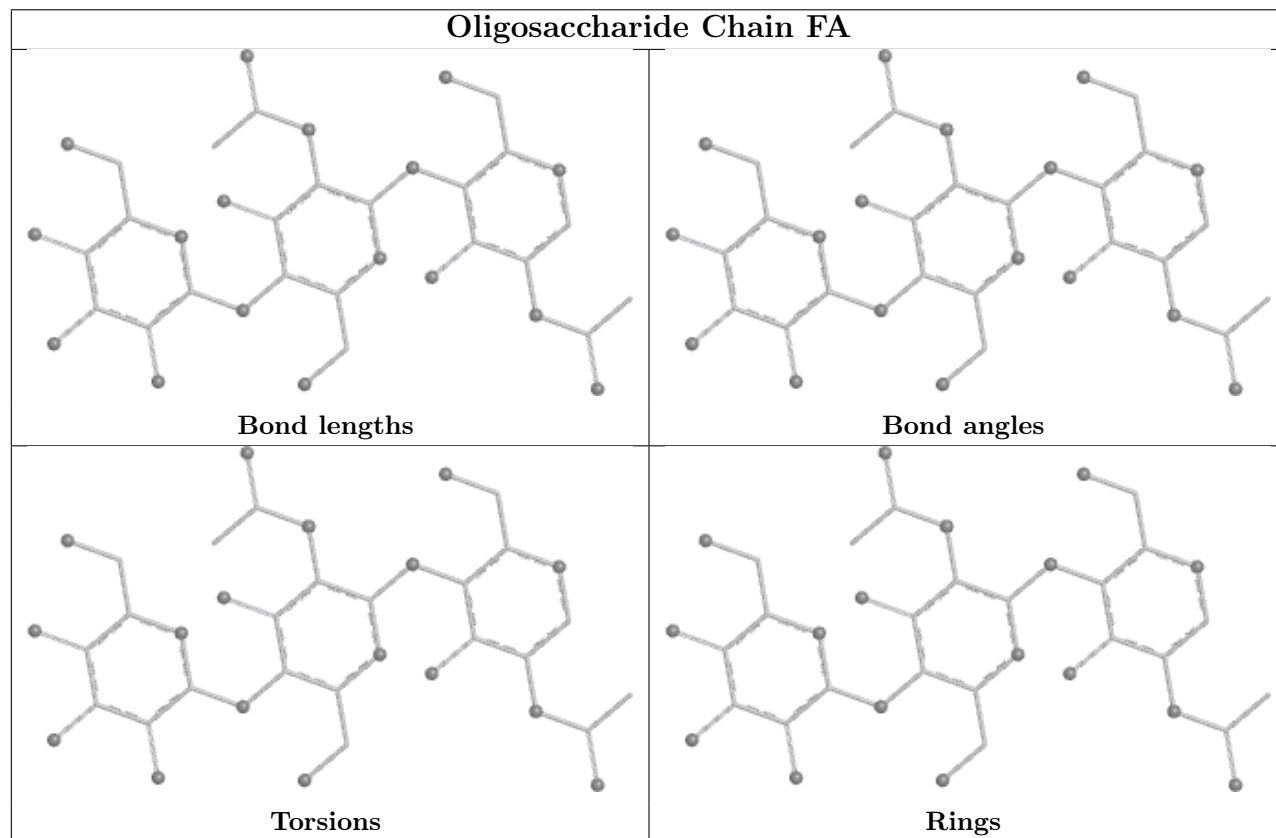
Oligosaccharide Chain DA



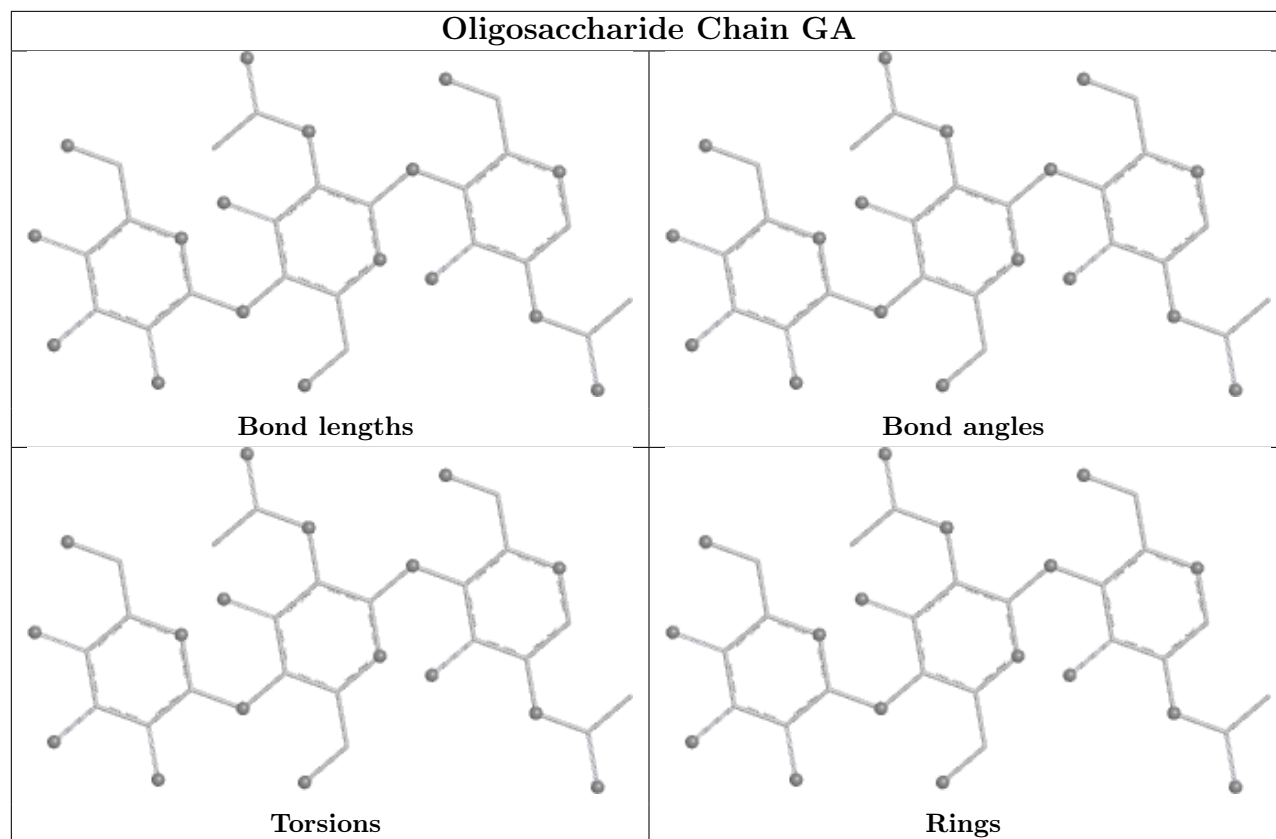
Oligosaccharide Chain EA



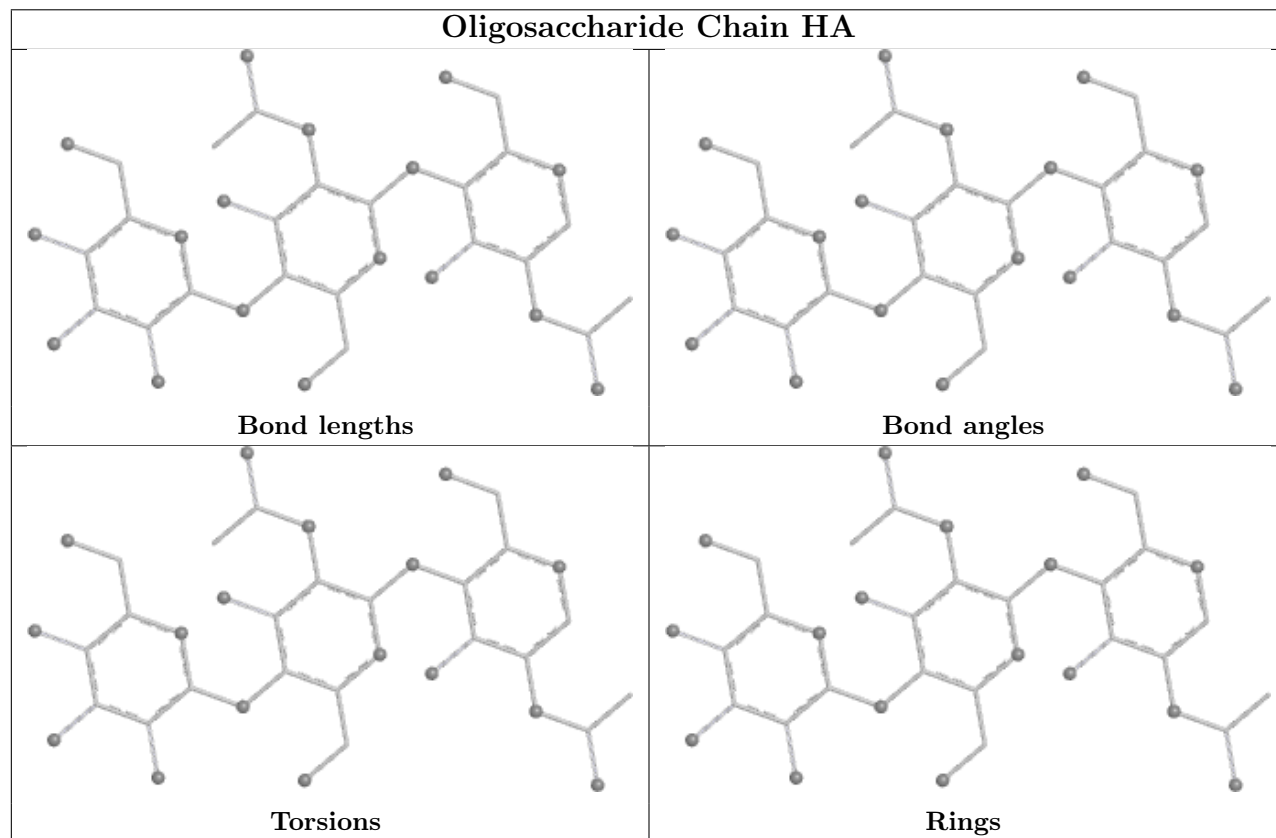
Oligosaccharide Chain FA



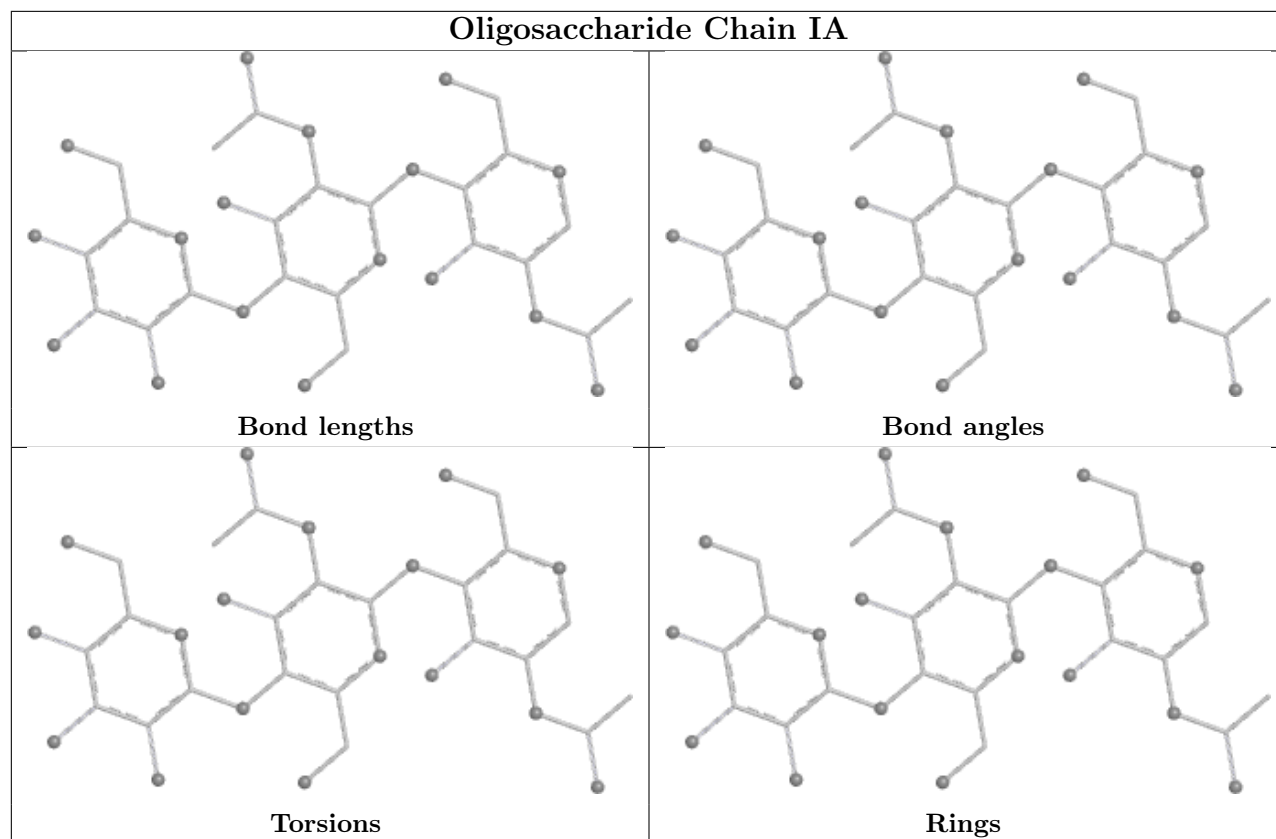
Oligosaccharide Chain GA



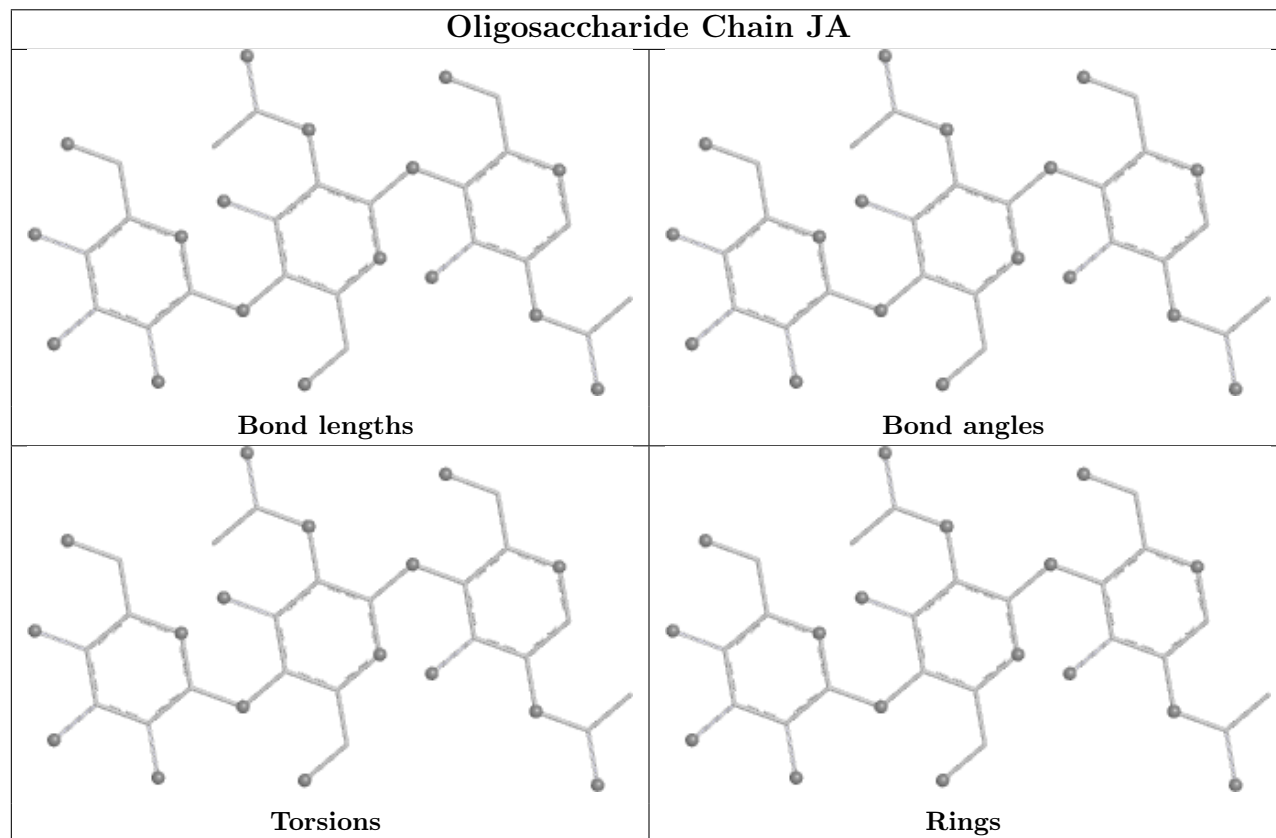
Oligosaccharide Chain HA



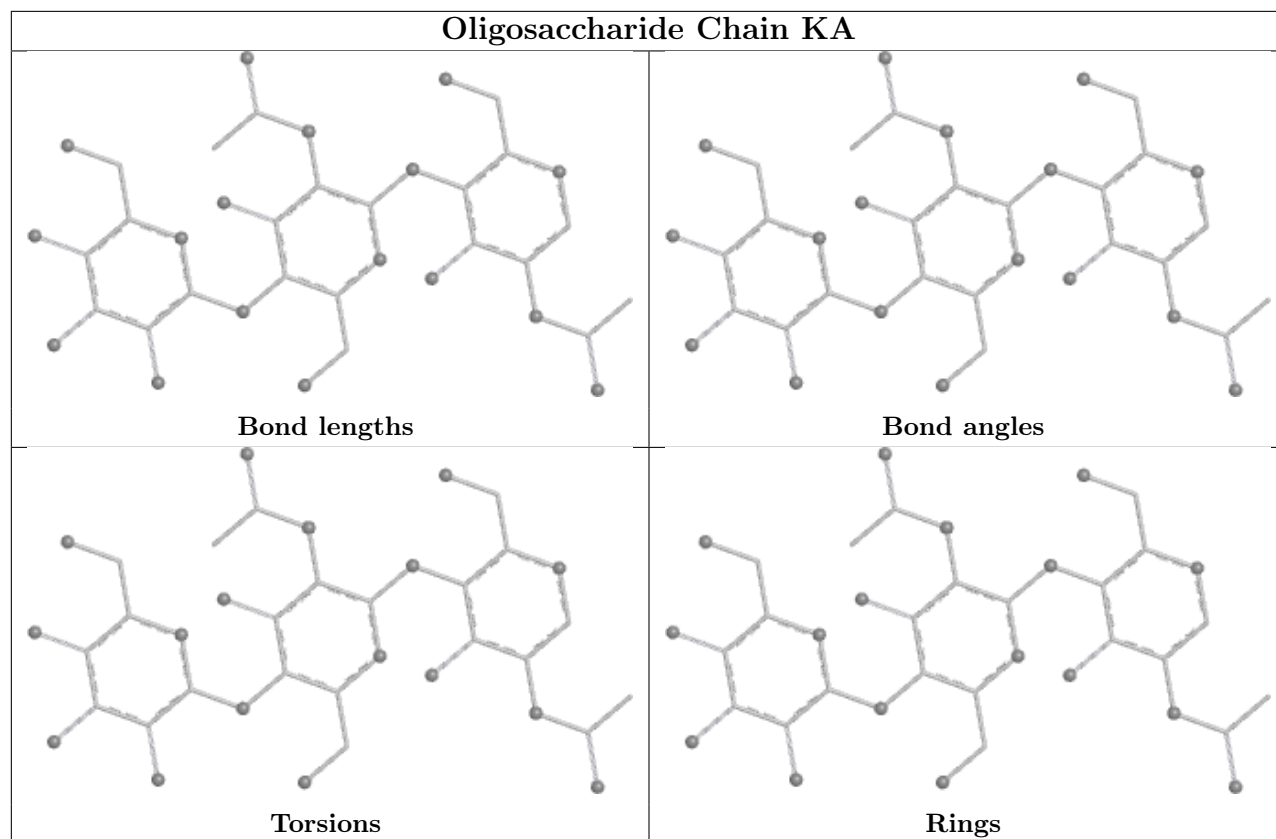
Oligosaccharide Chain IA



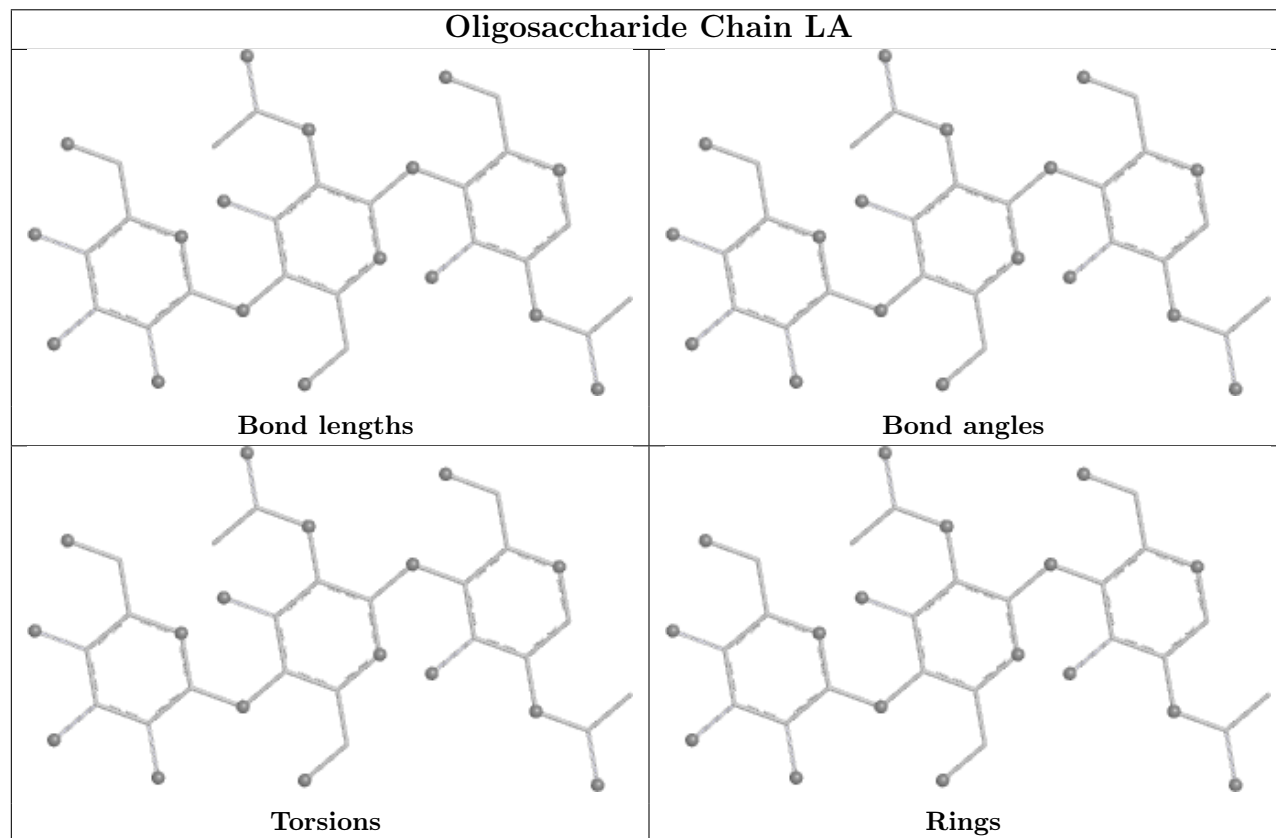
Oligosaccharide Chain JA

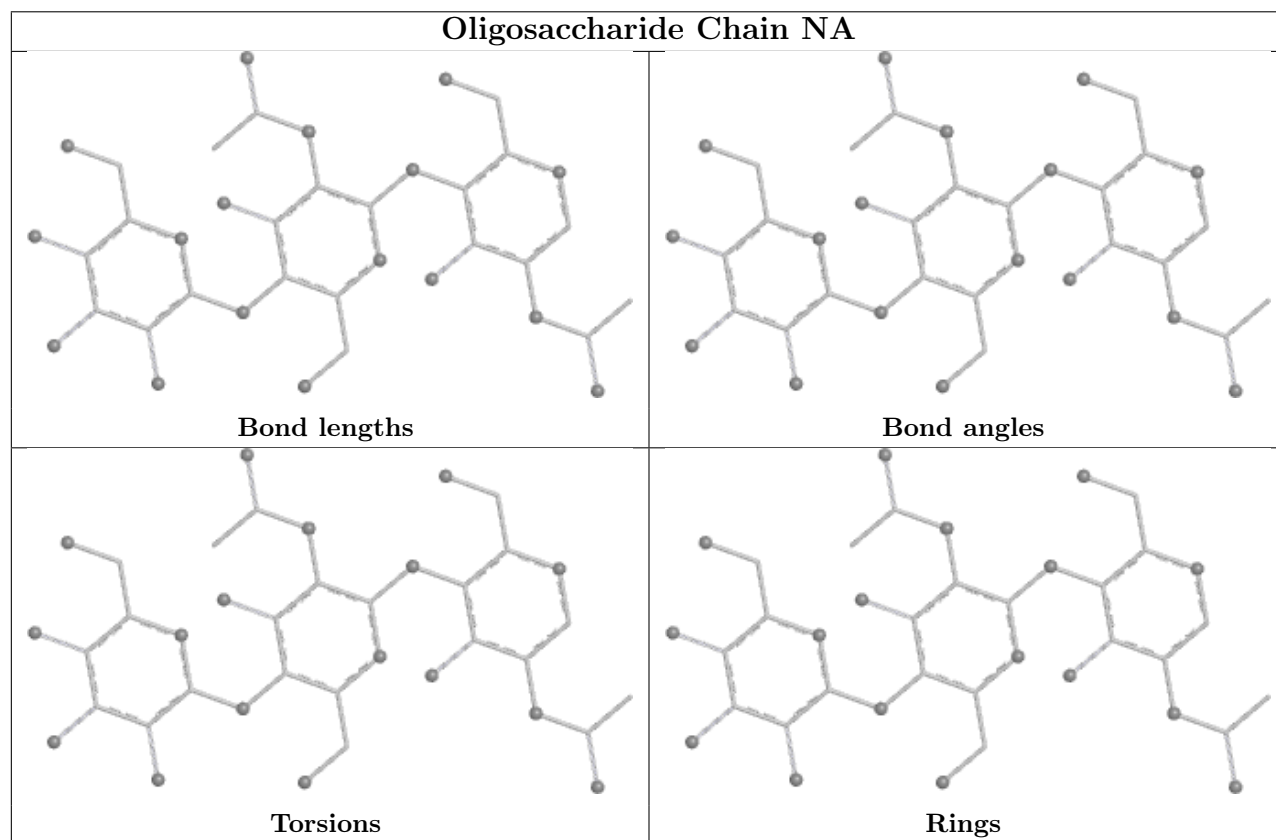
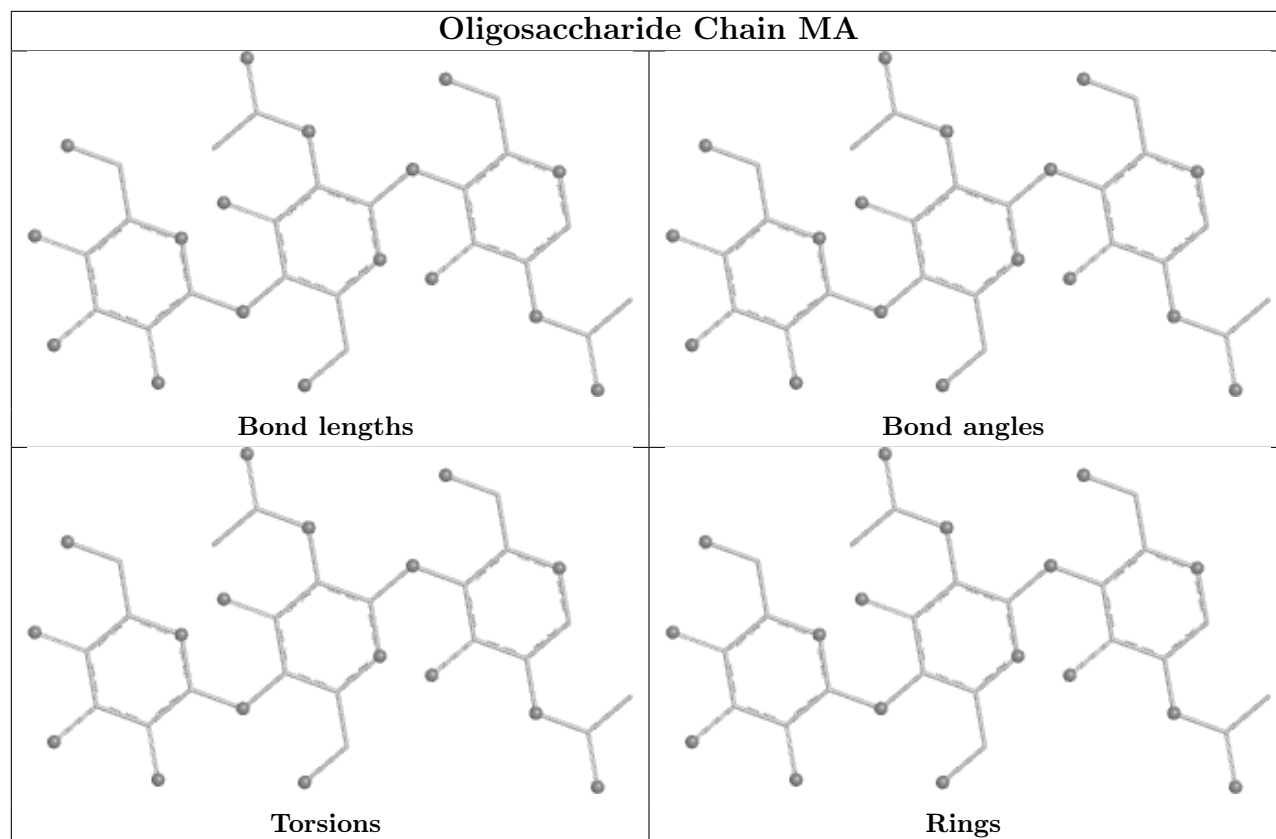


Oligosaccharide Chain KA

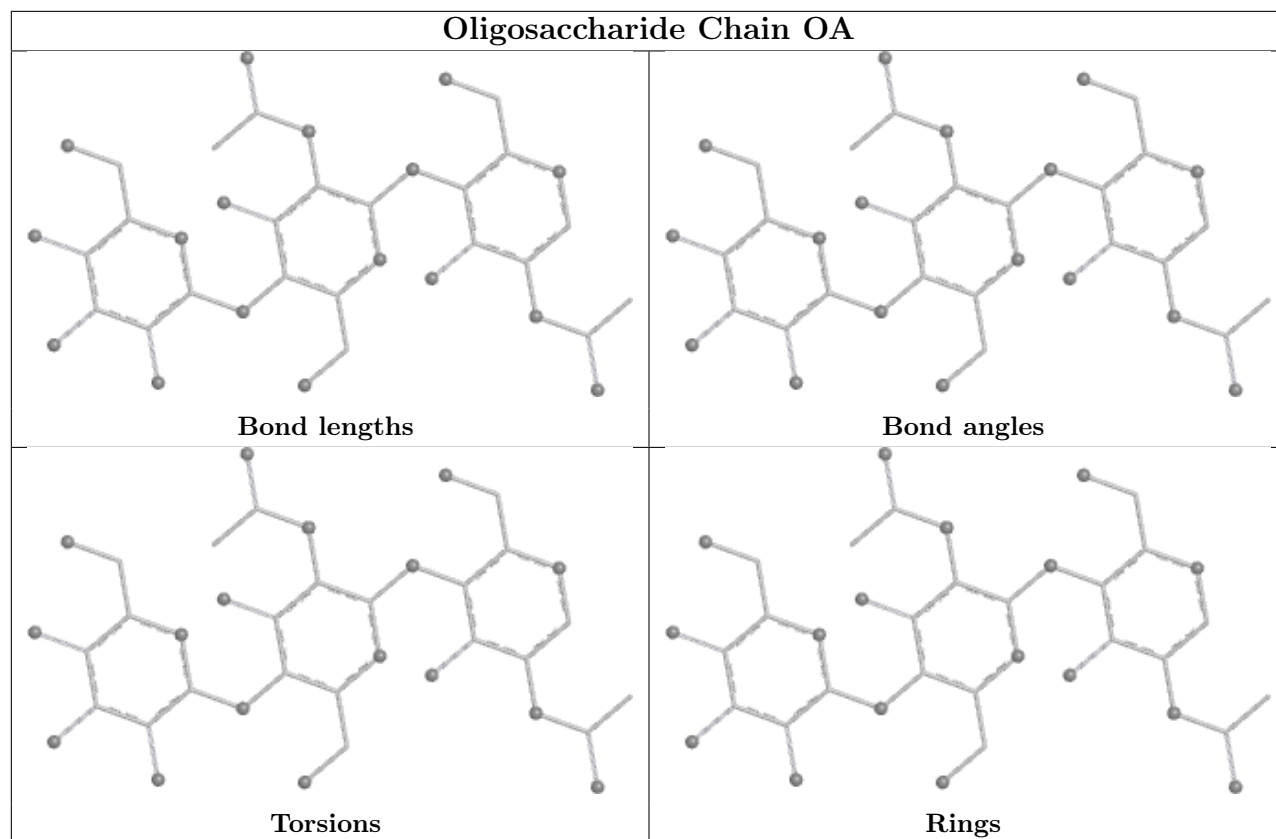


Oligosaccharide Chain LA

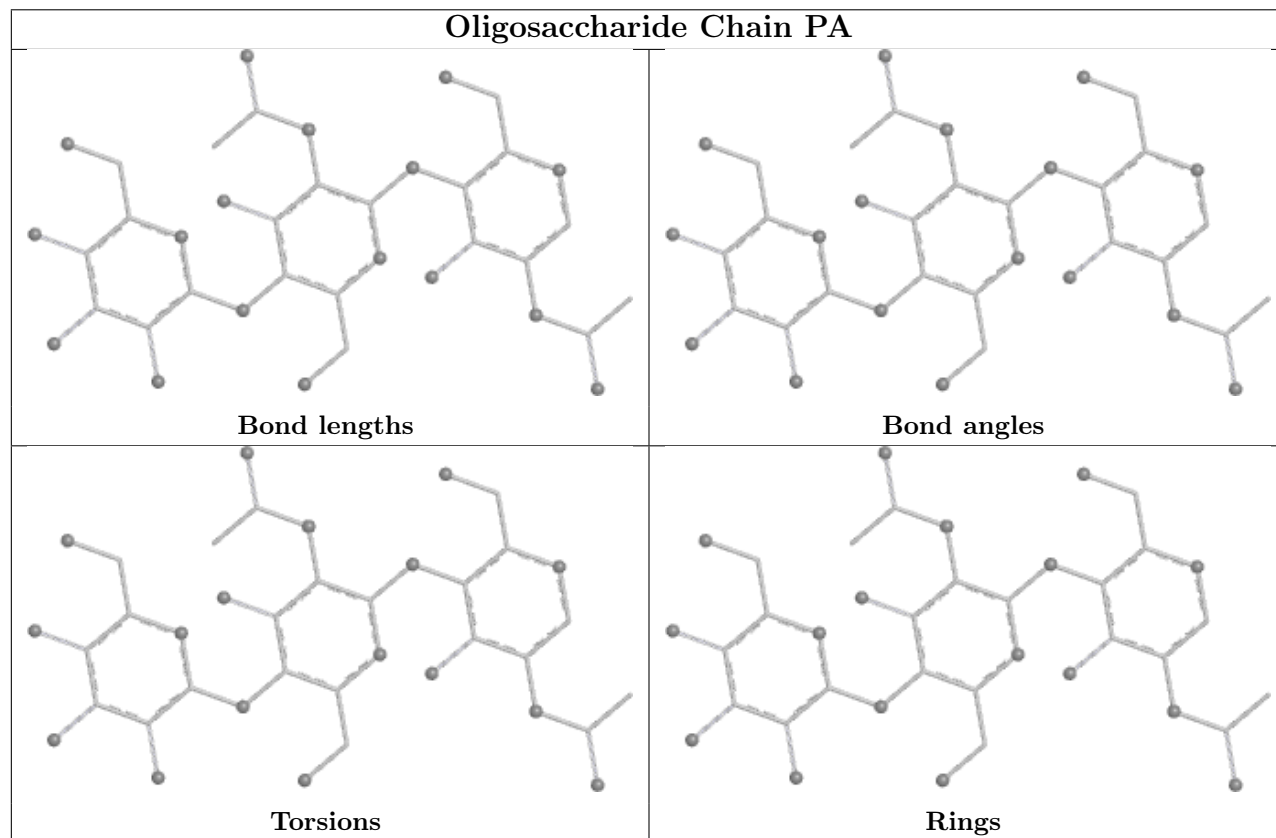




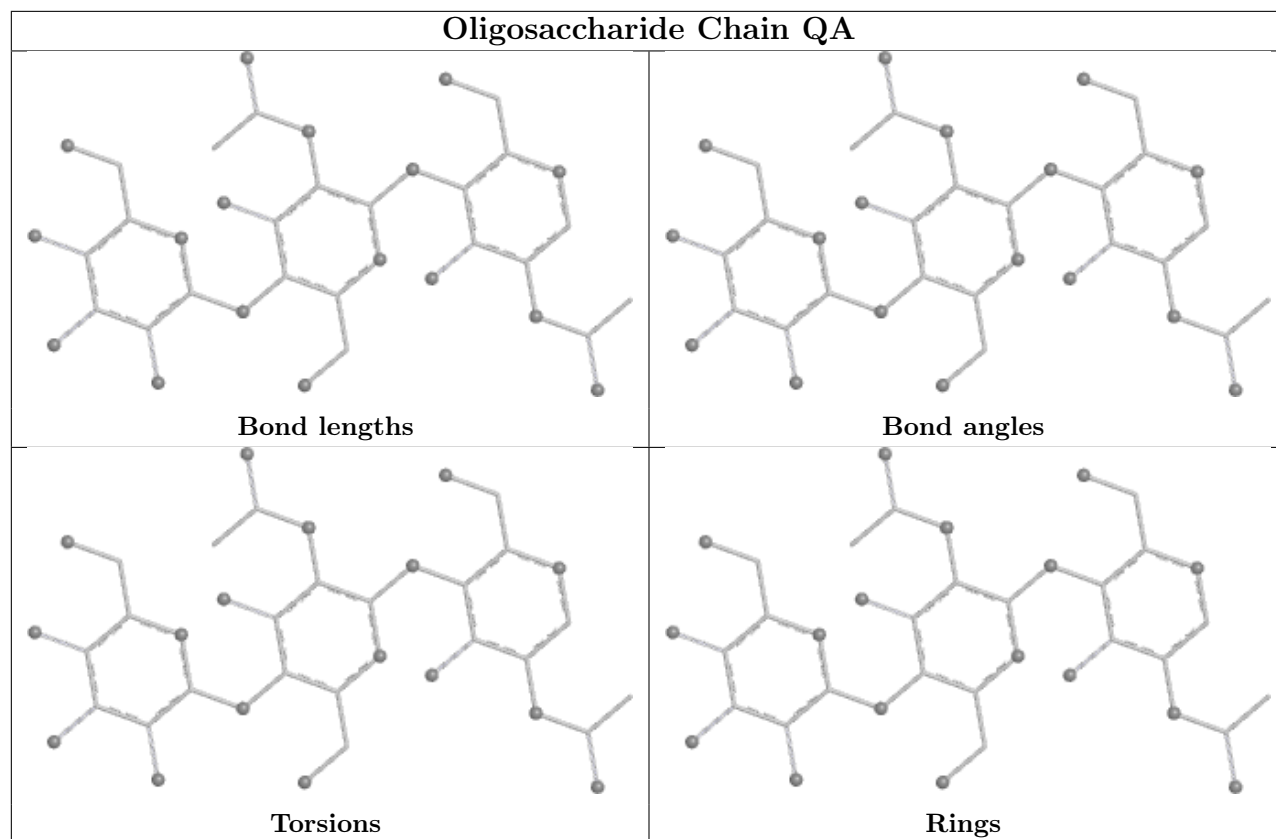
Oligosaccharide Chain OA



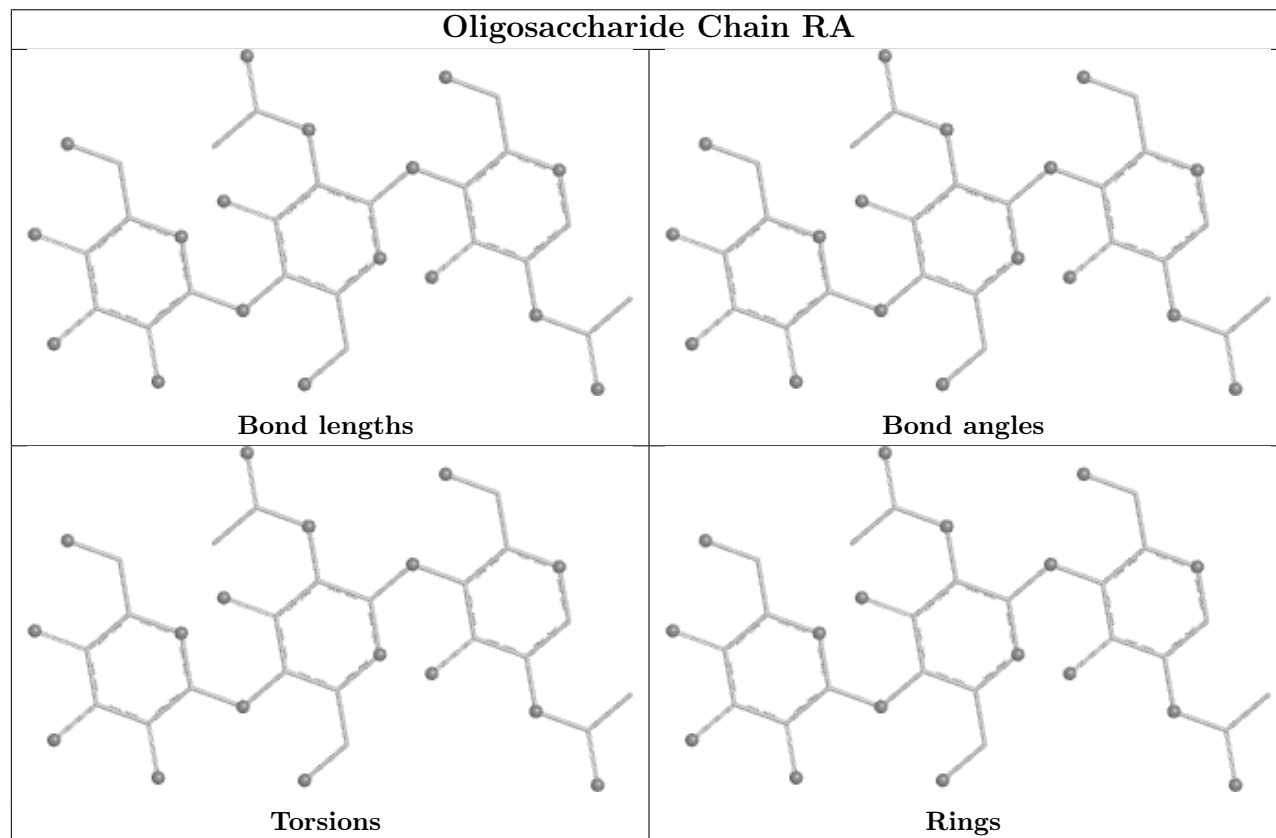
Oligosaccharide Chain PA

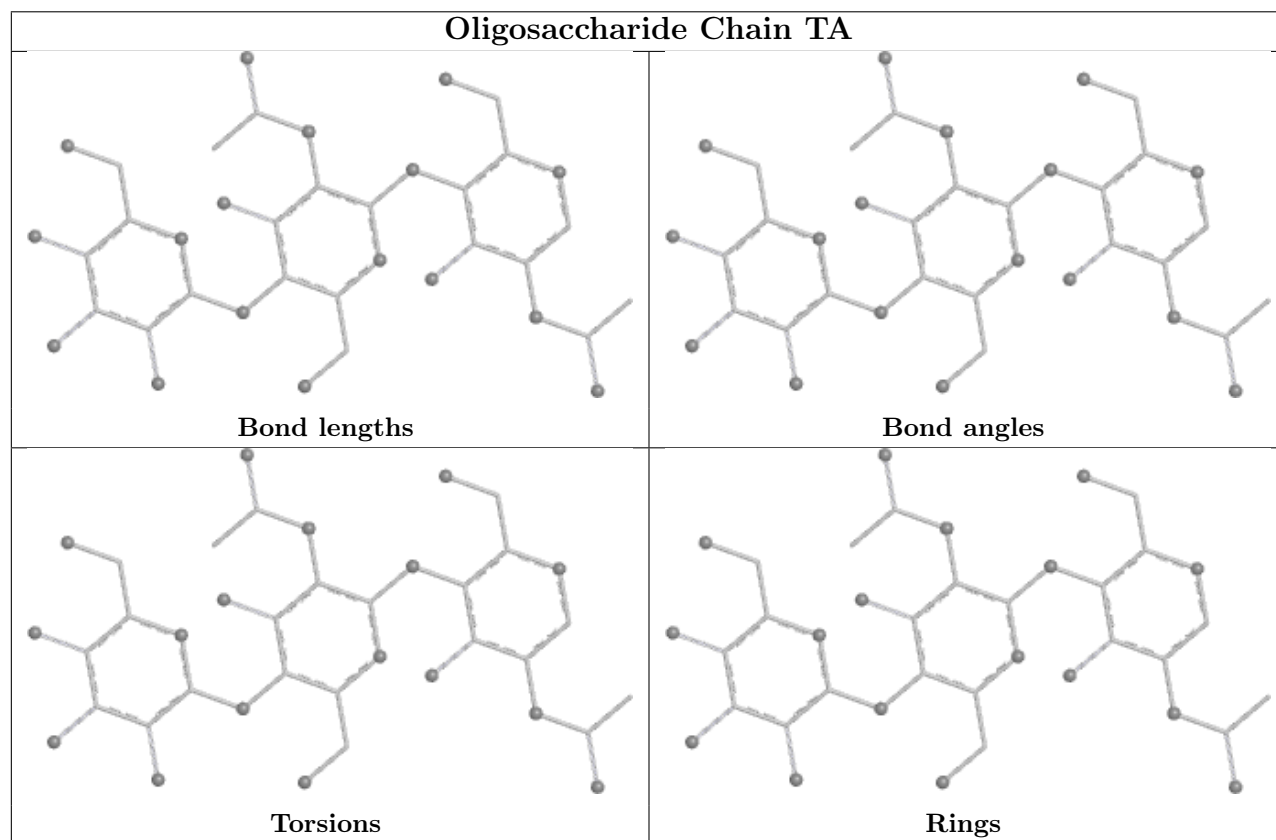
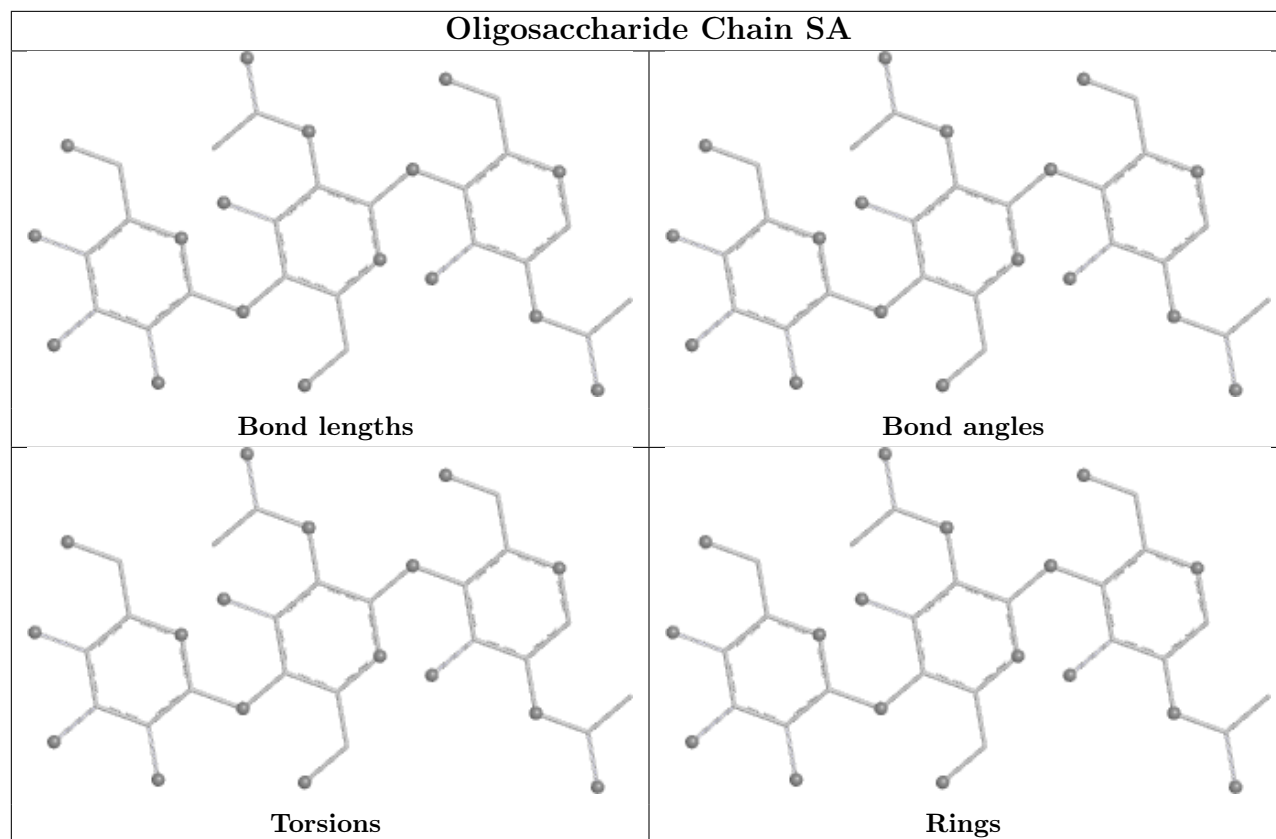


Oligosaccharide Chain QA

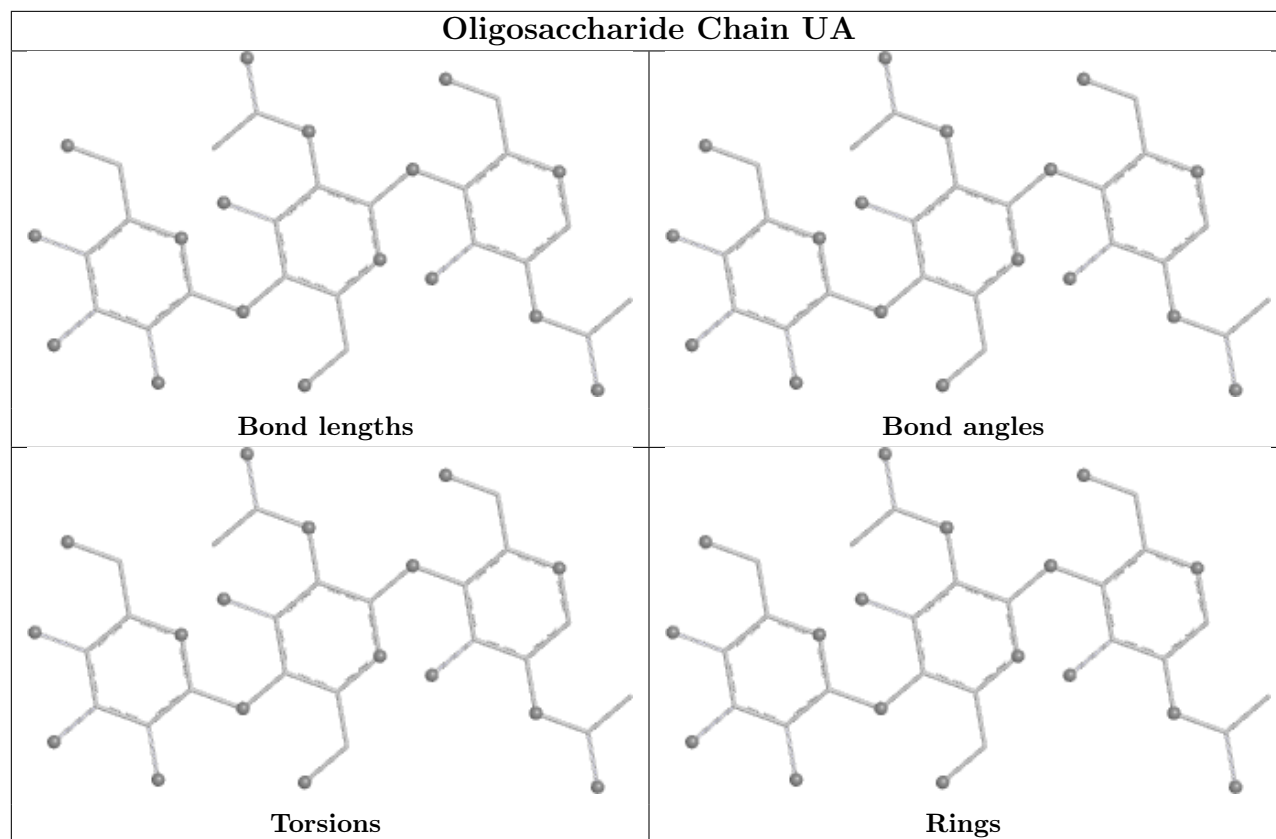


Oligosaccharide Chain RA

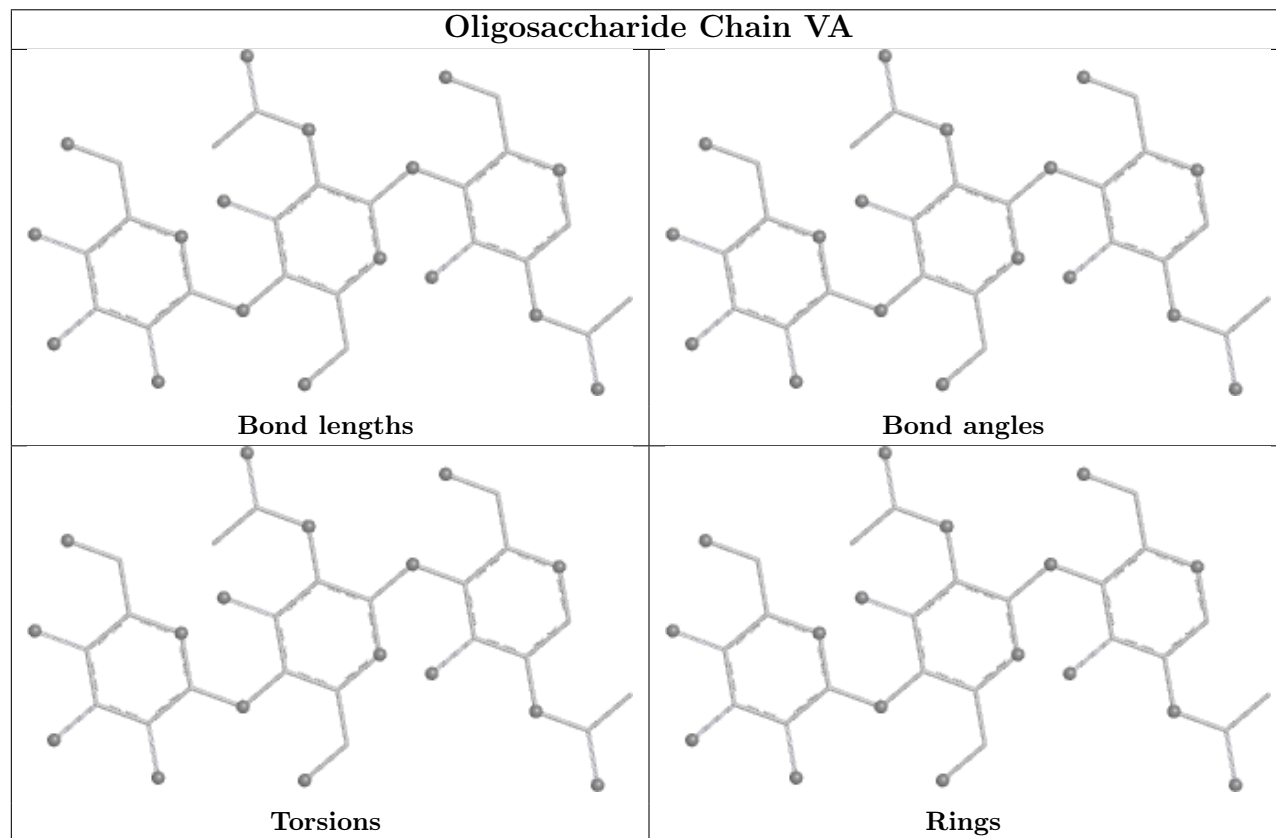




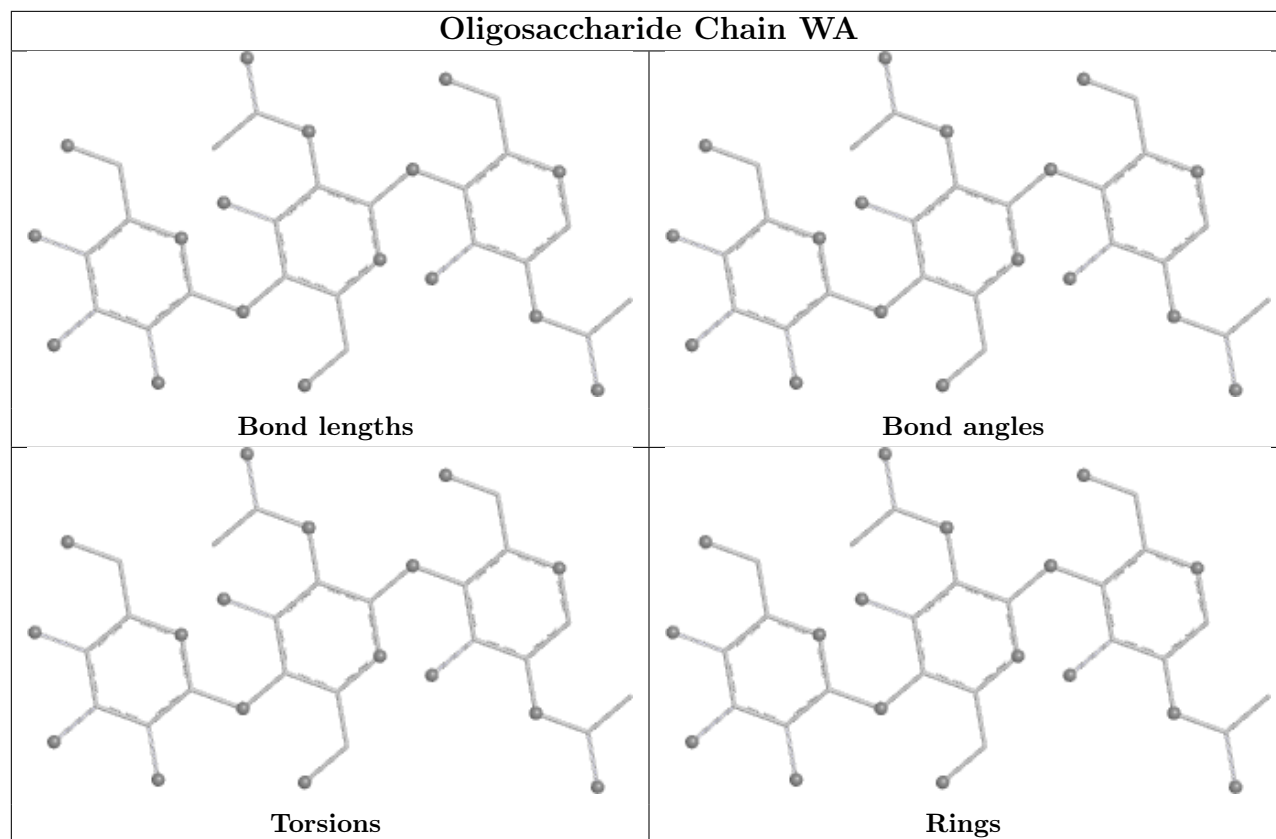
Oligosaccharide Chain UA



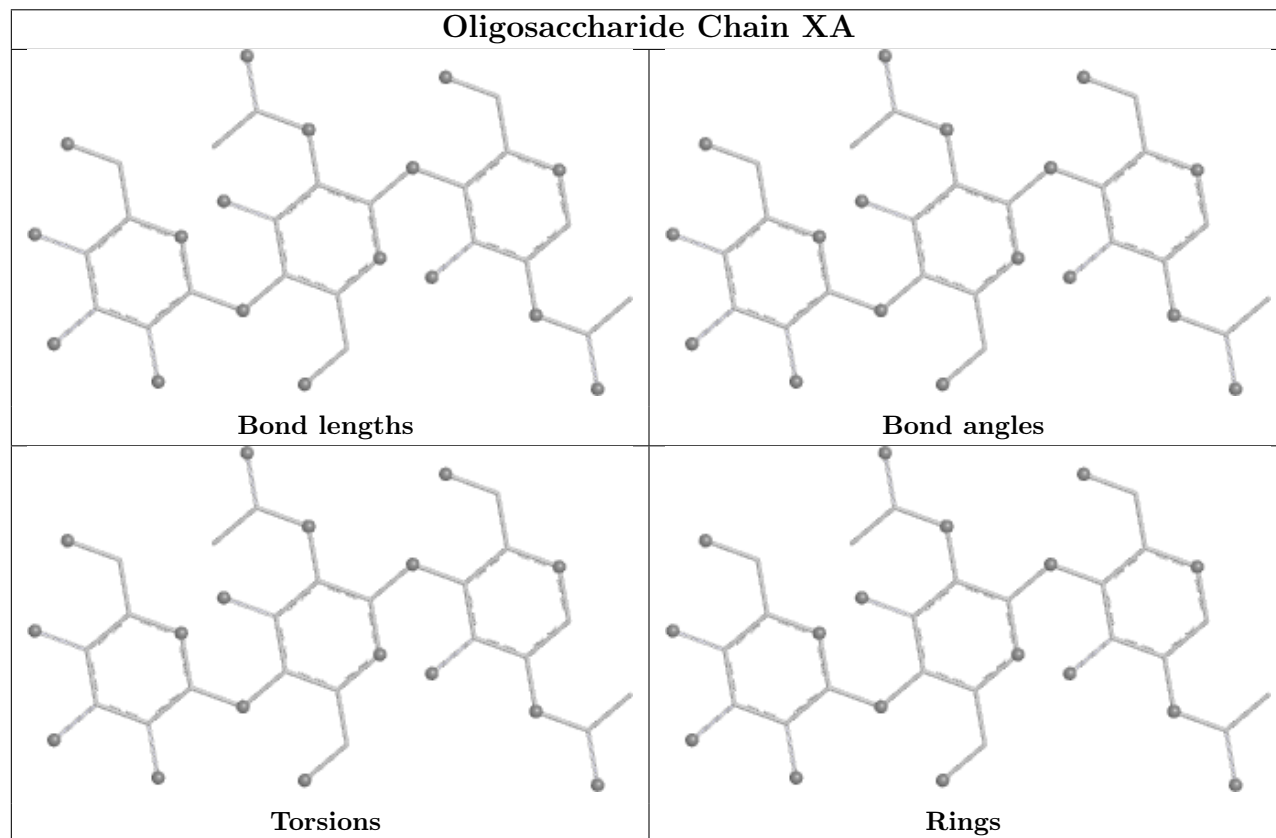
Oligosaccharide Chain VA



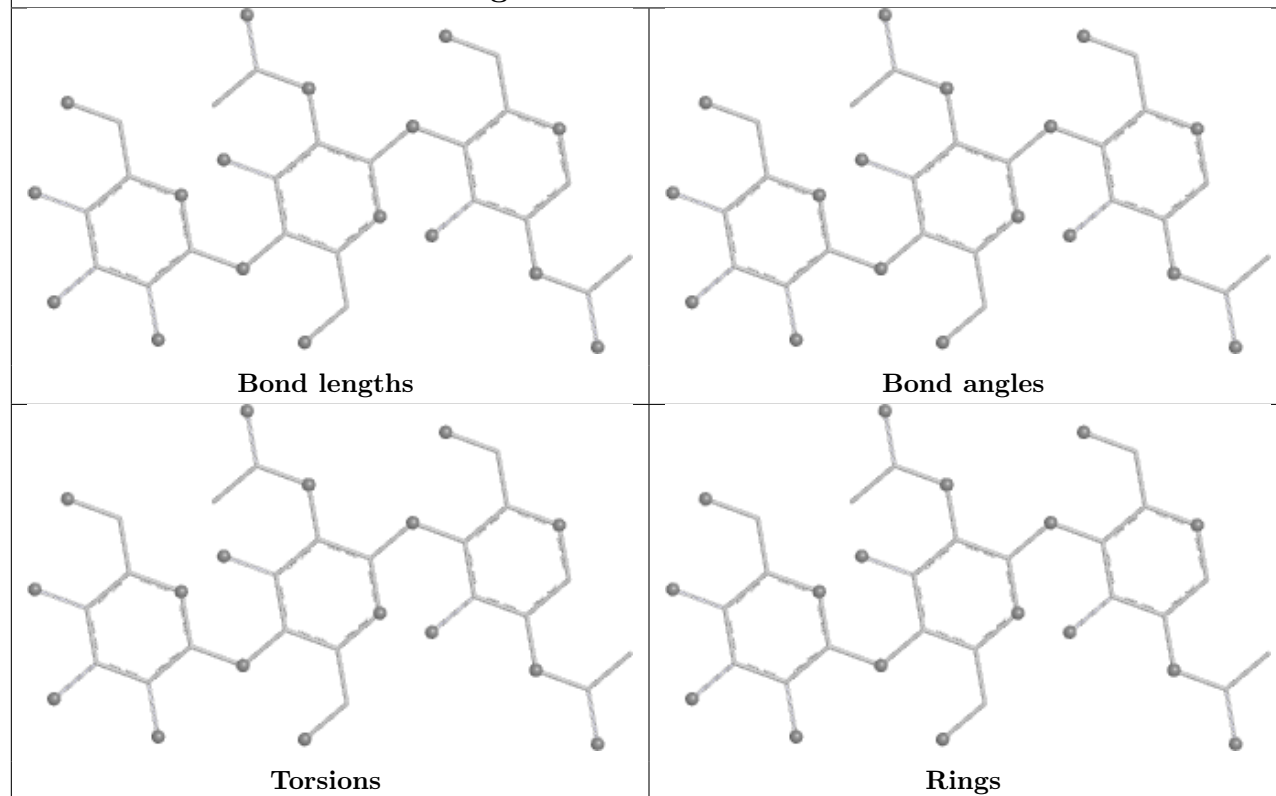
Oligosaccharide Chain WA



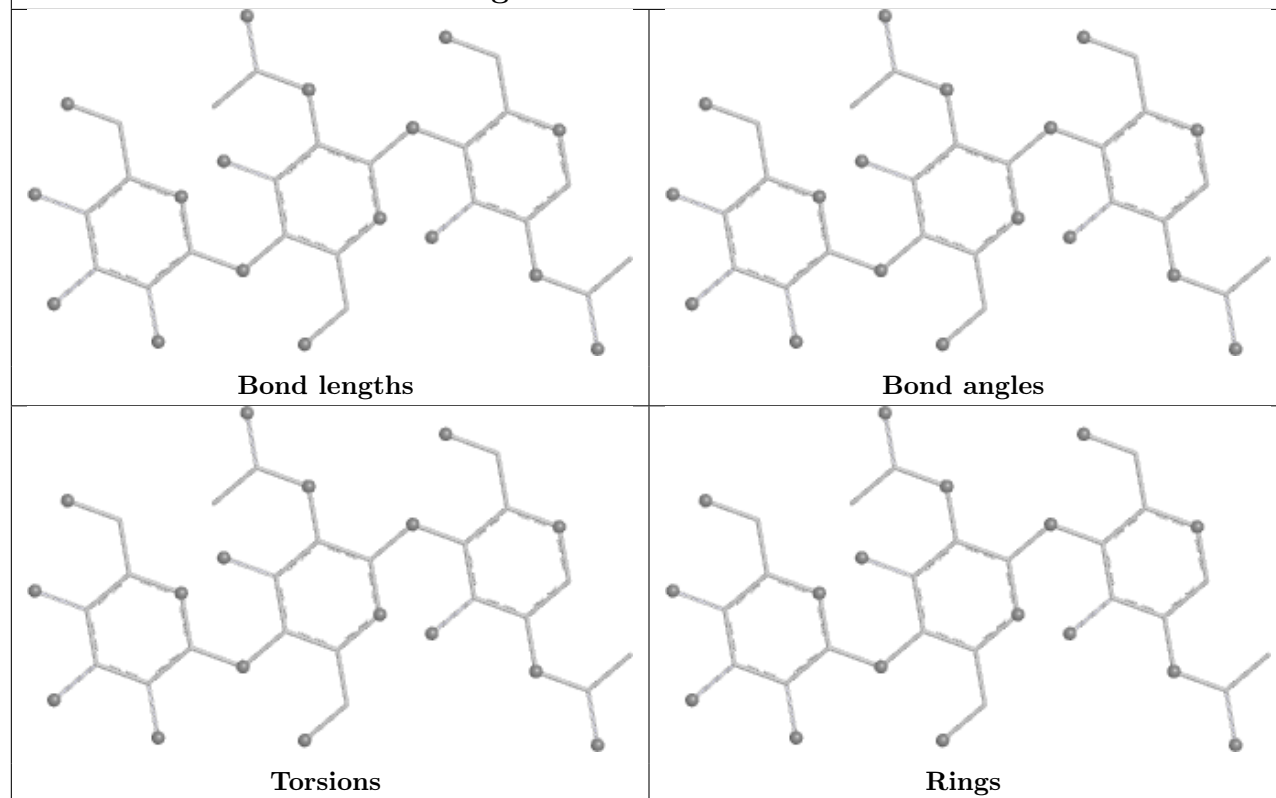
Oligosaccharide Chain XA

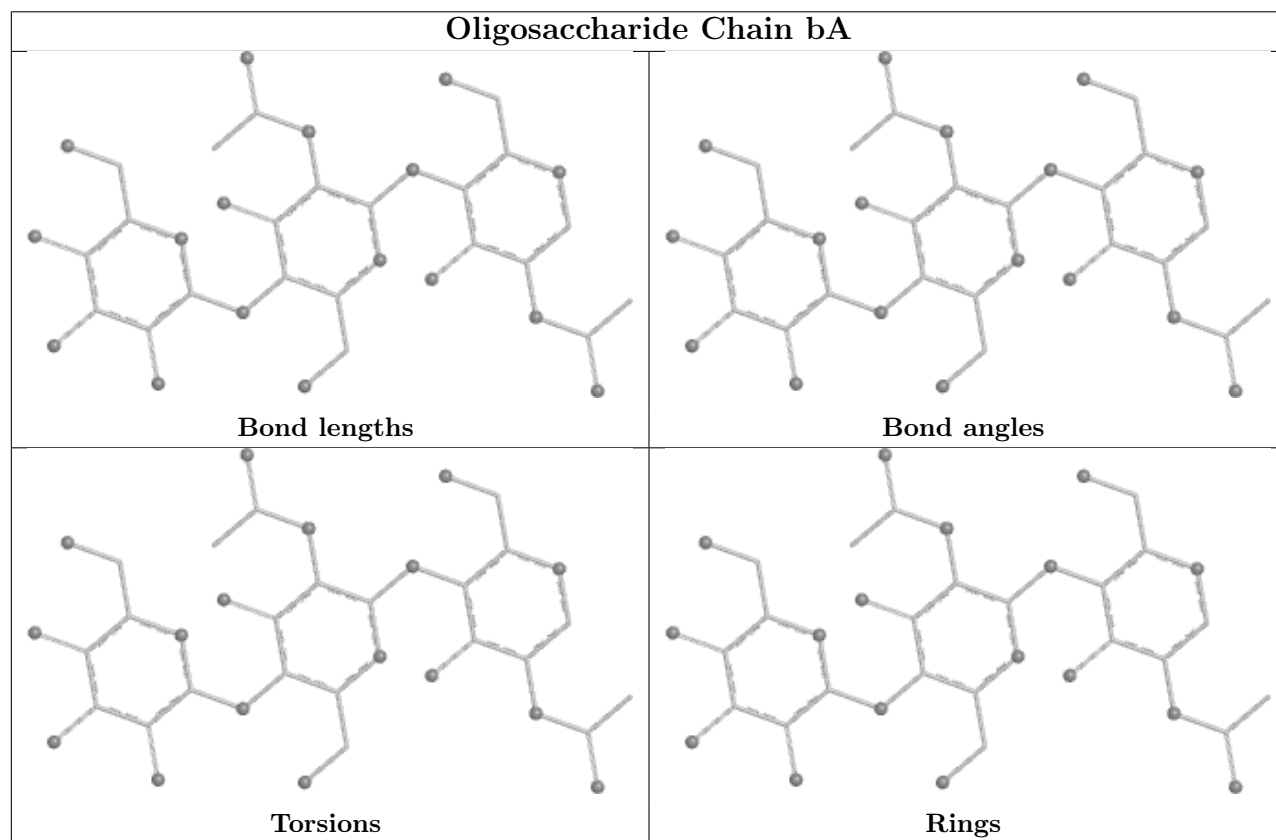
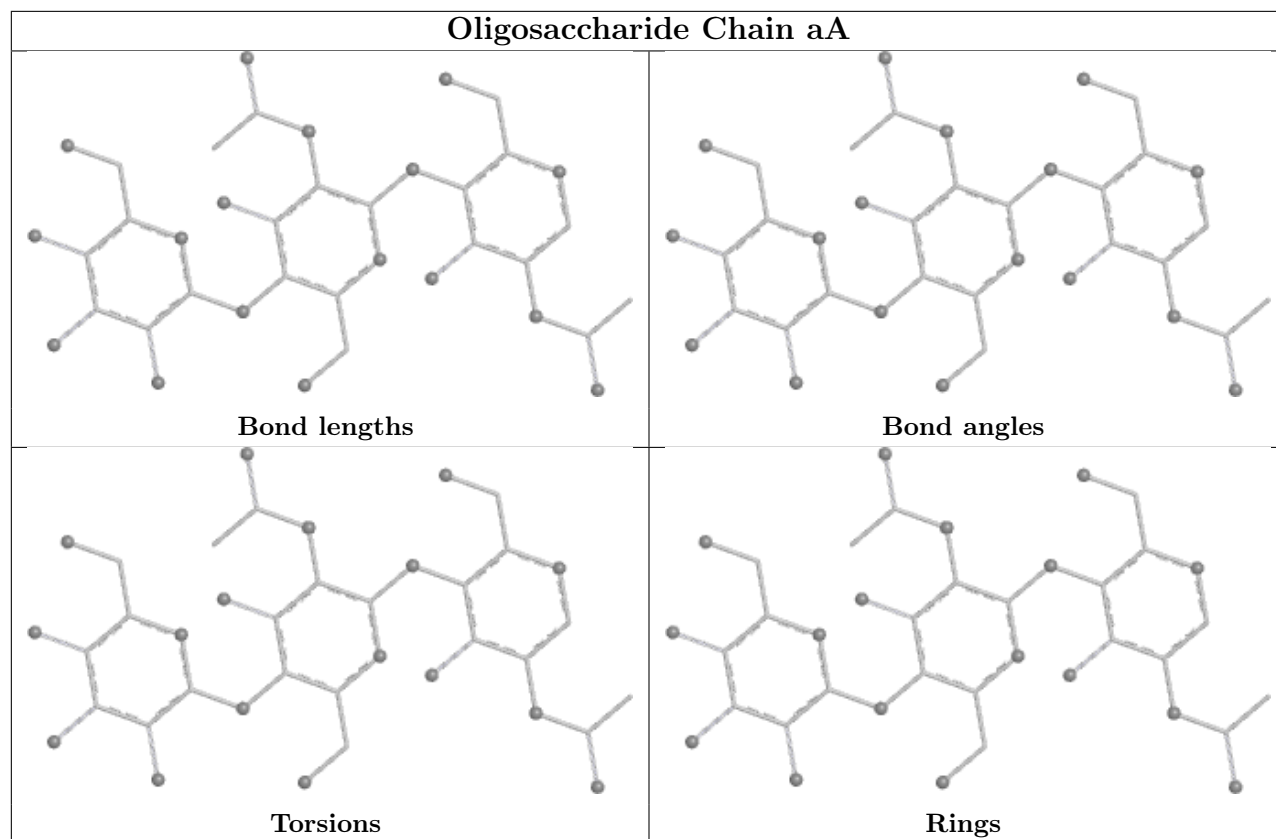


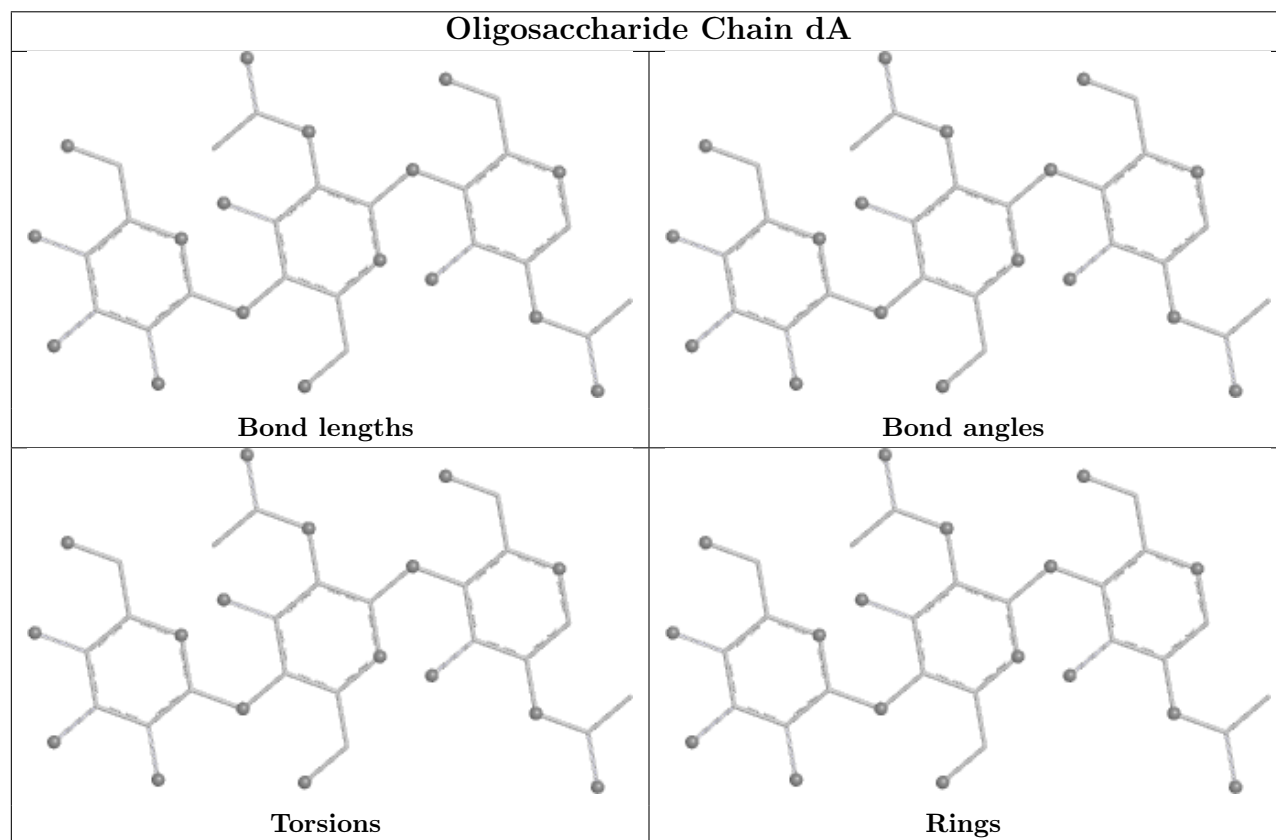
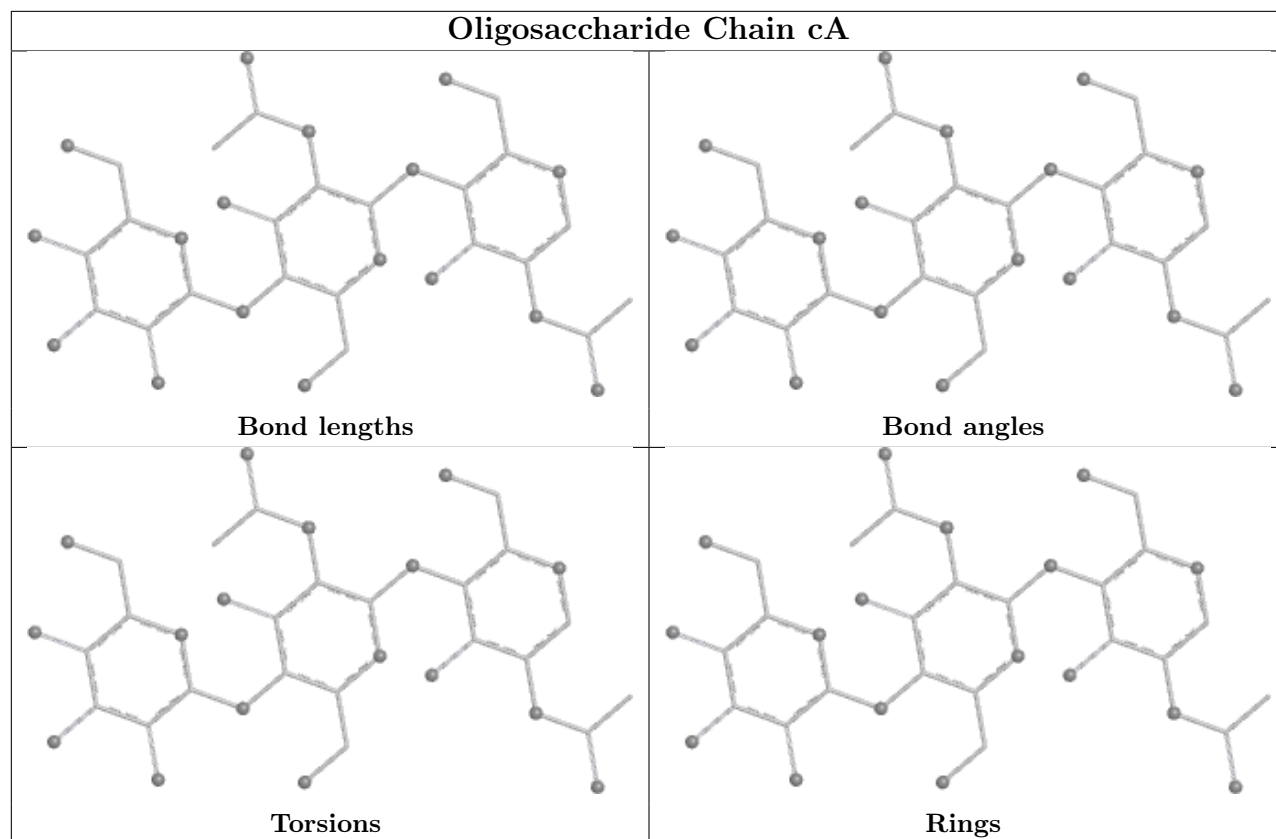
Oligosaccharide Chain YA

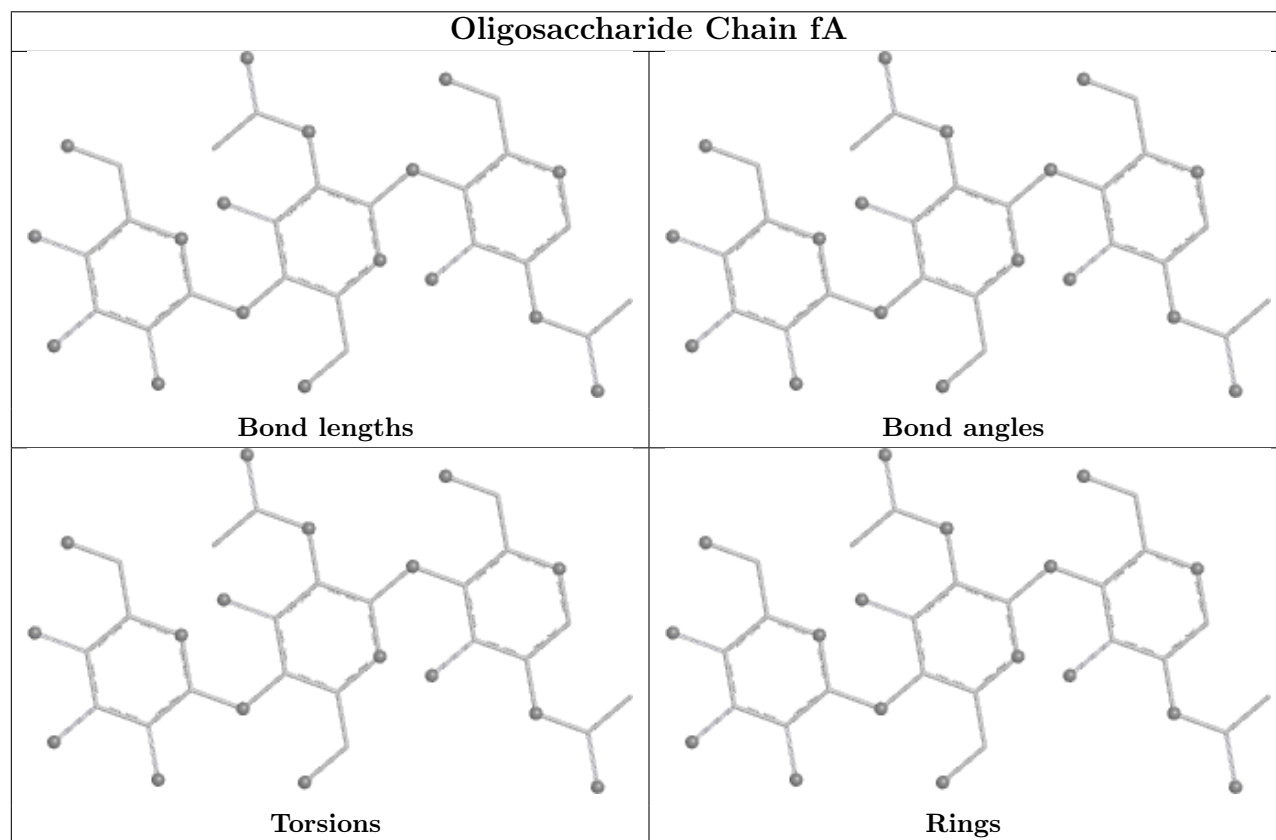
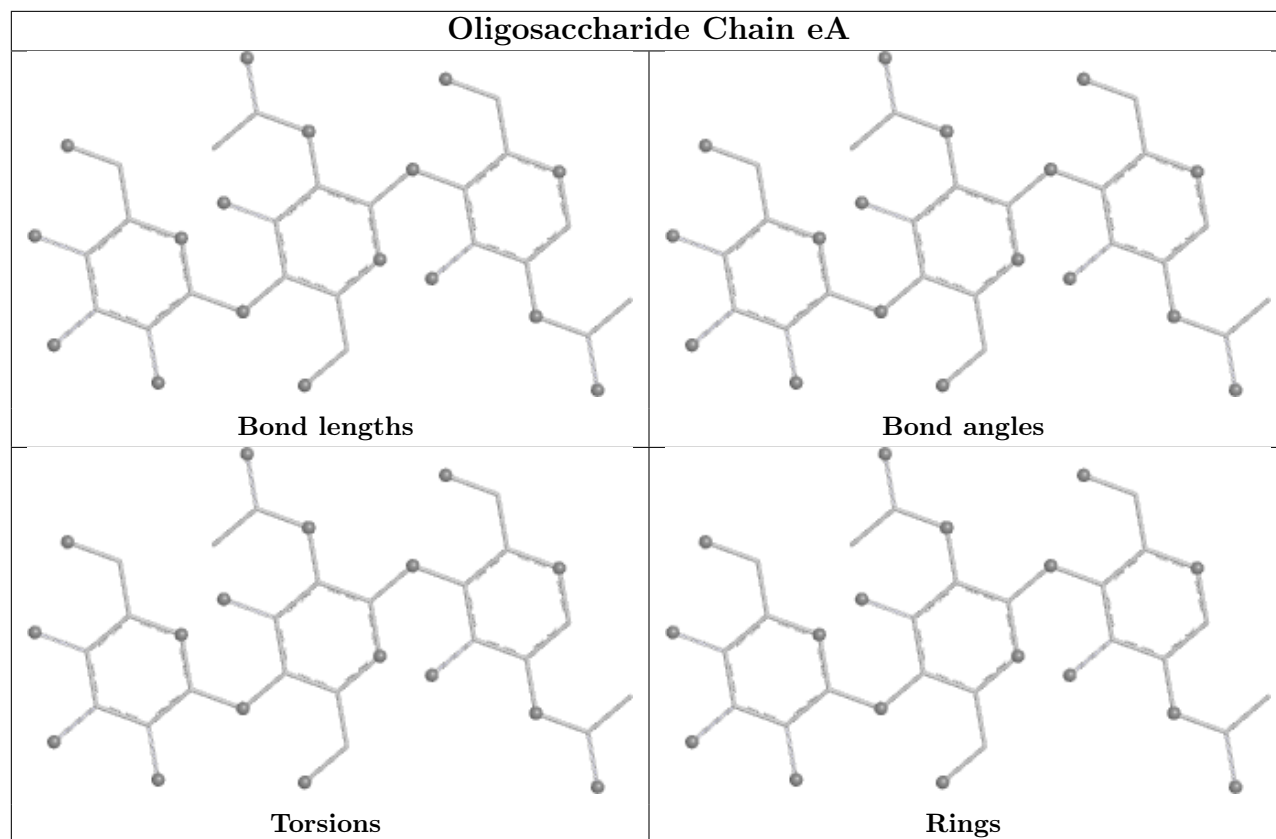


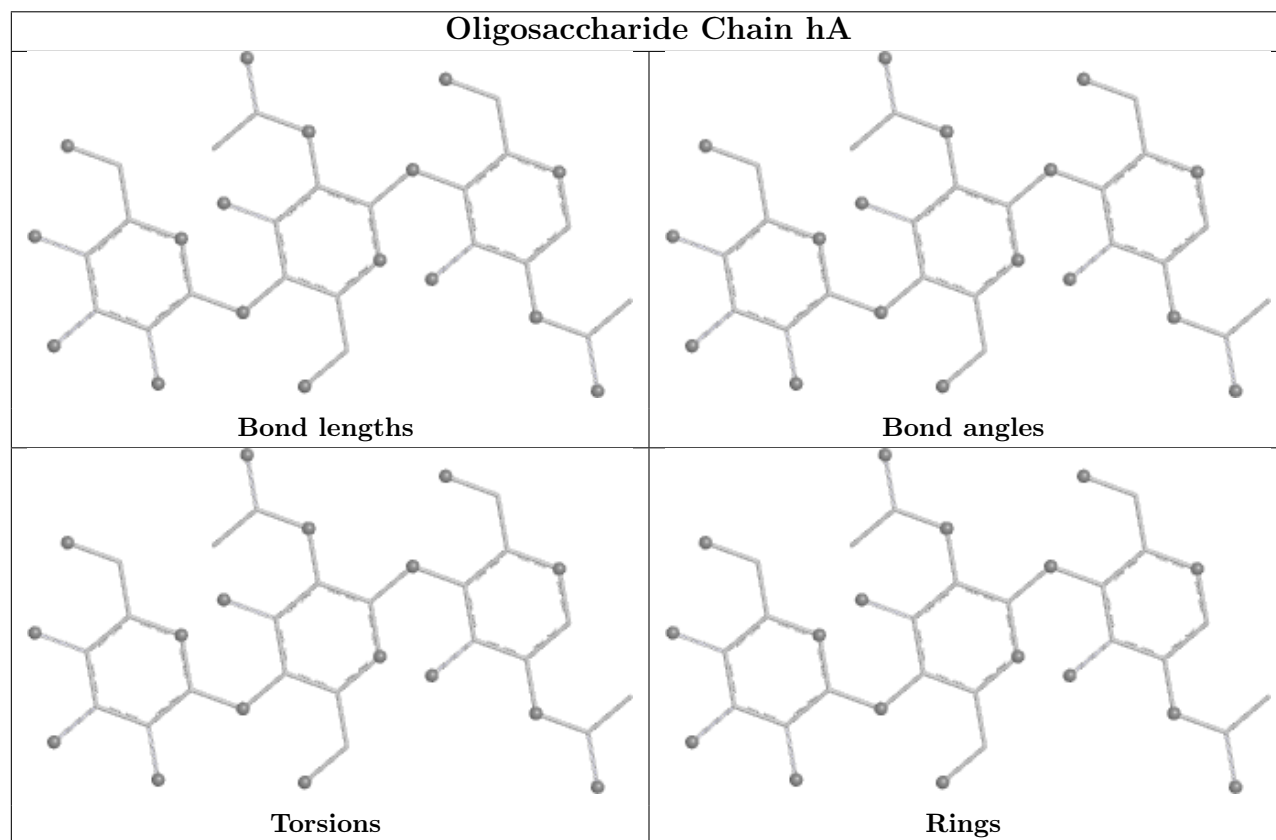
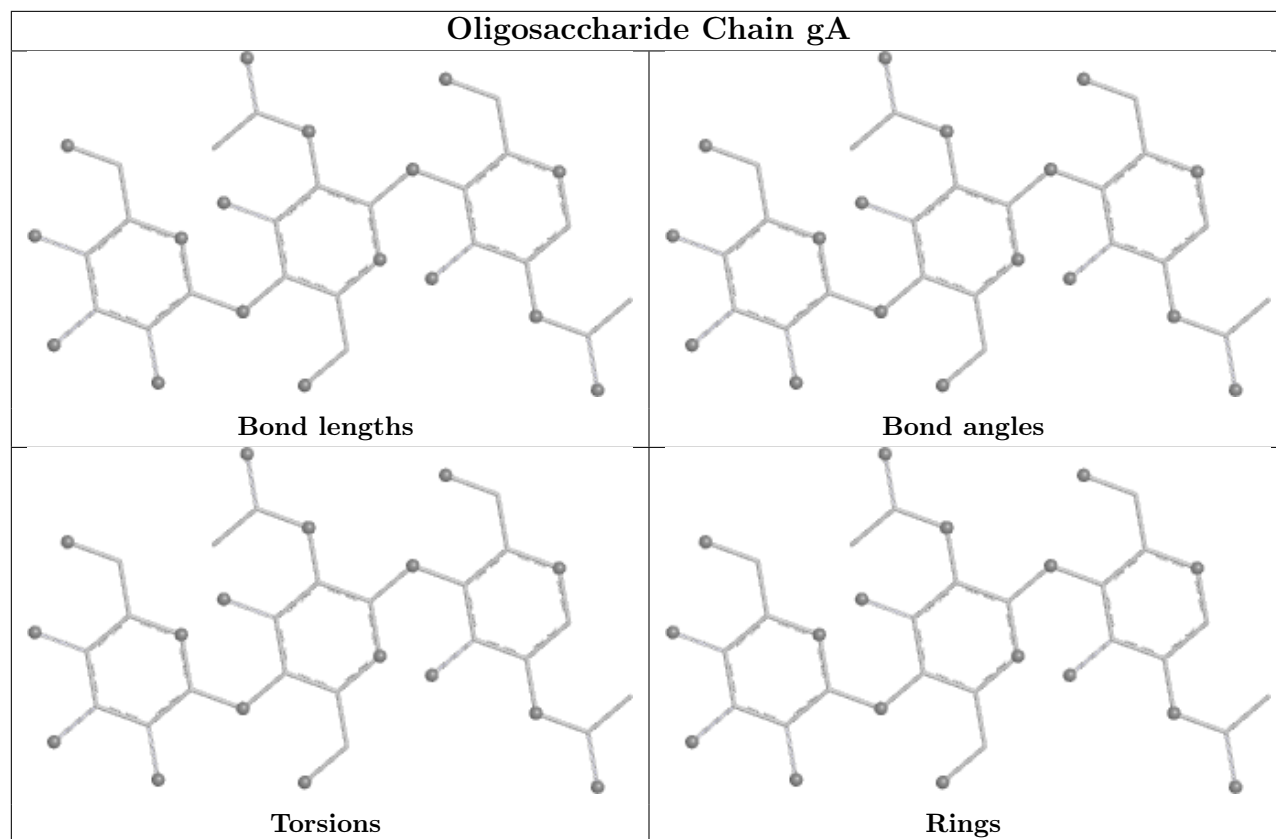
Oligosaccharide Chain ZA

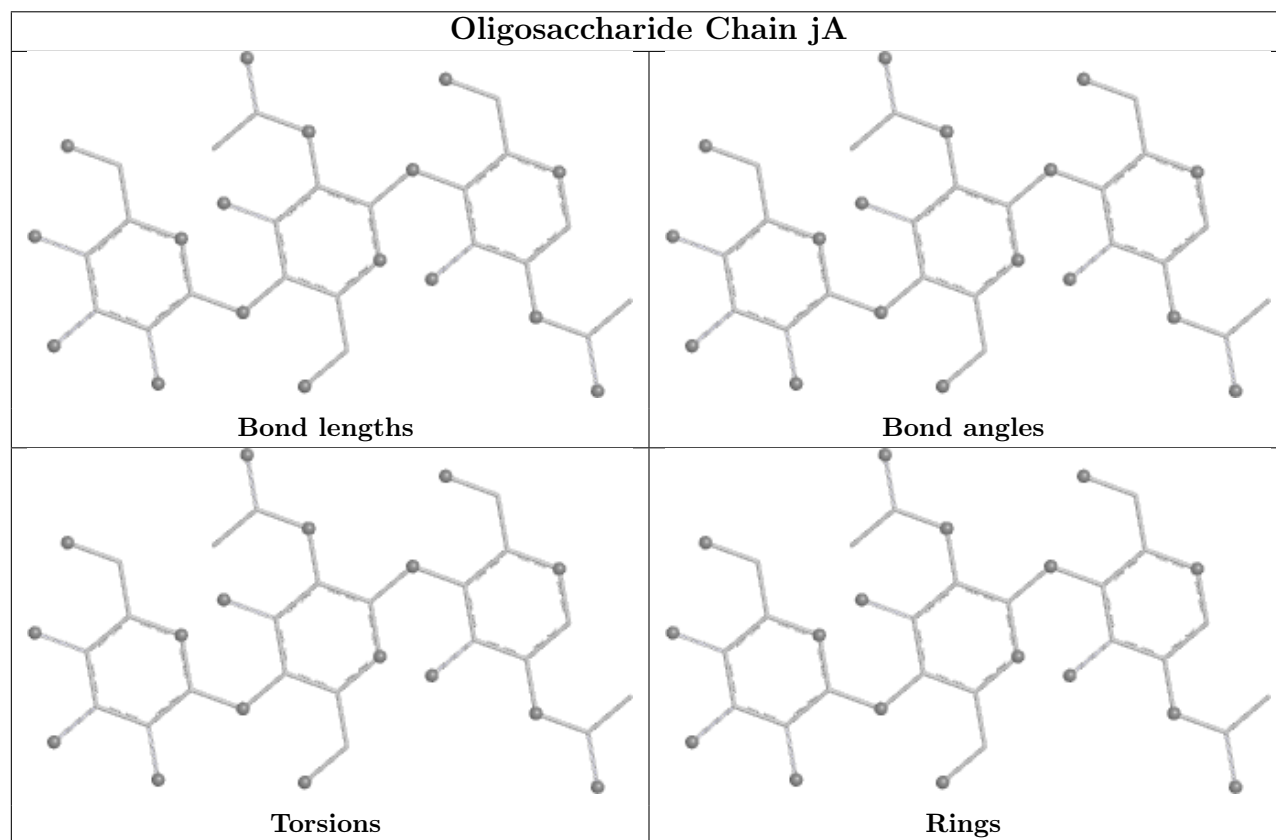
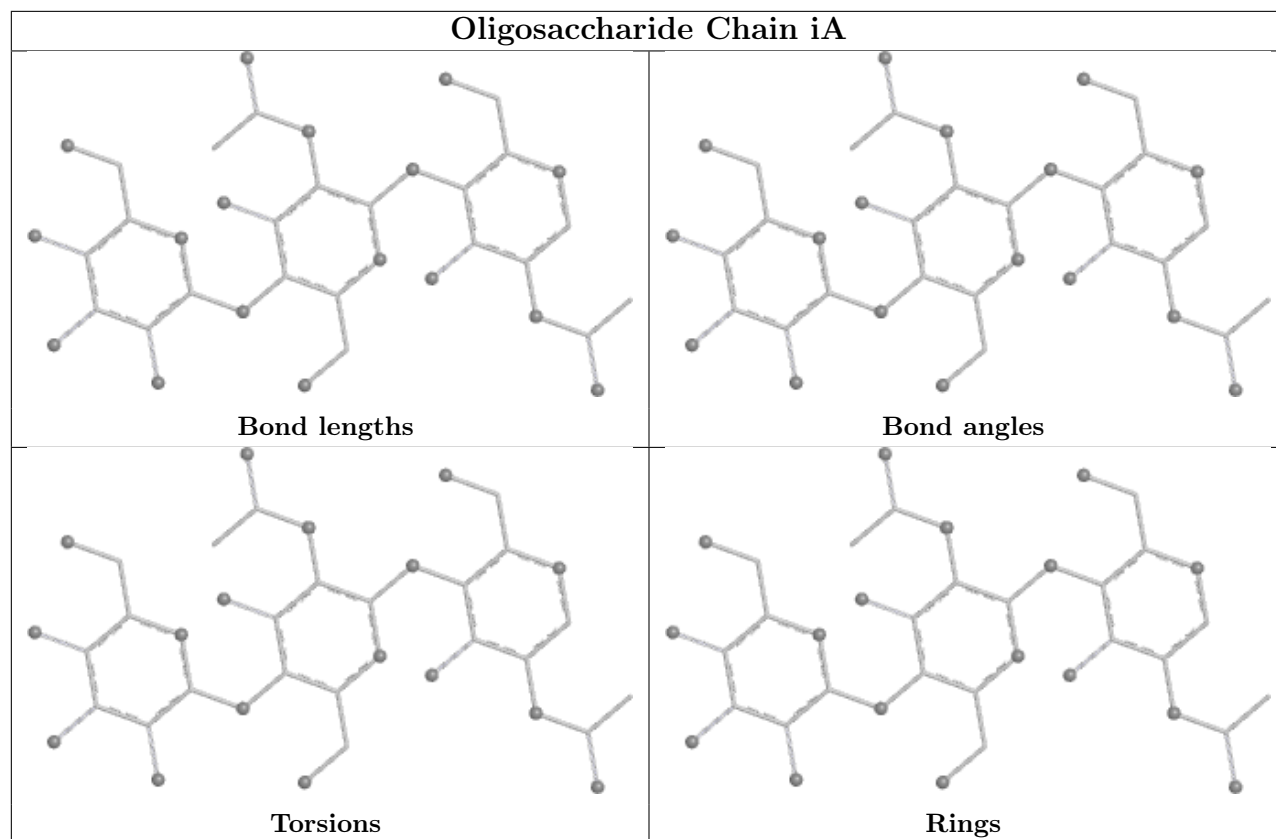




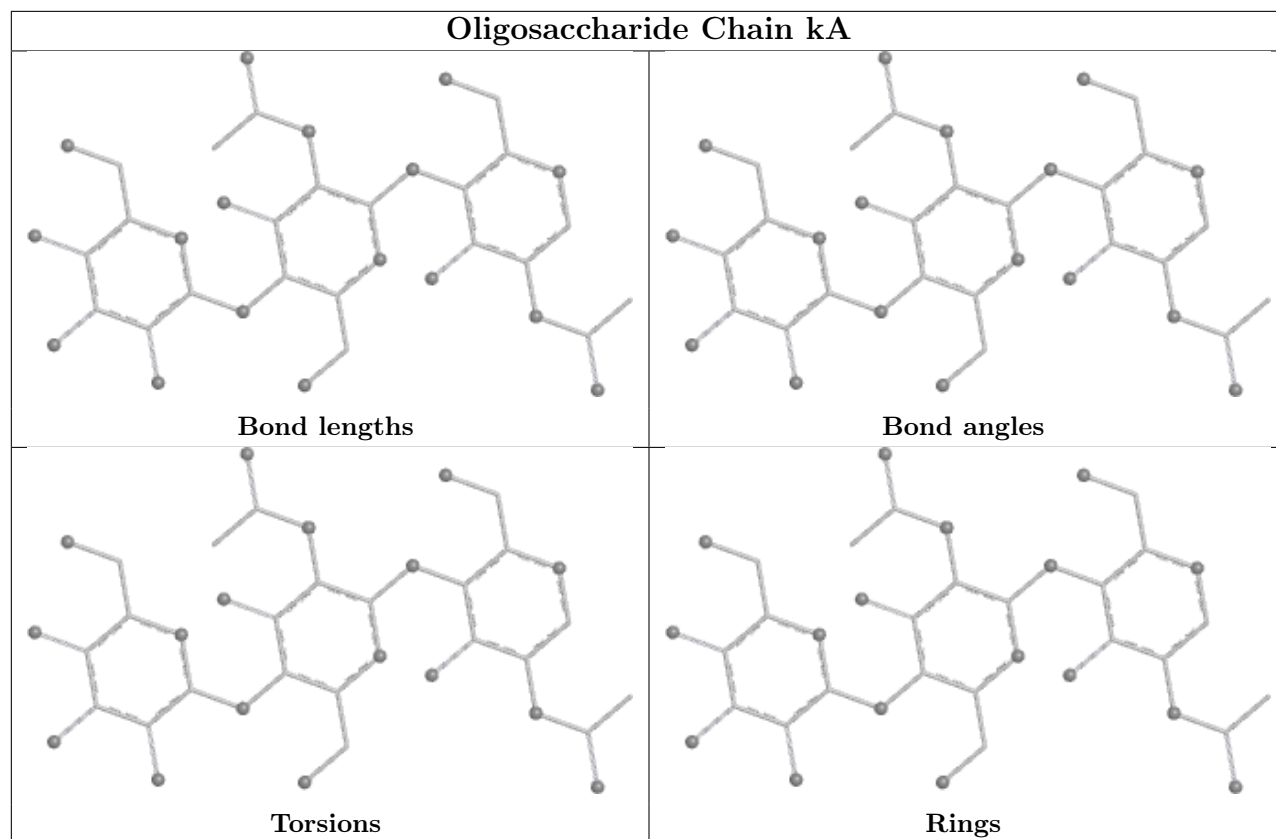




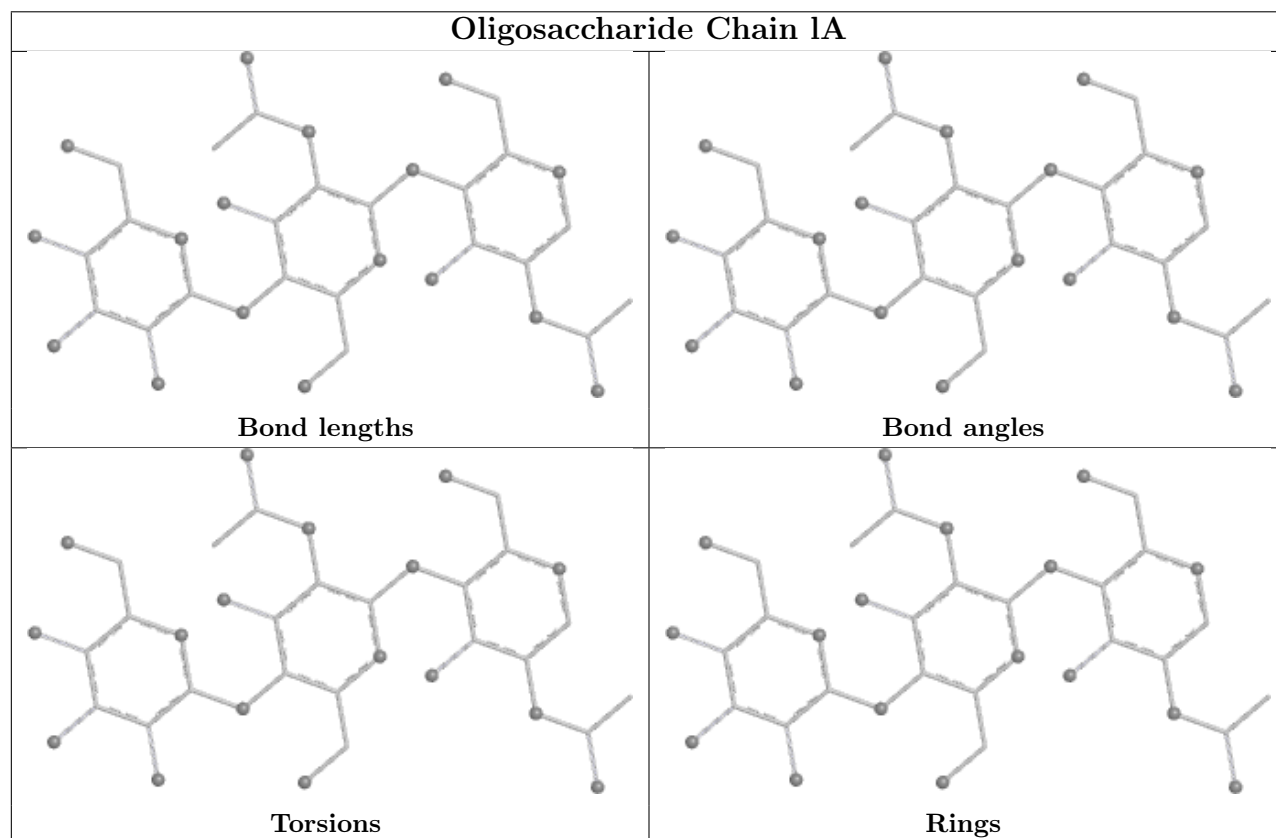


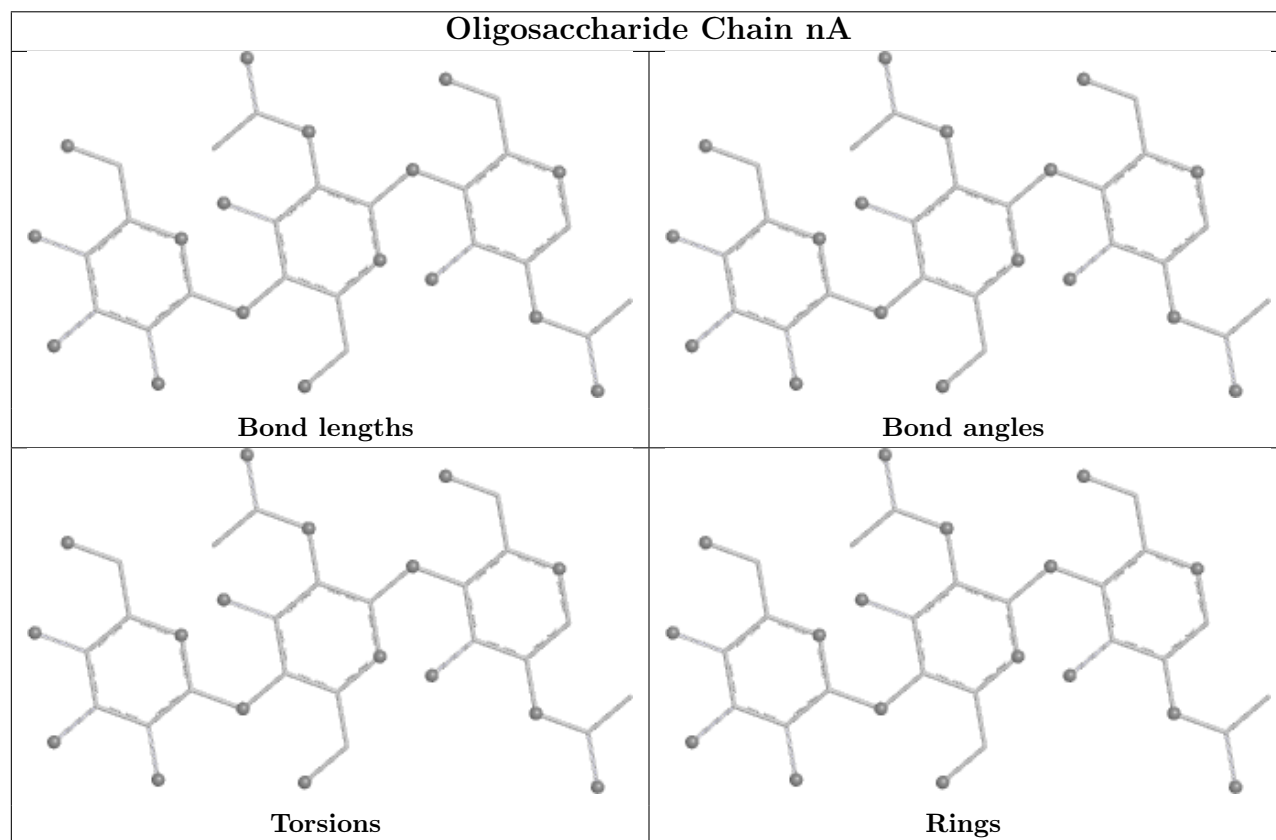
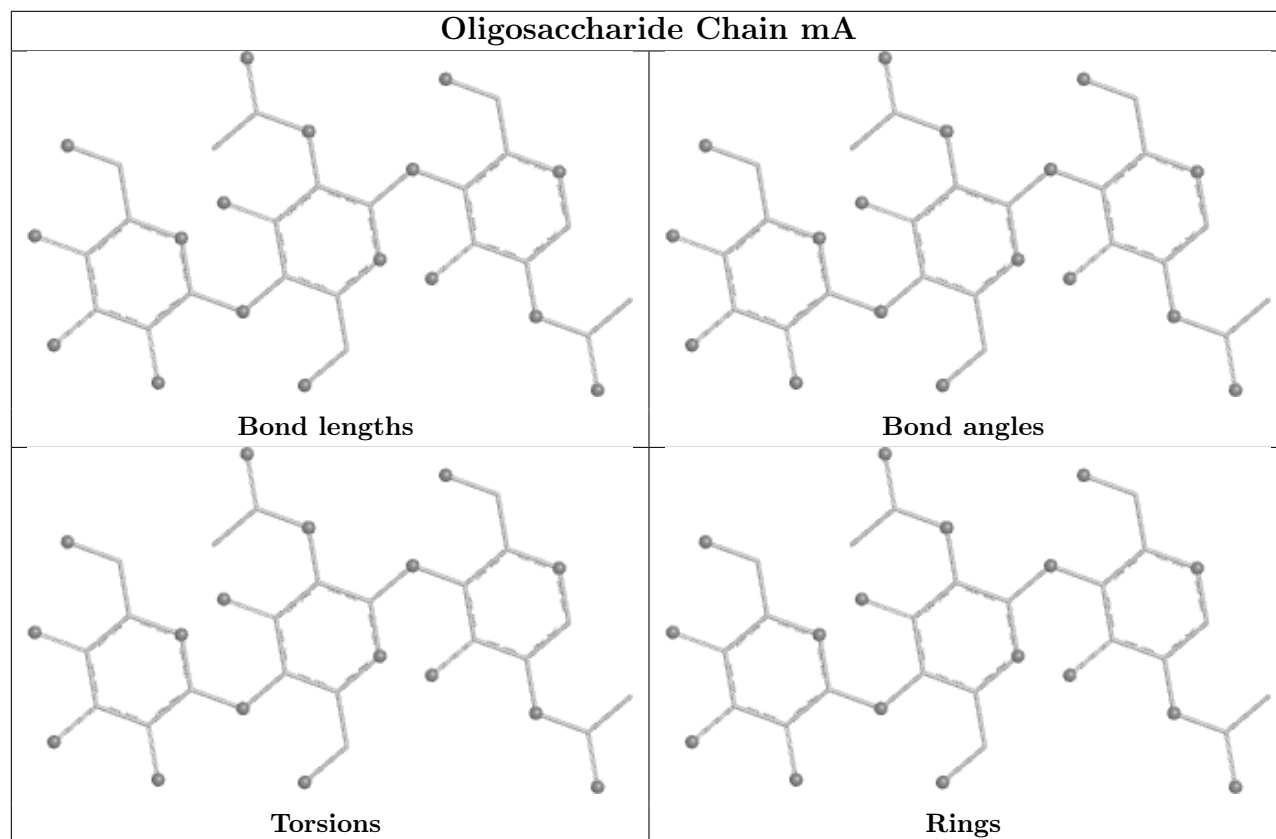


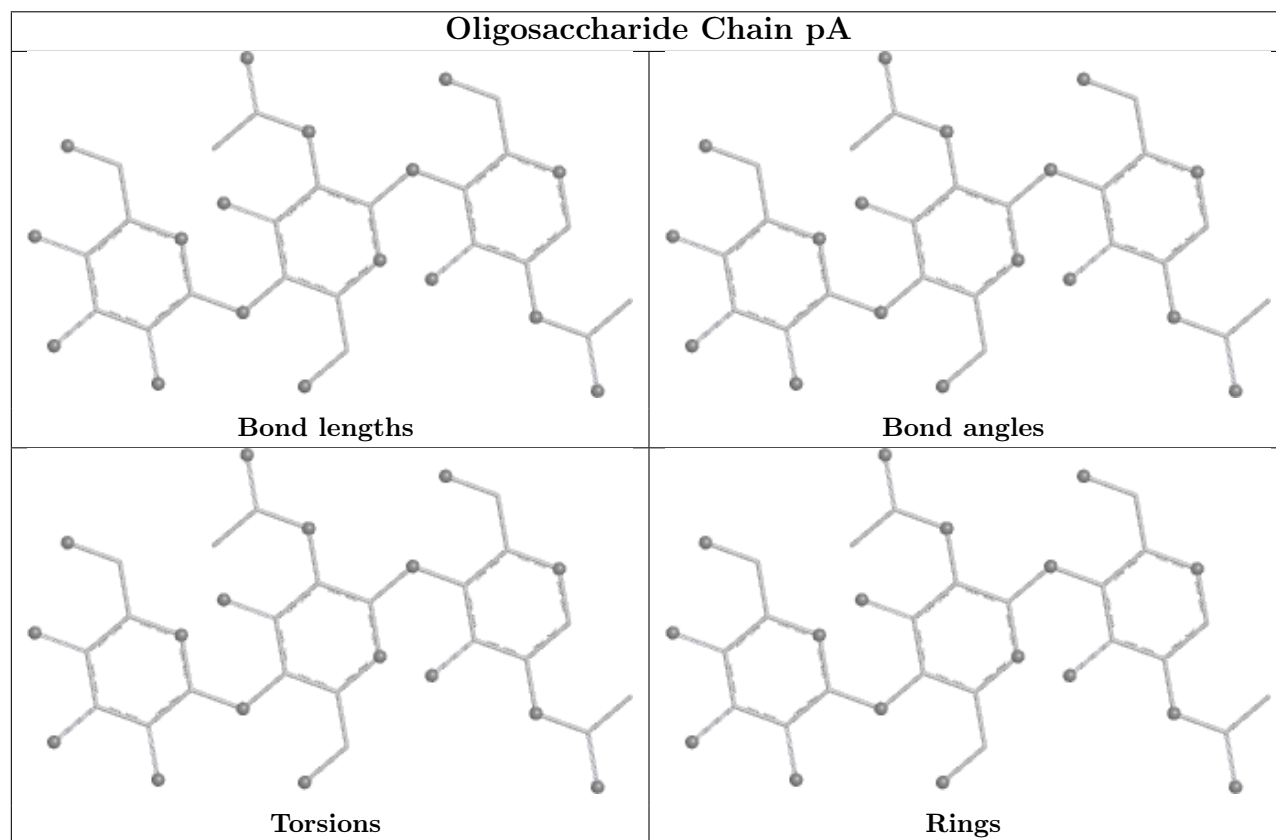
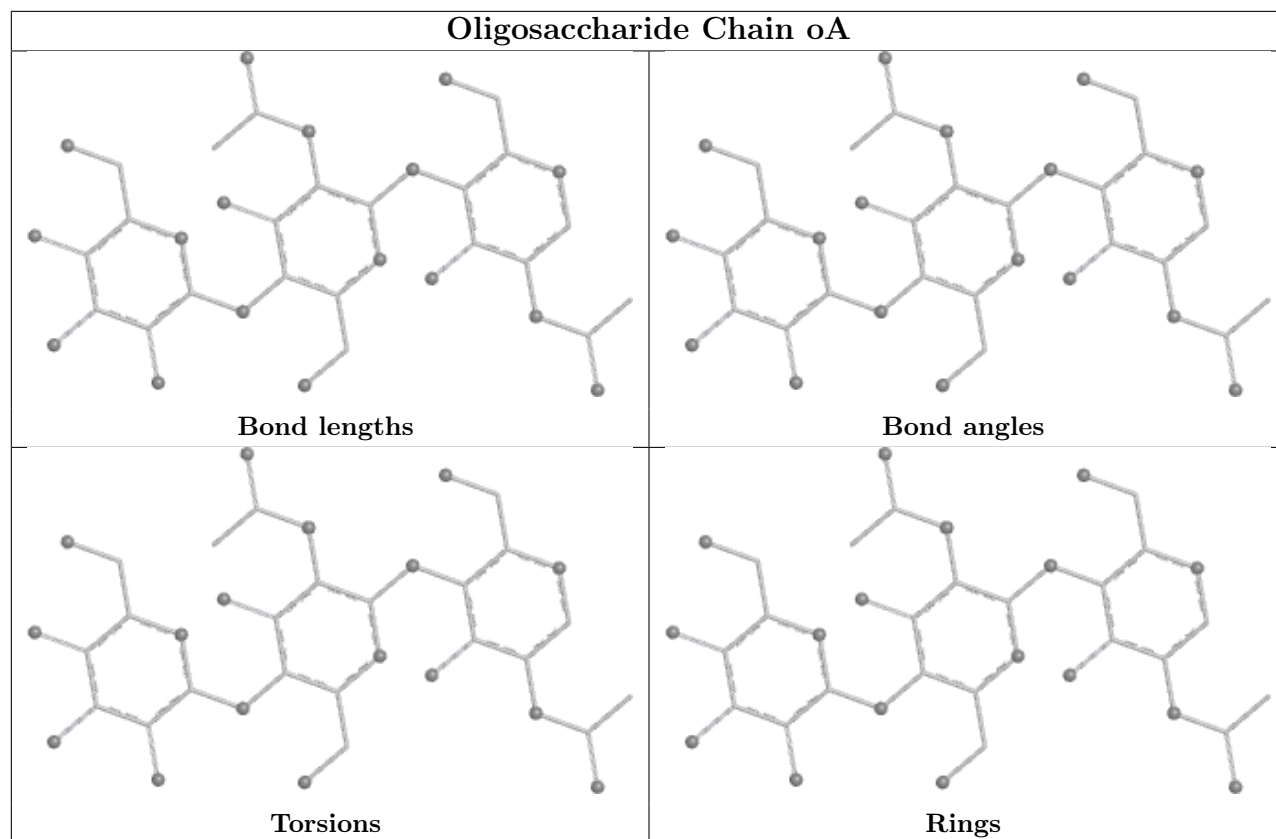
Oligosaccharide Chain kA



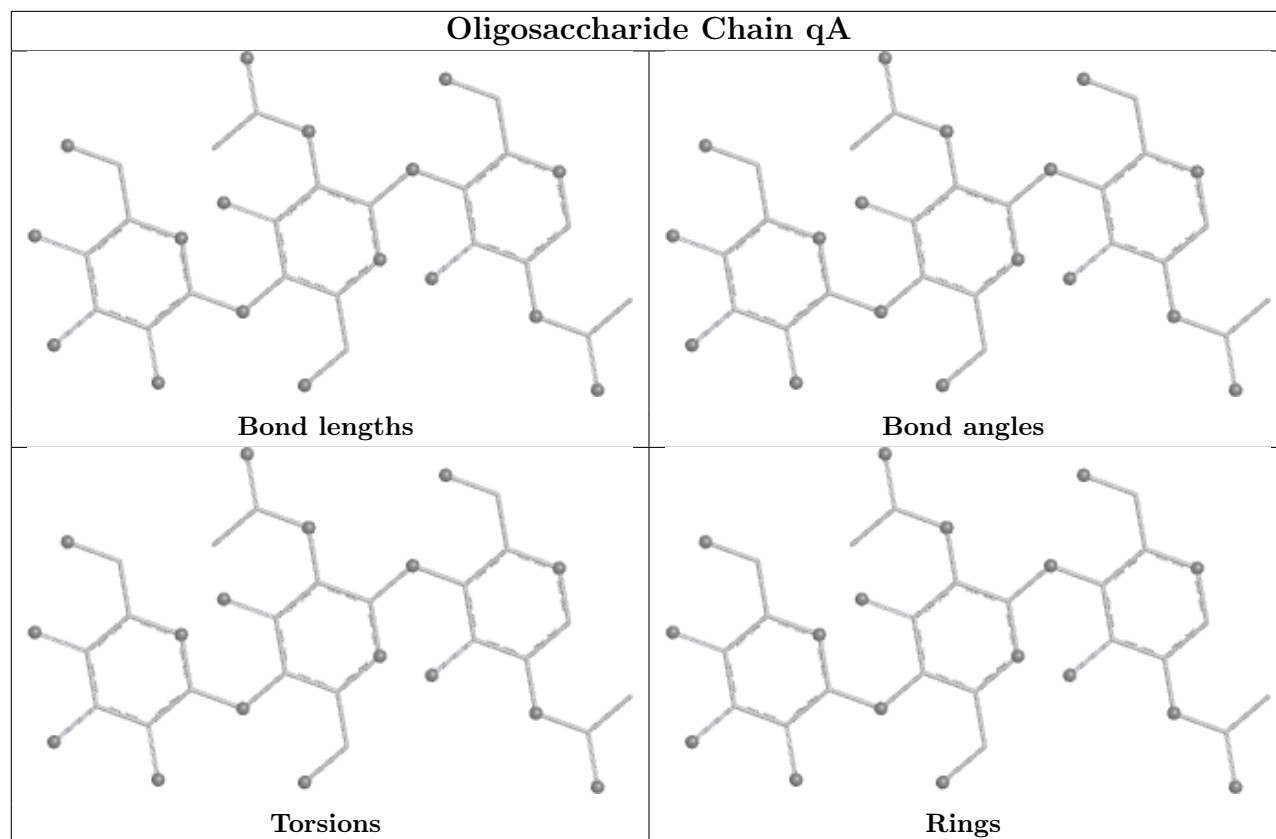
Oligosaccharide Chain lA



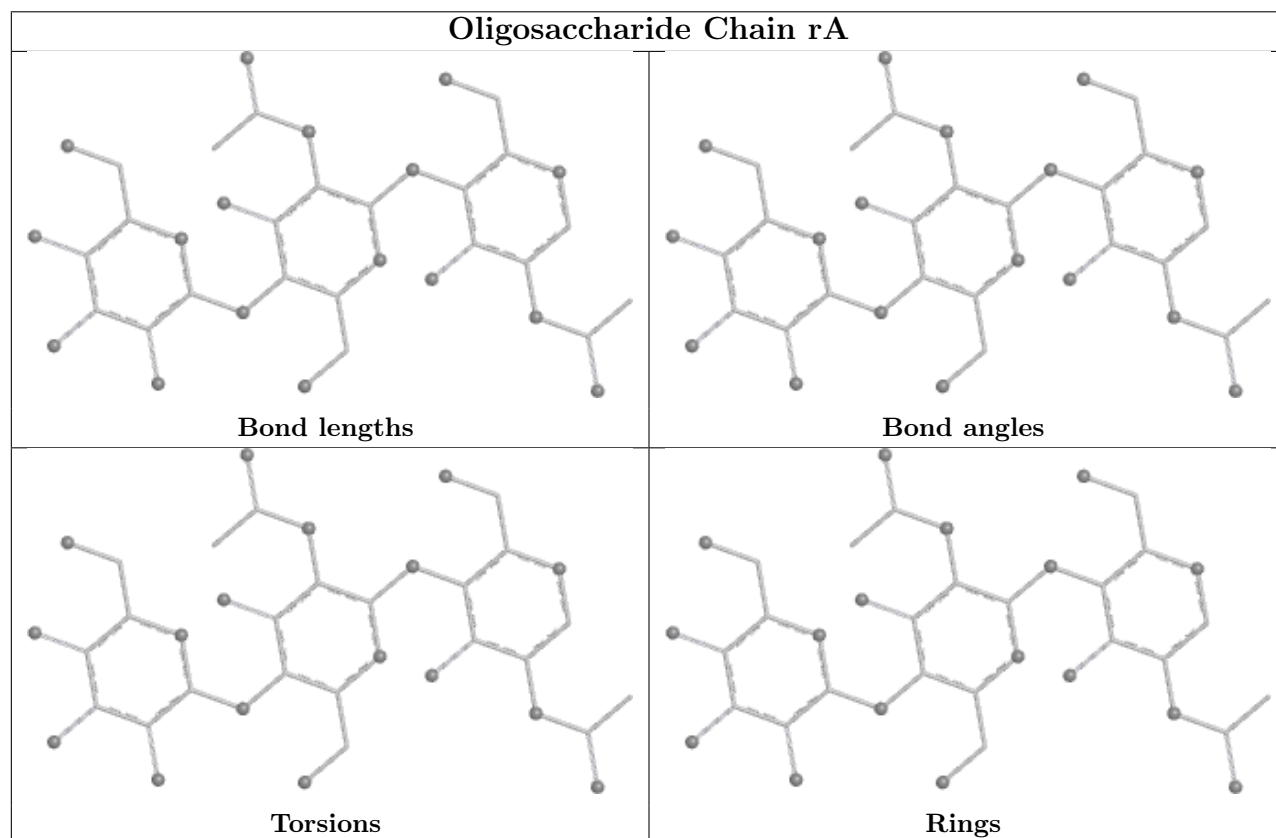


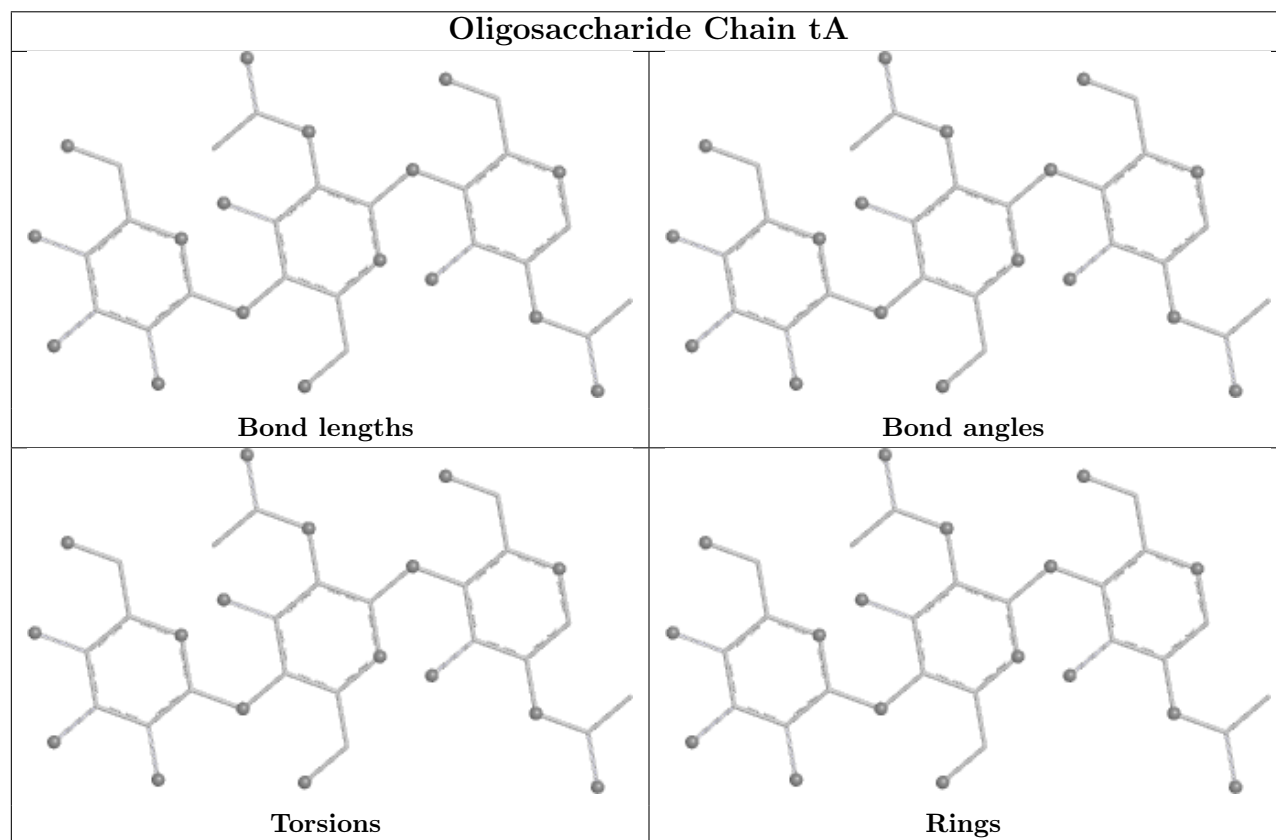
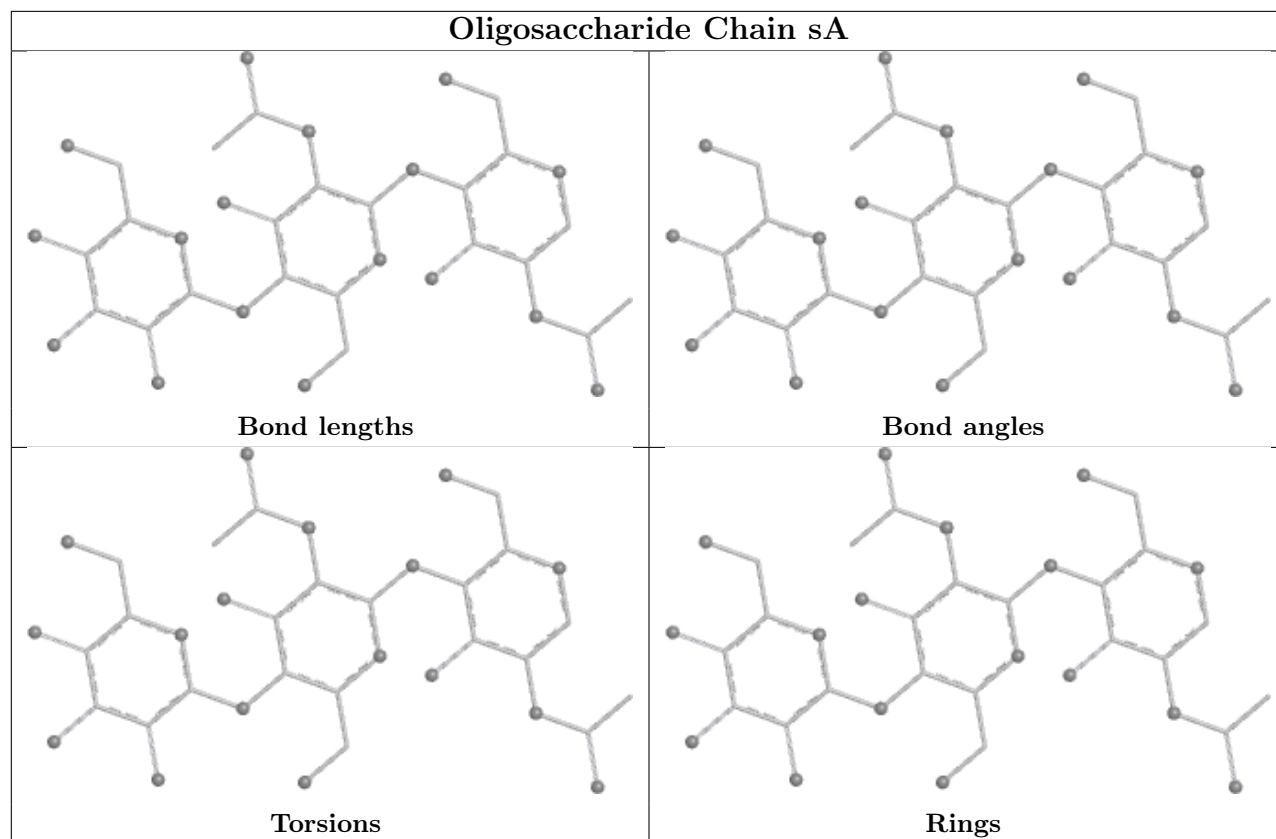


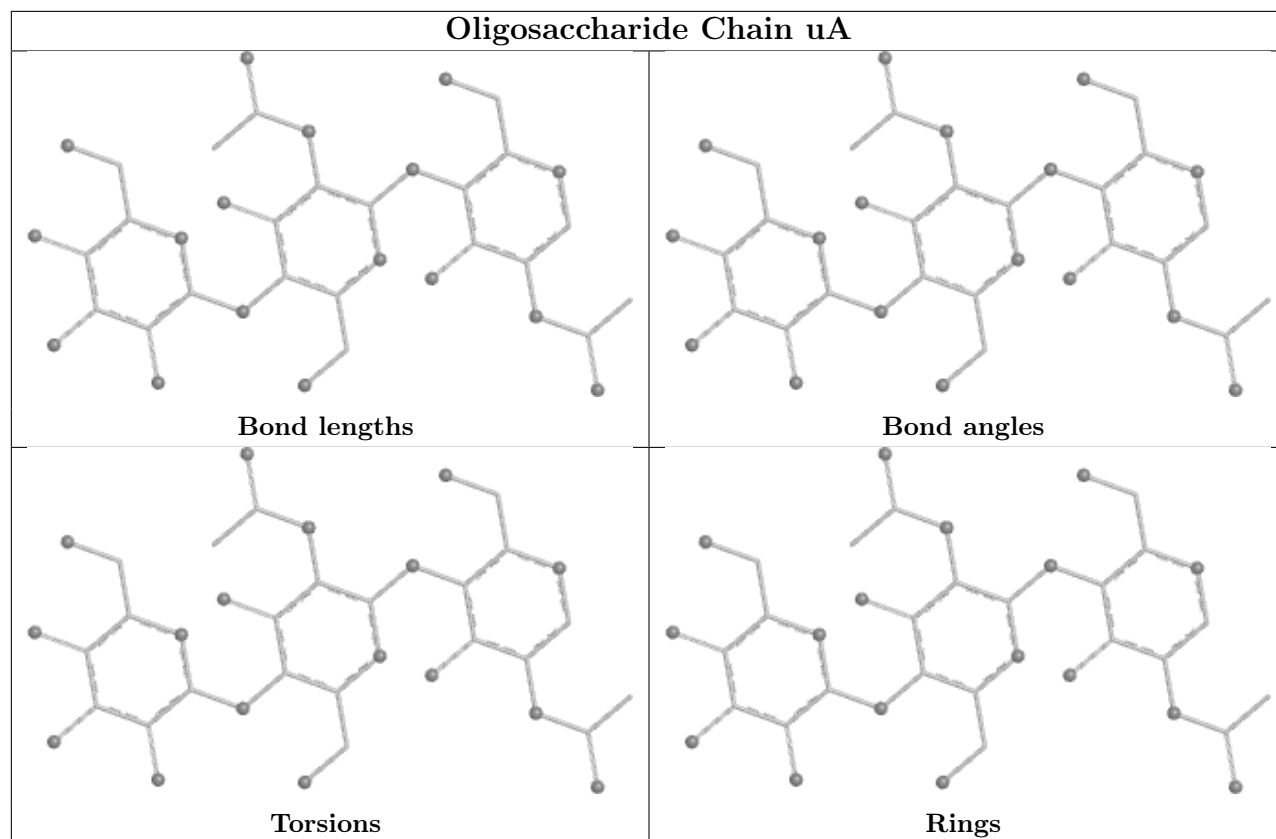
Oligosaccharide Chain qA



Oligosaccharide Chain rA







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.

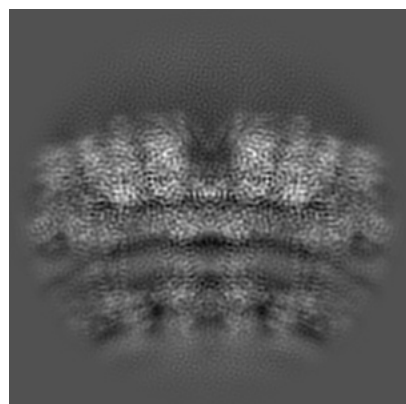
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39620. These allow visual inspection of the internal detail of the map and identification of artifacts.

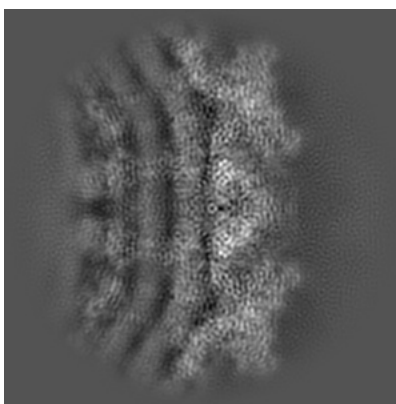
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

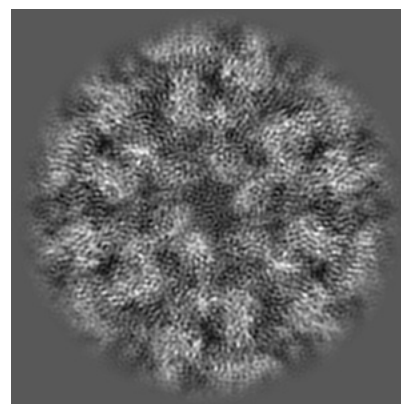
6.1.1 Primary map



X

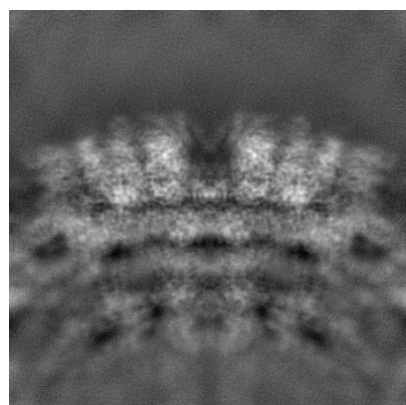


Y

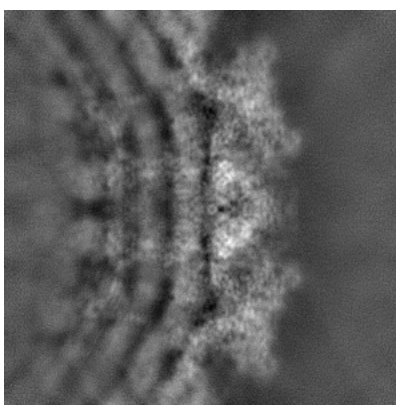


Z

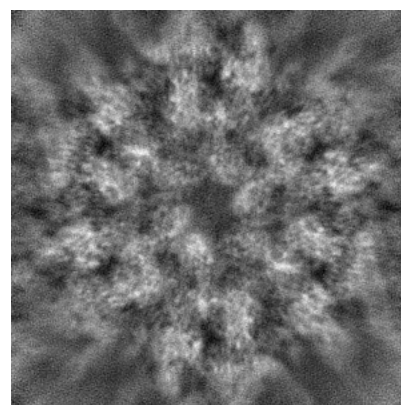
6.1.2 Raw map



X



Y

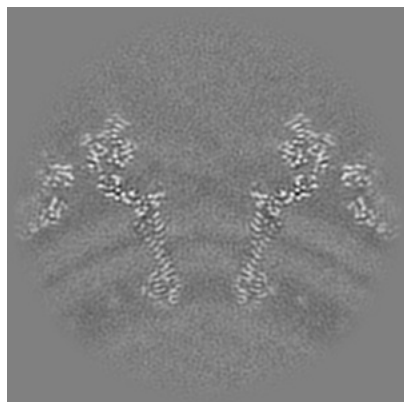


Z

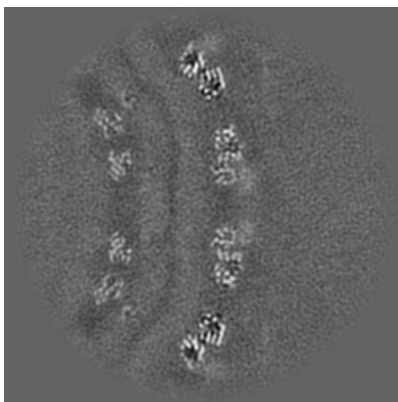
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

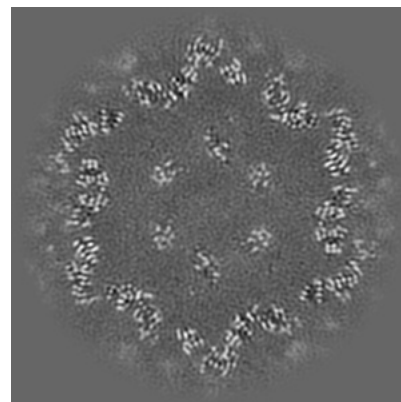
6.2.1 Primary map



X Index: 160

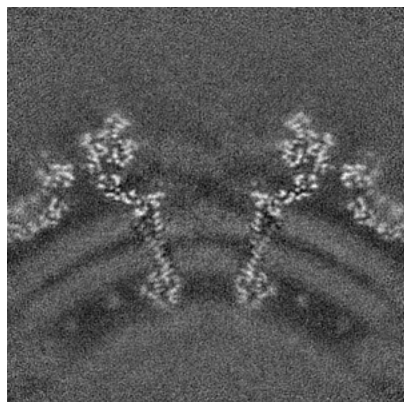


Y Index: 160

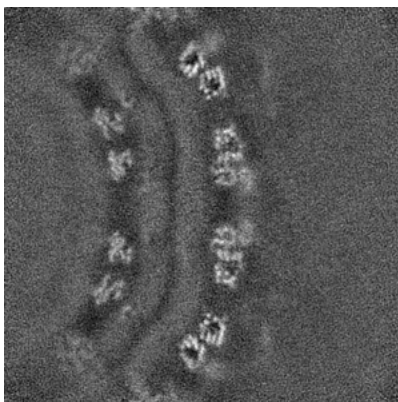


Z Index: 160

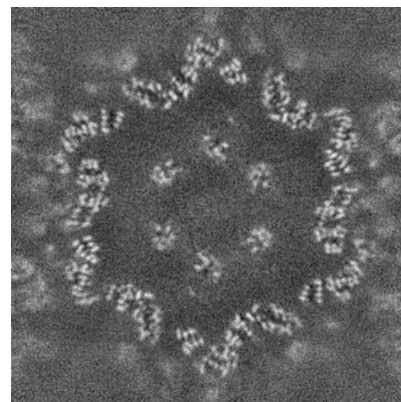
6.2.2 Raw map



X Index: 160



Y Index: 160

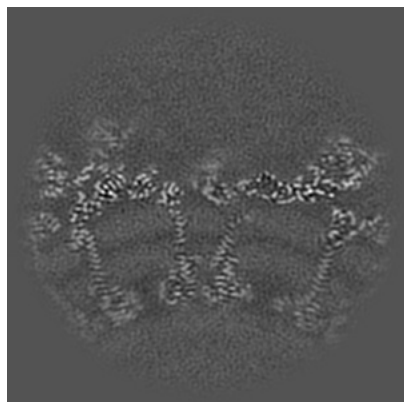


Z Index: 160

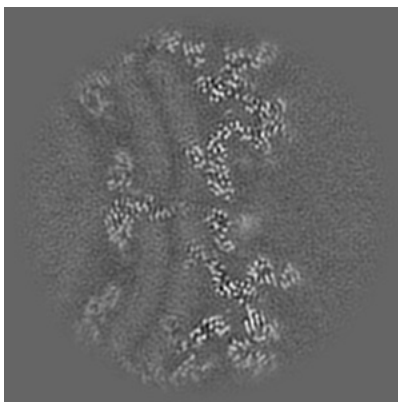
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

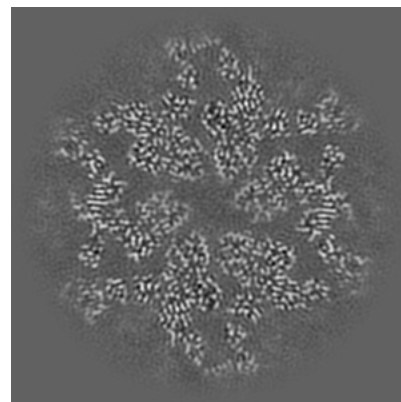
6.3.1 Primary map



X Index: 188

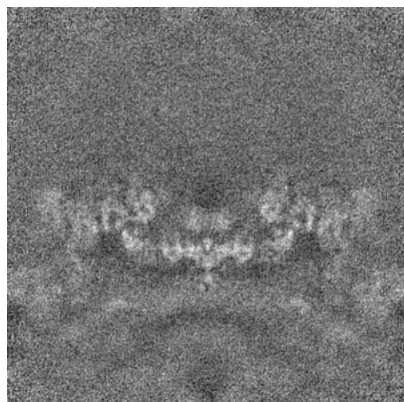


Y Index: 127

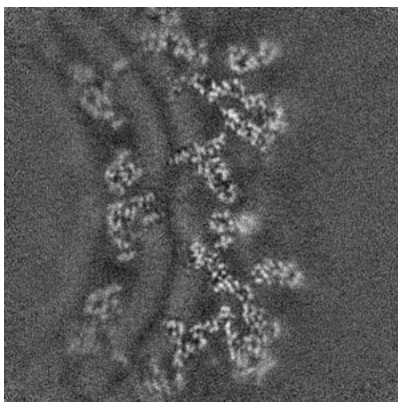


Z Index: 172

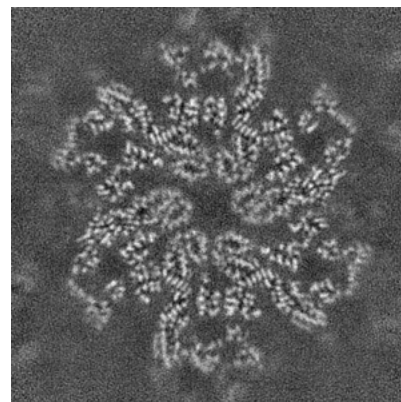
6.3.2 Raw map



X Index: 0



Y Index: 131

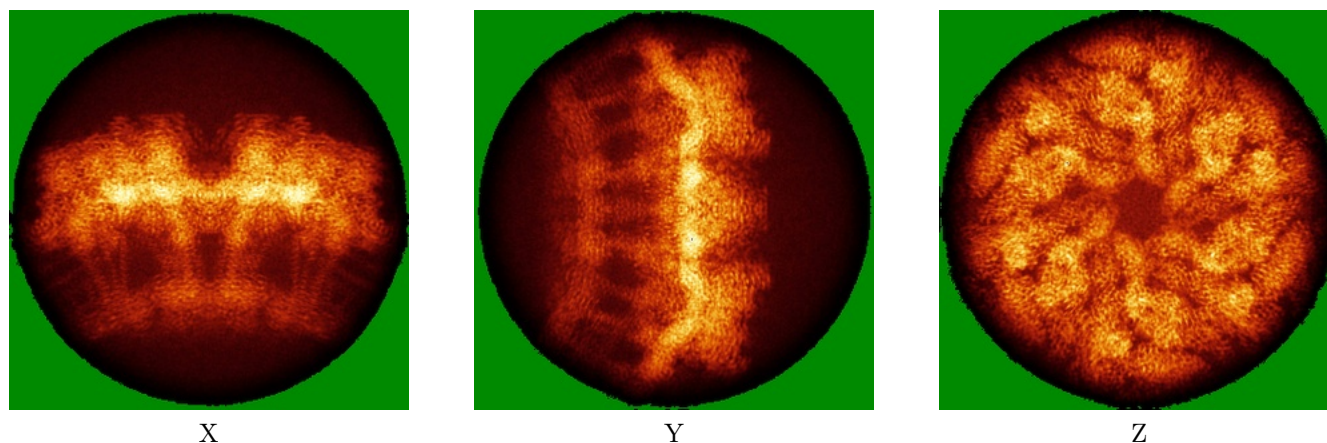


Z Index: 177

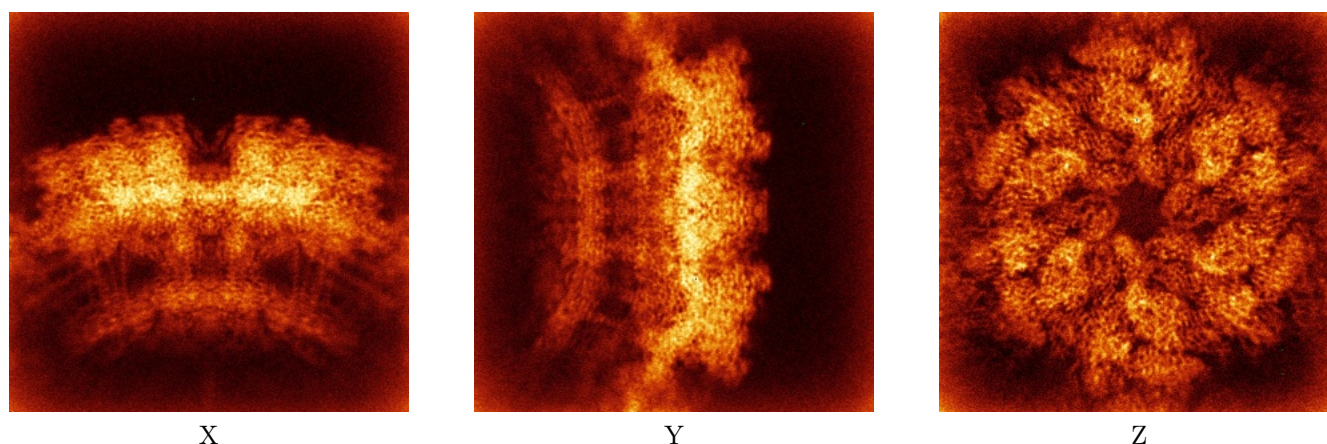
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

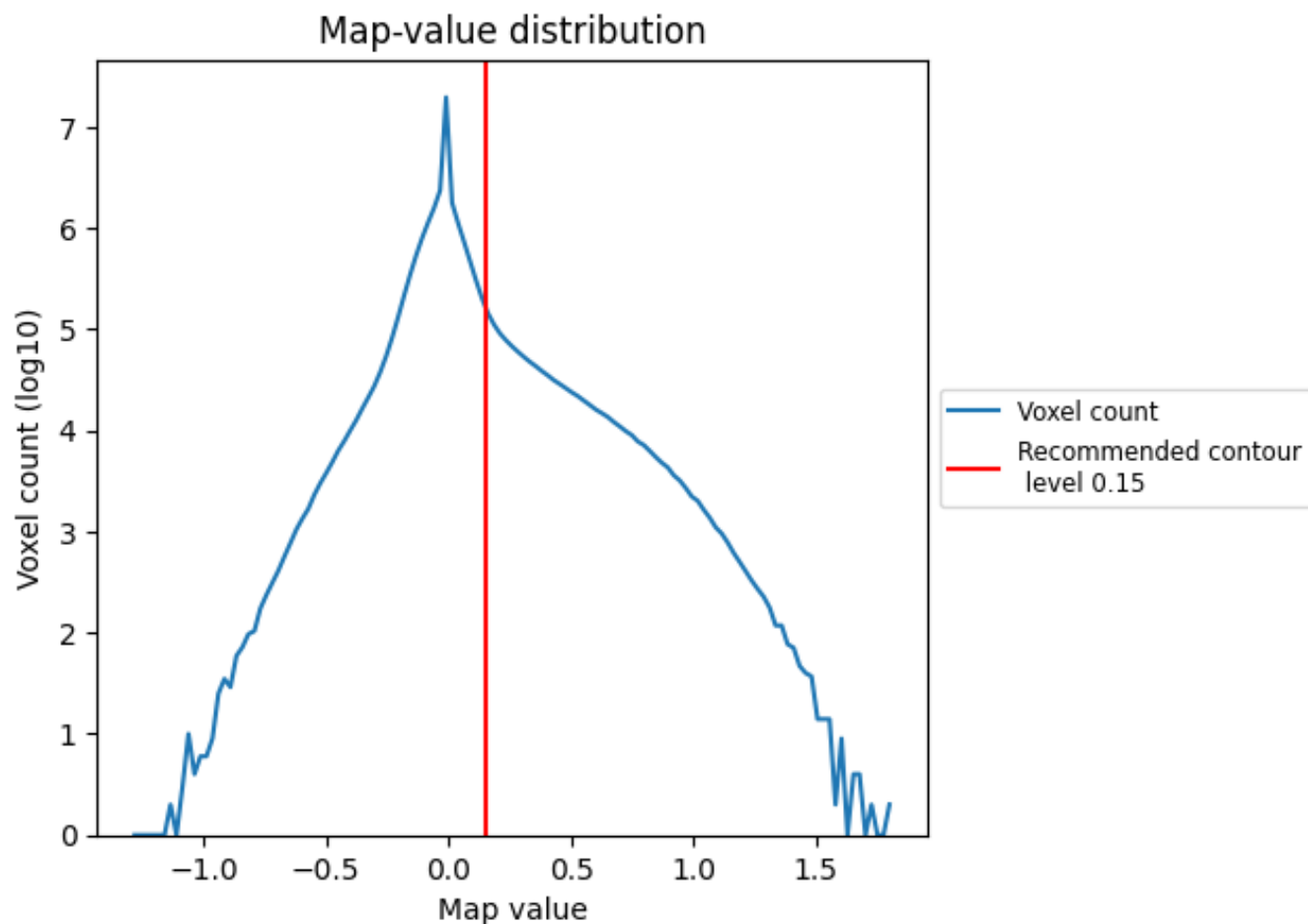
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

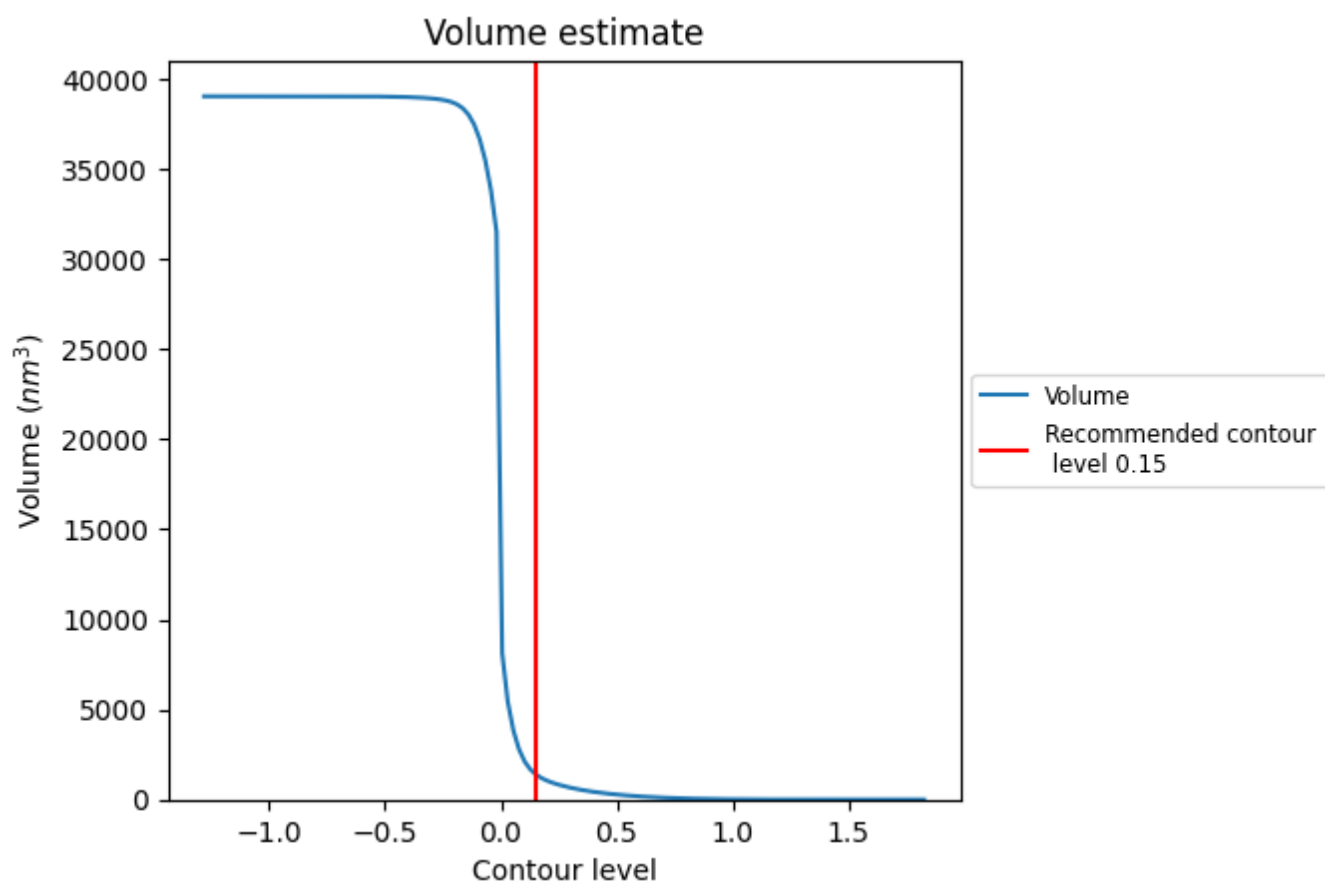
This section contains the results of statistical analysis of the map.

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.

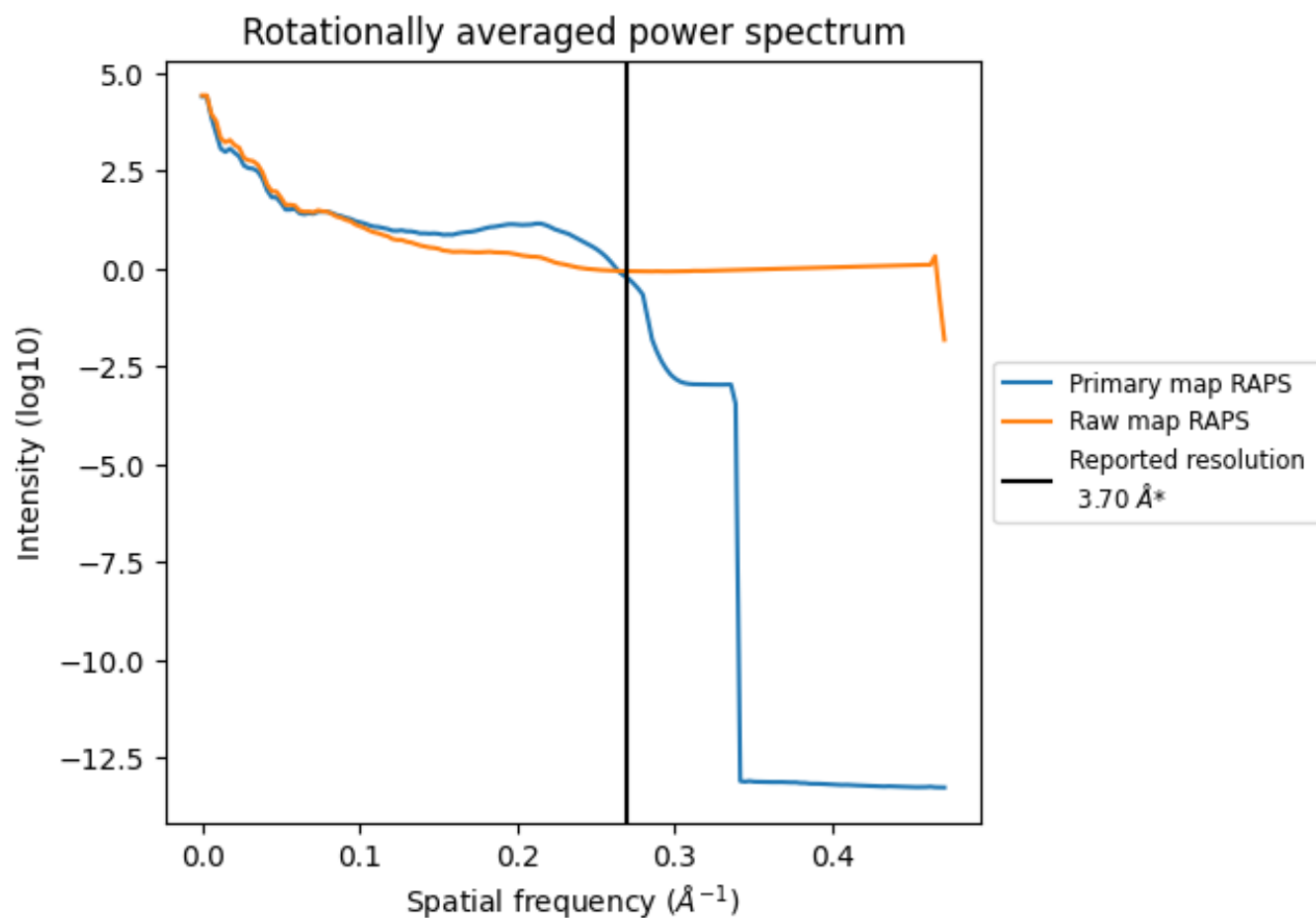
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1404 nm³; this corresponds to an approximate mass of 1268 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 ⓘ

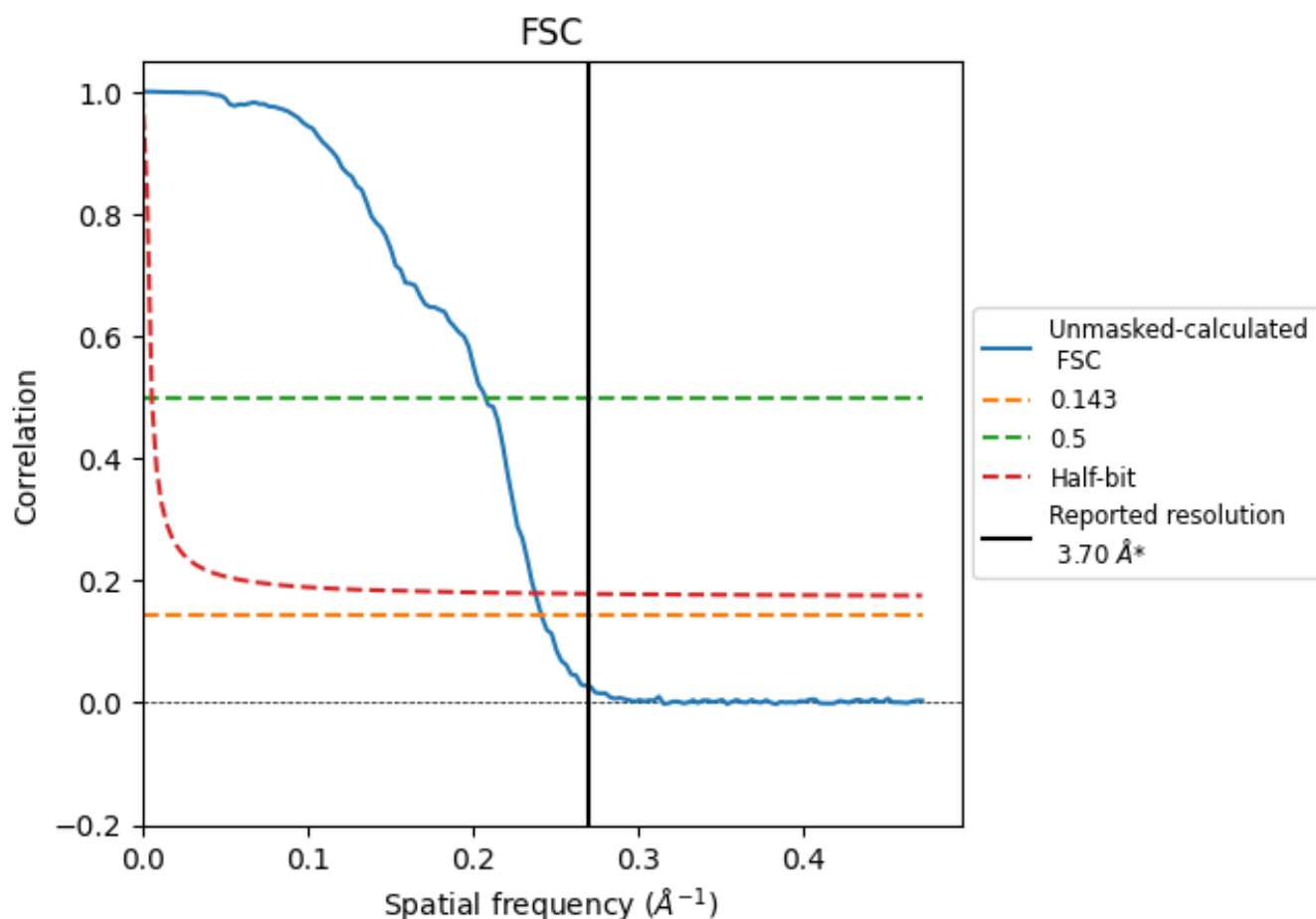


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

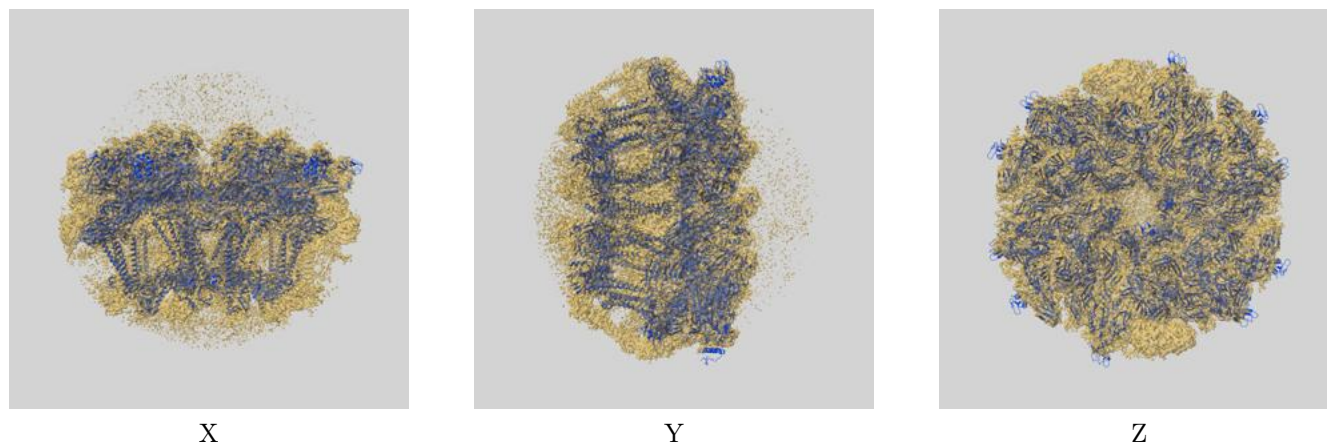
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	4.82	4.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

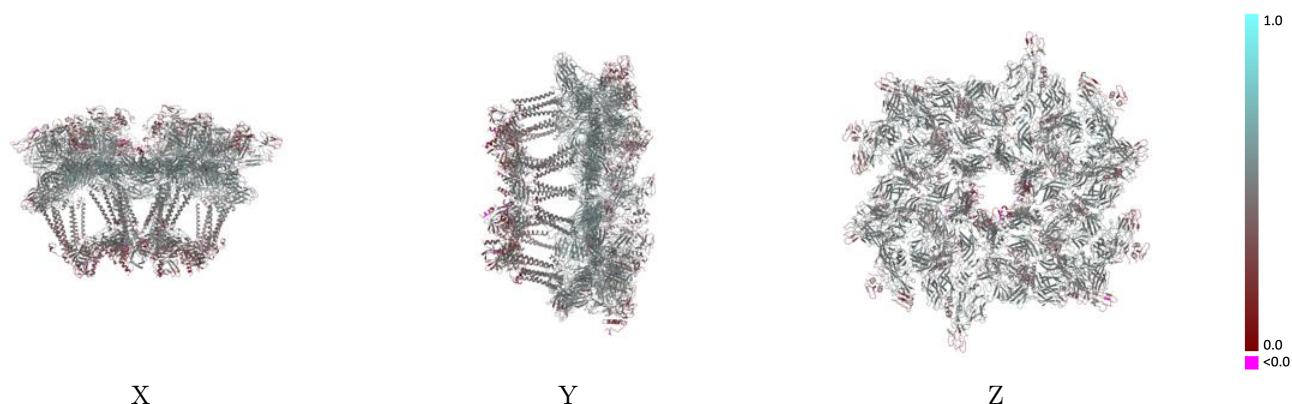
This section contains information regarding the fit between EMDB map EMD-39620 and PDB model 8YW2. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



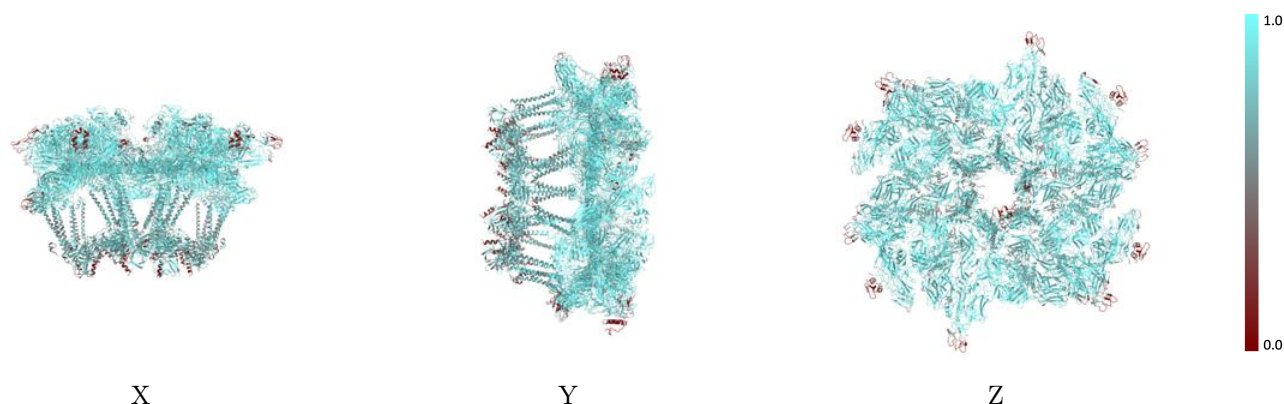
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



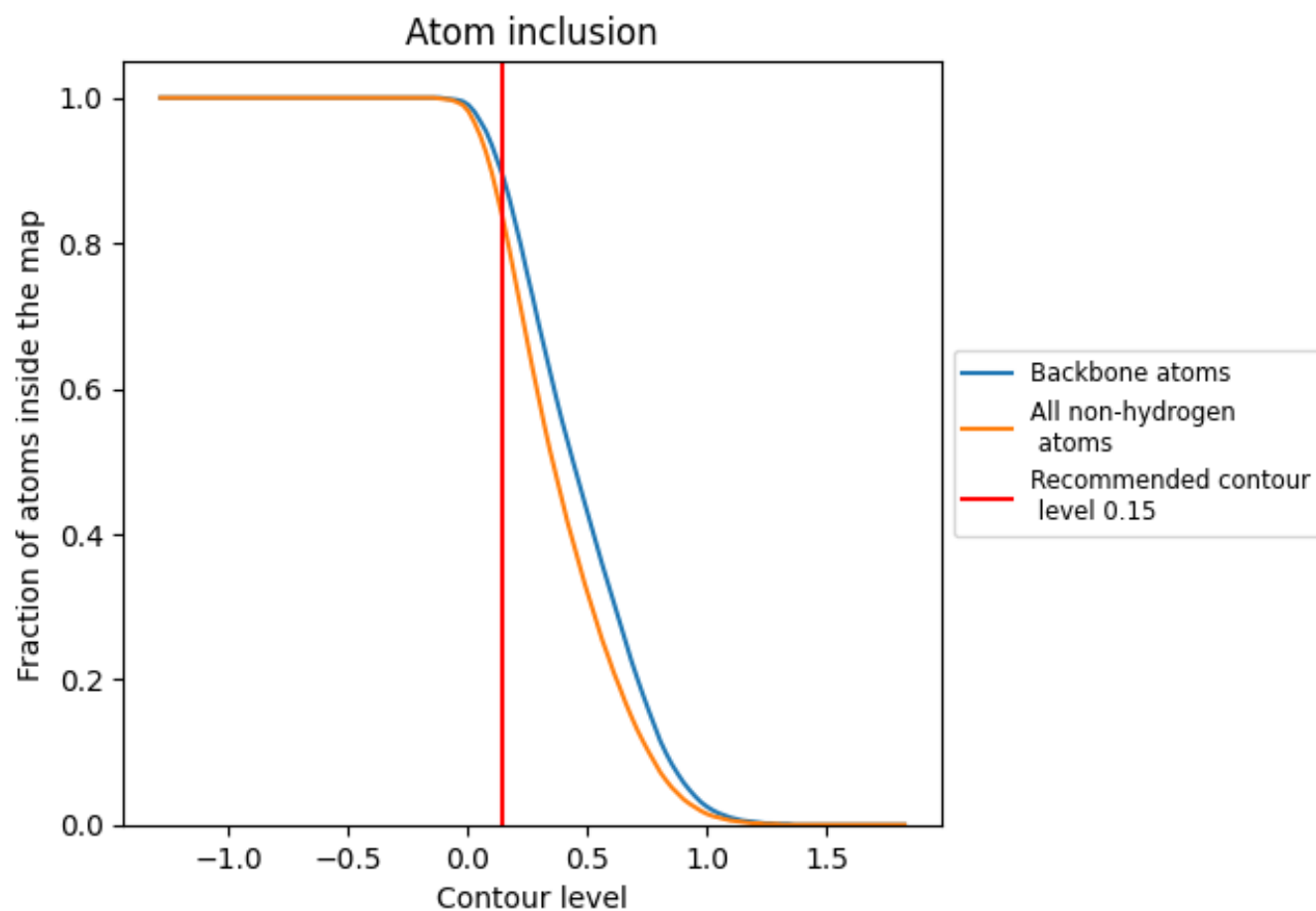
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.4670
0	 0.8230	 0.4150
1	 0.7890	 0.4550
2	 0.7320	 0.4030
3	 0.7460	 0.4480
4	 0.9230	 0.5120
5	 0.8010	 0.4780
6	 0.9100	 0.5070
7	 0.8960	 0.4780
8	 0.8530	 0.4600
9	 0.8950	 0.4760
A	 0.4770	 0.1720
AA	 0.1290	 0.2760
AB	 0.7950	 0.4150
AC	 0.7150	 0.4170
AD	 0.5910	 0.3640
AE	 0.5920	 0.3640
B	 0.8450	 0.4710
BA	 0.6150	 0.3090
C	 0.6920	 0.3730
CA	 0.7950	 0.4230
D	 0.7710	 0.4400
DA	 0.8460	 0.4480
E	 0.9060	 0.5060
EA	 0.6670	 0.3430
F	 0.9210	 0.5130
FA	 0.6920	 0.3490
G	 0.8010	 0.4700
GA	 0.8460	 0.3790
H	 0.9040	 0.5080
HA	 0.8970	 0.4570
I	 0.8990	 0.4760
IA	 0.7690	 0.4030
J	 0.8490	 0.4610
JA	 0.5380	 0.4160



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Chain	Atom inclusion	Q-score
K	 0.8860	 0.4770
KA	 0.6670	 0.4200
L	 0.7670	 0.3680
LA	 0.6150	 0.3970
M	 0.1390	 0.2730
MA	 0.5900	 0.3100
N	 0.7340	 0.3580
NA	 0.6410	 0.3380
O	 0.6900	 0.4170
OA	 0.8720	 0.4030
P	 0.6010	 0.3680
PA	 0.9230	 0.4480
Q	 0.6450	 0.3750
QA	 0.6920	 0.3350
R	 0.8920	 0.4800
RA	 0.5900	 0.3420
S	 0.7520	 0.4070
SA	 0.8210	 0.3880
T	 0.6310	 0.3800
TA	 0.8210	 0.4420
U	 0.8520	 0.4970
UA	 0.7690	 0.4020
V	 0.9140	 0.5050
VA	 0.8720	 0.4850
W	 0.9220	 0.5140
WA	 0.6670	 0.3890
X	 0.8620	 0.4650
XA	 0.5380	 0.2470
Y	 0.8590	 0.4770
YA	 0.7180	 0.3670
Z	 0.8290	 0.4660
ZA	 0.7690	 0.3530
a	 0.1440	 0.2800
aA	 0.7180	 0.4010
b	 0.7470	 0.4070
bA	 0.6920	 0.3460
c	 0.7670	 0.4080
cA	 0.6670	 0.3310
d	 0.6680	 0.4020
dA	 0.8720	 0.4580
e	 0.7360	 0.4370
eA	 0.3850	 0.4240

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Chain	Atom inclusion	Q-score
f	 0.7620	 0.4460
fA	 0.7180	 0.4060
g	 0.7870	 0.4150
gA	 0.5900	 0.3420
h	 0.9150	 0.5140
hA	 0.8210	 0.4180
i	 0.9030	 0.5080
iA	 1.0000	 0.4840
j	 0.8920	 0.4780
jA	 0.7690	 0.4140
k	 0.5900	 0.2680
kA	 0.7180	 0.4020
l	 0.7670	 0.4030
lA	 0.6150	 0.2790
m	 0.9140	 0.5140
mA	 0.6150	 0.3140
n	 0.6400	 0.3570
nA	 0.8460	 0.4450
o	 0.8580	 0.4990
oA	 0.8460	 0.4500
p	 0.9040	 0.5020
pA	 0.7440	 0.3710
q	 0.9230	 0.5190
qA	 0.6410	 0.4120
r	 0.8700	 0.4750
rA	 0.7950	 0.4140
s	 0.8590	 0.4770
sA	 0.4100	 0.4420
t	 0.8340	 0.4700
tA	 0.8460	 0.3930
u	 0.1420	 0.2710
uA	 0.5380	 0.4020
v	 0.7420	 0.3710
w	 0.7170	 0.3870
x	 0.6770	 0.4070
y	 0.7540	 0.4430
z	 0.8460	 0.4770