



Full wwPDB EM Validation Report ⓘ

Nov 27, 2025 – 08:21 AM JST

PDB ID : 9J6D / pdb_00009j6d
EMDB ID : EMD-61168
Title : Structure of Chikungunya virus infectious particles, 2f block.
Authors : Han, X.; Ji, C.; Wang, F.; Tian, S.; Gao, F.G.; Yan, J.
Deposited on : 2024-08-15
Resolution : 3.11 Å(reported)

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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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

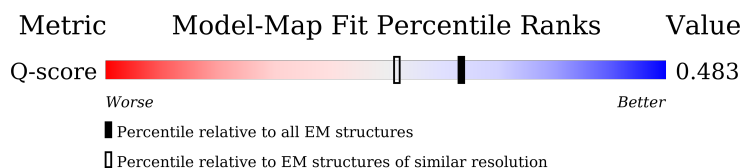
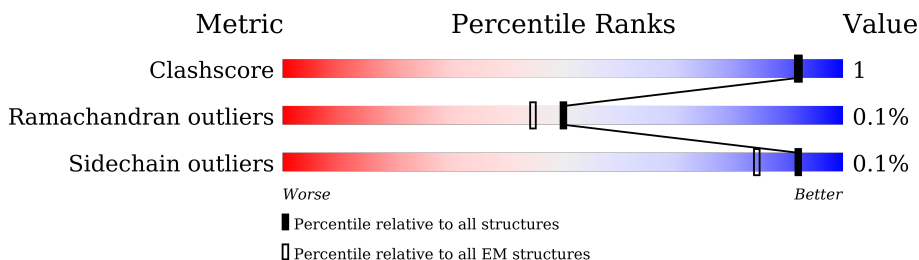
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14465 (2.61 - 3.61)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	U	55	<div> <div>85%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	V	55	<div> <div>71%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	W	55	<div> <div>89%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
1	X	55	<div> <div>96%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	A	439	
2	B	439	
2	C	439	
2	D	439	
3	E	414	
3	F	414	
3	G	414	
3	H	414	
4	I	151	
4	J	151	
4	K	151	
4	L	151	
5	M	4	
5	N	4	
5	O	4	
5	P	4	
6	Q	3	
6	R	3	
6	S	3	
6	T	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	N	1	X	-	-	-
6	BMA	Q	3	X	-	-	-
6	BMA	R	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BMA	S	3	X	-	-	-
6	BMA	T	3	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 32993 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 chikungunya E3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	55	Total	C	N	O	S	0	0
			427	268	67	83	9		
1	V	55	Total	C	N	O	S	0	0
			427	268	67	83	9		
1	W	55	Total	C	N	O	S	0	0
			427	268	67	83	9		
1	X	55	Total	C	N	O	S	0	0
			427	268	67	83	9		

- Molecule 2 is a protein called chikungunya virus E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	439	Total	C	N	O	S	0	0
			3327	2106	556	638	27		
2	B	439	Total	C	N	O	S	0	0
			3327	2106	556	638	27		
2	C	439	Total	C	N	O	S	0	0
			3327	2106	556	638	27		
2	D	439	Total	C	N	O	S	0	0
			3327	2106	556	638	27		

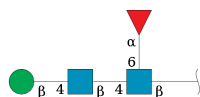
- Molecule 3 is a protein called chikungunya E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	413	Total	C	N	O	S	0	0
			3249	2039	582	600	28		
3	F	414	Total	C	N	O	S	0	0
			3257	2045	583	601	28		
3	G	414	Total	C	N	O	S	0	0
			3257	2045	583	601	28		
3	H	412	Total	C	N	O	S	0	0
			3238	2032	580	598	28		

- Molecule 4 is a protein called CHIKV capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
4	J	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
4	K	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
4	L	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	4	Total	C	N	O	0	0
			49	28	2	19		
5	N	4	Total	C	N	O	0	0
			49	28	2	19		
5	O	4	Total	C	N	O	0	0
			49	28	2	19		
5	P	4	Total	C	N	O	0	0
			49	28	2	19		

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

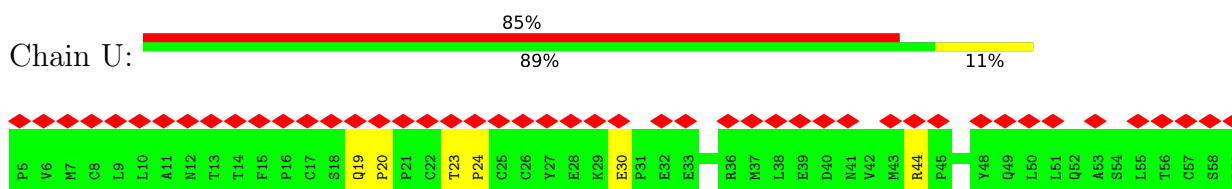


Mol	Chain	Residues	Atoms				AltConf	Trace
6	Q	3	Total	C	N	O	0	0
			39	22	2	15		
6	R	3	Total	C	N	O	0	0
			39	22	2	15		
6	S	3	Total	C	N	O	0	0
			39	22	2	15		
6	T	3	Total	C	N	O	0	0
			39	22	2	15		

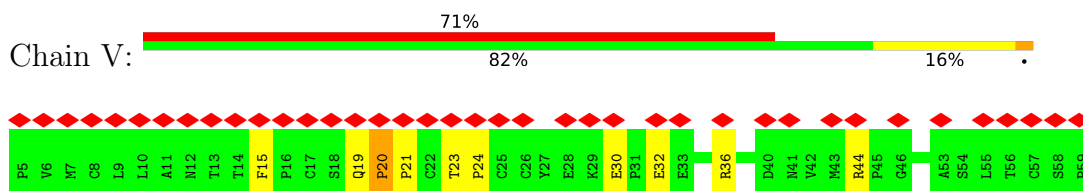
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

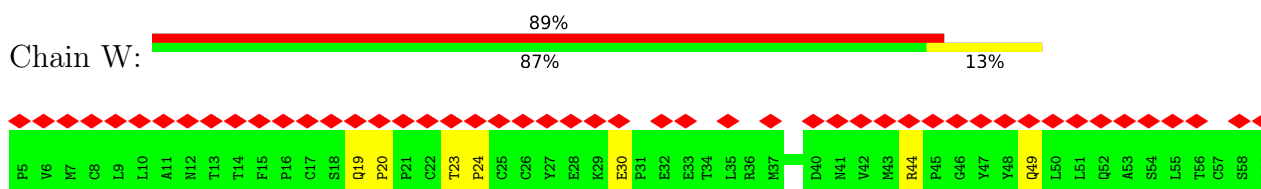
- Molecule 1: chikungunya E3



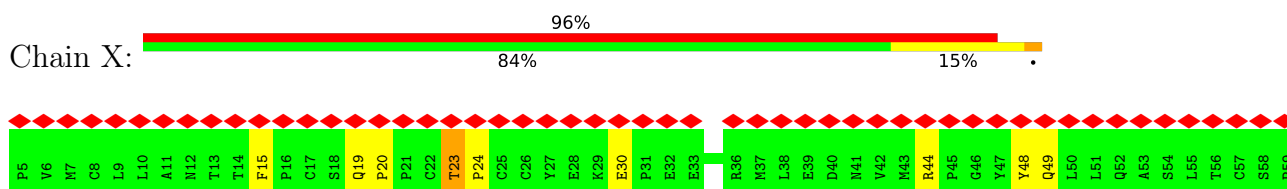
- Molecule 1: chikungunya E3



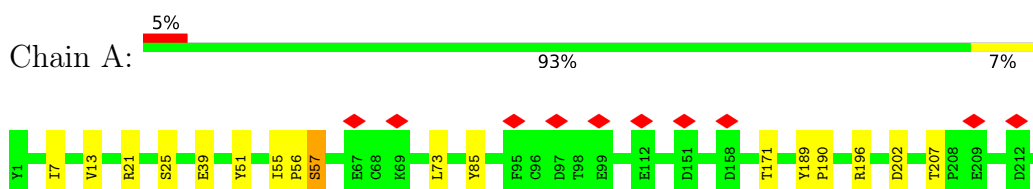
- Molecule 1: chikungunya E3

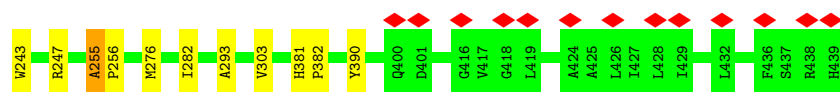


- Molecule 1: chikungunya E3

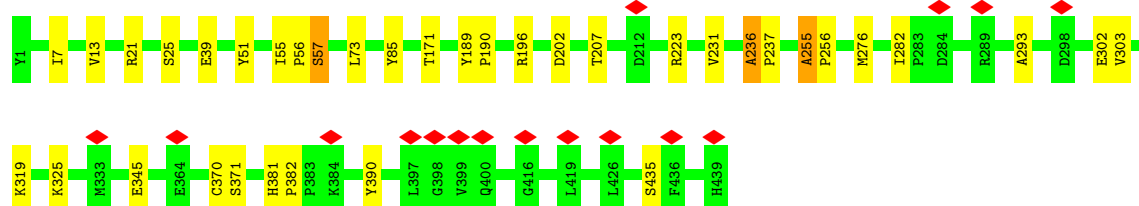


- Molecule 2: chikungunya virus E1

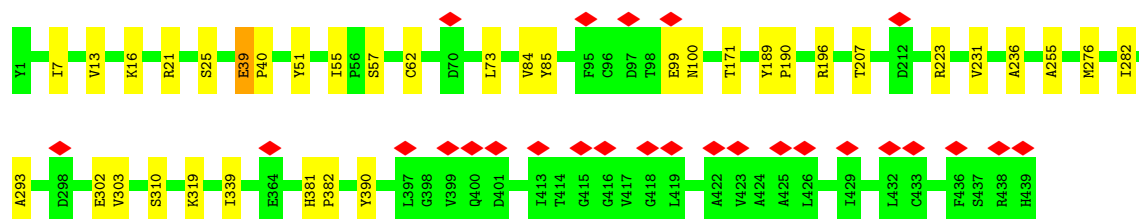




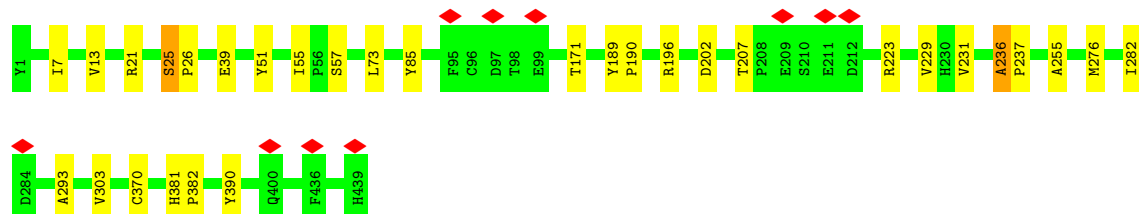
- Molecule 2: chikungunya virus E1



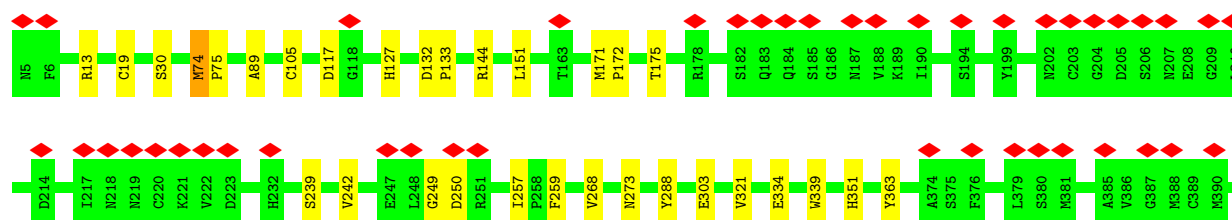
- Molecule 2: chikungunya virus E1



- Molecule 2: chikungunya virus E1

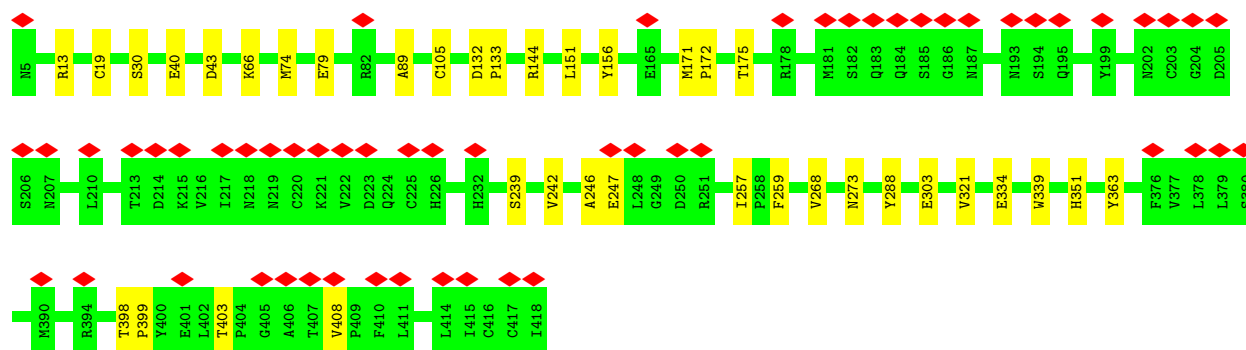
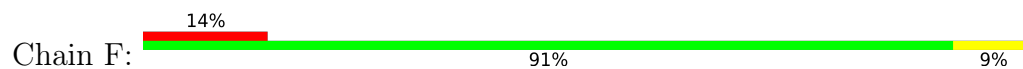


- Molecule 3: chikungunya E2

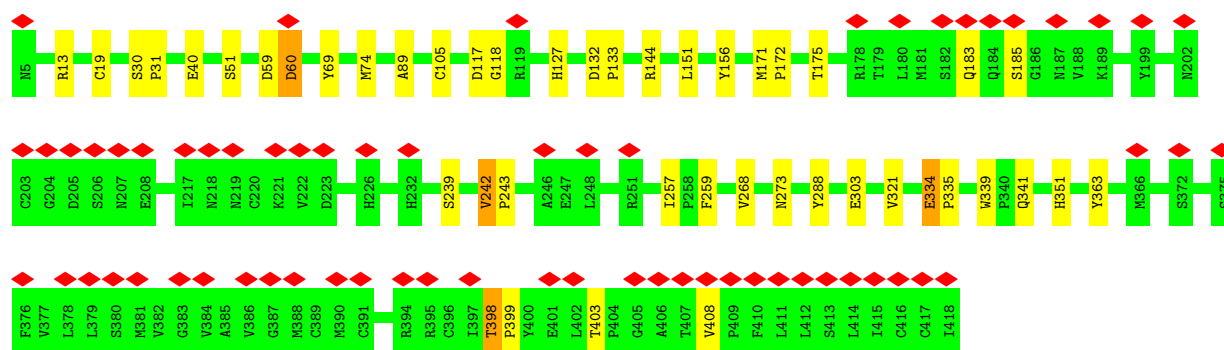
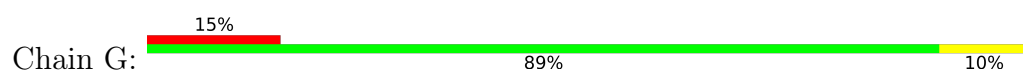




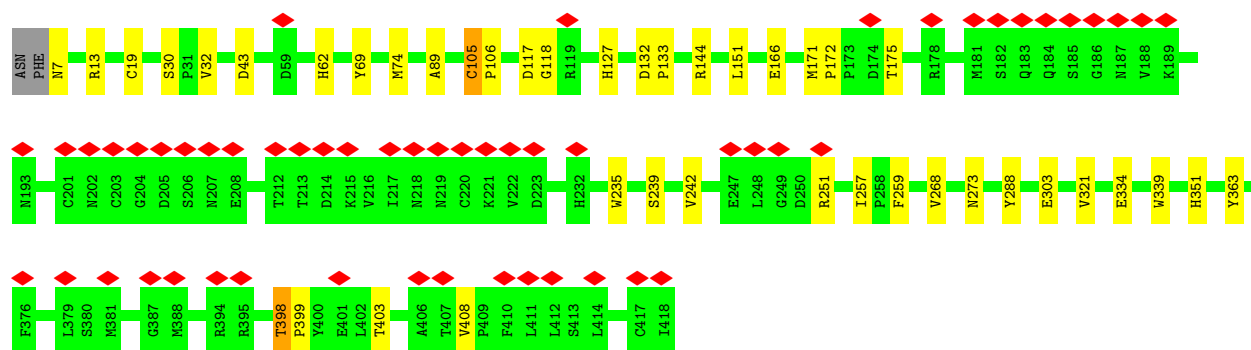
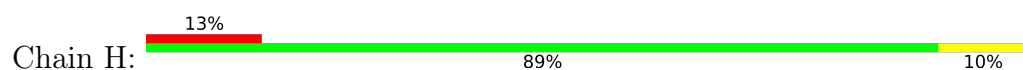
- Molecule 3: chikungunya E2



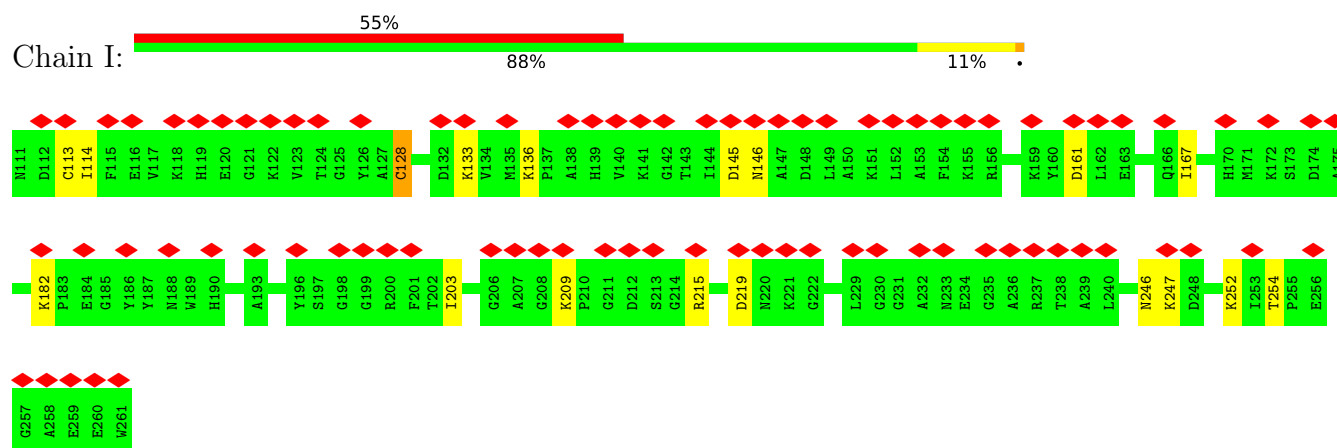
- Molecule 3: chikungunya E2



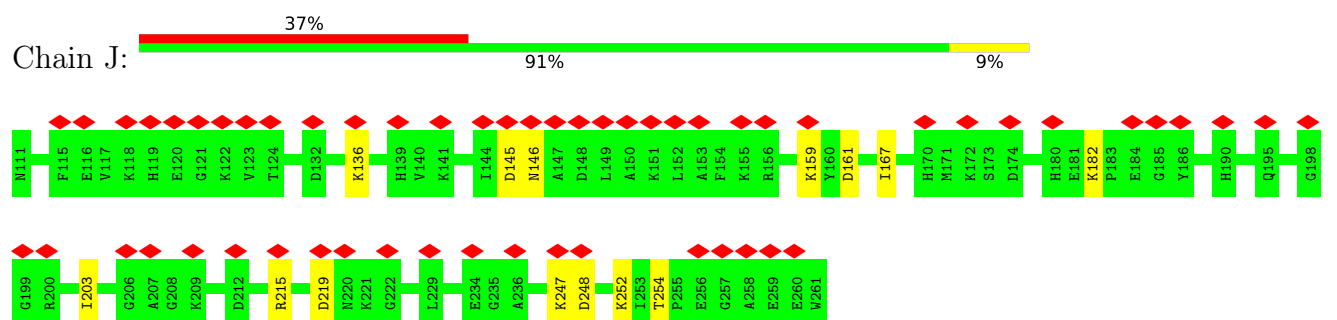
- Molecule 3: chikungunya E2



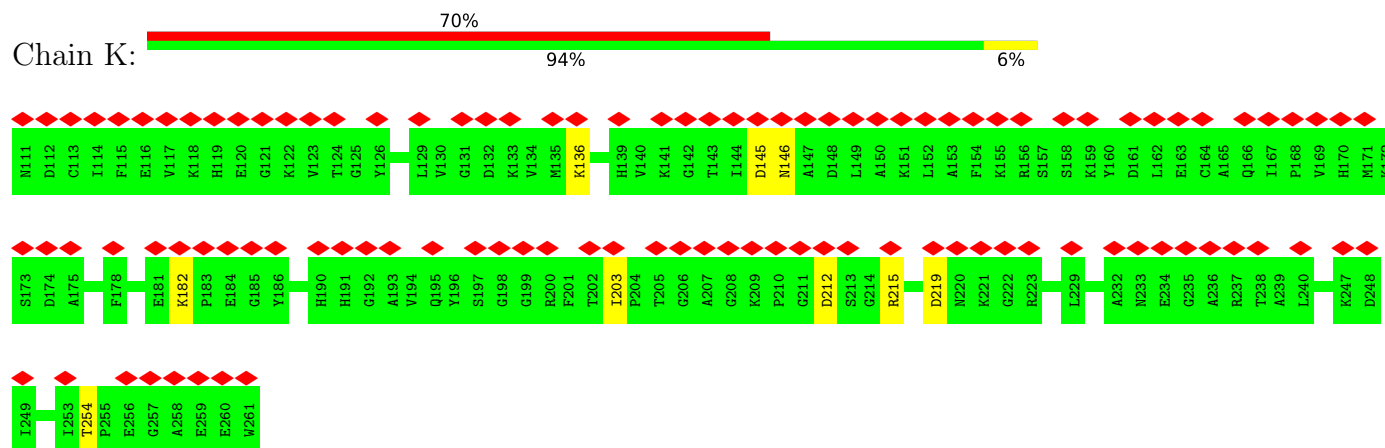
- Molecule 4: CHIKV capsid protein



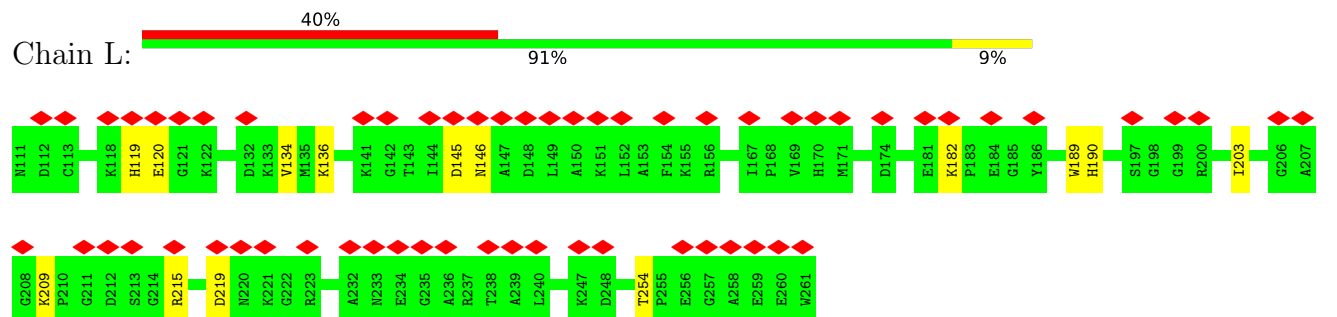
• Molecule 4: CHIKV capsid protein



• Molecule 4: CHIKV capsid protein



• Molecule 4: CHIKV capsid protein



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 



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

Chain Q: 



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

Chain R: 



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1618503	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.896	Depositor
Minimum map value	-0.480	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	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, FUC

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	U	0.63	0/438	1.16	8/598 (1.3%)
1	V	0.64	0/438	1.09	10/598 (1.7%)
1	W	0.62	0/438	1.08	8/598 (1.3%)
1	X	0.61	0/438	1.07	10/598 (1.7%)
2	A	0.61	0/3409	1.01	50/4651 (1.1%)
2	B	0.61	0/3409	0.99	50/4651 (1.1%)
2	C	0.62	0/3409	0.98	50/4651 (1.1%)
2	D	0.62	0/3409	1.00	50/4651 (1.1%)
3	E	0.63	0/3336	1.05	60/4546 (1.3%)
3	F	0.63	0/3344	1.04	56/4557 (1.2%)
3	G	0.64	0/3344	1.05	60/4557 (1.3%)
3	H	0.63	0/3324	1.06	60/4530 (1.3%)
4	I	0.63	0/1184	0.95	15/1599 (0.9%)
4	J	0.64	0/1184	0.96	12/1599 (0.8%)
4	K	0.64	0/1184	0.94	10/1599 (0.6%)
4	L	0.65	0/1184	0.92	12/1599 (0.8%)
All	All	0.63	0/33472	1.02	521/45582 (1.1%)

There are no bond length outliers.

All (521) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	19	GLN	CA-C-N	9.83	126.83	119.66
1	U	19	GLN	C-N-CA	9.83	126.83	119.66
2	A	189	TYR	CA-C-N	8.94	126.09	119.66
2	A	189	TYR	C-N-CA	8.94	126.09	119.66
2	D	189	TYR	CA-C-N	8.85	126.12	119.66
2	D	189	TYR	C-N-CA	8.85	126.12	119.66
2	B	381	HIS	CA-C-N	8.32	125.65	119.66
2	B	381	HIS	C-N-CA	8.32	125.65	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	381	HIS	CA-C-N	8.22	125.58	119.66
2	A	381	HIS	C-N-CA	8.22	125.58	119.66
3	F	172	PRO	CA-C-N	8.12	128.06	120.03
3	F	172	PRO	C-N-CA	8.12	128.06	120.03
3	H	105	CYS	CA-C-N	8.00	128.02	119.78
3	H	105	CYS	C-N-CA	8.00	128.02	119.78
3	F	144	ARG	CA-C-N	7.95	128.39	120.52
3	F	144	ARG	C-N-CA	7.95	128.39	120.52
2	C	381	HIS	CA-C-N	7.94	125.38	119.66
2	C	381	HIS	C-N-CA	7.94	125.38	119.66
3	E	105	CYS	CA-C-N	7.82	127.83	119.78
3	E	105	CYS	C-N-CA	7.82	127.83	119.78
3	G	30	SER	CA-C-N	7.79	127.43	119.56
3	G	30	SER	C-N-CA	7.79	127.43	119.56
3	H	30	SER	CA-C-N	7.78	127.42	119.56
3	H	30	SER	C-N-CA	7.78	127.42	119.56
3	E	321	VAL	CA-C-N	7.76	127.71	120.03
3	E	321	VAL	C-N-CA	7.76	127.71	120.03
3	F	105	CYS	CA-C-N	7.75	127.76	119.78
3	F	105	CYS	C-N-CA	7.75	127.76	119.78
3	H	171	MET	CA-C-N	7.72	125.22	119.66
3	H	171	MET	C-N-CA	7.72	125.22	119.66
2	B	382	PRO	CA-C-N	7.71	127.66	120.03
2	B	382	PRO	C-N-CA	7.71	127.66	120.03
3	G	144	ARG	CA-C-N	7.60	127.76	120.31
3	G	144	ARG	C-N-CA	7.60	127.76	120.31
3	F	13	ARG	CA-C-N	7.56	127.56	119.78
3	F	13	ARG	C-N-CA	7.56	127.56	119.78
3	G	171	MET	CA-C-N	7.55	125.10	119.66
3	G	171	MET	C-N-CA	7.55	125.10	119.66
2	D	382	PRO	CA-C-N	7.53	127.49	120.03
2	D	382	PRO	C-N-CA	7.53	127.49	120.03
2	D	255	ALA	CA-C-N	7.53	127.97	119.92
2	D	255	ALA	C-N-CA	7.53	127.97	119.92
3	H	13	ARG	CA-C-N	7.50	127.50	119.78
3	H	13	ARG	C-N-CA	7.50	127.50	119.78
3	H	403	THR	CA-C-N	7.48	127.19	119.56
3	H	403	THR	C-N-CA	7.48	127.19	119.56
3	F	30	SER	CA-C-N	7.47	127.10	119.56
3	F	30	SER	C-N-CA	7.47	127.10	119.56
3	E	30	SER	CA-C-N	7.46	127.09	119.56
3	E	30	SER	C-N-CA	7.46	127.09	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	255	ALA	CA-C-N	7.44	127.88	119.92
2	A	255	ALA	C-N-CA	7.44	127.88	119.92
3	E	13	ARG	CA-C-N	7.42	127.43	119.78
3	E	13	ARG	C-N-CA	7.42	127.43	119.78
2	C	255	ALA	CA-C-N	7.38	127.83	120.52
2	C	255	ALA	C-N-CA	7.38	127.83	120.52
3	G	363	TYR	CA-C-N	7.37	127.07	119.56
3	G	363	TYR	C-N-CA	7.37	127.07	119.56
3	E	144	ARG	CA-C-N	7.36	127.53	120.31
3	E	144	ARG	C-N-CA	7.36	127.53	120.31
2	B	255	ALA	CA-C-N	7.36	127.79	119.92
2	B	255	ALA	C-N-CA	7.36	127.79	119.92
4	I	254	THR	CA-C-N	7.35	127.35	119.78
4	I	254	THR	C-N-CA	7.35	127.35	119.78
4	K	215	ARG	CA-C-N	7.34	127.26	119.85
4	K	215	ARG	C-N-CA	7.34	127.26	119.85
3	E	172	PRO	CA-C-N	7.32	127.28	120.03
3	E	172	PRO	C-N-CA	7.32	127.28	120.03
3	G	172	PRO	CA-C-N	7.32	127.27	120.03
3	G	172	PRO	C-N-CA	7.32	127.27	120.03
3	H	144	ARG	CA-C-N	7.27	127.44	120.31
3	H	144	ARG	C-N-CA	7.27	127.44	120.31
1	V	44	ARG	CA-C-N	7.27	126.90	119.56
1	V	44	ARG	C-N-CA	7.27	126.90	119.56
3	E	363	TYR	CA-C-N	7.26	126.97	119.56
3	E	363	TYR	C-N-CA	7.26	126.97	119.56
3	H	363	TYR	CA-C-N	7.23	126.87	119.56
3	H	363	TYR	C-N-CA	7.23	126.87	119.56
2	A	382	PRO	CA-C-N	7.19	127.11	119.85
2	A	382	PRO	C-N-CA	7.19	127.11	119.85
2	C	196	ARG	CA-C-N	7.14	126.90	119.76
2	C	196	ARG	C-N-CA	7.14	126.90	119.76
2	C	382	PRO	CA-C-N	7.13	127.06	119.85
2	C	382	PRO	C-N-CA	7.13	127.06	119.85
2	B	73	LEU	CA-C-N	7.12	127.44	119.32
2	B	73	LEU	C-N-CA	7.12	127.44	119.32
2	D	85	TYR	CA-C-N	7.12	127.04	119.85
2	D	85	TYR	C-N-CA	7.12	127.04	119.85
2	C	73	LEU	CA-C-N	7.09	127.40	119.32
2	C	73	LEU	C-N-CA	7.09	127.40	119.32
2	A	390	TYR	CA-C-N	7.06	126.98	119.85
2	A	390	TYR	C-N-CA	7.06	126.98	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	85	TYR	CA-C-N	7.06	126.98	119.85
2	C	85	TYR	C-N-CA	7.06	126.98	119.85
3	G	259	PHE	CA-C-N	7.04	126.96	119.85
3	G	259	PHE	C-N-CA	7.04	126.96	119.85
3	G	105	CYS	CA-C-N	7.04	126.96	119.85
3	G	105	CYS	C-N-CA	7.04	126.96	119.85
2	A	73	LEU	CA-C-N	7.03	127.33	119.32
2	A	73	LEU	C-N-CA	7.03	127.33	119.32
2	C	190	PRO	CA-C-N	7.02	126.99	119.76
2	C	190	PRO	C-N-CA	7.02	126.99	119.76
2	D	73	LEU	CA-C-N	7.02	127.32	119.32
2	D	73	LEU	C-N-CA	7.02	127.32	119.32
3	G	74	MET	CA-C-N	7.01	127.00	119.78
3	G	74	MET	C-N-CA	7.01	127.00	119.78
2	A	85	TYR	CA-C-N	6.99	126.91	119.85
2	A	85	TYR	C-N-CA	6.99	126.91	119.85
3	H	268	VAL	CA-C-N	6.99	126.95	120.03
3	H	268	VAL	C-N-CA	6.99	126.95	120.03
2	D	196	ARG	CA-C-N	6.98	126.95	119.76
2	D	196	ARG	C-N-CA	6.98	126.95	119.76
1	X	44	ARG	CA-C-N	6.98	126.61	119.56
1	X	44	ARG	C-N-CA	6.98	126.61	119.56
1	U	20	PRO	CA-C-N	6.98	126.95	119.28
1	U	20	PRO	C-N-CA	6.98	126.95	119.28
3	H	175	THR	CA-C-N	6.95	126.92	119.76
3	H	175	THR	C-N-CA	6.95	126.92	119.76
2	D	223	ARG	CA-C-N	6.93	126.92	119.78
2	D	223	ARG	C-N-CA	6.93	126.92	119.78
3	E	74	MET	CA-C-N	6.93	126.92	119.78
3	E	74	MET	C-N-CA	6.93	126.92	119.78
4	L	254	THR	CA-C-N	6.92	126.91	119.78
4	L	254	THR	C-N-CA	6.92	126.91	119.78
3	G	303	GLU	CA-C-N	6.92	126.55	119.56
3	G	303	GLU	C-N-CA	6.92	126.55	119.56
1	W	44	ARG	CA-C-N	6.89	126.52	119.56
1	W	44	ARG	C-N-CA	6.89	126.52	119.56
2	B	390	TYR	CA-C-N	6.86	126.78	119.85
2	B	390	TYR	C-N-CA	6.86	126.78	119.85
2	B	85	TYR	CA-C-N	6.85	126.61	119.76
2	B	85	TYR	C-N-CA	6.85	126.61	119.76
2	D	276	MET	CA-C-N	6.83	126.80	119.76
2	D	276	MET	C-N-CA	6.83	126.80	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	172	PRO	CA-C-N	6.83	126.79	120.03
3	H	172	PRO	C-N-CA	6.83	126.79	120.03
3	F	74	MET	CA-C-N	6.82	126.78	120.03
3	F	74	MET	C-N-CA	6.82	126.78	120.03
3	E	175	THR	CA-C-N	6.81	126.78	119.76
3	E	175	THR	C-N-CA	6.81	126.78	119.76
3	G	13	ARG	CA-C-N	6.79	126.75	120.03
3	G	13	ARG	C-N-CA	6.79	126.75	120.03
3	H	259	PHE	CA-C-N	6.79	126.71	119.85
3	H	259	PHE	C-N-CA	6.79	126.71	119.85
3	H	303	GLU	CA-C-N	6.77	126.39	119.56
3	H	303	GLU	C-N-CA	6.77	126.39	119.56
2	C	390	TYR	CA-C-N	6.75	126.67	119.85
2	C	390	TYR	C-N-CA	6.75	126.67	119.85
2	D	390	TYR	CA-C-N	6.75	126.67	119.85
2	D	390	TYR	C-N-CA	6.75	126.67	119.85
3	F	239	SER	CA-C-N	6.75	126.89	119.87
3	F	239	SER	C-N-CA	6.75	126.89	119.87
3	H	257	ILE	CA-C-N	6.74	126.71	120.03
3	H	257	ILE	C-N-CA	6.74	126.71	120.03
3	E	273	ASN	CA-C-N	6.74	126.66	119.85
3	E	273	ASN	C-N-CA	6.74	126.66	119.85
1	U	44	ARG	CA-C-N	6.72	126.35	119.56
1	U	44	ARG	C-N-CA	6.72	126.35	119.56
2	D	190	PRO	CA-C-N	6.72	126.68	119.76
2	D	190	PRO	C-N-CA	6.72	126.68	119.76
3	E	268	VAL	CA-C-N	6.72	126.68	120.03
3	E	268	VAL	C-N-CA	6.72	126.68	120.03
3	F	268	VAL	CA-C-N	6.71	126.67	120.03
3	F	268	VAL	C-N-CA	6.71	126.67	120.03
3	G	273	ASN	CA-C-N	6.70	126.87	120.31
3	G	273	ASN	C-N-CA	6.70	126.87	120.31
2	C	55	ILE	CA-C-N	6.69	126.67	119.78
2	C	55	ILE	C-N-CA	6.69	126.67	119.78
2	C	171	THR	CA-C-N	6.67	126.30	119.56
2	C	171	THR	C-N-CA	6.67	126.30	119.56
2	D	7	ILE	CA-C-N	6.67	126.66	119.78
2	D	7	ILE	C-N-CA	6.67	126.66	119.78
3	G	268	VAL	CA-C-N	6.66	126.62	120.03
3	G	268	VAL	C-N-CA	6.66	126.62	120.03
1	X	19	GLN	CA-C-N	6.66	127.24	120.38
1	X	19	GLN	C-N-CA	6.66	127.24	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	259	PHE	CA-C-N	6.65	126.57	119.85
3	E	259	PHE	C-N-CA	6.65	126.57	119.85
3	F	259	PHE	CA-C-N	6.65	126.57	119.85
3	F	259	PHE	C-N-CA	6.65	126.57	119.85
4	K	254	THR	CA-C-N	6.62	126.58	119.76
4	K	254	THR	C-N-CA	6.62	126.58	119.76
3	E	239	SER	CA-C-N	6.62	126.76	119.87
3	E	239	SER	C-N-CA	6.62	126.76	119.87
2	A	190	PRO	CA-C-N	6.62	126.60	119.78
2	A	190	PRO	C-N-CA	6.62	126.60	119.78
3	G	339	TRP	CA-C-N	6.62	126.53	119.85
3	G	339	TRP	C-N-CA	6.62	126.53	119.85
3	H	239	SER	CA-C-N	6.62	126.75	119.87
3	H	239	SER	C-N-CA	6.62	126.75	119.87
2	C	303	VAL	CA-C-N	6.60	126.85	119.32
2	C	303	VAL	C-N-CA	6.60	126.85	119.32
2	D	171	THR	CA-C-N	6.60	126.23	119.56
2	D	171	THR	C-N-CA	6.60	126.23	119.56
2	B	196	ARG	CA-C-N	6.60	126.56	119.76
2	B	196	ARG	C-N-CA	6.60	126.56	119.76
2	A	223	ARG	CA-C-N	6.60	126.52	119.85
2	A	223	ARG	C-N-CA	6.60	126.52	119.85
3	G	321	VAL	CA-C-N	6.60	127.05	120.52
3	G	321	VAL	C-N-CA	6.60	127.05	120.52
3	H	19	CYS	CA-C-N	6.58	126.27	119.56
3	H	19	CYS	C-N-CA	6.58	126.27	119.56
3	E	334	GLU	CA-C-N	6.58	126.53	119.76
3	E	334	GLU	C-N-CA	6.58	126.53	119.76
2	D	236	ALA	CA-C-N	6.57	126.54	119.78
2	D	236	ALA	C-N-CA	6.57	126.54	119.78
3	H	74	MET	CA-C-N	6.57	126.54	119.78
3	H	74	MET	C-N-CA	6.57	126.54	119.78
3	H	321	VAL	CA-C-N	6.57	127.02	120.52
3	H	321	VAL	C-N-CA	6.57	127.02	120.52
3	F	133	PRO	CA-C-N	6.56	126.48	119.85
3	F	133	PRO	C-N-CA	6.56	126.48	119.85
2	B	55	ILE	CA-C-N	6.56	126.54	119.78
2	B	55	ILE	C-N-CA	6.56	126.54	119.78
3	G	239	SER	CA-C-N	6.55	126.68	119.87
3	G	239	SER	C-N-CA	6.55	126.68	119.87
2	B	276	MET	CA-C-N	6.55	126.50	119.76
2	B	276	MET	C-N-CA	6.55	126.50	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	ARG	CA-C-N	6.53	126.44	119.85
2	B	223	ARG	C-N-CA	6.53	126.44	119.85
2	A	293	ALA	CA-C-N	6.53	126.48	119.76
2	A	293	ALA	C-N-CA	6.53	126.48	119.76
1	W	19	GLN	CA-C-N	6.53	127.10	120.38
1	W	19	GLN	C-N-CA	6.53	127.10	120.38
3	F	273	ASN	CA-C-N	6.52	126.49	119.78
3	F	273	ASN	C-N-CA	6.52	126.49	119.78
3	F	257	ILE	CA-C-N	6.51	126.48	120.03
3	F	257	ILE	C-N-CA	6.51	126.48	120.03
3	H	273	ASN	CA-C-N	6.51	126.48	120.03
3	H	273	ASN	C-N-CA	6.51	126.48	120.03
3	E	339	TRP	CA-C-N	6.50	126.42	119.85
3	E	339	TRP	C-N-CA	6.50	126.42	119.85
4	I	215	ARG	CA-C-N	6.50	127.03	120.14
4	I	215	ARG	C-N-CA	6.50	127.03	120.14
3	E	303	GLU	CA-C-N	6.50	126.19	119.56
3	E	303	GLU	C-N-CA	6.50	126.19	119.56
2	A	25	SER	CA-C-N	6.49	126.40	119.85
2	A	25	SER	C-N-CA	6.49	126.40	119.85
3	E	403	THR	CA-C-N	6.49	126.17	119.56
3	E	403	THR	C-N-CA	6.49	126.17	119.56
3	F	321	VAL	CA-C-N	6.48	126.94	120.52
3	F	321	VAL	C-N-CA	6.48	126.94	120.52
3	G	175	THR	CA-C-N	6.48	126.24	119.76
3	G	175	THR	C-N-CA	6.48	126.24	119.76
2	A	55	ILE	CA-C-N	6.48	126.45	119.78
2	A	55	ILE	C-N-CA	6.48	126.45	119.78
2	A	196	ARG	CA-C-N	6.47	126.43	119.76
2	A	196	ARG	C-N-CA	6.47	126.43	119.76
3	E	257	ILE	CA-C-N	6.47	126.44	120.03
3	E	257	ILE	C-N-CA	6.47	126.44	120.03
2	D	55	ILE	CA-C-N	6.46	126.44	119.78
2	D	55	ILE	C-N-CA	6.46	126.44	119.78
3	F	303	GLU	CA-C-N	6.46	126.03	119.19
3	F	303	GLU	C-N-CA	6.46	126.03	119.19
3	G	257	ILE	CA-C-N	6.46	126.42	120.03
3	G	257	ILE	C-N-CA	6.46	126.42	120.03
2	B	171	THR	CA-C-N	6.45	126.08	119.56
2	B	171	THR	C-N-CA	6.45	126.08	119.56
3	H	288	TYR	CA-C-N	6.44	126.36	119.85
3	H	288	TYR	C-N-CA	6.44	126.36	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	57	SER	CA-C-N	6.44	126.36	119.85
2	D	57	SER	C-N-CA	6.44	126.36	119.85
2	D	303	VAL	CA-C-N	6.44	126.07	119.56
2	D	303	VAL	C-N-CA	6.44	126.07	119.56
4	I	167	ILE	CA-C-N	6.44	126.47	119.90
4	I	167	ILE	C-N-CA	6.44	126.47	119.90
4	J	215	ARG	CA-C-N	6.44	126.35	119.85
4	J	215	ARG	C-N-CA	6.44	126.35	119.85
1	V	30	GLU	CA-C-N	6.43	126.01	119.19
1	V	30	GLU	C-N-CA	6.43	126.01	119.19
2	B	190	PRO	CA-C-N	6.43	126.41	119.78
2	B	190	PRO	C-N-CA	6.43	126.41	119.78
2	C	223	ARG	CA-C-N	6.43	126.35	119.85
2	C	223	ARG	C-N-CA	6.43	126.35	119.85
3	E	133	PRO	CA-C-N	6.43	126.35	119.85
3	E	133	PRO	C-N-CA	6.43	126.35	119.85
2	A	13	VAL	CA-C-N	6.42	126.18	119.76
2	A	13	VAL	C-N-CA	6.42	126.18	119.76
2	A	171	THR	CA-C-N	6.42	126.05	119.56
2	A	171	THR	C-N-CA	6.42	126.05	119.56
3	F	175	THR	CA-C-N	6.40	126.16	119.76
3	F	175	THR	C-N-CA	6.40	126.16	119.76
3	F	19	CYS	CA-C-N	6.40	126.32	119.28
3	F	19	CYS	C-N-CA	6.40	126.32	119.28
2	A	39	GLU	CA-C-N	6.39	126.31	119.85
2	A	39	GLU	C-N-CA	6.39	126.31	119.85
3	G	133	PRO	CA-C-N	6.39	126.31	119.85
3	G	133	PRO	C-N-CA	6.39	126.31	119.85
2	A	303	VAL	CA-C-N	6.39	126.02	119.56
2	A	303	VAL	C-N-CA	6.39	126.02	119.56
3	H	242	VAL	CA-C-N	6.39	126.31	119.85
3	H	242	VAL	C-N-CA	6.39	126.31	119.85
1	W	20	PRO	CA-C-N	6.38	126.07	119.56
1	W	20	PRO	C-N-CA	6.38	126.07	119.56
2	B	293	ALA	CA-C-N	6.38	126.33	119.76
2	B	293	ALA	C-N-CA	6.38	126.33	119.76
4	J	254	THR	CA-C-N	6.37	126.32	119.76
4	J	254	THR	C-N-CA	6.37	126.32	119.76
2	B	57	SER	CA-C-N	6.36	126.12	119.76
2	B	57	SER	C-N-CA	6.36	126.12	119.76
3	E	242	VAL	CA-C-N	6.36	126.27	119.85
3	E	242	VAL	C-N-CA	6.36	126.27	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	293	ALA	CA-C-N	6.35	126.30	119.76
2	C	293	ALA	C-N-CA	6.35	126.30	119.76
4	I	136	LYS	CA-C-N	6.34	126.29	119.76
4	I	136	LYS	C-N-CA	6.34	126.29	119.76
3	H	133	PRO	CA-C-N	6.33	126.25	119.85
3	H	133	PRO	C-N-CA	6.33	126.25	119.85
4	L	182	LYS	CA-C-N	6.33	126.25	119.85
4	L	182	LYS	C-N-CA	6.33	126.25	119.85
2	B	303	VAL	CA-C-N	6.33	126.54	119.32
2	B	303	VAL	C-N-CA	6.33	126.54	119.32
3	E	151	LEU	CA-C-N	6.33	126.28	119.76
3	E	151	LEU	C-N-CA	6.33	126.28	119.76
4	I	182	LYS	CA-C-N	6.32	126.24	119.85
4	I	182	LYS	C-N-CA	6.32	126.24	119.85
2	B	7	ILE	CA-C-N	6.32	126.29	119.78
2	B	7	ILE	C-N-CA	6.32	126.29	119.78
2	C	13	VAL	CA-C-N	6.31	126.07	119.76
2	C	13	VAL	C-N-CA	6.31	126.07	119.76
2	C	57	SER	CA-C-N	6.30	126.06	119.76
2	C	57	SER	C-N-CA	6.30	126.06	119.76
2	B	13	VAL	CA-C-N	6.29	126.05	119.76
2	B	13	VAL	C-N-CA	6.29	126.05	119.76
3	F	334	GLU	CA-C-N	6.27	126.22	119.76
3	F	334	GLU	C-N-CA	6.27	126.22	119.76
2	B	236	ALA	CA-C-N	6.25	126.21	119.78
2	B	236	ALA	C-N-CA	6.25	126.21	119.78
2	B	25	SER	CA-C-N	6.23	126.18	119.76
2	B	25	SER	C-N-CA	6.23	126.18	119.76
2	A	7	ILE	CA-C-N	6.23	126.18	119.76
2	A	7	ILE	C-N-CA	6.23	126.18	119.76
3	F	151	LEU	CA-C-N	6.22	126.17	119.76
3	F	151	LEU	C-N-CA	6.22	126.17	119.76
4	L	215	ARG	CA-C-N	6.21	126.72	120.14
4	L	215	ARG	C-N-CA	6.21	126.72	120.14
2	B	39	GLU	CA-C-N	6.20	126.11	119.85
2	B	39	GLU	C-N-CA	6.20	126.11	119.85
4	J	182	LYS	CA-C-N	6.19	126.11	119.85
4	J	182	LYS	C-N-CA	6.19	126.11	119.85
3	F	242	VAL	CA-C-N	6.17	126.09	119.85
3	F	242	VAL	C-N-CA	6.17	126.09	119.85
1	X	30	GLU	CA-C-N	6.17	125.73	119.19
1	X	30	GLU	C-N-CA	6.17	125.73	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	182	LYS	CA-C-N	6.15	126.07	119.85
4	K	182	LYS	C-N-CA	6.15	126.07	119.85
2	A	282	ILE	CA-C-N	6.15	126.06	119.85
2	A	282	ILE	C-N-CA	6.15	126.06	119.85
1	X	20	PRO	CA-C-N	6.15	125.83	119.56
1	X	20	PRO	C-N-CA	6.15	125.83	119.56
3	F	363	TYR	CA-C-N	6.14	126.32	119.32
3	F	363	TYR	C-N-CA	6.14	126.32	119.32
3	G	334	GLU	CA-C-N	6.12	126.07	119.76
3	G	334	GLU	C-N-CA	6.12	126.07	119.76
2	A	236	ALA	CA-C-N	6.12	126.08	119.78
2	A	236	ALA	C-N-CA	6.12	126.08	119.78
1	V	19	GLN	CA-C-N	6.11	126.67	120.38
1	V	19	GLN	C-N-CA	6.11	126.67	120.38
2	D	13	VAL	CA-C-N	6.11	125.87	119.76
2	D	13	VAL	C-N-CA	6.11	125.87	119.76
2	B	231	VAL	CA-C-N	6.10	126.61	120.14
2	B	231	VAL	C-N-CA	6.10	126.61	120.14
2	D	293	ALA	CA-C-N	6.10	126.05	119.76
2	D	293	ALA	C-N-CA	6.10	126.05	119.76
3	E	288	TYR	CA-C-N	6.10	126.01	119.85
3	E	288	TYR	C-N-CA	6.10	126.01	119.85
2	A	207	THR	CA-C-N	6.10	126.27	119.32
2	A	207	THR	C-N-CA	6.10	126.27	119.32
3	G	288	TYR	CA-C-N	6.10	126.01	119.85
3	G	288	TYR	C-N-CA	6.10	126.01	119.85
3	H	334	GLU	CA-C-N	6.10	126.04	119.76
3	H	334	GLU	C-N-CA	6.10	126.04	119.76
2	C	189	TYR	CA-C-N	6.10	126.66	120.38
2	C	189	TYR	C-N-CA	6.10	126.66	120.38
2	C	282	ILE	CA-C-N	6.09	126.01	119.85
2	C	282	ILE	C-N-CA	6.09	126.01	119.85
3	F	408	VAL	CA-C-N	6.09	126.01	119.85
3	F	408	VAL	C-N-CA	6.09	126.01	119.85
3	E	19	CYS	CA-C-N	6.09	125.98	119.28
3	E	19	CYS	C-N-CA	6.09	125.98	119.28
2	C	236	ALA	CA-C-N	6.08	126.04	119.78
2	C	236	ALA	C-N-CA	6.08	126.04	119.78
3	G	242	VAL	CA-C-N	6.07	126.03	119.78
3	G	242	VAL	C-N-CA	6.07	126.03	119.78
2	C	39	GLU	CA-C-N	6.06	125.82	119.76
2	C	39	GLU	C-N-CA	6.06	125.82	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	276	MET	CA-C-N	6.05	126.00	119.76
2	C	276	MET	C-N-CA	6.05	126.00	119.76
2	D	282	ILE	CA-C-N	6.04	125.95	119.85
2	D	282	ILE	C-N-CA	6.04	125.95	119.85
2	D	231	VAL	CA-C-N	6.04	126.54	120.14
2	D	231	VAL	C-N-CA	6.04	126.54	120.14
3	H	151	LEU	CA-C-N	6.03	125.97	119.76
3	H	151	LEU	C-N-CA	6.03	125.97	119.76
4	J	167	ILE	CA-C-N	6.03	125.97	119.76
4	J	167	ILE	C-N-CA	6.03	125.97	119.76
3	H	408	VAL	CA-C-N	6.02	126.04	119.90
3	H	408	VAL	C-N-CA	6.02	126.04	119.90
3	E	408	VAL	CA-C-N	6.01	126.03	119.90
3	E	408	VAL	C-N-CA	6.01	126.03	119.90
2	B	282	ILE	CA-C-N	6.01	125.92	119.85
2	B	282	ILE	C-N-CA	6.01	125.92	119.85
2	A	276	MET	CA-C-N	5.99	125.75	119.76
2	A	276	MET	C-N-CA	5.99	125.75	119.76
4	L	203	ILE	CA-C-N	5.99	125.93	119.76
4	L	203	ILE	C-N-CA	5.99	125.93	119.76
3	G	408	VAL	CA-C-N	5.99	126.01	119.90
3	G	408	VAL	C-N-CA	5.99	126.01	119.90
2	D	25	SER	CA-C-N	5.97	125.99	119.90
2	D	25	SER	C-N-CA	5.97	125.99	119.90
2	D	39	GLU	CA-C-N	5.95	125.71	119.76
2	D	39	GLU	C-N-CA	5.95	125.71	119.76
2	A	57	SER	CA-C-N	5.94	125.85	119.85
2	A	57	SER	C-N-CA	5.94	125.85	119.85
3	G	151	LEU	CA-C-N	5.93	126.24	119.83
3	G	151	LEU	C-N-CA	5.93	126.24	119.83
3	G	19	CYS	CA-C-N	5.92	125.80	119.28
3	G	19	CYS	C-N-CA	5.92	125.80	119.28
2	D	207	THR	CA-C-N	5.89	125.57	119.56
2	D	207	THR	C-N-CA	5.89	125.57	119.56
3	F	171	MET	CA-C-N	5.89	126.44	120.38
3	F	171	MET	C-N-CA	5.89	126.44	120.38
2	C	231	VAL	CA-C-N	5.85	125.76	119.85
2	C	231	VAL	C-N-CA	5.85	125.76	119.85
4	I	114	ILE	N-CA-C	5.84	116.60	108.89
2	A	231	VAL	CA-C-N	5.83	126.32	120.14
2	A	231	VAL	C-N-CA	5.83	126.32	120.14
3	F	403	THR	CA-C-N	5.83	125.74	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	403	THR	C-N-CA	5.83	125.74	119.85
3	H	89	ALA	CA-C-N	5.83	125.84	119.90
3	H	89	ALA	C-N-CA	5.83	125.84	119.90
2	C	7	ILE	CA-C-N	5.82	125.83	119.90
2	C	7	ILE	C-N-CA	5.82	125.83	119.90
4	J	136	LYS	CA-C-N	5.82	125.75	119.76
4	J	136	LYS	C-N-CA	5.82	125.75	119.76
2	C	25	SER	CA-C-N	5.80	125.81	119.90
2	C	25	SER	C-N-CA	5.80	125.81	119.90
3	H	351	HIS	CA-C-N	5.79	125.92	119.32
3	H	351	HIS	C-N-CA	5.79	125.92	119.32
3	F	351	HIS	CA-C-N	5.79	125.92	119.32
3	F	351	HIS	C-N-CA	5.79	125.92	119.32
3	F	132	ASP	CA-C-N	5.78	126.34	120.38
3	F	132	ASP	C-N-CA	5.78	126.34	120.38
3	F	89	ALA	CA-C-N	5.78	125.80	119.90
3	F	89	ALA	C-N-CA	5.78	125.80	119.90
3	G	403	THR	CA-C-N	5.78	126.07	119.83
3	G	403	THR	C-N-CA	5.78	126.07	119.83
3	F	288	TYR	CA-C-N	5.76	125.52	119.76
3	F	288	TYR	C-N-CA	5.76	125.52	119.76
3	E	351	HIS	CA-C-N	5.72	125.84	119.32
3	E	351	HIS	C-N-CA	5.72	125.84	119.32
2	A	21	ARG	CA-C-N	5.71	126.04	119.93
2	A	21	ARG	C-N-CA	5.71	126.04	119.93
1	V	20	PRO	CA-C-N	5.70	126.08	119.47
1	V	20	PRO	C-N-CA	5.70	126.08	119.47
3	F	339	TRP	CA-C-N	5.69	126.17	120.14
3	F	339	TRP	C-N-CA	5.69	126.17	120.14
4	J	203	ILE	CA-C-N	5.69	125.62	119.76
4	J	203	ILE	C-N-CA	5.69	125.62	119.76
3	E	398	THR	CA-C-N	5.69	125.36	119.56
3	E	398	THR	C-N-CA	5.69	125.36	119.56
3	H	339	TRP	CA-C-N	5.68	126.17	120.14
3	H	339	TRP	C-N-CA	5.68	126.17	120.14
1	W	30	GLU	CA-C-N	5.68	125.53	119.28
1	W	30	GLU	C-N-CA	5.68	125.53	119.28
4	K	203	ILE	CA-C-N	5.68	125.61	119.76
4	K	203	ILE	C-N-CA	5.68	125.61	119.76
2	B	189	TYR	CA-C-N	5.65	126.20	120.38
2	B	189	TYR	C-N-CA	5.65	126.20	120.38
3	E	171	MET	CA-C-N	5.65	126.20	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	171	MET	C-N-CA	5.65	126.20	120.38
3	E	89	ALA	CA-C-N	5.61	125.62	119.90
3	E	89	ALA	C-N-CA	5.61	125.62	119.90
3	G	351	HIS	CA-C-N	5.60	125.70	119.32
3	G	351	HIS	C-N-CA	5.60	125.70	119.32
3	H	132	ASP	CA-C-N	5.57	126.12	120.38
3	H	132	ASP	C-N-CA	5.57	126.12	120.38
3	E	132	ASP	CA-C-N	5.57	126.11	120.38
3	E	132	ASP	C-N-CA	5.57	126.11	120.38
3	G	398	THR	CA-C-N	5.53	125.20	119.56
3	G	398	THR	C-N-CA	5.53	125.20	119.56
4	L	136	LYS	CA-C-N	5.52	125.80	119.83
4	L	136	LYS	C-N-CA	5.52	125.80	119.83
3	G	132	ASP	CA-C-N	5.50	126.05	120.38
3	G	132	ASP	C-N-CA	5.50	126.05	120.38
4	I	203	ILE	CA-C-N	5.46	125.39	119.76
4	I	203	ILE	C-N-CA	5.46	125.39	119.76
3	G	127	HIS	CA-C-N	5.46	125.22	119.76
3	G	127	HIS	C-N-CA	5.46	125.22	119.76
3	H	398	THR	CA-C-N	5.40	125.07	119.56
3	H	398	THR	C-N-CA	5.40	125.07	119.56
1	U	30	GLU	CA-C-N	5.38	125.19	119.28
1	U	30	GLU	C-N-CA	5.38	125.19	119.28
2	C	21	ARG	CA-C-N	5.30	125.60	119.93
2	C	21	ARG	C-N-CA	5.30	125.60	119.93
4	I	209	LYS	CA-C-N	5.29	125.30	119.90
4	I	209	LYS	C-N-CA	5.29	125.30	119.90
2	D	381	HIS	CA-C-N	5.28	125.81	120.38
2	D	381	HIS	C-N-CA	5.28	125.81	120.38
2	D	21	ARG	CA-C-N	5.26	125.55	119.93
2	D	21	ARG	C-N-CA	5.26	125.55	119.93
3	H	127	HIS	CA-C-N	5.23	125.53	119.93
3	H	127	HIS	C-N-CA	5.23	125.53	119.93
1	V	15	PHE	CA-C-N	5.23	125.48	119.83
1	V	15	PHE	C-N-CA	5.23	125.48	119.83
1	X	15	PHE	CA-C-N	5.22	125.47	119.83
1	X	15	PHE	C-N-CA	5.22	125.47	119.83
2	B	207	THR	CA-C-N	5.21	125.51	119.47
2	B	207	THR	C-N-CA	5.21	125.51	119.47
2	C	207	THR	CA-C-N	5.18	125.48	119.47
2	C	207	THR	C-N-CA	5.18	125.48	119.47
4	K	136	LYS	CA-C-N	5.14	125.38	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	136	LYS	C-N-CA	5.14	125.38	119.83
2	B	21	ARG	CA-C-N	5.12	125.41	119.93
2	B	21	ARG	C-N-CA	5.12	125.41	119.93
3	G	89	ALA	CA-C-N	5.08	125.37	119.93
3	G	89	ALA	C-N-CA	5.08	125.37	119.93
4	L	209	LYS	CA-C-N	5.08	125.36	119.93
4	L	209	LYS	C-N-CA	5.08	125.36	119.93
3	E	127	HIS	CA-C-N	5.02	125.25	119.83
3	E	127	HIS	C-N-CA	5.02	125.25	119.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	427	0	410	4	0
1	V	427	0	410	4	0
1	W	427	0	410	3	0
1	X	427	0	410	6	0
2	A	3327	0	3247	6	0
2	B	3327	0	3249	9	0
2	C	3327	0	3247	7	0
2	D	3327	0	3249	5	0
3	E	3249	0	3178	4	0
3	F	3257	0	3189	5	0
3	G	3257	0	3189	10	0
3	H	3238	0	3174	9	0
4	I	1156	0	1135	5	0
4	J	1156	0	1135	5	0
4	K	1156	0	1135	3	0
4	L	1156	0	1135	6	0
5	M	49	0	43	0	0
5	N	49	0	43	0	0
5	O	49	0	43	0	0
5	P	49	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	39	0	34	0	0
6	R	39	0	34	0	0
6	S	39	0	34	0	0
6	T	39	0	34	0	0
All	All	32993	0	32210	88	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 1.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:7:ASN:N	3:H:62:HIS:HE2	1.93	0.66
1:U:23:THR:N	1:U:24:PRO:CD	2.58	0.66
1:X:23:THR:H	1:X:24:PRO:CD	2.09	0.65
1:V:23:THR:N	1:V:24:PRO:CD	2.60	0.64
1:W:23:THR:N	1:W:24:PRO:CD	2.61	0.63
3:G:40:GLU:OE1	3:G:156:TYR:OH	2.16	0.63
1:W:23:THR:N	1:W:24:PRO:HD2	2.15	0.62
3:H:69:TYR:OH	3:H:117:ASP:OD1	2.14	0.61
1:U:23:THR:H	1:U:24:PRO:CD	2.18	0.56
1:X:23:THR:H	1:X:24:PRO:HD2	1.70	0.56
1:X:23:THR:N	1:X:24:PRO:CD	2.69	0.55
3:F:40:GLU:OE1	3:F:156:TYR:OH	2.24	0.54
1:U:23:THR:H	1:U:24:PRO:HD3	1.72	0.54
3:H:166:GLU:OE1	1:X:48:TYR:OH	2.25	0.54
4:L:119:HIS:CG	4:L:120:GLU:N	2.78	0.52
2:B:325:LYS:NZ	2:B:345:GLU:OE2	2.40	0.52
3:F:66:LYS:NZ	3:F:79:GLU:OE2	2.42	0.52
1:U:23:THR:N	1:U:24:PRO:HD2	2.25	0.51
4:L:119:HIS:CG	4:L:120:GLU:H	2.27	0.51
3:E:249:GLY:O	3:E:250:ASP:C	2.51	0.51
3:E:398:THR:N	3:E:399:PRO:CD	2.76	0.49
4:L:119:HIS:ND1	4:L:120:GLU:N	2.61	0.49
2:B:435:SER:O	4:J:159:LYS:NZ	2.46	0.48
2:D:202:ASP:N	2:D:202:ASP:OD1	2.45	0.48
3:E:117:ASP:OD1	3:E:117:ASP:C	2.57	0.48
4:J:145:ASP:OD1	4:J:146:ASN:N	2.46	0.48
2:C:99:GLU:N	2:C:99:GLU:OE1	2.47	0.48
3:G:398:THR:N	3:G:399:PRO:CD	2.77	0.48
1:V:23:THR:N	1:V:24:PRO:HD2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:69:TYR:OH	3:G:117:ASP:OD1	2.14	0.47
4:I:161:ASP:OD2	4:I:252:LYS:NZ	2.42	0.47
2:D:229:VAL:HG12	2:D:229:VAL:O	2.16	0.46
1:W:49:GLN:OE1	1:W:49:GLN:N	2.48	0.46
3:F:246:ALA:O	3:F:247:GLU:C	2.59	0.46
3:G:117:ASP:OD1	3:G:118:GLY:N	2.45	0.46
3:H:398:THR:N	3:H:399:PRO:CD	2.78	0.46
2:B:51:TYR:CD1	2:B:51:TYR:C	2.94	0.45
2:D:51:TYR:C	2:D:51:TYR:CD1	2.95	0.45
4:K:212:ASP:C	4:K:212:ASP:OD1	2.59	0.44
2:A:51:TYR:C	2:A:51:TYR:CD1	2.95	0.44
4:J:161:ASP:OD2	4:J:252:LYS:NZ	2.44	0.44
1:X:49:GLN:OE1	1:X:49:GLN:N	2.50	0.44
3:H:32:VAL:O	3:H:32:VAL:HG22	2.17	0.44
4:I:246:ASN:OD1	4:I:247:LYS:N	2.50	0.44
2:C:16:LYS:NZ	2:C:339:ILE:O	2.51	0.44
2:C:51:TYR:CD1	2:C:51:TYR:C	2.96	0.44
3:H:117:ASP:OD1	3:H:118:GLY:N	2.47	0.44
2:C:310:SER:CB	3:G:341:GLN:HE22	2.32	0.43
4:J:219:ASP:OD1	4:J:219:ASP:C	2.61	0.43
4:L:189:TRP:O	4:L:190:HIS:HB3	2.19	0.43
4:I:219:ASP:OD1	4:I:219:ASP:C	2.62	0.43
2:C:302:GLU:OE2	2:C:319:LYS:NZ	2.52	0.43
2:D:25:SER:HA	2:D:26:PRO:HD3	1.89	0.43
3:H:105:CYS:HA	3:H:106:PRO:HD3	1.89	0.43
3:H:235:TRP:HE1	3:H:251:ARG:CD	2.31	0.43
4:I:145:ASP:OD1	4:I:146:ASN:N	2.52	0.43
2:B:236:ALA:HA	2:B:237:PRO:HD3	1.90	0.42
4:L:145:ASP:OD1	4:L:146:ASN:N	2.52	0.42
4:L:219:ASP:OD1	4:L:219:ASP:C	2.62	0.42
3:F:398:THR:HB	3:F:399:PRO:HD3	2.01	0.42
4:K:145:ASP:OD1	4:K:146:ASN:N	2.52	0.42
2:B:255:ALA:HA	2:B:256:PRO:HD3	1.86	0.42
1:V:32:GLU:O	1:V:36:ARG:HG2	2.20	0.42
3:G:31:PRO:O	3:G:51:SER:OG	2.38	0.41
3:F:43:ASP:OD1	3:F:43:ASP:C	2.63	0.41
4:J:247:LYS:NZ	4:J:248:ASP:OD2	2.51	0.41
2:A:255:ALA:HA	2:A:256:PRO:HD3	1.87	0.41
2:A:202:ASP:OD1	2:A:202:ASP:N	2.53	0.41
3:G:183:GLN:HG2	3:G:185:SER:H	1.85	0.41
3:H:43:ASP:OD1	3:H:43:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:334:GLU:HA	3:G:335:PRO:HD3	1.89	0.41
4:K:219:ASP:OD1	4:K:219:ASP:C	2.64	0.41
2:A:56:PRO:O	2:A:57:SER:C	2.63	0.41
3:E:74:MET:HA	3:E:75:PRO:HD3	1.93	0.41
3:G:59:ASP:O	3:G:60:ASP:C	2.63	0.41
3:G:242:VAL:HA	3:G:243:PRO:HD3	1.86	0.41
1:X:23:THR:N	1:X:24:PRO:HD2	2.34	0.41
2:B:56:PRO:O	2:B:57:SER:C	2.64	0.41
2:B:202:ASP:OD1	2:B:202:ASP:N	2.52	0.41
2:A:243:TRP:O	2:A:247:ARG:HG3	2.21	0.40
2:C:39:GLU:HA	2:C:40:PRO:HD2	1.94	0.40
4:I:113:CYS:SG	4:I:128:CYS:CB	3.08	0.40
2:C:84:VAL:O	2:C:100:ASN:HB2	2.21	0.40
1:V:20:PRO:HA	1:V:21:PRO:HD3	1.94	0.40
2:B:370:CYS:O	2:B:371:SER:HB2	2.21	0.40
2:D:236:ALA:HA	2:D:237:PRO:HD3	1.93	0.40
2:A:236:ALA:HA	2:A:237:PRO:HD3	1.89	0.40
2:B:302:GLU:OE2	2:B:319:LYS:NZ	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
1	V	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
1	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
1	X	53/55 (96%)	50 (94%)	2 (4%)	1 (2%)	6	26
2	A	437/439 (100%)	432 (99%)	5 (1%)	0	100	100
2	B	437/439 (100%)	433 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	437/439 (100%)	429 (98%)	7 (2%)	1 (0%)	44	73
2	D	437/439 (100%)	432 (99%)	4 (1%)	1 (0%)	44	73
3	E	411/414 (99%)	402 (98%)	9 (2%)	0	100	100
3	F	412/414 (100%)	404 (98%)	8 (2%)	0	100	100
3	G	412/414 (100%)	406 (98%)	5 (1%)	1 (0%)	44	73
3	H	410/414 (99%)	403 (98%)	7 (2%)	0	100	100
4	I	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
4	J	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
4	K	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
4	L	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
All	All	4201/4236 (99%)	4126 (98%)	71 (2%)	4 (0%)	50	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	370	CYS
3	G	60	ASP
1	X	23	THR
2	C	62	CYS

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	U	52/52 (100%)	52 (100%)	0	100	100
1	V	52/52 (100%)	52 (100%)	0	100	100
1	W	52/52 (100%)	52 (100%)	0	100	100
1	X	52/52 (100%)	52 (100%)	0	100	100
2	A	369/369 (100%)	369 (100%)	0	100	100
2	B	369/369 (100%)	369 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	369/369 (100%)	369 (100%)	0	100	100
2	D	369/369 (100%)	369 (100%)	0	100	100
3	E	365/366 (100%)	365 (100%)	0	100	100
3	F	366/366 (100%)	366 (100%)	0	100	100
3	G	366/366 (100%)	366 (100%)	0	100	100
3	H	364/366 (100%)	364 (100%)	0	100	100
4	I	120/120 (100%)	118 (98%)	2 (2%)	56	76
4	J	120/120 (100%)	120 (100%)	0	100	100
4	K	120/120 (100%)	120 (100%)	0	100	100
4	L	120/120 (100%)	119 (99%)	1 (1%)	79	89
All	All	3625/3628 (100%)	3622 (100%)	3 (0%)	92	97

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

Mol	Chain	Res	Type
4	I	128	CYS
4	I	133	LYS
4	L	134	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	252	GLN
2	B	252	GLN
2	C	138	GLN
2	C	222	GLN
2	C	252	GLN
2	C	253	HIS
2	C	368	GLN
3	E	146	GLN
3	E	184	GLN
3	F	146	GLN
3	F	187	ASN
3	F	202	ASN
3	F	224	GLN
3	F	349	HIS
3	G	127	HIS

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Mol	Chain	Res	Type
3	G	146	GLN
3	G	207	ASN
4	K	191	HIS
4	L	191	HIS
1	X	19	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 ⓘ

28 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	$\# Z > 2$
5	NAG	M	1	5,2	14,14,15	0.82	1 (7%)	17,19,21	1.31	2 (11%)
5	NAG	M	2	5	14,14,15	0.83	1 (7%)	17,19,21	1.04	2 (11%)
5	BMA	M	3	5	11,11,12	0.83	0	15,15,17	0.63	0
5	FUC	M	4	5	10,10,11	0.84	0	14,14,16	0.54	0
5	NAG	N	1	5,2	14,14,15	0.85	1 (7%)	17,19,21	1.40	3 (17%)
5	NAG	N	2	5	14,14,15	0.88	1 (7%)	17,19,21	1.12	2 (11%)
5	BMA	N	3	5	11,11,12	0.86	0	15,15,17	0.59	0
5	FUC	N	4	5	10,10,11	0.86	0	14,14,16	0.50	0
5	NAG	O	1	5,2	14,14,15	0.81	1 (7%)	17,19,21	1.28	2 (11%)
5	NAG	O	2	5	14,14,15	0.85	1 (7%)	17,19,21	0.97	1 (5%)
5	BMA	O	3	5	11,11,12	0.84	0	15,15,17	0.62	0
5	FUC	O	4	5	10,10,11	0.86	0	14,14,16	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	P	1	5,2	14,14,15	0.80	1 (7%)	17,19,21	1.25	2 (11%)
5	NAG	P	2	5	14,14,15	0.84	1 (7%)	17,19,21	1.02	1 (5%)
5	BMA	P	3	5	11,11,12	0.85	0	15,15,17	0.61	0
5	FUC	P	4	5	10,10,11	0.84	0	14,14,16	0.49	0
6	NAG	Q	1	6,3	14,14,15	0.90	1 (7%)	17,19,21	1.03	1 (5%)
6	NAG	Q	2	6	14,14,15	0.94	1 (7%)	17,19,21	1.18	2 (11%)
6	BMA	Q	3	6	11,11,12	0.87	0	15,15,17	0.88	2 (13%)
6	NAG	R	1	6,3	14,14,15	0.90	1 (7%)	17,19,21	1.02	1 (5%)
6	NAG	R	2	6	14,14,15	0.91	1 (7%)	17,19,21	1.24	2 (11%)
6	BMA	R	3	6	11,11,12	0.86	0	15,15,17	0.89	2 (13%)
6	NAG	S	1	6,3	14,14,15	0.89	1 (7%)	17,19,21	1.05	2 (11%)
6	NAG	S	2	6	14,14,15	0.95	1 (7%)	17,19,21	1.28	2 (11%)
6	BMA	S	3	6	11,11,12	0.88	0	15,15,17	0.88	2 (13%)
6	NAG	T	1	6,3	14,14,15	0.91	1 (7%)	17,19,21	1.04	1 (5%)
6	NAG	T	2	6	14,14,15	0.96	1 (7%)	17,19,21	1.22	2 (11%)
6	BMA	T	3	6	11,11,12	0.89	0	15,15,17	0.85	1 (6%)

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
5	NAG	M	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	FUC	M	4	5	-	-	0/1/1/1
5	NAG	N	1	5,2	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	1/2/19/22	0/1/1/1
5	FUC	N	4	5	-	-	0/1/1/1
5	NAG	O	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
5	FUC	O	4	5	-	-	0/1/1/1
5	NAG	P	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	1/2/19/22	0/1/1/1
5	FUC	P	4	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	Q	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	3	6	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	R	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	S	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	BMA	S	3	6	1/1/4/5	1/2/19/22	0/1/1/1
6	NAG	T	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	1/1/4/5	0/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	1	NAG	C1-C2	2.75	1.56	1.52
6	T	1	NAG	C1-C2	2.74	1.56	1.52
6	Q	1	NAG	C1-C2	2.71	1.56	1.52
6	S	1	NAG	C1-C2	2.54	1.56	1.52
6	S	2	NAG	C1-C2	2.53	1.56	1.52
5	M	1	NAG	C1-C2	2.52	1.56	1.52
5	N	1	NAG	C1-C2	2.48	1.56	1.52
6	Q	2	NAG	C1-C2	2.45	1.56	1.52
6	T	2	NAG	C1-C2	2.45	1.56	1.52
5	P	1	NAG	C1-C2	2.43	1.56	1.52
5	N	2	NAG	C1-C2	2.42	1.55	1.52
5	O	1	NAG	C1-C2	2.39	1.55	1.52
5	P	2	NAG	C1-C2	2.38	1.55	1.52
5	O	2	NAG	C1-C2	2.35	1.55	1.52
6	R	2	NAG	C1-C2	2.32	1.55	1.52
5	M	2	NAG	C1-C2	2.21	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1	NAG	C2-N2-C7	-3.01	118.62	122.90
5	N	1	NAG	C2-N2-C7	-2.84	118.86	122.90
5	O	1	NAG	C2-N2-C7	-2.82	118.89	122.90
5	P	1	NAG	C2-N2-C7	-2.78	118.95	122.90
5	O	1	NAG	C8-C7-N2	2.78	120.80	116.10
5	P	1	NAG	C8-C7-N2	2.63	120.55	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	2	NAG	C8-C7-N2	2.61	120.51	116.10
5	M	1	NAG	C8-C7-N2	2.55	120.41	116.10
5	N	1	NAG	C8-C7-N2	2.53	120.39	116.10
6	R	2	NAG	C8-C7-N2	2.53	120.38	116.10
6	T	2	NAG	C8-C7-N2	2.52	120.37	116.10
6	Q	2	NAG	C8-C7-N2	2.52	120.36	116.10
6	S	2	NAG	C8-C7-N2	2.52	120.36	116.10
6	S	1	NAG	C8-C7-N2	2.50	120.33	116.10
5	P	2	NAG	C8-C7-N2	2.47	120.29	116.10
5	M	2	NAG	C8-C7-N2	2.45	120.25	116.10
5	O	2	NAG	C8-C7-N2	2.44	120.23	116.10
6	R	1	NAG	C8-C7-N2	2.41	120.18	116.10
6	Q	1	NAG	C8-C7-N2	2.41	120.17	116.10
5	N	2	NAG	C2-N2-C7	-2.37	119.52	122.90
6	T	1	NAG	C8-C7-N2	2.33	120.05	116.10
5	N	1	NAG	C3-C4-C5	-2.31	106.12	110.24
6	S	3	BMA	O5-C1-C2	2.26	114.26	110.77
6	T	2	NAG	C2-N2-C7	-2.25	119.70	122.90
6	Q	2	NAG	C2-N2-C7	-2.23	119.73	122.90
6	S	2	NAG	C2-N2-C7	-2.20	119.78	122.90
5	M	2	NAG	C2-N2-C7	-2.19	119.79	122.90
6	R	2	NAG	C2-N2-C7	-2.17	119.81	122.90
6	R	3	BMA	C1-C2-C3	-2.17	107.00	109.67
6	S	1	NAG	C2-N2-C7	-2.13	119.87	122.90
6	R	3	BMA	O5-C1-C2	2.12	114.04	110.77
6	Q	3	BMA	O5-C1-C2	2.12	114.04	110.77
6	Q	3	BMA	C1-C2-C3	-2.11	107.08	109.67
6	T	3	BMA	O5-C1-C2	2.07	113.96	110.77
6	S	3	BMA	C1-C2-C3	-2.03	107.17	109.67

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	N	1	NAG	C1
6	Q	3	BMA	C1
6	R	3	BMA	C1
6	S	3	BMA	C1
6	T	3	BMA	C1

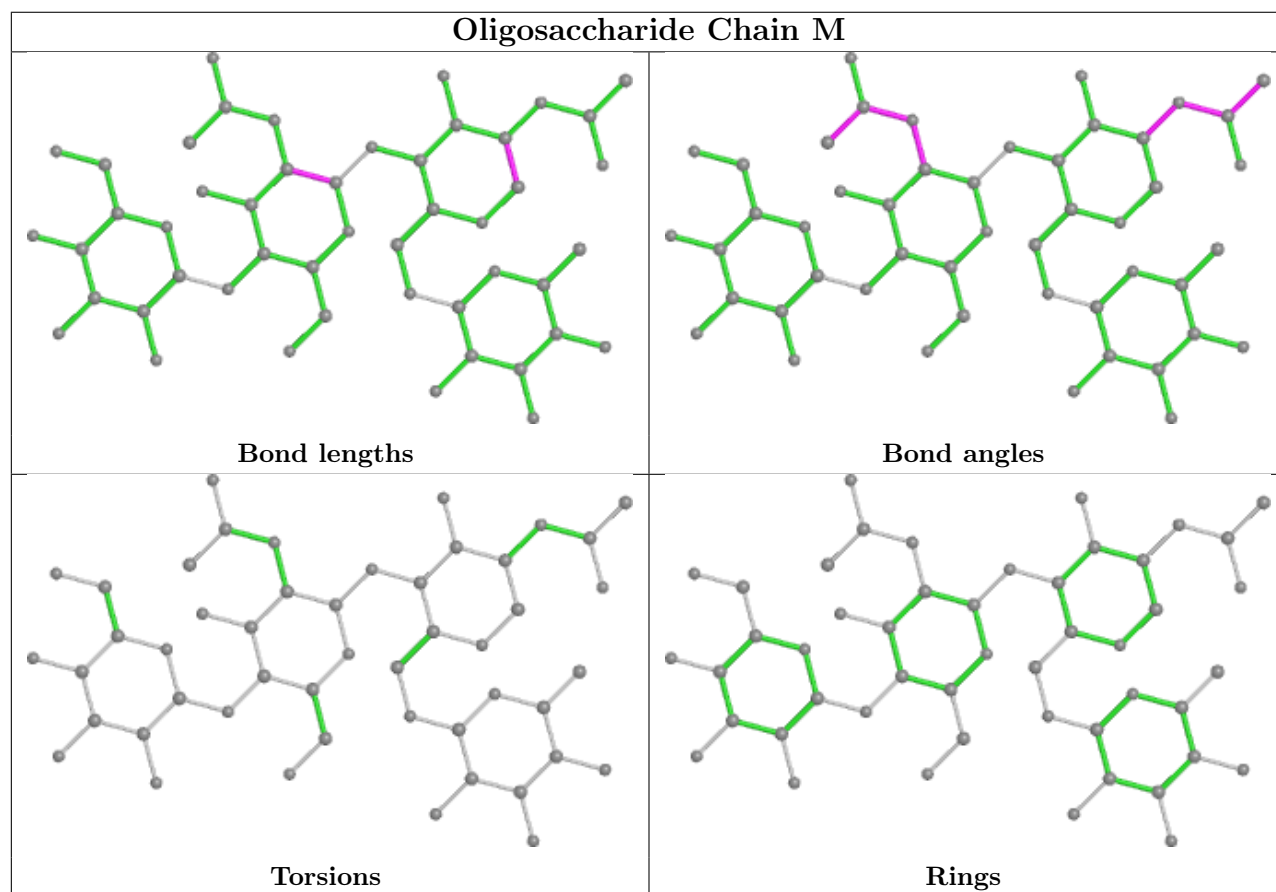
All (4) torsion outliers are listed below:

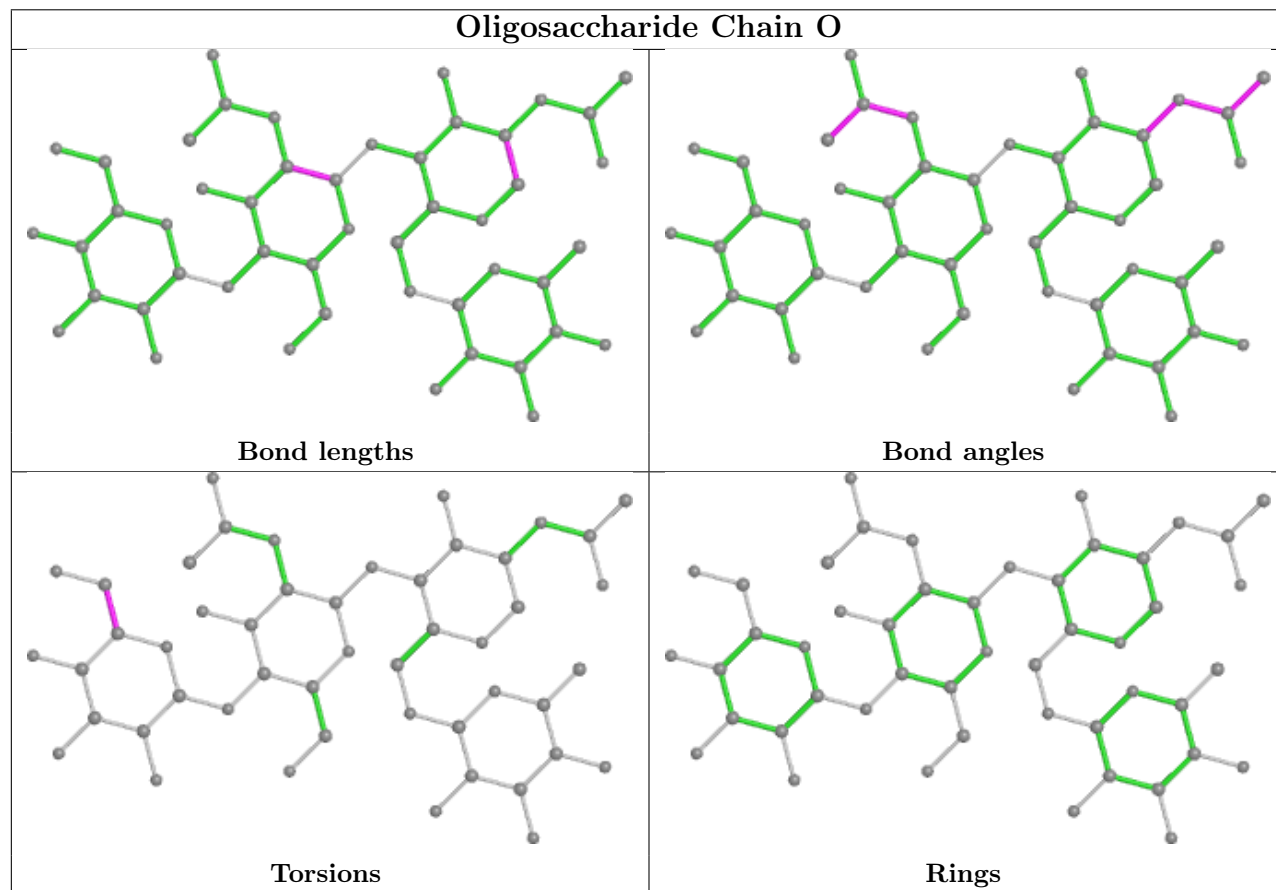
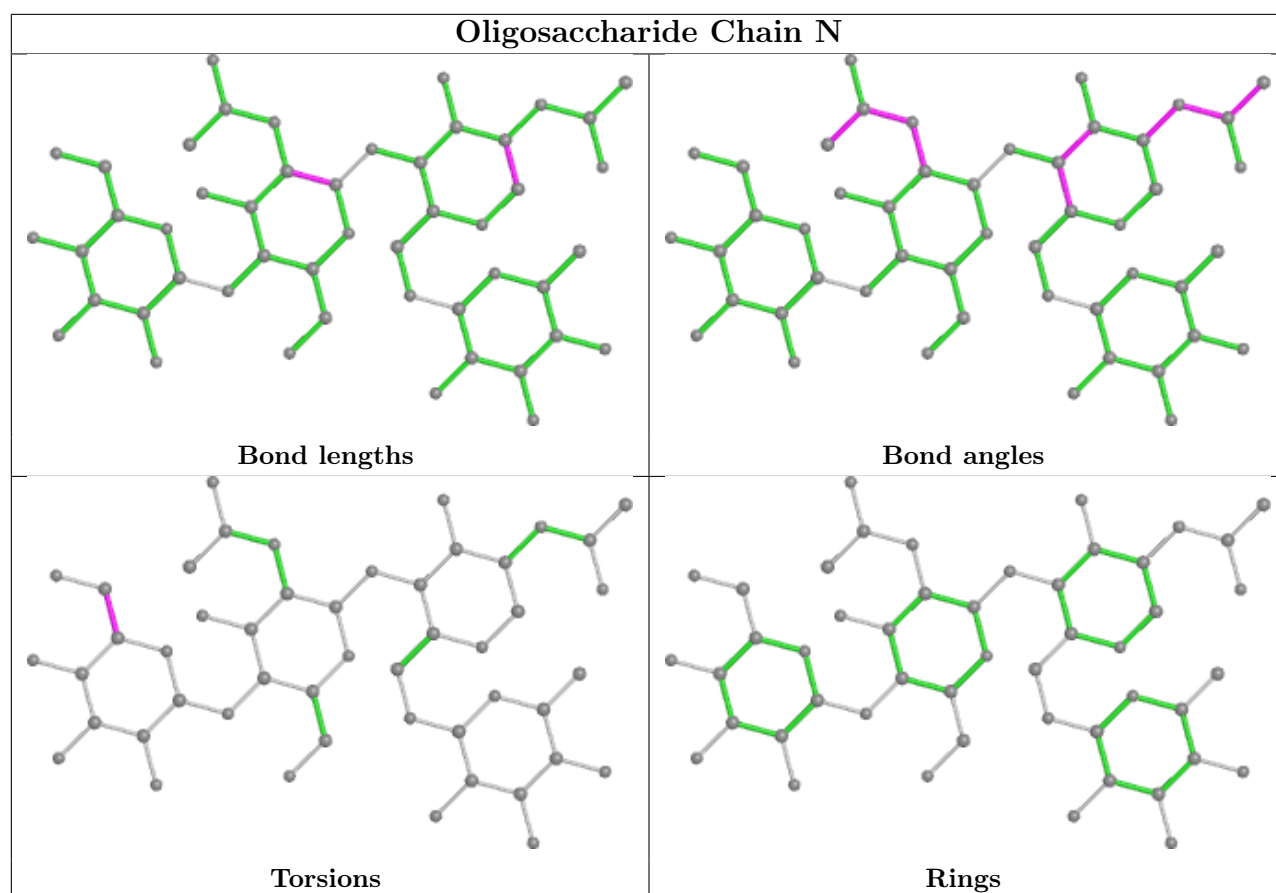
Mol	Chain	Res	Type	Atoms
5	N	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6

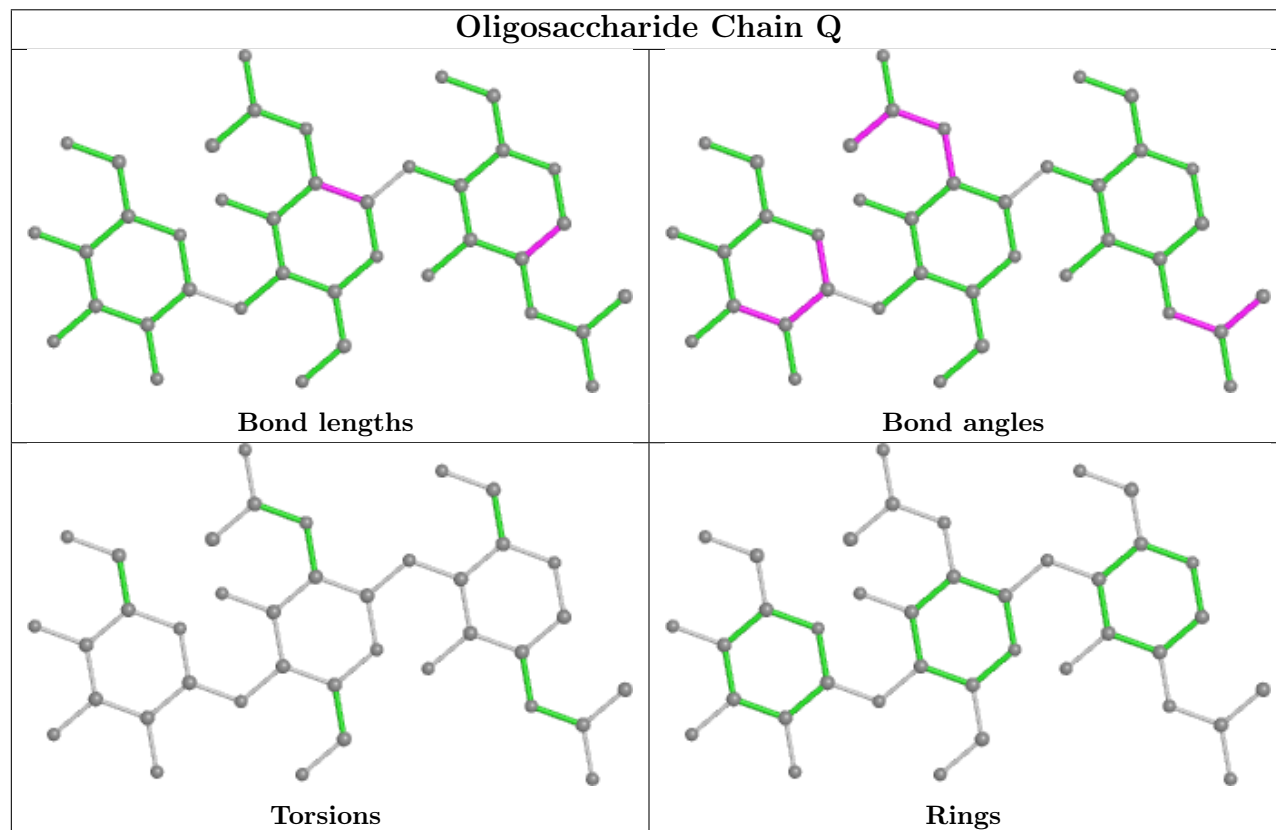
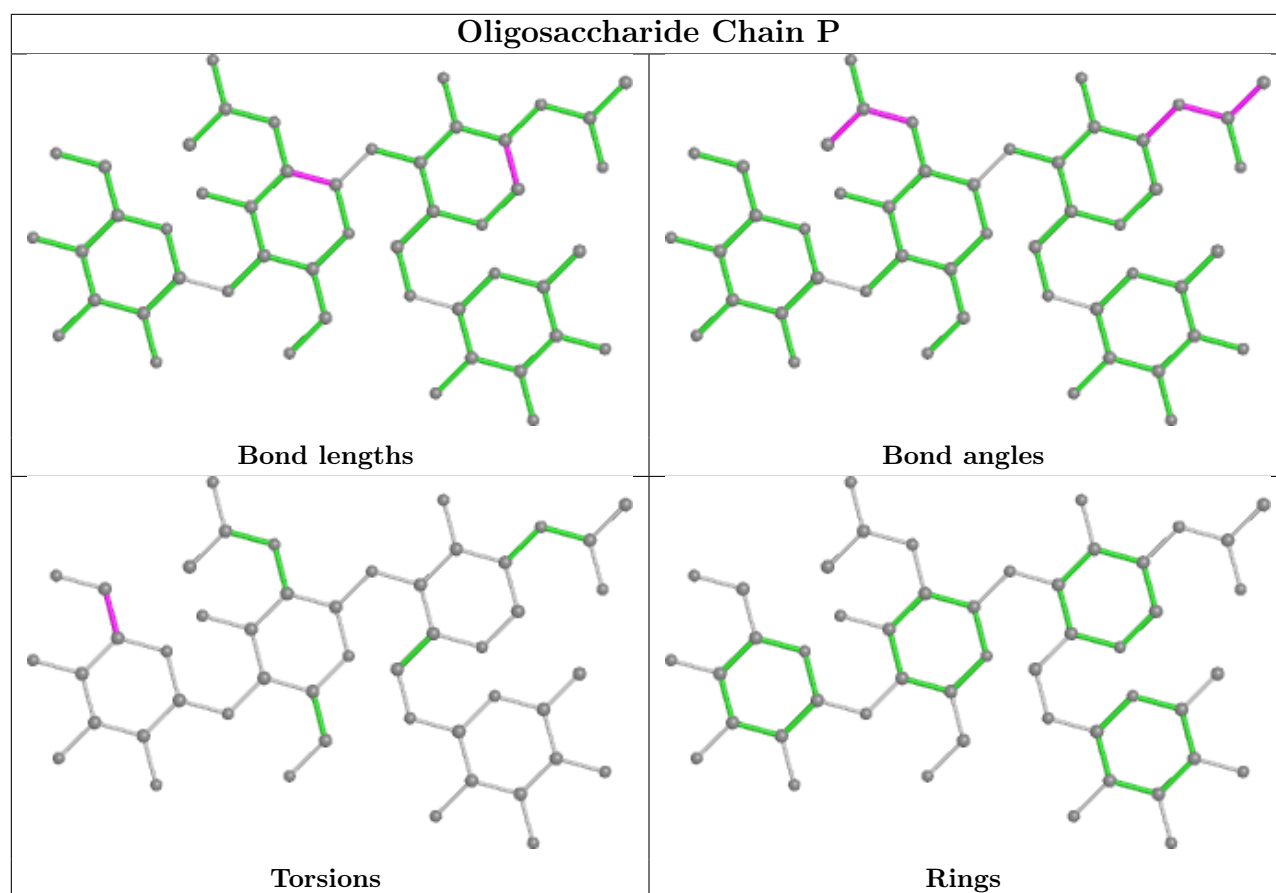
There are no ring outliers.

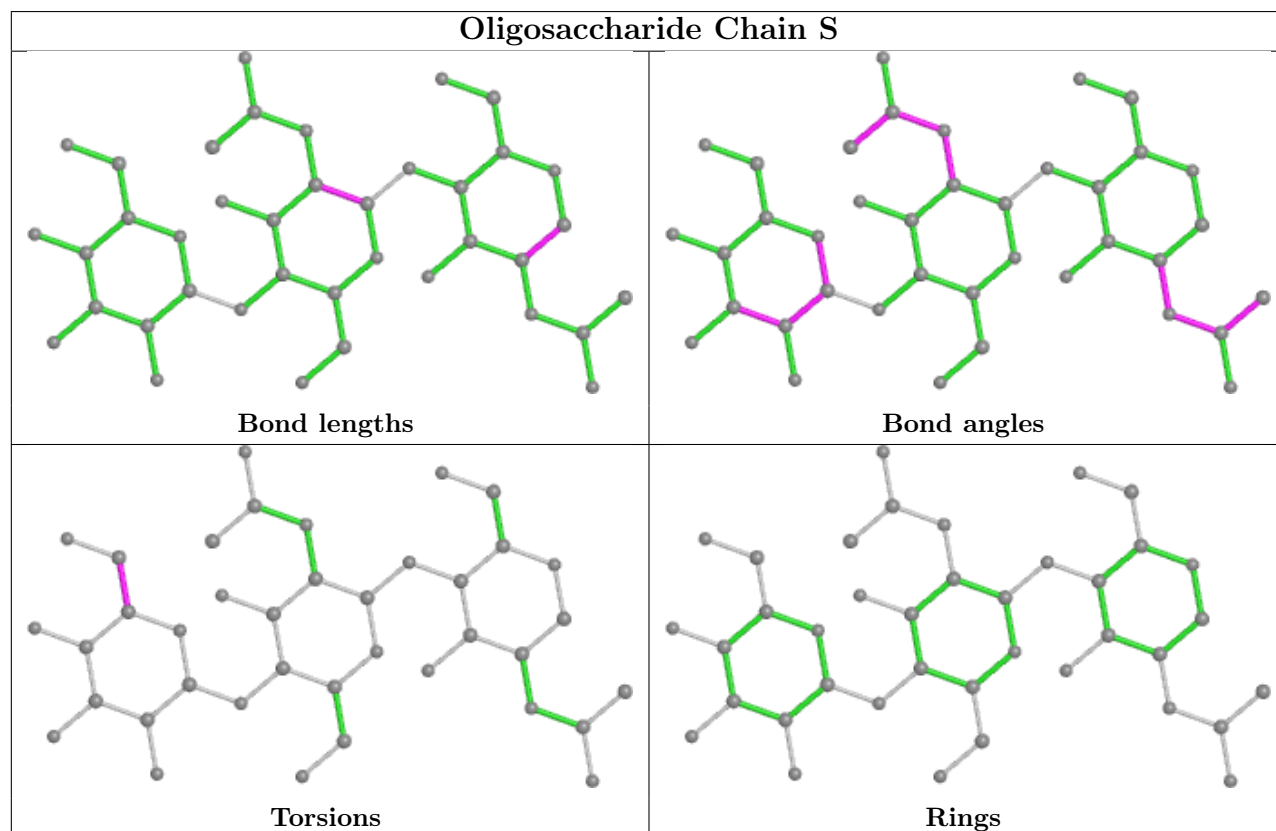
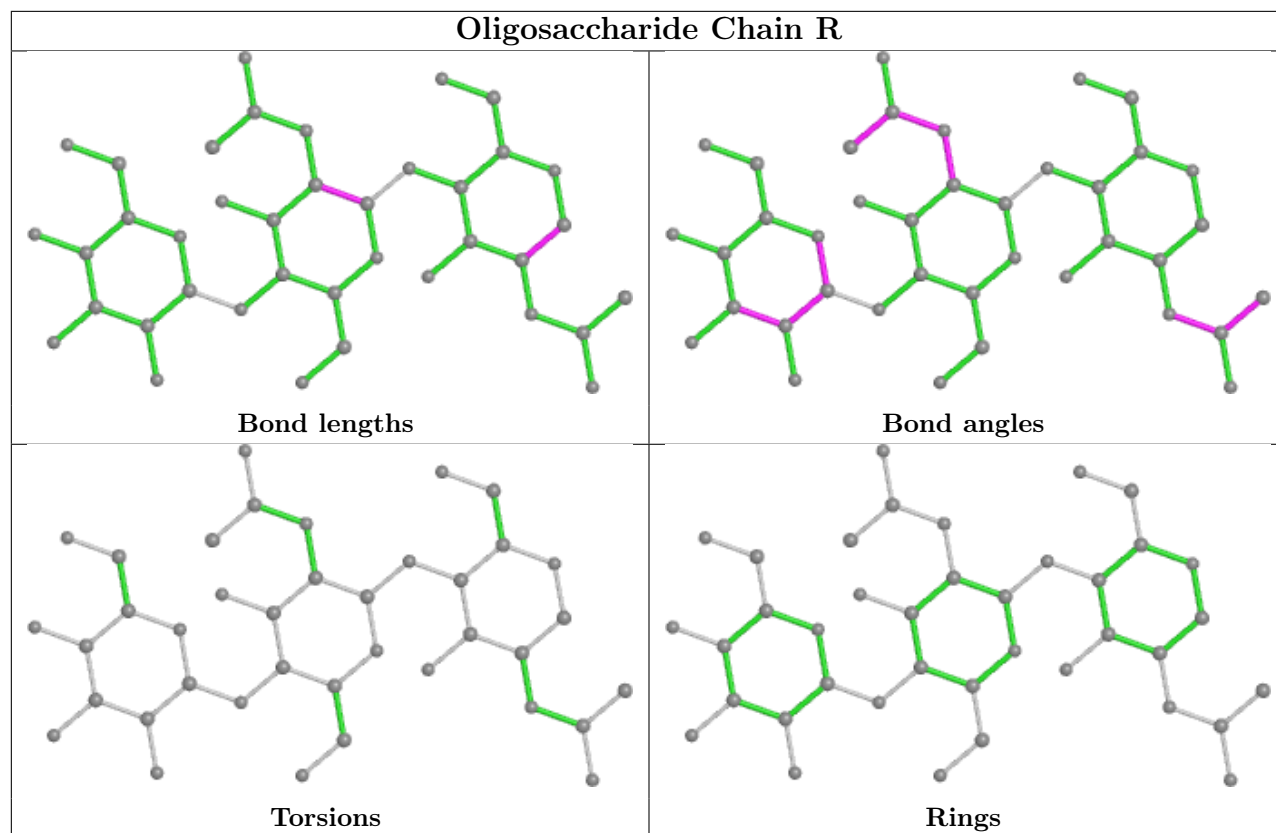
No monomer is involved in short contacts.

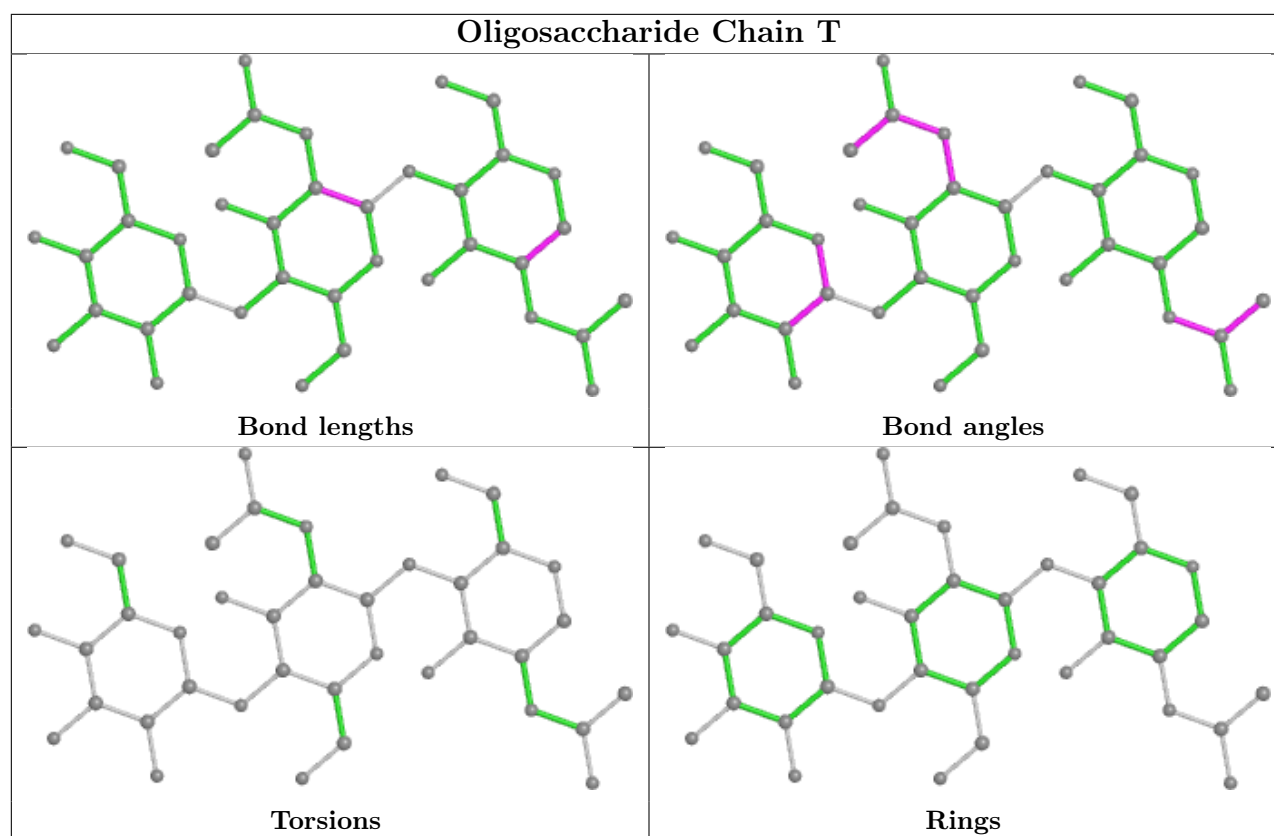
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

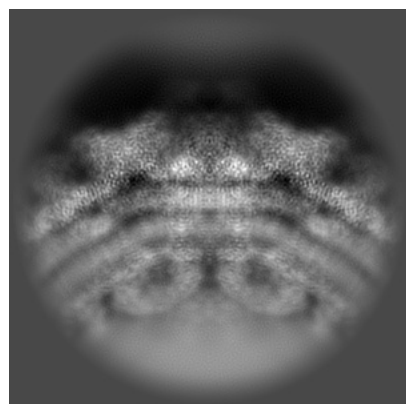
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61168. These allow visual inspection of the internal detail of the map and identification of artifacts.

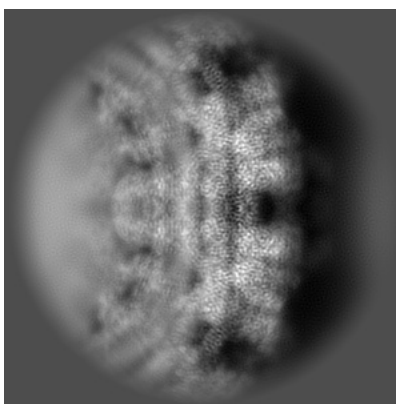
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

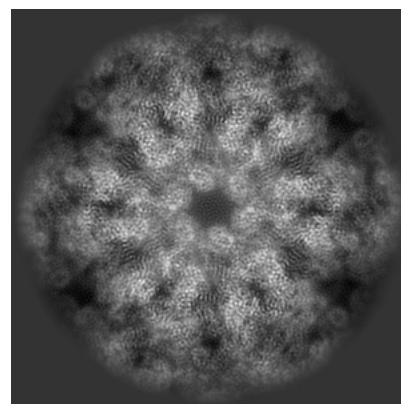
6.1.1 Primary map



X

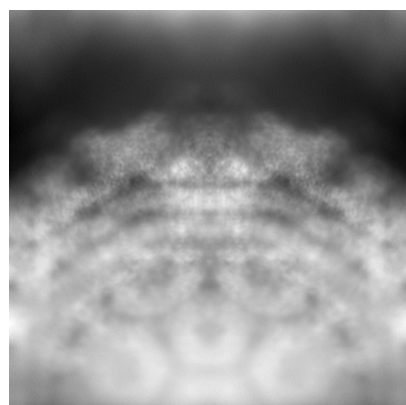


Y

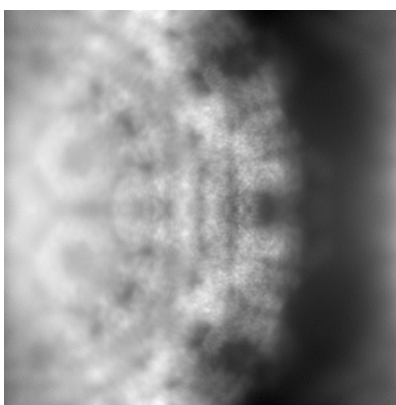


Z

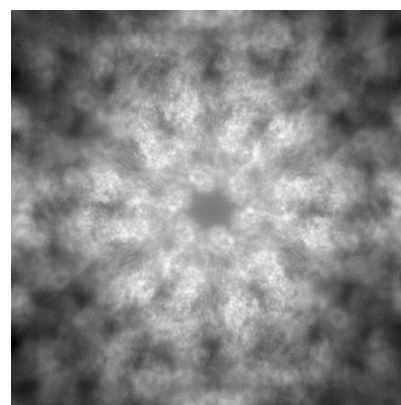
6.1.2 Raw map



X



Y

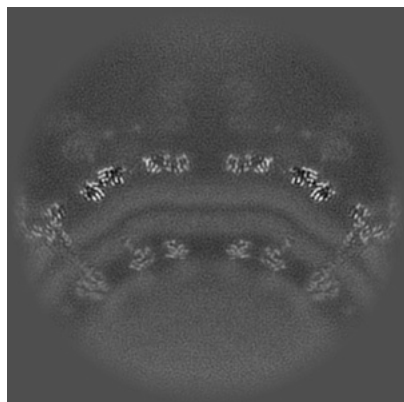


Z

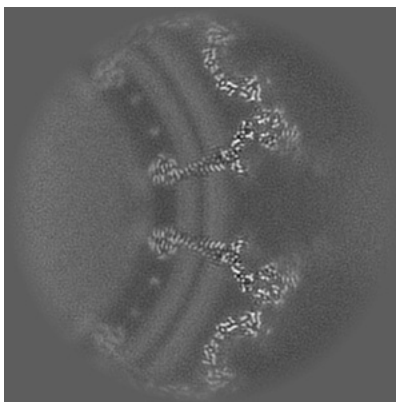
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

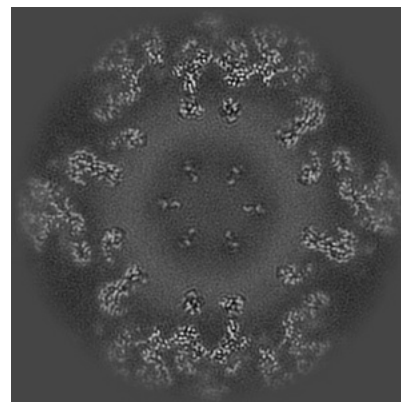
6.2.1 Primary map



X Index: 160

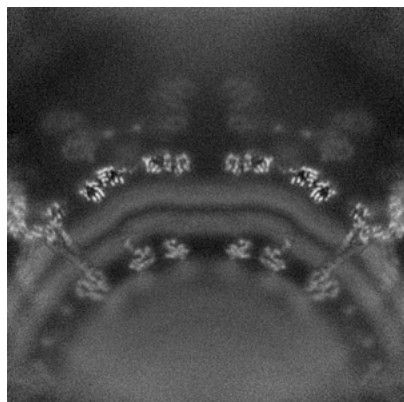


Y Index: 160

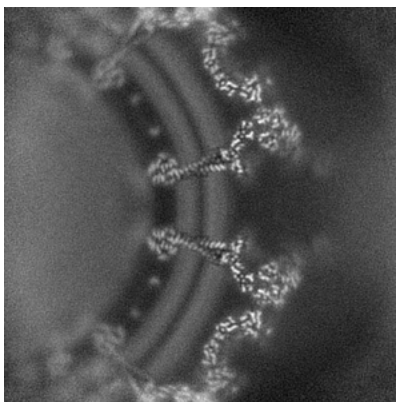


Z Index: 160

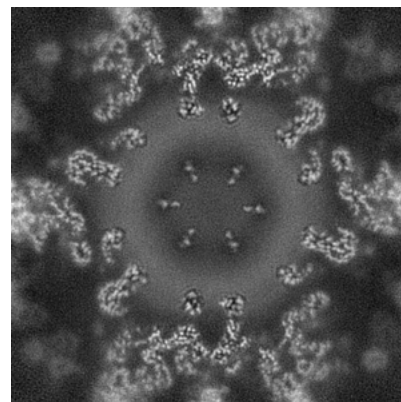
6.2.2 Raw map



X Index: 160



Y Index: 160

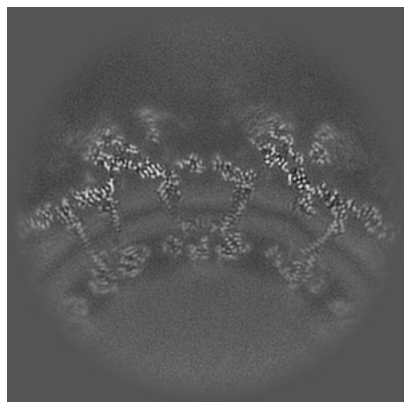


Z Index: 160

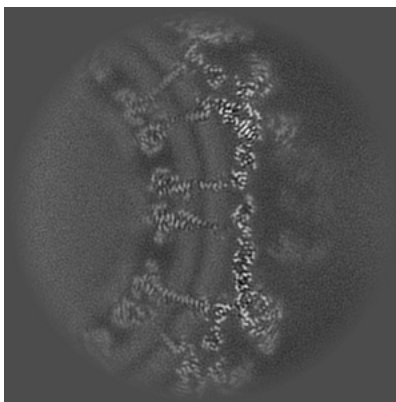
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

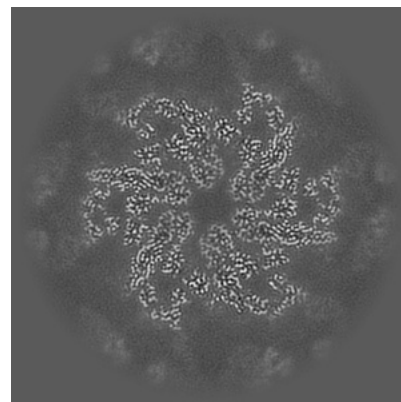
6.3.1 Primary map



X Index: 180

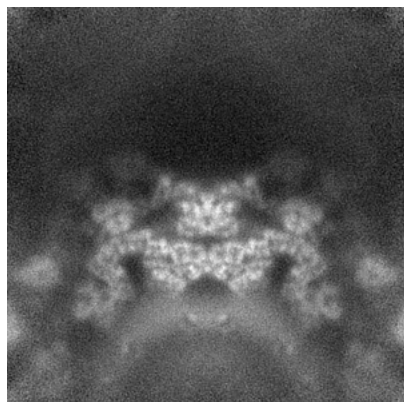


Y Index: 181

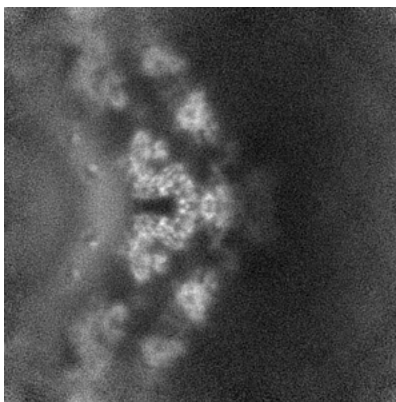


Z Index: 191

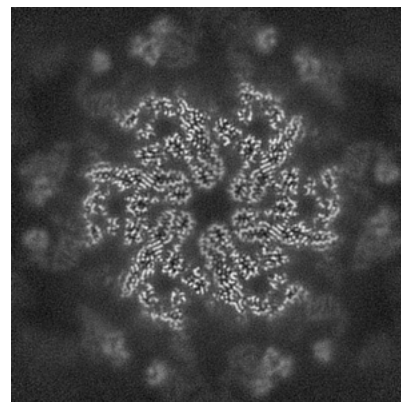
6.3.2 Raw map



X Index: 0



Y Index: 0

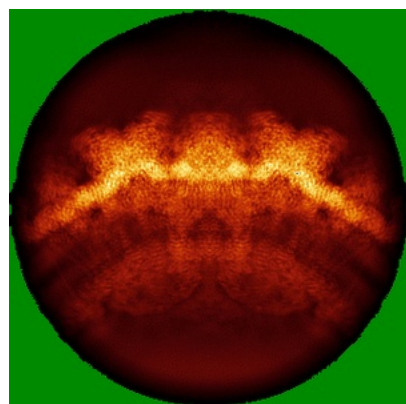


Z Index: 192

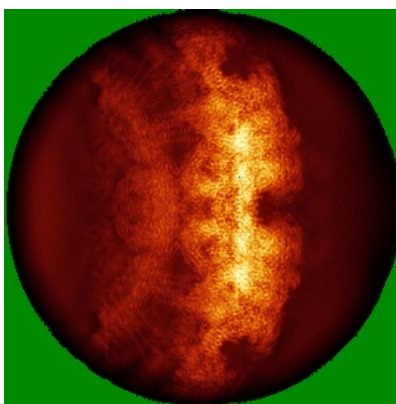
The images above show the largest variance slices of the map in three orthogonal directions.

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

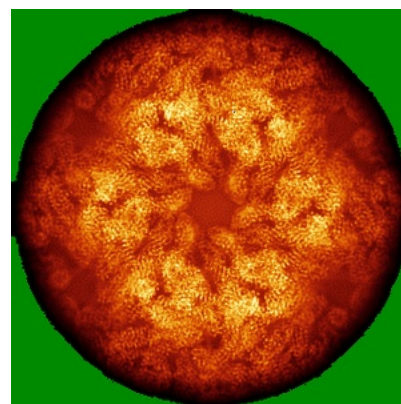
6.4.1 Primary map



X

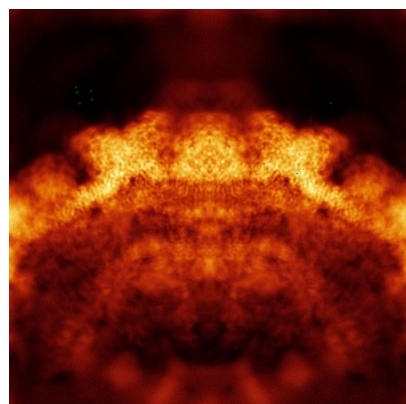


Y

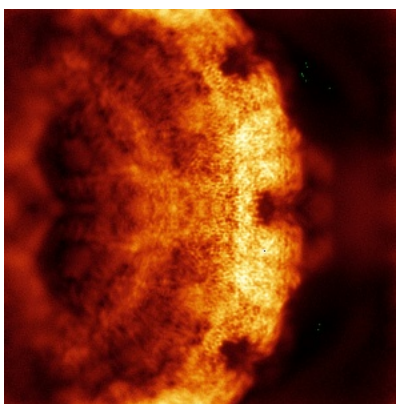


Z

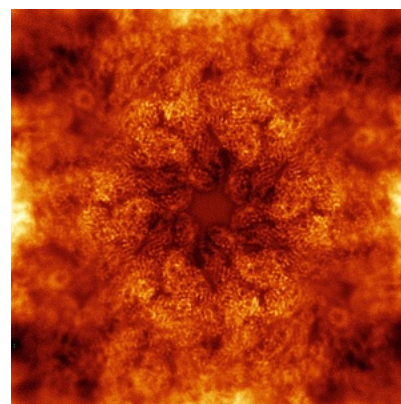
6.4.2 Raw map



X



Y



Z

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

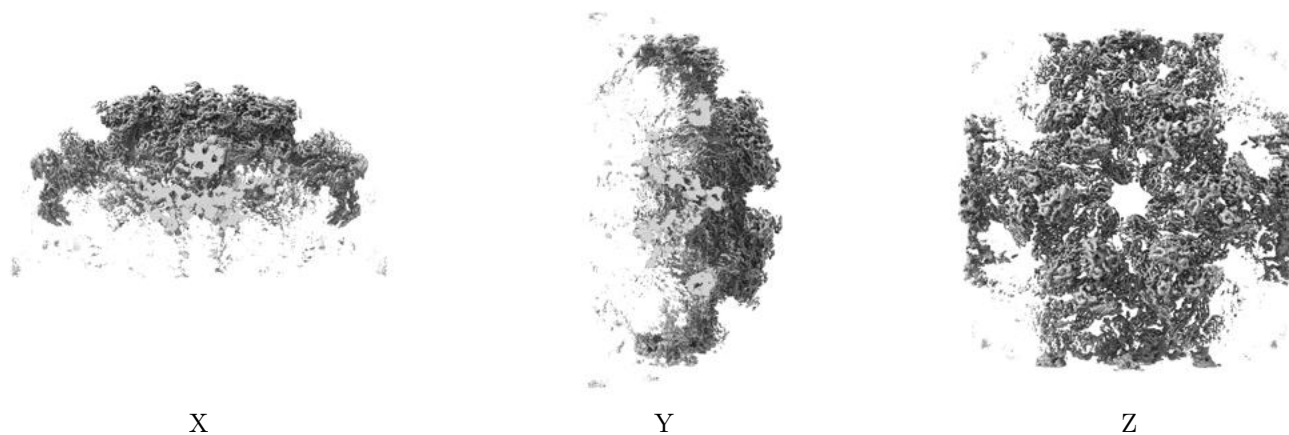
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

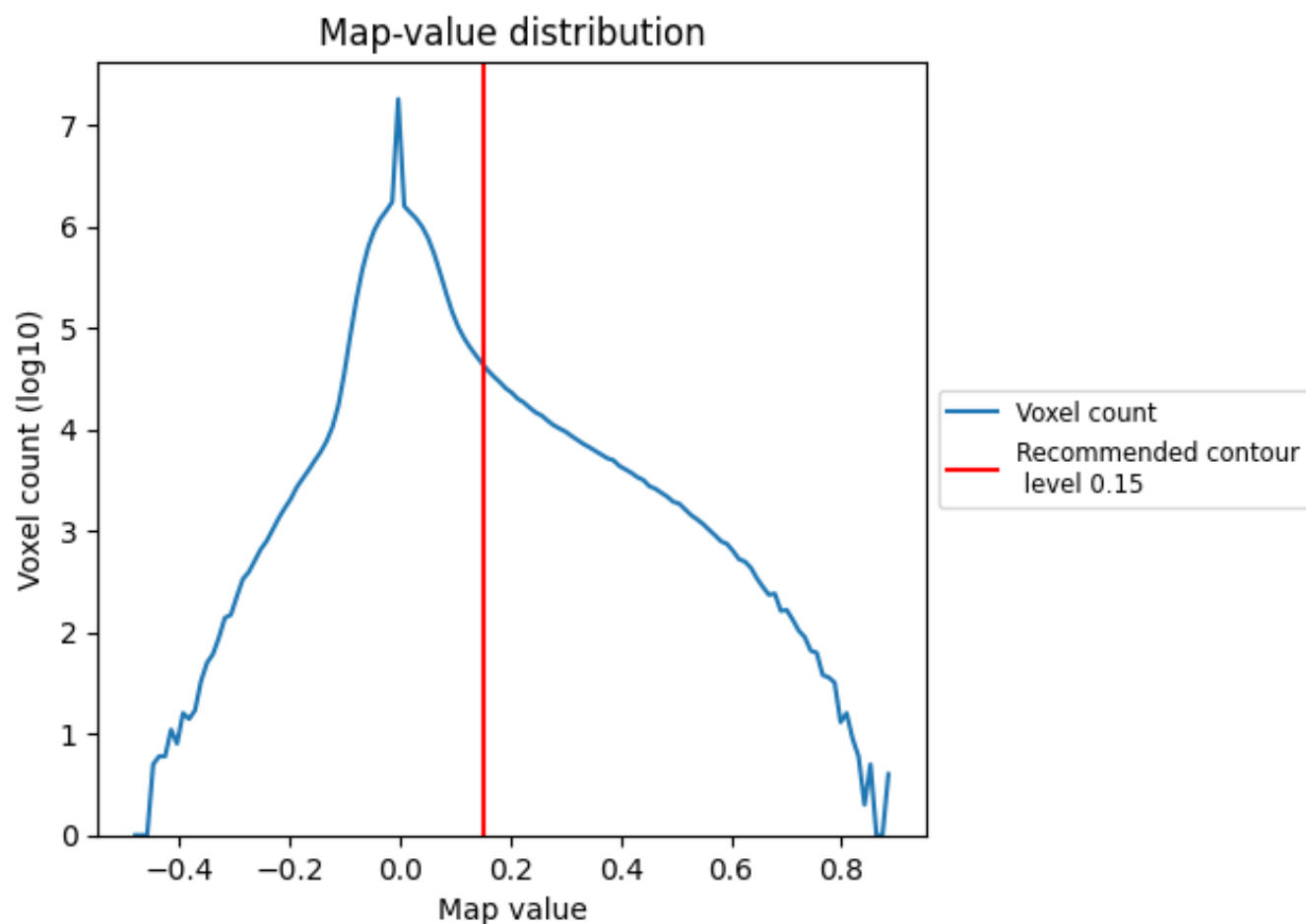
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

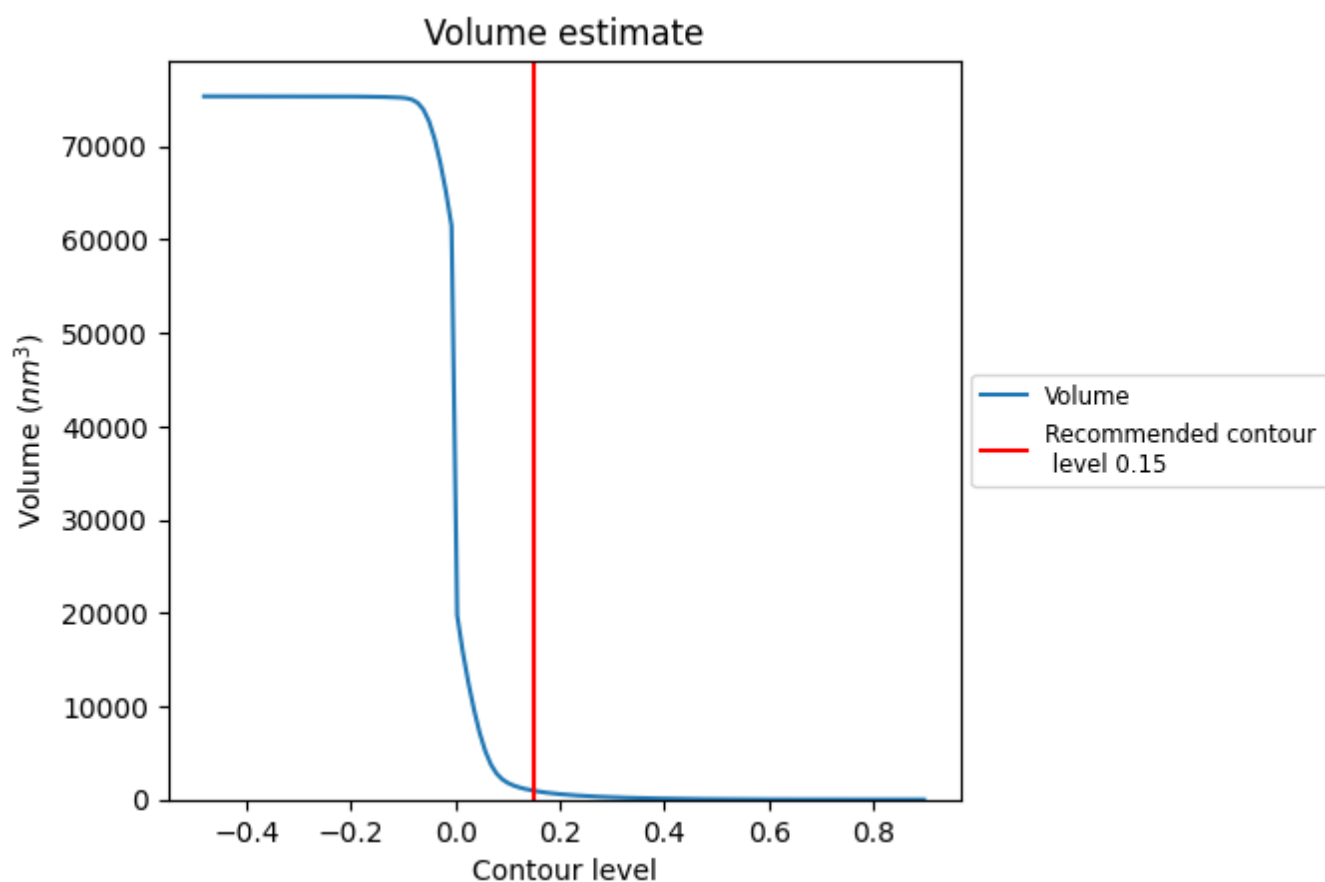
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

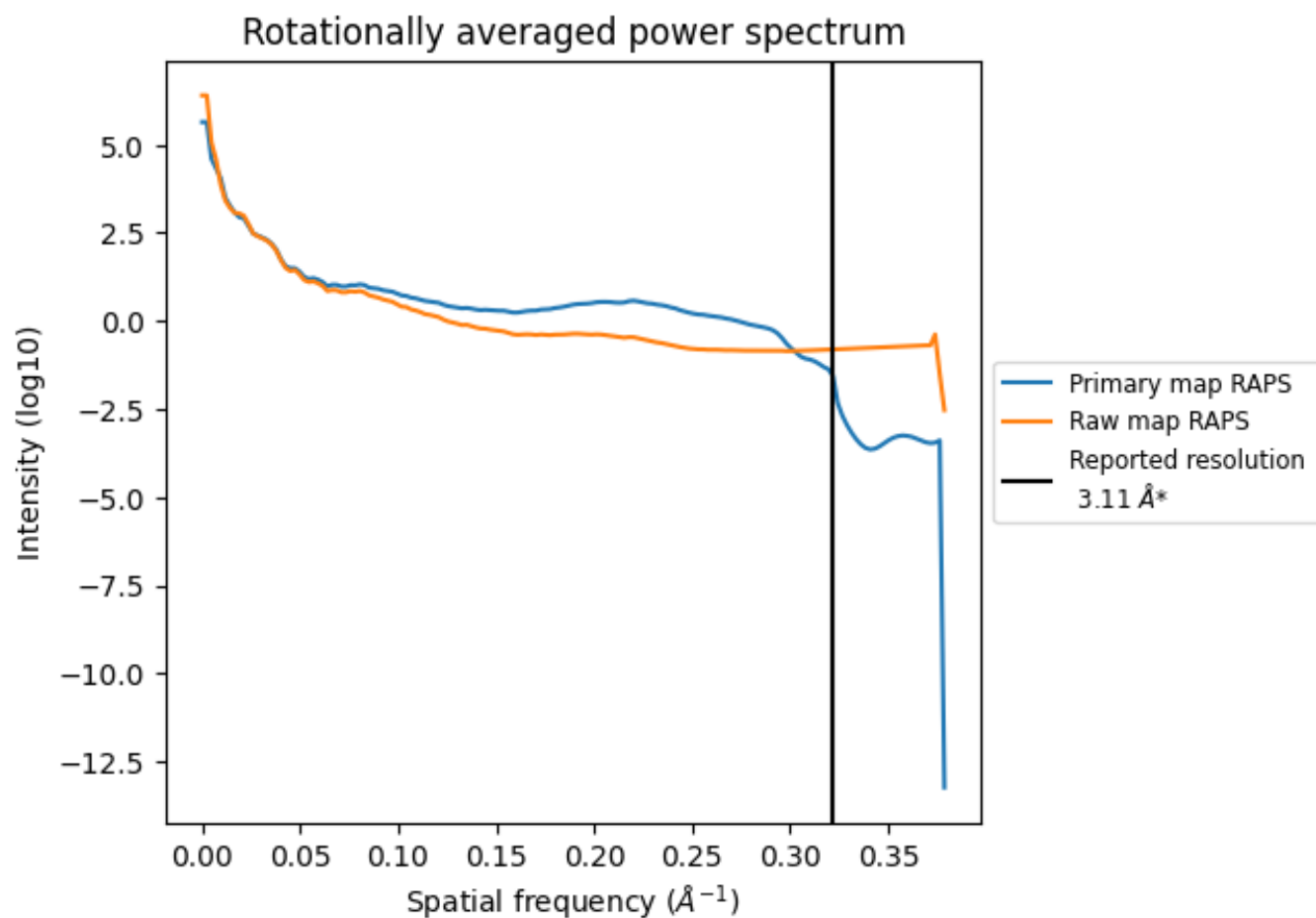
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 948 nm³; this corresponds to an approximate mass of 856 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

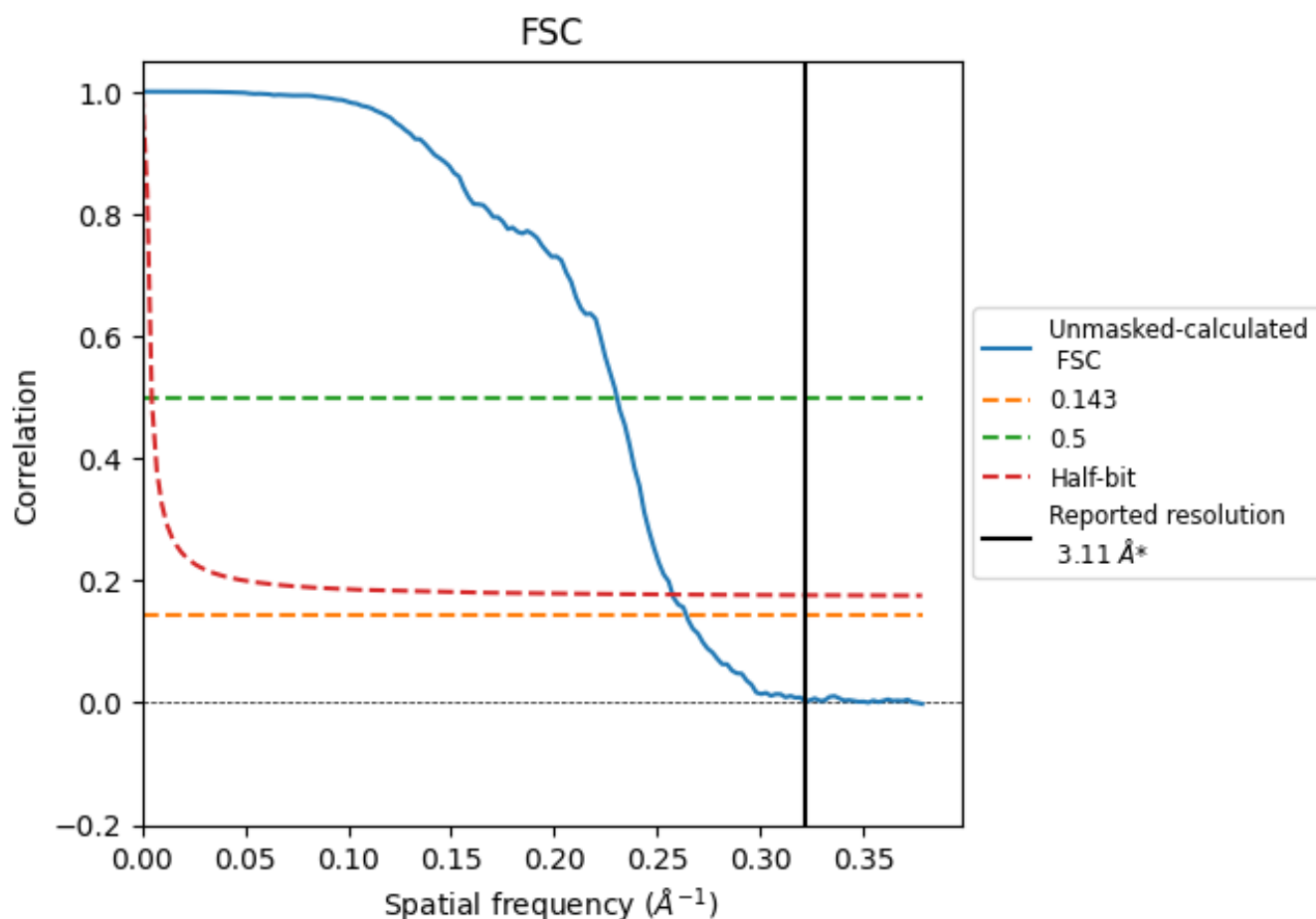


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.322 \AA^{-1}

8.2 Resolution estimates [i](#)

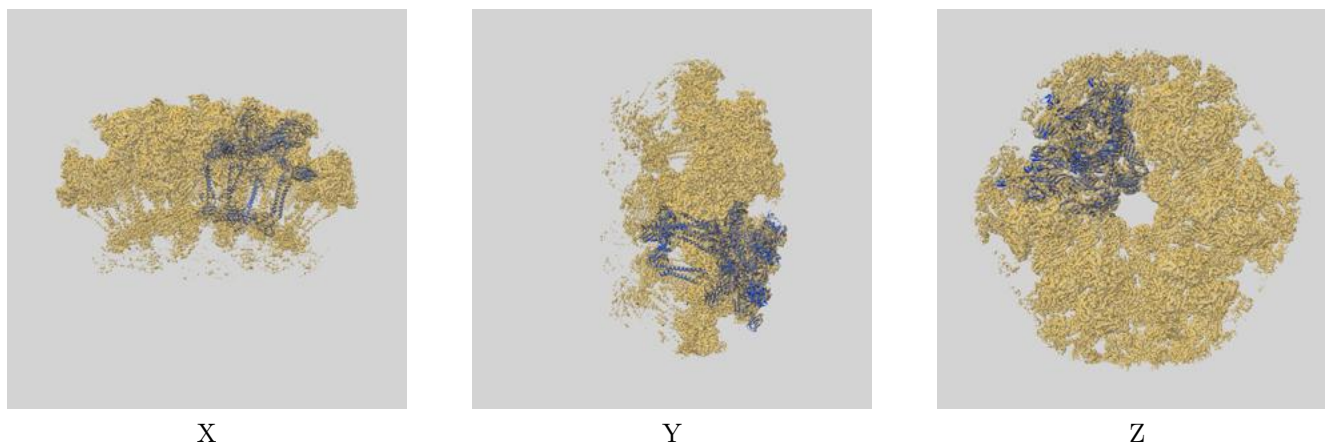
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.79	4.34	3.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 3.11 by more than 10 %

9 Map-model fit [i](#)

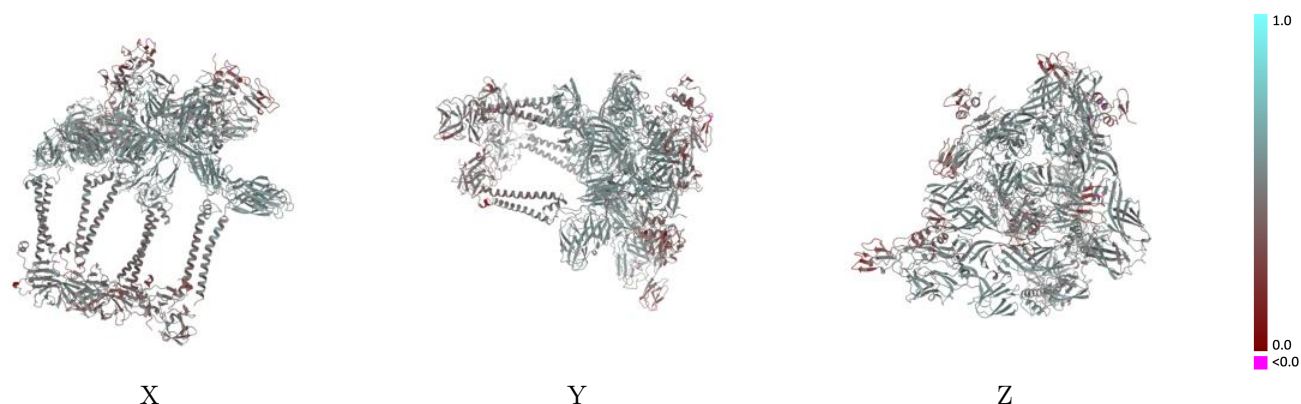
This section contains information regarding the fit between EMDB map EMD-61168 and PDB model 9J6D. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



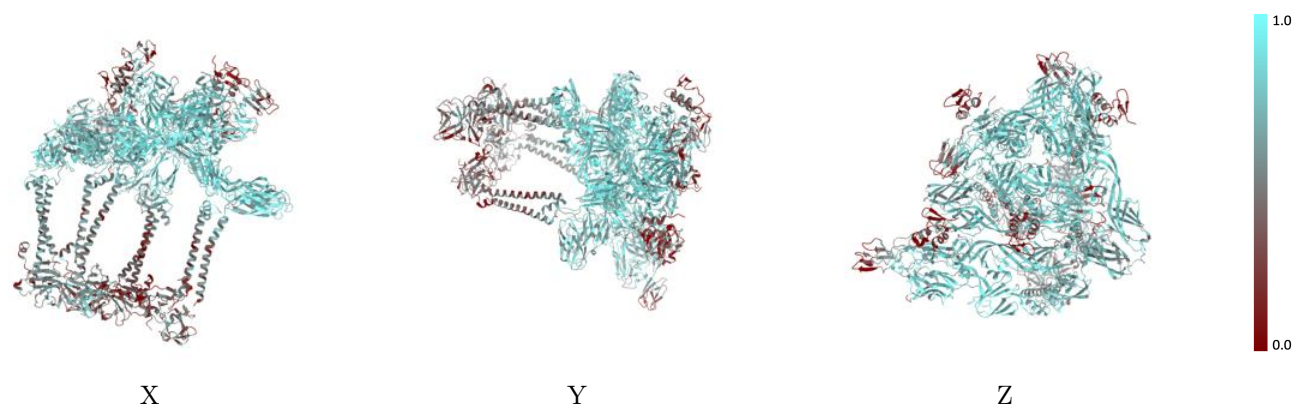
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



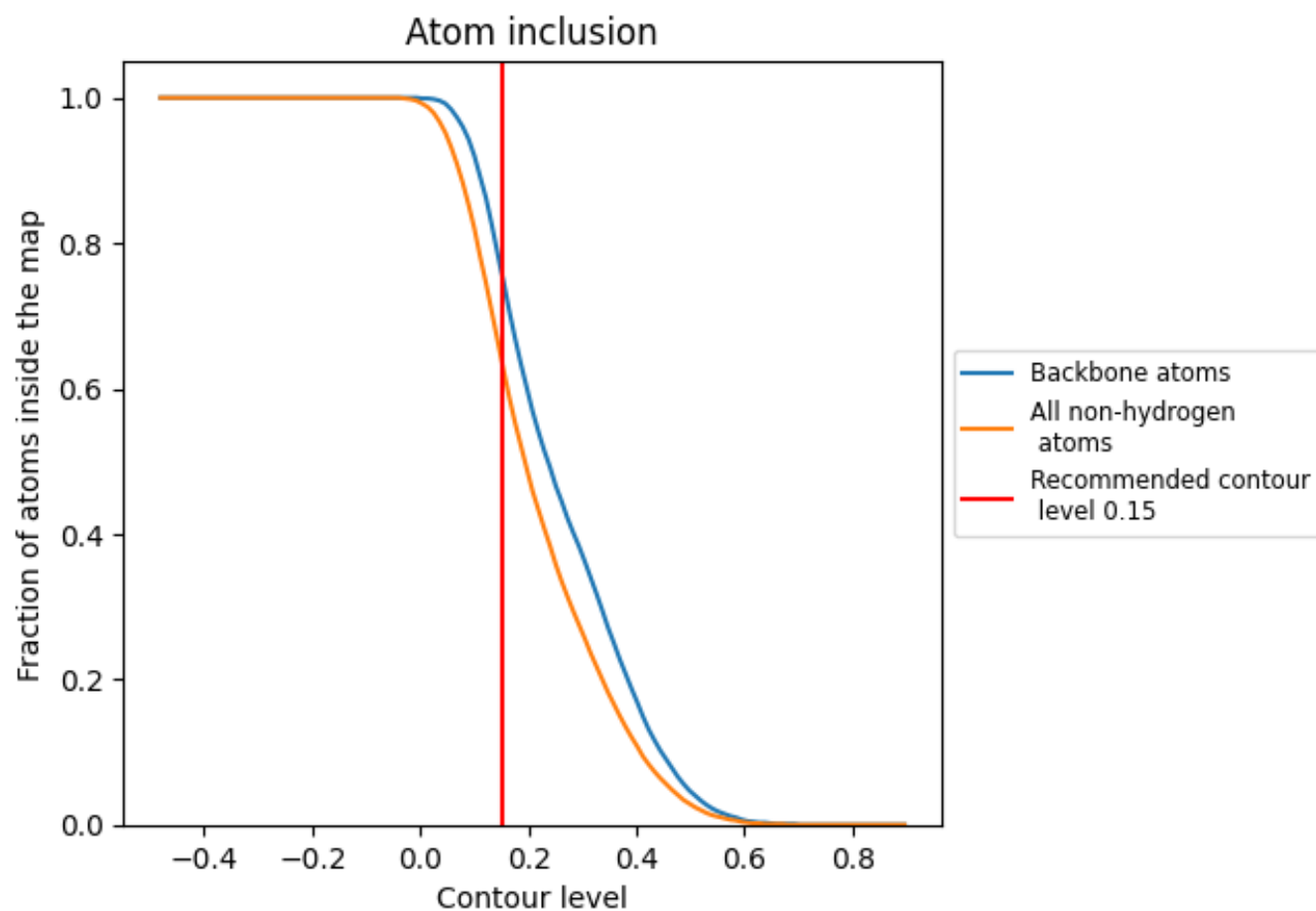
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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



















































9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6390	 0.4830
A	 0.7610	 0.5180
B	 0.7330	 0.5100
C	 0.7330	 0.5180
D	 0.7480	 0.5180
E	 0.6980	 0.4880
F	 0.6940	 0.4890
G	 0.6780	 0.4820
H	 0.6830	 0.4840
I	 0.3740	 0.4270
J	 0.4670	 0.4470
K	 0.2860	 0.3930
L	 0.4520	 0.4510
M	 0.4900	 0.4410
N	 0.3270	 0.4060
O	 0.3470	 0.3520
P	 0.3880	 0.3510
Q	 0.3590	 0.3960
R	 0.3080	 0.4570
S	 0.0510	 0.4090
T	 0.2050	 0.4080
U	 0.1830	 0.3680
V	 0.2430	 0.3620
W	 0.1620	 0.3570
X	 0.1480	 0.3510

