



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:29 AM UTC

PDB ID : 8YVZ / pdb_00008yvz
EMDB ID : EMD-39617
Title : Semliki Forest virus viron
Authors : Wang, J.; Zheng, T.; Yang, D.
Deposited on : 2024-03-29
Resolution : 3.45 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

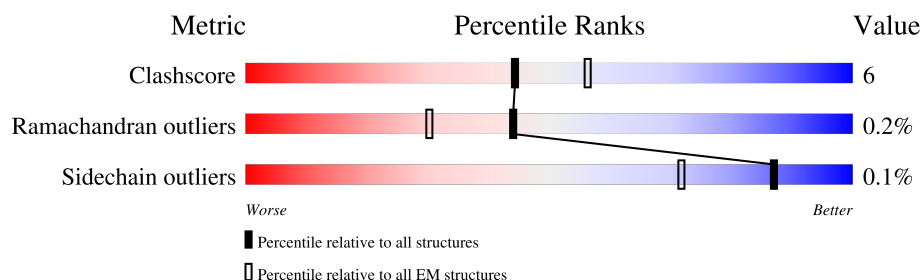
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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.



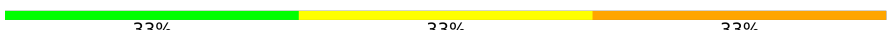
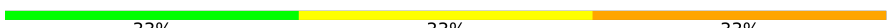
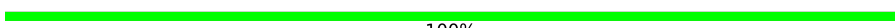
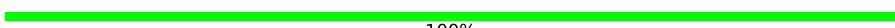
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	438	88% 12%
1	F	438	91% 8%
1	G	438	90% 10%
1	H	438	89% 11%
2	B	418	82% 18%
2	I	418	80% 20%
2	J	418	78% 22%
2	K	418	75% 24% .
3	C	52	79% 21%

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Mol	Chain	Length	Quality of chain
3	L	52	 75%25%
3	M	52	 79%21%
3	N	52	 81%19%
4	D	161	 84%16%
4	O	161	 83%17%
4	P	161	 88%12%
4	Q	161	 89%11%
5	E	44	 86%14%
5	R	44	 89%11%
5	S	44	 89%11%
5	T	44	 84%16%
6	U	3	 67%33%
6	V	3	 33%33%33%
6	W	3	 33%67%
6	X	3	 67%33%
6	Y	3	 33%33%33%
6	Z	3	 100%
6	a	3	 67%33%
6	b	3	 100%
6	c	3	 67%33%
6	d	3	 67%33%
6	e	3	 100%
6	f	3	 67%33%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 34740 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 E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
1	F	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
1	G	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
1	H	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		

- Molecule 2 is a protein called Spike glycoprotein E2.

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

- Molecule 3 is a protein called Spike glycoprotein E3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
3	L	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
3	M	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
3	N	52	Total	C	N	O	S	0	0
			404	252	67	77	8		

- Molecule 4 is a protein called capsid protein, partial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
4	O	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
4	P	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
4	Q	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		

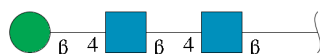
- Molecule 5 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	44	Total	C	N	O	S	0	0
			328	186	62	73	7		
5	R	44	Total	C	N	O	S	0	0
			328	186	62	73	7		
5	S	44	Total	C	N	O	S	0	0
			328	186	62	73	7		
5	T	44	Total	C	N	O	S	0	0
			328	186	62	73	7		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	108	GLY	-	expression tag	UNP P98155
E	109	SER	-	expression tag	UNP P98155
R	108	GLY	-	expression tag	UNP P98155
R	109	SER	-	expression tag	UNP P98155
S	108	GLY	-	expression tag	UNP P98155
S	109	SER	-	expression tag	UNP P98155
T	108	GLY	-	expression tag	UNP P98155
T	109	SER	-	expression tag	UNP P98155

- 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	U	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	V	3	Total	C	N	O	0	0
			39	22	2	15		
6	W	3	Total	C	N	O	0	0
			39	22	2	15		
6	X	3	Total	C	N	O	0	0
			39	22	2	15		
6	Y	3	Total	C	N	O	0	0
			39	22	2	15		
6	Z	3	Total	C	N	O	0	0
			39	22	2	15		
6	a	3	Total	C	N	O	0	0
			39	22	2	15		
6	b	3	Total	C	N	O	0	0
			39	22	2	15		
6	c	3	Total	C	N	O	0	0
			39	22	2	15		
6	d	3	Total	C	N	O	0	0
			39	22	2	15		
6	e	3	Total	C	N	O	0	0
			39	22	2	15		
6	f	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

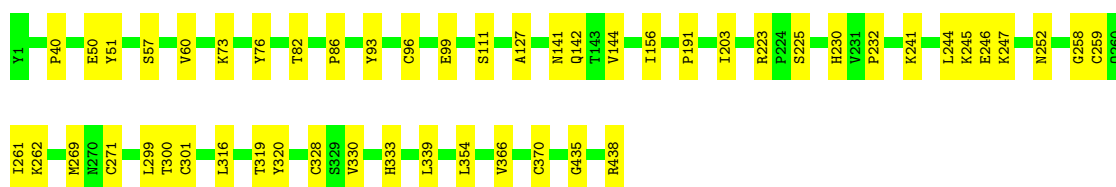
Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total	Ca	0
			1	1	
7	R	1	Total	Ca	0
			1	1	
7	S	1	Total	Ca	0
			1	1	
7	T	1	Total	Ca	0
			1	1	

3 Residue-property plots

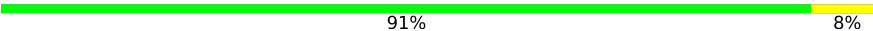
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

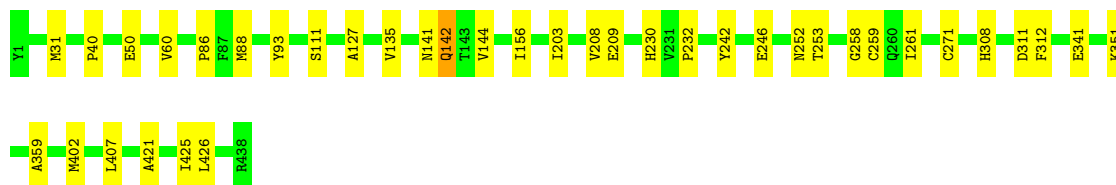
- Molecule 1: Spike glycoprotein E1

Chain A: 



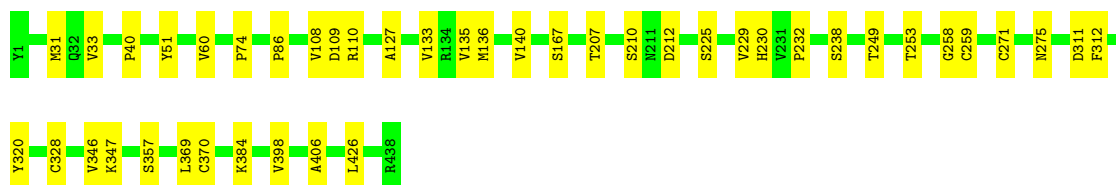
- Molecule 1: Spike glycoprotein E1

Chain F: 



- Molecule 1: Spike glycoprotein E1

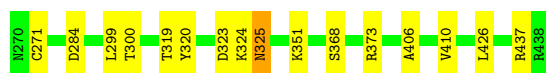
Chain G: 



- Molecule 1: Spike glycoprotein E1

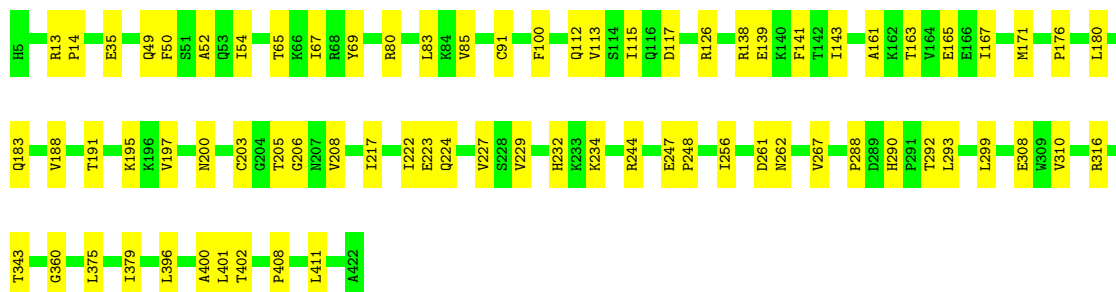
Chain H: 





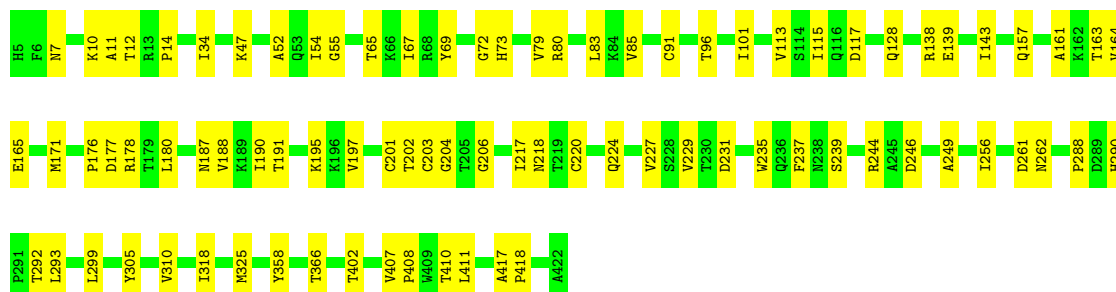
• Molecule 2: Spike glycoprotein E2

Chain B: 82% 18%



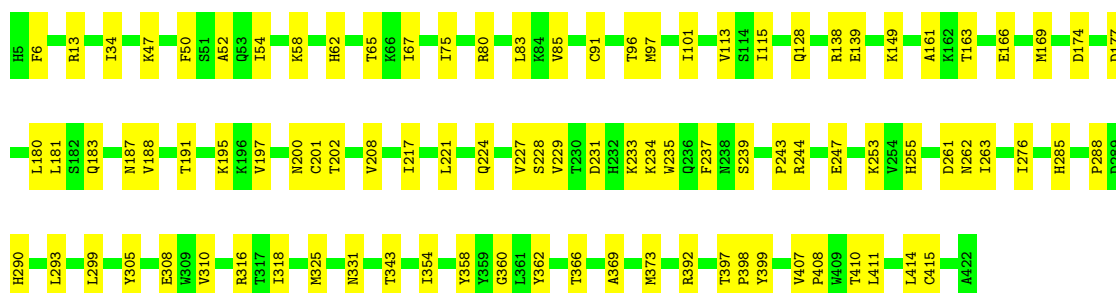
• Molecule 2: Spike glycoprotein E2

Chain I: 80% 20%



• Molecule 2: Spike glycoprotein E2

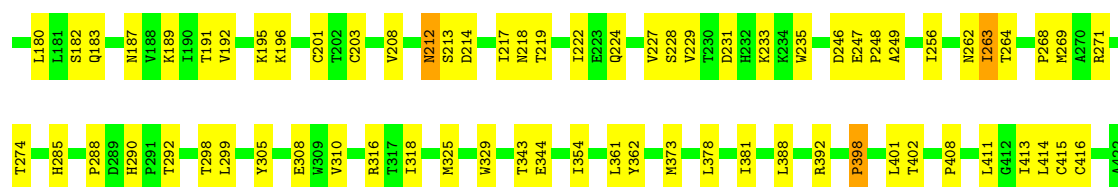
Chain J: 78% 22%



• Molecule 2: Spike glycoprotein E2

Chain K: 75% 24%





• Molecule 3: Spike glycoprotein E3

Chain C: 79% (green), 21% (yellow)



• Molecule 3: Spike glycoprotein E3

Chain L: 75% (green), 25% (yellow)



• Molecule 3: Spike glycoprotein E3

Chain M: 79% (green), 21% (yellow)



• Molecule 3: Spike glycoprotein E3

Chain N: 81% (green), 19% (yellow)



• Molecule 4: capsid protein, partial

Chain D: 84% (green), 16% (yellow)



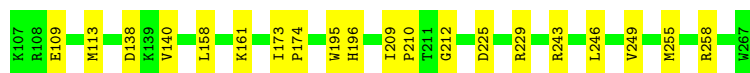
• Molecule 4: capsid protein, partial

Chain O: 83% (green), 17% (yellow)



• Molecule 4: capsid protein, partial

Chain P:  88% 12%



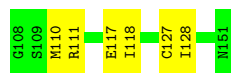
- Molecule 4: capsid protein, partial

Chain Q:  89% 11%



- Molecule 5: Very low-density lipoprotein receptor

Chain E:  86% 14%



- Molecule 5: Very low-density lipoprotein receptor

Chain R:  89% 11%



- Molecule 5: Very low-density lipoprotein receptor

Chain S:  89% 11%



- Molecule 5: Very low-density lipoprotein receptor

Chain T:  84% 16%

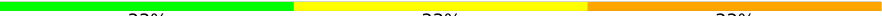


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  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 V:  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 W:  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 X:  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 Y:  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 Z:  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 a:  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 b:  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 c:  67% 33%

MAG1
MAG2
BMA3

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

Chain d:  67% 33%

MAG1
MAG2
BMA3

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

Chain e:  100%

MAG1
MAG2
BMA3

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

Chain f:  67% 33%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43127	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

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, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/3416	0.32	0/4660
1	F	0.15	0/3416	0.31	0/4660
1	G	0.14	0/3416	0.29	0/4660
1	H	0.16	0/3416	0.29	0/4660
2	B	0.15	0/3354	0.34	0/4574
2	I	0.15	0/3354	0.34	0/4574
2	J	0.15	0/3354	0.34	0/4574
2	K	0.17	0/3354	0.37	1/4574 (0.0%)
3	C	0.11	0/413	0.29	0/563
3	L	0.10	0/413	0.28	0/563
3	M	0.09	0/413	0.27	0/563
3	N	0.10	0/413	0.31	0/563
4	D	0.11	0/1273	0.27	0/1714
4	O	0.09	0/1273	0.21	0/1714
4	P	0.09	0/1273	0.24	0/1714
4	Q	0.10	0/1273	0.26	0/1714
5	E	0.12	0/332	0.47	0/446
5	R	0.16	0/332	0.49	0/446
5	S	0.13	0/332	0.54	0/446
5	T	0.14	0/332	0.51	1/446 (0.2%)
All	All	0.14	0/35152	0.32	2/47828 (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
2	K	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	398	PRO	CA-N-CD	-5.92	103.71	112.00
5	T	118	ILE	N-CA-C	-5.50	107.91	113.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	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	A	3330	0	3247	29	0
1	F	3330	0	3247	23	0
1	G	3330	0	3247	29	0
1	H	3330	0	3247	36	0
2	B	3260	0	3172	47	0
2	I	3260	0	3172	54	0
2	J	3260	0	3172	73	0
2	K	3260	0	3172	76	0
3	C	404	0	377	6	0
3	L	404	0	377	8	0
3	M	404	0	377	11	0
3	N	404	0	377	6	0
4	D	1245	0	1229	17	0
4	O	1245	0	1229	16	0
4	P	1245	0	1229	14	0
4	Q	1245	0	1229	12	0
5	E	328	0	275	4	0
5	R	328	0	275	4	0
5	S	328	0	275	4	0
5	T	328	0	275	4	0
6	U	39	0	34	0	0
6	V	39	0	34	2	0
6	W	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	X	39	0	34	0	0
6	Y	39	0	34	2	0
6	Z	39	0	34	0	0
6	a	39	0	34	1	0
6	b	39	0	34	0	0
6	c	39	0	34	0	0
6	d	39	0	34	1	0
6	e	39	0	34	0	0
6	f	39	0	34	1	0
7	E	1	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
All	All	34740	0	33608	439	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 6.

All (439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:CYS:SG	2:B:224:GLN:NE2	2.56	0.78
4:Q:140:VAL:HG23	4:Q:173:ILE:HG22	1.67	0.76
2:B:180:LEU:HD12	2:B:227:VAL:HG11	1.67	0.75
1:F:311:ASP:OD1	1:F:312:PHE:N	2.18	0.75
5:T:114:ARG:HG2	5:T:115:ILE:H	1.50	0.75
2:I:408:PRO:HA	2:I:411:LEU:HB3	1.70	0.74
1:G:229:VAL:HG11	2:J:243:PRO:HG3	1.69	0.73
5:T:133:ARG:NH1	5:T:134:CYS:SG	2.62	0.73
2:J:392:ARG:HG2	2:J:414:LEU:HD12	1.71	0.72
2:K:263:ILE:HG13	2:K:264:THR:H	1.55	0.71
2:I:55:GLY:H	2:I:67:ILE:HG22	1.54	0.71
2:K:408:PRO:HA	2:K:411:LEU:HB3	1.73	0.70
2:K:87:THR:HG22	2:K:88:SER:H	1.57	0.70
2:J:139:GLU:OE1	2:J:290:HIS:NE2	2.25	0.69
2:B:408:PRO:HA	2:B:411:LEU:HB3	1.75	0.67
1:H:259:CYS:HB3	1:H:271:CYS:HA	1.77	0.67
2:B:308:GLU:OE1	2:B:316:ARG:NH1	2.26	0.66
4:O:140:VAL:HG23	4:O:173:ILE:HG22	1.77	0.66
1:F:253:THR:HG23	2:I:305:TYR:HE1	1.60	0.66
2:K:183:GLN:NE2	2:K:187:ASN:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:TYR:HB3	2:I:176:PRO:HG3	1.77	0.65
2:J:255:HIS:HE1	3:M:49:TYR:CZ	2.13	0.65
2:B:83:LEU:HB2	2:B:115:ILE:HD12	1.79	0.65
4:Q:239:ASN:HA	4:Q:244:THR:HG22	1.79	0.65
3:L:33:GLU:O	3:L:37:ARG:HG2	1.97	0.65
2:J:80:ARG:NH2	2:J:96:THR:OG1	2.29	0.64
2:K:180:LEU:HD12	2:K:227:VAL:HG11	1.79	0.64
2:B:85:VAL:HG23	2:B:91:CYS:HB2	1.80	0.64
1:F:259:CYS:HB3	1:F:271:CYS:HA	1.80	0.64
2:K:139:GLU:OE1	2:K:290:HIS:NE2	2.26	0.64
1:G:259:CYS:HB3	1:G:271:CYS:HA	1.79	0.64
2:J:85:VAL:HG23	2:J:91:CYS:HB2	1.80	0.64
2:J:255:HIS:CE1	3:M:49:TYR:CZ	2.86	0.64
2:K:235:TRP:NE1	3:N:40:GLU:OE2	2.28	0.64
2:J:83:LEU:HB2	2:J:115:ILE:HD12	1.80	0.63
2:K:401:LEU:HB2	4:Q:256:VAL:HG21	1.80	0.63
2:K:80:ARG:NH2	2:K:96:THR:OG1	2.30	0.63
2:J:65:THR:O	2:J:80:ARG:N	2.32	0.63
2:J:169:MET:HB3	2:J:235:TRP:HB3	1.81	0.63
1:G:207:THR:HG22	1:G:210:SER:HB2	1.81	0.63
1:G:40:PRO:HA	1:G:127:ALA:HA	1.80	0.62
4:O:186:HIS:O	4:O:188:LYS:NZ	2.30	0.62
2:I:65:THR:O	2:I:80:ARG:N	2.33	0.62
2:J:85:VAL:HG12	2:J:113:VAL:HG12	1.80	0.62
3:L:38:MET:O	3:L:42:ASN:ND2	2.33	0.62
1:A:141:ASN:O	1:A:142:GLN:HG3	1.99	0.62
3:C:9:CYS:N	3:C:18:CYS:SG	2.73	0.62
2:I:80:ARG:NH2	2:I:96:THR:OG1	2.28	0.62
3:N:9:CYS:N	3:N:18:CYS:SG	2.73	0.62
1:A:259:CYS:HB3	1:A:271:CYS:HA	1.82	0.61
2:B:13:ARG:HD2	2:B:234:LYS:HG3	1.82	0.61
2:I:7:ASN:HB3	2:I:10:LYS:HE2	1.82	0.61
2:J:180:LEU:HD11	2:J:227:VAL:HG11	1.82	0.61
2:B:261:ASP:OD1	2:B:262:ASN:N	2.31	0.61
1:H:93:TYR:HB3	2:K:176:PRO:HG3	1.82	0.61
4:O:154:ASP:HA	4:O:157:LYS:HE3	1.83	0.61
2:I:67:ILE:HD11	2:I:115:ILE:HD13	1.83	0.61
2:J:244:ARG:HH21	2:J:247:GLU:HG3	1.65	0.61
5:E:110:MET:HG2	5:E:111:ARG:HG2	1.83	0.61
4:O:234:VAL:HA	4:O:248:VAL:HG12	1.83	0.60
2:B:139:GLU:OE1	2:B:290:HIS:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:THR:O	2:B:80:ARG:N	2.35	0.60
1:H:253:THR:HG23	2:K:305:TYR:HE1	1.67	0.60
3:M:11:LEU:HD12	3:M:38:MET:HG3	1.84	0.60
2:B:171:MET:HE1	2:B:232:HIS:HB3	1.84	0.60
1:G:312:PHE:HA	1:G:357:SER:HB2	1.84	0.60
2:I:180:LEU:HB2	2:I:227:VAL:HG21	1.83	0.59
3:C:10:VAL:HG13	3:C:45:ARG:HH12	1.68	0.59
2:J:174:ASP:HB3	2:J:228:SER:HB3	1.85	0.59
3:M:9:CYS:N	3:M:18:CYS:SG	2.76	0.59
2:I:318:ILE:HD12	2:I:325:MET:HE1	1.83	0.59
1:H:323:ASP:OD1	1:H:324:LYS:N	2.36	0.59
2:K:398:PRO:HB3	4:Q:255:MET:HE1	1.85	0.58
1:H:300:THR:OG1	1:H:319:THR:OG1	2.22	0.58
2:K:65:THR:O	2:K:80:ARG:N	2.34	0.58
1:A:244:LEU:O	1:A:247:LYS:NZ	2.36	0.58
4:O:209:ILE:HG22	4:O:212:GLY:H	1.68	0.58
4:D:126:GLU:OE2	4:D:128:LYS:NZ	2.35	0.58
2:J:408:PRO:HA	2:J:411:LEU:HB3	1.85	0.57
3:N:36:LEU:HA	3:N:39:LEU:HD12	1.87	0.57
2:B:85:VAL:HG12	2:B:113:VAL:HG12	1.85	0.57
6:Y:2:NAG:H3	6:Y:2:NAG:H83	1.86	0.57
2:J:200:ASN:HA	2:J:208:VAL:HG12	1.86	0.57
6:V:2:NAG:H83	6:V:2:NAG:H3	1.86	0.57
2:B:247:GLU:HG3	2:B:248:PRO:HD3	1.86	0.57
1:H:325:ASN:C	1:H:325:ASN:HD22	2.10	0.57
2:I:261:ASP:OD1	2:I:262:ASN:N	2.37	0.56
2:B:197:VAL:HB	2:B:227:VAL:HG13	1.86	0.56
1:A:245:LYS:HG3	1:A:246:GLU:HG2	1.87	0.56
4:P:255:MET:HE2	4:P:255:MET:HA	1.87	0.56
1:A:60:VAL:HG11	1:A:86:PRO:HG2	1.88	0.56
1:H:60:VAL:HG11	1:H:86:PRO:HG2	1.87	0.56
2:I:54:ILE:HD12	2:I:96:THR:HG23	1.88	0.56
4:D:140:VAL:HG23	4:D:173:ILE:HG22	1.87	0.55
1:G:230:HIS:CD2	1:G:232:PRO:HG3	2.41	0.55
2:B:112:GLN:HB3	2:B:126:ARG:HB3	1.88	0.55
2:K:288:PRO:HG3	2:K:310:VAL:HG12	1.88	0.55
2:K:392:ARG:NH2	2:K:415:CYS:O	2.39	0.55
1:A:300:THR:OG1	1:A:319:THR:OG1	2.24	0.55
2:K:165:GLU:HB2	2:K:256:ILE:HG12	1.89	0.55
6:a:1:NAG:H83	6:a:1:NAG:H3	1.89	0.55
2:B:54:ILE:HG22	2:B:67:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:HIS:CD2	1:H:232:PRO:HG3	2.43	0.54
2:I:187:ASN:HB3	2:I:218:ASN:HA	1.89	0.54
2:I:244:ARG:HH11	2:I:249:ALA:HB2	1.73	0.54
2:B:50:PHE:HB3	2:B:52:ALA:H	1.73	0.54
3:M:8:MET:SD	3:M:8:MET:N	2.81	0.54
1:F:50:GLU:O	1:F:111:SER:HB3	2.08	0.54
2:J:261:ASP:OD1	2:J:262:ASN:N	2.37	0.54
1:F:208:VAL:HG13	1:F:209:GLU:HG2	1.90	0.53
2:J:50:PHE:CZ	2:J:101:ILE:HD11	2.43	0.53
4:O:210:PRO:HA	4:O:243:ARG:HE	1.73	0.53
1:F:60:VAL:HG11	1:F:86:PRO:HG2	1.91	0.53
3:L:9:CYS:N	3:L:18:CYS:SG	2.80	0.53
2:I:407:VAL:O	2:I:410:THR:N	2.42	0.53
2:I:85:VAL:HG13	2:I:91:CYS:HB2	1.91	0.53
2:K:262:ASN:O	2:K:263:ILE:HG22	2.07	0.53
2:I:54:ILE:HG22	2:I:67:ILE:HD12	1.91	0.53
1:F:230:HIS:CD2	1:F:232:PRO:HG3	2.43	0.53
2:K:263:ILE:HG13	2:K:264:THR:N	2.23	0.53
1:A:230:HIS:CD2	1:A:232:PRO:HG3	2.44	0.53
2:K:169:MET:HB3	2:K:235:TRP:HB3	1.91	0.53
2:K:274:THR:HB	2:K:285:HIS:HB2	1.91	0.53
2:B:67:ILE:HD13	2:B:115:ILE:HD13	1.90	0.52
3:C:8:MET:N	3:C:8:MET:SD	2.82	0.52
2:B:195:LYS:HB3	2:B:229:VAL:HG13	1.91	0.52
1:H:21:ARG:HG3	1:H:22:PRO:HD2	1.91	0.52
1:H:258:GLY:HA3	2:K:299:LEU:HB2	1.91	0.52
1:A:40:PRO:HA	1:A:127:ALA:HA	1.91	0.52
4:P:138:ASP:OD2	4:Q:206:ARG:NH2	2.42	0.52
2:B:401:LEU:HB2	4:D:256:VAL:HG21	1.92	0.52
1:A:435:GLY:HA2	1:A:438:ARG:HD2	1.92	0.52
4:D:185:THR:HB	4:D:229:ARG:HD2	1.91	0.52
1:F:40:PRO:HA	1:F:127:ALA:HA	1.90	0.52
1:G:320:TYR:OH	1:G:347:LYS:N	2.39	0.52
2:B:288:PRO:HG3	2:B:310:VAL:HG12	1.92	0.52
2:I:188:VAL:H	2:I:217:ILE:HG22	1.75	0.52
2:J:397:THR:HA	4:P:161:LYS:NZ	2.25	0.52
2:I:54:ILE:HA	2:I:67:ILE:HB	1.92	0.51
4:P:210:PRO:HA	4:P:243:ARG:HE	1.75	0.51
1:A:93:TYR:HB3	2:B:176:PRO:HG3	1.91	0.51
2:J:398:PRO:HB2	4:P:255:MET:HE1	1.91	0.51
4:D:108:ARG:HH21	4:D:226:ASN:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:54:ILE:HG22	2:K:67:ILE:HB	1.92	0.51
4:P:195:TRP:CD1	4:P:196:HIS:H	2.28	0.51
2:I:165:GLU:HB3	2:I:256:ILE:HG12	1.92	0.51
2:J:166:GLU:OE1	3:M:49:TYR:OH	2.28	0.51
2:J:392:ARG:NH1	2:J:415:CYS:O	2.37	0.51
2:I:180:LEU:HD22	2:I:191:THR:HB	1.93	0.51
2:J:358:TYR:O	2:J:366:THR:OG1	2.23	0.51
2:K:361:LEU:HB3	2:K:362:TYR:CD1	2.45	0.51
1:H:51:TYR:HB3	1:H:203:ILE:HD13	1.92	0.51
1:H:437:ARG:HH11	2:J:408:PRO:HB3	1.76	0.51
3:N:8:MET:SD	3:N:8:MET:N	2.84	0.51
3:L:8:MET:O	3:L:45:ARG:NH2	2.44	0.50
4:D:186:HIS:O	4:D:188:LYS:NZ	2.38	0.50
4:O:143:PRO:HB2	4:O:146:VAL:HG12	1.93	0.50
4:D:225:ASP:N	4:D:229:ARG:O	2.42	0.50
2:J:6:PHE:CE1	3:M:53:GLN:HA	2.46	0.50
2:K:180:LEU:HD22	2:K:191:THR:HB	1.93	0.50
3:L:50:ASP:OD1	3:L:51:LEU:N	2.44	0.50
1:A:316:LEU:HB3	1:A:354:LEU:HB2	1.92	0.50
2:K:14:PRO:HB3	2:K:52:ALA:HA	1.94	0.50
2:J:50:PHE:HB3	2:J:52:ALA:H	1.77	0.50
2:K:196:LYS:HD2	2:K:231:ASP:HB2	1.94	0.50
5:S:110:MET:SD	5:S:111:ARG:N	2.85	0.50
2:I:139:GLU:OE1	2:I:290:HIS:NE2	2.45	0.50
2:K:34:ILE:HD11	2:K:113:VAL:HG22	1.93	0.50
5:E:117:GLU:HG2	5:E:127:CYS:HB3	1.94	0.50
1:G:33:VAL:HA	1:G:133:VAL:HG12	1.94	0.49
2:I:69:TYR:OH	2:I:117:ASP:OD1	2.23	0.49
2:K:32:VAL:HG12	2:K:32:VAL:O	2.12	0.49
2:J:188:VAL:HG22	2:J:217:ILE:H	1.77	0.49
2:J:308:GLU:OE1	2:J:316:ARG:NH1	2.45	0.49
1:A:299:LEU:HD12	1:A:320:TYR:HB3	1.93	0.49
1:A:330:VAL:HG12	1:A:339:LEU:HD13	1.93	0.49
4:D:116:GLU:OE1	4:D:196:HIS:ND1	2.45	0.49
2:B:188:VAL:HG22	2:B:217:ILE:HG22	1.94	0.49
2:I:288:PRO:HG3	2:I:310:VAL:HG12	1.94	0.49
1:F:31:MET:HG2	1:F:135:VAL:HG22	1.94	0.49
2:I:83:LEU:HD21	2:I:101:ILE:HD12	1.95	0.49
2:K:50:PHE:CZ	2:K:101:ILE:HD11	2.48	0.49
2:J:253:LYS:HG2	3:M:48:TYR:CE2	2.47	0.49
5:E:110:MET:O	5:E:111:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:118:ILE:HD11	5:S:128:ILE:HD11	1.95	0.49
2:I:14:PRO:HB3	2:I:52:ALA:HA	1.95	0.49
2:K:308:GLU:OE1	2:K:316:ARG:NH1	2.45	0.49
1:G:225:SER:H	1:G:230:HIS:CE1	2.32	0.48
2:K:378:LEU:HA	2:K:381:ILE:HG22	1.96	0.48
4:D:210:PRO:HA	4:D:243:ARG:HE	1.78	0.48
2:J:183:GLN:NE2	2:J:187:ASN:O	2.46	0.48
4:O:209:ILE:HB	4:O:244:THR:HB	1.95	0.48
4:D:219:SER:OG	4:D:267:TRP:O	2.26	0.48
1:H:225:SER:H	1:H:230:HIS:CE1	2.31	0.48
2:K:290:HIS:O	2:K:292:THR:HG23	2.14	0.48
3:M:21:PRO:HG2	3:M:24:VAL:HG23	1.95	0.48
4:P:210:PRO:HA	4:P:243:ARG:NE	2.28	0.48
4:Q:173:ILE:HD11	4:Q:178:ARG:HG2	1.95	0.48
1:F:341:GLU:N	1:F:341:GLU:OE1	2.47	0.48
1:G:249:THR:HA	2:J:305:TYR:OH	2.13	0.48
2:J:195:LYS:HB3	2:J:229:VAL:HG13	1.95	0.48
1:A:225:SER:H	1:A:230:HIS:CE1	2.32	0.48
4:D:136:VAL:HB	4:D:141:MET:HE3	1.95	0.48
2:I:358:TYR:O	2:I:366:THR:OG1	2.23	0.48
2:J:276:ILE:HD12	2:J:285:HIS:HE2	1.79	0.48
4:P:140:VAL:HG23	4:P:173:ILE:HG22	1.95	0.48
1:A:258:GLY:HA3	2:B:299:LEU:HB2	1.96	0.48
2:K:149:LYS:HG3	2:K:269:MET:SD	2.54	0.48
2:K:413:ILE:HG22	2:K:414:LEU:HD12	1.95	0.48
1:F:258:GLY:HA3	2:I:299:LEU:HB2	1.94	0.48
2:B:14:PRO:HB3	2:B:52:ALA:HA	1.96	0.47
2:K:145:PRO:HG3	2:K:268:PRO:HB3	1.95	0.47
2:K:192:VAL:HG21	2:K:213:SER:HA	1.96	0.47
4:O:195:TRP:CD1	4:O:196:HIS:H	2.31	0.47
1:H:299:LEU:HD12	1:H:320:TYR:HB3	1.94	0.47
2:J:67:ILE:HD11	2:J:115:ILE:HD13	1.95	0.47
1:G:406:ALA:HB2	2:J:354:ILE:HG21	1.95	0.47
1:H:21:ARG:NH1	1:H:284:ASP:OD1	2.35	0.47
2:J:138:ARG:CZ	2:J:293:LEU:HD23	2.45	0.47
1:A:82:THR:O	1:A:223:ARG:NH2	2.47	0.47
1:G:210:SER:OG	1:G:212:ASP:OD1	2.29	0.47
5:R:120:CYS:HB2	5:R:128:ILE:HG12	1.96	0.47
2:B:375:LEU:O	2:B:379:ILE:HG12	2.15	0.47
1:A:191:PRO:HB3	1:H:151:ASP:HA	1.97	0.47
1:F:242:TYR:O	1:F:246:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:402:MET:HA	1:F:407:LEU:HD12	1.97	0.47
2:J:183:GLN:HG2	2:J:221:LEU:HB3	1.96	0.47
6:W:1:NAG:O6	6:W:2:NAG:N2	2.47	0.47
2:B:200:ASN:HA	2:B:208:VAL:HG12	1.97	0.47
2:K:195:LYS:HB3	2:K:229:VAL:HG13	1.96	0.47
3:M:38:MET:HE2	3:M:38:MET:HB3	1.80	0.47
4:O:247:SER:HB2	4:O:261:PRO:HD2	1.96	0.47
3:C:37:ARG:N	3:C:37:ARG:HD2	2.30	0.46
2:I:47:LYS:NZ	2:I:256:ILE:HD12	2.30	0.46
5:S:110:MET:SD	5:S:111:ARG:HB2	2.55	0.46
1:H:40:PRO:HA	1:H:127:ALA:HA	1.96	0.46
2:K:212:ASN:O	2:K:212:ASN:ND2	2.45	0.46
1:A:241:LYS:HD3	1:A:241:LYS:HA	1.74	0.46
2:I:203:CYS:HB3	2:I:220:CYS:HB3	1.60	0.46
2:I:246:ASP:N	2:I:246:ASP:OD1	2.47	0.46
1:H:202:ASP:OD1	1:H:202:ASP:N	2.48	0.46
2:K:134:GLN:HA	2:K:134:GLN:OE1	2.15	0.46
5:T:111:ARG:NH1	5:T:127:CYS:SG	2.87	0.46
2:B:180:LEU:HD22	2:B:191:THR:HB	1.98	0.46
1:G:60:VAL:HG11	1:G:86:PRO:HG2	1.97	0.46
1:H:113:VAL:HG22	1:H:116:HIS:HB2	1.96	0.46
2:K:217:ILE:HG23	2:K:219:THR:H	1.81	0.46
1:H:115:ARG:HB3	1:H:115:ARG:NH1	2.30	0.46
2:K:56:ILE:HG21	2:K:68:ARG:HH21	1.81	0.46
1:F:426:LEU:HD23	1:F:426:LEU:HA	1.84	0.46
1:G:31:MET:HG2	1:G:135:VAL:HG22	1.97	0.46
1:H:144:VAL:HG21	1:H:156:ILE:HD11	1.97	0.46
4:O:108:ARG:NH2	4:O:226:ASN:OD1	2.49	0.46
2:K:392:ARG:HH21	2:K:416:CYS:HA	1.81	0.46
2:B:35:GLU:HB2	2:B:49:GLN:HG2	1.98	0.46
2:K:6:PHE:CE2	3:N:53:GLN:HA	2.51	0.45
1:A:51:TYR:HB3	1:A:203:ILE:HD13	1.97	0.45
2:B:69:TYR:OH	2:B:117:ASP:OD1	2.17	0.45
2:K:35:GLU:HB2	2:K:49:GLN:HG2	1.98	0.45
5:R:117:GLU:HG3	5:R:128:ILE:O	2.16	0.45
1:H:325:ASN:C	1:H:325:ASN:ND2	2.74	0.45
1:H:368:SER:HB3	1:H:373:ARG:HD3	1.98	0.45
2:K:201:CYS:HA	2:K:224:GLN:HG3	1.99	0.45
2:B:290:HIS:O	2:B:292:THR:HG23	2.16	0.45
2:I:204:GLY:C	2:I:206:GLY:H	2.24	0.45
2:J:54:ILE:HD12	2:J:96:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:209:ILE:HG22	4:P:212:GLY:H	1.81	0.45
5:S:128:ILE:HB	5:S:132:TRP:HE3	1.82	0.45
1:G:225:SER:H	1:G:230:HIS:HE1	1.64	0.45
2:K:246:ASP:CG	2:K:248:PRO:HD2	2.41	0.45
4:P:249:VAL:HG22	4:P:258:ARG:HG3	1.99	0.45
4:Q:216:PRO:HA	4:Q:267:TRP:HB3	1.98	0.45
1:A:73:LYS:HB2	1:A:76:TYR:HB2	1.98	0.45
1:G:109:ASP:OD1	1:G:110:ARG:N	2.50	0.45
2:I:195:LYS:HB3	2:I:229:VAL:HG13	1.99	0.45
2:J:177:ASP:HB3	2:J:180:LEU:HD22	1.98	0.45
5:R:117:GLU:CD	5:R:127:CYS:HB3	2.42	0.45
1:A:328:CYS:HB3	1:A:370:CYS:H	1.82	0.45
4:Q:124:LYS:HE3	4:Q:124:LYS:HB3	1.77	0.45
1:G:258:GLY:HA3	2:J:299:LEU:HB2	1.99	0.45
2:K:149:LYS:HB3	2:K:149:LYS:HE2	1.68	0.45
6:V:1:NAG:H61	6:V:2:NAG:H82	1.99	0.45
5:T:114:ARG:CG	5:T:115:ILE:H	2.25	0.44
1:H:225:SER:H	1:H:230:HIS:HE1	1.65	0.44
2:I:12:THR:HA	2:I:235:TRP:O	2.17	0.44
2:I:72:GLY:O	2:I:73:HIS:ND1	2.50	0.44
5:R:118:ILE:HG13	5:R:120:CYS:H	1.82	0.44
2:I:138:ARG:CZ	2:I:293:LEU:HD23	2.47	0.44
2:J:197:VAL:HB	2:J:227:VAL:HG13	1.99	0.44
1:G:426:LEU:HD23	1:G:426:LEU:HA	1.84	0.44
2:I:34:ILE:HD11	2:I:113:VAL:HG22	1.98	0.44
1:A:262:LYS:HD2	1:A:269:MET:SD	2.58	0.44
2:B:183:GLN:HB2	2:B:222:ILE:HG23	1.98	0.44
2:I:290:HIS:O	2:I:292:THR:HG23	2.18	0.44
2:J:201:CYS:HA	2:J:224:GLN:HG3	2.00	0.44
2:K:63:ASP:OD1	2:K:64:TYR:N	2.51	0.44
2:B:400:ALA:O	4:D:139:LYS:HE3	2.17	0.44
1:H:146:VAL:HG11	1:H:163:PHE:CD1	2.52	0.44
4:Q:124:LYS:HA	4:Q:129:VAL:HA	1.99	0.44
1:A:96:CYS:HB3	1:A:99:GLU:HG2	1.98	0.44
4:O:210:PRO:HA	4:O:243:ARG:NE	2.33	0.44
2:B:100:PHE:HZ	2:B:167:ILE:HD11	1.83	0.44
4:P:109:GLU:O	4:P:113:MET:HG2	2.18	0.44
1:H:437:ARG:HA	1:H:437:ARG:HD3	1.69	0.44
2:K:139:GLU:HB3	2:K:290:HIS:CD2	2.53	0.44
2:B:67:ILE:CD1	2:B:115:ILE:HD13	2.48	0.43
1:H:245:LYS:HB2	1:H:245:LYS:HE3	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:208:VAL:HG21	6:d:1:NAG:H81	1.99	0.43
1:G:346:VAL:HG11	1:G:369:LEU:HD21	2.00	0.43
2:I:190:ILE:HG21	2:I:197:VAL:HG11	2.01	0.43
2:K:47:LYS:HA	2:K:101:ILE:O	2.18	0.43
2:K:167:ILE:HD11	2:K:256:ILE:HG22	2.00	0.43
2:K:343:THR:OG1	2:K:344:GLU:N	2.48	0.43
1:G:167:SER:HB3	1:G:275:ASN:H	1.83	0.43
2:K:183:GLN:HB2	2:K:222:ILE:HD11	2.00	0.43
3:L:24:VAL:HA	3:L:25:PRO:HA	1.85	0.43
2:B:161:ALA:O	2:B:163:THR:HG23	2.19	0.43
2:B:165:GLU:HB2	2:B:256:ILE:HG12	2.01	0.43
2:I:201:CYS:HA	2:I:224:GLN:O	2.19	0.43
2:J:181:LEU:HD23	2:J:181:LEU:HA	1.86	0.43
2:K:174:ASP:HB2	2:K:228:SER:HB3	2.01	0.43
2:K:212:ASN:HD22	2:K:212:ASN:C	2.26	0.43
2:J:399:TYR:HE2	2:J:407:VAL:HG23	1.83	0.43
1:G:311:ASP:OD1	1:G:311:ASP:N	2.50	0.43
1:H:228:MET:HE2	1:H:230:HIS:CE1	2.54	0.43
1:H:262:LYS:HD2	1:H:269:MET:SD	2.58	0.43
1:H:325:ASN:ND2	1:H:325:ASN:O	2.43	0.43
1:H:351:LYS:HB2	1:H:351:LYS:HE2	1.84	0.43
4:O:123:VAL:HG22	4:O:150:ILE:HG12	2.00	0.43
2:I:417:ALA:HB3	2:I:418:PRO:HD3	2.01	0.43
2:K:402:THR:O	4:Q:139:LYS:NZ	2.41	0.43
1:A:301:CYS:SG	1:A:316:LEU:HD11	2.58	0.43
4:D:122:GLU:HG2	4:D:132:TYR:HE1	1.84	0.43
1:G:398:VAL:HG21	2:J:362:TYR:OH	2.19	0.43
2:I:11:ALA:O	2:I:235:TRP:N	2.51	0.43
2:I:402:THR:HG23	4:O:256:VAL:HG23	2.00	0.43
2:J:308:GLU:CD	2:J:316:ARG:HH12	2.26	0.43
3:N:33:GLU:OE1	3:N:37:ARG:NH2	2.32	0.43
2:I:177:ASP:OD1	2:I:178:ARG:N	2.52	0.43
2:I:197:VAL:HG21	2:I:227:VAL:HG13	2.01	0.43
2:J:255:HIS:HE1	3:M:49:TYR:CE2	2.36	0.43
1:A:333:HIS:HB2	1:A:366:VAL:HG13	2.01	0.42
2:B:402:THR:HG23	4:D:256:VAL:HG23	2.01	0.42
2:K:271:ARG:O	2:K:329:TRP:NE1	2.48	0.42
4:P:209:ILE:HD11	4:P:246:LEU:HD11	2.01	0.42
4:Q:225:ASP:OD2	4:Q:229:ARG:NH2	2.50	0.42
1:F:308:HIS:HB2	1:F:359:ALA:HA	2.01	0.42
1:G:259:CYS:HB3	1:G:271:CYS:CA	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:202:THR:HB	2:I:224:GLN:HG2	2.01	0.42
2:J:13:ARG:HB3	2:J:234:LYS:HD3	2.02	0.42
2:K:203:CYS:SG	2:K:224:GLN:HG2	2.59	0.42
2:J:180:LEU:HB2	2:J:191:THR:HB	2.00	0.42
2:K:87:THR:HG23	2:K:110:PHE:O	2.19	0.42
4:D:209:ILE:HD11	4:D:246:LEU:HD11	2.02	0.42
2:J:67:ILE:CD1	2:J:115:ILE:HD13	2.49	0.42
2:J:202:THR:H	2:J:224:GLN:CD	2.28	0.42
2:J:369:ALA:O	2:J:373:MET:HG3	2.20	0.42
4:O:252:ASN:OD1	4:O:253:LYS:N	2.46	0.42
2:B:205:THR:OG1	2:B:206:GLY:N	2.53	0.42
2:J:316:ARG:HA	2:J:316:ARG:HD3	1.85	0.42
2:K:298:THR:HA	2:K:325:MET:HB3	2.01	0.42
2:K:299:LEU:HD12	2:K:299:LEU:O	2.20	0.42
5:E:118:ILE:HD11	5:E:128:ILE:HD11	2.01	0.42
1:F:203:ILE:O	1:F:203:ILE:HG13	2.19	0.42
1:H:426:LEU:HD23	1:H:426:LEU:HA	1.87	0.42
2:J:47:LYS:HA	2:J:101:ILE:O	2.20	0.42
2:K:231:ASP:O	2:K:233:LYS:NZ	2.50	0.42
1:A:252:ASN:ND2	1:A:261:ILE:HB	2.35	0.42
2:B:143:ILE:HD11	2:I:128:GLN:N	2.34	0.42
2:B:165:GLU:CB	2:B:256:ILE:HG12	2.49	0.42
2:I:79:VAL:O	2:I:115:ILE:HD11	2.19	0.42
2:J:62:HIS:CE1	2:J:97:MET:HE1	2.54	0.42
2:J:139:GLU:HG3	2:J:331:ASN:OD1	2.20	0.42
2:J:237:PHE:HD2	2:J:239:SER:HB2	1.83	0.42
3:C:11:LEU:O	3:C:13:ASN:N	2.52	0.42
2:I:171:MET:SD	3:L:37:ARG:NH1	2.90	0.42
2:J:253:LYS:HE2	2:J:253:LYS:HB3	1.88	0.42
2:K:343:THR:HB	2:K:361:LEU:HD12	2.00	0.42
2:K:180:LEU:HB2	2:K:227:VAL:HG21	2.02	0.42
2:K:213:SER:OG	2:K:214:ASP:N	2.52	0.42
2:K:318:ILE:HD12	2:K:325:MET:CE	2.50	0.42
1:F:351:LYS:HB3	1:F:351:LYS:HE3	1.71	0.41
2:J:34:ILE:HD11	2:J:113:VAL:HG22	2.02	0.41
2:J:318:ILE:HD12	2:J:325:MET:HE1	2.01	0.41
2:K:208:VAL:HG11	6:f:1:NAG:O7	2.20	0.41
1:F:421:ALA:O	1:F:425:ILE:HG12	2.20	0.41
1:H:50:GLU:O	1:H:111:SER:HB3	2.20	0.41
2:K:47:LYS:NZ	2:K:256:ILE:HD12	2.34	0.41
2:B:223:GLU:CD	2:B:224:GLN:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:LYS:HE3	4:D:147:LYS:HB3	1.90	0.41
1:H:406:ALA:HB2	2:K:354:ILE:HG21	2.01	0.41
2:J:149:LYS:HB3	2:J:149:LYS:HE2	1.67	0.41
6:Y:1:NAG:H4	6:Y:2:NAG:H2	1.82	0.41
1:A:50:GLU:O	1:A:111:SER:HB3	2.20	0.41
1:G:253:THR:HG23	2:J:305:TYR:HE1	1.86	0.41
1:H:410:VAL:HG22	2:K:373:MET:HE1	2.03	0.41
2:J:183:GLN:CD	2:J:221:LEU:HD22	2.45	0.41
2:K:388:LEU:HD23	2:K:388:LEU:HA	1.88	0.41
2:B:138:ARG:CZ	2:B:293:LEU:HD23	2.51	0.41
4:D:210:PRO:HA	4:D:243:ARG:NE	2.35	0.41
1:F:88:MET:HE2	1:F:88:MET:HB3	1.91	0.41
1:G:74:PRO:HG2	1:G:108:VAL:O	2.20	0.41
1:G:328:CYS:HB3	1:G:370:CYS:H	1.85	0.41
2:J:58:LYS:HD3	2:J:75:ILE:O	2.20	0.41
2:K:316:ARG:HD3	2:K:316:ARG:HA	1.79	0.41
4:O:124:LYS:HE3	4:O:151:ASP:HB2	2.03	0.41
3:C:53:GLN:O	3:C:57:THR:OG1	2.36	0.41
1:G:51:TYR:CE2	1:G:238:SER:HA	2.55	0.41
1:G:384:LYS:HD3	1:G:384:LYS:HA	1.91	0.41
2:J:407:VAL:O	2:J:410:THR:N	2.53	0.41
1:G:136:MET:HA	1:G:140:VAL:O	2.21	0.41
1:H:82:THR:O	1:H:223:ARG:NH2	2.53	0.41
4:P:225:ASP:N	4:P:229:ARG:O	2.48	0.41
2:B:396:LEU:HD23	2:B:396:LEU:HA	1.90	0.41
1:F:252:ASN:ND2	1:F:261:ILE:HB	2.36	0.41
2:I:237:PHE:HD2	2:I:239:SER:HB2	1.85	0.41
2:J:288:PRO:HG3	2:J:310:VAL:HG12	2.03	0.41
1:F:141:ASN:O	1:F:142:GLN:CB	2.68	0.41
2:J:161:ALA:O	2:J:163:THR:HG23	2.21	0.41
4:Q:250:THR:OG1	4:Q:251:TRP:N	2.53	0.41
2:B:141:PHE:CE1	2:B:267:VAL:HG12	2.56	0.40
2:B:343:THR:OG1	2:B:360:GLY:HA3	2.21	0.40
2:J:231:ASP:O	2:J:233:LYS:N	2.51	0.40
1:A:57:SER:O	2:B:244:ARG:NH1	2.54	0.40
2:I:161:ALA:O	2:I:163:THR:HG23	2.21	0.40
2:I:195:LYS:HD2	2:I:229:VAL:HG21	2.03	0.40
2:K:50:PHE:CE1	2:K:101:ILE:HD11	2.57	0.40
3:L:21:PRO:HG2	3:L:24:VAL:HG23	2.03	0.40
2:J:318:ILE:HD12	2:J:325:MET:CE	2.51	0.40
2:J:343:THR:OG1	2:J:360:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:12:THR:HA	2:K:235:TRP:O	2.21	0.40
2:K:187:ASN:HB3	2:K:218:ASN:HA	2.02	0.40
4:P:158:LEU:HD11	4:P:174:PRO:HD3	2.03	0.40
1:A:144:VAL:HG21	1:A:156:ILE:HD11	2.02	0.40
1:F:144:VAL:HG21	1:F:156:ILE:HD11	2.04	0.40
2:I:177:ASP:O	2:I:227:VAL:HB	2.21	0.40
2:K:182:SER:HB2	2:K:189:LYS:HB2	2.03	0.40
2:I:143:ILE:HG12	2:J:128:GLN:HB2	2.04	0.40
2:J:166:GLU:OE2	2:J:253:LYS:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/438 (100%)	415 (95%)	21 (5%)	0	100	100
1	F	436/438 (100%)	412 (94%)	23 (5%)	1 (0%)	43	74
1	G	436/438 (100%)	408 (94%)	28 (6%)	0	100	100
1	H	436/438 (100%)	412 (94%)	24 (6%)	0	100	100
2	B	416/418 (100%)	378 (91%)	38 (9%)	0	100	100
2	I	416/418 (100%)	369 (89%)	45 (11%)	2 (0%)	24	57
2	J	416/418 (100%)	374 (90%)	41 (10%)	1 (0%)	43	74
2	K	416/418 (100%)	370 (89%)	44 (11%)	2 (0%)	24	57
3	C	50/52 (96%)	49 (98%)	0	1 (2%)	6	32
3	L	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
3	M	50/52 (96%)	49 (98%)	0	1 (2%)	6	32
3	N	50/52 (96%)	49 (98%)	0	1 (2%)	6	32
4	D	159/161 (99%)	156 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
4	P	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
4	Q	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	E	42/44 (96%)	36 (86%)	6 (14%)	0	100	100
5	R	42/44 (96%)	36 (86%)	6 (14%)	0	100	100
5	S	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
5	T	42/44 (96%)	35 (83%)	7 (17%)	0	100	100
All	All	4412/4452 (99%)	4100 (93%)	303 (7%)	9 (0%)	44	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	142	GLN
2	J	263	ILE
2	K	263	ILE
3	C	12	ALA
3	M	12	ALA
2	I	231	ASP
3	N	12	ALA
2	K	249	ALA
2	I	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	A	372/372 (100%)	372 (100%)	0	100	100
1	F	372/372 (100%)	372 (100%)	0	100	100
1	G	372/372 (100%)	372 (100%)	0	100	100
1	H	372/372 (100%)	371 (100%)	1 (0%)	86	83
2	B	356/356 (100%)	356 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	356/356 (100%)	355 (100%)	1 (0%)	86	83
2	J	356/356 (100%)	356 (100%)	0	100	100
2	K	356/356 (100%)	355 (100%)	1 (0%)	86	83
3	C	45/45 (100%)	45 (100%)	0	100	100
3	L	45/45 (100%)	45 (100%)	0	100	100
3	M	45/45 (100%)	45 (100%)	0	100	100
3	N	45/45 (100%)	45 (100%)	0	100	100
4	D	132/132 (100%)	132 (100%)	0	100	100
4	O	132/132 (100%)	132 (100%)	0	100	100
4	P	132/132 (100%)	132 (100%)	0	100	100
4	Q	132/132 (100%)	132 (100%)	0	100	100
5	E	38/38 (100%)	38 (100%)	0	100	100
5	R	38/38 (100%)	38 (100%)	0	100	100
5	S	38/38 (100%)	38 (100%)	0	100	100
5	T	38/38 (100%)	38 (100%)	0	100	100
All	All	3772/3772 (100%)	3769 (100%)	3 (0%)	87	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	325	ASN
2	I	157	GLN
2	K	212	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	43	ASN
2	B	62	HIS
2	B	184	GLN
3	C	13	ASN
3	C	30	ASN
4	D	194	ASN
1	F	43	ASN
1	F	331	HIS

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Mol	Chain	Res	Type
1	F	394	HIS
1	G	196	GLN
1	G	230	HIS
1	G	235	GLN
1	H	43	ASN
1	H	196	GLN
1	H	230	HIS
1	H	325	ASN
1	H	394	HIS
2	I	130	HIS
2	I	131	HIS
2	I	304	GLN
2	I	306	HIS
2	I	340	GLN
2	I	421	HIS
2	J	61	ASN
2	J	255	HIS
2	J	277	HIS
2	K	26	HIS
2	K	62	HIS
2	K	120	ASN
2	K	130	HIS
2	K	131	HIS
2	K	348	HIS
2	K	352	HIS
2	K	421	HIS
3	M	13	ASN
3	N	42	ASN
4	P	192	HIS
4	P	194	ASN
4	Q	186	HIS

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 ⓘ

36 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	U	1	1,6	14,14,15	0.20	0	17,19,21	0.67	1 (5%)
6	NAG	U	2	6	14,14,15	0.21	0	17,19,21	0.43	0
6	BMA	U	3	6	11,11,12	0.58	0	15,15,17	0.69	0
6	NAG	V	1	2,6	14,14,15	0.32	0	17,19,21	0.57	0
6	NAG	V	2	6	14,14,15	0.45	0	17,19,21	1.34	2 (11%)
6	BMA	V	3	6	11,11,12	0.54	0	15,15,17	0.84	0
6	NAG	W	1	2,6	14,14,15	0.23	0	17,19,21	0.40	0
6	NAG	W	2	6	14,14,15	0.23	0	17,19,21	0.48	0
6	BMA	W	3	6	11,11,12	0.54	0	15,15,17	0.74	0
6	NAG	X	1	1,6	14,14,15	0.22	0	17,19,21	0.62	1 (5%)
6	NAG	X	2	6	14,14,15	0.23	0	17,19,21	0.40	0
6	BMA	X	3	6	11,11,12	0.54	0	15,15,17	0.70	0
6	NAG	Y	1	1,6	14,14,15	0.28	0	17,19,21	0.58	0
6	NAG	Y	2	6	14,14,15	0.77	1 (7%)	17,19,21	1.36	2 (11%)
6	BMA	Y	3	6	11,11,12	0.65	0	15,15,17	0.81	0
6	NAG	Z	1	1,6	14,14,15	0.19	0	17,19,21	0.53	0
6	NAG	Z	2	6	14,14,15	0.31	0	17,19,21	0.45	0
6	BMA	Z	3	6	11,11,12	0.54	0	15,15,17	0.67	0
6	NAG	a	1	2,6	14,14,15	0.39	0	17,19,21	1.35	2 (11%)
6	NAG	a	2	6	14,14,15	0.24	0	17,19,21	0.44	0
6	BMA	a	3	6	11,11,12	0.52	0	15,15,17	0.67	0
6	NAG	b	1	2,6	14,14,15	0.18	0	17,19,21	0.44	0
6	NAG	b	2	6	14,14,15	0.20	0	17,19,21	0.43	0
6	BMA	b	3	6	11,11,12	0.58	0	15,15,17	0.69	0
6	NAG	c	1	2,6	14,14,15	0.48	0	17,19,21	0.66	0
6	NAG	c	2	6	14,14,15	0.22	0	17,19,21	0.59	0
6	BMA	c	3	6	11,11,12	0.55	0	15,15,17	0.93	1 (6%)
6	NAG	d	1	2,6	14,14,15	0.18	0	17,19,21	0.59	0
6	NAG	d	2	6	14,14,15	0.21	0	17,19,21	0.46	0
6	BMA	d	3	6	11,11,12	0.63	0	15,15,17	0.68	0
6	NAG	e	1	2,6	14,14,15	0.23	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	e	2	6	14,14,15	0.19	0	17,19,21	0.45	0
6	BMA	e	3	6	11,11,12	0.53	0	15,15,17	0.86	0
6	NAG	f	1	2,6	14,14,15	0.17	0	17,19,21	0.46	0
6	NAG	f	2	6	14,14,15	0.18	0	17,19,21	0.46	0
6	BMA	f	3	6	11,11,12	0.56	0	15,15,17	0.79	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	U	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	1/6/23/26	0/1/1/1
6	BMA	U	3	6	-	1/2/19/22	0/1/1/1
6	NAG	V	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	6/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
6	NAG	W	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	0/6/23/26	0/1/1/1
6	BMA	W	3	6	-	0/2/19/22	0/1/1/1
6	NAG	X	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	0/6/23/26	0/1/1/1
6	BMA	X	3	6	-	1/2/19/22	0/1/1/1
6	NAG	Y	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	4/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	1/2/19/22	0/1/1/1
6	NAG	Z	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	1/2/19/22	0/1/1/1
6	NAG	a	1	2,6	-	6/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	BMA	a	3	6	-	0/2/19/22	0/1/1/1
6	NAG	b	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	b	2	6	-	4/6/23/26	0/1/1/1
6	BMA	b	3	6	-	1/2/19/22	0/1/1/1
6	NAG	c	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	c	2	6	-	0/6/23/26	0/1/1/1
6	BMA	c	3	6	-	1/2/19/22	0/1/1/1
6	NAG	d	1	2,6	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	d	2	6	-	1/6/23/26	0/1/1/1
6	BMA	d	3	6	-	0/2/19/22	0/1/1/1
6	NAG	e	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	e	2	6	-	1/6/23/26	0/1/1/1
6	BMA	e	3	6	-	0/2/19/22	0/1/1/1
6	NAG	f	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	f	2	6	-	3/6/23/26	0/1/1/1
6	BMA	f	3	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	2	NAG	C1-C2	2.68	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	2	NAG	C2-N2-C7	4.58	129.04	122.90
6	a	1	NAG	C2-N2-C7	4.53	128.98	122.90
6	Y	2	NAG	C2-N2-C7	4.50	128.94	122.90
6	V	2	NAG	C1-C2-N2	2.22	113.93	110.43
6	a	1	NAG	C1-C2-N2	2.22	113.93	110.43
6	Y	2	NAG	C1-C2-N2	2.19	113.89	110.43
6	c	3	BMA	C1-O5-C5	2.09	114.98	112.19
6	U	1	NAG	C1-O5-C5	2.08	114.97	112.19
6	X	1	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	a	2	NAG	O5-C5-C6-O6
6	d	1	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	b	2	NAG	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	V	3	BMA	O5-C5-C6-O6
6	d	1	NAG	C4-C5-C6-O6
6	b	2	NAG	C4-C5-C6-O6
6	Y	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
6	c	1	NAG	C4-C5-C6-O6
6	a	1	NAG	C4-C5-C6-O6
6	Y	1	NAG	C4-C5-C6-O6
6	f	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
6	V	2	NAG	C8-C7-N2-C2
6	V	2	NAG	O7-C7-N2-C2
6	Y	2	NAG	C8-C7-N2-C2
6	Y	2	NAG	O7-C7-N2-C2
6	Z	2	NAG	C8-C7-N2-C2
6	Z	2	NAG	O7-C7-N2-C2
6	a	1	NAG	C8-C7-N2-C2
6	a	1	NAG	O7-C7-N2-C2
6	b	2	NAG	C8-C7-N2-C2
6	b	2	NAG	O7-C7-N2-C2
6	e	1	NAG	C8-C7-N2-C2
6	e	1	NAG	O7-C7-N2-C2
6	f	1	NAG	C8-C7-N2-C2
6	f	1	NAG	O7-C7-N2-C2
6	f	2	NAG	C8-C7-N2-C2
6	f	2	NAG	O7-C7-N2-C2
6	V	2	NAG	O5-C5-C6-O6
6	X	3	BMA	O5-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
6	b	3	BMA	O5-C5-C6-O6
6	c	3	BMA	O5-C5-C6-O6
6	Z	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	d	2	NAG	O5-C5-C6-O6
6	W	1	NAG	O5-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
6	Y	3	BMA	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	c	1	NAG	C3-C2-N2-C7

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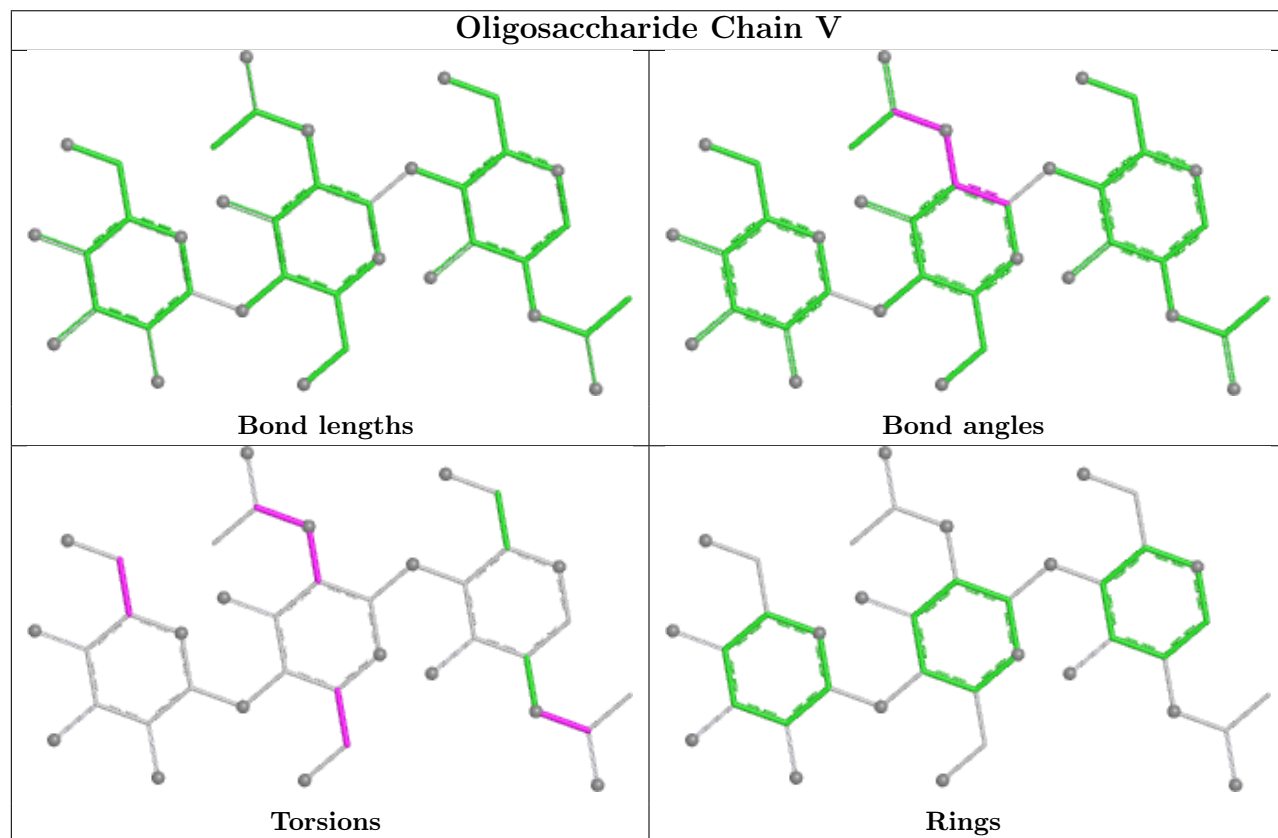
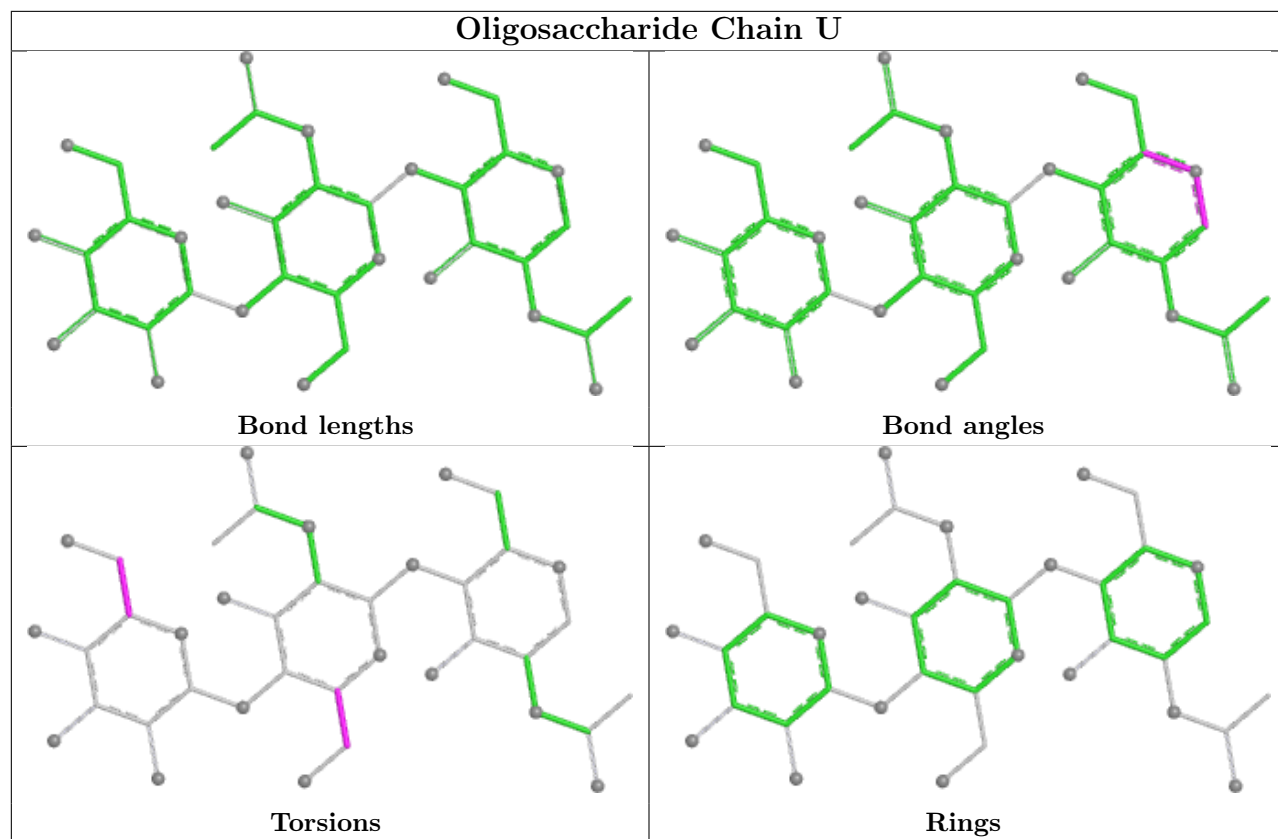
Mol	Chain	Res	Type	Atoms
6	d	1	NAG	C3-C2-N2-C7
6	U	2	NAG	O5-C5-C6-O6
6	V	2	NAG	C1-C2-N2-C7
6	W	1	NAG	C1-C2-N2-C7
6	Y	2	NAG	C1-C2-N2-C7
6	a	1	NAG	C1-C2-N2-C7
6	c	1	NAG	C1-C2-N2-C7
6	d	1	NAG	C1-C2-N2-C7
6	e	1	NAG	C4-C5-C6-O6
6	V	3	BMA	C4-C5-C6-O6
6	V	2	NAG	C3-C2-N2-C7
6	Y	2	NAG	C3-C2-N2-C7
6	a	1	NAG	C3-C2-N2-C7

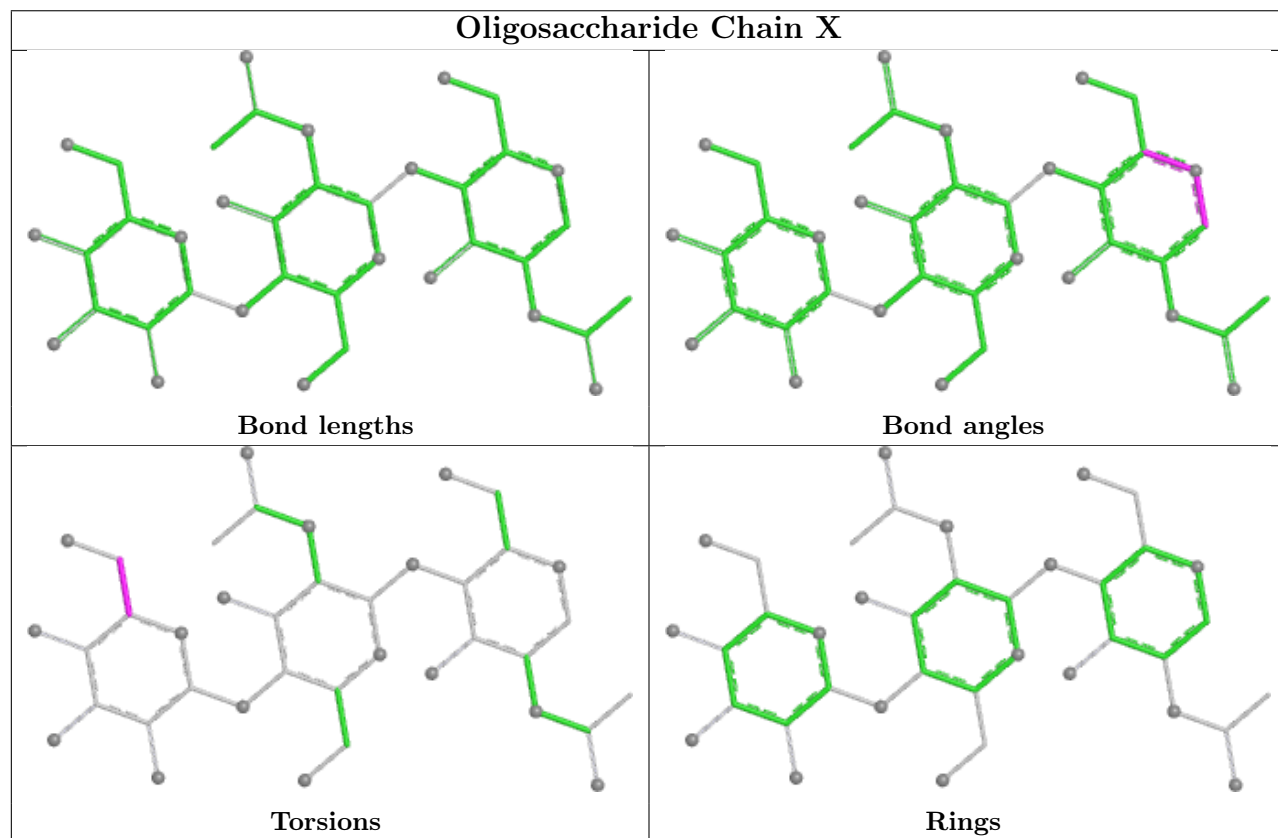
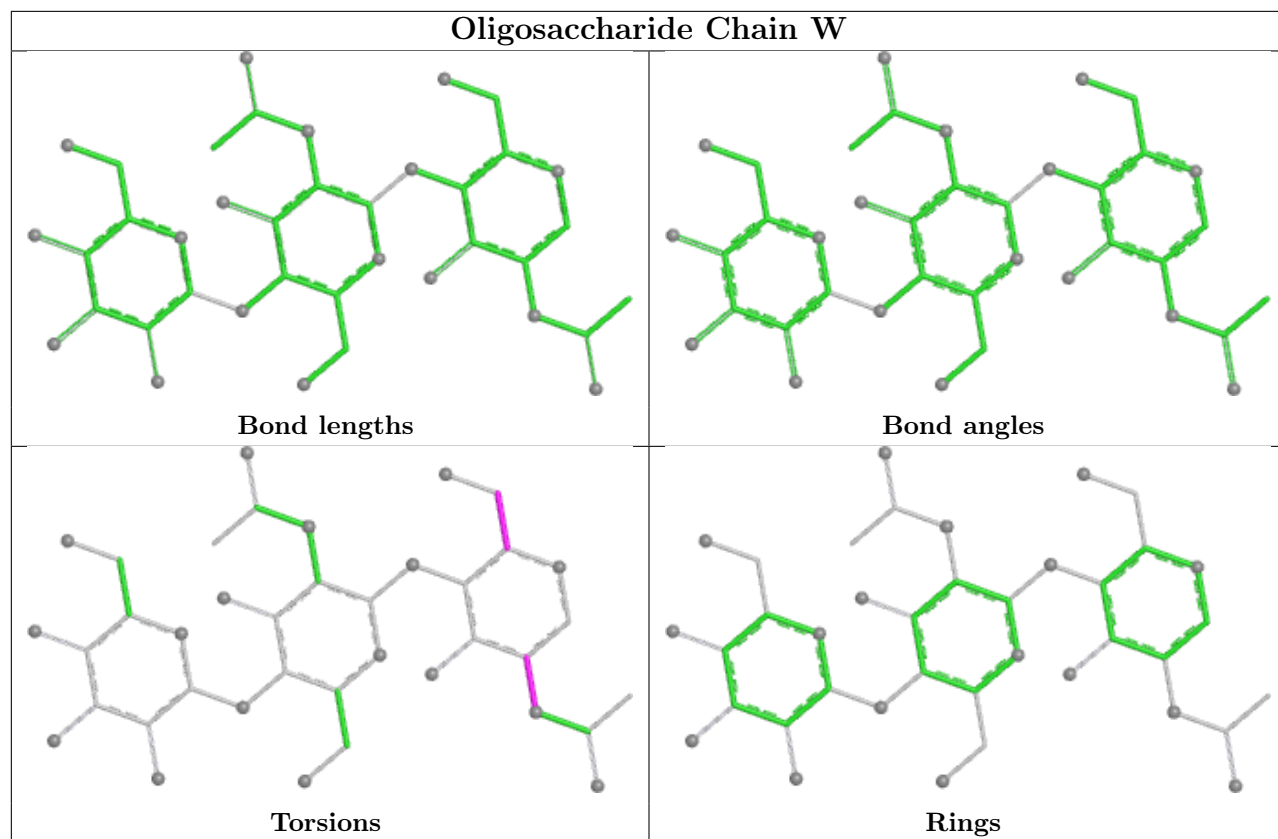
There are no ring outliers.

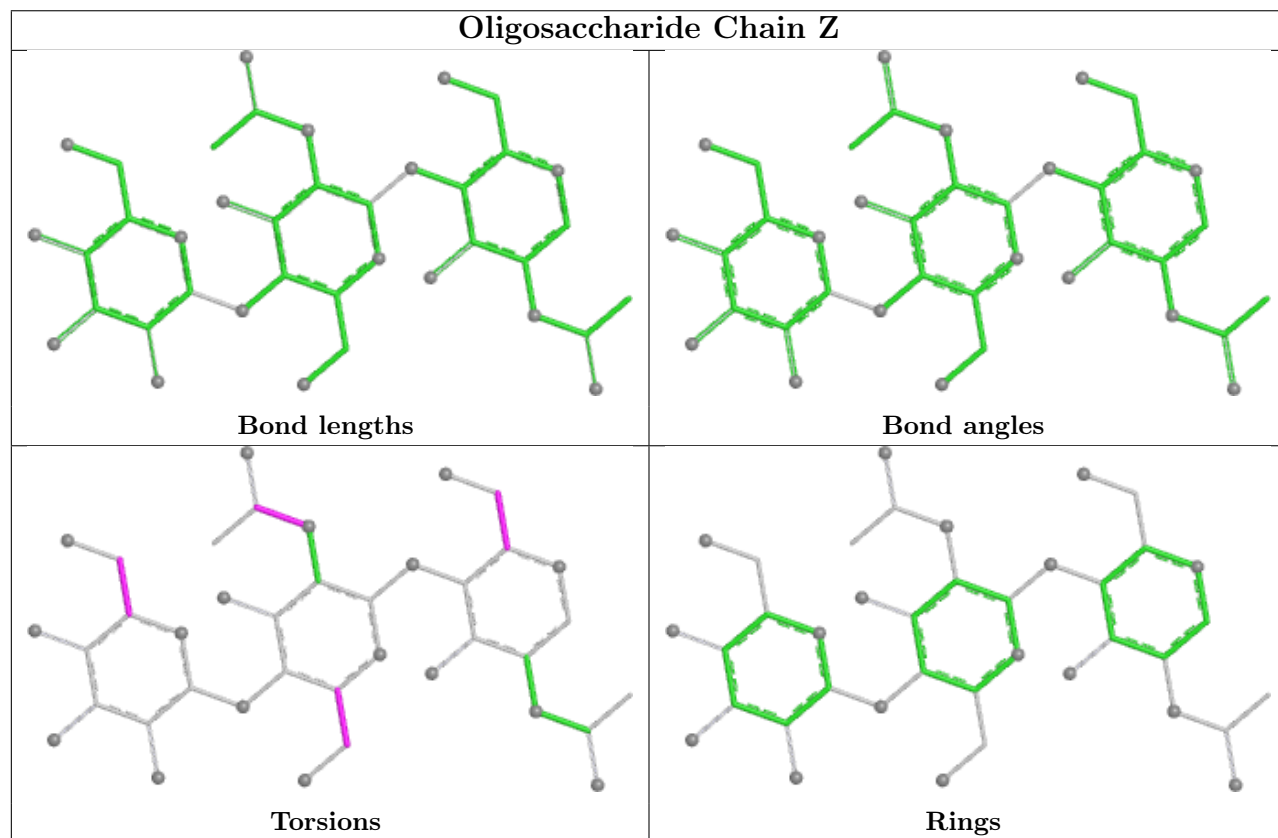
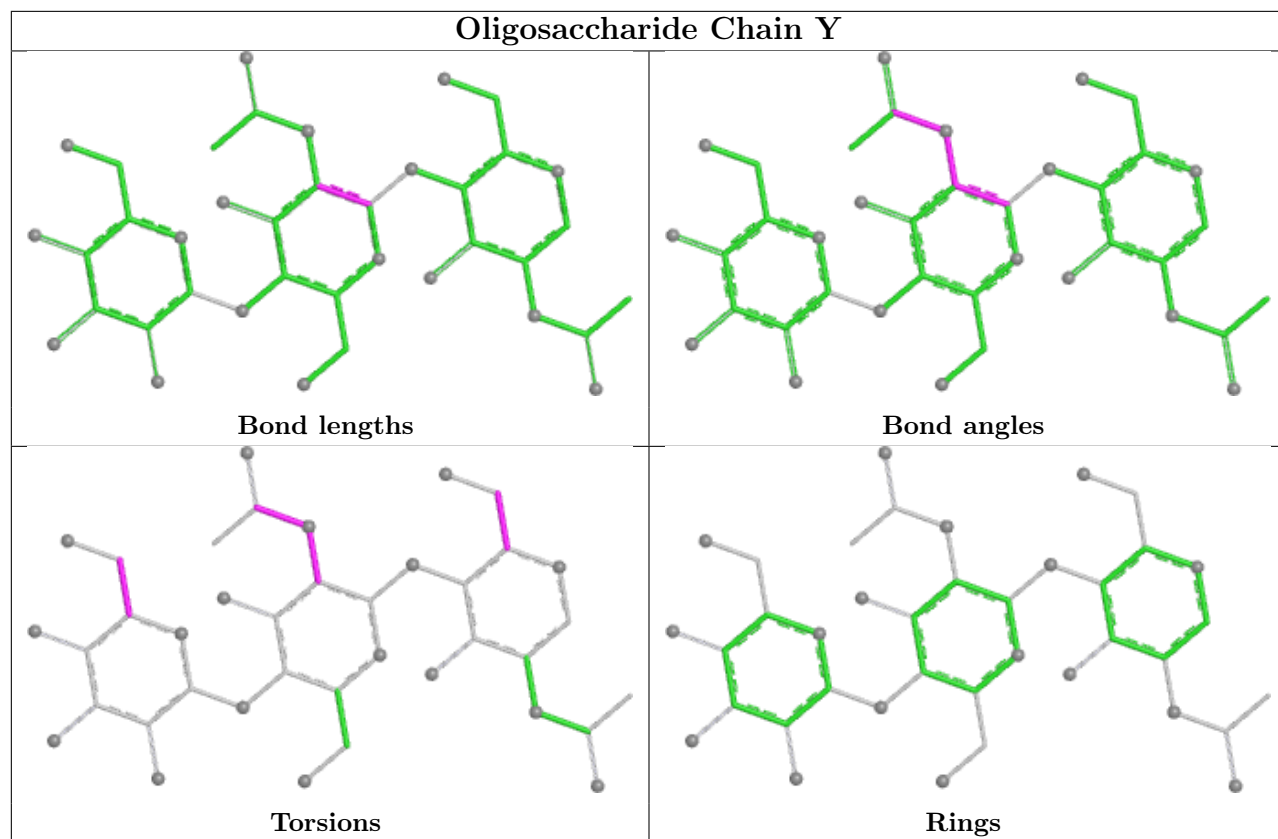
9 monomers are involved in 8 short contacts:

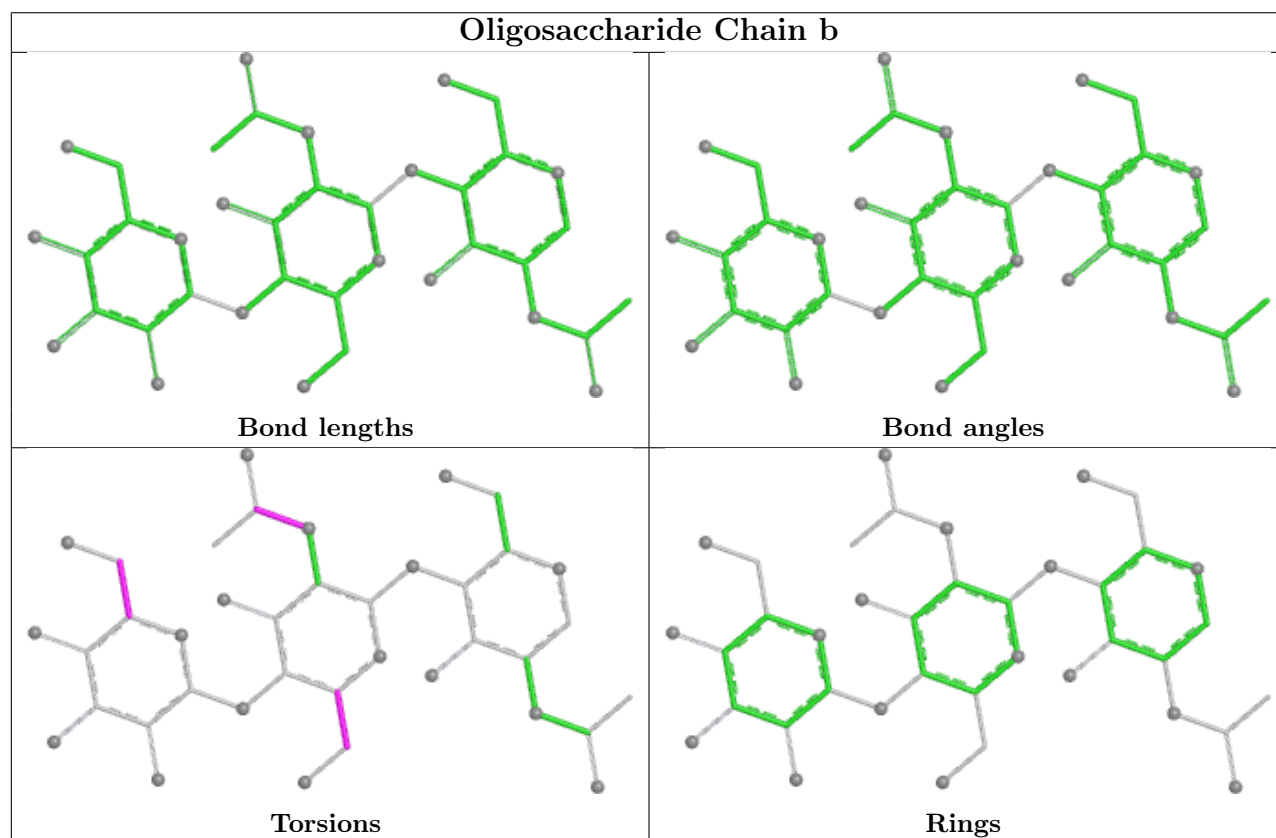
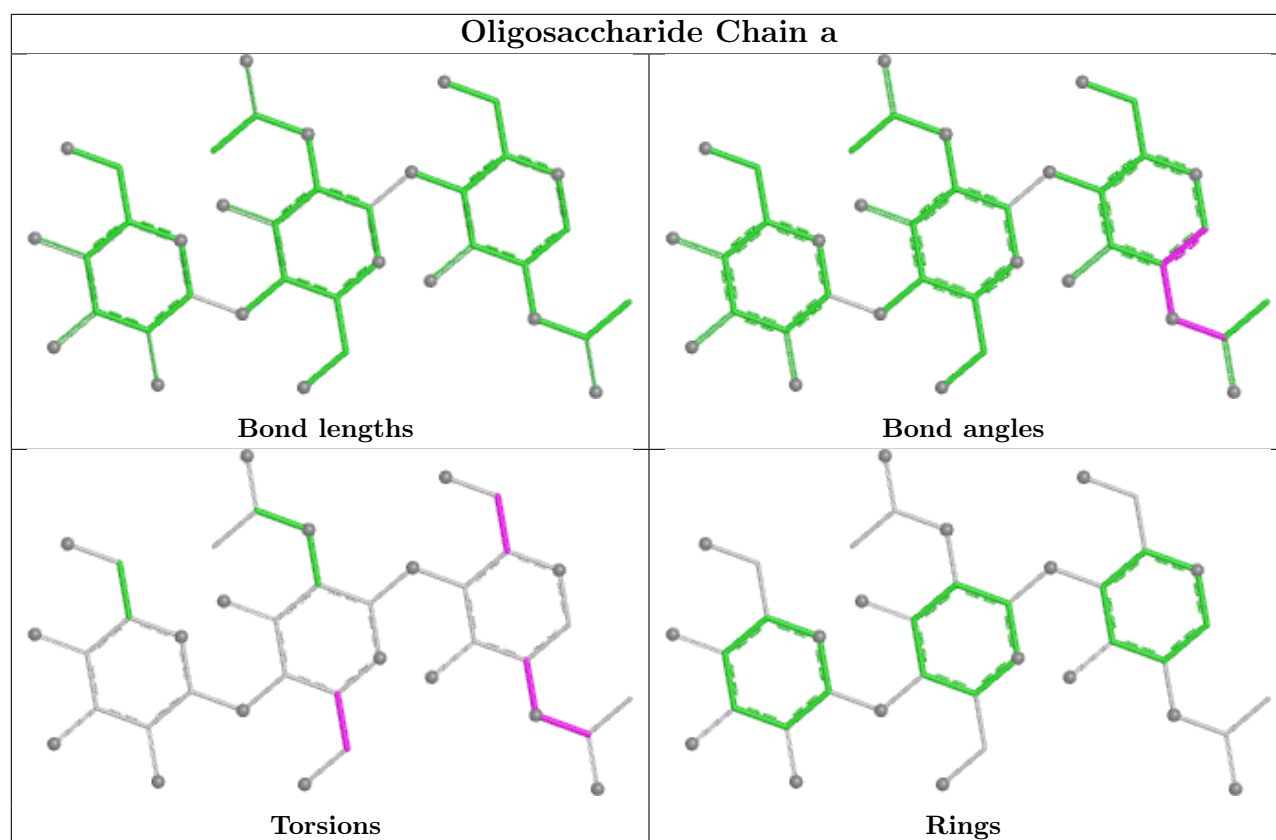
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	W	1	NAG	1	0
6	a	1	NAG	1	0
6	Y	1	NAG	1	0
6	Y	2	NAG	2	0
6	f	1	NAG	1	0
6	V	1	NAG	1	0
6	V	2	NAG	2	0
6	d	1	NAG	1	0
6	W	2	NAG	1	0

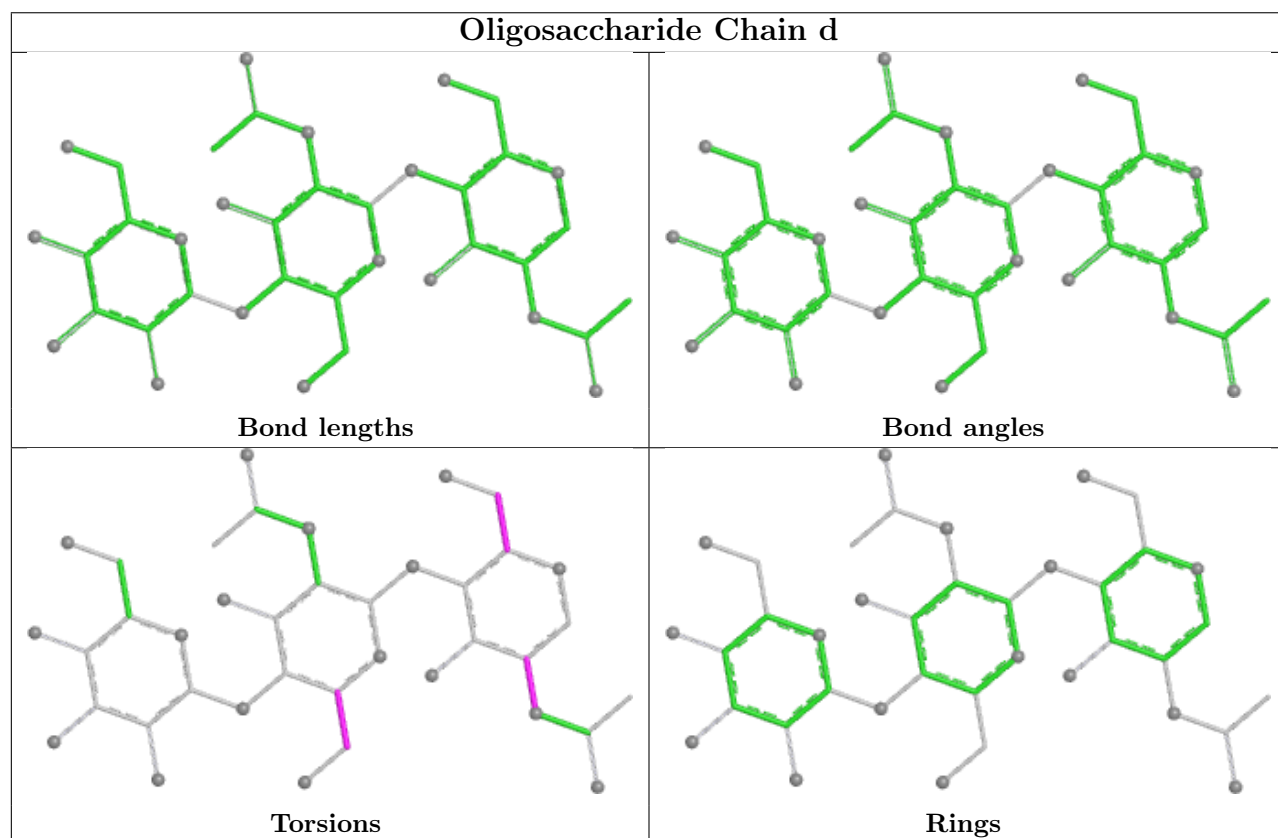
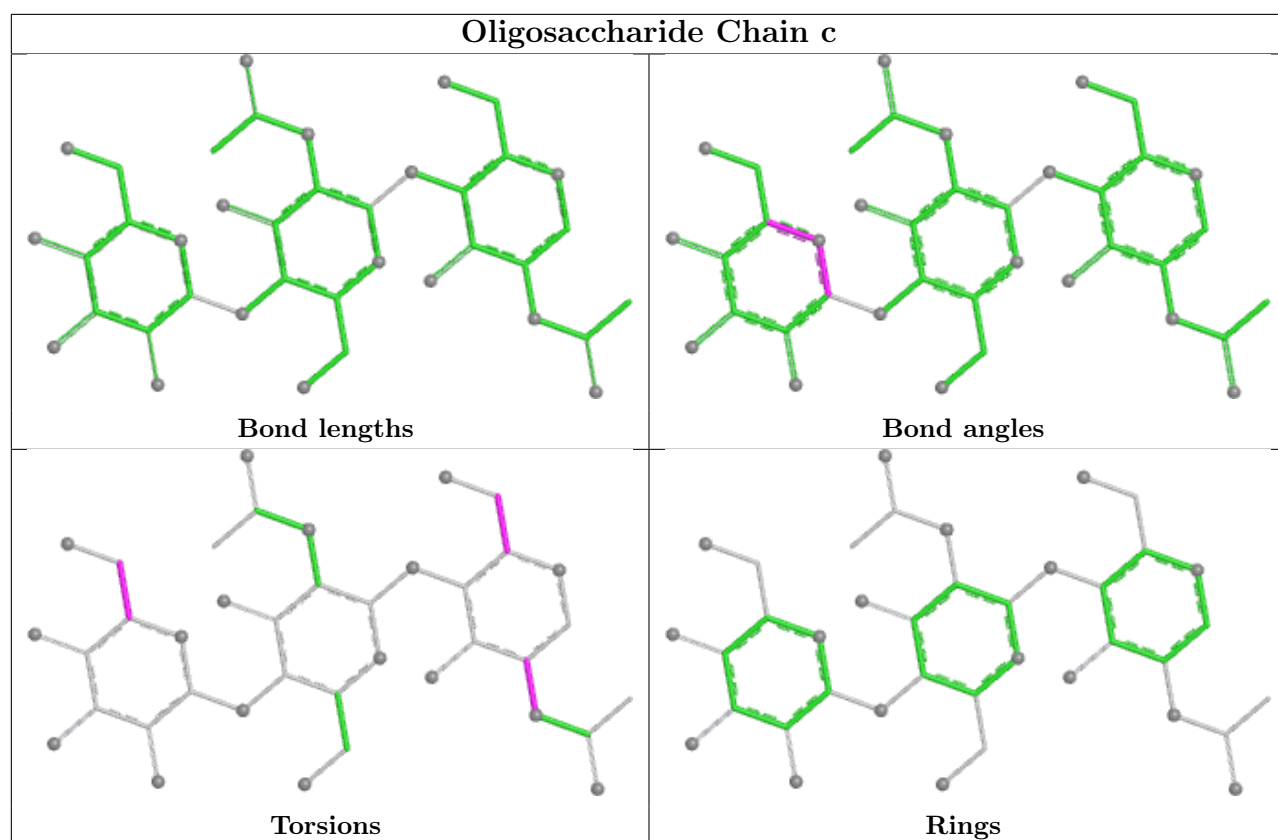
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

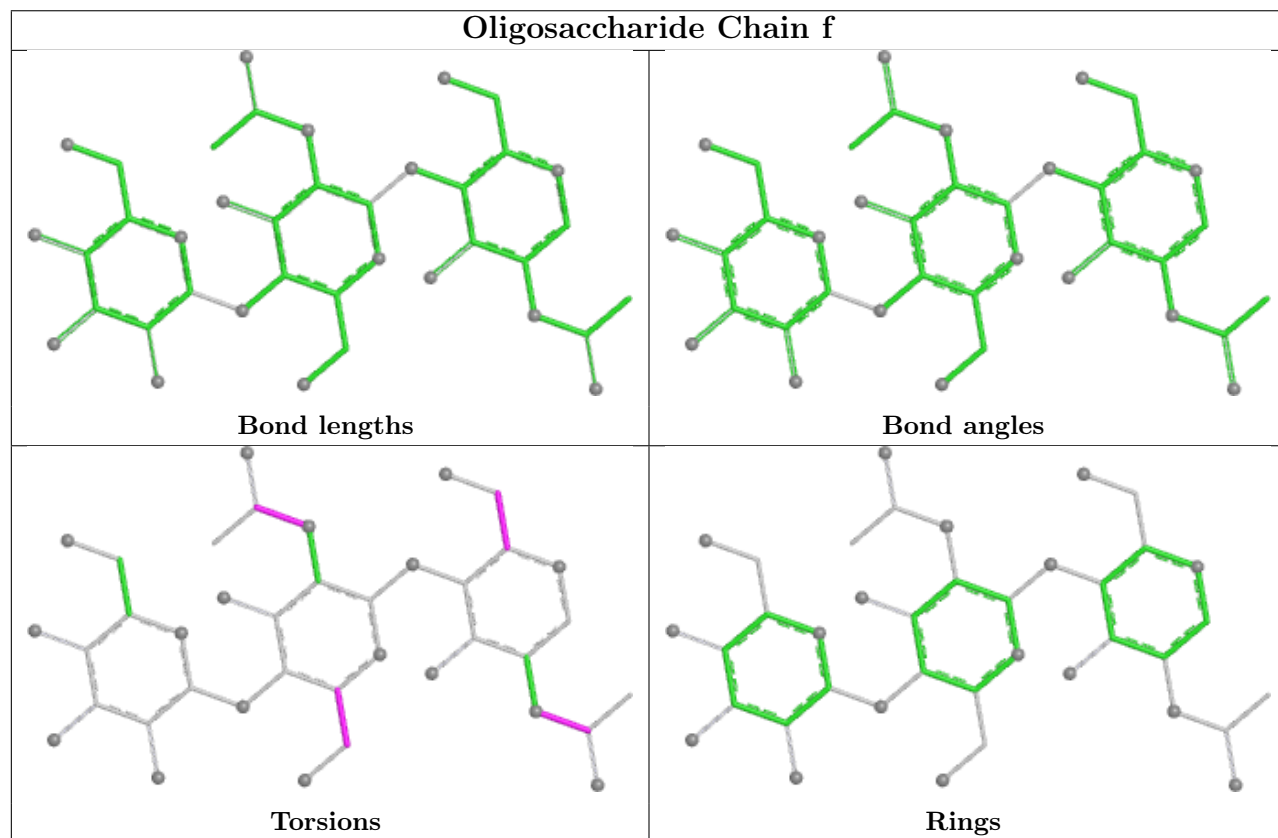
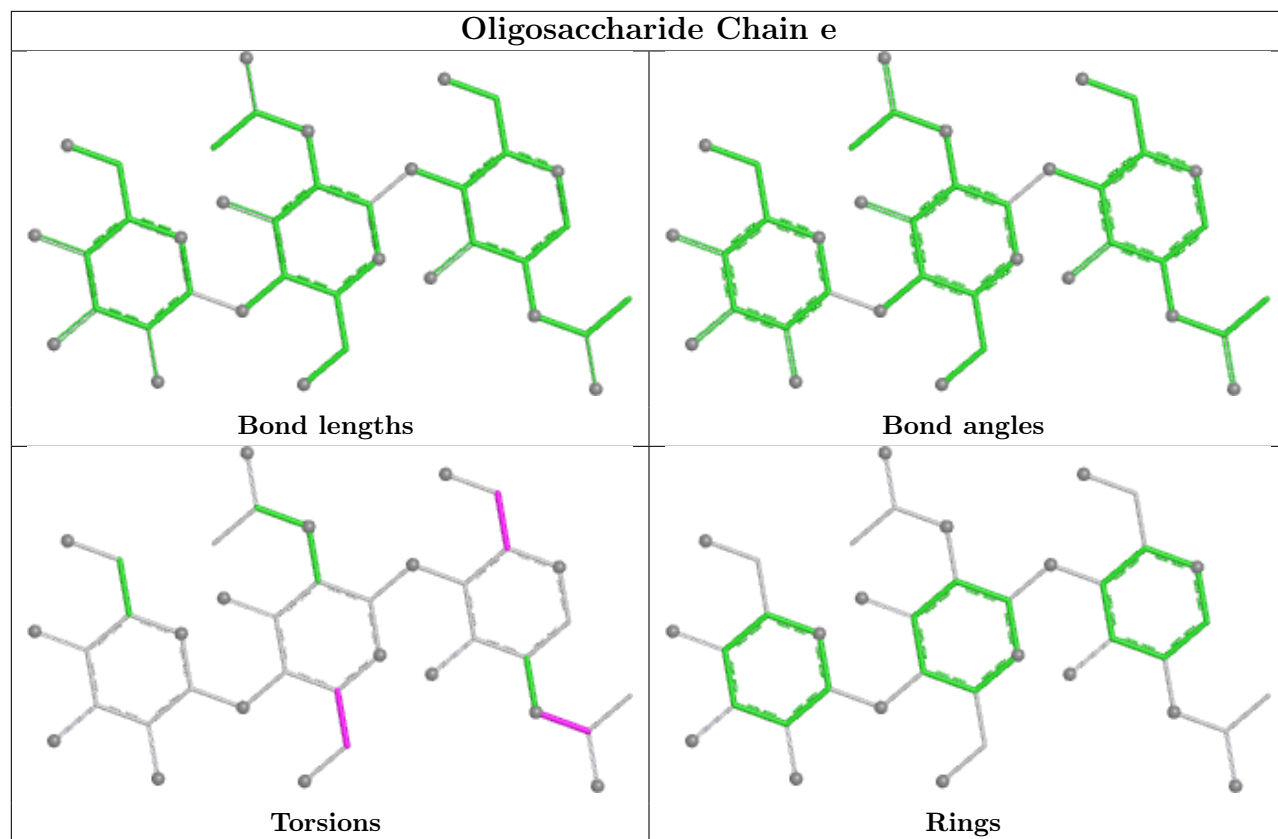












5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39617. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.