



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:03 PM UTC

PDB ID : 7THT / pdb_00007tht
EMDB ID : EMD-25904
Title : CryoEM structure of SARS-CoV-2 S protein in complex with Receptor Binding Domain antibody DH1042
Authors : Manne, K.; May, A.; Acharya, P.
Deposited on : 2022-01-12
Resolution : 3.42 Å (reported)
Based on initial models : 7EAN, 6VYB

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

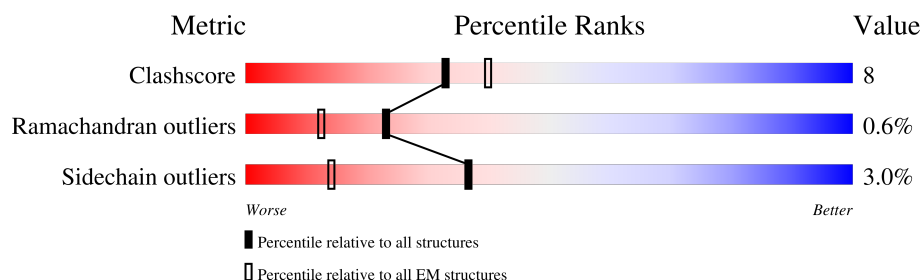
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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.



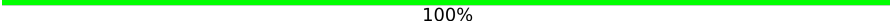
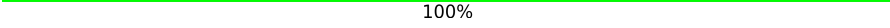
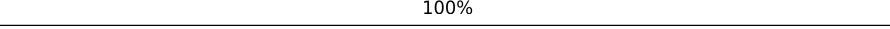
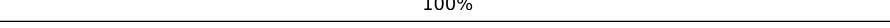
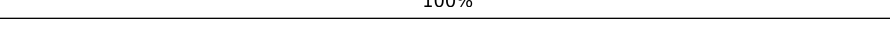
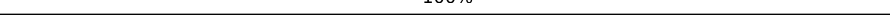
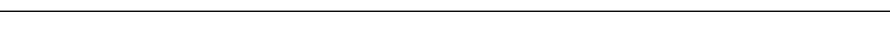
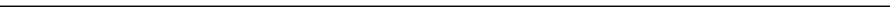
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	C	1121	82% 5% • 12%
1	S	1121	80% 7% •• 12%
1	V	1121	77% 8% • 12%
2	H	122	98% •
2	a	122	98% •
2	d	122	86% 11% •
3	L	106	97% •
3	b	106	96% •
3	c	106	95% 5%

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Mol	Chain	Length	Quality of chain
4	A	3	 67%33%
5	B	2	 100%
5	D	2	 100%
5	E	2	 100%
5	F	2	 100%
5	G	2	 100%
5	I	2	 100%
5	J	2	 100%
5	K	2	 100%
5	M	2	 100%
5	N	2	 100%
5	O	2	 100%
5	W	2	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 28900 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	991	Total	C	N	O	S	0	0
			7620	4877	1268	1441	34		
1	V	986	Total	C	N	O	S	0	0
			7587	4856	1260	1437	34		
1	C	990	Total	C	N	O	S	0	0
			7606	4872	1270	1430	34		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	607	GLU	GLN	conflict	UNP P0DTC2
S	986	PRO	LYS	conflict	UNP P0DTC2
S	987	PRO	VAL	conflict	UNP P0DTC2
V	607	GLU	GLN	conflict	UNP P0DTC2
V	986	PRO	LYS	conflict	UNP P0DTC2
V	987	PRO	VAL	conflict	UNP P0DTC2
C	607	GLU	GLN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

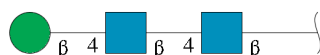
- Molecule 2 is a protein called DH1042 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	122	Total	C	N	O	S	0	0
			946	597	159	184	6		
2	a	122	Total	C	N	O	S	0	0
			946	597	159	184	6		
2	d	122	Total	C	N	O	S	0	0
			946	597	159	184	6		

- Molecule 3 is a protein called DH1042 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	106	Total	C	N	O	S	0	0
			804	504	132	165	3		
3	c	106	Total	C	N	O	S	0	0
			804	504	132	165	3		
3	b	106	Total	C	N	O	S	0	0
			804	504	132	165	3		

- Molecule 4 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
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



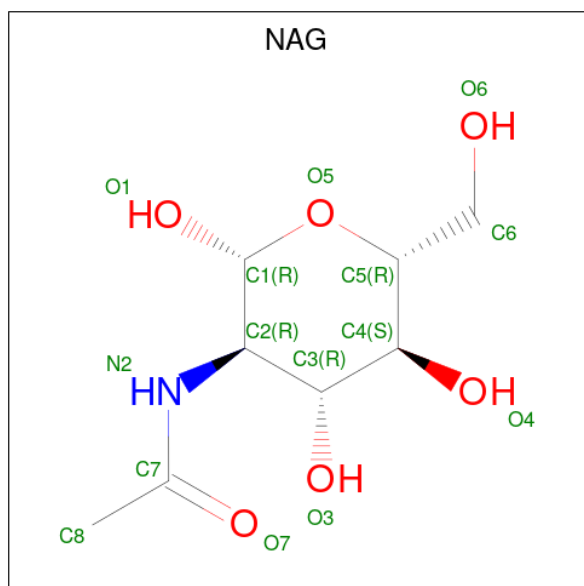
Mol	Chain	Residues	Atoms				AltConf	Trace
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				AltConf
6	S	1	Total	C	N	O	0
			14	8	1	5	
6	S	1	Total	C	N	O	0
			14	8	1	5	
6	S	1	Total	C	N	O	0
			14	8	1	5	
6	V	1	Total	C	N	O	0
			14	8	1	5	
6	V	1	Total	C	N	O	0
			14	8	1	5	
6	V	1	Total	C	N	O	0
			14	8	1	5	
6	V	1	Total	C	N	O	0
			14	8	1	5	
6	V	1	Total	C	N	O	0
			14	8	1	5	
6	V	1	Total	C	N	O	0
			14	8	1	5	
6	V	1	Total	C	N	O	0
			14	8	1	5	
6	V	1	Total	C	N	O	0
			14	8	1	5	
6	V	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

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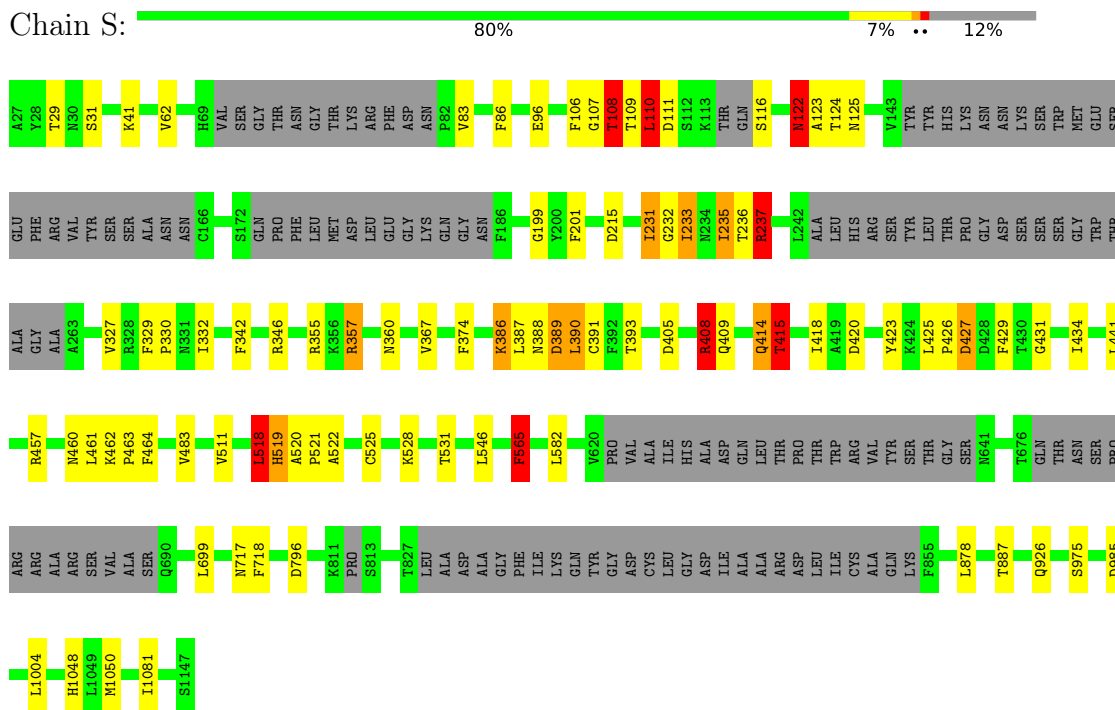
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

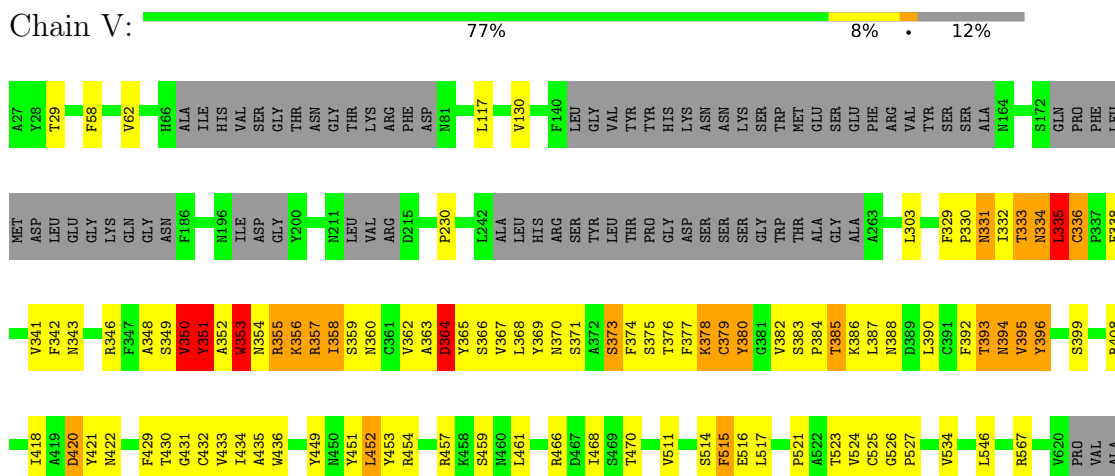
3 Residue-property plots

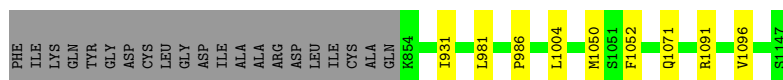
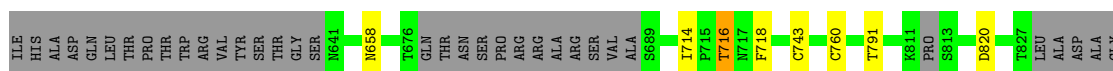
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



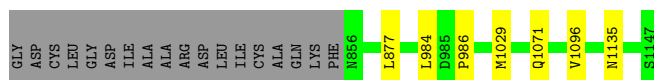
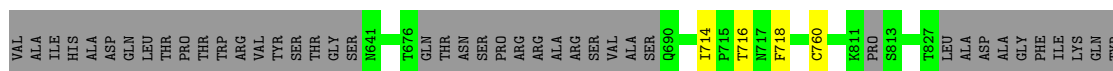
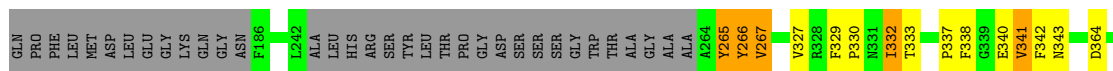
- Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein

Chain C: 82% 5% • 12%



• Molecule 2: DH1042 heavy chain

Chain H: 98% •



• Molecule 2: DH1042 heavy chain

Chain a: 98% •

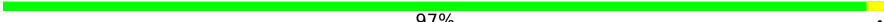


• Molecule 2: DH1042 heavy chain

Chain d: 86% 11% •

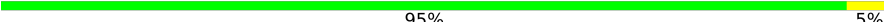


• Molecule 3: DH1042 light chain

Chain L:  97%

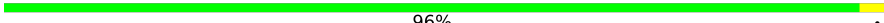


- Molecule 3: DH1042 light chain

Chain c:  95% 5%



- Molecule 3: DH1042 light chain

Chain b:  96%



- Molecule 4: 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%

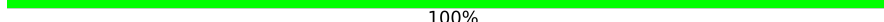


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175460	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.02	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	C	0.75	3/7777 (0.0%)	1.27	9/10596 (0.1%)
1	S	0.76	4/7790 (0.1%)	1.28	23/10611 (0.2%)
1	V	0.77	3/7757 (0.0%)	1.28	15/10565 (0.1%)
2	H	0.83	0/966	1.36	0/1307
2	a	0.82	0/966	1.30	1/1307 (0.1%)
2	d	0.86	0/966	1.35	1/1307 (0.1%)
3	L	0.84	0/823	1.36	0/1118
3	b	0.82	0/823	1.36	0/1118
3	c	0.82	0/823	1.35	1/1118 (0.1%)
All	All	0.78	10/28691 (0.0%)	1.29	50/39047 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	329	PHE	C-O	-7.71	1.14	1.24
1	C	266	TYR	C-O	-7.23	1.15	1.23
1	S	717	ASN	C-O	-6.92	1.17	1.24
1	S	518	LEU	N-CA	6.43	1.54	1.46
1	C	332	ILE	C-O	-6.26	1.17	1.24
1	S	414	GLN	C-O	-6.02	1.16	1.23
1	S	408	ARG	C-O	-5.75	1.15	1.24
1	C	267	VAL	C-O	-5.39	1.17	1.24
1	V	330	PRO	C-O	-5.24	1.17	1.23
1	V	353	TRP	N-CA	5.01	1.49	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	495	TYR	CB-CA-C	-10.63	94.19	110.88
1	C	333	THR	CB-CA-C	-9.59	93.43	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	415	THR	CB-CA-C	8.85	124.41	109.80
1	V	335	LEU	N-CA-C	-8.32	97.16	109.15
1	S	565	PHE	CA-CB-CG	8.18	121.98	113.80
1	S	237	ARG	CB-CA-C	-7.96	96.28	111.48
1	S	357	ARG	CG-CD-NE	-7.86	94.71	112.00
2	d	93	ALA	N-CA-C	7.70	121.52	109.96
1	V	333	THR	CB-CA-C	-7.48	95.53	110.42
3	c	70	ASP	CA-CB-CG	7.48	120.08	112.60
1	S	389	ASP	N-CA-CB	-7.40	99.53	110.49
1	S	389	ASP	CB-CA-C	7.37	122.40	110.09
1	V	334	ASN	CB-CA-C	7.27	123.40	111.41
1	S	717	ASN	CB-CA-C	-6.54	99.37	114.41
1	V	452	LEU	CA-C-N	6.52	132.80	122.62
1	V	452	LEU	C-N-CA	6.52	132.80	122.62
1	V	331	ASN	CB-CG-ND2	6.48	126.12	116.40
1	C	342	PHE	CB-CA-C	-6.45	98.76	109.99
1	V	330	PRO	CA-C-O	-6.44	113.83	122.08
1	V	452	LEU	CA-C-O	-6.42	114.14	121.58
1	C	986	PRO	N-CA-C	6.02	118.05	110.70
1	S	386	LYS	CA-C-N	5.96	132.93	121.54
1	S	386	LYS	C-N-CA	5.96	132.93	121.54
1	S	414	GLN	CA-C-O	-5.94	113.98	120.81
1	S	1048	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	V	743	CYS	N-CA-CB	-5.67	102.86	111.19
1	S	390	LEU	CB-CA-C	-5.66	98.69	109.66
1	V	335	LEU	CA-C-O	-5.63	113.92	120.62
1	S	357	ARG	CB-CG-CD	-5.63	98.35	111.30
1	V	515	PHE	CA-CB-CG	5.55	119.35	113.80
1	C	392	PHE	CA-C-N	5.55	128.03	120.54
1	C	392	PHE	C-N-CA	5.55	128.03	120.54
1	V	534	VAL	N-CA-C	5.54	112.14	106.21
1	S	108	THR	CB-CA-C	-5.49	102.08	109.16
1	S	389	ASP	CA-C-N	5.48	132.02	122.81
1	S	389	ASP	C-N-CA	5.48	132.02	122.81
1	C	343	ASN	CA-CB-CG	-5.39	107.20	112.60
1	S	518	LEU	N-CA-C	5.38	122.26	110.80
1	S	796	ASP	CA-CB-CG	5.35	117.95	112.60
2	a	29	PHE	CA-CB-CG	5.22	119.02	113.80
1	V	58	PHE	CA-CB-CG	5.20	119.00	113.80
1	S	388	ASN	CA-CB-CG	5.19	117.79	112.60
1	C	559	PHE	CA-CB-CG	5.17	118.97	113.80
1	V	986	PRO	N-CA-C	5.16	116.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	215	ASP	CA-CB-CG	5.15	117.75	112.60
1	V	331	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	S	1050	MET	N-CA-CB	-5.15	103.73	111.56
1	S	405	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	405	ASP	CA-CB-CG	5.03	117.62	112.60
1	S	460	ASN	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7606	0	7342	75	0
1	S	7620	0	7364	106	0
1	V	7587	0	7307	256	0
2	H	946	0	926	0	0
2	a	946	0	926	0	0
2	d	946	0	924	45	0
3	L	804	0	781	1	0
3	b	804	0	781	2	0
3	c	804	0	781	1	0
4	A	39	0	34	5	0
5	B	28	0	25	3	0
5	D	28	0	25	0	0
5	E	28	0	25	0	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	K	28	0	25	0	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	W	28	0	25	0	0
6	C	154	0	143	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	140	0	130	4	0
6	V	168	0	156	4	0
All	All	28900	0	27895	476	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 8.

All (476) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:380:TYR:CD2	1:V:429:PHE:HE2	1.16	1.64
1:V:353:TRP:CZ3	1:V:466:ARG:CD	1.81	1.61
1:V:353:TRP:CZ3	1:V:466:ARG:HD2	1.35	1.58
1:S:357:ARG:HH22	1:V:230:PRO:CB	0.98	1.56
1:S:83:VAL:CG1	1:S:237:ARG:HD3	1.25	1.56
1:V:336:CYS:H	1:V:363:ALA:CB	0.94	1.53
1:V:380:TYR:CD2	1:V:429:PHE:CE2	1.93	1.53
1:V:331:ASN:ND2	6:V:1204:NAG:C1	1.71	1.53
1:C:403:ARG:HB2	1:C:495:TYR:CE2	1.40	1.52
1:V:336:CYS:N	1:V:363:ALA:CB	1.78	1.45
2:d:94:ARG:NH1	2:d:102:VAL:CB	1.79	1.41
2:d:96:MET:HE3	2:d:99:ARG:CB	1.48	1.41
1:C:403:ARG:CB	1:C:495:TYR:CE2	2.08	1.35
1:V:421:TYR:CD1	1:V:457:ARG:HB3	1.63	1.34
1:C:337:PRO:O	1:C:341:VAL:CG1	1.75	1.33
1:V:336:CYS:N	1:V:363:ALA:HB2	1.34	1.33
1:V:350:VAL:CG1	1:V:453:TYR:HA	1.59	1.30
1:S:357:ARG:NH2	1:V:230:PRO:HB2	0.99	1.30
1:C:403:ARG:CB	1:C:495:TYR:HE2	1.43	1.27
1:V:362:VAL:CG1	1:V:526:GLY:O	1.82	1.26
2:d:96:MET:CE	2:d:99:ARG:HB2	1.64	1.26
1:V:353:TRP:CZ3	1:V:466:ARG:NE	2.03	1.24
1:V:382:VAL:HG11	1:V:515:PHE:CE2	1.73	1.23
1:S:386:LYS:NZ	1:V:981:LEU:O	1.68	1.22
2:d:94:ARG:NH1	2:d:102:VAL:HB	0.89	1.20
1:S:83:VAL:CG1	1:S:237:ARG:CD	2.20	1.20
1:V:422:ASN:O	1:V:461:LEU:HD11	1.39	1.20
1:V:342:PHE:CD1	1:V:511:VAL:HG21	1.77	1.19
1:V:353:TRP:CH2	1:V:466:ARG:CG	2.27	1.18
1:V:342:PHE:CE1	1:V:511:VAL:CB	2.28	1.17
1:V:342:PHE:CE1	1:V:511:VAL:HG21	1.81	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:362:VAL:HG11	1:V:526:GLY:O	1.42	1.14
1:V:350:VAL:HG11	1:V:453:TYR:HA	1.18	1.13
1:V:365:TYR:CD2	1:V:527:PRO:HG3	1.81	1.13
1:S:83:VAL:HG13	1:S:237:ARG:HD3	1.32	1.12
1:S:106:PHE:HB3	1:S:235:ILE:HG21	1.32	1.11
1:V:350:VAL:HG11	1:V:453:TYR:CA	1.80	1.11
1:C:337:PRO:O	1:C:341:VAL:HG12	0.94	1.11
2:d:94:ARG:HH12	2:d:102:VAL:CB	1.51	1.11
1:V:374:PHE:CD1	1:V:434:ILE:HG21	1.86	1.10
1:V:362:VAL:HG22	1:V:525:CYS:HB2	1.34	1.10
1:C:329:PHE:CE2	1:C:391:CYS:SG	2.45	1.10
1:C:452:LEU:HD23	1:C:494:SER:HB2	1.32	1.10
1:V:336:CYS:N	1:V:363:ALA:HB1	1.57	1.10
1:V:342:PHE:CE1	1:V:511:VAL:CG2	2.33	1.10
1:V:395:VAL:HG11	1:V:515:PHE:CD1	1.85	1.10
1:V:353:TRP:CE3	1:V:466:ARG:NE	2.15	1.09
1:V:422:ASN:HD21	1:V:454:ARG:HB3	1.13	1.09
1:V:342:PHE:HE1	1:V:511:VAL:HB	1.07	1.09
1:S:83:VAL:HG11	1:S:237:ARG:CD	1.81	1.08
1:V:422:ASN:O	1:V:461:LEU:CD1	2.02	1.08
1:V:342:PHE:CE1	1:V:511:VAL:HB	1.88	1.07
1:V:342:PHE:CZ	1:V:511:VAL:HG11	1.90	1.07
1:V:353:TRP:CH2	1:V:466:ARG:HG3	1.87	1.07
1:V:374:PHE:HD1	1:V:434:ILE:CG2	1.67	1.07
1:V:371:SER:HB2	1:V:374:PHE:HD2	1.15	1.07
1:V:374:PHE:CD1	1:V:434:ILE:CG2	2.38	1.06
1:S:409:GLN:CD	1:S:418:ILE:HG22	1.80	1.05
1:C:329:PHE:HE2	1:C:391:CYS:SG	1.78	1.05
1:V:380:TYR:O	1:V:430:THR:HA	1.55	1.05
1:S:357:ARG:HH22	1:V:230:PRO:HB3	1.13	1.04
2:d:94:ARG:HH12	2:d:102:VAL:CG2	1.69	1.04
1:V:382:VAL:HG11	1:V:515:PHE:CD2	1.91	1.04
1:C:403:ARG:HB3	1:C:495:TYR:HE2	1.22	1.04
1:S:116:SER:N	1:S:233:ILE:CD1	2.20	1.03
1:V:342:PHE:HE1	1:V:511:VAL:CB	1.65	1.03
1:S:409:GLN:OE1	1:S:418:ILE:HG22	1.60	1.01
1:V:353:TRP:CH2	1:V:466:ARG:CD	2.44	1.01
1:V:376:THR:O	1:V:434:ILE:HA	1.58	1.01
1:S:985:ASP:OD2	1:C:383:SER:OG	1.79	1.01
1:V:371:SER:HB2	1:V:374:PHE:CD2	1.96	1.01
1:V:336:CYS:H	1:V:363:ALA:HB1	1.12	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:380:TYR:CE2	1:V:429:PHE:HE2	1.80	1.00
1:S:83:VAL:HG11	1:S:237:ARG:HD3	1.00	0.99
1:C:716:THR:HG22	1:C:1071:GLN:O	1.61	0.99
1:S:236:THR:HG21	5:B:1:NAG:H62	1.45	0.98
1:V:365:TYR:HD2	1:V:527:PRO:HG3	1.21	0.98
1:V:421:TYR:CD1	1:V:457:ARG:CB	2.47	0.97
1:V:380:TYR:HD2	1:V:429:PHE:CE2	1.75	0.97
1:C:338:PHE:HA	1:C:341:VAL:HG13	1.47	0.97
1:V:358:ILE:HD13	1:V:358:ILE:H	1.30	0.97
1:V:353:TRP:HH2	1:V:466:ARG:HB2	1.29	0.96
1:V:350:VAL:HG11	1:V:453:TYR:CB	1.96	0.96
1:V:353:TRP:CH2	1:V:466:ARG:HD2	1.98	0.96
2:d:96:MET:CE	2:d:99:ARG:CB	2.34	0.95
2:d:4:LEU:HD11	2:d:94:ARG:HD2	1.45	0.95
1:S:357:ARG:NH2	1:V:230:PRO:CB	1.76	0.94
1:V:357:ARG:H	1:V:357:ARG:HE	1.15	0.94
1:V:422:ASN:ND2	1:V:454:ARG:HB3	1.82	0.94
1:S:106:PHE:HB3	1:S:235:ILE:CG2	1.96	0.94
1:S:332:ILE:HD11	1:S:360:ASN:OD1	1.67	0.94
1:V:353:TRP:CZ3	1:V:466:ARG:CG	2.47	0.93
2:d:96:MET:CG	2:d:99:ARG:HB3	1.99	0.93
1:S:409:GLN:OE1	1:S:418:ILE:CG2	2.16	0.93
1:C:452:LEU:CD2	1:C:494:SER:HB2	1.98	0.92
2:d:2:VAL:HG13	2:d:94:ARG:NH2	1.85	0.92
2:d:36:TRP:CZ3	2:d:92:CYS:HB3	2.04	0.92
1:V:350:VAL:CG1	1:V:453:TYR:CA	2.44	0.92
1:V:380:TYR:CG	1:V:429:PHE:CE2	2.59	0.90
1:V:395:VAL:HG22	1:V:514:SER:O	1.48	0.89
1:S:342:PHE:CE1	1:S:511:VAL:HG21	2.07	0.88
1:V:331:ASN:CG	6:V:1204:NAG:C1	2.47	0.88
1:C:337:PRO:C	1:C:341:VAL:HG12	1.99	0.88
1:V:388:ASN:O	1:V:526:GLY:HA3	1.74	0.88
1:V:350:VAL:HG13	1:V:453:TYR:HA	1.53	0.88
1:V:362:VAL:HG13	1:V:526:GLY:O	1.74	0.88
1:V:375:SER:N	1:V:435:ALA:O	2.07	0.88
1:S:415:THR:OG1	1:S:420:ASP:OD1	1.91	0.87
1:V:365:TYR:HA	1:V:527:PRO:CG	2.05	0.87
1:C:403:ARG:HB3	1:C:495:TYR:CE2	1.99	0.86
1:V:377:PHE:CD1	1:V:432:CYS:SG	2.70	0.85
1:V:342:PHE:CZ	1:V:511:VAL:CG1	2.60	0.85
1:V:353:TRP:CH2	1:V:466:ARG:CB	2.60	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:353:TRP:CH2	1:V:466:ARG:HB2	2.12	0.85
1:V:421:TYR:CD1	1:V:459:SER:O	2.30	0.84
1:S:409:GLN:CD	1:S:418:ILE:CG2	2.51	0.83
1:C:337:PRO:C	1:C:341:VAL:CG1	2.51	0.83
1:V:353:TRP:HZ3	1:V:466:ARG:CD	1.41	0.83
1:V:380:TYR:OH	1:V:433:VAL:N	2.10	0.83
1:C:64:TRP:CD1	1:C:266:TYR:CE1	2.67	0.83
1:V:380:TYR:CG	1:V:429:PHE:HE2	1.90	0.83
1:S:83:VAL:HG12	1:S:237:ARG:HD3	1.59	0.83
1:S:109:THR:O	1:S:111:ASP:N	2.09	0.83
1:V:421:TYR:CE1	1:V:457:ARG:HB3	2.13	0.82
1:V:353:TRP:HE3	1:V:466:ARG:HE	1.26	0.82
1:V:374:PHE:CE1	1:V:434:ILE:HG21	2.14	0.82
1:V:716:THR:HG22	1:V:1071:GLN:O	1.80	0.82
3:c:13:ALA:O	3:c:106:ILE:OXT	1.97	0.82
1:V:392:PHE:CE1	1:V:516:GLU:N	2.46	0.81
2:d:2:VAL:HG13	2:d:94:ARG:HH21	1.44	0.81
1:S:357:ARG:HH21	1:V:230:PRO:HB2	1.37	0.81
1:V:382:VAL:CG1	1:V:515:PHE:CE2	2.61	0.81
1:V:421:TYR:CE1	1:V:459:SER:O	2.34	0.81
1:V:356:LYS:HE3	1:V:396:TYR:HA	1.62	0.81
1:V:365:TYR:HA	1:V:527:PRO:HD3	1.62	0.81
1:S:116:SER:N	1:S:233:ILE:HD11	1.94	0.81
2:d:35:SER:OG	2:d:93:ALA:O	1.98	0.80
1:C:338:PHE:HA	1:C:341:VAL:CG1	2.11	0.80
2:d:2:VAL:CG1	2:d:94:ARG:HH21	1.95	0.80
1:V:421:TYR:CE1	1:V:459:SER:C	2.60	0.79
2:d:94:ARG:CZ	2:d:102:VAL:HB	2.05	0.79
1:V:350:VAL:HG12	1:V:452:LEU:O	1.81	0.79
1:V:336:CYS:H	1:V:363:ALA:HB2	0.63	0.79
1:V:365:TYR:HA	1:V:527:PRO:CD	2.12	0.79
2:d:94:ARG:HH12	2:d:102:VAL:HB	1.05	0.79
1:V:380:TYR:CE2	1:V:429:PHE:CE2	2.62	0.79
1:V:380:TYR:O	1:V:430:THR:CA	2.30	0.79
1:V:342:PHE:CE1	1:V:511:VAL:CG1	2.66	0.78
1:S:108:THR:HG23	1:S:236:THR:CG2	2.13	0.78
1:V:380:TYR:CD2	1:V:431:GLY:C	2.62	0.78
2:d:4:LEU:HD11	2:d:94:ARG:CD	2.14	0.78
1:V:359:SER:O	1:V:523:THR:HB	1.83	0.78
1:S:386:LYS:O	1:S:389:ASP:HB2	1.84	0.78
1:V:354:ASN:OD1	1:V:399:SER:OG	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:377:PHE:CE1	1:V:432:CYS:SG	2.76	0.78
1:V:353:TRP:HZ3	1:V:466:ARG:HD2	0.74	0.77
1:S:408:ARG:H	1:S:408:ARG:HD3	1.46	0.77
1:V:350:VAL:HG21	1:V:422:ASN:OD1	1.83	0.77
1:V:342:PHE:CD1	1:V:511:VAL:CG2	2.59	0.77
1:V:395:VAL:CG2	1:V:514:SER:O	2.30	0.77
2:d:94:ARG:HH11	2:d:102:VAL:HB	0.95	0.77
4:A:1:NAG:O7	4:A:1:NAG:O3	2.03	0.77
1:V:358:ILE:HG22	1:V:524:VAL:HG21	1.67	0.76
1:C:519:HIS:O	1:C:565:PHE:HE2	1.67	0.76
1:S:926:GLN:NE2	4:A:1:NAG:H82	1.99	0.76
1:V:358:ILE:HG13	1:V:393:THR:O	1.85	0.76
1:V:421:TYR:HE1	1:V:459:SER:C	1.94	0.76
1:C:338:PHE:CA	1:C:341:VAL:HG13	2.15	0.76
1:C:403:ARG:HB2	1:C:495:TYR:CD2	2.17	0.76
1:V:342:PHE:CE1	1:V:511:VAL:HG11	2.21	0.75
2:d:96:MET:HE3	2:d:99:ARG:CG	2.16	0.74
1:S:125:ASN:OD1	6:S:1208:NAG:O6	2.04	0.74
1:V:365:TYR:CD2	1:V:527:PRO:CG	2.66	0.74
2:d:96:MET:HG3	2:d:99:ARG:HB3	1.68	0.74
1:S:386:LYS:O	1:S:389:ASP:OD2	2.05	0.73
1:S:985:ASP:CG	1:C:383:SER:OG	2.31	0.73
1:S:985:ASP:CG	1:C:383:SER:HG	1.96	0.73
1:V:331:ASN:ND2	6:V:1204:NAG:O5	2.23	0.72
1:V:394:ASN:O	1:V:516:GLU:HB3	1.89	0.72
1:S:108:THR:HG23	1:S:236:THR:HG23	1.69	0.72
1:V:365:TYR:CA	1:V:527:PRO:HD3	2.20	0.72
1:V:392:PHE:CZ	1:V:515:PHE:HB3	2.25	0.72
1:C:519:HIS:O	1:C:565:PHE:CE2	2.43	0.72
1:V:352:ALA:HB1	1:V:466:ARG:CZ	2.20	0.71
2:d:2:VAL:CG1	2:d:94:ARG:NH2	2.52	0.71
1:S:107:GLY:O	1:S:236:THR:N	2.19	0.71
1:V:395:VAL:HG11	1:V:515:PHE:HD1	1.52	0.71
1:V:358:ILE:HB	1:V:524:VAL:HG23	1.72	0.71
1:V:392:PHE:CZ	1:V:516:GLU:N	2.58	0.71
1:C:452:LEU:HD23	1:C:494:SER:CB	2.16	0.71
1:V:355:ARG:NH1	1:V:355:ARG:HG3	2.06	0.71
1:S:393:THR:HG21	1:S:518:LEU:HD11	1.73	0.71
1:V:358:ILE:HD13	1:V:358:ILE:N	2.06	0.71
1:V:387:LEU:C	1:V:387:LEU:HD23	2.16	0.71
1:V:716:THR:CG2	1:V:1071:GLN:O	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:421:TYR:HB3	1:V:457:ARG:HD2	1.73	0.70
2:d:95:TYR:HD2	2:d:100(D):TYR:H	1.40	0.69
1:V:355:ARG:HG3	1:V:355:ARG:HH11	1.57	0.69
3:b:13:ALA:O	3:b:106:ILE:OXT	2.11	0.69
1:V:395:VAL:CG1	1:V:515:PHE:CD1	2.72	0.69
3:L:13:ALA:O	3:L:106:ILE:OXT	2.10	0.69
1:V:377:PHE:HD1	1:V:432:CYS:SG	2.16	0.69
1:V:352:ALA:HB1	1:V:466:ARG:NH1	2.09	0.68
1:C:403:ARG:N	1:C:495:TYR:OH	2.19	0.68
1:V:357:ARG:H	1:V:357:ARG:NE	1.91	0.68
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.75	0.68
1:V:365:TYR:HA	1:V:527:PRO:HG3	1.75	0.68
1:V:422:ASN:C	1:V:461:LEU:HD11	2.20	0.67
1:C:332:ILE:C	1:C:332:ILE:HD12	2.18	0.67
1:V:353:TRP:CZ2	1:V:466:ARG:HG3	2.30	0.67
1:S:31:SER:HB3	1:S:62:VAL:HG11	1.76	0.66
1:V:382:VAL:CG1	1:V:515:PHE:CD2	2.76	0.66
1:V:365:TYR:N	1:V:527:PRO:HD3	2.11	0.66
1:S:374:PHE:CG	1:S:434:ILE:HD11	2.32	0.65
1:S:329:PHE:HB3	1:S:330:PRO:HD2	1.78	0.65
1:V:371:SER:CB	1:V:374:PHE:CD2	2.75	0.65
1:V:349:SER:OG	1:V:451:TYR:HA	1.96	0.65
2:d:36:TRP:CE3	2:d:92:CYS:HB3	2.32	0.65
1:V:380:TYR:O	1:V:431:GLY:N	2.29	0.64
1:V:362:VAL:HG13	1:V:525:CYS:C	2.22	0.64
1:V:364:ASP:CB	1:V:526:GLY:HA2	2.27	0.64
1:S:985:ASP:CG	1:C:383:SER:CB	2.71	0.64
1:S:462:LYS:HB3	1:S:463:PRO:HD2	1.80	0.64
1:S:409:GLN:OE1	1:S:418:ILE:HG23	1.98	0.64
1:V:392:PHE:CZ	1:V:517:LEU:CD1	2.81	0.64
1:V:368:LEU:HA	1:V:374:PHE:CE2	2.33	0.63
1:V:355:ARG:HH11	1:V:355:ARG:CG	2.12	0.63
1:S:332:ILE:CD1	1:S:360:ASN:OD1	2.46	0.63
1:S:386:LYS:O	1:S:389:ASP:CB	2.46	0.62
1:V:380:TYR:CD2	1:V:429:PHE:CZ	2.81	0.62
1:V:368:LEU:HD22	1:V:374:PHE:CZ	2.34	0.62
1:C:338:PHE:CA	1:C:341:VAL:CG1	2.76	0.62
1:C:392:PHE:HB3	1:C:516:GLU:O	2.00	0.62
1:V:421:TYR:HD1	1:V:459:SER:O	1.82	0.61
1:V:348:ALA:HB3	1:V:353:TRP:HA	1.81	0.61
1:V:331:ASN:OD1	6:V:1204:NAG:C1	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:VAL:HG12	1:C:329:PHE:HD1	1.64	0.61
2:d:96:MET:HE3	2:d:99:ARG:HB2	0.71	0.61
1:S:386:LYS:O	1:S:389:ASP:CG	2.44	0.61
1:C:403:ARG:CB	1:C:495:TYR:CZ	2.80	0.61
1:V:362:VAL:CG1	1:V:526:GLY:C	2.72	0.61
1:V:365:TYR:H	1:V:527:PRO:HD3	1.65	0.61
1:S:116:SER:N	1:S:233:ILE:HD12	2.14	0.60
1:V:374:PHE:HD1	1:V:434:ILE:HG22	1.61	0.60
1:V:366:SER:OG	1:V:388:ASN:HB3	2.01	0.60
5:B:1:NAG:H3	5:B:2:NAG:H83	1.84	0.60
1:S:408:ARG:HD3	1:S:408:ARG:N	2.16	0.59
2:d:96:MET:HG2	2:d:99:ARG:NE	2.16	0.59
1:C:327:VAL:CG1	1:C:329:PHE:CE1	2.85	0.59
1:S:357:ARG:NH2	1:V:230:PRO:CA	2.64	0.59
1:V:380:TYR:CE2	1:V:432:CYS:N	2.70	0.59
1:C:332:ILE:HD12	1:C:332:ILE:O	2.03	0.59
1:V:62:VAL:O	1:V:62:VAL:HG23	2.03	0.58
1:V:352:ALA:HB2	1:V:468:ILE:HG22	1.85	0.58
1:S:201:PHE:CE2	1:S:235:ILE:CD1	2.86	0.58
1:S:427:ASP:OD1	1:S:427:ASP:N	2.35	0.58
1:S:109:THR:O	1:S:109:THR:HG22	2.01	0.58
1:S:520:ALA:N	1:S:521:PRO:HD3	2.18	0.58
1:S:108:THR:HG23	1:S:236:THR:HG21	1.85	0.57
1:V:353:TRP:N	1:V:353:TRP:CD2	2.72	0.57
1:V:358:ILE:HB	1:V:523:THR:OG1	2.03	0.57
5:B:2:NAG:O7	5:B:2:NAG:H3	2.04	0.57
1:V:379:CYS:HB3	1:V:382:VAL:HG23	1.86	0.57
2:d:95:TYR:N	2:d:95:TYR:CD1	2.71	0.57
6:S:1208:NAG:O3	6:S:1208:NAG:H82	2.03	0.57
1:S:342:PHE:CE1	1:S:511:VAL:CG2	2.86	0.57
1:V:357:ARG:HE	1:V:357:ARG:N	1.95	0.57
1:V:364:ASP:HB2	1:V:526:GLY:HA2	1.87	0.57
1:C:453:TYR:CZ	1:C:493:GLN:HG2	2.40	0.57
1:S:233:ILE:HG23	1:S:235:ILE:HG12	1.87	0.57
1:V:375:SER:HB2	1:V:436:TRP:HA	1.87	0.57
6:S:1210:NAG:O7	6:S:1210:NAG:O3	2.21	0.56
1:V:392:PHE:HE1	1:V:516:GLU:H	1.52	0.56
1:V:449:TYR:CE1	2:d:96:MET:HE1	2.40	0.56
1:V:353:TRP:C	1:V:466:ARG:HH21	2.14	0.56
1:C:327:VAL:CG1	1:C:329:PHE:CD1	2.88	0.56
1:V:422:ASN:O	1:V:461:LEU:HD13	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:116:SER:N	1:S:233:ILE:HD13	2.17	0.56
1:S:237:ARG:NH1	1:S:237:ARG:HG3	2.20	0.56
1:V:382:VAL:HG11	1:V:515:PHE:HE2	1.60	0.56
1:S:423:TYR:CE2	1:S:425:LEU:HD21	2.41	0.55
1:V:420:ASP:O	1:V:461:LEU:HD23	2.05	0.55
1:S:201:PHE:CD2	1:S:235:ILE:HD11	2.40	0.55
1:V:336:CYS:CA	1:V:363:ALA:CB	2.81	0.55
2:d:33:ALA:O	2:d:94:ARG:HB2	2.06	0.55
1:C:327:VAL:HG12	1:C:329:PHE:CD1	2.41	0.55
1:V:369:TYR:HA	1:V:377:PHE:CE2	2.42	0.55
2:d:96:MET:SD	2:d:99:ARG:HB3	2.46	0.55
1:S:718:PHE:CD1	1:S:718:PHE:C	2.85	0.55
2:d:96:MET:HB3	2:d:99:ARG:NH2	2.22	0.55
1:C:64:TRP:CD1	1:C:266:TYR:CD1	2.94	0.55
1:V:718:PHE:C	1:V:718:PHE:CD1	2.85	0.55
1:V:341:VAL:O	1:V:341:VAL:HG22	2.06	0.55
1:V:362:VAL:HG13	1:V:525:CYS:O	2.07	0.55
1:C:265:TYR:CD1	1:C:265:TYR:C	2.84	0.54
1:C:718:PHE:CD1	1:C:718:PHE:C	2.85	0.54
1:C:64:TRP:HD1	1:C:266:TYR:CD1	2.25	0.54
1:C:329:PHE:CD2	1:C:391:CYS:SG	2.99	0.54
1:V:392:PHE:CE2	1:V:517:LEU:HD11	2.42	0.54
1:V:1050:MET:HE2	1:V:1052:PHE:CE1	2.42	0.54
1:V:373:SER:O	1:V:436:TRP:HB3	2.07	0.54
1:V:380:TYR:CG	1:V:429:PHE:CD2	2.94	0.54
2:d:96:MET:CE	2:d:99:ARG:HG3	2.37	0.54
2:d:34:ILE:HA	2:d:94:ARG:HA	1.88	0.54
1:S:86:PHE:HB3	1:S:236:THR:O	2.08	0.54
1:V:350:VAL:HG11	1:V:453:TYR:HB3	1.86	0.53
1:C:452:LEU:HA	1:C:494:SER:HA	1.90	0.53
1:V:355:ARG:HH21	1:V:396:TYR:HB2	1.74	0.53
2:d:94:ARG:HH12	2:d:102:VAL:HG23	1.69	0.52
1:S:122:ASN:O	1:S:124:THR:N	2.42	0.52
1:S:201:PHE:HD2	1:S:235:ILE:HD11	1.74	0.52
1:S:426:PRO:CG	1:S:464:PHE:CE2	2.92	0.52
1:V:378:LYS:O	1:V:432:CYS:HA	2.09	0.52
1:S:329:PHE:HB3	1:S:330:PRO:CD	2.40	0.52
1:S:926:GLN:HE21	4:A:1:NAG:H82	1.71	0.52
1:S:83:VAL:HG13	1:S:237:ARG:CD	2.16	0.52
1:S:391:CYS:SG	1:S:525:CYS:HA	2.49	0.52
1:V:377:PHE:HE1	1:V:432:CYS:SG	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:LEU:CD2	1:C:494:SER:CB	2.82	0.52
1:S:199:GLY:HA2	1:S:232:GLY:HA2	1.92	0.52
1:C:453:TYR:CE1	1:C:493:GLN:HG2	2.44	0.52
1:S:29:THR:O	1:S:62:VAL:HG22	2.10	0.51
1:V:353:TRP:O	1:V:466:ARG:NH2	2.41	0.51
1:S:391:CYS:HB3	1:S:522:ALA:HB1	1.91	0.51
1:V:380:TYR:CB	1:V:429:PHE:CD2	2.93	0.51
1:S:201:PHE:CD2	1:S:235:ILE:CD1	2.93	0.51
1:V:380:TYR:CE2	1:V:431:GLY:C	2.88	0.51
1:V:388:ASN:HB2	1:V:527:PRO:HD2	1.93	0.51
1:C:599:THR:HG22	1:C:601:GLY:H	1.74	0.51
1:V:392:PHE:CZ	1:V:517:LEU:HD12	2.44	0.51
1:V:395:VAL:CG1	1:V:515:PHE:HD1	2.16	0.51
1:C:403:ARG:N	1:C:495:TYR:CZ	2.78	0.51
1:V:420:ASP:O	1:V:461:LEU:CD2	2.59	0.51
2:d:96:MET:HG2	2:d:99:ARG:HB3	1.91	0.50
1:S:107:GLY:N	1:S:235:ILE:HG22	2.26	0.50
1:V:421:TYR:C	1:V:461:LEU:HD22	2.37	0.50
1:V:355:ARG:NH2	1:V:396:TYR:HB2	2.27	0.50
1:C:327:VAL:HG13	1:C:329:PHE:CE1	2.47	0.50
1:S:426:PRO:HG3	1:S:464:PHE:CE2	2.46	0.50
1:V:380:TYR:HD2	1:V:431:GLY:CA	2.25	0.50
2:d:96:MET:SD	2:d:99:ARG:CB	3.00	0.50
1:S:106:PHE:CB	1:S:235:ILE:CG2	2.83	0.49
1:V:332:ILE:HD11	1:V:527:PRO:HA	1.93	0.49
1:V:388:ASN:O	1:V:526:GLY:CA	2.55	0.49
1:S:41:LYS:HD3	1:C:519:HIS:CD2	2.47	0.49
1:S:332:ILE:HD13	1:S:360:ASN:C	2.37	0.49
1:V:387:LEU:C	1:V:387:LEU:CD2	2.85	0.49
1:C:327:VAL:CG1	1:C:329:PHE:HE1	2.26	0.49
1:S:107:GLY:N	1:S:235:ILE:CG2	2.76	0.49
1:S:519:HIS:O	1:S:565:PHE:CZ	2.66	0.49
1:V:353:TRP:CZ3	1:V:466:ARG:HG3	2.27	0.49
1:S:355:ARG:NH2	1:S:464:PHE:CD1	2.80	0.49
1:V:368:LEU:HD22	1:V:374:PHE:HZ	1.76	0.49
1:V:422:ASN:C	1:V:461:LEU:CD1	2.80	0.49
2:d:95:TYR:CD2	2:d:100(D):TYR:N	2.64	0.49
1:V:29:THR:O	1:V:62:VAL:HG22	2.12	0.49
1:V:380:TYR:CD2	1:V:431:GLY:CA	2.96	0.48
2:d:96:MET:CG	2:d:99:ARG:NE	2.76	0.48
1:C:327:VAL:HG13	1:C:329:PHE:HE1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LEU:HD22	1:C:493:GLN:HB3	1.94	0.48
1:C:62:VAL:HG23	1:C:62:VAL:O	2.14	0.48
6:S:1207:NAG:O6	6:S:1207:NAG:O4	2.30	0.48
2:d:96:MET:CG	2:d:99:ARG:CB	2.84	0.48
1:V:379:CYS:SG	1:V:384:PRO:HD3	2.54	0.48
2:d:94:ARG:HH11	2:d:102:VAL:CB	1.87	0.48
1:V:377:PHE:HE1	1:V:432:CYS:HG	1.55	0.48
1:V:394:ASN:O	1:V:394:ASN:ND2	2.45	0.48
1:V:338:PHE:O	1:V:341:VAL:HG12	2.14	0.48
1:S:926:GLN:HE22	4:A:1:NAG:H82	1.78	0.48
1:V:422:ASN:HD21	1:V:454:ARG:CB	2.03	0.47
1:C:390:LEU:HD22	1:C:390:LEU:N	2.29	0.47
1:V:396:TYR:CD1	1:V:396:TYR:N	2.80	0.47
1:V:364:ASP:HB3	1:V:526:GLY:HA2	1.96	0.47
1:V:371:SER:CB	1:V:374:PHE:HD2	2.03	0.47
1:C:265:TYR:CG	1:C:265:TYR:O	2.67	0.47
1:C:364:ASP:HB2	1:C:527:PRO:HG3	1.97	0.47
1:S:409:GLN:CB	1:S:418:ILE:CG2	2.93	0.47
2:d:96:MET:CE	2:d:99:ARG:CG	2.83	0.47
1:S:237:ARG:CG	1:S:237:ARG:HH11	2.28	0.47
1:V:358:ILE:HG22	1:V:524:VAL:CG2	2.42	0.47
1:V:378:LYS:HB2	1:V:378:LYS:HE2	1.44	0.47
1:V:353:TRP:N	1:V:466:ARG:HH21	2.12	0.47
1:V:383:SER:HB3	1:V:386:LYS:HG3	1.97	0.47
1:V:335:LEU:HD13	1:V:335:LEU:N	2.29	0.47
1:V:353:TRP:HB2	1:V:354:ASN:H	1.56	0.47
1:V:395:VAL:CB	1:V:514:SER:O	2.63	0.47
1:S:408:ARG:N	1:S:408:ARG:CD	2.73	0.47
1:V:421:TYR:CG	1:V:457:ARG:CB	2.97	0.47
1:C:329:PHE:HD2	1:C:525:CYS:HB3	1.80	0.47
1:C:105:ILE:HD12	1:C:135:PHE:CE1	2.50	0.46
2:d:95:TYR:N	2:d:95:TYR:HD1	2.13	0.46
1:V:335:LEU:HA	1:V:363:ALA:HA	1.97	0.46
1:V:350:VAL:CG2	1:V:422:ASN:CG	2.88	0.46
1:V:352:ALA:CB	1:V:468:ILE:HG22	2.45	0.46
1:V:373:SER:O	1:V:436:TRP:CB	2.63	0.46
1:S:237:ARG:NH1	1:S:237:ARG:CG	2.77	0.46
1:V:350:VAL:CG2	1:V:422:ASN:HB3	2.45	0.46
1:S:233:ILE:CG2	1:S:235:ILE:HG12	2.44	0.46
1:V:350:VAL:CG2	1:V:422:ASN:OD1	2.58	0.46
1:S:110:LEU:HD21	1:S:237:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:332:ILE:CD1	1:V:527:PRO:HA	2.45	0.46
1:V:355:ARG:HD2	1:V:355:ARG:HA	1.62	0.46
1:V:353:TRP:N	1:V:466:ARG:NH2	2.63	0.46
1:S:29:THR:OG1	1:S:62:VAL:HG23	2.16	0.46
1:S:31:SER:HB3	1:S:62:VAL:CG1	2.46	0.46
1:V:421:TYR:HD1	1:V:457:ARG:HB3	1.60	0.46
1:S:41:LYS:HD3	1:C:519:HIS:NE2	2.32	0.45
1:V:335:LEU:N	1:V:335:LEU:CD1	2.79	0.45
1:V:392:PHE:CE2	1:V:515:PHE:HB3	2.51	0.45
1:S:342:PHE:CZ	1:S:511:VAL:CG2	3.00	0.45
1:V:353:TRP:CE3	1:V:353:TRP:N	2.76	0.45
1:V:358:ILE:N	1:V:358:ILE:CD1	2.73	0.45
1:S:374:PHE:CD1	1:S:434:ILE:HD11	2.52	0.45
1:S:387:LEU:C	1:S:389:ASP:H	2.24	0.45
1:C:265:TYR:CD1	1:C:265:TYR:O	2.70	0.45
1:C:714:ILE:HD12	1:C:1096:VAL:HG11	1.99	0.45
1:S:718:PHE:CD1	1:S:718:PHE:O	2.70	0.45
1:V:375:SER:CB	1:V:435:ALA:O	2.65	0.45
1:V:395:VAL:HG12	1:V:395:VAL:O	2.18	0.44
2:d:96:MET:HE2	2:d:99:ARG:HG3	1.98	0.44
1:S:107:GLY:O	1:S:235:ILE:HA	2.16	0.44
1:V:335:LEU:C	1:V:363:ALA:CB	2.76	0.44
1:V:714:ILE:HD12	1:V:1096:VAL:HG11	1.99	0.44
1:V:375:SER:CA	1:V:435:ALA:O	2.66	0.44
1:V:369:TYR:HA	1:V:377:PHE:HE2	1.80	0.44
1:V:385:THR:H	1:V:385:THR:HG1	1.50	0.44
1:V:470:THR:HG21	2:d:54:PHE:CZ	2.53	0.44
1:S:83:VAL:HG12	1:S:237:ARG:CD	2.30	0.44
1:V:360:ASN:C	1:V:523:THR:O	2.60	0.44
1:V:393:THR:CG2	1:V:521:PRO:O	2.61	0.44
1:V:421:TYR:HD1	1:V:457:ARG:HD3	1.83	0.44
1:S:393:THR:CG2	1:S:518:LEU:HD11	2.45	0.44
1:V:357:ARG:NE	1:V:357:ARG:N	2.60	0.43
1:V:422:ASN:N	1:V:461:LEU:HD22	2.32	0.43
1:S:519:HIS:O	1:S:565:PHE:HZ	2.01	0.43
1:C:387:LEU:HA	1:C:390:LEU:HD23	1.98	0.43
1:S:926:GLN:HE21	4:A:1:NAG:C8	2.31	0.43
1:C:877:LEU:HD13	1:C:1029:MET:SD	2.58	0.43
1:S:327:VAL:CG1	1:S:329:PHE:CE2	3.02	0.43
1:V:368:LEU:N	1:V:368:LEU:HD23	2.34	0.43
1:V:380:TYR:OH	1:V:432:CYS:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:380:TYR:HB2	1:V:429:PHE:CD2	2.54	0.43
1:V:380:TYR:C	1:V:430:THR:HA	2.38	0.43
1:V:394:ASN:ND2	1:V:516:GLU:O	2.52	0.43
1:S:408:ARG:HH11	1:S:408:ARG:HD2	1.65	0.43
1:C:329:PHE:CD2	1:C:525:CYS:HB3	2.54	0.43
1:C:390:LEU:N	1:C:390:LEU:CD2	2.82	0.43
1:S:106:PHE:CB	1:S:235:ILE:HG21	2.24	0.42
1:S:332:ILE:HD13	1:S:360:ASN:HA	2.00	0.42
1:V:360:ASN:HA	1:V:523:THR:HB	2.01	0.42
1:V:352:ALA:HB2	1:V:468:ILE:CG2	2.50	0.42
1:V:364:ASP:CB	1:V:526:GLY:CA	2.95	0.42
1:V:364:ASP:HB2	1:V:526:GLY:CA	2.48	0.42
1:V:359:SER:O	1:V:523:THR:CB	2.61	0.42
1:V:359:SER:C	1:V:523:THR:HB	2.43	0.42
1:V:418:ILE:O	1:V:422:ASN:HB2	2.19	0.42
1:C:338:PHE:C	1:C:341:VAL:HG13	2.44	0.42
1:C:404:GLY:HA3	1:C:508:TYR:CE1	2.55	0.42
1:V:395:VAL:CA	1:V:514:SER:O	2.68	0.41
1:C:389:ASP:OD1	1:C:389:ASP:N	2.51	0.41
1:V:449:TYR:CZ	2:d:96:MET:HE1	2.55	0.41
1:C:31:SER:HB3	1:C:62:VAL:HG13	2.01	0.41
1:V:382:VAL:CG1	1:V:515:PHE:HE2	2.22	0.41
1:S:429:PHE:CZ	1:S:431:GLY:HA3	2.55	0.41
1:V:363:ALA:N	1:V:525:CYS:O	2.53	0.41
1:C:92:PHE:CE2	1:C:265:TYR:CE1	3.09	0.41
1:V:392:PHE:CZ	1:V:517:LEU:HD11	2.55	0.41
1:C:329:PHE:HD2	1:C:525:CYS:SG	2.44	0.41
1:C:493:GLN:O	1:C:493:GLN:CG	2.68	0.41
1:C:329:PHE:CD2	1:C:525:CYS:SG	3.14	0.41
2:d:34:ILE:HG13	2:d:94:ARG:HB3	2.02	0.41
1:S:699:LEU:H	1:S:699:LEU:HD12	1.86	0.40
1:V:349:SER:HB2	1:V:351:TYR:HE1	1.86	0.40
1:C:341:VAL:O	1:C:341:VAL:CG2	2.68	0.40
3:b:23:CYS:SG	3:b:88:CYS:SG	3.10	0.40
1:V:395:VAL:CG1	1:V:395:VAL:O	2.69	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	C	972/1121 (87%)	904 (93%)	62 (6%)	6 (1%)	21	49
1	S	971/1121 (87%)	899 (93%)	65 (7%)	7 (1%)	18	47
1	V	964/1121 (86%)	895 (93%)	64 (7%)	5 (0%)	24	54
2	H	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
2	a	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
2	d	120/122 (98%)	107 (89%)	12 (10%)	1 (1%)	16	44
3	L	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
3	b	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
3	c	104/106 (98%)	98 (94%)	5 (5%)	1 (1%)	12	39
All	All	3579/4047 (88%)	3320 (93%)	239 (7%)	20 (1%)	23	49

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	110	LEU
1	S	122	ASN
1	S	518	LEU
1	S	528	LYS
1	V	364	ASP
1	C	112	SER
1	S	123	ALA
1	V	350	VAL
1	V	420	ASP
1	C	604	THR
2	d	83	ARG
1	S	582	LEU
1	V	351	TYR
1	V	1091	ARG
3	c	60	SER
1	C	582	LEU

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Mol	Chain	Res	Type
1	C	123	ALA
1	C	614	ASP
1	C	476	GLY
1	S	231	ILE

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	C	827/972 (85%)	812 (98%)	15 (2%)	51	66
1	S	833/972 (86%)	804 (96%)	29 (4%)	32	55
1	V	830/972 (85%)	791 (95%)	39 (5%)	23	49
2	H	101/101 (100%)	99 (98%)	2 (2%)	48	65
2	a	101/101 (100%)	100 (99%)	1 (1%)	68	74
2	d	101/101 (100%)	97 (96%)	4 (4%)	28	52
3	L	92/92 (100%)	91 (99%)	1 (1%)	65	73
3	b	92/92 (100%)	92 (100%)	0	100	100
3	c	92/92 (100%)	91 (99%)	1 (1%)	65	73
All	All	3069/3495 (88%)	2977 (97%)	92 (3%)	37	59

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	96	GLU
1	S	108	THR
1	S	110	LEU
1	S	122	ASN
1	S	231	ILE
1	S	233	ILE
1	S	235	ILE
1	S	237	ARG
1	S	346	ARG
1	S	367	VAL

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Mol	Chain	Res	Type
1	S	390	LEU
1	S	408	ARG
1	S	414	GLN
1	S	415	THR
1	S	427	ASP
1	S	441	LEU
1	S	457	ARG
1	S	461	LEU
1	S	483	VAL
1	S	518	LEU
1	S	519	HIS
1	S	531	THR
1	S	546	LEU
1	S	565	PHE
1	S	878	LEU
1	S	887	THR
1	S	975	SER
1	S	1004	LEU
1	S	1081	ILE
1	V	117	LEU
1	V	130	VAL
1	V	303	LEU
1	V	333	THR
1	V	334	ASN
1	V	335	LEU
1	V	336	CYS
1	V	343	ASN
1	V	346	ARG
1	V	350	VAL
1	V	351	TYR
1	V	353	TRP
1	V	355	ARG
1	V	356	LYS
1	V	357	ARG
1	V	358	ILE
1	V	364	ASP
1	V	367	VAL
1	V	370	ASN
1	V	373	SER
1	V	378	LYS
1	V	379	CYS
1	V	380	TYR

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Mol	Chain	Res	Type
1	V	385	THR
1	V	390	LEU
1	V	393	THR
1	V	394	ASN
1	V	395	VAL
1	V	396	TYR
1	V	408	ARG
1	V	546	LEU
1	V	567	ARG
1	V	658	ASN
1	V	716	THR
1	V	760	CYS
1	V	791	THR
1	V	820	ASP
1	V	931	ILE
1	V	1004	LEU
1	C	265	TYR
1	C	267	VAL
1	C	340	GLU
1	C	341	VAL
1	C	389	ASP
1	C	392	PHE
1	C	474	GLN
1	C	493	GLN
1	C	501	ASN
1	C	546	LEU
1	C	572	THR
1	C	578	ASP
1	C	760	CYS
1	C	984	LEU
1	C	1135	ASN
2	H	18	VAL
2	H	99	ARG
3	L	4	MET
2	a	67	VAL
3	c	33	LEU
2	d	85	GLU
2	d	94	ARG
2	d	95	TYR
2	d	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	49	HIS
1	S	211	ASN
1	S	481	ASN
1	S	536	ASN
1	S	606	ASN
1	S	690	GLN
1	S	755	GLN
1	S	919	ASN
1	S	926	GLN
1	S	1002	GLN
1	S	1005	GLN
1	S	1108	ASN
1	S	1135	ASN
1	V	188	ASN
1	V	314	GLN
1	V	317	ASN
1	V	370	ASN
1	V	414	GLN
1	V	422	ASN
1	V	460	ASN
1	V	506	GLN
1	V	540	ASN
1	V	606	ASN
1	V	762	GLN
1	V	784	GLN
1	V	804	GLN
1	V	957	GLN
1	V	969	ASN
1	V	1002	GLN
1	V	1005	GLN
1	V	1108	ASN
1	C	49	HIS
1	C	99	ASN
1	C	188	ASN
1	C	196	ASN
1	C	460	ASN
1	C	481	ASN
1	C	501	ASN
1	C	690	GLN
1	C	764	ASN
1	C	804	GLN
1	C	969	ASN
1	C	1002	GLN

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Mol	Chain	Res	Type
2	H	39	GLN
3	L	38	GLN
3	L	79	GLN
3	c	38	GLN
2	d	39	GLN
3	b	34	ASN
3	b	38	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 ⓘ

27 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	$\# Z > 2$
4	NAG	A	1	4,1	14,14,15	2.54	5 (35%)	17,19,21	2.45	5 (29%)
4	NAG	A	2	4	14,14,15	0.72	0	17,19,21	2.20	5 (29%)
4	BMA	A	3	4	11,11,12	0.42	0	15,15,17	1.87	4 (26%)
5	NAG	B	1	5,1	14,14,15	0.54	0	17,19,21	2.32	6 (35%)
5	NAG	B	2	5	14,14,15	0.43	0	17,19,21	1.17	2 (11%)
5	NAG	D	1	5,1	14,14,15	0.28	0	17,19,21	0.64	0
5	NAG	D	2	5	14,14,15	0.28	0	17,19,21	0.68	0
5	NAG	E	1	5,1	14,14,15	0.28	0	17,19,21	0.69	0
5	NAG	E	2	5	14,14,15	0.27	0	17,19,21	0.61	0
5	NAG	F	1	5,1	14,14,15	1.20	1 (7%)	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	2	5	14,14,15	1.23	1 (7%)	17,19,21	0.84	1 (5%)
5	NAG	G	1	5,1	14,14,15	1.23	1 (7%)	17,19,21	0.90	2 (11%)
5	NAG	G	2	5	14,14,15	1.20	1 (7%)	17,19,21	0.84	1 (5%)
5	NAG	I	1	5,1	14,14,15	1.17	1 (7%)	17,19,21	0.65	0
5	NAG	I	2	5	14,14,15	1.24	1 (7%)	17,19,21	0.73	0
5	NAG	J	1	5,1	14,14,15	1.28	1 (7%)	17,19,21	0.95	1 (5%)
5	NAG	J	2	5	14,14,15	1.24	1 (7%)	17,19,21	0.78	0
5	NAG	K	1	5,1	14,14,15	1.21	1 (7%)	17,19,21	0.68	0
5	NAG	K	2	5	14,14,15	1.21	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	M	1	5,1	14,14,15	1.20	2 (14%)	17,19,21	0.71	0
5	NAG	M	2	5	14,14,15	1.25	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	N	1	5,1	14,14,15	1.26	1 (7%)	17,19,21	0.79	0
5	NAG	N	2	5	14,14,15	1.22	1 (7%)	17,19,21	0.76	0
5	NAG	O	1	5,1	14,14,15	1.23	2 (14%)	17,19,21	0.65	0
5	NAG	O	2	5	14,14,15	1.27	2 (14%)	17,19,21	0.78	1 (5%)
5	NAG	W	1	5,1	14,14,15	1.19	1 (7%)	17,19,21	0.76	0
5	NAG	W	2	5	14,14,15	1.28	1 (7%)	17,19,21	1.04	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	A	2	4	-	4/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1
5	NAG	B	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	B	2	5	-	3/6/23/26	0/1/1/1
5	NAG	D	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	D	2	5	-	1/6/23/26	0/1/1/1
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	NAG	G	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	O5-C1	-5.32	1.34	1.43
4	A	1	NAG	C1-C2	-4.65	1.46	1.52
4	A	1	NAG	O5-C5	-3.73	1.36	1.43
4	A	1	NAG	C2-N2	-3.12	1.41	1.46
5	J	2	NAG	O5-C5	2.84	1.49	1.43
5	I	2	NAG	O5-C5	2.83	1.48	1.43
5	W	2	NAG	O5-C5	2.81	1.48	1.43
5	N	2	NAG	O5-C5	2.79	1.48	1.43
5	F	2	NAG	O5-C5	2.76	1.48	1.43
5	J	1	NAG	O5-C5	2.76	1.48	1.43
5	M	2	NAG	O5-C5	2.74	1.48	1.43
5	G	2	NAG	O5-C5	2.69	1.48	1.43
5	N	1	NAG	O5-C5	2.63	1.48	1.43
5	K	2	NAG	O5-C5	2.62	1.48	1.43
5	O	2	NAG	O5-C5	2.49	1.48	1.43
5	G	1	NAG	O5-C5	2.48	1.48	1.43
5	W	1	NAG	O5-C5	2.32	1.47	1.43
5	O	1	NAG	O5-C5	2.30	1.47	1.43
5	K	1	NAG	O5-C5	2.29	1.47	1.43
5	M	1	NAG	O5-C5	2.24	1.47	1.43
5	I	1	NAG	O5-C5	2.20	1.47	1.43
5	F	1	NAG	O5-C5	2.20	1.47	1.43
5	O	2	NAG	O5-C1	2.19	1.47	1.43
4	A	1	NAG	C3-C2	-2.17	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	O4-C4	2.11	1.48	1.43
5	O	1	NAG	O4-C4	2.02	1.48	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	O4-C4-C3	6.34	125.32	110.38
5	B	1	NAG	C1-C2-N2	-5.37	101.97	110.43
4	A	2	NAG	O3-C3-C4	-4.94	98.73	110.38
4	A	1	NAG	O5-C5-C6	-4.61	98.69	107.66
5	B	1	NAG	C1-O5-C5	4.37	118.05	112.19
5	B	1	NAG	O4-C4-C5	4.26	119.81	109.32
4	A	2	NAG	O3-C3-C2	-4.16	100.75	109.40
4	A	2	NAG	C2-N2-C7	4.01	128.27	122.90
4	A	1	NAG	C1-C2-N2	-3.81	104.42	110.43
4	A	3	BMA	O5-C1-C2	-3.36	102.77	110.79
4	A	3	BMA	C1-O5-C5	3.32	116.64	112.19
5	B	1	NAG	O3-C3-C4	-3.25	102.72	110.38
4	A	3	BMA	O2-C2-C3	-3.02	103.90	110.15
4	A	1	NAG	C4-C3-C2	-2.95	106.70	111.02
5	M	2	NAG	C1-O5-C5	2.76	115.88	112.19
5	G	2	NAG	C1-O5-C5	2.59	115.65	112.19
5	B	2	NAG	O5-C1-C2	-2.54	107.36	111.29
4	A	2	NAG	C1-O5-C5	2.51	115.55	112.19
4	A	1	NAG	O5-C5-C4	-2.46	104.85	110.83
5	W	2	NAG	C1-O5-C5	2.45	115.46	112.19
4	A	3	BMA	C2-C3-C4	-2.44	106.56	110.86
5	B	2	NAG	C1-O5-C5	2.40	115.41	112.19
5	O	2	NAG	C1-O5-C5	2.34	115.33	112.19
5	F	2	NAG	C1-O5-C5	2.32	115.30	112.19
5	B	1	NAG	O5-C5-C6	2.25	112.04	107.66
5	B	1	NAG	O5-C1-C2	-2.23	107.85	111.29
5	J	1	NAG	C1-O5-C5	2.19	115.12	112.19
5	K	2	NAG	C1-O5-C5	2.19	115.12	112.19
5	G	1	NAG	C3-C4-C5	2.12	114.08	110.23
4	A	2	NAG	C6-C5-C4	-2.09	107.89	113.02
5	G	1	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

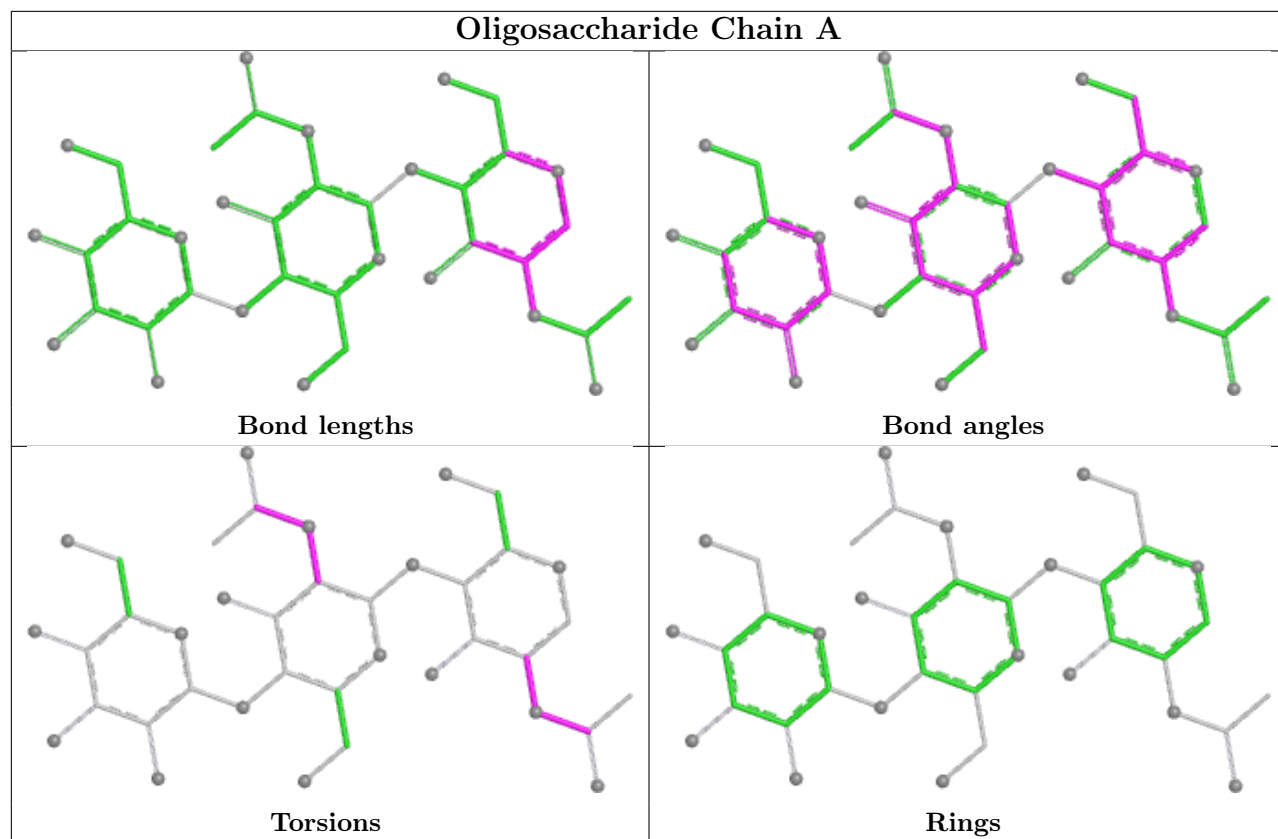
Mol	Chain	Res	Type	Atoms
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
5	B	1	NAG	C1-C2-N2-C7
5	D	1	NAG	C1-C2-N2-C7
5	D	2	NAG	C1-C2-N2-C7
5	B	1	NAG	C4-C5-C6-O6
5	B	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C8-C7-N2-C2
5	B	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
5	B	1	NAG	O7-C7-N2-C2
5	O	2	NAG	O5-C5-C6-O6
4	A	1	NAG	C3-C2-N2-C7
5	B	2	NAG	C3-C2-N2-C7
5	W	2	NAG	C1-C2-N2-C7
4	A	2	NAG	C3-C2-N2-C7
5	B	2	NAG	C8-C7-N2-C2
5	B	2	NAG	O7-C7-N2-C2
4	A	2	NAG	C1-C2-N2-C7
5	W	2	NAG	C3-C2-N2-C7
5	D	1	NAG	C8-C7-N2-C2
5	D	1	NAG	O7-C7-N2-C2

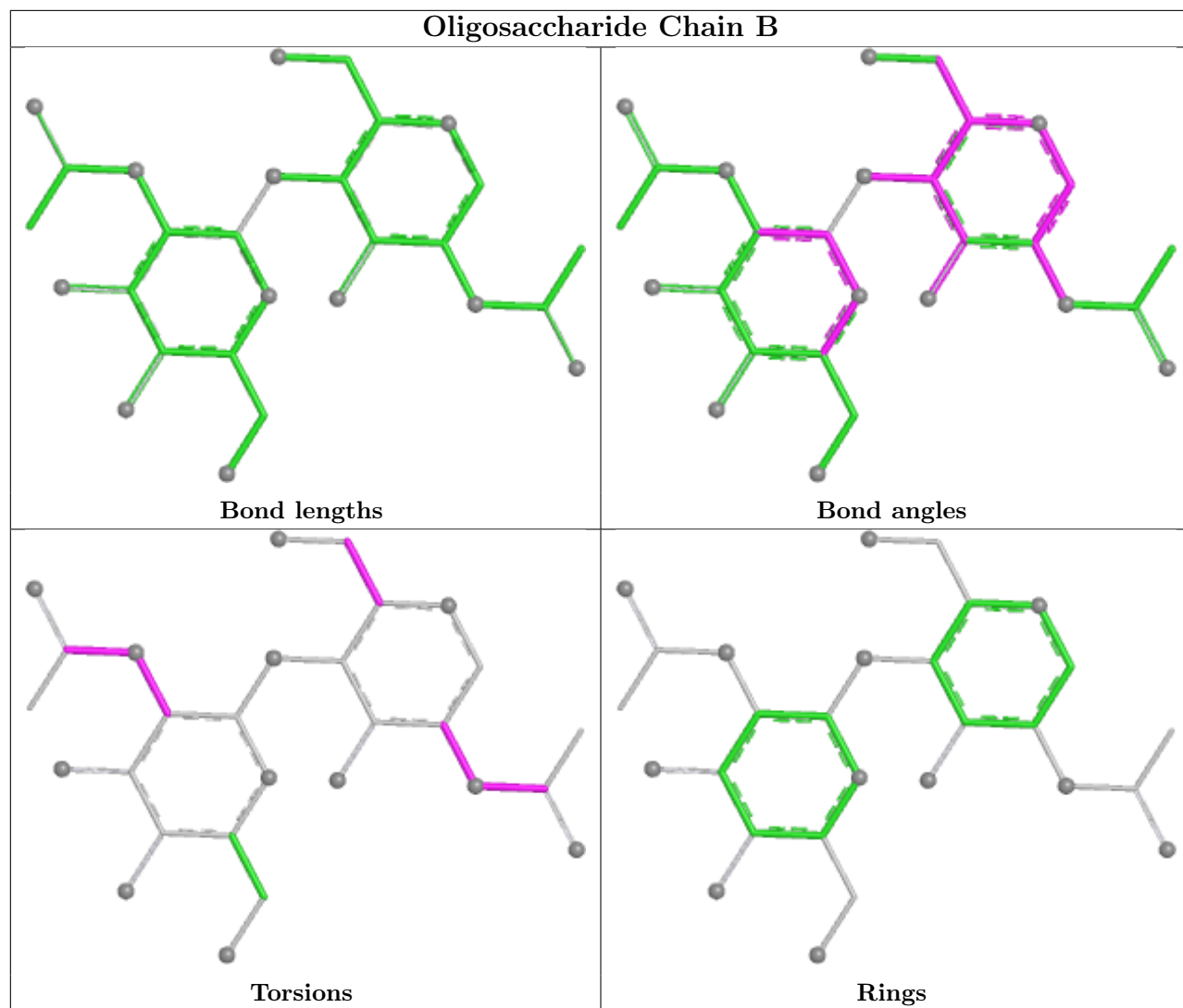
There are no ring outliers.

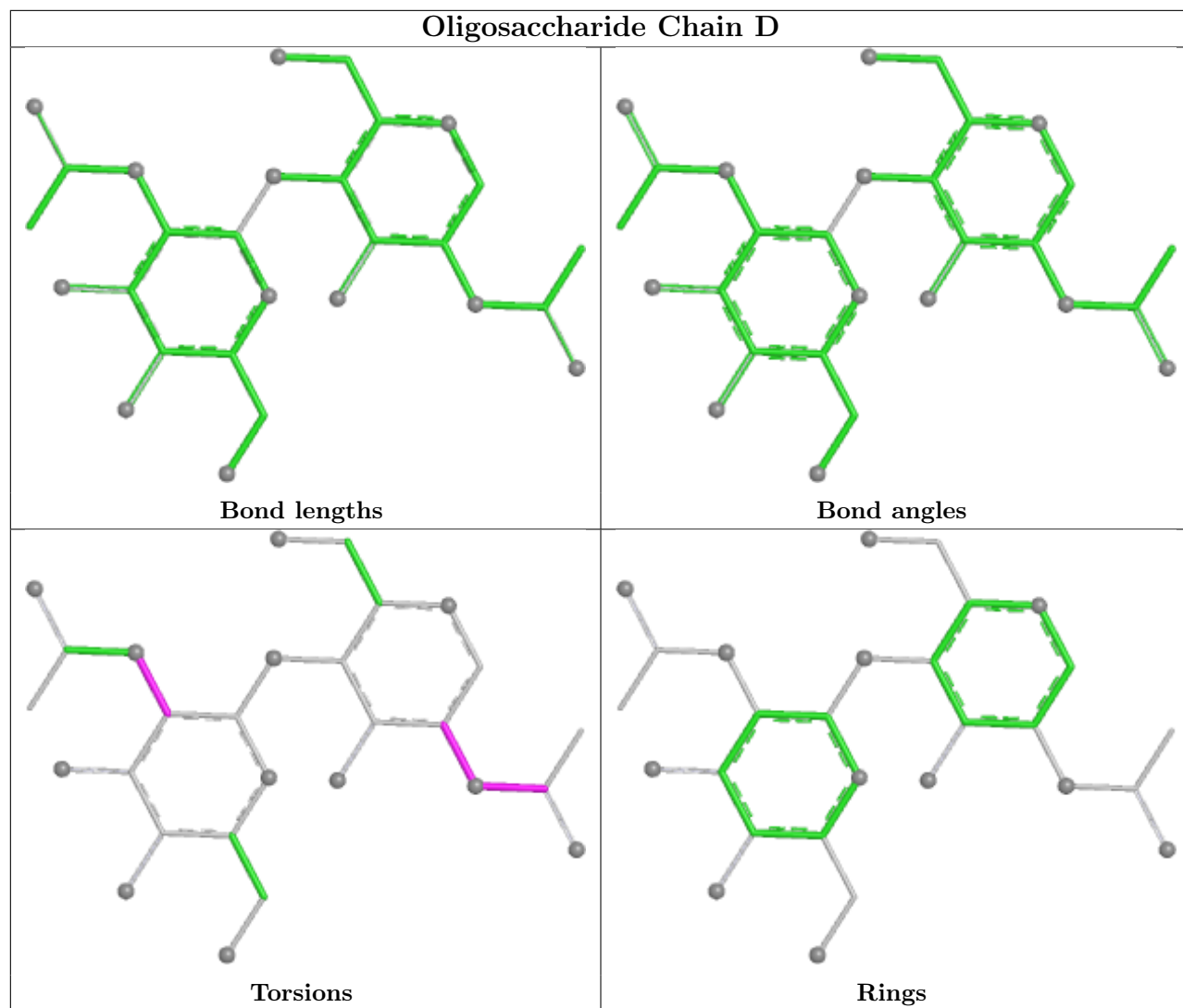
3 monomers are involved in 8 short contacts:

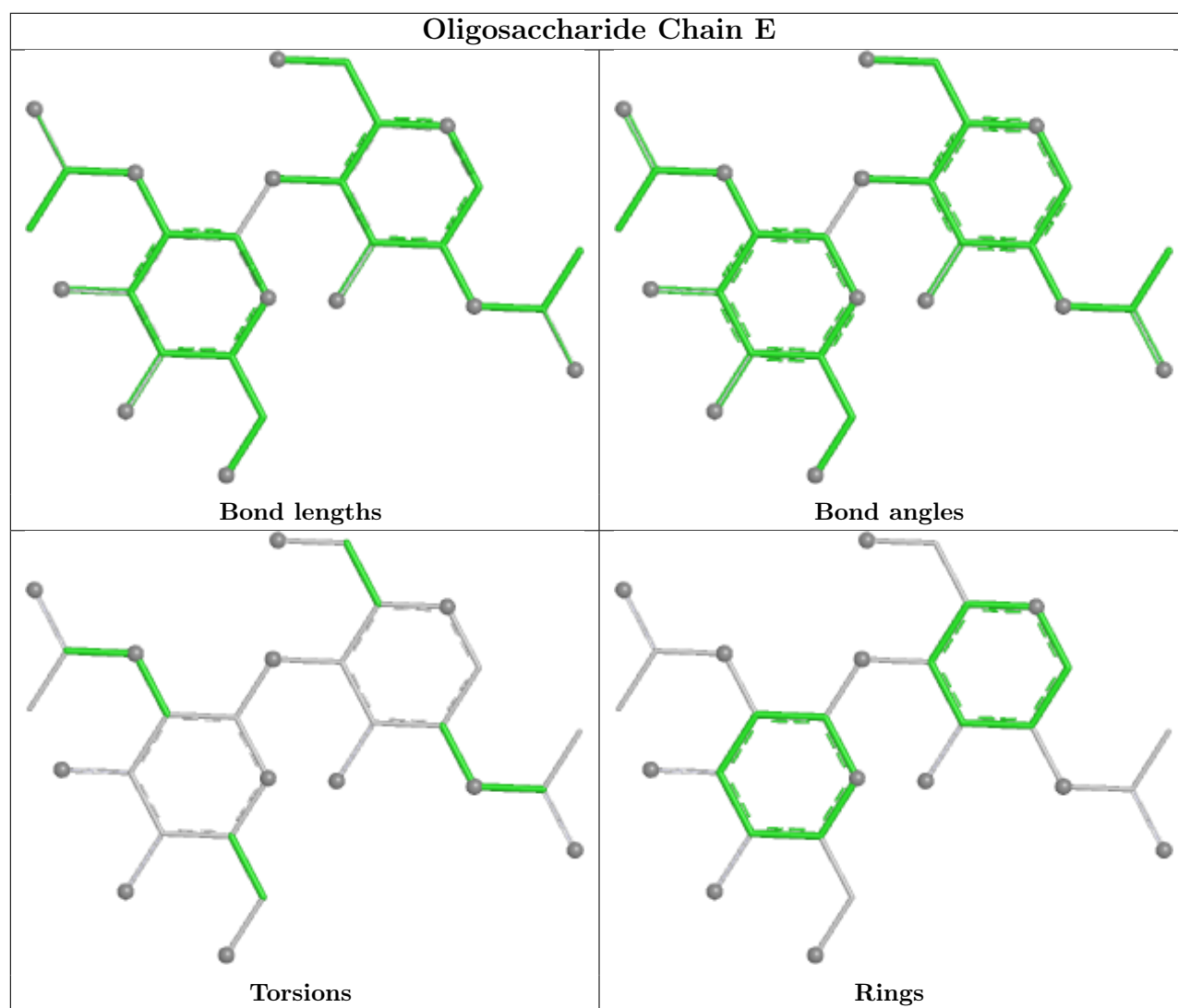
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	5	0
5	B	1	NAG	2	0
5	B	2	NAG	2	0

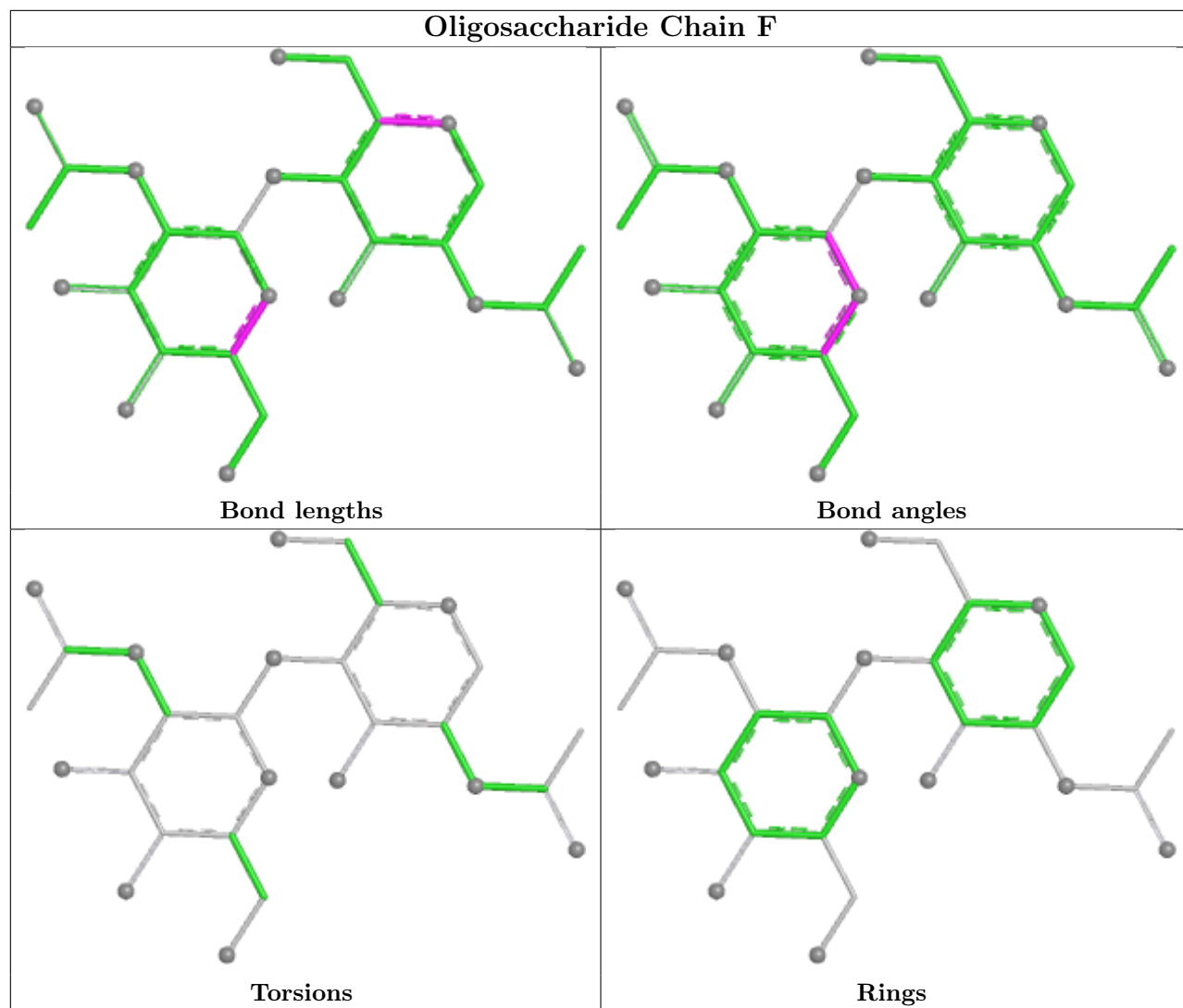
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

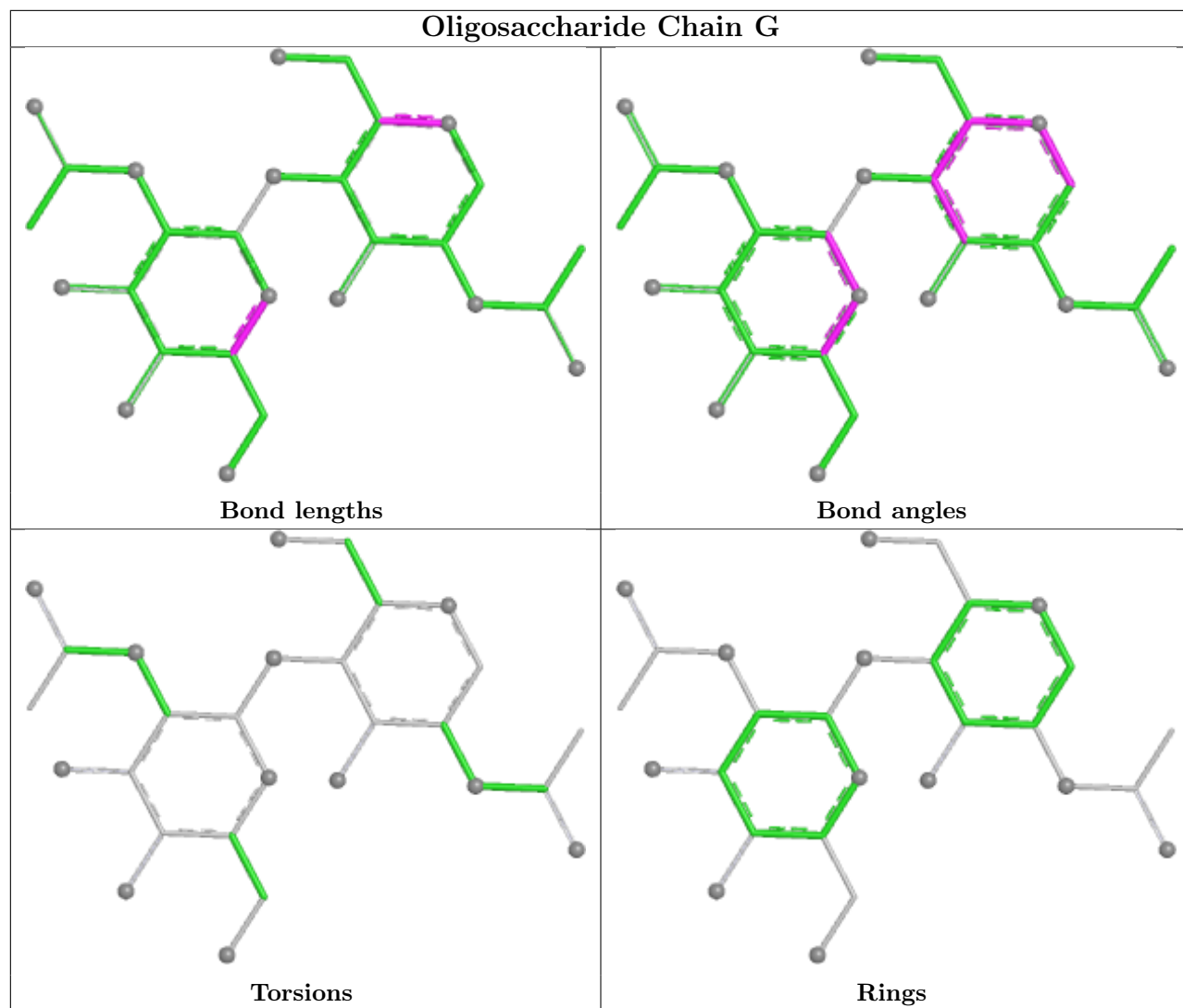


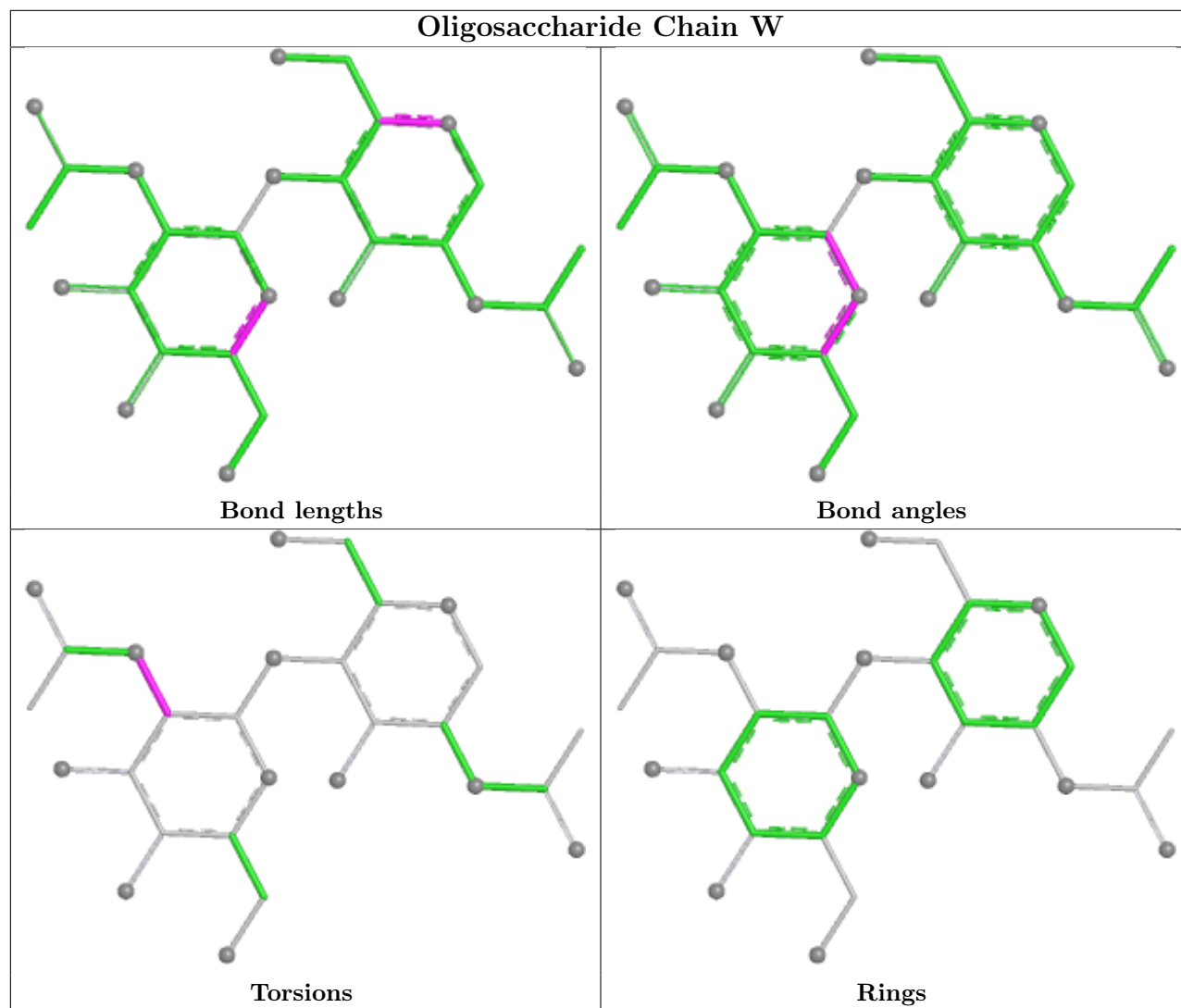


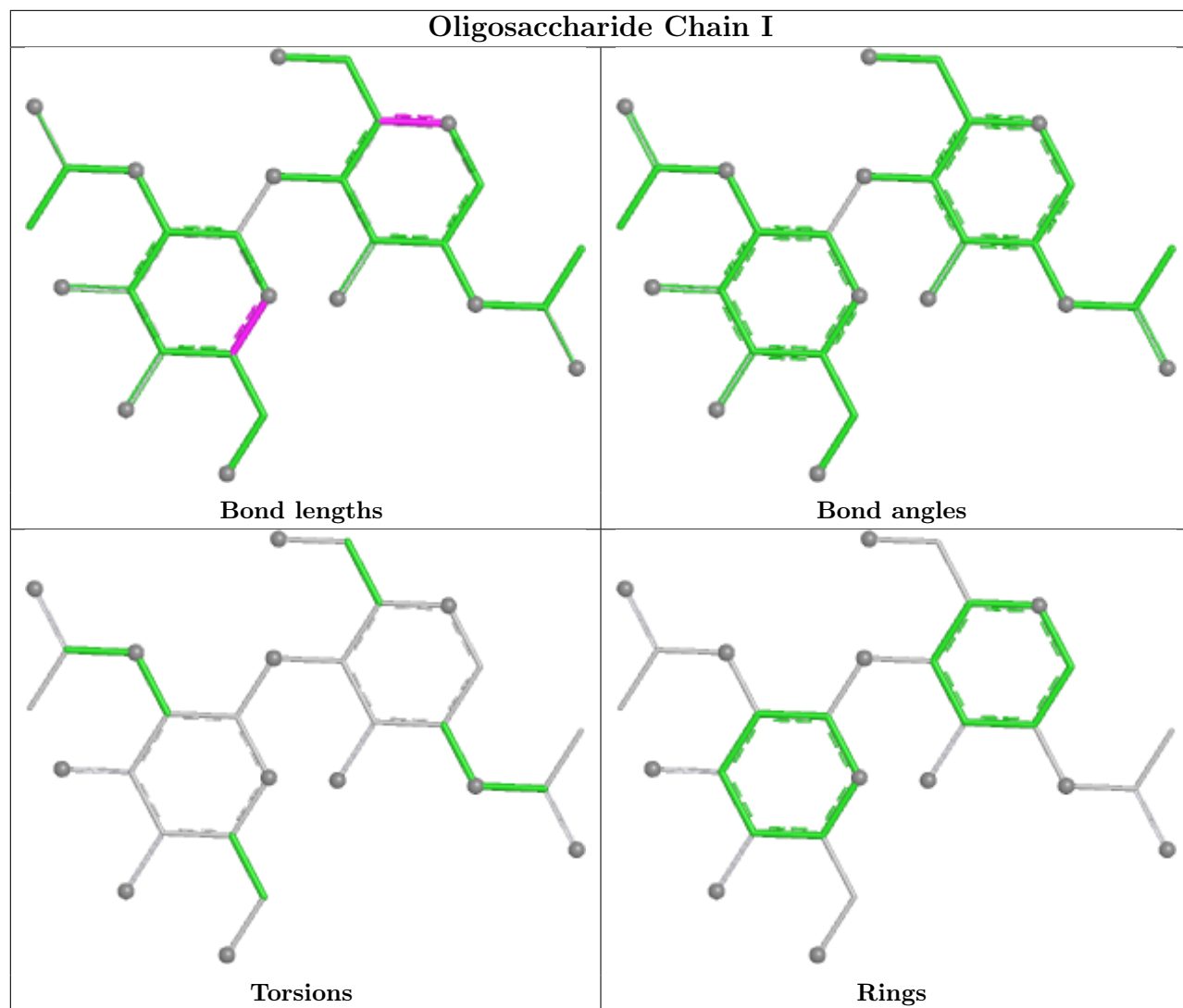


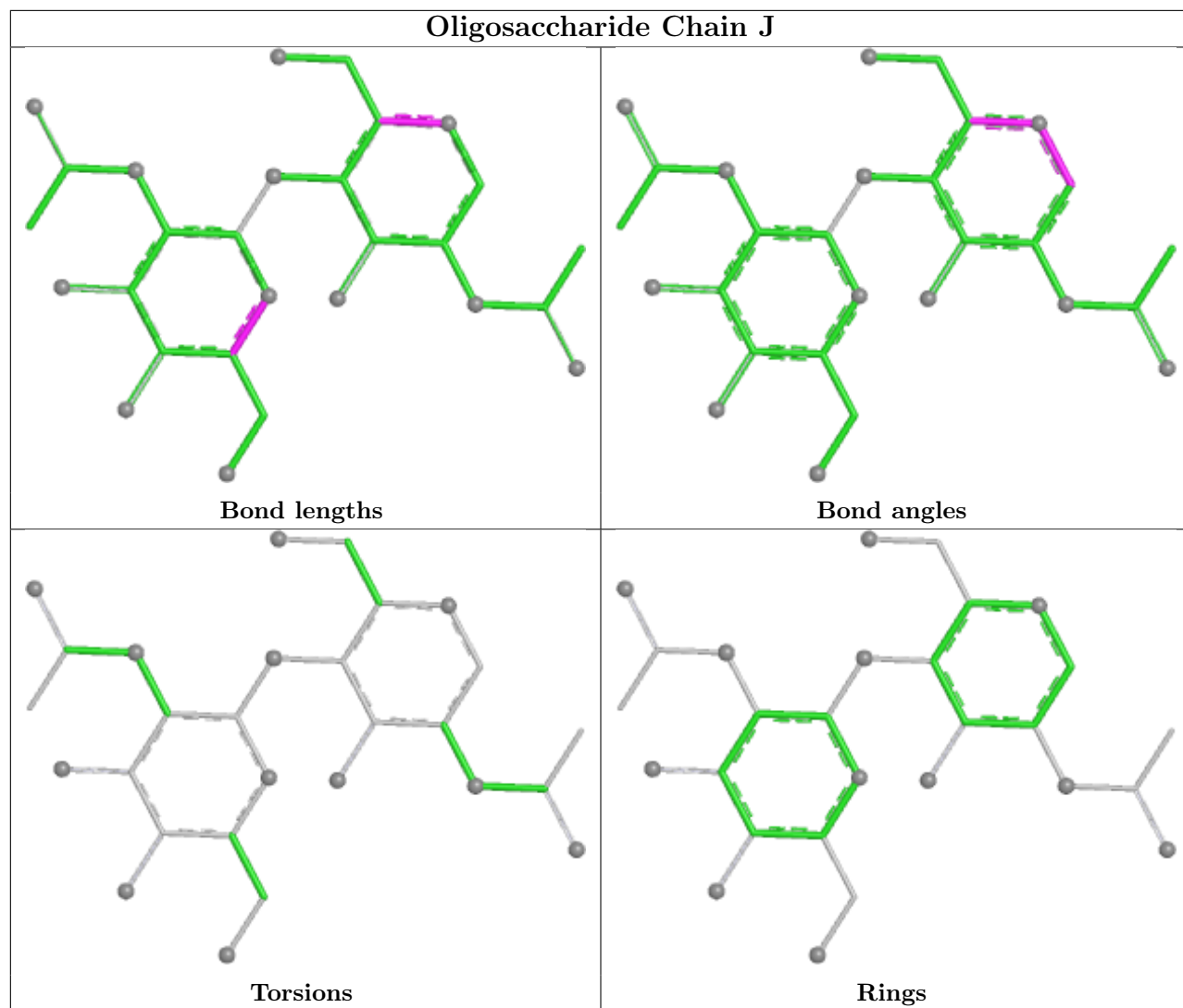


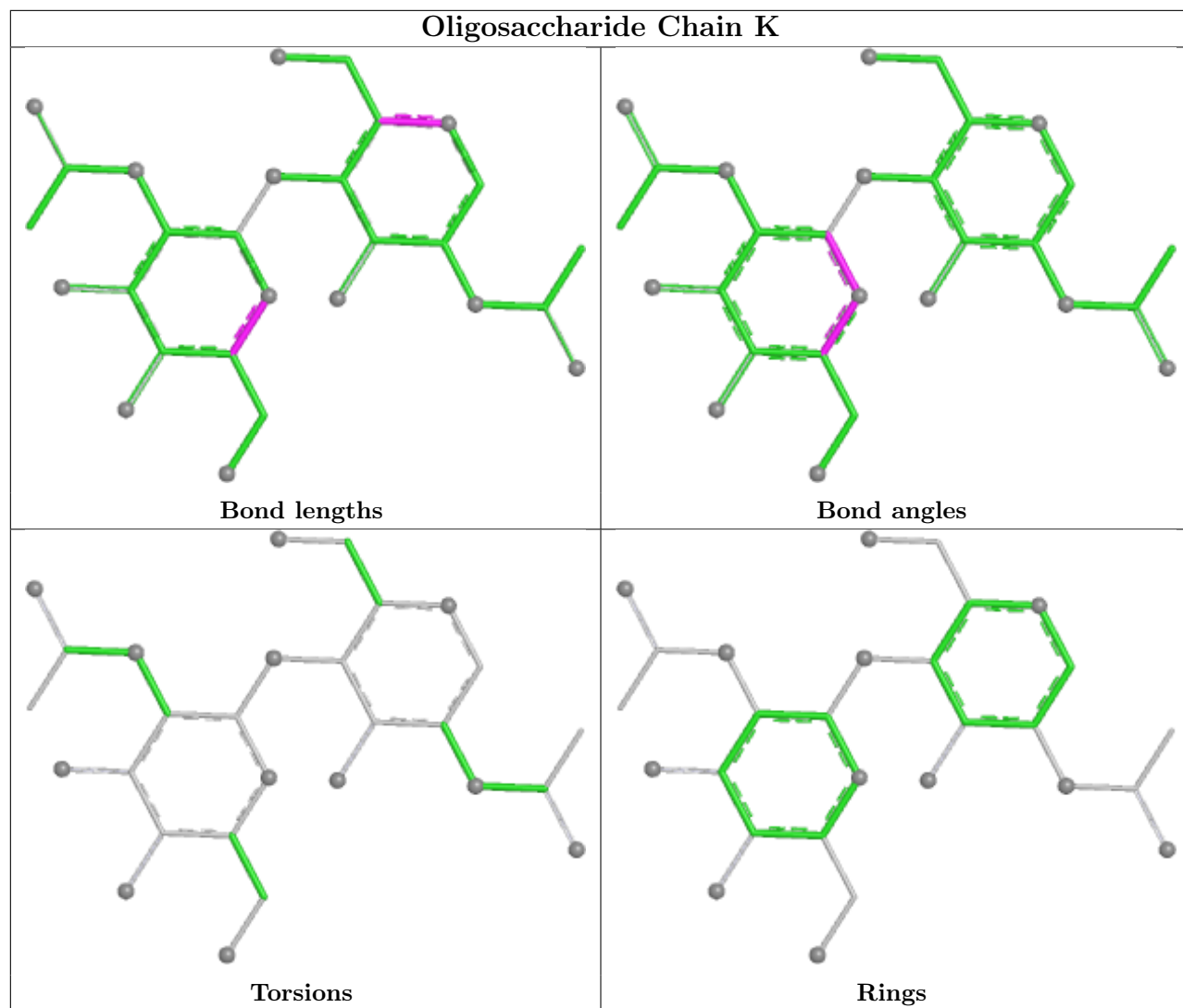


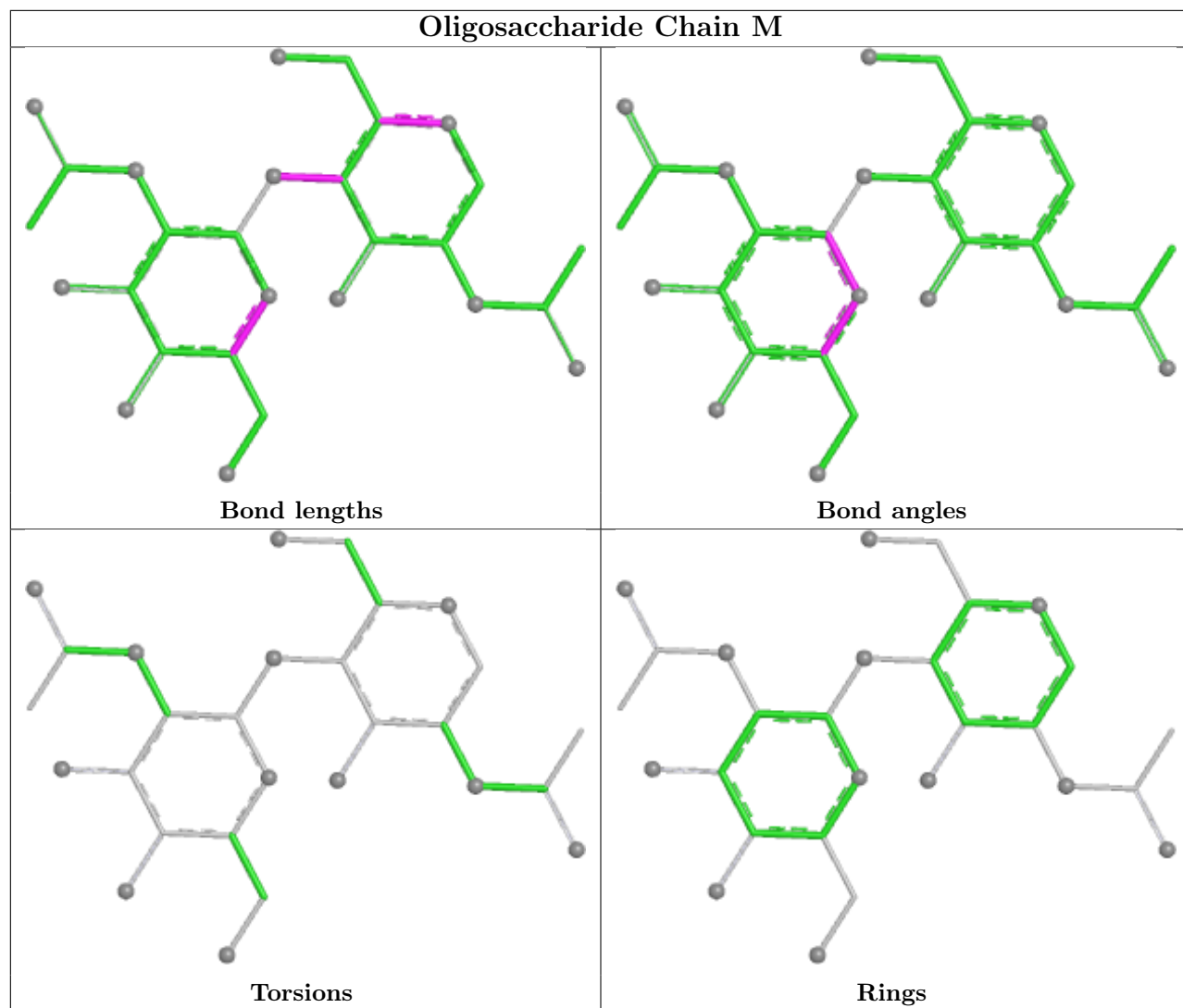


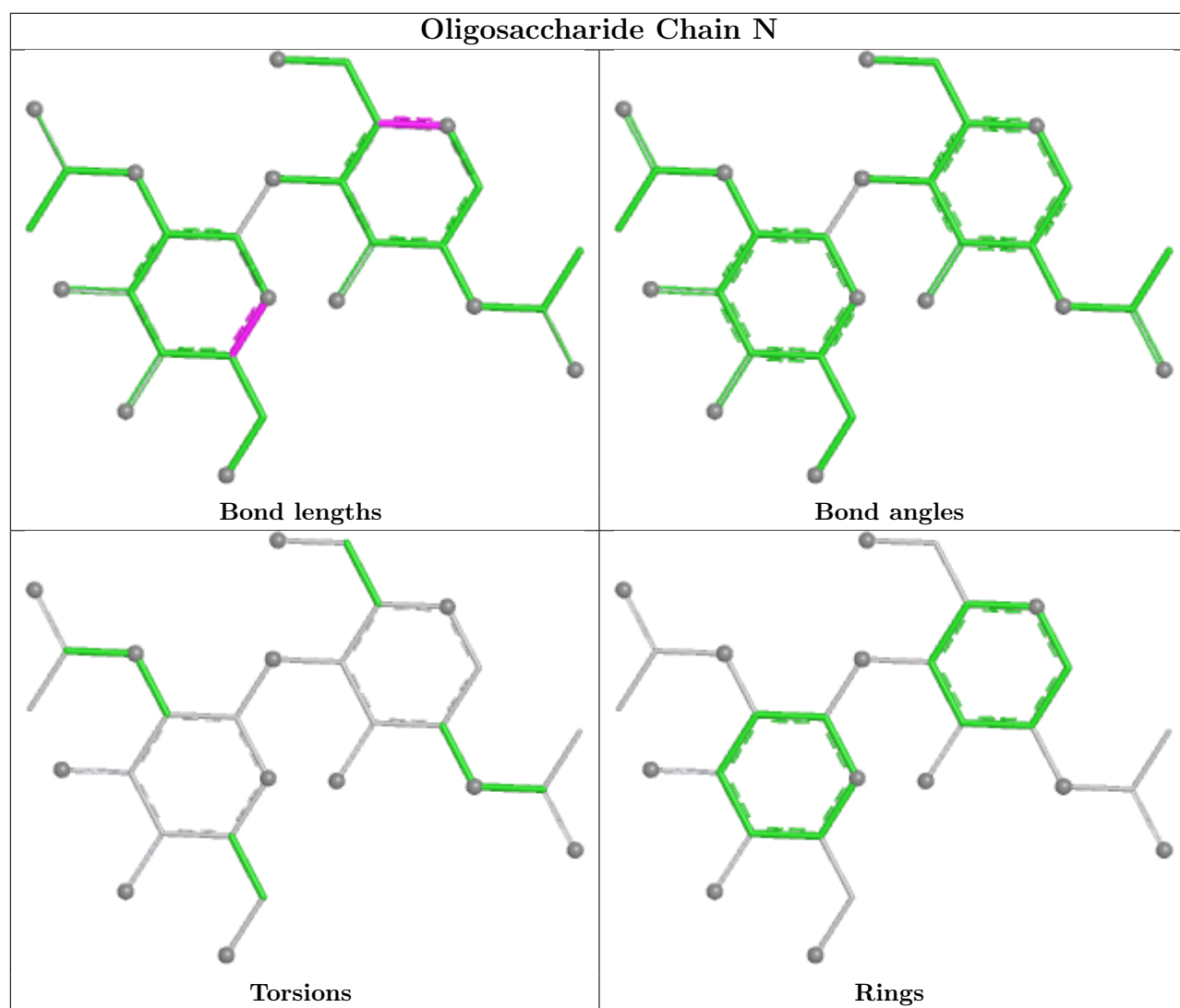


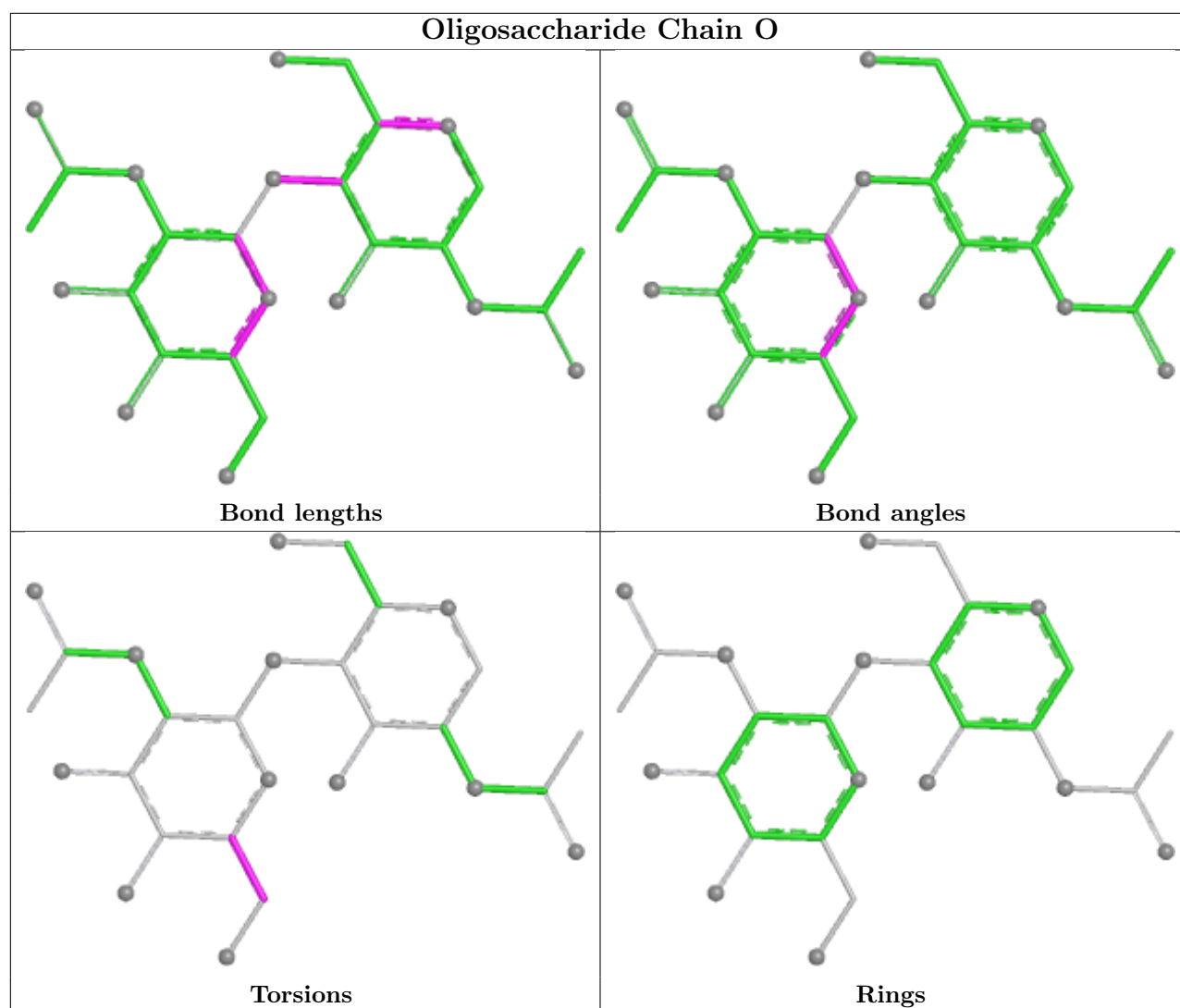












5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	1210	1	14,14,15	1.34	3 (21%)	17,19,21	0.90	1 (5%)
6	NAG	V	1208	1	14,14,15	1.22	1 (7%)	17,19,21	0.77	1 (5%)
6	NAG	V	1212	1	14,14,15	0.34	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	V	1201	1	14,14,15	1.29	3 (21%)	17,19,21	1.10	1 (5%)
6	NAG	S	1209	1	14,14,15	0.30	0	17,19,21	0.64	0
6	NAG	V	1211	1	14,14,15	0.32	0	17,19,21	0.65	0
6	NAG	V	1205	1	14,14,15	1.47	3 (21%)	17,19,21	0.72	0
6	NAG	V	1203	1	14,14,15	1.26	2 (14%)	17,19,21	0.81	1 (5%)
6	NAG	S	1205	1	14,14,15	1.20	1 (7%)	17,19,21	0.75	0
6	NAG	S	1203	1	14,14,15	1.22	1 (7%)	17,19,21	0.69	0
6	NAG	C	1201	1	14,14,15	1.42	2 (14%)	17,19,21	0.71	0
6	NAG	V	1202	1	14,14,15	1.26	2 (14%)	17,19,21	0.75	1 (5%)
6	NAG	C	1207	1	14,14,15	1.28	1 (7%)	17,19,21	0.72	0
6	NAG	V	1206	1	14,14,15	1.27	2 (14%)	17,19,21	0.78	1 (5%)
6	NAG	S	1208	1	14,14,15	0.27	0	17,19,21	0.71	0
6	NAG	S	1206	1	14,14,15	1.26	3 (21%)	17,19,21	1.08	1 (5%)
6	NAG	V	1210	1	14,14,15	1.31	2 (14%)	17,19,21	0.63	0
6	NAG	S	1204	1	14,14,15	1.32	3 (21%)	17,19,21	0.81	1 (5%)
6	NAG	C	1208	1	14,14,15	1.20	2 (14%)	17,19,21	1.05	1 (5%)
6	NAG	V	1207	1	14,14,15	1.32	2 (14%)	17,19,21	0.80	1 (5%)
6	NAG	C	1203	1	14,14,15	1.36	1 (7%)	17,19,21	0.72	1 (5%)
6	NAG	S	1207	1	14,14,15	0.31	0	17,19,21	0.95	0
6	NAG	C	1204	1	14,14,15	1.27	1 (7%)	17,19,21	0.81	1 (5%)
6	NAG	V	1209	1	14,14,15	1.23	1 (7%)	17,19,21	0.80	1 (5%)
6	NAG	S	1202	1	14,14,15	1.30	2 (14%)	17,19,21	0.90	1 (5%)
6	NAG	C	1211	1	14,14,15	0.30	0	17,19,21	0.65	0
6	NAG	S	1201	1	14,14,15	1.26	1 (7%)	17,19,21	0.86	1 (5%)
6	NAG	C	1202	1	14,14,15	1.31	2 (14%)	17,19,21	0.61	0
6	NAG	V	1204	-	14,14,15	1.23	1 (7%)	17,19,21	0.74	1 (5%)
6	NAG	S	1210	1	14,14,15	0.51	0	17,19,21	2.40	6 (35%)
6	NAG	C	1209	1	14,14,15	1.23	1 (7%)	17,19,21	0.99	1 (5%)
6	NAG	C	1206	1	14,14,15	1.32	3 (21%)	17,19,21	0.99	1 (5%)
6	NAG	C	1205	1	14,14,15	1.40	3 (21%)	17,19,21	0.90	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1210	1	-	1/6/23/26	0/1/1/1
6	NAG	V	1208	1	-	1/6/23/26	0/1/1/1
6	NAG	V	1212	1	-	2/6/23/26	0/1/1/1
6	NAG	V	1201	1	-	1/6/23/26	0/1/1/1
6	NAG	S	1209	1	-	2/6/23/26	0/1/1/1
6	NAG	V	1211	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1205	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1203	1	-	0/6/23/26	0/1/1/1
6	NAG	S	1205	1	-	1/6/23/26	0/1/1/1
6	NAG	S	1203	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1201	1	-	1/6/23/26	0/1/1/1
6	NAG	V	1202	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1206	1	-	0/6/23/26	0/1/1/1
6	NAG	S	1208	1	-	6/6/23/26	0/1/1/1
6	NAG	S	1206	1	-	1/6/23/26	0/1/1/1
6	NAG	V	1210	1	-	1/6/23/26	0/1/1/1
6	NAG	S	1204	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1208	1	-	2/6/23/26	0/1/1/1
6	NAG	V	1207	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1203	1	-	0/6/23/26	0/1/1/1
6	NAG	S	1207	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1209	1	-	0/6/23/26	0/1/1/1
6	NAG	S	1202	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1211	1	-	3/6/23/26	0/1/1/1
6	NAG	S	1201	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1202	1	-	1/6/23/26	0/1/1/1
6	NAG	V	1204	-	-	0/6/23/26	0/1/1/1
6	NAG	S	1210	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1209	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1206	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1205	1	-	0/6/23/26	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1205	NAG	O5-C5	3.17	1.49	1.43
6	C	1203	NAG	O5-C5	3.13	1.49	1.43
6	C	1201	NAG	O5-C5	2.90	1.49	1.43
6	C	1207	NAG	O5-C5	2.88	1.49	1.43
6	C	1205	NAG	O5-C5	2.87	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1204	NAG	O5-C5	2.87	1.49	1.43
6	S	1204	NAG	O5-C5	2.85	1.49	1.43
6	S	1201	NAG	O5-C5	2.83	1.48	1.43
6	S	1202	NAG	O5-C5	2.78	1.48	1.43
6	V	1207	NAG	O5-C5	2.77	1.48	1.43
6	C	1201	NAG	O5-C1	2.77	1.48	1.43
6	C	1210	NAG	O5-C5	2.76	1.48	1.43
6	V	1204	NAG	O5-C5	2.76	1.48	1.43
6	V	1203	NAG	O5-C5	2.74	1.48	1.43
6	V	1209	NAG	O5-C5	2.74	1.48	1.43
6	C	1209	NAG	O5-C5	2.70	1.48	1.43
6	C	1206	NAG	O5-C5	2.66	1.48	1.43
6	S	1206	NAG	O5-C5	2.65	1.48	1.43
6	V	1208	NAG	O5-C5	2.62	1.48	1.43
6	C	1205	NAG	C1-C2	2.62	1.55	1.52
6	C	1202	NAG	O5-C5	2.60	1.48	1.43
6	V	1206	NAG	C1-C2	2.58	1.55	1.52
6	V	1210	NAG	O5-C5	2.57	1.48	1.43
6	S	1205	NAG	O5-C5	2.57	1.48	1.43
6	V	1205	NAG	O5-C1	2.48	1.47	1.43
6	V	1205	NAG	C1-C2	2.48	1.55	1.52
6	V	1206	NAG	O5-C5	2.47	1.48	1.43
6	V	1201	NAG	C1-C2	2.43	1.55	1.52
6	V	1201	NAG	O5-C5	2.42	1.48	1.43
6	V	1202	NAG	O5-C5	2.41	1.48	1.43
6	S	1203	NAG	O5-C5	2.41	1.48	1.43
6	C	1206	NAG	C1-C2	2.40	1.55	1.52
6	C	1210	NAG	C1-C2	2.35	1.55	1.52
6	C	1208	NAG	O5-C5	2.33	1.48	1.43
6	V	1207	NAG	C1-C2	2.25	1.55	1.52
6	S	1204	NAG	C1-C2	2.20	1.55	1.52
6	C	1208	NAG	C1-C2	2.19	1.55	1.52
6	S	1202	NAG	C1-C2	2.19	1.55	1.52
6	V	1210	NAG	C1-C2	2.17	1.55	1.52
6	S	1206	NAG	C1-C2	2.17	1.55	1.52
6	C	1205	NAG	O5-C1	2.10	1.47	1.43
6	C	1206	NAG	O5-C1	2.10	1.47	1.43
6	C	1202	NAG	C1-C2	2.08	1.55	1.52
6	V	1202	NAG	C1-C2	2.07	1.55	1.52
6	V	1201	NAG	O5-C1	2.04	1.47	1.43
6	S	1206	NAG	O5-C1	2.02	1.47	1.43
6	C	1210	NAG	O5-C1	2.02	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1203	NAG	C1-C2	2.01	1.55	1.52
6	S	1204	NAG	O5-C1	2.01	1.47	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	1210	NAG	C1-C2-N2	4.73	117.88	110.43
6	S	1210	NAG	C2-N2-C7	-4.65	116.67	122.90
6	S	1210	NAG	O5-C1-C2	-4.24	104.73	111.29
6	S	1210	NAG	C4-C3-C2	-3.94	105.25	111.02
6	V	1201	NAG	C1-O5-C5	3.91	117.43	112.19
6	S	1206	NAG	C1-O5-C5	3.81	117.30	112.19
6	C	1208	NAG	C1-O5-C5	3.77	117.23	112.19
6	C	1209	NAG	C1-O5-C5	3.48	116.85	112.19
6	S	1210	NAG	C6-C5-C4	-3.35	104.79	113.02
6	C	1206	NAG	C1-O5-C5	3.33	116.65	112.19
6	S	1202	NAG	C1-O5-C5	2.76	115.89	112.19
6	S	1201	NAG	C1-O5-C5	2.73	115.85	112.19
6	V	1202	NAG	C1-O5-C5	2.61	115.69	112.19
6	S	1204	NAG	C1-O5-C5	2.53	115.57	112.19
6	V	1209	NAG	C1-O5-C5	2.49	115.52	112.19
6	V	1207	NAG	C1-O5-C5	2.46	115.48	112.19
6	V	1212	NAG	C2-N2-C7	-2.43	119.65	122.90
6	V	1208	NAG	C1-O5-C5	2.40	115.40	112.19
6	C	1205	NAG	C1-O5-C5	2.40	115.40	112.19
6	C	1204	NAG	C1-O5-C5	2.37	115.36	112.19
6	S	1210	NAG	C1-O5-C5	2.35	115.33	112.19
6	V	1206	NAG	C1-O5-C5	2.26	115.22	112.19
6	V	1203	NAG	C1-O5-C5	2.25	115.19	112.19
6	C	1203	NAG	C1-O5-C5	2.11	115.02	112.19
6	C	1210	NAG	C1-O5-C5	2.06	114.94	112.19
6	V	1204	NAG	C1-O5-C5	2.05	114.94	112.19

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	S	1208	NAG	C8-C7-N2-C2
6	S	1208	NAG	O7-C7-N2-C2
6	V	1212	NAG	C8-C7-N2-C2
6	V	1212	NAG	O7-C7-N2-C2
6	S	1210	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	S	1210	NAG	O7-C7-N2-C2
6	C	1211	NAG	C8-C7-N2-C2
6	C	1211	NAG	O7-C7-N2-C2
6	S	1207	NAG	O5-C5-C6-O6
6	C	1210	NAG	O5-C5-C6-O6
6	S	1205	NAG	O5-C5-C6-O6
6	S	1206	NAG	O5-C5-C6-O6
6	C	1211	NAG	O5-C5-C6-O6
6	V	1202	NAG	O5-C5-C6-O6
6	V	1210	NAG	O5-C5-C6-O6
6	V	1208	NAG	O5-C5-C6-O6
6	V	1201	NAG	O5-C5-C6-O6
6	C	1202	NAG	O5-C5-C6-O6
6	S	1203	NAG	O5-C5-C6-O6
6	C	1201	NAG	O5-C5-C6-O6
6	S	1208	NAG	C1-C2-N2-C7
6	S	1208	NAG	C4-C5-C6-O6
6	S	1208	NAG	O5-C5-C6-O6
6	S	1209	NAG	C8-C7-N2-C2
6	S	1208	NAG	C3-C2-N2-C7
6	S	1204	NAG	C1-C2-N2-C7
6	V	1207	NAG	C1-C2-N2-C7
6	S	1209	NAG	O7-C7-N2-C2
6	C	1208	NAG	C4-C5-C6-O6
6	C	1208	NAG	O5-C5-C6-O6
6	S	1207	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	1208	NAG	2	0
6	S	1207	NAG	1	0
6	V	1204	NAG	4	0
6	S	1210	NAG	1	0

5.7 Other polymers [i](#)

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-25904. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

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.