



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:47 PM UTC

PDB ID : 6YI5 / pdb_00006yi5
EMDB ID : EMD-10810
Title : In-situ structure of the trimeric HEF from influenza C by flexible fitting into a cryo-ET map.
Authors : Halldorsson, S.; Rosenthal, P.B.
Deposited on : 2020-03-31
Resolution : 9.10 Å(reported)
Based on initial model : 1FLC

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

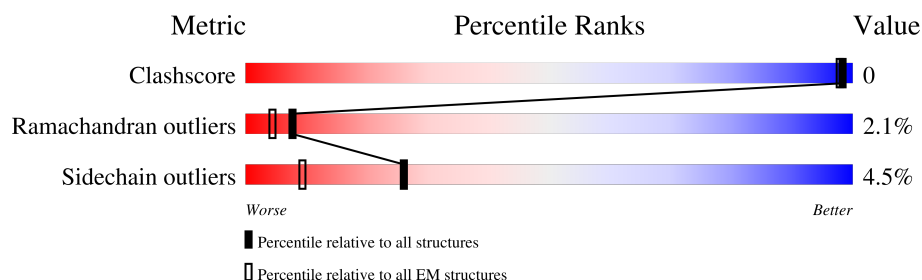
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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.



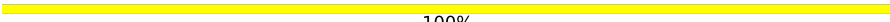
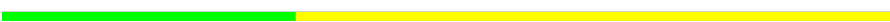
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	432	87% 11% ..
1	C	432	88% 10% .
1	E	432	90% 9% .
2	B	175	81% 10% . 7%
2	D	175	82% 7% . 7%
2	F	175	83% 8% . 7%
3	G	3	33% 67%
3	H	3	100%
3	J	3	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	K	3	 100%
3	M	3	 67%33%
3	N	3	 100%
4	I	3	 33%67%
4	L	3	 67%33%
4	O	3	 33%67%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14061 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.

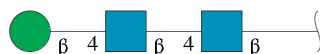
- Molecule 1 is a protein called Hemagglutinin-esterase-fusion glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	427	Total	C	N	O	S	0	0
			3339	2113	565	636	25		
1	E	427	Total	C	N	O	S	0	0
			3339	2113	565	636	25		
1	C	427	Total	C	N	O	S	0	0
			3339	2113	565	636	25		

- Molecule 2 is a protein called Hemagglutinin-esterase-fusion glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1231	776	206	246	3		
2	F	162	Total	C	N	O	S	0	0
			1231	776	206	246	3		
2	D	162	Total	C	N	O	S	0	0
			1231	776	206	246	3		

- Molecule 3 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.



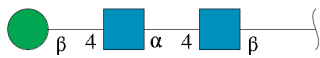
Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

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

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

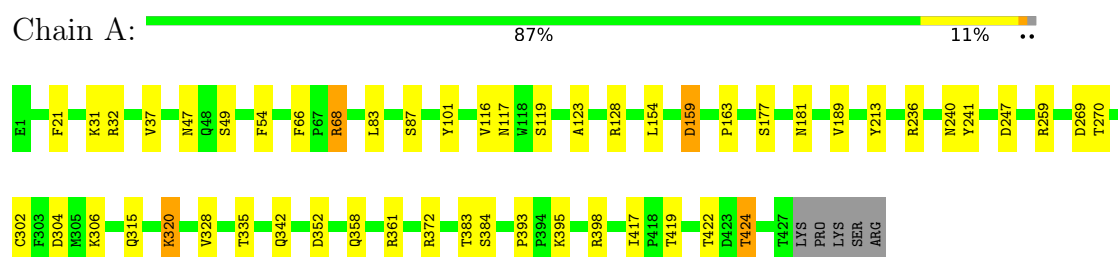


Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	3	Total	C	N	O	0	0
			39	22	2	15		
4	L	3	Total	C	N	O	0	0
			39	22	2	15		
4	O	3	Total	C	N	O	0	0
			39	22	2	15		

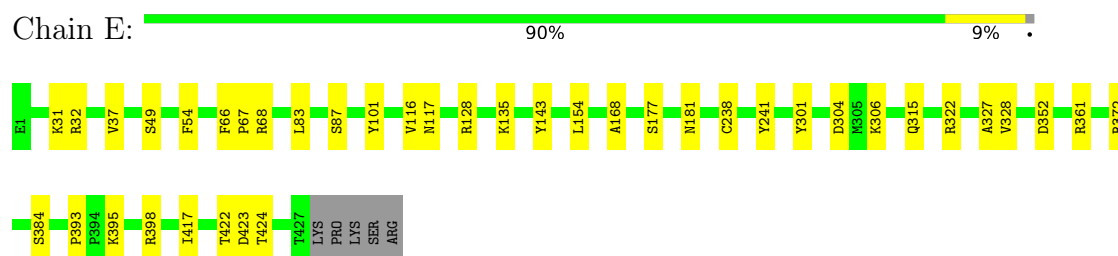
3 Residue-property plots [i](#)

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.

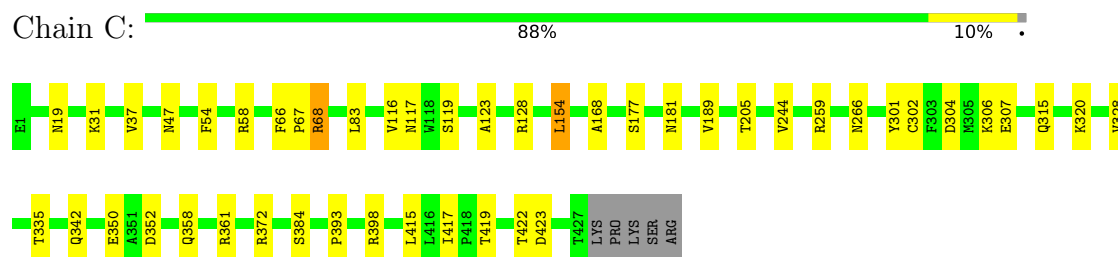
- Molecule 1: Hemagglutinin-esterase-fusion glycoprotein



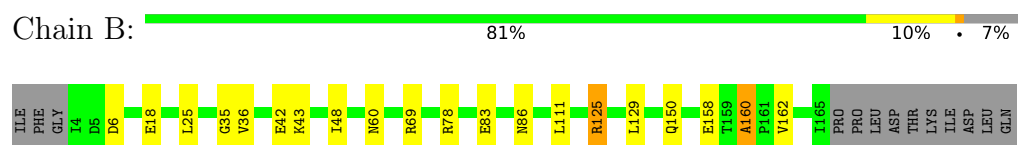
- Molecule 1: Hemagglutinin-esterase-fusion glycoprotein



- Molecule 1: Hemagglutinin-esterase-fusion glycoprotein



- Molecule 2: Hemagglutinin-esterase-fusion glycoprotein



- Molecule 2: Hemagglutinin-esterase-fusion glycoprotein

Chain F:  83% 8% • 7%



- Molecule 2: Hemagglutinin-esterase-fusion glycoprotein

Chain D:  82% 7% • 7%

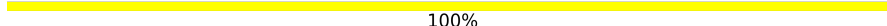


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%

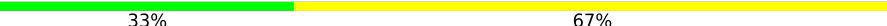


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

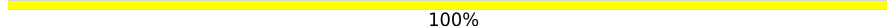


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 67%



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

Chain K:  100%



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

Chain M:  67% 33%



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

Chain N:  100%

MAG1
MAG2
BMA3

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

Chain I:  33% 67%

MAG1
NDG2
BMA3

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

Chain L:  67% 33%

MAG1
NDG2
BMA3

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

Chain O:  33% 67%

MAG1
NDG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	14057	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.57	Depositor
Minimum defocus (nm)	2.5	Depositor
Maximum defocus (nm)	4.5	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 QUANTUM (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, NDG

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	0.89	0/3420	1.47	23/4622 (0.5%)
1	C	0.89	0/3420	1.47	24/4622 (0.5%)
1	E	0.89	0/3420	1.48	30/4622 (0.6%)
2	B	0.91	0/1244	1.66	13/1682 (0.8%)
2	D	1.06	4/1244 (0.3%)	1.94	25/1682 (1.5%)
2	F	0.89	0/1244	1.67	11/1682 (0.7%)
All	All	0.91	4/13992 (0.0%)	1.56	126/18912 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	C	0	5
1	E	0	6
2	B	0	2
2	D	0	2
2	F	0	2
All	All	0	25

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	44	GLY	CA-C	6.42	1.59	1.51
2	D	43	LYS	N-CA	5.73	1.53	1.46
2	D	43	LYS	C-N	5.66	1.40	1.34
2	D	44	GLY	C-N	5.50	1.41	1.33

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	43	LYS	N-CA-C	15.03	133.34	112.45
2	D	43	LYS	CA-C-N	13.38	137.19	120.34
2	D	43	LYS	C-N-CA	13.38	137.19	120.34
2	D	45	PHE	CA-CB-CG	11.93	125.73	113.80
2	D	43	LYS	N-CA-CB	-10.81	94.15	110.26
2	D	48	ILE	CA-C-N	10.41	131.75	119.99
2	D	48	ILE	C-N-CA	10.41	131.75	119.99
2	D	44	GLY	O-C-N	-9.56	111.35	122.34
1	A	352	ASP	CA-CB-CG	8.96	121.56	112.60
1	C	393	PRO	N-CA-C	8.70	121.32	110.70
1	A	393	PRO	N-CA-C	8.57	121.16	110.70
1	E	393	PRO	N-CA-C	8.55	121.13	110.70
1	C	306	LYS	N-CA-C	8.24	120.04	111.14
2	F	86	ASN	CA-CB-CG	8.18	120.78	112.60
2	D	44	GLY	N-CA-C	-7.75	102.23	113.86
1	A	159	ASP	CA-CB-CG	7.61	120.21	112.60
1	C	304	ASP	CA-CB-CG	7.46	120.06	112.60
2	D	46	GLU	N-CA-C	7.37	121.18	111.75
2	B	48	ILE	CA-C-N	7.34	128.28	119.99
2	B	48	ILE	C-N-CA	7.34	128.28	119.99
2	D	69	ARG	N-CA-C	7.17	118.88	111.14
1	A	116	VAL	N-CA-C	7.15	118.77	110.62
2	D	42	GLU	CA-C-O	7.14	130.72	120.51
1	E	116	VAL	N-CA-C	7.12	118.74	110.62
2	D	45	PHE	N-CA-CB	7.02	120.44	110.12
2	B	162	VAL	N-CA-C	7.01	116.60	108.96
1	C	54	PHE	CA-CB-CG	-7.00	106.80	113.80
1	A	304	ASP	CA-CB-CG	6.91	119.51	112.60
2	F	48	ILE	CA-C-N	6.80	127.67	119.99
2	F	48	ILE	C-N-CA	6.80	127.67	119.99
1	E	306	LYS	N-CA-C	6.72	118.61	111.28
1	E	54	PHE	CA-CB-CG	-6.69	107.11	113.80
1	A	306	LYS	N-CA-C	6.63	118.30	111.14
1	E	304	ASP	CA-CB-CG	6.61	119.21	112.60
1	C	116	VAL	N-CA-C	6.48	118.00	110.62
1	E	68	ARG	CA-C-N	6.46	129.57	120.28
1	E	68	ARG	C-N-CA	6.46	129.57	120.28
2	F	150	GLN	CA-C-N	6.42	128.88	120.28
2	F	150	GLN	C-N-CA	6.42	128.88	120.28
2	B	150	GLN	CA-C-N	6.40	128.86	120.28
2	B	150	GLN	C-N-CA	6.40	128.86	120.28
2	B	86	ASN	CA-CB-CG	6.37	118.97	112.60
2	B	69	ARG	N-CA-C	6.34	117.99	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	PHE	CA-CB-CG	-6.26	107.54	113.80
2	D	46	GLU	CA-C-O	6.25	127.20	120.20
1	E	328	VAL	CA-C-N	6.12	129.29	120.79
1	E	328	VAL	C-N-CA	6.12	129.29	120.79
2	F	162	VAL	N-CA-C	6.03	115.54	108.96
2	D	18	GLU	N-CA-C	6.02	117.85	111.28
1	C	422	THR	CA-C-N	6.02	128.26	120.44
1	C	422	THR	C-N-CA	6.02	128.26	120.44
1	C	352	ASP	CA-CB-CG	6.00	118.61	112.60
2	D	45	PHE	CB-CA-C	-5.97	100.87	110.79
1	C	352	ASP	N-CA-C	-5.94	100.36	108.38
2	D	45	PHE	O-C-N	-5.87	115.90	122.12
1	A	352	ASP	N-CA-C	-5.85	100.48	108.38
2	D	45	PHE	N-CA-C	-5.82	104.94	111.28
1	E	352	ASP	N-CA-C	-5.81	100.54	108.38
1	E	352	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	168	ALA	N-CA-C	5.78	118.44	110.35
1	A	68	ARG	CA-C-N	5.76	129.81	120.60
1	A	68	ARG	C-N-CA	5.76	129.81	120.60
2	D	150	GLN	CA-C-N	5.76	127.99	120.28
2	D	150	GLN	C-N-CA	5.76	127.99	120.28
1	E	238	CYS	N-CA-C	5.75	117.55	111.28
2	F	6	ASP	CA-CB-CG	5.75	118.35	112.60
2	F	36	VAL	N-CA-C	5.71	117.86	109.63
1	C	19	ASN	CA-CB-CG	5.66	118.26	112.60
1	C	123	ALA	N-CA-C	5.63	119.20	111.54
1	A	320	LYS	N-CA-C	5.63	118.51	110.24
1	A	123	ALA	N-CA-C	5.60	117.46	110.91
2	F	82	LEU	N-CA-C	5.57	117.79	111.11
1	A	119	SER	CA-C-O	-5.55	116.14	121.08
2	F	60	ASN	CA-C-N	5.46	127.92	120.77
2	F	60	ASN	C-N-CA	5.46	127.92	120.77
1	A	117	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	422	THR	CA-C-N	5.44	127.57	120.28
1	A	422	THR	C-N-CA	5.44	127.57	120.28
1	C	417	ILE	CA-C-N	5.43	125.19	119.76
1	C	417	ILE	C-N-CA	5.43	125.19	119.76
1	E	327	ALA	CA-C-N	5.42	127.88	120.77
1	E	327	ALA	C-N-CA	5.42	127.88	120.77
1	E	417	ILE	CA-C-N	5.40	125.16	119.76
1	E	417	ILE	C-N-CA	5.40	125.16	119.76
2	B	60	ASN	CA-C-N	5.39	127.83	120.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60	ASN	C-N-CA	5.39	127.83	120.77
1	C	393	PRO	CA-C-O	-5.39	112.75	120.56
1	E	168	ALA	N-CA-C	5.38	117.89	110.35
2	D	60	ASN	CA-C-N	5.33	127.76	120.77
2	D	60	ASN	C-N-CA	5.33	127.76	120.77
2	B	36	VAL	N-CA-C	5.32	116.55	109.37
1	E	143	TYR	CA-C-N	5.31	128.17	120.79
1	E	143	TYR	C-N-CA	5.31	128.17	120.79
2	B	125	ARG	N-CA-C	5.29	117.05	111.28
1	A	417	ILE	CA-C-N	5.28	125.04	119.76
1	A	417	ILE	C-N-CA	5.28	125.04	119.76
2	D	158	GLU	CA-C-N	5.28	128.34	120.95
2	D	158	GLU	C-N-CA	5.28	128.34	120.95
1	E	67	PRO	CA-C-N	5.27	127.61	120.65
1	E	67	PRO	C-N-CA	5.27	127.61	120.65
1	C	328	VAL	CA-C-N	5.26	128.11	120.79
1	C	328	VAL	C-N-CA	5.26	128.11	120.79
1	C	423	ASP	CA-C-N	5.25	131.57	121.54
1	C	423	ASP	C-N-CA	5.25	131.57	121.54
1	E	117	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	240	ASN	CA-CB-CG	-5.21	107.39	112.60
1	C	117	ASN	CA-CB-CG	-5.16	107.44	112.60
1	C	67	PRO	CA-C-N	5.12	127.41	120.65
1	C	67	PRO	C-N-CA	5.12	127.41	120.65
1	A	328	VAL	CA-C-N	5.12	127.91	120.79
1	A	328	VAL	C-N-CA	5.12	127.91	120.79
1	A	163	PRO	CA-C-N	5.11	127.83	120.38
1	A	163	PRO	C-N-CA	5.11	127.83	120.38
1	E	424	THR	N-CA-C	5.09	121.63	110.80
1	E	393	PRO	CA-C-O	-5.08	113.19	120.56
1	C	58	ARG	NE-CZ-NH2	-5.08	114.62	119.20
1	E	423	ASP	CA-C-N	5.07	131.22	121.54
1	E	423	ASP	C-N-CA	5.07	131.22	121.54
1	C	119	SER	CA-C-O	-5.05	116.58	121.08
2	B	35	GLY	N-CA-C	5.04	119.01	112.25
2	D	125	ARG	N-CA-C	5.04	116.78	111.28
1	E	422	THR	CA-C-N	5.03	127.02	120.28
1	E	422	THR	C-N-CA	5.03	127.02	120.28
1	E	135	LYS	CA-C-N	5.02	127.77	120.79
1	E	135	LYS	C-N-CA	5.02	127.77	120.79
2	B	160	ALA	N-CA-C	5.01	120.89	109.81

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	TYR	Sidechain
1	A	213	TYR	Sidechain
1	A	241	TYR	Sidechain
1	A	259	ARG	Sidechain
1	A	361	ARG	Sidechain
1	A	372	ARG	Sidechain
1	A	398	ARG	Sidechain
1	A	68	ARG	Sidechain
2	B	125	ARG	Sidechain
2	B	78	ARG	Sidechain
1	C	259	ARG	Sidechain
1	C	361	ARG	Sidechain
1	C	372	ARG	Sidechain
1	C	398	ARG	Sidechain
1	C	68	ARG	Sidechain
2	D	125	ARG	Sidechain
2	D	45	PHE	Sidechain
1	E	101	TYR	Sidechain
1	E	241	TYR	Sidechain
1	E	322	ARG	Sidechain
1	E	361	ARG	Sidechain
1	E	372	ARG	Sidechain
1	E	398	ARG	Sidechain
2	F	125	ARG	Sidechain
2	F	69	ARG	Sidechain

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	3339	0	3253	2	0
1	C	3339	0	3253	2	0
1	E	3339	0	3253	1	0
2	B	1231	0	1241	0	0
2	D	1231	0	1241	1	0
2	F	1231	0	1241	1	0
3	G	39	0	34	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	39	0	34	0	0
3	J	39	0	34	0	0
3	K	39	0	34	0	0
3	M	39	0	34	0	0
3	N	39	0	34	0	0
4	I	39	0	33	0	0
4	L	39	0	33	1	0
4	O	39	0	33	0	0
All	All	14061	0	13785	7	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 0.

All (7) 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:D:44:GLY:O	2:D:47:LYS:HB3	2.11	0.51
1:E:154:LEU:HD23	1:E:301:TYR:CE1	2.50	0.46
1:C:154:LEU:HD23	1:C:301:TYR:CE1	2.53	0.43
2:F:132:GLU:H	2:F:132:GLU:CD	2.26	0.43
1:A:236:ARG:HH22	1:A:269:ASP:CG	2.27	0.43
1:C:68:ARG:HH21	1:C:350:GLU:CD	2.27	0.42
1:A:21:PHE:CE1	4:L:1:NAG:H82	2.55	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	425/432 (98%)	380 (89%)	35 (8%)	10 (2%)	4 27
1	C	425/432 (98%)	384 (90%)	33 (8%)	8 (2%)	6 32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	425/432 (98%)	380 (89%)	36 (8%)	9 (2%)	5	30
2	B	160/175 (91%)	140 (88%)	17 (11%)	3 (2%)	6	32
2	D	160/175 (91%)	140 (88%)	16 (10%)	4 (2%)	4	26
2	F	160/175 (91%)	139 (87%)	18 (11%)	3 (2%)	6	32
All	All	1755/1821 (96%)	1563 (89%)	155 (9%)	37 (2%)	8	30

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	384	SER
1	E	384	SER
1	C	181	ASN
1	A	83	LEU
2	B	42	GLU
1	E	181	ASN
2	F	42	GLU
1	C	266	ASN
1	C	384	SER
1	A	49	SER
1	E	83	LEU
2	F	158	GLU
2	D	42	GLU
1	A	128	ARG
1	A	177	SER
1	A	315	GLN
2	B	6	ASP
1	E	128	ARG
1	C	177	SER
2	D	6	ASP
2	D	34	GLY
1	A	87	SER
1	A	424	THR
2	B	160	ALA
1	E	49	SER
1	E	87	SER
1	E	315	GLN
1	C	83	LEU
1	C	315	GLN
1	A	66	PHE
1	E	66	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	177	SER
2	F	160	ALA
1	C	128	ARG
2	D	160	ALA
1	C	66	PHE

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	368/374 (98%)	350 (95%)	18 (5%)	22	43
1	C	369/374 (99%)	354 (96%)	15 (4%)	27	49
1	E	94/374 (25%)	90 (96%)	4 (4%)	26	47
2	B	135/147 (92%)	128 (95%)	7 (5%)	21	42
2	D	135/147 (92%)	130 (96%)	5 (4%)	30	51
2	F	83/147 (56%)	79 (95%)	4 (5%)	23	44
All	All	1184/1563 (76%)	1131 (96%)	53 (4%)	26	46

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	32	ARG
1	A	37	VAL
1	A	47	ASN
1	A	154	LEU
1	A	159	ASP
1	A	189	VAL
1	A	247	ASP
1	A	270	THR
1	A	302	CYS
1	A	320	LYS
1	A	335	THR
1	A	342	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	358	GLN
1	A	383	THR
1	A	395	LYS
1	A	419	THR
1	A	424	THR
2	B	18	GLU
2	B	25	LEU
2	B	43	LYS
2	B	83	GLU
2	B	111	LEU
2	B	129	LEU
2	B	158	GLU
1	E	31	LYS
1	E	32	ARG
1	E	37	VAL
1	E	395	LYS
2	F	43	LYS
2	F	129	LEU
2	F	132	GLU
2	F	158	GLU
1	C	31	LYS
1	C	37	VAL
1	C	47	ASN
1	C	154	LEU
1	C	189	VAL
1	C	205	THR
1	C	244	VAL
1	C	302	CYS
1	C	307	GLU
1	C	320	LYS
1	C	335	THR
1	C	342	GLN
1	C	358	GLN
1	C	415	LEU
1	C	419	THR
2	D	25	LEU
2	D	46	GLU
2	D	129	LEU
2	D	132	GLU
2	D	158	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	121	HIS
1	A	176	ASN
1	A	209	GLN
1	A	234	ASN
2	F	150	GLN
1	C	18	HIS
1	C	19	ASN
1	C	141	ASN
1	C	279	GLN
1	C	330	GLN
2	D	143	ASN
2	D	150	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
3	NAG	G	1	1,3	14,14,15	0.22	0	17,19,21	0.76	0
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	1.17	1 (5%)
3	BMA	G	3	3	11,11,12	0.20	0	15,15,17	1.06	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.36	0	17,19,21	1.00	1 (5%)
3	NAG	H	2	3	14,14,15	0.28	0	17,19,21	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	H	3	3	11,11,12	0.20	0	15,15,17	0.84	1 (6%)
4	NAG	I	1	2,4	14,14,15	0.38	0	17,19,21	0.98	1 (5%)
4	NDG	I	2	4	14,14,15	0.35	0	17,19,21	1.31	3 (17%)
4	BMA	I	3	4	11,11,12	0.29	0	15,15,17	0.57	0
3	NAG	J	1	1,3	14,14,15	0.22	0	17,19,21	0.96	1 (5%)
3	NAG	J	2	3	14,14,15	0.27	0	17,19,21	1.22	2 (11%)
3	BMA	J	3	3	11,11,12	0.18	0	15,15,17	0.78	0
3	NAG	K	1	1,3	14,14,15	0.24	0	17,19,21	1.07	1 (5%)
3	NAG	K	2	3	14,14,15	0.33	0	17,19,21	1.30	3 (17%)
3	BMA	K	3	3	11,11,12	0.26	0	15,15,17	1.11	1 (6%)
4	NAG	L	1	2,4	14,14,15	0.39	0	17,19,21	0.91	0
4	NDG	L	2	4	14,14,15	0.38	0	17,19,21	1.12	0
4	BMA	L	3	4	11,11,12	0.26	0	15,15,17	0.67	0
3	NAG	M	1	1,3	14,14,15	0.23	0	17,19,21	0.94	0
3	NAG	M	2	3	14,14,15	0.40	0	17,19,21	1.22	2 (11%)
3	BMA	M	3	3	11,11,12	0.37	0	15,15,17	0.95	0
3	NAG	N	1	1,3	14,14,15	0.26	0	17,19,21	1.23	2 (11%)
3	NAG	N	2	3	14,14,15	0.31	0	17,19,21	1.34	2 (11%)
3	BMA	N	3	3	11,11,12	0.27	0	15,15,17	0.96	1 (6%)
4	NAG	O	1	2,4	14,14,15	0.42	0	17,19,21	0.93	1 (5%)
4	NDG	O	2	4	14,14,15	0.41	0	17,19,21	1.42	3 (17%)
4	BMA	O	3	4	11,11,12	0.24	0	15,15,17	0.67	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
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
4	NAG	I	1	2,4	-	0/6/23/26	0/1/1/1
4	NDG	I	2	4	-	1/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
4	NAG	L	1	2,4	-	0/6/23/26	0/1/1/1
4	NDG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
4	NAG	O	1	2,4	-	0/6/23/26	0/1/1/1
4	NDG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	O5-C1-C2	-4.31	104.61	111.29
3	N	2	NAG	O5-C1-C2	-4.18	104.82	111.29
3	N	1	NAG	O5-C1-C2	-3.88	105.28	111.29
3	K	1	NAG	O5-C1-C2	-3.58	105.76	111.29
3	H	1	NAG	O5-C1-C2	-3.52	105.85	111.29
3	M	2	NAG	O5-C1-C2	-3.45	105.96	111.29
3	J	2	NAG	O5-C5-C6	-3.32	101.20	107.66
3	K	3	BMA	O5-C1-C2	-2.90	103.86	110.79
3	K	2	NAG	C2-N2-C7	2.89	126.77	122.90
3	M	2	NAG	O5-C5-C6	-2.83	102.15	107.66
3	G	2	NAG	O5-C1-C2	-2.75	107.03	111.29
3	H	2	NAG	C1-C2-N2	2.73	114.73	110.43
3	N	3	BMA	O5-C1-C2	-2.65	104.46	110.79
4	I	2	NDG	C3-C4-C5	-2.64	105.45	110.23
3	K	2	NAG	O5-C1-C2	-2.53	107.38	111.29
4	O	2	NDG	C3-C4-C5	-2.48	105.73	110.23
3	G	3	BMA	O5-C1-C2	-2.40	105.06	110.79
4	O	2	NDG	C4-C3-C2	-2.32	107.62	111.02
4	I	2	NDG	O5-C5-C4	-2.30	105.24	110.83
3	K	2	NAG	C4-C3-C2	2.23	114.29	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NDG	C4-C3-C2	-2.17	107.84	111.02
4	I	1	NAG	C3-C4-C5	-2.16	106.31	110.23
4	O	1	NAG	O5-C1-C2	-2.16	107.95	111.29
3	N	1	NAG	C1-C2-N2	2.13	113.79	110.43
3	J	1	NAG	C3-C4-C5	-2.10	106.42	110.23
3	J	2	NAG	O5-C1-C2	-2.10	108.05	111.29
3	N	2	NAG	C4-C3-C2	2.09	114.08	111.02
4	O	2	NDG	C1-O5-C5	2.07	114.95	112.19
3	H	3	BMA	O5-C1-C2	-2.06	105.87	110.79

There are no chirality outliers.

All (11) torsion outliers are listed below:

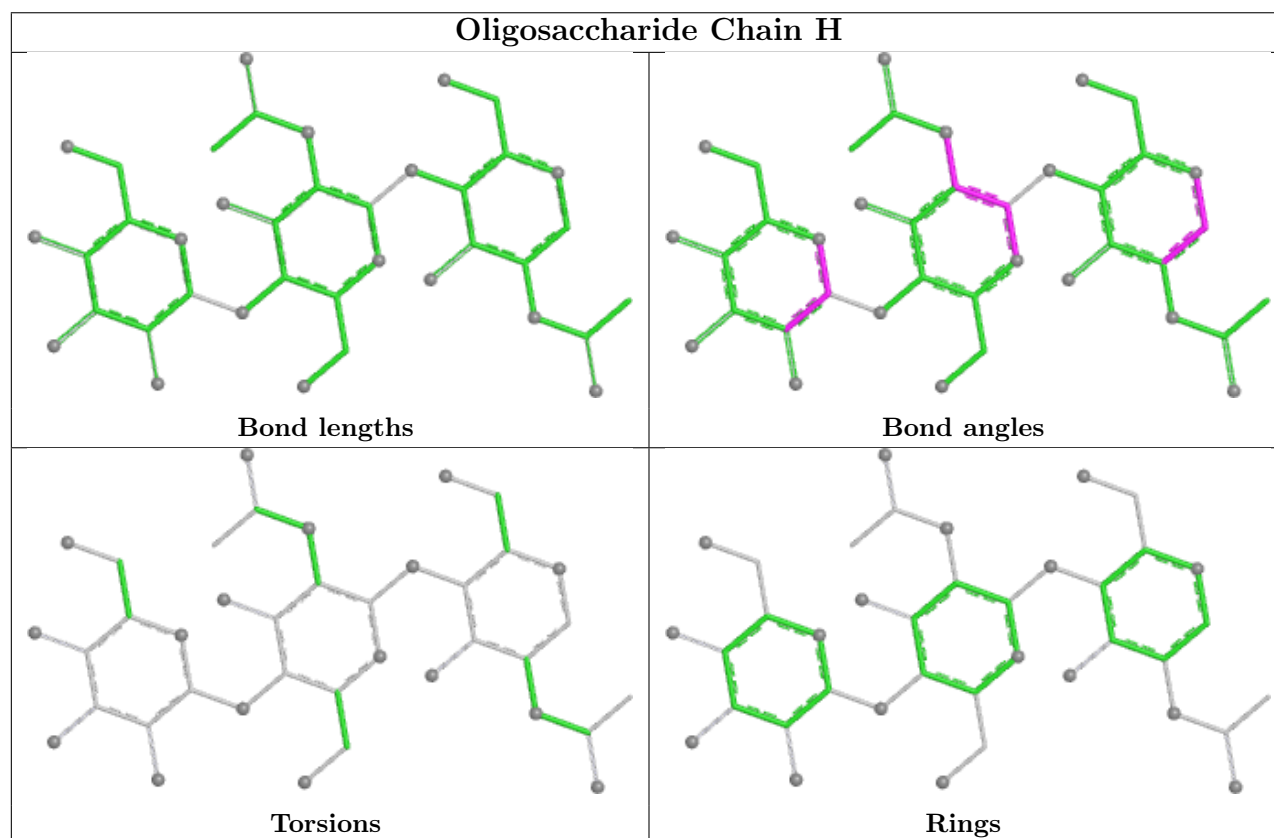
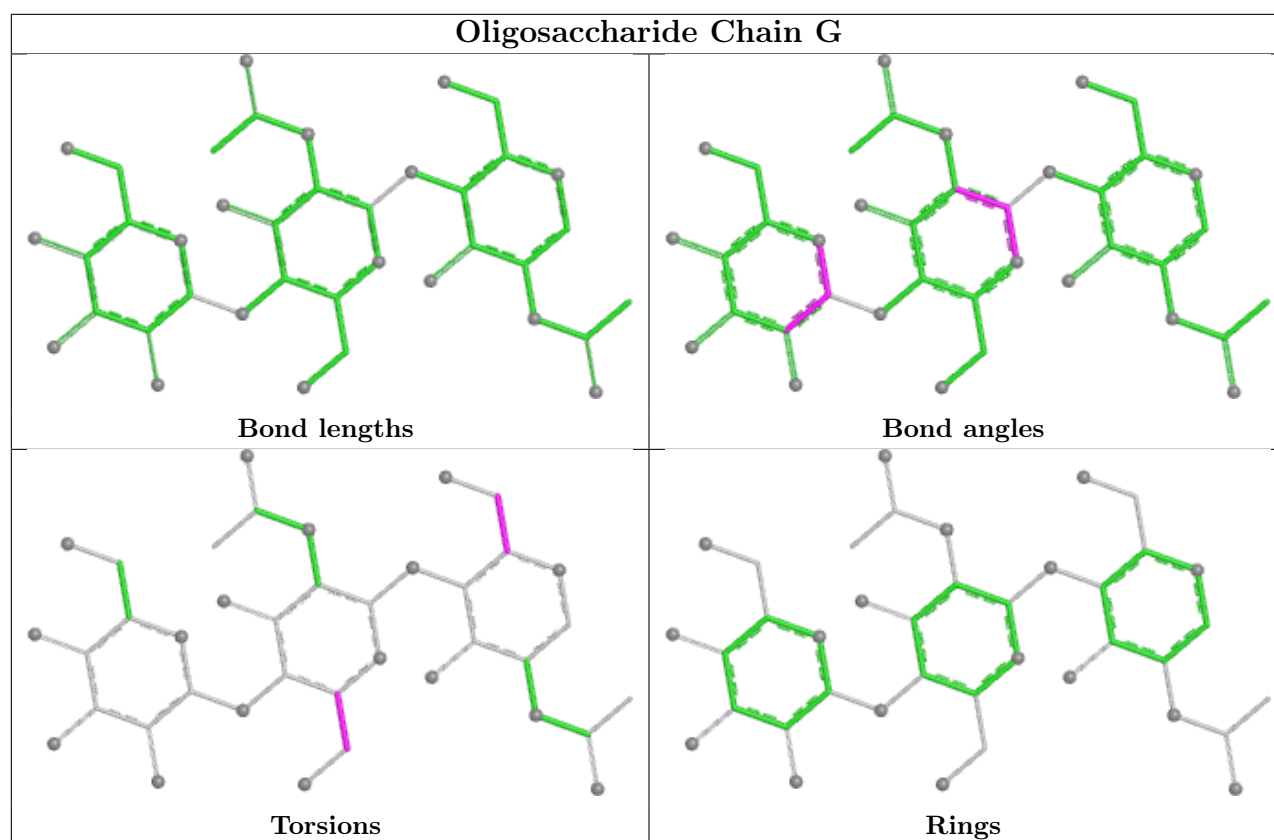
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C3-C2-N2-C7
4	I	2	NDG	C4-C5-C6-O6

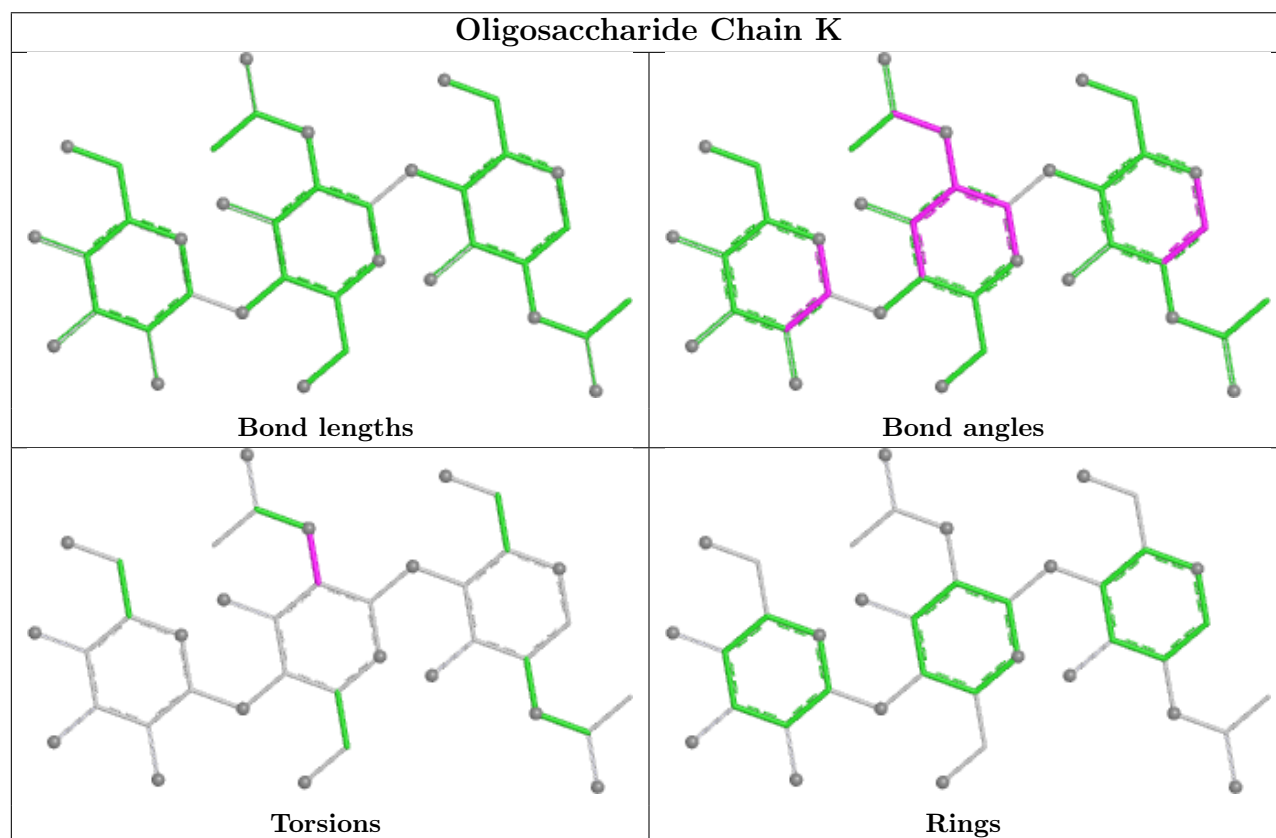
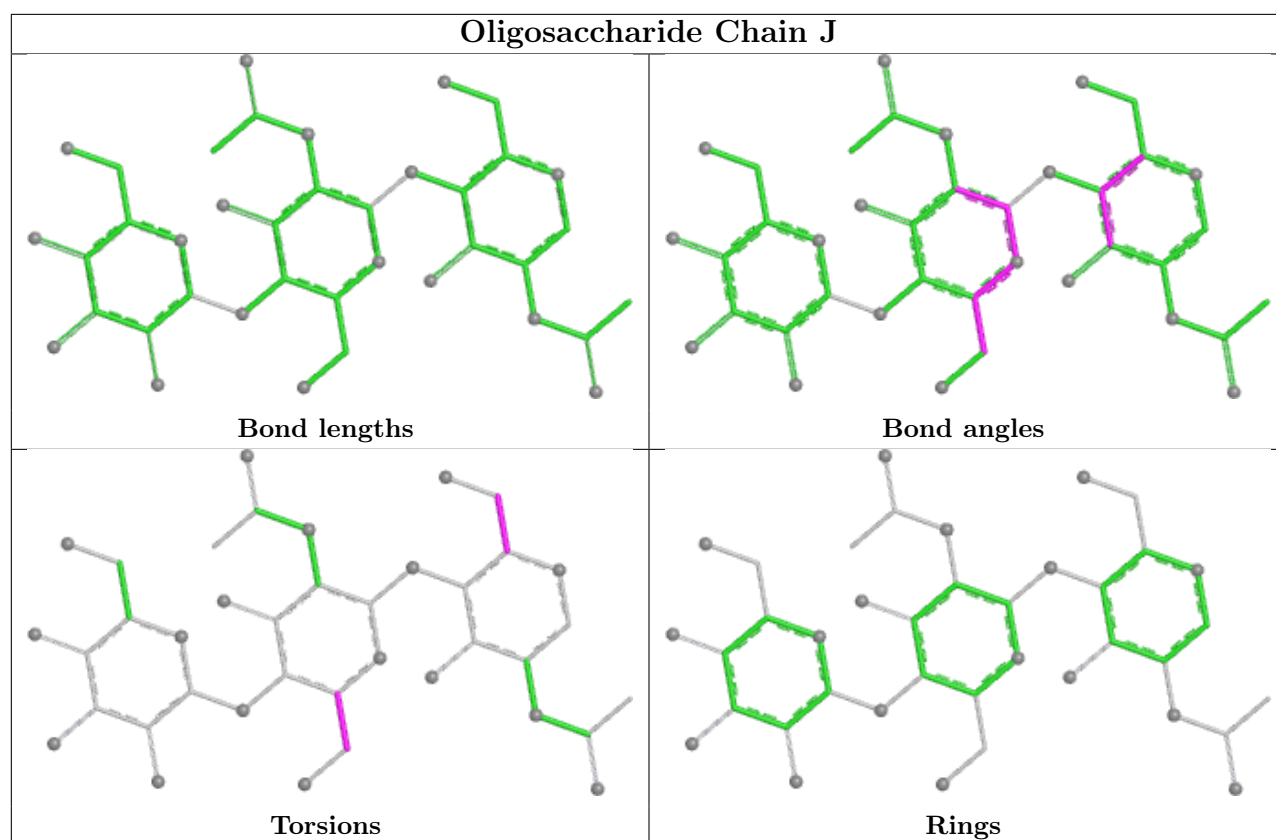
There are no ring outliers.

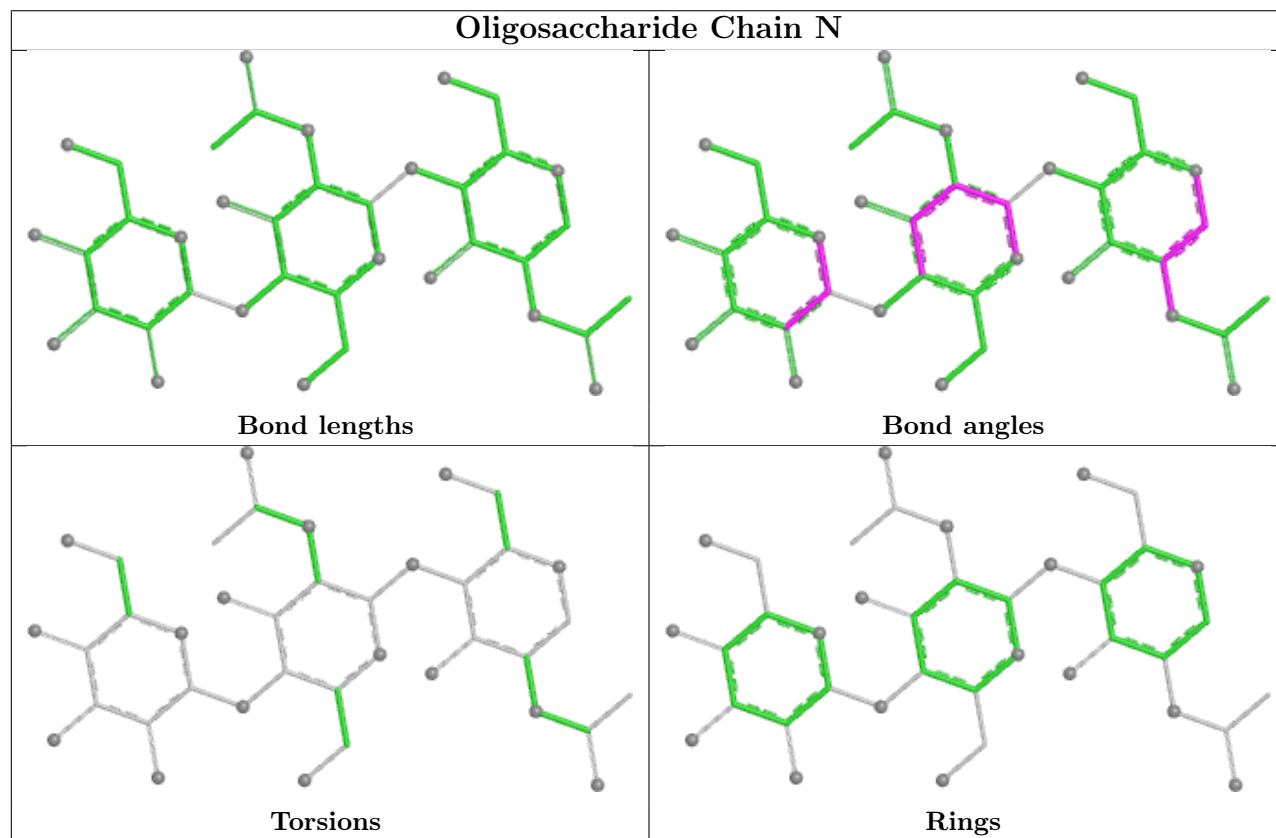
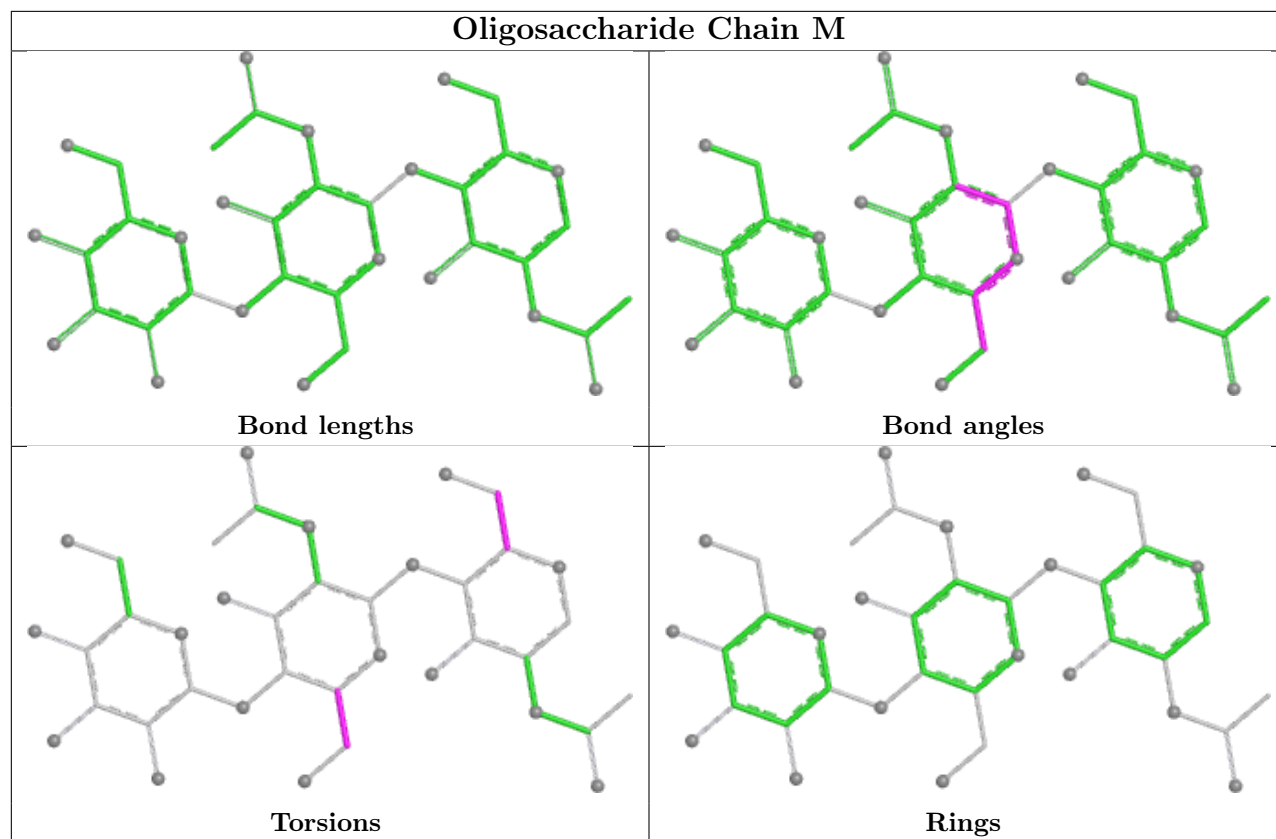
1 monomer is involved in 1 short contact:

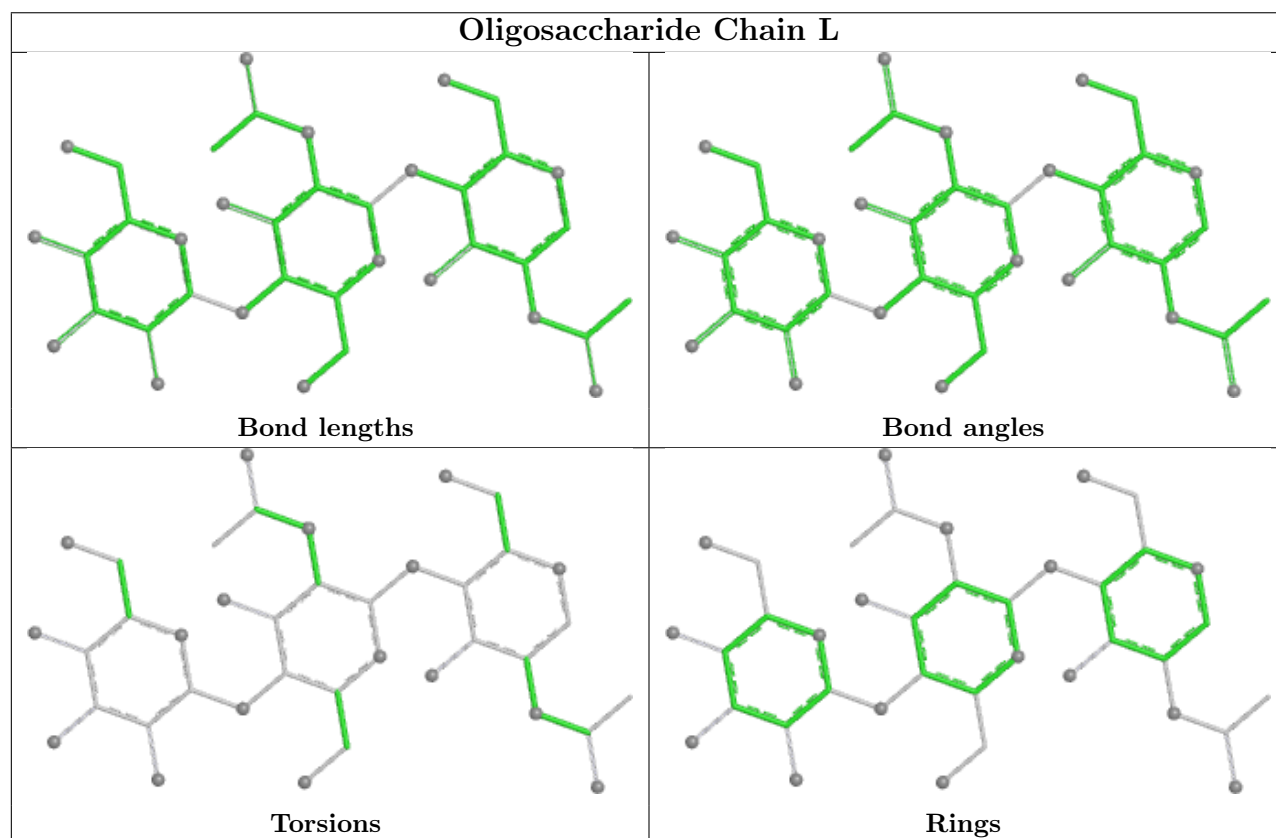
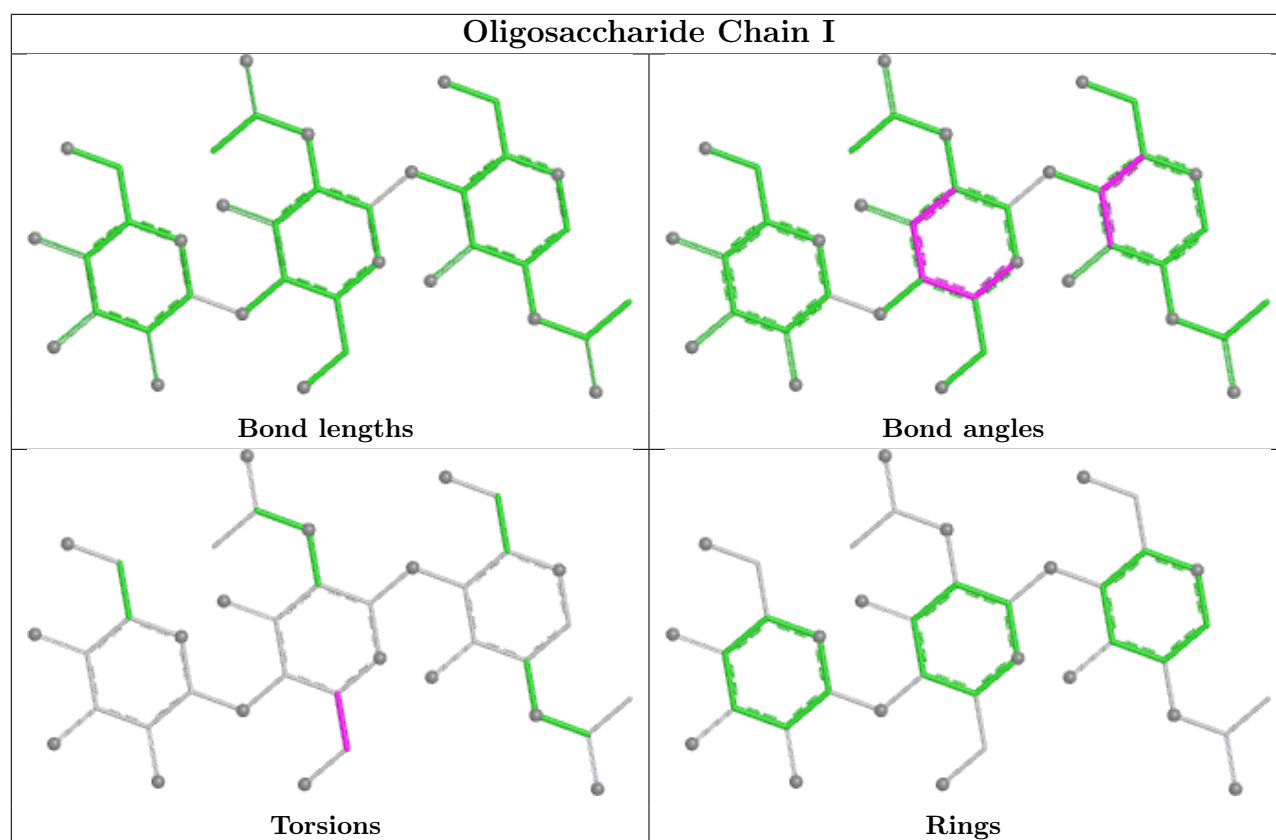
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1	NAG	1	0

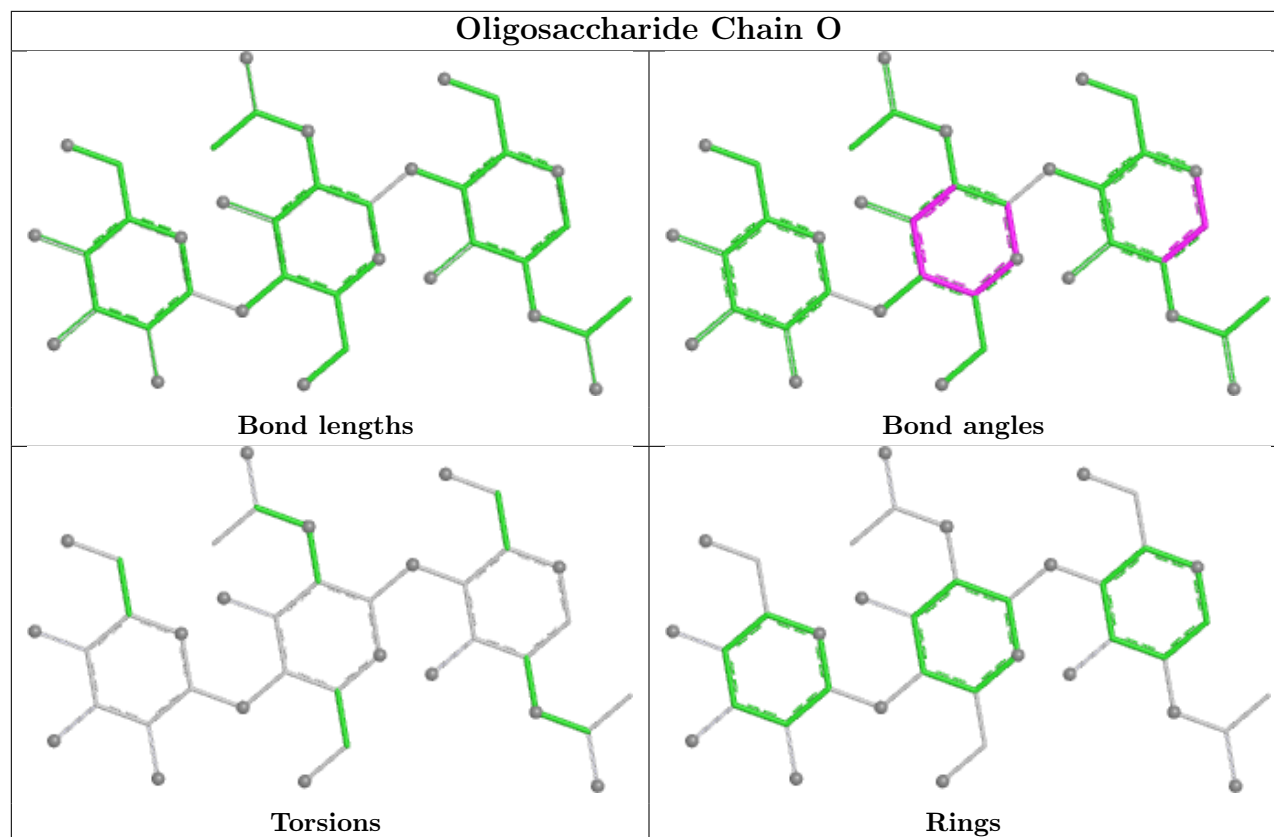
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10810. 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.