



Full wwPDB EM Validation Report ⓘ

Nov 5, 2025 – 04:26 PM JST

PDB ID : 9IYI / pdb_00009iyi
EMDB ID : EMD-60997
Title : VLP structure of Chikungunya virus complexed with C34 Fab, 2f block.
Authors : Han, X.; Ji, C.; Wang, F.; Tian, S.; Gao, F.G.; Yan, J.
Deposited on : 2024-07-30
Resolution : 3.73 Å(reported)
Based on initial models : 8FCG, 6JO8

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:

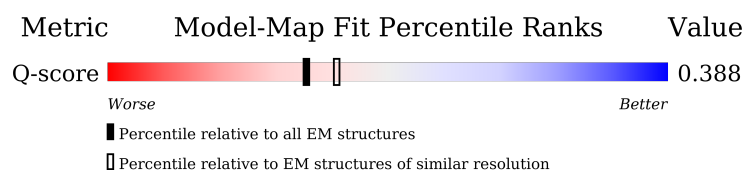
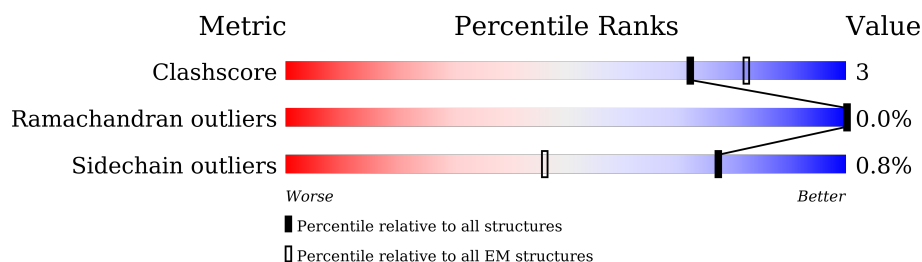
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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 3.73 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	10415 (3.23 - 4.23)

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	M	264	<div> <div>42%</div> <div> <div></div> <div>80%</div> <div>5% •</div> <div>15%</div> </div> </div>
1	O	264	<div> <div>82%</div> <div> <div></div> <div>76%</div> <div>8% •</div> <div>15%</div> </div> </div>
1	Q	264	<div> <div>18%</div> <div> <div></div> <div>79%</div> <div>5% •</div> <div>15%</div> </div> </div>
1	S	264	<div> <div>14%</div> <div> <div></div> <div>79%</div> <div>5% •</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	N	241	
2	P	241	
2	R	241	
2	T	241	
3	A	439	
3	B	439	
3	C	439	
3	D	439	
4	E	419	
4	F	419	
4	G	419	
4	H	419	
5	I	151	
5	J	151	
5	K	151	
5	L	151	
6	U	6	
7	V	4	
8	W	3	
9	X	4	
10	Y	2	

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
10	NAG	Y	1	X	-	-	-
11	CLR	C	501	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLR	D	501	-	-	X	-
11	CLR	F	501	-	-	X	-
6	NAG	U	1	X	-	-	-
6	NAG	U	2	X	-	-	-
6	MAN	U	3	X	-	-	-
7	NAG	V	1	X	-	-	-
7	FUC	V	4	X	-	-	-
8	NAG	W	2	X	-	-	-
9	NAG	X	2	X	-	-	-
9	BMA	X	3	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 44589 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 C34 Fab, Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	224	Total	C	N	O	S	0	0
			1671	1047	282	334	8		
1	Q	224	Total	C	N	O	S	0	0
			1671	1047	282	334	8		
1	O	224	Total	C	N	O	S	0	0
			1671	1047	282	334	8		
1	M	224	Total	C	N	O	S	0	0
			1671	1047	282	334	8		

- Molecule 2 is a protein called C34 Fab, Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	211	Total	C	N	O	S	0	0
			1631	1022	276	329	4		
2	R	211	Total	C	N	O	S	0	0
			1631	1022	276	329	4		
2	P	211	Total	C	N	O	S	0	0
			1631	1022	276	329	4		
2	N	211	Total	C	N	O	S	0	0
			1631	1022	276	329	4		

- Molecule 3 is a protein called CHIKV E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		
3	B	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		
3	C	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		
3	D	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	LYS	GLU	conflict	UNP A0A286S4J4
B	211	LYS	GLU	conflict	UNP A0A286S4J4
C	211	LYS	GLU	conflict	UNP A0A286S4J4
D	211	LYS	GLU	conflict	UNP A0A286S4J4

- Molecule 4 is a protein called Structural polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	419	Total	C	N	O	S	0	0
			3282	2062	584	607	29		
4	F	419	Total	C	N	O	S	0	0
			3282	2062	584	607	29		
4	G	419	Total	C	N	O	S	0	0
			3282	2062	584	607	29		
4	H	417	Total	C	N	O	S	0	0
			3263	2049	581	604	29		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	60	ASP	GLY	conflict	UNP D7R9A2
E	211	THR	ILE	conflict	UNP D7R9A2
E	312	MET	THR	conflict	UNP D7R9A2
F	60	ASP	GLY	conflict	UNP D7R9A2
F	211	THR	ILE	conflict	UNP D7R9A2
F	312	MET	THR	conflict	UNP D7R9A2
G	60	ASP	GLY	conflict	UNP D7R9A2
G	211	THR	ILE	conflict	UNP D7R9A2
G	312	MET	THR	conflict	UNP D7R9A2
H	60	ASP	GLY	conflict	UNP D7R9A2
H	211	THR	ILE	conflict	UNP D7R9A2
H	312	MET	THR	conflict	UNP D7R9A2

- Molecule 5 is a protein called CHIKV capsid protein.

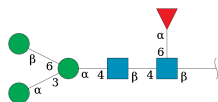
Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
5	J	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
5	K	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		

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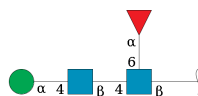
Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-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.



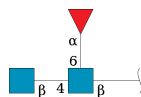
Mol	Chain	Residues	Atoms				AltConf	Trace
6	U	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 7 is an oligosaccharide called alpha-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.



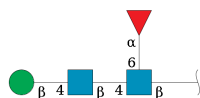
Mol	Chain	Residues	Atoms				AltConf	Trace
7	V	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 8 is an oligosaccharide called 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
8	W	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 9 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.



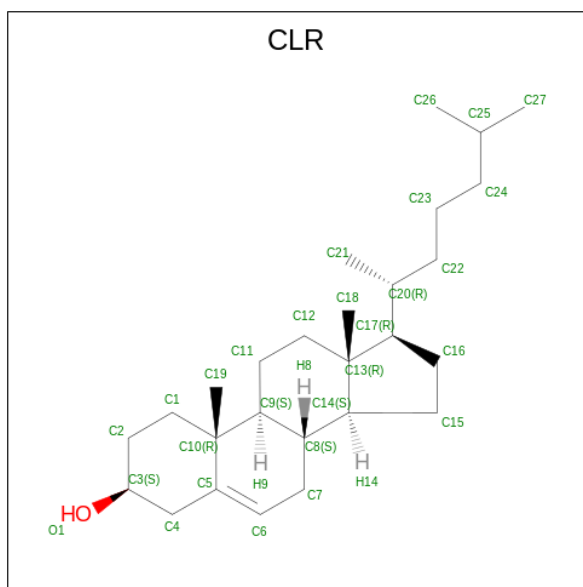
Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	Y	2	Total	C	N	O	0	0
			29	16	2	11		

- Molecule 11 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	C	O	0
			28	27	1	
11	D	1	Total	C	O	0
			28	27	1	

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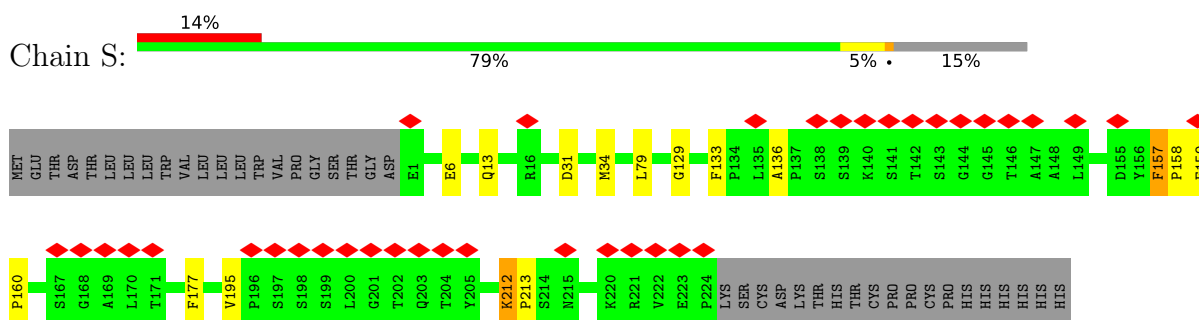
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Mol	Chain	Residues	Atoms			AltConf
11	E	1	Total	C	O	0
			28	27	1	
11	F	1	Total	C	O	0
			28	27	1	

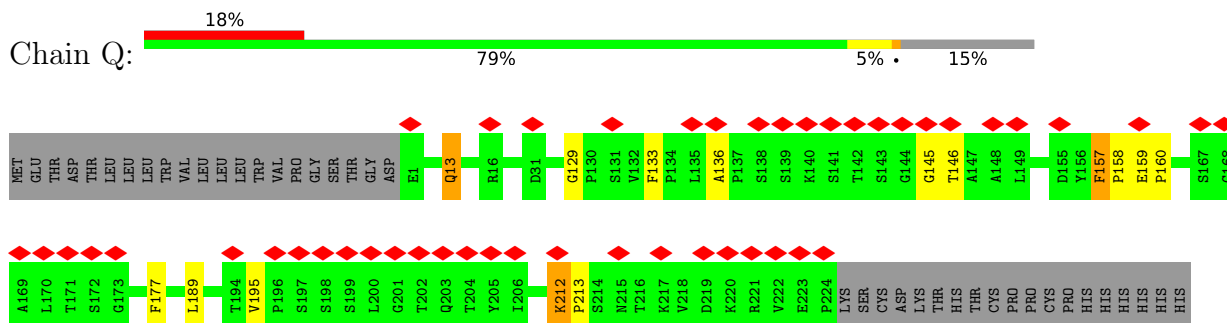
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: C34 Fab, Heavy Chain

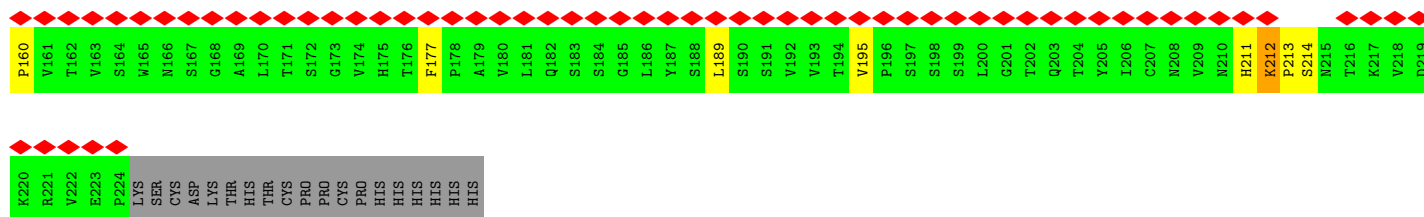


- Molecule 1: C34 Fab, Heavy Chain

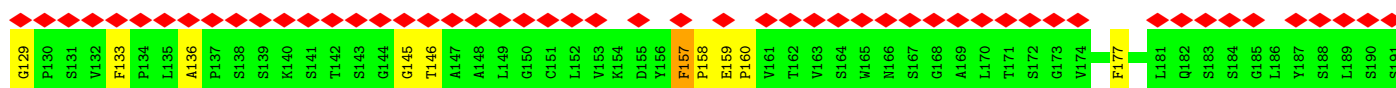
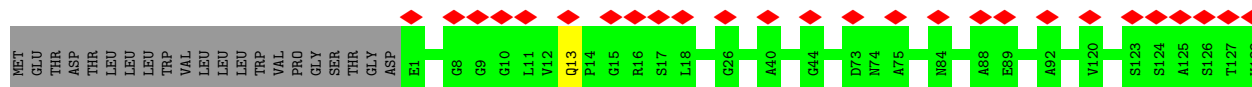
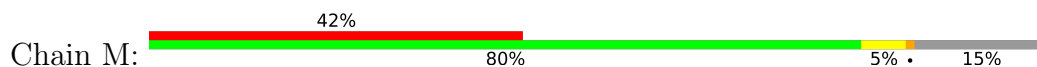


- Molecule 1: C34 Fab, Heavy Chain

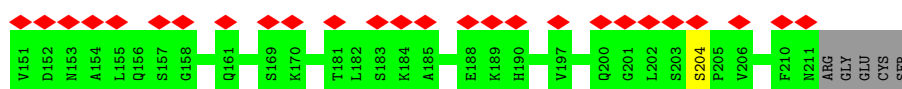
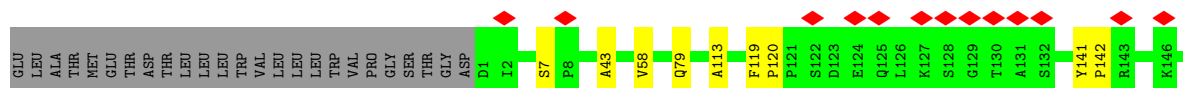
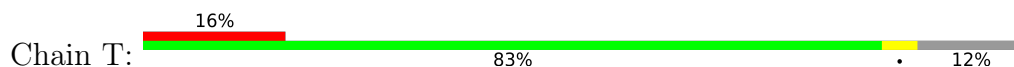




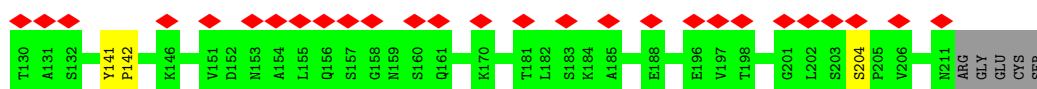
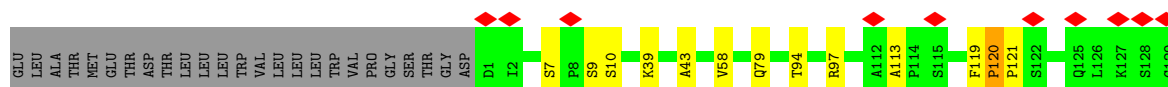
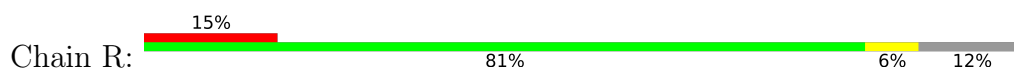
• Molecule 1: C34 Fab, Heavy Chain



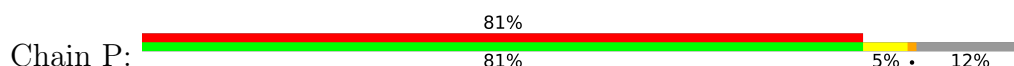
• Molecule 2: C34 Fab, Light Chain

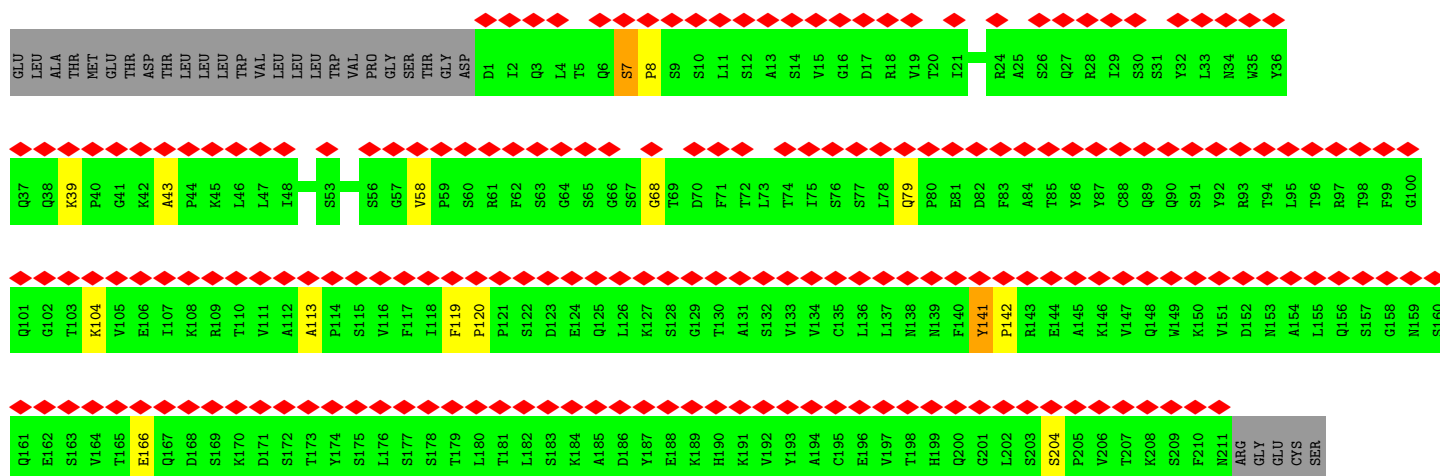


• Molecule 2: C34 Fab, Light Chain

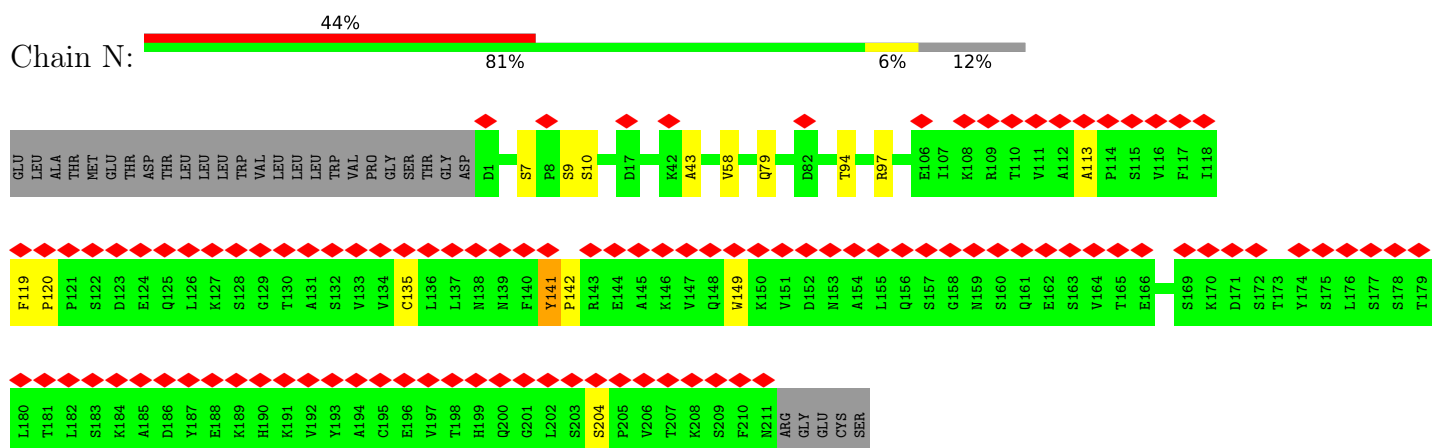


• Molecule 2: C34 Fab, Light Chain

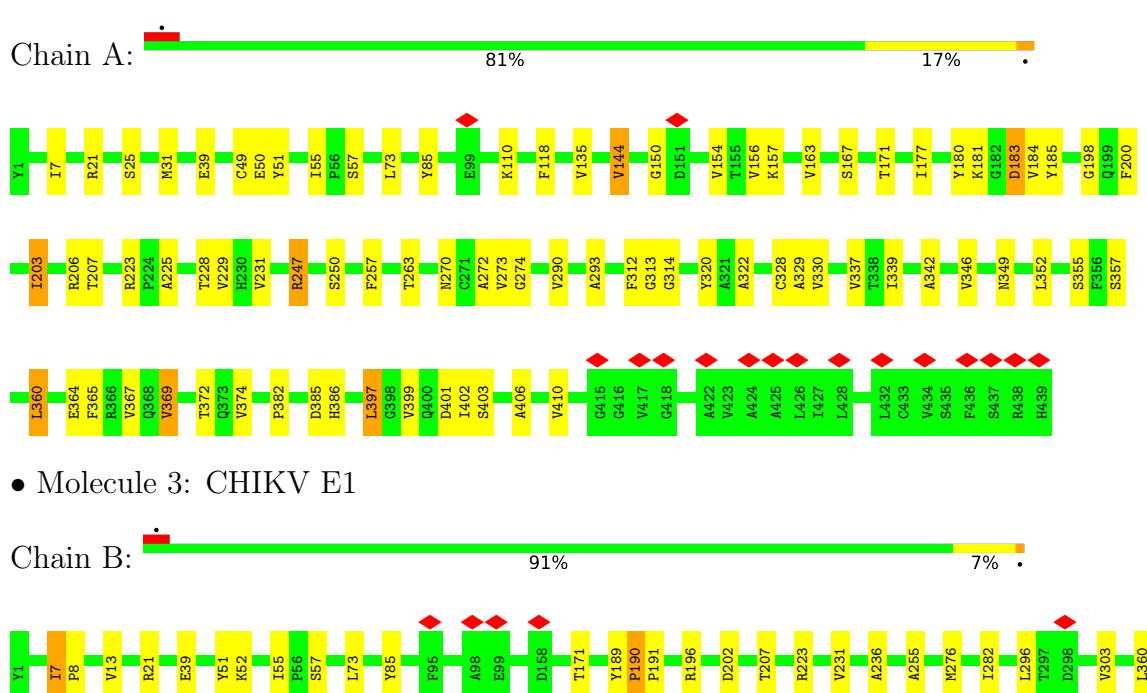


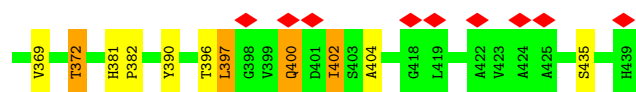


• Molecule 2: C34 Fab, Light Chain

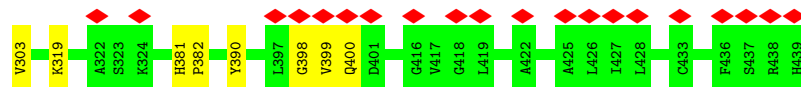
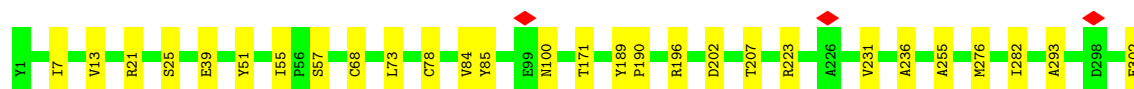


• Molecule 3: CHIKV E1

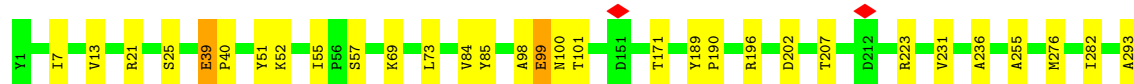
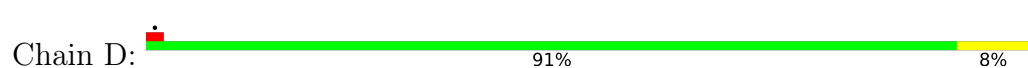




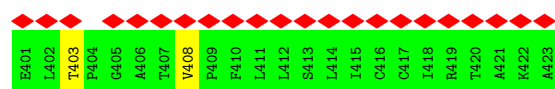
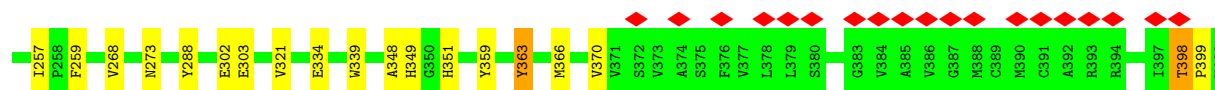
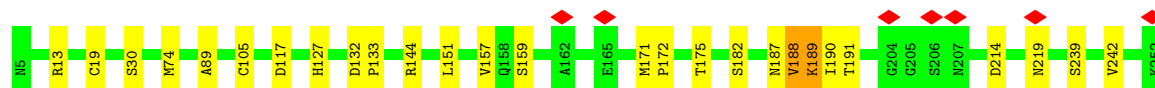
- Molecule 3: CHIKV E1



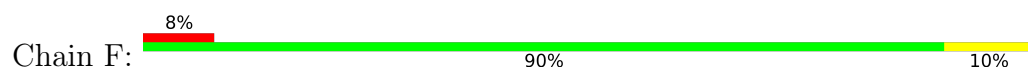
- Molecule 3: CHIKV E1

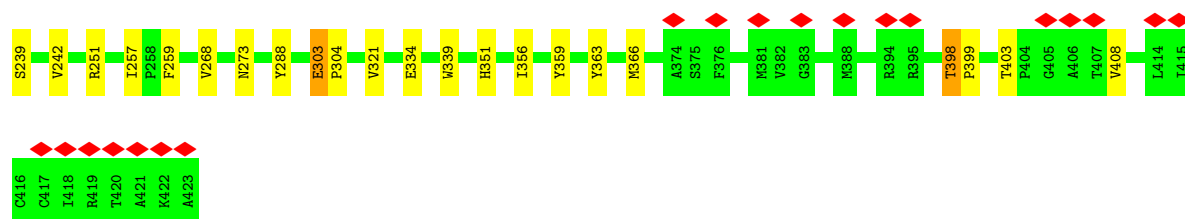


- Molecule 4: Structural polyprotein

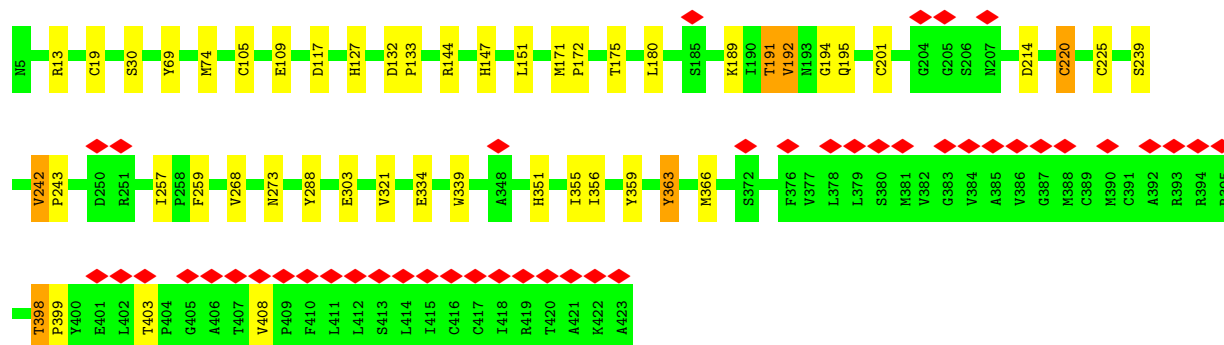
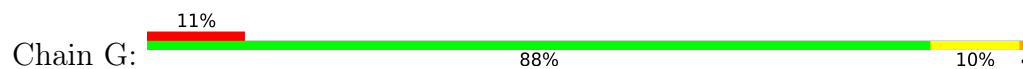


- Molecule 4: Structural polyprotein

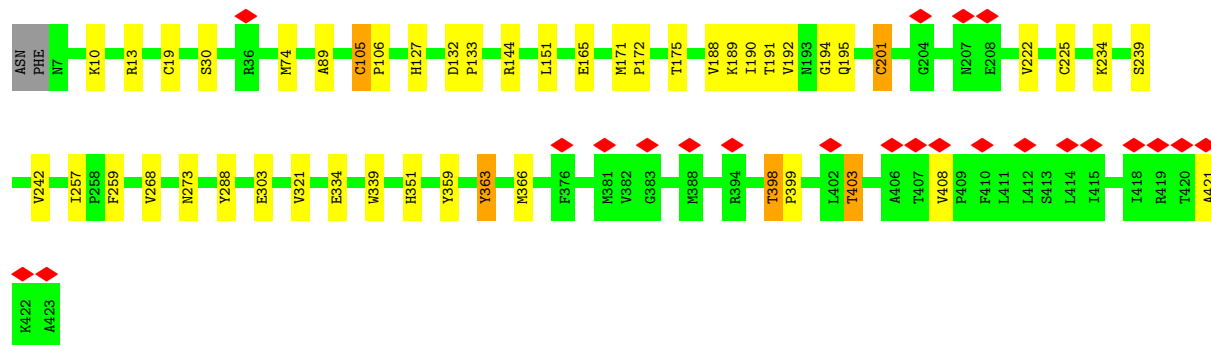
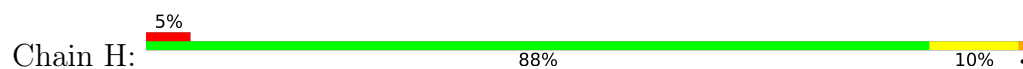




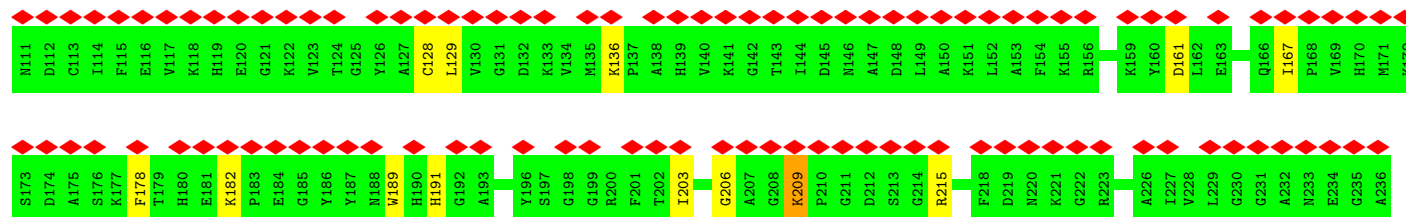
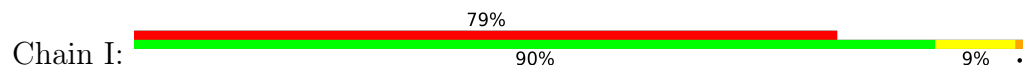
• Molecule 4: Structural polyprotein

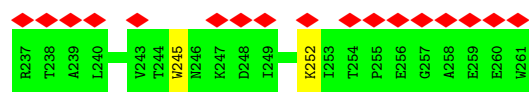


• Molecule 4: Structural polyprotein

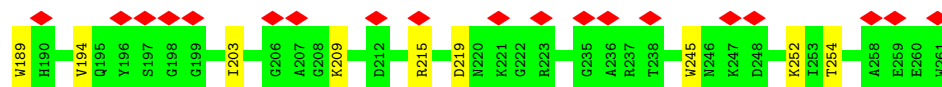
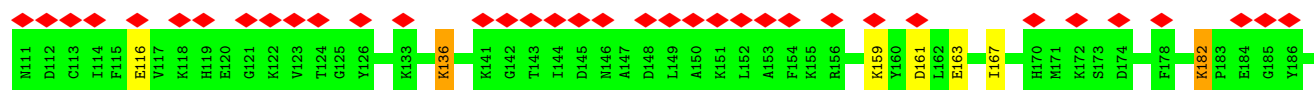
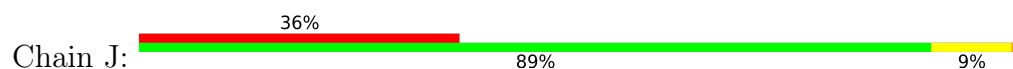


• Molecule 5: CHIKV capsid protein

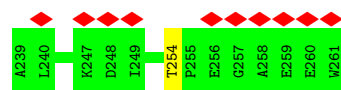
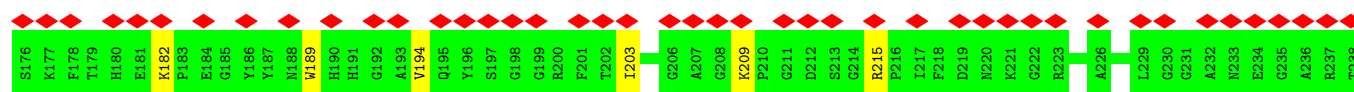




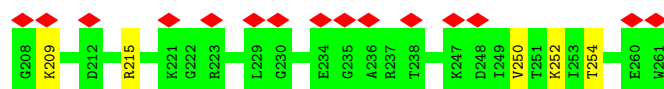
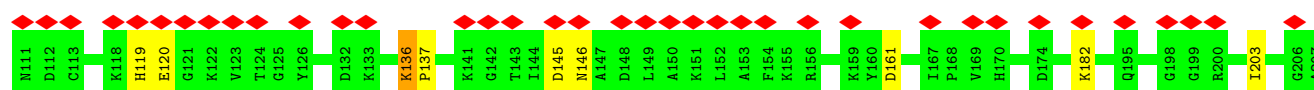
• Molecule 5: CHIKV capsid protein



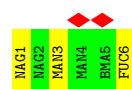
• Molecule 5: CHIKV capsid protein




• Molecule 5: CHIKV capsid protein



• Molecule 6: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-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



- Molecule 7: α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain V: 



- Molecule 8: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain W: 



- Molecule 9: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain X: 



- Molecule 10: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Y: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	491507	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.944	Depositor
Minimum map value	-0.596	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.135	Depositor
Map size (\AA)	493.12003, 493.12003, 493.12003	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	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: CLR, NAG, MAN, BMA, 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	M	0.54	0/1711	0.94	16/2329 (0.7%)
1	O	0.55	0/1711	0.93	16/2329 (0.7%)
1	Q	0.55	0/1711	0.92	16/2329 (0.7%)
1	S	0.55	0/1711	0.94	16/2329 (0.7%)
2	N	0.53	0/1665	0.92	18/2259 (0.8%)
2	P	0.52	0/1665	0.93	20/2259 (0.9%)
2	R	0.53	0/1665	0.94	18/2259 (0.8%)
2	T	0.53	0/1665	0.94	16/2259 (0.7%)
3	A	1.03	0/3407	1.23	38/4649 (0.8%)
3	B	0.57	0/3407	1.02	48/4649 (1.0%)
3	C	0.54	0/3407	1.00	51/4649 (1.1%)
3	D	0.57	0/3407	1.04	53/4649 (1.1%)
4	E	0.57	0/3369	1.09	62/4589 (1.4%)
4	F	0.56	0/3369	1.07	61/4589 (1.3%)
4	G	0.58	0/3369	1.11	62/4589 (1.4%)
4	H	0.57	0/3349	1.09	62/4562 (1.4%)
5	I	0.57	0/1184	0.94	12/1599 (0.8%)
5	J	0.58	0/1184	0.94	14/1599 (0.9%)
5	K	0.58	0/1184	0.93	12/1599 (0.8%)
5	L	0.57	0/1184	0.92	12/1599 (0.8%)
All	All	0.61	0/45324	1.03	623/61673 (1.0%)

There are no bond length outliers.

All (623) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	313	GLY	N-CA-C	12.63	128.94	112.77
4	G	189	LYS	N-CA-C	11.29	123.67	111.36
3	A	386	HIS	N-CA-C	10.07	122.33	111.36
4	F	132	ASP	CA-C-N	9.66	126.71	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	132	ASP	C-N-CA	9.66	126.71	119.66
4	G	132	ASP	CA-C-N	9.65	126.70	119.66
4	G	132	ASP	C-N-CA	9.65	126.70	119.66
2	T	119	PHE	CA-C-N	9.65	126.70	119.66
2	T	119	PHE	C-N-CA	9.65	126.70	119.66
2	R	119	PHE	CA-C-N	9.55	126.63	119.66
2	R	119	PHE	C-N-CA	9.55	126.63	119.66
3	D	189	TYR	CA-C-N	9.54	126.53	119.66
3	D	189	TYR	C-N-CA	9.54	126.53	119.66
4	E	132	ASP	CA-C-N	9.47	126.57	119.66
4	E	132	ASP	C-N-CA	9.47	126.57	119.66
4	H	132	ASP	CA-C-N	9.40	126.52	119.66
4	H	132	ASP	C-N-CA	9.40	126.52	119.66
4	E	189	LYS	N-CA-C	8.61	120.75	111.36
1	O	129	GLY	CA-C-N	8.20	128.14	119.85
1	O	129	GLY	C-N-CA	8.20	128.14	119.85
1	S	129	GLY	CA-C-N	8.15	128.09	119.85
1	S	129	GLY	C-N-CA	8.15	128.09	119.85
4	F	172	PRO	CA-C-N	8.13	128.08	120.03
4	F	172	PRO	C-N-CA	8.13	128.08	120.03
4	G	172	PRO	CA-C-N	7.99	127.88	120.21
4	G	172	PRO	C-N-CA	7.99	127.88	120.21
4	H	105	CYS	CA-C-N	7.95	127.96	119.78
4	H	105	CYS	C-N-CA	7.95	127.96	119.78
4	F	105	CYS	CA-C-N	7.92	127.94	119.78
4	F	105	CYS	C-N-CA	7.92	127.94	119.78
1	Q	129	GLY	CA-C-N	7.92	127.84	119.85
1	Q	129	GLY	C-N-CA	7.92	127.84	119.85
1	M	129	GLY	CA-C-N	7.87	127.80	119.85
1	M	129	GLY	C-N-CA	7.87	127.80	119.85
4	G	144	ARG	CA-C-N	7.83	127.98	120.31
4	G	144	ARG	C-N-CA	7.83	127.98	120.31
4	E	363	TYR	CA-C-N	7.82	127.54	119.56
4	E	363	TYR	C-N-CA	7.82	127.54	119.56
3	D	382	PRO	CA-C-N	7.82	127.77	120.03
3	D	382	PRO	C-N-CA	7.82	127.77	120.03
4	H	363	TYR	CA-C-N	7.81	127.45	119.56
4	H	363	TYR	C-N-CA	7.81	127.45	119.56
4	E	105	CYS	CA-C-N	7.81	127.83	119.78
4	E	105	CYS	C-N-CA	7.81	127.83	119.78
4	E	242	VAL	CA-C-N	7.81	127.82	119.78
4	E	242	VAL	C-N-CA	7.81	127.82	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	382	PRO	CA-C-N	7.76	127.72	120.03
3	C	382	PRO	C-N-CA	7.76	127.72	120.03
4	E	321	VAL	CA-C-N	7.75	127.70	120.03
4	E	321	VAL	C-N-CA	7.75	127.70	120.03
3	D	190	PRO	CA-C-N	7.68	127.61	119.85
3	D	190	PRO	C-N-CA	7.68	127.61	119.85
4	G	13	ARG	CA-C-N	7.68	127.69	119.78
4	G	13	ARG	C-N-CA	7.68	127.69	119.78
3	C	255	ALA	CA-C-N	7.63	128.08	120.52
3	C	255	ALA	C-N-CA	7.63	128.08	120.52
3	B	255	ALA	CA-C-N	7.63	128.08	120.52
3	B	255	ALA	C-N-CA	7.63	128.08	120.52
2	N	113	ALA	CA-C-N	7.58	127.50	119.85
2	N	113	ALA	C-N-CA	7.58	127.50	119.85
4	F	144	ARG	CA-C-N	7.54	127.70	120.31
4	F	144	ARG	C-N-CA	7.54	127.70	120.31
3	D	255	ALA	CA-C-N	7.52	127.96	119.92
3	D	255	ALA	C-N-CA	7.52	127.96	119.92
3	B	382	PRO	CA-C-N	7.51	127.44	119.85
3	B	382	PRO	C-N-CA	7.51	127.44	119.85
3	C	190	PRO	CA-C-N	7.49	127.50	119.78
3	C	190	PRO	C-N-CA	7.49	127.50	119.78
4	F	13	ARG	CA-C-N	7.47	127.48	119.78
4	F	13	ARG	C-N-CA	7.47	127.48	119.78
4	F	74	MET	CA-C-N	7.45	127.41	120.03
4	F	74	MET	C-N-CA	7.45	127.41	120.03
4	G	191	THR	N-CA-C	7.40	120.27	111.02
4	G	105	CYS	CA-C-N	7.39	127.31	119.85
4	G	105	CYS	C-N-CA	7.39	127.31	119.85
4	G	239	SER	CA-C-N	7.38	127.06	119.82
4	G	239	SER	C-N-CA	7.38	127.06	119.82
4	F	321	VAL	CA-C-N	7.38	127.54	120.31
4	F	321	VAL	C-N-CA	7.38	127.54	120.31
4	H	268	VAL	CA-C-N	7.37	127.33	120.03
4	H	268	VAL	C-N-CA	7.37	127.33	120.03
3	A	382	PRO	N-CA-C	7.37	118.46	110.58
4	E	268	VAL	CA-C-N	7.37	127.32	120.03
4	E	268	VAL	C-N-CA	7.37	127.32	120.03
4	E	172	PRO	CA-C-N	7.36	127.32	120.03
4	E	172	PRO	C-N-CA	7.36	127.32	120.03
4	F	268	VAL	CA-C-N	7.35	127.31	120.03
4	F	268	VAL	C-N-CA	7.35	127.31	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	259	PHE	CA-C-N	7.33	127.29	120.03
4	E	259	PHE	C-N-CA	7.33	127.29	120.03
4	H	189	LYS	N-CA-C	7.32	119.34	111.36
5	I	215	ARG	CA-C-N	7.30	127.22	119.85
5	I	215	ARG	C-N-CA	7.30	127.22	119.85
4	H	172	PRO	CA-C-N	7.30	127.25	120.03
4	H	172	PRO	C-N-CA	7.30	127.25	120.03
3	C	85	TYR	CA-C-N	7.28	127.21	119.85
3	C	85	TYR	C-N-CA	7.28	127.21	119.85
4	G	268	VAL	CA-C-N	7.28	127.24	120.03
4	G	268	VAL	C-N-CA	7.28	127.24	120.03
4	H	133	PRO	CA-C-N	7.27	127.23	120.03
4	H	133	PRO	C-N-CA	7.27	127.23	120.03
4	H	321	VAL	CA-C-N	7.27	127.44	120.31
4	H	321	VAL	C-N-CA	7.27	127.44	120.31
2	R	7	SER	CA-C-N	7.26	126.96	119.56
2	R	7	SER	C-N-CA	7.26	126.96	119.56
4	F	133	PRO	CA-C-N	7.26	127.21	120.03
4	F	133	PRO	C-N-CA	7.26	127.21	120.03
5	L	215	ARG	CA-C-N	7.26	127.42	120.31
5	L	215	ARG	C-N-CA	7.26	127.42	120.31
3	A	150	GLY	N-CA-C	-7.25	104.56	115.00
4	G	30	SER	CA-C-N	7.24	127.40	119.87
4	G	30	SER	C-N-CA	7.24	127.40	119.87
4	H	30	SER	CA-C-N	7.23	127.39	119.87
4	H	30	SER	C-N-CA	7.23	127.39	119.87
4	G	273	ASN	CA-C-N	7.23	127.18	120.03
4	G	273	ASN	C-N-CA	7.23	127.18	120.03
4	G	133	PRO	CA-C-N	7.22	127.18	120.03
4	G	133	PRO	C-N-CA	7.22	127.18	120.03
2	P	113	ALA	CA-C-N	7.22	127.14	119.85
2	P	113	ALA	C-N-CA	7.22	127.14	119.85
3	D	85	TYR	CA-C-N	7.21	127.14	119.85
3	D	85	TYR	C-N-CA	7.21	127.14	119.85
3	A	85	TYR	CA-C-N	7.18	127.10	119.85
3	A	85	TYR	C-N-CA	7.18	127.10	119.85
3	C	196	ARG	CA-C-N	7.17	126.93	119.76
3	C	196	ARG	C-N-CA	7.17	126.93	119.76
4	F	30	SER	CA-C-N	7.17	126.81	119.56
4	F	30	SER	C-N-CA	7.17	126.81	119.56
3	B	55	ILE	CA-C-N	7.17	127.17	119.78
3	B	55	ILE	C-N-CA	7.17	127.17	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	175	THR	CA-C-N	7.17	127.14	119.76
4	G	175	THR	C-N-CA	7.17	127.14	119.76
4	H	239	SER	CA-C-N	7.17	126.85	119.82
4	H	239	SER	C-N-CA	7.17	126.85	119.82
5	L	209	LYS	CA-C-N	7.16	127.13	119.76
5	L	209	LYS	C-N-CA	7.16	127.13	119.76
3	C	55	ILE	CA-C-N	7.15	127.14	119.78
3	C	55	ILE	C-N-CA	7.15	127.14	119.78
4	F	257	ILE	CA-C-N	7.13	127.06	120.21
4	F	257	ILE	C-N-CA	7.13	127.06	120.21
4	E	257	ILE	CA-C-N	7.13	127.05	120.21
4	E	257	ILE	C-N-CA	7.13	127.05	120.21
3	B	85	TYR	CA-C-N	7.12	127.05	119.85
3	B	85	TYR	C-N-CA	7.12	127.05	119.85
4	E	133	PRO	CA-C-N	7.11	127.03	119.85
4	E	133	PRO	C-N-CA	7.11	127.03	119.85
4	H	144	ARG	CA-C-N	7.11	127.07	120.03
4	H	144	ARG	C-N-CA	7.11	127.07	120.03
3	D	171	THR	CA-C-N	7.10	126.73	119.56
3	D	171	THR	C-N-CA	7.10	126.73	119.56
3	D	223	ARG	CA-C-N	7.10	127.02	119.85
3	D	223	ARG	C-N-CA	7.10	127.02	119.85
4	E	144	ARG	CA-C-N	7.09	127.26	120.31
4	E	144	ARG	C-N-CA	7.09	127.26	120.31
3	B	223	ARG	CA-C-N	7.09	127.01	119.85
3	B	223	ARG	C-N-CA	7.09	127.01	119.85
4	G	259	PHE	CA-C-N	7.08	127.04	120.03
4	G	259	PHE	C-N-CA	7.08	127.04	120.03
4	E	175	THR	CA-C-N	7.08	127.05	119.76
4	E	175	THR	C-N-CA	7.08	127.05	119.76
3	A	7	ILE	CA-C-N	7.08	127.11	119.89
3	A	7	ILE	C-N-CA	7.08	127.11	119.89
1	O	177	PHE	CA-C-N	7.07	127.04	119.76
1	O	177	PHE	C-N-CA	7.07	127.04	119.76
3	D	7	ILE	CA-C-N	7.06	127.06	119.78
3	D	7	ILE	C-N-CA	7.06	127.06	119.78
3	B	282	ILE	CA-C-N	7.06	127.03	119.76
3	B	282	ILE	C-N-CA	7.06	127.03	119.76
4	H	257	ILE	CA-C-N	7.05	126.98	120.21
4	H	257	ILE	C-N-CA	7.05	126.98	120.21
3	B	7	ILE	CA-C-N	7.05	127.04	119.78
3	B	7	ILE	C-N-CA	7.05	127.04	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	215	ARG	CA-C-N	7.04	127.21	120.31
5	K	215	ARG	C-N-CA	7.04	127.21	120.31
2	R	113	ALA	CA-C-N	7.03	126.95	119.85
2	R	113	ALA	C-N-CA	7.03	126.95	119.85
4	E	13	ARG	CA-C-N	7.03	127.02	119.78
4	E	13	ARG	C-N-CA	7.03	127.02	119.78
4	G	74	MET	CA-C-N	7.03	127.02	119.78
4	G	74	MET	C-N-CA	7.03	127.02	119.78
4	G	192	VAL	N-CA-C	7.03	117.79	110.62
2	T	113	ALA	CA-C-N	7.03	126.95	119.85
2	T	113	ALA	C-N-CA	7.03	126.95	119.85
4	H	175	THR	CA-C-N	7.02	126.99	119.76
4	H	175	THR	C-N-CA	7.02	126.99	119.76
4	E	30	SER	CA-C-N	7.01	126.64	119.56
4	E	30	SER	C-N-CA	7.01	126.64	119.56
4	H	74	MET	CA-C-N	7.00	126.99	119.78
4	H	74	MET	C-N-CA	7.00	126.99	119.78
4	E	74	MET	CA-C-N	6.99	126.98	119.78
4	E	74	MET	C-N-CA	6.99	126.98	119.78
5	K	254	THR	CA-C-N	6.99	126.98	119.78
5	K	254	THR	C-N-CA	6.99	126.98	119.78
4	F	334	GLU	CA-C-N	6.96	126.87	119.85
4	F	334	GLU	C-N-CA	6.96	126.87	119.85
3	C	282	ILE	CA-C-N	6.94	126.91	119.76
3	C	282	ILE	C-N-CA	6.94	126.91	119.76
4	F	239	SER	CA-C-N	6.93	127.07	119.87
4	F	239	SER	C-N-CA	6.93	127.07	119.87
1	M	133	PHE	CA-C-N	6.92	126.68	119.76
1	M	133	PHE	C-N-CA	6.92	126.68	119.76
1	M	13	GLN	CA-C-N	6.92	126.91	119.78
1	M	13	GLN	C-N-CA	6.92	126.91	119.78
4	G	242	VAL	CA-C-N	6.92	126.88	119.76
4	G	242	VAL	C-N-CA	6.92	126.88	119.76
4	E	403	THR	CA-C-N	6.91	126.61	119.56
4	E	403	THR	C-N-CA	6.91	126.61	119.56
4	G	257	ILE	CA-C-N	6.91	126.87	120.03
4	G	257	ILE	C-N-CA	6.91	126.87	120.03
2	N	120	PRO	CA-C-N	6.91	126.90	119.78
2	N	120	PRO	C-N-CA	6.91	126.90	119.78
4	G	334	GLU	CA-C-N	6.90	126.82	119.85
4	G	334	GLU	C-N-CA	6.90	126.82	119.85
4	F	19	CYS	CA-C-N	6.89	126.52	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	19	CYS	C-N-CA	6.89	126.52	119.56
2	R	120	PRO	CA-C-N	6.89	126.86	119.76
2	R	120	PRO	C-N-CA	6.89	126.86	119.76
4	E	151	LEU	CA-C-N	6.89	126.86	119.76
4	E	151	LEU	C-N-CA	6.89	126.86	119.76
5	J	215	ARG	CA-C-N	6.89	126.87	119.78
5	J	215	ARG	C-N-CA	6.89	126.87	119.78
4	E	239	SER	CA-C-N	6.88	126.58	119.56
4	E	239	SER	C-N-CA	6.88	126.58	119.56
4	G	151	LEU	CA-C-N	6.88	126.64	119.76
4	G	151	LEU	C-N-CA	6.88	126.64	119.76
2	T	120	PRO	CA-C-N	6.88	126.84	119.76
2	T	120	PRO	C-N-CA	6.88	126.84	119.76
3	B	196	ARG	CA-C-N	6.86	126.83	119.76
3	B	196	ARG	C-N-CA	6.86	126.83	119.76
3	C	223	ARG	CA-C-N	6.86	126.82	120.03
3	C	223	ARG	C-N-CA	6.86	126.82	120.03
4	G	339	TRP	CA-C-N	6.85	126.77	119.85
4	G	339	TRP	C-N-CA	6.85	126.77	119.85
3	C	293	ALA	CA-C-N	6.85	126.83	119.78
3	C	293	ALA	C-N-CA	6.85	126.83	119.78
1	Q	136	ALA	CA-C-N	6.85	126.61	119.76
1	Q	136	ALA	C-N-CA	6.85	126.61	119.76
3	A	73	LEU	CA-C-N	6.84	127.12	119.32
3	A	73	LEU	C-N-CA	6.84	127.12	119.32
4	H	259	PHE	CA-C-N	6.84	126.75	119.85
4	H	259	PHE	C-N-CA	6.84	126.75	119.85
4	H	273	ASN	CA-C-N	6.83	126.79	120.03
4	H	273	ASN	C-N-CA	6.83	126.79	120.03
3	B	190	PRO	CA-C-N	6.83	126.81	119.78
3	B	190	PRO	C-N-CA	6.83	126.81	119.78
4	E	273	ASN	CA-C-N	6.82	126.73	119.85
4	E	273	ASN	C-N-CA	6.82	126.73	119.85
3	A	39	GLU	CA-C-N	6.81	126.72	119.85
3	A	39	GLU	C-N-CA	6.81	126.72	119.85
4	E	334	GLU	CA-C-N	6.81	126.73	119.85
4	E	334	GLU	C-N-CA	6.81	126.73	119.85
4	G	321	VAL	CA-C-N	6.79	127.25	120.52
4	G	321	VAL	C-N-CA	6.79	127.25	120.52
3	D	303	VAL	CA-C-N	6.79	126.42	119.56
3	D	303	VAL	C-N-CA	6.79	126.42	119.56
1	Q	177	PHE	CA-C-N	6.78	126.74	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	177	PHE	C-N-CA	6.78	126.74	119.76
4	F	339	TRP	CA-C-N	6.77	126.68	119.85
4	F	339	TRP	C-N-CA	6.77	126.68	119.85
3	C	7	ILE	CA-C-N	6.76	126.73	119.76
3	C	7	ILE	C-N-CA	6.76	126.73	119.76
3	D	73	LEU	CA-C-N	6.76	127.03	119.32
3	D	73	LEU	C-N-CA	6.76	127.03	119.32
3	C	276	MET	CA-C-N	6.76	126.72	119.76
3	C	276	MET	C-N-CA	6.76	126.72	119.76
5	I	182	LYS	CA-C-N	6.76	126.74	119.78
5	I	182	LYS	C-N-CA	6.76	126.74	119.78
5	L	182	LYS	CA-C-N	6.76	126.67	119.85
5	L	182	LYS	C-N-CA	6.76	126.67	119.85
5	K	209	LYS	CA-C-N	6.75	126.67	119.85
5	K	209	LYS	C-N-CA	6.75	126.67	119.85
1	O	136	ALA	CA-C-N	6.75	126.67	119.85
1	O	136	ALA	C-N-CA	6.75	126.67	119.85
3	D	293	ALA	CA-C-N	6.75	126.71	119.76
3	D	293	ALA	C-N-CA	6.75	126.71	119.76
3	C	39	GLU	CA-C-N	6.74	126.66	119.85
3	C	39	GLU	C-N-CA	6.74	126.66	119.85
4	F	259	PHE	CA-C-N	6.74	126.70	120.03
4	F	259	PHE	C-N-CA	6.74	126.70	120.03
1	M	136	ALA	CA-C-N	6.74	126.65	119.85
1	M	136	ALA	C-N-CA	6.74	126.65	119.85
3	B	171	THR	CA-C-N	6.72	126.35	119.56
3	B	171	THR	C-N-CA	6.72	126.35	119.56
3	B	39	GLU	CA-C-N	6.72	126.64	119.85
3	B	39	GLU	C-N-CA	6.72	126.64	119.85
4	F	273	ASN	CA-C-N	6.72	126.68	120.03
4	F	273	ASN	C-N-CA	6.72	126.68	120.03
5	I	167	ILE	CA-C-N	6.71	126.75	119.90
5	I	167	ILE	C-N-CA	6.71	126.75	119.90
2	P	43	ALA	CA-C-N	6.71	126.68	120.03
2	P	43	ALA	C-N-CA	6.71	126.68	120.03
2	P	120	PRO	CA-C-N	6.71	126.69	119.78
2	P	120	PRO	C-N-CA	6.71	126.69	119.78
2	P	58	VAL	CA-C-N	6.70	126.69	119.78
2	P	58	VAL	C-N-CA	6.70	126.69	119.78
4	G	408	VAL	CA-C-N	6.70	126.66	119.76
4	G	408	VAL	C-N-CA	6.70	126.66	119.76
5	J	254	THR	CA-C-N	6.70	126.68	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	254	THR	C-N-CA	6.70	126.68	119.78
4	H	151	LEU	CA-C-N	6.69	126.66	119.76
4	H	151	LEU	C-N-CA	6.69	126.66	119.76
4	H	288	TYR	CA-C-N	6.69	126.60	119.85
4	H	288	TYR	C-N-CA	6.69	126.60	119.85
3	C	390	TYR	CA-C-N	6.69	126.60	119.85
3	C	390	TYR	C-N-CA	6.69	126.60	119.85
3	A	206	ARG	N-CA-C	6.67	118.56	111.28
2	T	58	VAL	CA-C-N	6.66	126.64	119.78
2	T	58	VAL	C-N-CA	6.66	126.64	119.78
4	E	288	TYR	CA-C-N	6.66	126.57	119.85
4	E	288	TYR	C-N-CA	6.66	126.57	119.85
4	H	334	GLU	CA-C-N	6.66	126.57	119.85
4	H	334	GLU	C-N-CA	6.66	126.57	119.85
5	K	182	LYS	CA-C-N	6.66	126.57	119.85
5	K	182	LYS	C-N-CA	6.66	126.57	119.85
1	O	133	PHE	CA-C-N	6.66	126.62	119.76
1	O	133	PHE	C-N-CA	6.66	126.62	119.76
4	H	303	GLU	CA-C-N	6.65	126.24	119.19
4	H	303	GLU	C-N-CA	6.65	126.24	119.19
3	B	73	LEU	CA-C-N	6.65	126.90	119.32
3	B	73	LEU	C-N-CA	6.65	126.90	119.32
4	F	288	TYR	CA-C-N	6.65	126.57	119.85
4	F	288	TYR	C-N-CA	6.65	126.57	119.85
5	L	254	THR	CA-C-N	6.65	126.61	119.76
5	L	254	THR	C-N-CA	6.65	126.61	119.76
3	B	390	TYR	CA-C-N	6.65	126.56	119.85
3	B	390	TYR	C-N-CA	6.65	126.56	119.85
3	D	57	SER	CA-C-N	6.64	126.56	119.85
3	D	57	SER	C-N-CA	6.64	126.56	119.85
3	D	55	ILE	CA-C-N	6.64	126.61	120.03
3	D	55	ILE	C-N-CA	6.64	126.61	120.03
2	N	43	ALA	CA-C-N	6.64	126.56	119.85
2	N	43	ALA	C-N-CA	6.64	126.56	119.85
4	F	303	GLU	CA-C-N	6.62	126.24	119.56
4	F	303	GLU	C-N-CA	6.62	126.24	119.56
1	M	177	PHE	CA-C-N	6.61	126.57	119.76
1	M	177	PHE	C-N-CA	6.61	126.57	119.76
4	F	151	LEU	CA-C-N	6.61	126.57	119.76
4	F	151	LEU	C-N-CA	6.61	126.57	119.76
4	G	303	GLU	CA-C-N	6.61	126.23	119.56
4	G	303	GLU	C-N-CA	6.61	126.23	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	57	SER	CA-C-N	6.60	126.52	119.85
3	C	57	SER	C-N-CA	6.60	126.52	119.85
4	F	242	VAL	CA-C-N	6.60	126.51	119.85
4	F	242	VAL	C-N-CA	6.60	126.51	119.85
4	E	171	MET	CA-C-N	6.59	127.17	120.38
4	E	171	MET	C-N-CA	6.59	127.17	120.38
1	S	177	PHE	CA-C-N	6.59	126.55	119.76
1	S	177	PHE	C-N-CA	6.59	126.55	119.76
2	R	58	VAL	CA-C-N	6.59	126.61	119.89
2	R	58	VAL	C-N-CA	6.59	126.61	119.89
3	B	57	SER	CA-C-N	6.59	126.50	119.85
3	B	57	SER	C-N-CA	6.59	126.50	119.85
2	T	43	ALA	CA-C-N	6.58	126.53	119.76
2	T	43	ALA	C-N-CA	6.58	126.53	119.76
3	D	39	GLU	CA-C-N	6.58	126.49	119.85
3	D	39	GLU	C-N-CA	6.58	126.49	119.85
4	H	242	VAL	CA-C-N	6.58	126.49	119.85
4	H	242	VAL	C-N-CA	6.58	126.49	119.85
5	K	136	LYS	CA-C-N	6.57	126.53	119.76
5	K	136	LYS	C-N-CA	6.57	126.53	119.76
2	P	7	SER	CA-C-N	6.56	126.80	119.32
2	P	7	SER	C-N-CA	6.56	126.80	119.32
3	A	57	SER	CA-C-N	6.56	126.47	119.85
3	A	57	SER	C-N-CA	6.56	126.47	119.85
4	H	19	CYS	CA-C-N	6.55	126.13	119.19
4	H	19	CYS	C-N-CA	6.55	126.13	119.19
3	D	13	VAL	CA-C-N	6.54	126.45	119.85
3	D	13	VAL	C-N-CA	6.54	126.45	119.85
3	C	73	LEU	CA-C-N	6.53	126.77	119.32
3	C	73	LEU	C-N-CA	6.53	126.77	119.32
3	D	390	TYR	CA-C-N	6.52	126.44	119.85
3	D	390	TYR	C-N-CA	6.52	126.44	119.85
3	C	236	ALA	CA-C-N	6.51	126.49	119.78
3	C	236	ALA	C-N-CA	6.51	126.49	119.78
1	S	133	PHE	CA-C-N	6.50	126.42	119.85
1	S	133	PHE	C-N-CA	6.50	126.42	119.85
3	C	171	THR	CA-C-N	6.50	126.63	119.87
3	C	171	THR	C-N-CA	6.50	126.63	119.87
3	C	303	VAL	CA-C-N	6.50	126.73	119.32
3	C	303	VAL	C-N-CA	6.50	126.73	119.32
2	N	119	PHE	CA-C-N	6.49	127.06	120.38
2	N	119	PHE	C-N-CA	6.49	127.06	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	136	ALA	CA-C-N	6.47	126.23	119.76
1	S	136	ALA	C-N-CA	6.47	126.23	119.76
2	R	43	ALA	CA-C-N	6.46	126.38	119.85
2	R	43	ALA	C-N-CA	6.46	126.38	119.85
2	T	7	SER	CA-C-N	6.46	126.69	119.32
2	T	7	SER	C-N-CA	6.46	126.69	119.32
5	L	203	ILE	CA-C-N	6.46	126.41	119.76
5	L	203	ILE	C-N-CA	6.46	126.41	119.76
5	J	167	ILE	CA-C-N	6.46	126.41	119.76
5	J	167	ILE	C-N-CA	6.46	126.41	119.76
4	H	13	ARG	CA-C-N	6.45	126.36	119.85
4	H	13	ARG	C-N-CA	6.45	126.36	119.85
1	Q	133	PHE	CA-C-N	6.43	126.35	119.85
1	Q	133	PHE	C-N-CA	6.43	126.35	119.85
5	K	203	ILE	CA-C-N	6.43	126.40	119.78
5	K	203	ILE	C-N-CA	6.43	126.40	119.78
3	B	236	ALA	CA-C-N	6.42	126.39	119.78
3	B	236	ALA	C-N-CA	6.42	126.39	119.78
4	E	408	VAL	CA-C-N	6.41	126.36	119.76
4	E	408	VAL	C-N-CA	6.41	126.36	119.76
4	E	19	CYS	CA-C-N	6.40	126.31	119.28
4	E	19	CYS	C-N-CA	6.40	126.31	119.28
4	H	408	VAL	CA-C-N	6.40	126.42	119.90
4	H	408	VAL	C-N-CA	6.40	126.42	119.90
4	G	19	CYS	CA-C-N	6.39	126.31	119.28
4	G	19	CYS	C-N-CA	6.39	126.31	119.28
3	A	247	ARG	N-CA-C	6.38	118.23	111.28
3	D	236	ALA	CA-C-N	6.38	126.35	119.78
3	D	236	ALA	C-N-CA	6.38	126.35	119.78
3	D	196	ARG	CA-C-N	6.36	126.31	119.76
3	D	196	ARG	C-N-CA	6.36	126.31	119.76
3	C	231	VAL	CA-C-N	6.35	126.27	119.85
3	C	231	VAL	C-N-CA	6.35	126.27	119.85
3	A	55	ILE	CA-C-N	6.35	126.71	119.92
3	A	55	ILE	C-N-CA	6.35	126.71	119.92
5	J	182	LYS	CA-C-N	6.33	126.25	119.85
5	J	182	LYS	C-N-CA	6.33	126.25	119.85
4	E	303	GLU	CA-C-N	6.30	125.99	119.56
4	E	303	GLU	C-N-CA	6.30	125.99	119.56
2	N	58	VAL	CA-C-N	6.30	126.22	119.85
2	N	58	VAL	C-N-CA	6.30	126.22	119.85
1	M	212	LYS	CA-C-N	6.30	125.98	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	212	LYS	C-N-CA	6.30	125.98	119.56
1	S	212	LYS	CA-C-N	6.29	125.98	119.56
1	S	212	LYS	C-N-CA	6.29	125.98	119.56
5	I	136	LYS	CA-C-N	6.29	126.24	119.76
5	I	136	LYS	C-N-CA	6.29	126.24	119.76
4	G	220	CYS	N-CA-C	6.29	118.64	110.53
3	A	21	ARG	CA-C-N	6.28	126.31	119.90
3	A	21	ARG	C-N-CA	6.28	126.31	119.90
3	A	270	ASN	N-CA-C	6.28	120.28	112.24
3	D	276	MET	CA-C-N	6.28	126.61	119.83
3	D	276	MET	C-N-CA	6.28	126.61	119.83
4	F	175	THR	CA-C-N	6.28	126.19	119.85
4	F	175	THR	C-N-CA	6.28	126.19	119.85
2	P	119	PHE	CA-C-N	6.27	126.84	120.38
2	P	119	PHE	C-N-CA	6.27	126.84	120.38
2	T	204	SER	CA-C-N	6.25	126.20	119.76
2	T	204	SER	C-N-CA	6.25	126.20	119.76
2	N	79	GLN	CA-C-N	6.25	126.15	119.28
2	N	79	GLN	C-N-CA	6.25	126.15	119.28
2	P	79	GLN	CA-C-N	6.23	126.14	119.28
2	P	79	GLN	C-N-CA	6.23	126.14	119.28
3	D	369	VAL	N-CA-C	6.22	116.38	110.53
1	Q	212	LYS	CA-C-N	6.22	125.91	119.56
1	Q	212	LYS	C-N-CA	6.22	125.91	119.56
4	G	288	TYR	CA-C-N	6.22	126.13	119.85
4	G	288	TYR	C-N-CA	6.22	126.13	119.85
2	T	79	GLN	CA-C-N	6.21	126.11	119.28
2	T	79	GLN	C-N-CA	6.21	126.11	119.28
3	B	303	VAL	CA-C-N	6.21	126.40	119.32
3	B	303	VAL	C-N-CA	6.21	126.40	119.32
5	L	136	LYS	CA-C-N	6.21	126.15	119.76
5	L	136	LYS	C-N-CA	6.21	126.15	119.76
4	H	171	MET	CA-C-N	6.20	126.77	120.38
4	H	171	MET	C-N-CA	6.20	126.77	120.38
3	A	274	GLY	N-CA-C	6.19	123.73	112.58
2	N	204	SER	CA-C-N	6.19	126.13	119.76
2	N	204	SER	C-N-CA	6.19	126.13	119.76
4	F	363	TYR	CA-C-N	6.18	126.08	119.28
4	F	363	TYR	C-N-CA	6.18	126.08	119.28
5	J	136	LYS	CA-C-N	6.18	126.13	119.76
5	J	136	LYS	C-N-CA	6.18	126.13	119.76
4	G	363	TYR	CA-C-N	6.17	126.07	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	363	TYR	C-N-CA	6.17	126.07	119.28
4	E	351	HIS	CA-C-N	6.16	126.35	119.32
4	E	351	HIS	C-N-CA	6.16	126.35	119.32
3	A	25	SER	CA-C-N	6.16	126.10	119.76
3	A	25	SER	C-N-CA	6.16	126.10	119.76
3	D	282	ILE	CA-C-N	6.15	126.06	119.85
3	D	282	ILE	C-N-CA	6.15	126.06	119.85
1	O	157	PHE	CA-C-N	6.14	126.11	119.78
1	O	157	PHE	C-N-CA	6.14	126.11	119.78
3	D	21	ARG	CA-C-N	6.14	126.16	119.90
3	D	21	ARG	C-N-CA	6.14	126.16	119.90
3	C	189	TYR	CA-C-N	6.14	126.70	120.38
3	C	189	TYR	C-N-CA	6.14	126.70	120.38
2	P	204	SER	CA-C-N	6.11	126.13	119.90
2	P	204	SER	C-N-CA	6.11	126.13	119.90
2	N	7	SER	CA-C-N	6.10	126.27	119.32
2	N	7	SER	C-N-CA	6.10	126.27	119.32
2	R	204	SER	CA-C-N	6.09	126.11	119.90
2	R	204	SER	C-N-CA	6.09	126.11	119.90
3	B	276	MET	CA-C-N	6.09	126.40	119.83
3	B	276	MET	C-N-CA	6.09	126.40	119.83
4	F	351	HIS	CA-C-N	6.09	126.26	119.32
4	F	351	HIS	C-N-CA	6.09	126.26	119.32
1	Q	13	GLN	CA-C-N	6.07	126.01	119.76
1	Q	13	GLN	C-N-CA	6.07	126.01	119.76
4	F	171	MET	CA-C-N	6.04	126.61	120.38
4	F	171	MET	C-N-CA	6.04	126.61	120.38
3	A	167	SER	N-CA-C	6.04	117.86	111.28
4	E	127	HIS	CA-C-N	6.03	125.79	119.76
4	E	127	HIS	C-N-CA	6.03	125.79	119.76
5	I	209	LYS	CA-C-N	6.03	126.05	119.90
5	I	209	LYS	C-N-CA	6.03	126.05	119.90
4	F	408	VAL	CA-C-N	6.02	125.93	119.85
4	F	408	VAL	C-N-CA	6.02	125.93	119.85
3	C	25	SER	CA-C-N	6.00	126.02	119.90
3	C	25	SER	C-N-CA	6.00	126.02	119.90
3	D	25	SER	CA-C-N	5.99	126.01	119.90
3	D	25	SER	C-N-CA	5.99	126.01	119.90
1	O	195	VAL	CA-C-N	5.97	125.91	119.76
1	O	195	VAL	C-N-CA	5.97	125.91	119.76
4	E	339	TRP	CA-C-N	5.96	126.45	120.14
4	E	339	TRP	C-N-CA	5.96	126.45	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	342	ALA	N-CA-C	5.94	117.55	111.14
3	D	98	ALA	N-CA-C	5.94	117.83	111.36
3	A	402	ILE	N-CA-C	-5.93	99.16	108.95
5	J	203	ILE	CA-C-N	5.93	125.87	119.76
5	J	203	ILE	C-N-CA	5.93	125.87	119.76
4	H	339	TRP	CA-C-N	5.93	126.43	120.14
4	H	339	TRP	C-N-CA	5.93	126.43	120.14
3	C	13	VAL	CA-C-N	5.91	126.40	120.14
3	C	13	VAL	C-N-CA	5.91	126.40	120.14
1	O	212	LYS	CA-C-N	5.90	125.52	119.56
1	O	212	LYS	C-N-CA	5.90	125.52	119.56
3	B	231	VAL	CA-C-N	5.89	126.38	120.14
3	B	231	VAL	C-N-CA	5.89	126.38	120.14
4	G	127	HIS	CA-C-N	5.87	125.63	119.76
4	G	127	HIS	C-N-CA	5.87	125.63	119.76
2	N	141	TYR	CA-C-N	5.86	125.77	119.85
2	N	141	TYR	C-N-CA	5.86	125.77	119.85
3	A	272	ALA	N-CA-C	5.86	118.41	109.62
4	G	351	HIS	CA-C-N	5.84	125.98	119.32
4	G	351	HIS	C-N-CA	5.84	125.98	119.32
4	H	403	THR	CA-C-N	5.83	125.59	119.76
4	H	403	THR	C-N-CA	5.83	125.59	119.76
3	B	13	VAL	CA-C-N	5.83	126.32	120.14
3	B	13	VAL	C-N-CA	5.83	126.32	120.14
3	B	189	TYR	CA-C-N	5.83	126.39	120.38
3	B	189	TYR	C-N-CA	5.83	126.39	120.38
4	G	171	MET	CA-C-N	5.81	126.37	120.38
4	G	171	MET	C-N-CA	5.81	126.37	120.38
2	R	79	GLN	CA-C-N	5.81	126.21	119.47
2	R	79	GLN	C-N-CA	5.81	126.21	119.47
3	D	381	HIS	CA-C-N	5.80	126.36	120.38
3	D	381	HIS	C-N-CA	5.80	126.36	120.38
4	H	351	HIS	CA-C-N	5.79	125.92	119.32
4	H	351	HIS	C-N-CA	5.79	125.92	119.32
3	C	21	ARG	CA-C-N	5.78	126.11	119.93
3	C	21	ARG	C-N-CA	5.78	126.11	119.93
3	D	207	THR	CA-C-N	5.77	126.16	119.47
3	D	207	THR	C-N-CA	5.77	126.16	119.47
1	S	13	GLN	CA-C-N	5.77	125.70	119.76
1	S	13	GLN	C-N-CA	5.77	125.70	119.76
4	F	403	THR	CA-C-N	5.77	125.78	119.90
4	F	403	THR	C-N-CA	5.77	125.78	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	203	ILE	CA-C-N	5.77	125.72	119.78
5	I	203	ILE	C-N-CA	5.77	125.72	119.78
4	F	127	HIS	CA-C-N	5.76	125.52	119.76
4	F	127	HIS	C-N-CA	5.76	125.52	119.76
3	C	381	HIS	CA-C-N	5.76	126.31	120.38
3	C	381	HIS	C-N-CA	5.76	126.31	120.38
3	D	231	VAL	CA-C-N	5.75	126.23	120.14
3	D	231	VAL	C-N-CA	5.75	126.23	120.14
3	B	21	ARG	CA-C-N	5.75	126.08	119.93
3	B	21	ARG	C-N-CA	5.75	126.08	119.93
1	O	13	GLN	CA-C-N	5.75	126.04	119.83
1	O	13	GLN	C-N-CA	5.75	126.04	119.83
4	H	398	THR	CA-C-N	5.74	125.42	119.56
4	H	398	THR	C-N-CA	5.74	125.42	119.56
3	A	198	GLY	N-CA-C	5.74	122.99	115.36
3	A	346	VAL	N-CA-C	5.70	116.08	108.11
4	E	398	THR	CA-C-N	5.69	125.36	119.56
4	E	398	THR	C-N-CA	5.69	125.36	119.56
3	B	381	HIS	CA-C-N	5.68	126.23	120.38
3	B	381	HIS	C-N-CA	5.68	126.23	120.38
3	C	207	THR	CA-C-N	5.67	126.05	119.47
3	C	207	THR	C-N-CA	5.67	126.05	119.47
3	B	396	THR	N-CA-C	5.64	117.97	110.53
4	E	188	VAL	N-CA-C	5.63	115.97	107.80
4	F	89	ALA	CA-C-N	5.63	125.64	119.90
4	F	89	ALA	C-N-CA	5.63	125.64	119.90
4	E	89	ALA	CA-C-N	5.55	125.56	119.90
4	E	89	ALA	C-N-CA	5.55	125.56	119.90
4	H	89	ALA	CA-C-N	5.55	125.56	119.90
4	H	89	ALA	C-N-CA	5.55	125.56	119.90
4	H	127	HIS	CA-C-N	5.54	125.81	119.83
4	H	127	HIS	C-N-CA	5.54	125.81	119.83
3	B	207	THR	CA-C-N	5.49	125.84	119.47
3	B	207	THR	C-N-CA	5.49	125.84	119.47
1	Q	195	VAL	CA-C-N	5.44	125.71	119.83
1	Q	195	VAL	C-N-CA	5.44	125.71	119.83
4	H	421	ALA	CB-CA-C	-5.41	110.32	116.54
3	D	373	GLN	N-CA-C	5.41	118.21	109.40
2	P	39	LYS	CA-C-N	5.39	125.70	119.93
2	P	39	LYS	C-N-CA	5.39	125.70	119.93
3	A	200	PHE	N-CA-C	-5.38	102.44	110.23
1	M	157	PHE	CA-C-N	5.37	125.28	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	157	PHE	C-N-CA	5.37	125.28	119.85
2	P	141	TYR	CA-C-N	5.35	125.27	119.76
2	P	141	TYR	C-N-CA	5.35	125.27	119.76
1	S	195	VAL	CA-C-N	5.35	125.65	119.93
1	S	195	VAL	C-N-CA	5.35	125.65	119.93
3	A	329	ALA	N-CA-C	5.33	117.59	108.90
4	F	251	ARG	CB-CA-C	-5.29	110.04	117.23
3	A	263	THR	N-CA-C	5.26	117.86	109.81
4	F	398	THR	CA-C-N	5.26	125.06	119.28
4	F	398	THR	C-N-CA	5.26	125.06	119.28
5	J	209	LYS	CA-C-N	5.26	125.26	119.90
5	J	209	LYS	C-N-CA	5.26	125.26	119.90
1	M	195	VAL	CA-C-N	5.23	125.48	119.83
1	M	195	VAL	C-N-CA	5.23	125.48	119.83
3	A	273	VAL	CB-CA-C	-5.23	102.70	110.33
1	S	157	PHE	CA-C-N	5.21	125.13	119.76
1	S	157	PHE	C-N-CA	5.21	125.13	119.76
1	Q	157	PHE	CA-C-N	5.21	125.15	119.78
1	Q	157	PHE	C-N-CA	5.21	125.15	119.78
3	A	293	ALA	N-CA-C	5.21	117.26	110.08
4	G	403	THR	CA-C-N	5.20	125.36	119.90
4	G	403	THR	C-N-CA	5.20	125.36	119.90
3	A	322	ALA	N-CA-C	5.15	117.84	109.24
3	A	314	GLY	N-CA-C	5.12	119.07	111.18
3	C	68	CYS	N-CA-C	5.07	117.67	109.40
3	A	223	ARG	N-CA-C	5.07	116.27	109.83
4	G	398	THR	CA-C-N	5.07	124.85	119.28
4	G	398	THR	C-N-CA	5.07	124.85	119.28
3	B	404	ALA	N-CA-C	5.05	116.84	110.33
2	R	39	LYS	CA-C-N	5.01	125.29	119.93
2	R	39	LYS	C-N-CA	5.01	125.29	119.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1671	0	1610	7	0
1	O	1671	0	1610	13	0
1	Q	1671	0	1610	8	0
1	S	1671	0	1610	7	0
2	N	1631	0	1598	5	0
2	P	1631	0	1598	5	0
2	R	1631	0	1598	4	0
2	T	1631	0	1598	1	0
3	A	3325	0	3253	26	0
3	B	3325	0	3253	11	0
3	C	3325	0	3252	19	0
3	D	3325	0	3253	13	0
4	E	3282	0	3221	13	0
4	F	3282	0	3222	48	0
4	G	3282	0	3222	40	0
4	H	3263	0	3207	36	0
5	I	1156	0	1133	7	0
5	J	1156	0	1135	7	0
5	K	1156	0	1135	1	0
5	L	1156	0	1135	7	0
6	U	71	0	61	0	0
7	V	49	0	43	0	0
8	W	38	0	34	0	0
9	X	49	0	43	0	0
10	Y	29	0	26	1	0
11	C	28	0	41	48	0
11	D	28	0	40	37	0
11	E	28	0	46	9	0
11	F	28	0	46	44	0
All	All	44589	0	43633	280	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 3.

All (280) 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)
11:D:501:CLR:H151	4:H:359:TYR:CD2	1.26	1.62
4:F:359:TYR:CD2	11:F:501:CLR:H151	1.37	1.58
4:F:359:TYR:CG	11:F:501:CLR:H151	1.03	1.54
4:F:359:TYR:CG	11:F:501:CLR:C15	1.91	1.51
11:D:501:CLR:C15	4:H:359:TYR:CD2	1.98	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:501:CLR:C16	4:H:359:TYR:CG	2.12	1.30
4:F:359:TYR:CD1	11:F:501:CLR:C15	2.16	1.29
11:D:501:CLR:H161	4:H:359:TYR:CG	1.69	1.25
11:D:501:CLR:C15	4:H:359:TYR:CG	2.21	1.24
11:D:501:CLR:H151	4:H:359:TYR:CG	1.74	1.22
4:F:359:TYR:CD1	11:F:501:CLR:H151	1.74	1.22
4:F:359:TYR:CD1	11:F:501:CLR:C16	2.21	1.22
3:C:400:GLN:OE1	11:C:501:CLR:C6	1.89	1.20
11:D:501:CLR:H161	4:H:359:TYR:CB	1.71	1.20
4:F:366:MET:HG3	11:F:501:CLR:H21	1.19	1.19
3:C:400:GLN:OE1	11:C:501:CLR:H6	1.42	1.18
3:D:399:VAL:CG2	11:D:501:CLR:H111	1.74	1.17
3:C:400:GLN:HA	11:C:501:CLR:H151	1.18	1.16
11:C:501:CLR:C19	4:G:366:MET:HG2	1.77	1.14
3:D:399:VAL:HG23	11:D:501:CLR:H111	1.19	1.13
3:C:398:GLY:O	11:C:501:CLR:H12	1.47	1.12
11:C:501:CLR:H192	4:G:366:MET:SD	1.91	1.10
11:C:501:CLR:C19	4:G:366:MET:CG	2.30	1.09
11:C:501:CLR:H191	4:G:366:MET:CG	1.81	1.09
3:C:400:GLN:HA	11:C:501:CLR:C15	1.83	1.08
3:C:399:VAL:HA	11:C:501:CLR:C6	1.78	1.07
11:C:501:CLR:H191	4:G:366:MET:HG2	1.11	1.06
11:D:501:CLR:C16	4:H:359:TYR:CD1	2.39	1.05
4:F:359:TYR:CD2	11:F:501:CLR:C15	2.24	1.02
11:C:501:CLR:C19	4:G:366:MET:SD	2.49	1.01
4:F:366:MET:HG3	11:F:501:CLR:C2	1.92	1.00
4:F:366:MET:CG	11:F:501:CLR:H21	1.92	0.99
4:F:359:TYR:CD1	11:F:501:CLR:H161	1.98	0.97
11:C:501:CLR:H42	4:G:366:MET:HE2	1.45	0.96
11:C:501:CLR:H192	4:G:366:MET:CE	1.95	0.96
3:D:399:VAL:HG23	11:D:501:CLR:C11	1.86	0.94
11:D:501:CLR:H151	4:H:359:TYR:HD2	1.21	0.93
11:C:501:CLR:H192	4:G:366:MET:HE2	1.50	0.93
11:D:501:CLR:H12	4:H:366:MET:CB	2.01	0.89
11:D:501:CLR:H162	4:H:359:TYR:CD1	2.07	0.89
11:D:501:CLR:H161	4:H:359:TYR:CD1	2.04	0.87
3:B:296:LEU:HB2	3:B:372:THR:HG21	1.55	0.87
3:C:399:VAL:CA	11:C:501:CLR:C6	2.53	0.86
11:D:501:CLR:H12	4:H:366:MET:HB2	1.57	0.86
11:D:501:CLR:H152	4:H:359:TYR:CD2	2.10	0.83
4:F:359:TYR:CG	11:F:501:CLR:C16	2.52	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:359:TYR:CE2	11:F:501:CLR:H72	2.13	0.83
11:D:501:CLR:C16	4:H:359:TYR:CB	2.51	0.82
4:F:366:MET:HB3	11:F:501:CLR:C1	2.10	0.82
3:A:360:LEU:HD21	3:A:401:ASP:HB3	1.61	0.82
3:A:312:PHE:HA	3:A:357:SER:HB3	1.62	0.81
11:C:501:CLR:H112	4:G:363:TYR:CG	2.15	0.81
4:F:366:MET:CB	11:F:501:CLR:H12	2.10	0.81
4:F:359:TYR:CE1	11:F:501:CLR:C15	2.64	0.81
11:D:501:CLR:H161	4:H:359:TYR:HB2	1.61	0.79
4:F:359:TYR:CE2	11:F:501:CLR:H151	2.14	0.79
5:I:178:PHE:HB2	5:I:245:TRP:CZ3	2.19	0.77
3:A:110:LYS:HG2	3:A:203:ILE:HD11	1.66	0.76
3:C:400:GLN:CA	11:C:501:CLR:H151	2.08	0.76
4:F:366:MET:CB	11:F:501:CLR:C1	2.65	0.75
4:F:366:MET:HB3	11:F:501:CLR:H11	1.67	0.75
11:D:501:CLR:C15	4:H:359:TYR:CE2	2.68	0.75
11:D:501:CLR:C1	4:H:366:MET:CB	2.64	0.75
3:B:360:LEU:HD23	3:B:397:LEU:HD21	1.69	0.75
4:F:359:TYR:CE2	11:F:501:CLR:C15	2.71	0.74
4:F:359:TYR:CD2	11:F:501:CLR:H72	2.23	0.74
4:F:359:TYR:CB	11:F:501:CLR:H151	2.12	0.73
3:C:400:GLN:CD	11:C:501:CLR:C6	2.64	0.71
11:D:501:CLR:H152	4:H:359:TYR:CE2	2.25	0.71
11:D:501:CLR:H71	4:H:363:TYR:CD2	2.27	0.70
1:O:211:HIS:HD1	1:O:214:SER:HG	1.37	0.70
4:F:359:TYR:CG	11:F:501:CLR:H161	2.25	0.69
3:A:177:ILE:HG23	3:A:184:VAL:HG13	1.74	0.68
3:A:51:TYR:HB3	3:A:203:ILE:HG21	1.76	0.68
4:F:366:MET:HB2	11:F:501:CLR:H12	1.76	0.66
4:F:359:TYR:CD2	11:F:501:CLR:C7	2.78	0.66
4:F:359:TYR:CD1	11:F:501:CLR:H162	2.27	0.66
11:C:501:CLR:C4	4:G:366:MET:HE2	2.25	0.64
3:D:399:VAL:CG2	11:D:501:CLR:C11	2.59	0.64
1:S:31:ASP:OD1	3:D:69:LYS:NZ	2.31	0.64
11:D:501:CLR:C1	4:H:366:MET:HB3	2.29	0.63
11:D:501:CLR:H11	4:H:366:MET:HB3	1.80	0.63
4:F:359:TYR:CE1	11:F:501:CLR:H152	2.33	0.62
4:F:359:TYR:CZ	11:F:501:CLR:H152	2.35	0.62
4:F:359:TYR:CB	11:F:501:CLR:C15	2.75	0.61
4:F:359:TYR:CB	11:F:501:CLR:H161	2.30	0.61
11:C:501:CLR:H192	4:G:366:MET:HG2	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:501:CLR:H151	4:H:359:TYR:CB	2.30	0.60
11:C:501:CLR:H112	4:G:363:TYR:CD2	2.36	0.60
5:I:178:PHE:HB2	5:I:245:TRP:HZ3	1.62	0.60
11:C:501:CLR:H191	4:G:366:MET:CB	2.32	0.60
4:F:359:TYR:HB2	11:F:501:CLR:H161	1.83	0.59
11:C:501:CLR:H25	4:G:356:ILE:CD1	2.33	0.59
11:C:501:CLR:H192	4:G:366:MET:CG	2.19	0.59
3:C:398:GLY:O	11:C:501:CLR:C1	2.38	0.58
11:C:501:CLR:H232	4:G:359:TYR:CD1	2.38	0.58
1:O:159:GLU:N	1:O:160:PRO:CD	2.68	0.56
3:A:399:VAL:HA	11:E:501:CLR:H12	1.88	0.56
11:C:501:CLR:C27	4:G:355:ILE:HG22	2.35	0.56
4:F:359:TYR:CZ	11:F:501:CLR:C15	2.88	0.56
1:M:159:GLU:N	1:M:160:PRO:CD	2.69	0.56
11:C:501:CLR:H271	4:G:355:ILE:HG22	1.88	0.55
1:Q:159:GLU:N	1:Q:160:PRO:CD	2.69	0.55
1:Q:212:LYS:N	1:Q:213:PRO:CD	2.70	0.55
1:S:212:LYS:N	1:S:213:PRO:CD	2.69	0.54
2:R:141:TYR:HB3	2:R:142:PRO:HD3	1.88	0.54
1:O:211:HIS:CE1	1:O:214:SER:HG	2.25	0.54
1:S:159:GLU:N	1:S:160:PRO:CD	2.71	0.54
1:M:212:LYS:N	1:M:213:PRO:CD	2.70	0.54
4:F:210:LEU:O	2:P:68:GLY:N	2.41	0.54
11:D:501:CLR:H161	4:H:359:TYR:HB3	1.79	0.54
4:G:191:THR:HA	4:G:214:ASP:OD1	2.08	0.54
4:F:359:TYR:HD1	11:F:501:CLR:H161	1.66	0.54
11:D:501:CLR:C15	4:H:359:TYR:CB	2.79	0.54
3:B:435:SER:O	5:J:159:LYS:NZ	2.41	0.53
3:A:328:CYS:SG	3:A:369:VAL:HG12	2.49	0.53
3:D:99:GLU:O	3:D:101:THR:HG23	2.10	0.52
3:B:397:LEU:HD22	3:B:402:ILE:HD12	1.92	0.52
3:A:144:VAL:HG11	3:A:156:VAL:HG22	1.92	0.52
11:C:501:CLR:H22	4:G:366:MET:HE2	1.92	0.51
3:C:398:GLY:O	11:C:501:CLR:H9	2.11	0.51
2:P:141:TYR:HB2	2:P:142:PRO:HD3	1.93	0.51
4:F:366:MET:CG	11:F:501:CLR:C2	2.71	0.51
3:C:400:GLN:HA	11:C:501:CLR:H152	1.88	0.51
4:E:366:MET:HB3	11:E:501:CLR:H6	1.92	0.51
4:F:366:MET:SD	11:F:501:CLR:H21	2.50	0.51
4:G:180:LEU:O	4:G:191:THR:HG22	2.10	0.51
2:T:141:TYR:HB3	2:T:142:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:302:GLU:OE2	3:C:319:LYS:NZ	2.44	0.50
11:D:501:CLR:C16	4:H:359:TYR:HB3	2.37	0.50
4:E:363:TYR:CD2	11:E:501:CLR:H192	2.46	0.50
4:F:211:THR:OG1	4:F:213:THR:O	2.29	0.50
3:A:49:CYS:SG	3:A:50:GLU:N	2.85	0.50
3:C:400:GLN:OE1	11:C:501:CLR:C7	2.59	0.50
3:D:399:VAL:HG21	11:D:501:CLR:H111	1.82	0.50
3:D:202:ASP:N	3:D:202:ASP:OD1	2.43	0.49
4:F:359:TYR:CE2	11:F:501:CLR:H152	2.43	0.49
11:D:501:CLR:C15	4:H:359:TYR:HB3	2.42	0.49
4:H:192:VAL:HG12	4:H:194:GLY:H	1.78	0.49
3:C:398:GLY:C	11:C:501:CLR:H9	2.38	0.49
3:A:225:ALA:HB2	4:G:147:HIS:CD2	2.48	0.48
11:C:501:CLR:C11	4:G:363:TYR:CG	2.93	0.48
4:H:403:THR:OG1	5:L:250:VAL:N	2.46	0.48
4:F:398:THR:N	4:F:399:PRO:CD	2.75	0.48
3:C:84:VAL:O	3:C:100:ASN:ND2	2.46	0.48
1:O:157:PHE:N	1:O:158:PRO:CD	2.76	0.48
3:A:185:TYR:OH	3:A:247:ARG:HD2	2.13	0.48
11:C:501:CLR:H22	4:G:366:MET:CE	2.44	0.48
4:F:359:TYR:CB	11:F:501:CLR:C16	2.90	0.48
11:C:501:CLR:H222	11:C:501:CLR:H162	1.77	0.48
11:C:501:CLR:H272	4:G:359:TYR:CD1	2.48	0.48
4:H:398:THR:N	4:H:399:PRO:CD	2.77	0.47
4:E:398:THR:N	4:E:399:PRO:CD	2.77	0.47
5:L:161:ASP:OD2	5:L:252:LYS:NZ	2.45	0.47
3:B:400:GLN:HA	11:F:501:CLR:C19	2.44	0.47
3:A:183:ASP:HB2	3:A:250:SER:HB2	1.96	0.47
3:C:399:VAL:HA	11:C:501:CLR:C5	2.37	0.47
11:C:501:CLR:H25	4:G:356:ILE:HD13	1.96	0.47
1:O:159:GLU:N	1:O:160:PRO:HD2	2.28	0.47
2:N:141:TYR:N	2:N:142:PRO:CD	2.77	0.47
11:C:501:CLR:H193	4:G:366:MET:SD	2.49	0.47
2:P:141:TYR:CB	2:P:142:PRO:HD3	2.45	0.47
5:L:119:HIS:CG	5:L:120:GLU:H	2.32	0.46
1:S:34:MET:HB3	1:S:79:LEU:HD22	1.97	0.46
5:L:119:HIS:CG	5:L:120:GLU:N	2.84	0.46
2:P:104:LYS:NZ	2:P:166:GLU:OE1	2.48	0.46
1:O:73:ASP:OD2	1:O:76:LYS:NZ	2.42	0.46
11:C:501:CLR:C12	4:G:363:TYR:CD2	2.98	0.46
1:O:212:LYS:HB3	1:O:213:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:TYR:CD1	3:C:51:TYR:C	2.94	0.45
1:O:29:PHE:O	1:O:72:ARG:NH2	2.49	0.45
4:E:157:VAL:HG12	4:E:159:SER:H	1.81	0.45
5:L:119:HIS:ND1	5:L:120:GLU:N	2.64	0.45
3:A:225:ALA:HB2	4:G:147:HIS:HD2	1.81	0.45
4:G:201:CYS:HB3	4:G:225:CYS:HA	1.98	0.45
4:G:398:THR:N	4:G:399:PRO:CD	2.79	0.45
4:E:370:VAL:HG21	11:E:501:CLR:H71	1.98	0.45
1:S:157:PHE:HB3	1:S:158:PRO:HD3	1.99	0.45
4:E:182:SER:HB3	4:E:189:LYS:HB2	1.98	0.45
2:R:94:THR:O	2:R:97:ARG:NH1	2.50	0.45
4:G:69:TYR:OH	4:G:117:ASP:OD1	2.22	0.45
11:D:501:CLR:H232	11:D:501:CLR:H211	1.63	0.45
4:H:201:CYS:HB3	4:H:225:CYS:HA	1.99	0.44
3:D:402:ILE:HG21	11:D:501:CLR:H6	1.98	0.44
11:F:501:CLR:H232	11:F:501:CLR:H211	1.63	0.44
1:M:157:PHE:HB3	1:M:158:PRO:HD3	1.99	0.44
11:C:501:CLR:H183	11:C:501:CLR:H20	1.86	0.44
11:E:501:CLR:H222	11:E:501:CLR:H162	1.62	0.44
11:D:501:CLR:H183	11:D:501:CLR:H20	1.81	0.44
5:J:182:LYS:NZ	5:J:245:TRP:O	2.50	0.44
11:C:501:CLR:H272	4:G:359:TYR:HD1	1.82	0.44
1:Q:157:PHE:HB3	1:Q:158:PRO:HD3	2.00	0.44
2:N:135:CYS:SG	2:N:149:TRP:CH2	3.11	0.44
3:C:202:ASP:OD1	3:C:202:ASP:N	2.48	0.44
4:E:348:ALA:C	4:E:349:HIS:CG	2.95	0.44
4:F:157:VAL:HG12	4:F:159:SER:H	1.83	0.44
4:E:359:TYR:CD2	11:E:501:CLR:H193	2.52	0.44
5:J:136:LYS:NZ	5:J:163:GLU:OE1	2.39	0.44
5:J:161:ASP:OD2	5:J:252:LYS:NZ	2.48	0.44
5:I:178:PHE:HB2	5:I:245:TRP:CH2	2.53	0.44
3:B:52:LYS:NZ	4:F:165:GLU:OE2	2.51	0.44
4:G:109:GLU:N	4:G:109:GLU:OE1	2.50	0.44
3:D:52:LYS:NZ	4:H:165:GLU:OE2	2.50	0.43
4:F:356:ILE:HD13	11:F:501:CLR:H221	2.00	0.43
3:A:51:TYR:CD1	3:A:51:TYR:C	2.96	0.43
3:B:190:PRO:HA	3:B:191:PRO:HD3	1.83	0.43
4:H:188:VAL:HG13	4:H:222:VAL:HG12	1.98	0.43
1:Q:157:PHE:N	1:Q:158:PRO:CD	2.81	0.43
5:J:116:GLU:OE1	5:J:116:GLU:N	2.50	0.43
2:R:120:PRO:HA	2:R:121:PRO:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:117:ASP:OD1	4:E:117:ASP:C	2.59	0.43
1:M:145:GLY:O	1:M:146:THR:HB	2.19	0.43
2:R:9:SER:OG	2:R:10:SER:N	2.51	0.43
3:A:180:TYR:CG	3:A:181:LYS:N	2.84	0.43
3:D:84:VAL:O	3:D:100:ASN:HB3	2.18	0.43
3:B:402:ILE:H	3:B:402:ILE:HG12	1.55	0.43
1:O:157:PHE:HB3	1:O:158:PRO:HD3	2.01	0.43
1:S:157:PHE:N	1:S:158:PRO:CD	2.82	0.43
4:F:359:TYR:HB3	11:F:501:CLR:H14	2.00	0.43
3:A:339:ILE:HD11	3:A:367:VAL:HG22	2.00	0.42
4:E:187:ASN:OD1	4:E:219:ASN:N	2.52	0.42
11:E:501:CLR:H8	11:E:501:CLR:H182	1.83	0.42
2:N:94:THR:O	2:N:97:ARG:NH1	2.52	0.42
3:A:257:PHE:CZ	4:E:302:GLU:HG3	2.54	0.42
4:E:370:VAL:CG1	11:E:501:CLR:H151	2.49	0.42
3:D:51:TYR:CD1	3:D:51:TYR:C	2.97	0.42
4:F:359:TYR:CD2	11:F:501:CLR:C14	3.01	0.42
4:H:10:LYS:O	4:H:234:LYS:NZ	2.51	0.42
5:I:161:ASP:OD2	5:I:252:LYS:NZ	2.47	0.42
5:K:189:TRP:CD1	5:K:194:VAL:HG23	2.53	0.42
1:M:159:GLU:N	1:M:160:PRO:HD2	2.34	0.42
5:I:128:CYS:SG	5:I:129:LEU:N	2.93	0.42
3:A:31:MET:HG2	3:A:135:VAL:HG22	2.01	0.42
3:A:337:VAL:HG21	3:A:365:PHE:HB3	2.00	0.42
11:C:501:CLR:H121	4:G:363:TYR:CD2	2.55	0.42
4:E:191:THR:HA	4:E:214:ASP:OD1	2.20	0.42
4:G:192:VAL:HG12	4:G:194:GLY:H	1.84	0.42
5:I:206:GLY:O	5:I:209:LYS:NZ	2.53	0.42
5:J:219:ASP:OD1	5:J:219:ASP:C	2.63	0.42
3:A:156:VAL:O	3:A:157:LYS:C	2.62	0.42
1:O:62:ASP:OD1	1:O:62:ASP:N	2.51	0.42
4:H:105:CYS:HA	4:H:106:PRO:HD3	1.91	0.42
5:I:189:TRP:NE1	5:I:191:HIS:O	2.52	0.42
5:L:145:ASP:OD1	5:L:146:ASN:N	2.53	0.42
11:D:501:CLR:H71	4:H:363:TYR:CG	2.55	0.41
2:N:141:TYR:HB2	2:N:142:PRO:HD3	2.03	0.41
2:N:9:SER:OG	2:N:10:SER:N	2.50	0.41
5:J:189:TRP:CD1	5:J:194:VAL:HG23	2.55	0.41
1:O:212:LYS:N	1:O:213:PRO:HD2	2.36	0.41
1:M:157:PHE:N	1:M:158:PRO:CD	2.83	0.41
3:B:202:ASP:OD1	3:B:202:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:366:MET:CG	11:F:501:CLR:C1	2.98	0.41
4:G:242:VAL:HA	4:G:243:PRO:HD3	1.91	0.41
1:O:13:GLN:HA	1:O:14:PRO:HD3	1.94	0.41
3:A:403:SER:O	3:A:406:ALA:HB3	2.20	0.41
11:C:501:CLR:C11	4:G:363:TYR:CD2	3.03	0.41
11:C:501:CLR:H193	11:C:501:CLR:H111	1.80	0.41
1:M:212:LYS:HB3	1:M:213:PRO:HD3	2.02	0.41
1:S:6:GLU:OE1	1:S:6:GLU:N	2.54	0.41
3:A:177:ILE:CG2	3:A:184:VAL:HG13	2.47	0.41
3:A:320:TYR:CD2	3:A:352:LEU:HD23	2.56	0.41
11:D:501:CLR:H232	11:D:501:CLR:H272	1.84	0.41
11:E:501:CLR:H211	11:E:501:CLR:H232	1.78	0.41
4:F:359:TYR:CD2	11:F:501:CLR:H71	2.55	0.41
5:L:136:LYS:HA	5:L:137:PRO:HD3	1.94	0.41
1:Q:145:GLY:O	1:Q:146:THR:HB	2.21	0.41
1:Q:159:GLU:N	1:Q:160:PRO:HD2	2.36	0.41
1:Q:212:LYS:HB2	1:Q:213:PRO:HD3	2.02	0.41
1:O:52:SER:OG	1:O:57:SER:N	2.52	0.41
3:D:39:GLU:HA	3:D:40:PRO:HD2	1.94	0.41
2:P:7:SER:HA	2:P:8:PRO:HD3	1.89	0.41
11:C:501:CLR:H232	11:C:501:CLR:H272	1.83	0.40
4:F:303:GLU:HA	4:F:304:PRO:HD2	1.95	0.40
3:A:118:PHE:HZ	10:Y:2:NAG:H2	1.86	0.40
3:B:7:ILE:HA	3:B:8:PRO:HD3	1.93	0.40
3:B:51:TYR:CD1	3:B:51:TYR:C	2.99	0.40
4:G:192:VAL:HG13	4:G:195:GLN:O	2.21	0.40
1:Q:13:GLN:OE1	1:Q:13:GLN:N	2.52	0.40
3:A:397:LEU:HD22	3:A:397:LEU:HA	1.78	0.40
3:A:406:ALA:O	3:A:410:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	222/264 (84%)	220 (99%)	2 (1%)	0	100	100
1	O	222/264 (84%)	219 (99%)	3 (1%)	0	100	100
1	Q	222/264 (84%)	220 (99%)	2 (1%)	0	100	100
1	S	222/264 (84%)	220 (99%)	2 (1%)	0	100	100
2	N	209/241 (87%)	206 (99%)	3 (1%)	0	100	100
2	P	209/241 (87%)	206 (99%)	3 (1%)	0	100	100
2	R	209/241 (87%)	206 (99%)	3 (1%)	0	100	100
2	T	209/241 (87%)	206 (99%)	3 (1%)	0	100	100
3	A	437/439 (100%)	430 (98%)	7 (2%)	0	100	100
3	B	437/439 (100%)	431 (99%)	5 (1%)	1 (0%)	44	72
3	C	437/439 (100%)	430 (98%)	7 (2%)	0	100	100
3	D	437/439 (100%)	431 (99%)	6 (1%)	0	100	100
4	E	417/419 (100%)	408 (98%)	9 (2%)	0	100	100
4	F	417/419 (100%)	410 (98%)	7 (2%)	0	100	100
4	G	417/419 (100%)	406 (97%)	11 (3%)	0	100	100
4	H	415/419 (99%)	409 (99%)	6 (1%)	0	100	100
5	I	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
5	J	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
5	K	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	19	51
5	L	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
All	All	5734/6056 (95%)	5646 (98%)	86 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	369	VAL
5	K	144	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	185/223 (83%)	185 (100%)	0	100	100
1	O	185/223 (83%)	184 (100%)	1 (0%)	86	92
1	Q	185/223 (83%)	184 (100%)	1 (0%)	86	92
1	S	185/223 (83%)	185 (100%)	0	100	100
2	N	187/213 (88%)	187 (100%)	0	100	100
2	P	187/213 (88%)	187 (100%)	0	100	100
2	R	187/213 (88%)	187 (100%)	0	100	100
2	T	187/213 (88%)	187 (100%)	0	100	100
3	A	366/366 (100%)	345 (94%)	21 (6%)	17	45
3	B	366/366 (100%)	362 (99%)	4 (1%)	70	80
3	C	366/366 (100%)	365 (100%)	1 (0%)	91	94
3	D	366/366 (100%)	363 (99%)	3 (1%)	79	85
4	E	369/369 (100%)	367 (100%)	2 (0%)	86	92
4	F	369/369 (100%)	369 (100%)	0	100	100
4	G	369/369 (100%)	368 (100%)	1 (0%)	91	94
4	H	367/369 (100%)	363 (99%)	4 (1%)	70	80
5	I	120/120 (100%)	120 (100%)	0	100	100
5	J	120/120 (100%)	120 (100%)	0	100	100
5	K	120/120 (100%)	120 (100%)	0	100	100
5	L	120/120 (100%)	120 (100%)	0	100	100
All	All	4906/5164 (95%)	4868 (99%)	38 (1%)	77	85

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	144	VAL
3	A	154	VAL
3	A	163	VAL
3	A	171	THR
3	A	183	ASP
3	A	203	ILE
3	A	207	THR
3	A	228	THR
3	A	229	VAL
3	A	231	VAL
3	A	290	VAL

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Mol	Chain	Res	Type
3	A	330	VAL
3	A	349	ASN
3	A	355	SER
3	A	360	LEU
3	A	364	GLU
3	A	369	VAL
3	A	372	THR
3	A	374	VAL
3	A	385	ASP
3	A	397	LEU
3	B	372	THR
3	B	397	LEU
3	B	400	GLN
3	B	402	ILE
3	C	78	CYS
3	D	99	GLU
3	D	369	VAL
3	D	372	THR
4	E	188	VAL
4	E	190	ILE
4	G	220	CYS
4	H	190	ILE
4	H	191	THR
4	H	195	GLN
4	H	201	CYS
1	Q	189	LEU
1	O	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	77	ASN
3	A	275	ASN
3	A	375	HIS
3	A	439	HIS
3	B	138	GLN
3	B	349	ASN
3	B	400	GLN
3	D	308	HIS
3	D	349	ASN
4	E	29	HIS
4	E	146	GLN

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Mol	Chain	Res	Type
4	E	184	GLN
4	E	333	ASN
4	F	146	GLN
4	F	184	GLN
4	F	187	ASN
4	G	29	HIS
4	G	184	GLN
4	G	218	ASN
4	H	184	GLN
1	Q	210	ASN
1	O	13	GLN
1	O	74	ASN
1	O	77	ASN
2	P	37	GLN
2	P	79	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 ⓘ

19 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	U	1	3,6	14,14,15	0.36	0	17,19,21	1.35	2 (11%)
6	NAG	U	2	6	14,14,15	0.33	0	17,19,21	0.76	0
6	MAN	U	3	6	11,11,12	0.35	0	15,15,17	1.81	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	U	4	6	11,11,12	0.25	0	15,15,17	0.60	0
6	BMA	U	5	6	11,11,12	0.27	0	15,15,17	0.79	0
6	FUC	U	6	6	10,10,11	0.33	0	14,14,16	0.94	1 (7%)
7	NAG	V	1	7,3	14,14,15	0.37	0	17,19,21	0.79	1 (5%)
7	NAG	V	2	7	14,14,15	0.31	0	17,19,21	0.64	0
7	MAN	V	3	7	11,11,12	0.18	0	15,15,17	0.70	0
7	FUC	V	4	7	10,10,11	0.23	0	14,14,16	0.69	0
8	NAG	W	1	8,3	14,14,15	0.47	0	17,19,21	1.96	4 (23%)
8	NAG	W	2	8	14,14,15	0.27	0	17,19,21	0.74	0
8	FUC	W	3	8	10,10,11	0.27	0	14,14,16	0.86	1 (7%)
9	NAG	X	1	3,9	14,14,15	0.45	0	17,19,21	2.05	5 (29%)
9	NAG	X	2	9	14,14,15	0.34	0	17,19,21	1.55	3 (17%)
9	BMA	X	3	9	11,11,12	0.25	0	15,15,17	0.67	0
9	FUC	X	4	9	10,10,11	0.26	0	14,14,16	0.76	1 (7%)
10	NAG	Y	1	10,4	14,14,15	0.65	0	17,19,21	1.79	4 (23%)
10	NAG	Y	2	10	15,15,15	0.41	0	21,21,21	1.00	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	U	1	3,6	1/1/5/7	6/6/23/26	0/1/1/1
6	NAG	U	2	6	1/1/5/7	2/6/23/26	0/1/1/1
6	MAN	U	3	6	1/1/4/5	1/2/19/22	0/1/1/1
6	MAN	U	4	6	-	0/2/19/22	1/1/1/1
6	BMA	U	5	6	-	0/2/19/22	0/1/1/1
6	FUC	U	6	6	-	-	0/1/1/1
7	NAG	V	1	7,3	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	V	2	7	-	5/6/23/26	0/1/1/1
7	MAN	V	3	7	-	0/2/19/22	1/1/1/1
7	FUC	V	4	7	1/1/4/5	-	0/1/1/1
8	NAG	W	1	8,3	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	1/1/5/7	2/6/23/26	0/1/1/1
8	FUC	W	3	8	-	-	0/1/1/1
9	NAG	X	1	3,9	-	4/6/23/26	0/1/1/1
9	NAG	X	2	9	1/1/5/7	0/6/23/26	0/1/1/1
9	BMA	X	3	9	1/1/4/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FUC	X	4	9	-	-	0/1/1/1
10	NAG	Y	1	10,4	1/1/5/7	4/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	X	1	NAG	O5-C1-C2	-5.27	102.97	111.29
6	U	3	MAN	O5-C1-C2	5.04	118.56	110.77
8	W	1	NAG	C1-O5-C5	5.00	118.97	112.19
8	W	1	NAG	C2-N2-C7	-4.67	116.25	122.90
10	Y	1	NAG	C4-C3-C2	-3.80	105.46	111.02
9	X	2	NAG	C1-O5-C5	3.73	117.25	112.19
9	X	1	NAG	C2-N2-C7	-3.56	117.83	122.90
10	Y	1	NAG	O4-C4-C3	3.52	118.50	110.35
6	U	1	NAG	C1-O5-C5	3.31	116.68	112.19
9	X	2	NAG	O5-C1-C2	3.22	116.38	111.29
9	X	2	NAG	C3-C4-C5	-3.09	104.73	110.24
6	U	3	MAN	O5-C5-C6	2.98	111.88	107.20
9	X	1	NAG	C1-O5-C5	2.80	115.99	112.19
10	Y	1	NAG	C3-C4-C5	-2.75	105.33	110.24
9	X	1	NAG	C6-C5-C4	-2.67	106.75	113.00
6	U	1	NAG	C4-C3-C2	2.63	114.88	111.02
6	U	6	FUC	O5-C1-C2	-2.51	106.90	110.77
8	W	1	NAG	C6-C5-C4	-2.49	107.17	113.00
10	Y	1	NAG	C1-C2-N2	2.45	114.68	110.49
9	X	1	NAG	C4-C3-C2	-2.44	107.44	111.02
10	Y	2	NAG	O1-C1-C2	-2.44	104.15	109.22
6	U	3	MAN	C3-C4-C5	-2.41	105.94	110.24
8	W	1	NAG	C3-C4-C5	2.27	114.28	110.24
8	W	3	FUC	O5-C1-C2	-2.20	107.38	110.77
7	V	1	NAG	O5-C5-C6	2.12	110.52	107.20
9	X	4	FUC	C1-C2-C3	2.10	112.25	109.67

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	U	1	NAG	C1
6	U	2	NAG	C1
6	U	3	MAN	C1

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Mol	Chain	Res	Type	Atom
7	V	1	NAG	C1
7	V	4	FUC	C1
8	W	2	NAG	C1
9	X	2	NAG	C1
9	X	3	BMA	C1
10	Y	1	NAG	C1

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	1	NAG	C1-C2-N2-C7
6	U	1	NAG	C8-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
7	V	1	NAG	C8-C7-N2-C2
7	V	1	NAG	O7-C7-N2-C2
8	W	1	NAG	C8-C7-N2-C2
8	W	1	NAG	O7-C7-N2-C2
8	W	2	NAG	C8-C7-N2-C2
8	W	2	NAG	O7-C7-N2-C2
10	Y	1	NAG	C3-C2-N2-C7
10	Y	1	NAG	C8-C7-N2-C2
10	Y	1	NAG	O7-C7-N2-C2
10	Y	2	NAG	C8-C7-N2-C2
10	Y	2	NAG	O7-C7-N2-C2
7	V	2	NAG	C1-C2-N2-C7
7	V	2	NAG	C8-C7-N2-C2
9	X	1	NAG	C8-C7-N2-C2
6	U	1	NAG	O5-C5-C6-O6
9	X	1	NAG	C4-C5-C6-O6
7	V	2	NAG	O7-C7-N2-C2
9	X	1	NAG	O7-C7-N2-C2
9	X	1	NAG	O5-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
6	U	1	NAG	C3-C2-N2-C7
7	V	2	NAG	C3-C2-N2-C7
6	U	3	MAN	C4-C5-C6-O6
10	Y	1	NAG	C4-C5-C6-O6

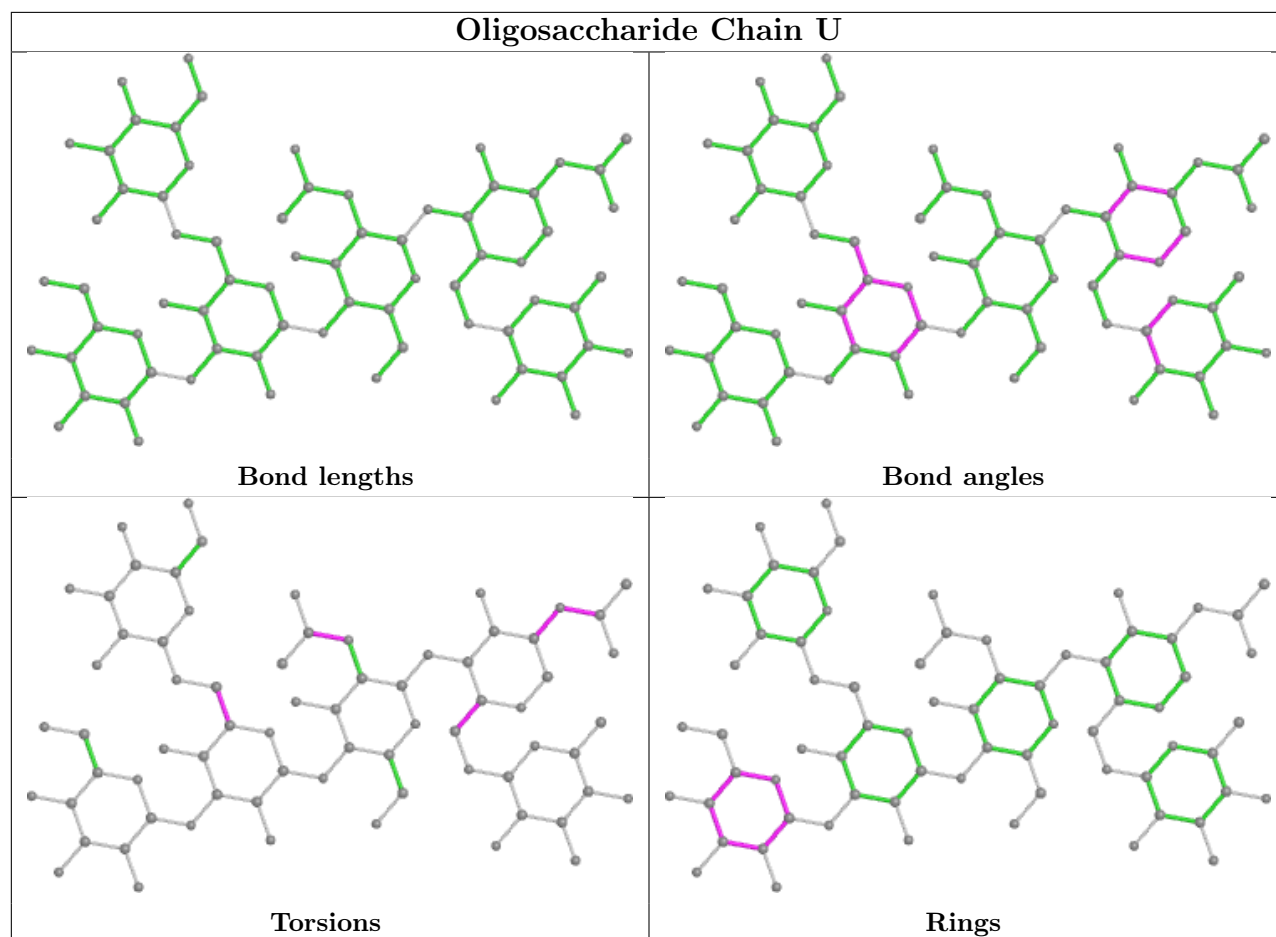
All (2) ring outliers are listed below:

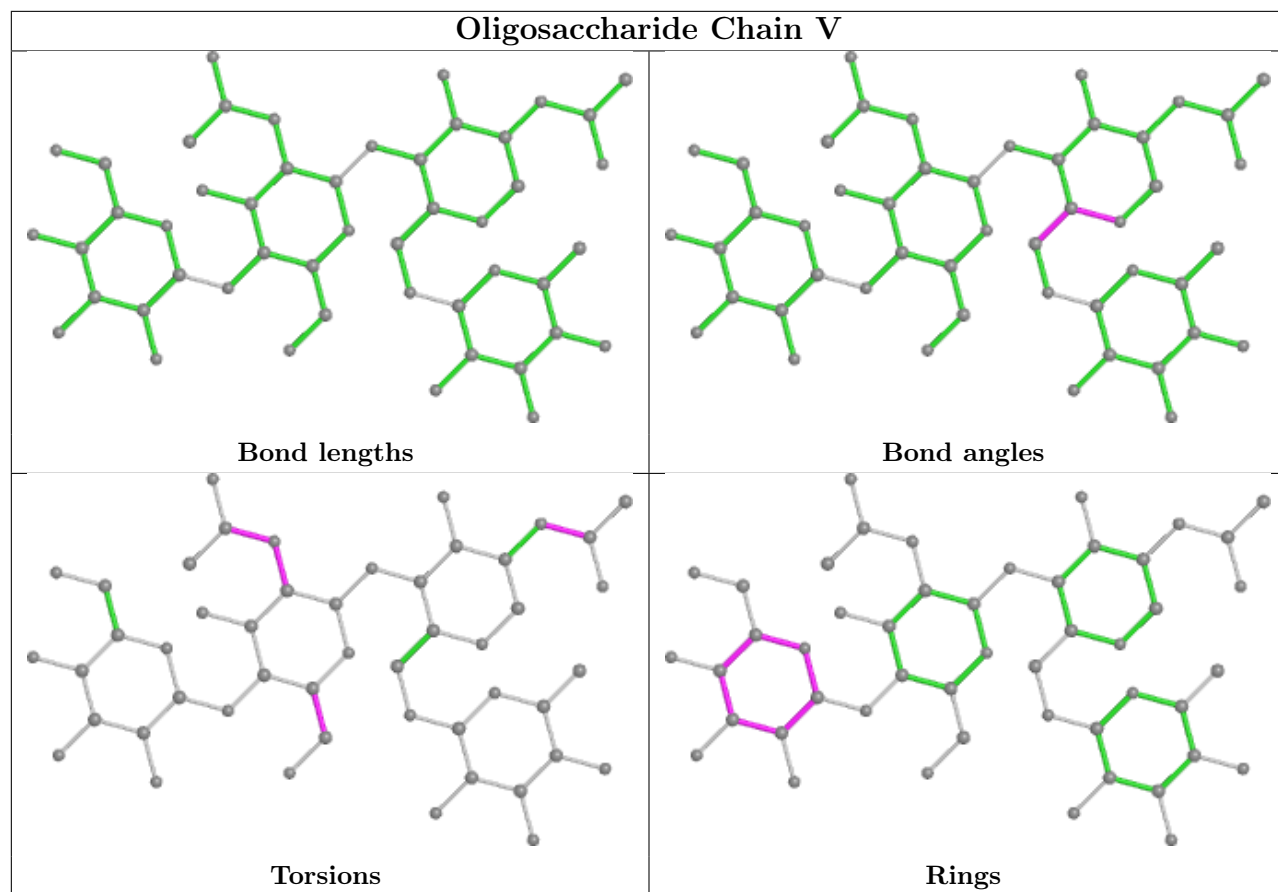
Mol	Chain	Res	Type	Atoms
6	U	4	MAN	C1-C2-C3-C4-C5-O5
7	V	3	MAN	C1-C2-C3-C4-C5-O5

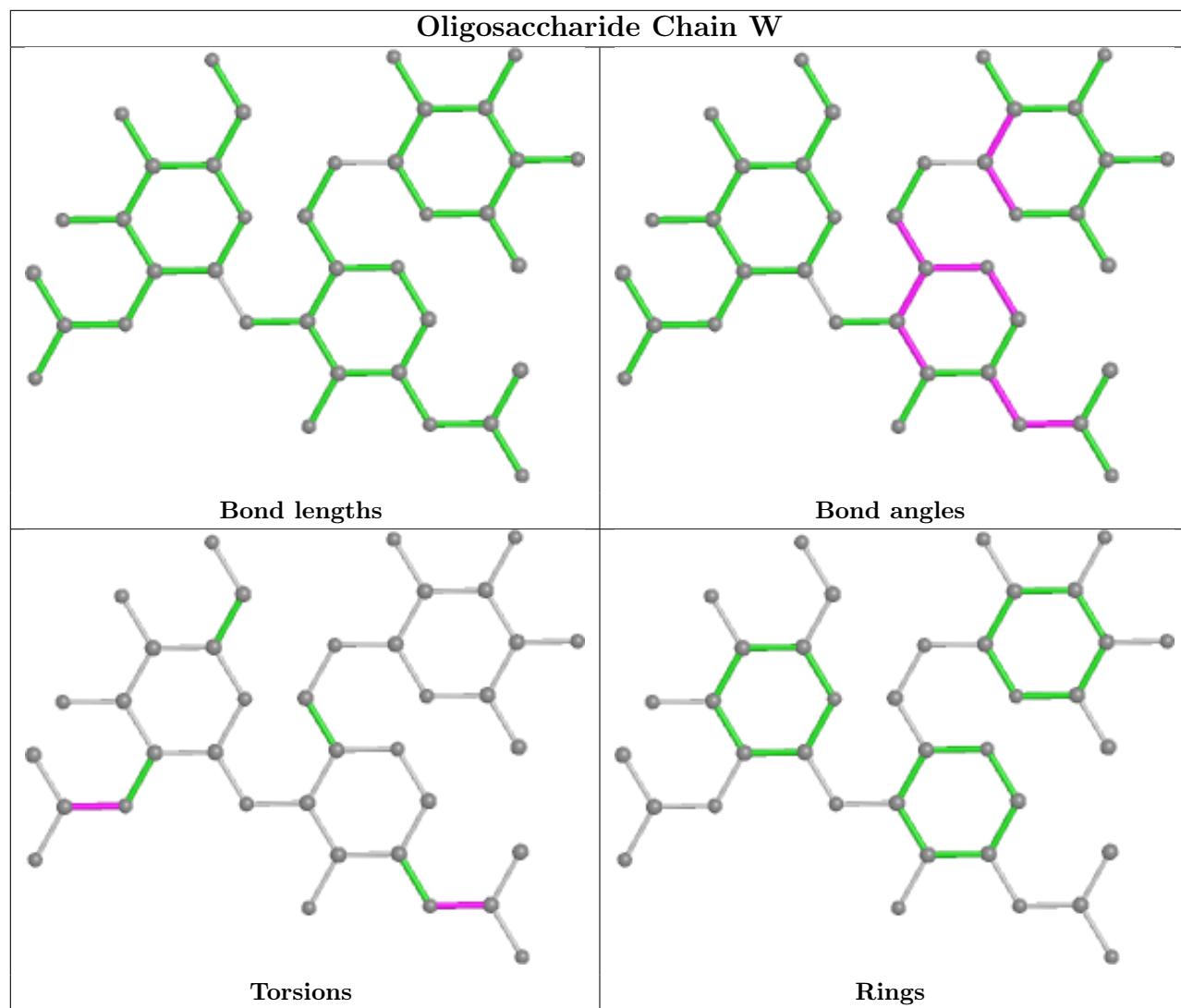
1 monomer is involved in 1 short contact:

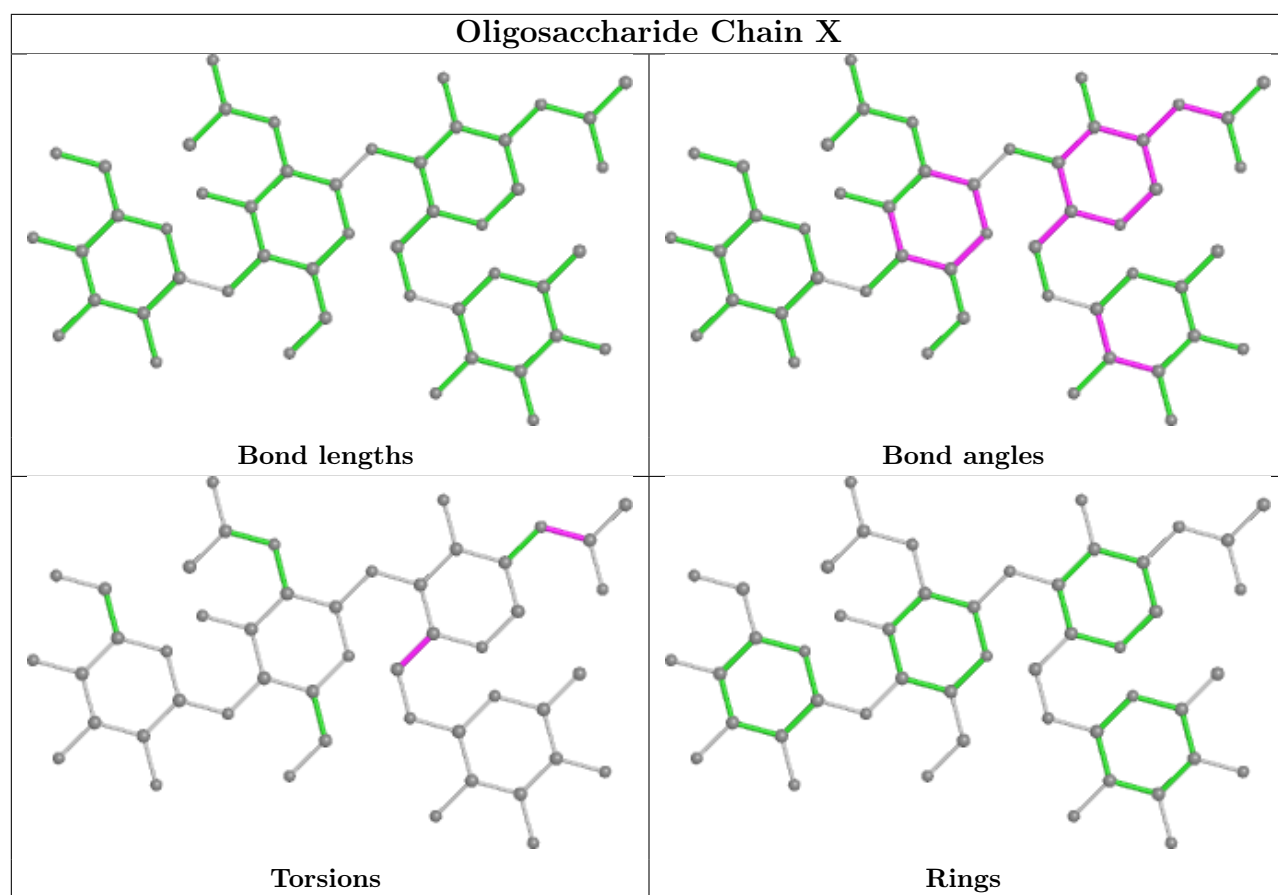
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Y	2	NAG	1	0

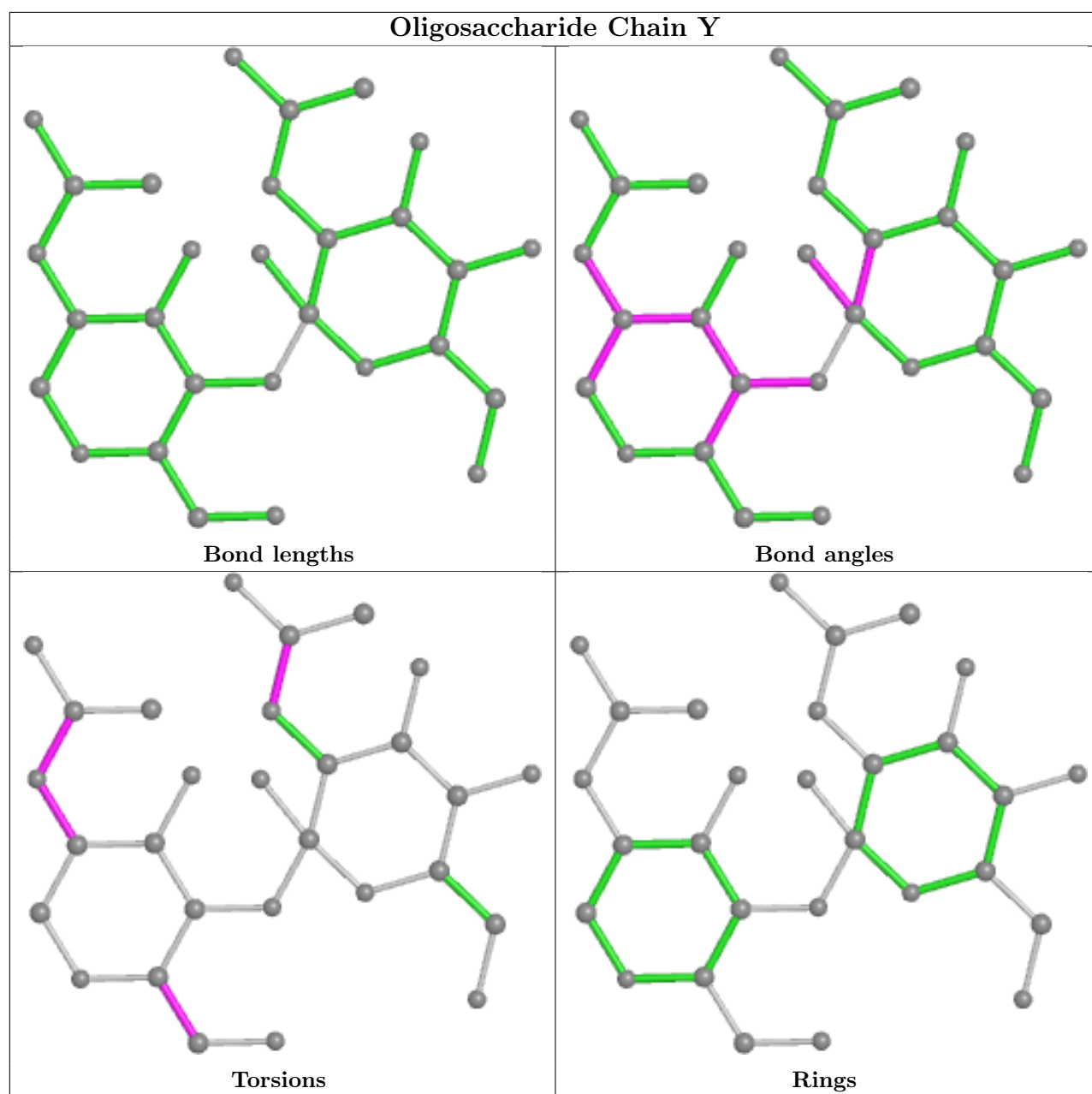
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLR	C	501	-	31,31,31	0.79	1 (3%)	48,48,48	1.15	6 (12%)
11	CLR	D	501	-	31,31,31	0.75	1 (3%)	48,48,48	1.31	7 (14%)
11	CLR	E	501	-	31,31,31	1.01	2 (6%)	48,48,48	1.64	13 (27%)
11	CLR	F	501	-	31,31,31	0.72	1 (3%)	48,48,48	1.32	8 (16%)

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
11	CLR	C	501	-	-	5/10/68/68	0/4/4/4
11	CLR	D	501	-	-	5/10/68/68	0/4/4/4
11	CLR	E	501	-	-	2/10/68/68	0/4/4/4
11	CLR	F	501	-	-	5/10/68/68	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	501	CLR	C13-C14	-2.44	1.50	1.55
11	D	501	CLR	C10-C9	-2.20	1.52	1.56
11	E	501	CLR	C19-C10	-2.18	1.50	1.54
11	C	501	CLR	C10-C9	-2.14	1.52	1.56
11	F	501	CLR	C10-C9	-2.08	1.52	1.56

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	501	CLR	C19-C10-C9	-4.11	106.78	111.68
11	D	501	CLR	C13-C17-C20	-3.61	113.84	119.49
11	F	501	CLR	C13-C17-C20	-3.60	113.84	119.49
11	E	501	CLR	C15-C14-C13	-3.08	100.13	103.84
11	E	501	CLR	C18-C13-C17	-3.02	106.07	111.71
11	E	501	CLR	C18-C13-C14	-2.95	106.21	111.71
11	E	501	CLR	C17-C13-C14	2.92	103.53	100.07
11	E	501	CLR	C11-C9-C8	-2.91	107.57	111.75
11	D	501	CLR	C11-C9-C10	-2.74	109.47	113.08
11	F	501	CLR	C17-C13-C14	2.73	103.31	100.07
11	F	501	CLR	C13-C14-C8	-2.62	110.50	114.38
11	E	501	CLR	C9-C10-C5	2.62	113.75	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	501	CLR	C11-C9-C10	-2.61	109.64	113.08
11	E	501	CLR	C16-C17-C20	-2.61	108.11	112.15
11	F	501	CLR	C11-C9-C10	-2.54	109.73	113.08
11	D	501	CLR	C23-C22-C20	-2.54	107.73	115.03
11	D	501	CLR	C17-C13-C14	2.54	103.08	100.07
11	C	501	CLR	C8-C7-C6	-2.47	109.18	112.73
11	D	501	CLR	C11-C12-C13	-2.40	108.67	112.78
11	C	501	CLR	C3-C4-C5	-2.38	107.98	112.03
11	F	501	CLR	C8-C7-C6	-2.33	109.38	112.73
11	E	501	CLR	C1-C10-C9	2.24	111.86	108.73
11	C	501	CLR	C19-C10-C9	-2.18	109.08	111.68
11	C	501	CLR	C11-C12-C13	-2.14	109.11	112.78
11	D	501	CLR	C13-C14-C8	-2.14	111.22	114.38
11	E	501	CLR	C13-C17-C20	-2.12	116.16	119.49
11	E	501	CLR	C13-C14-C8	-2.12	111.25	114.38
11	C	501	CLR	C11-C9-C10	-2.10	110.32	113.08
11	C	501	CLR	C13-C17-C20	-2.08	116.22	119.49
11	E	501	CLR	C18-C13-C12	2.02	113.79	110.59
11	F	501	CLR	C11-C12-C13	-2.02	109.31	112.78
11	F	501	CLR	C4-C5-C10	2.02	119.10	116.42
11	D	501	CLR	C8-C7-C6	-2.01	109.84	112.73
11	F	501	CLR	C19-C10-C9	-2.00	109.29	111.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	501	CLR	C13-C17-C20-C21
11	C	501	CLR	C16-C17-C20-C21
11	C	501	CLR	C16-C17-C20-C22
11	C	501	CLR	C13-C17-C20-C22
11	F	501	CLR	C13-C17-C20-C22
11	F	501	CLR	C16-C17-C20-C21
11	D	501	CLR	C13-C17-C20-C21
11	F	501	CLR	C13-C17-C20-C21
11	D	501	CLR	C16-C17-C20-C21
11	F	501	CLR	C16-C17-C20-C22
11	D	501	CLR	C13-C17-C20-C22
11	D	501	CLR	C16-C17-C20-C22
11	E	501	CLR	C13-C17-C20-C21
11	E	501	CLR	C13-C17-C20-C22
11	C	501	CLR	C21-C20-C22-C23

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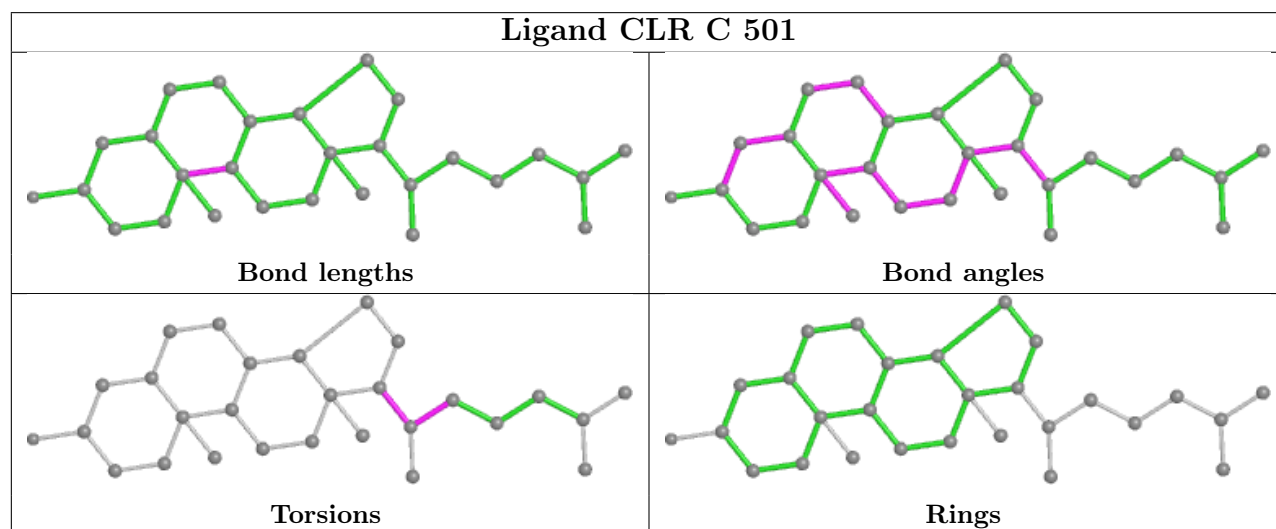
Mol	Chain	Res	Type	Atoms
11	D	501	CLR	C21-C20-C22-C23
11	F	501	CLR	C21-C20-C22-C23

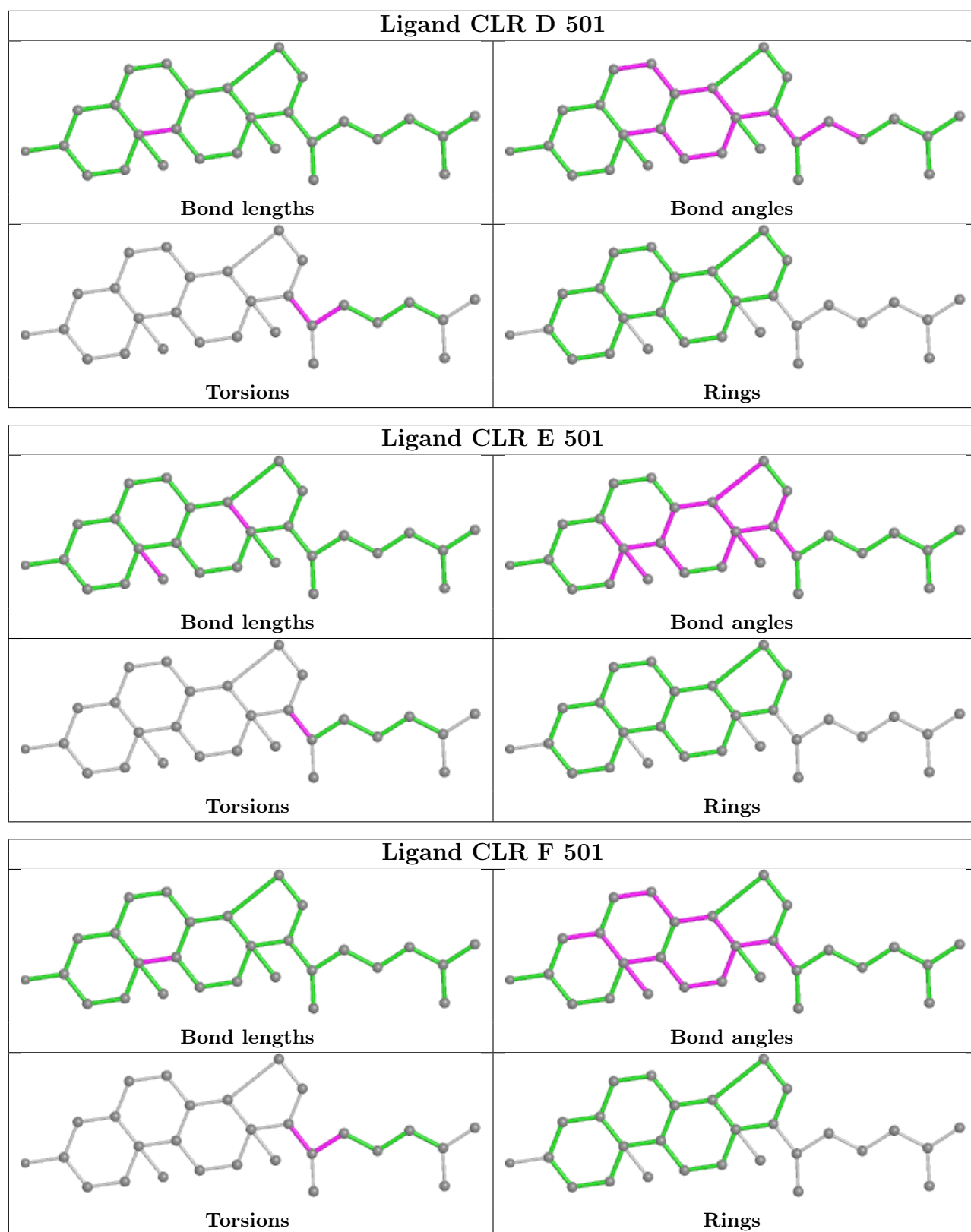
There are no ring outliers.

4 monomers are involved in 138 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	501	CLR	48	0
11	D	501	CLR	37	0
11	E	501	CLR	9	0
11	F	501	CLR	44	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

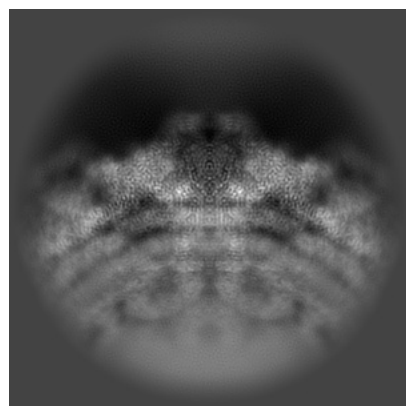
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60997. These allow visual inspection of the internal detail of the map and identification of artifacts.

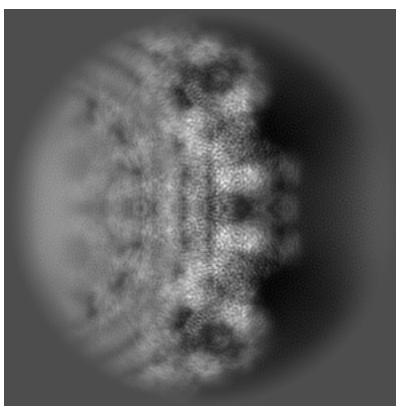
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

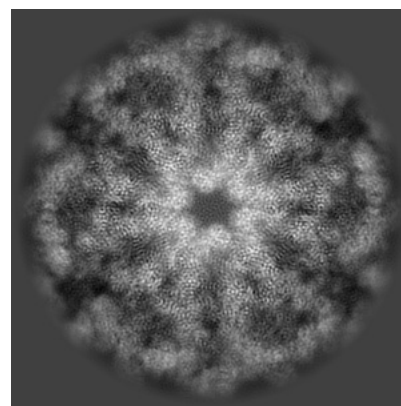
6.1.1 Primary map



X

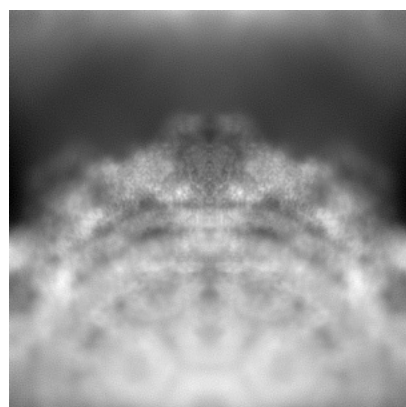


Y

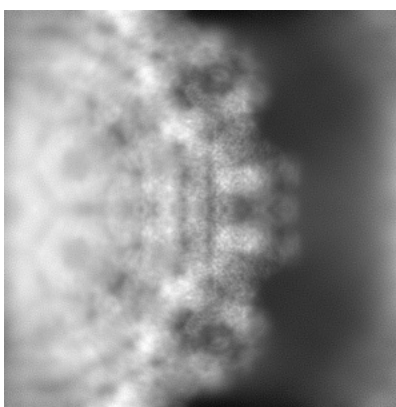


Z

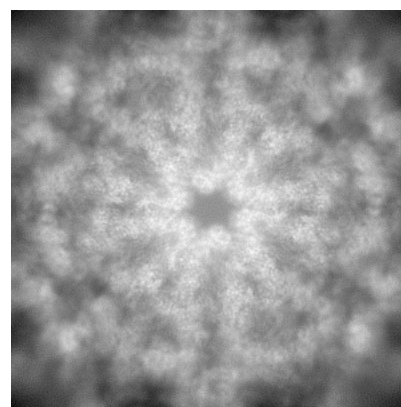
6.1.2 Raw map



X



Y

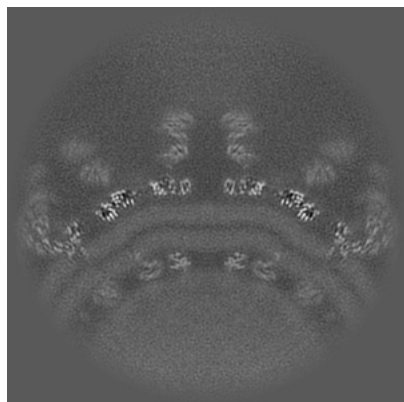


Z

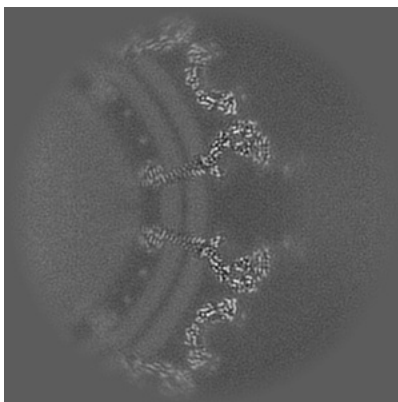
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

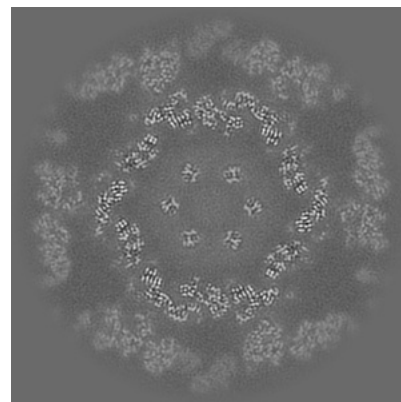
6.2.1 Primary map



X Index: 184

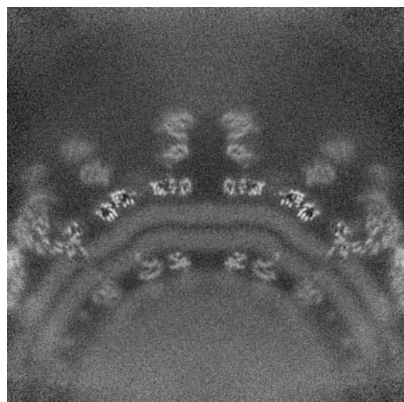


Y Index: 184

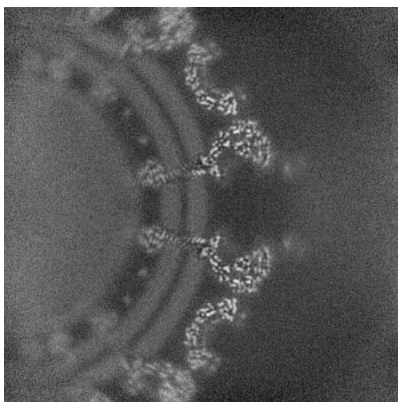


Z Index: 184

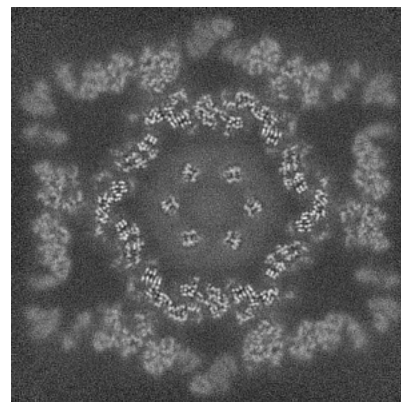
6.2.2 Raw map



X Index: 184



Y Index: 184

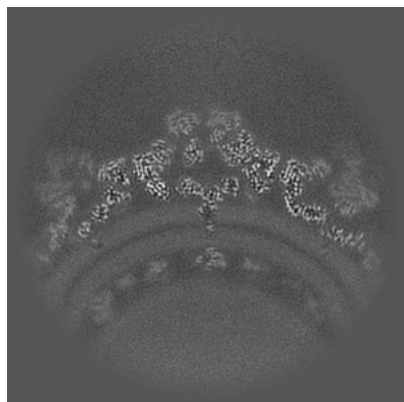


Z Index: 184

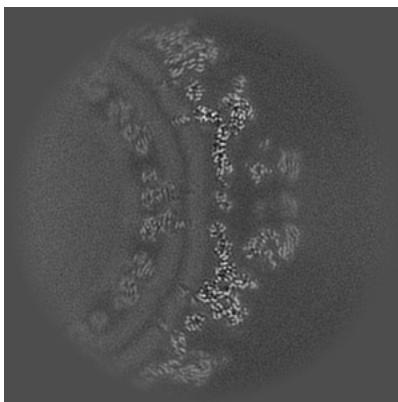
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

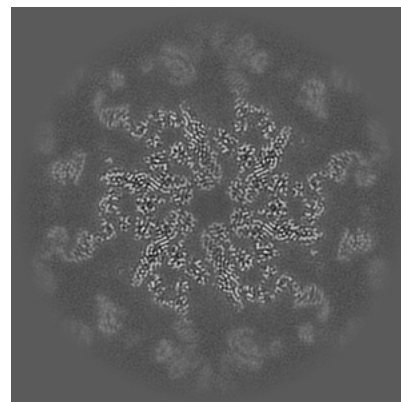
6.3.1 Primary map



X Index: 149

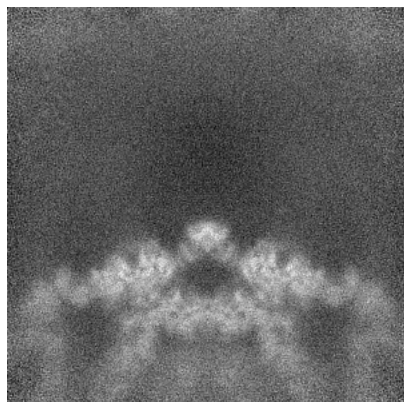


Y Index: 166

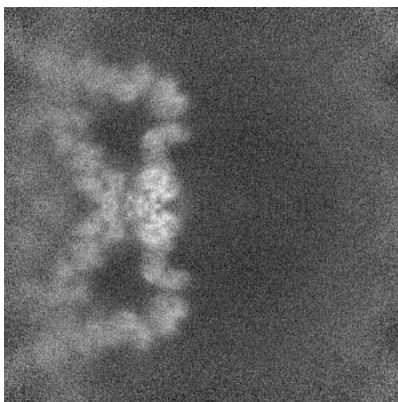


Z Index: 200

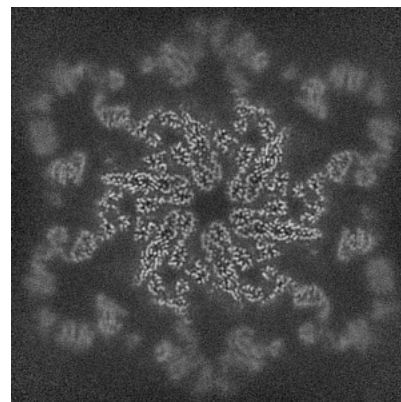
6.3.2 Raw map



X Index: 0



Y Index: 0

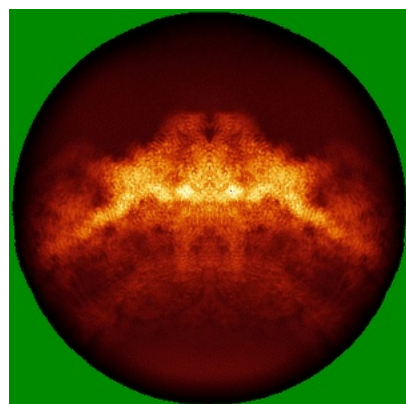


Z Index: 199

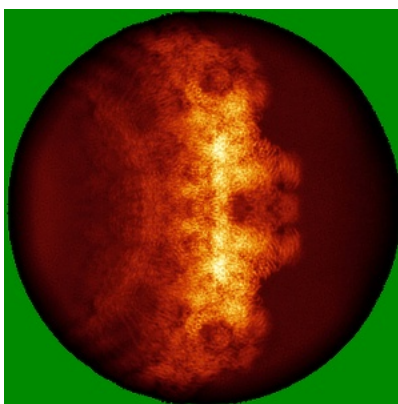
The images above show the largest variance slices of the map in three orthogonal directions.

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

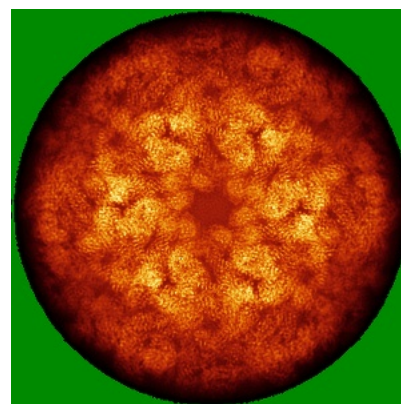
6.4.1 Primary map



X

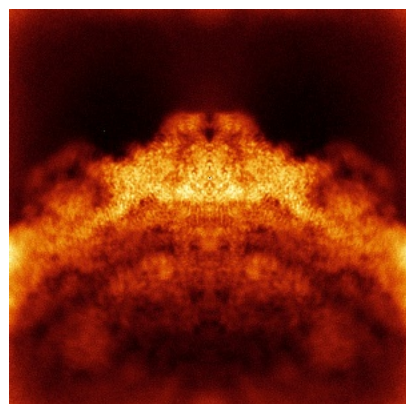


Y

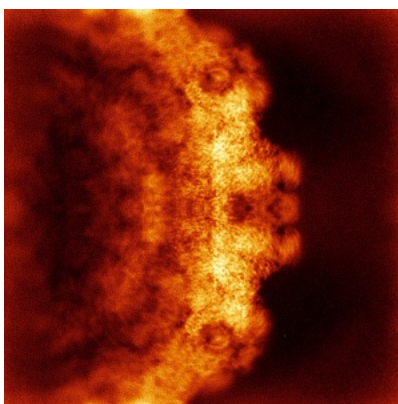


Z

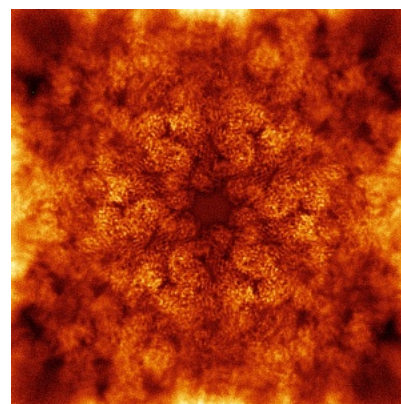
6.4.2 Raw map



X



Y

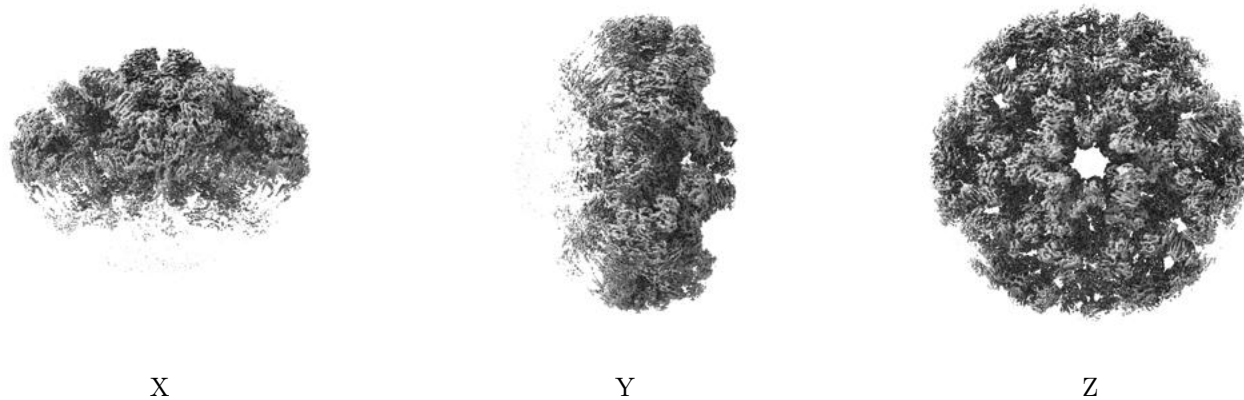


Z

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.

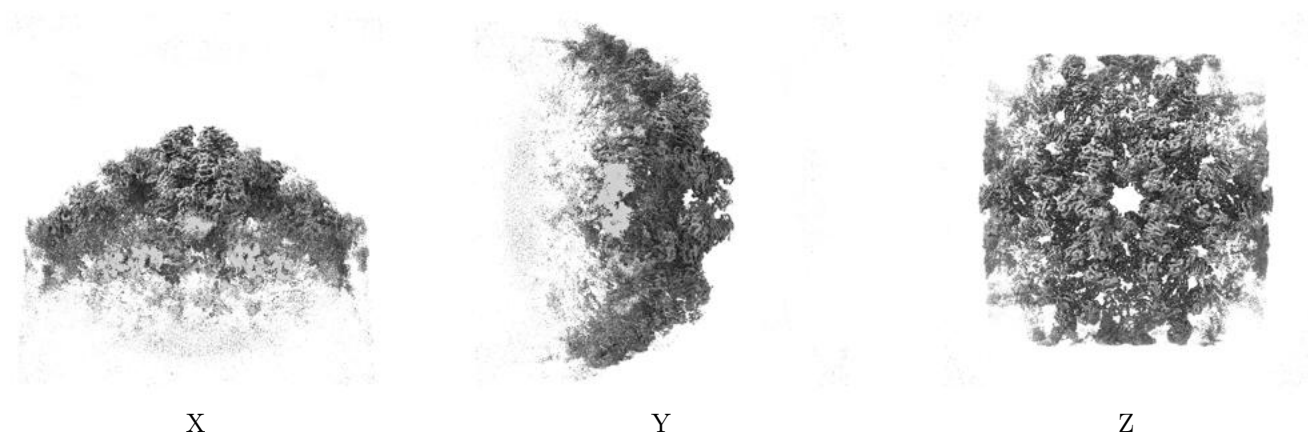
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.135. 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.

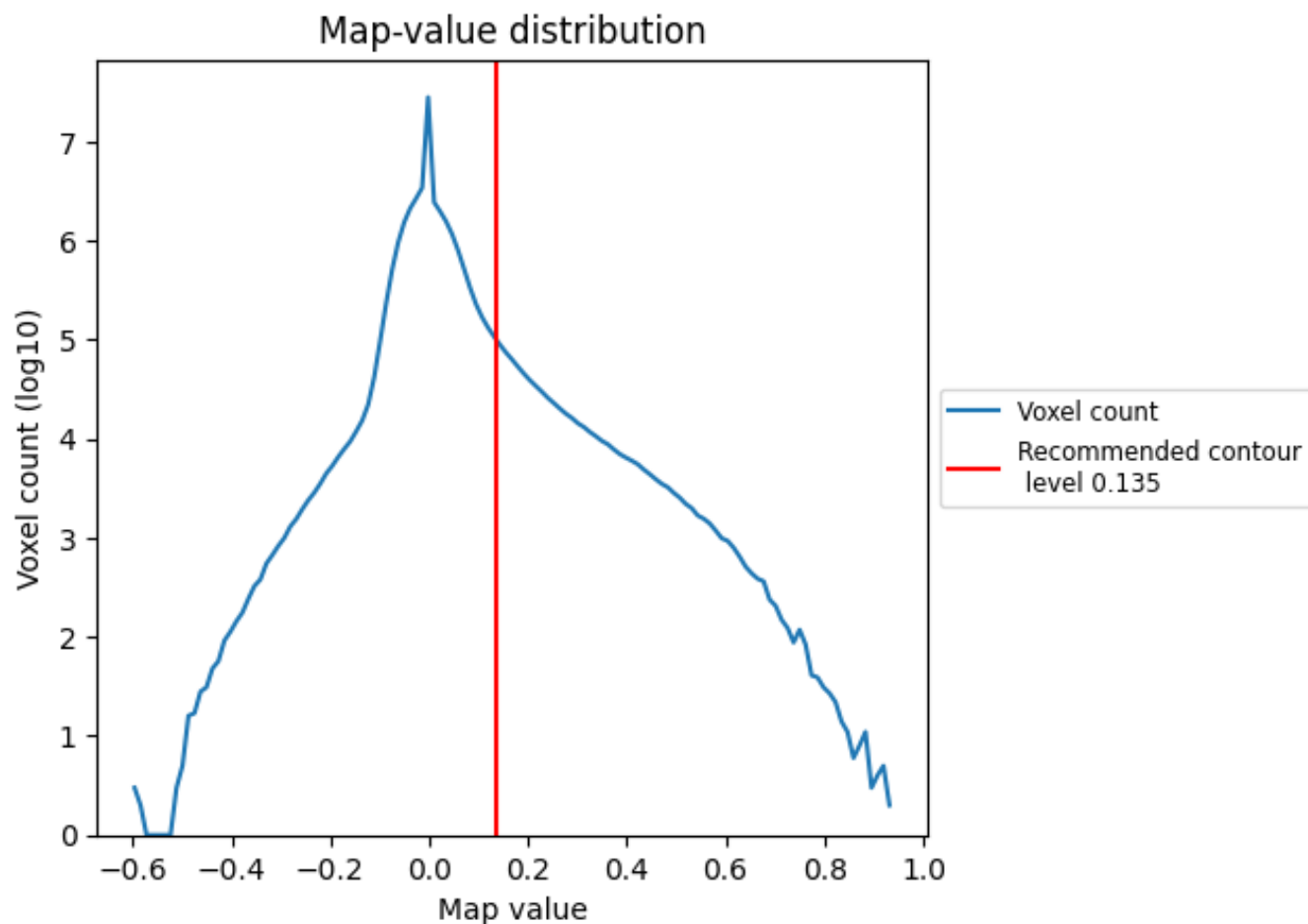
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

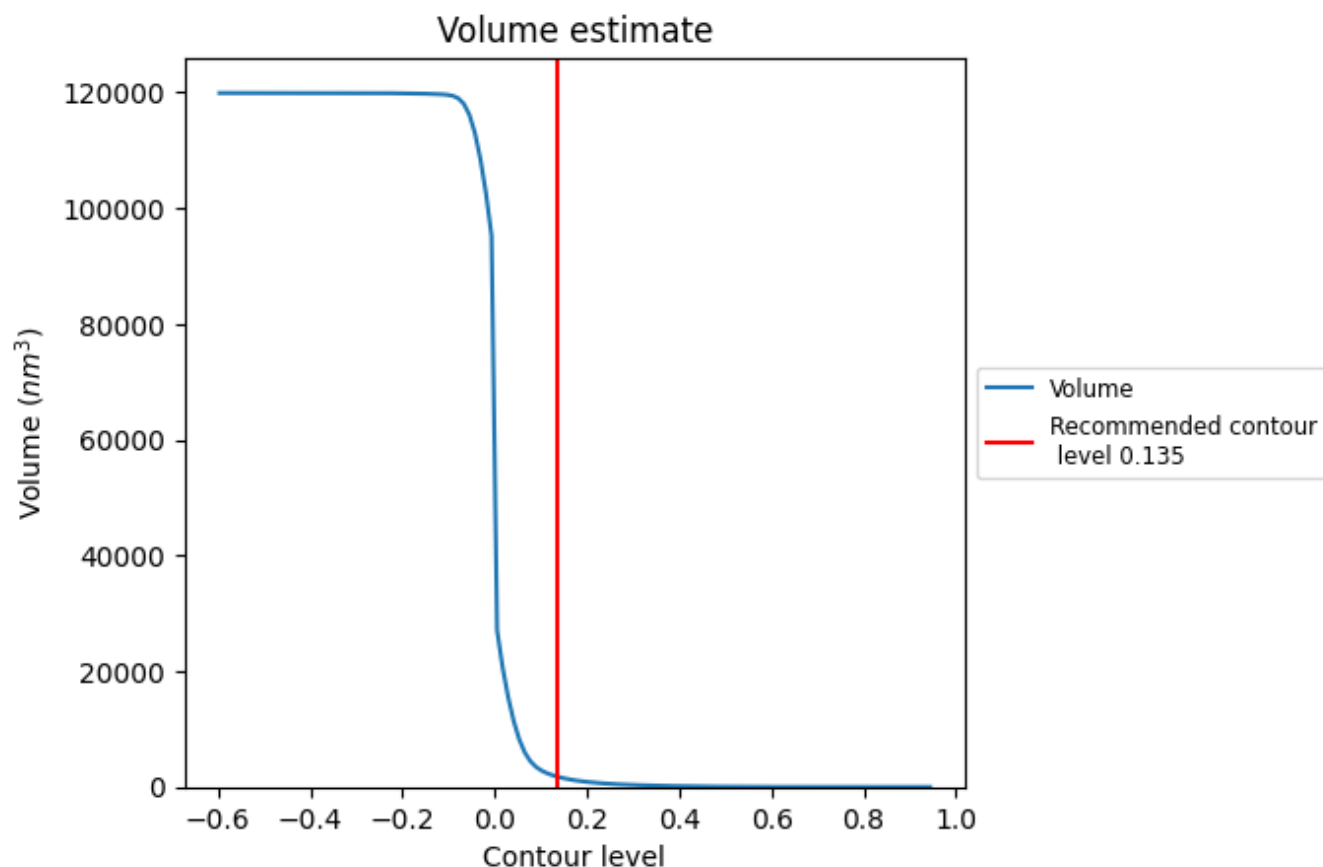
This section contains the results of statistical analysis of the map.

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.

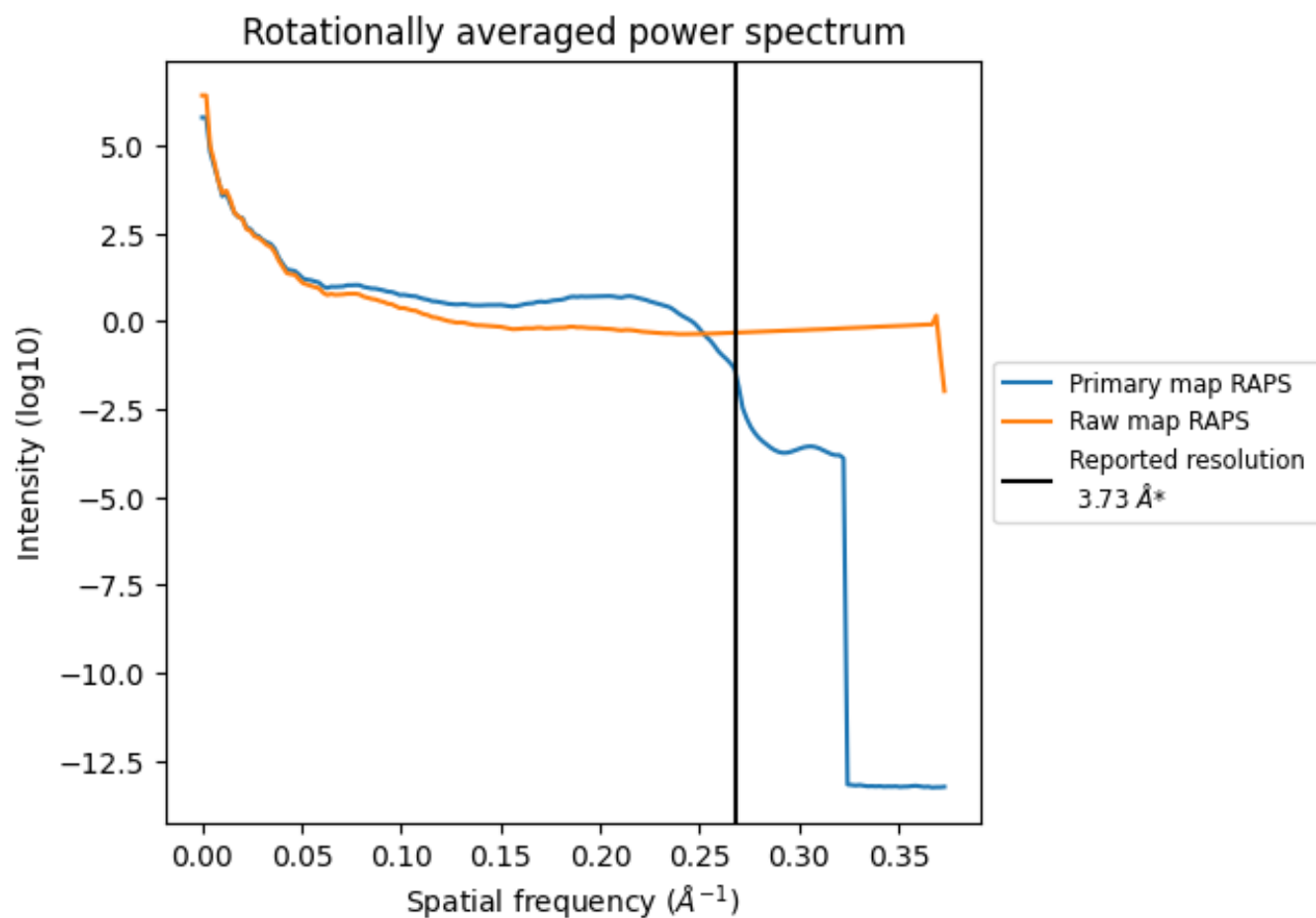
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1804 nm³; this corresponds to an approximate mass of 1629 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 ⓘ

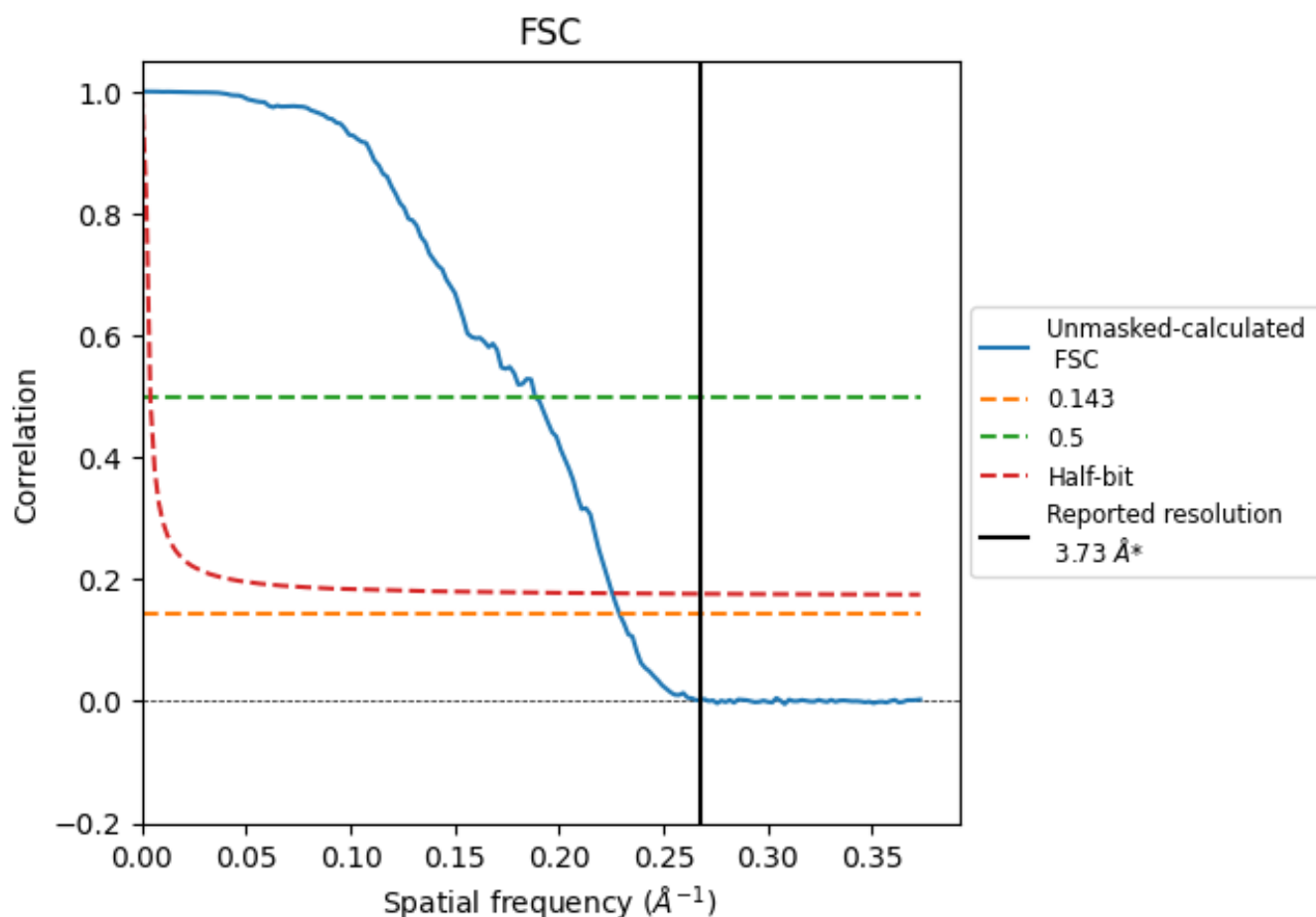


*Reported resolution corresponds to spatial frequency of 0.268 Å⁻¹

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 0.268 \AA^{-1}

8.2 Resolution estimates [i](#)

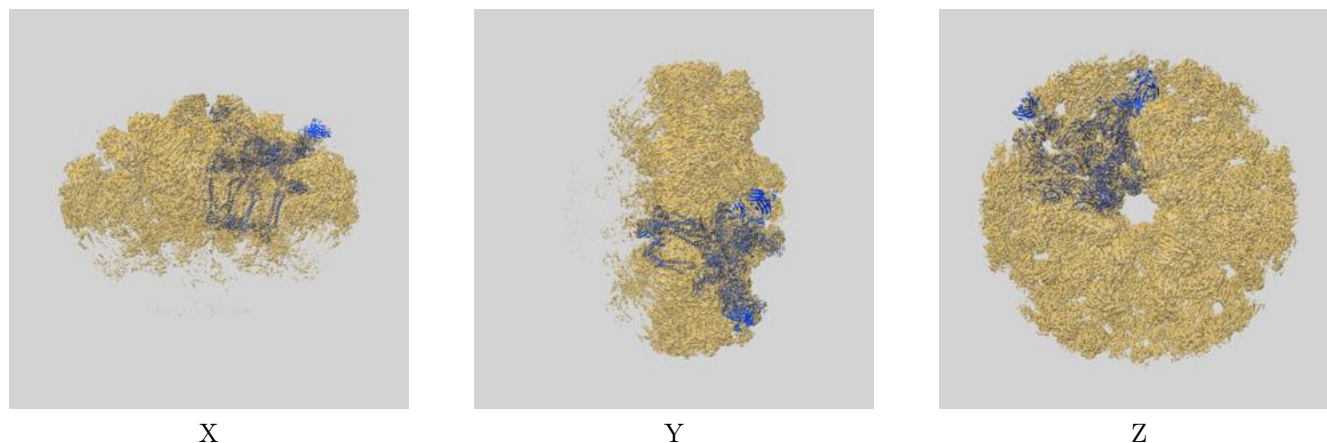
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	5.31	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 3.73 by more than 10 %

9 Map-model fit [i](#)

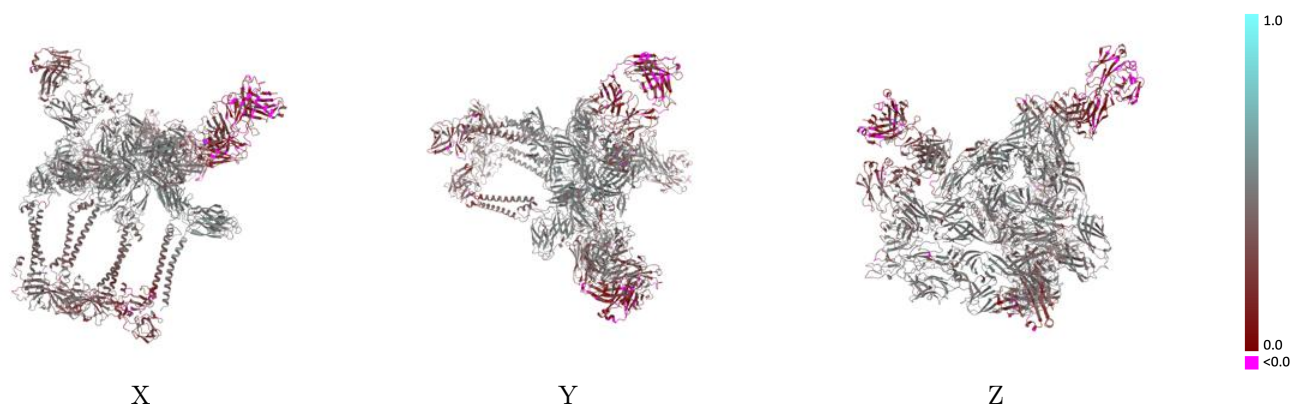
This section contains information regarding the fit between EMDB map EMD-60997 and PDB model 9IYI. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



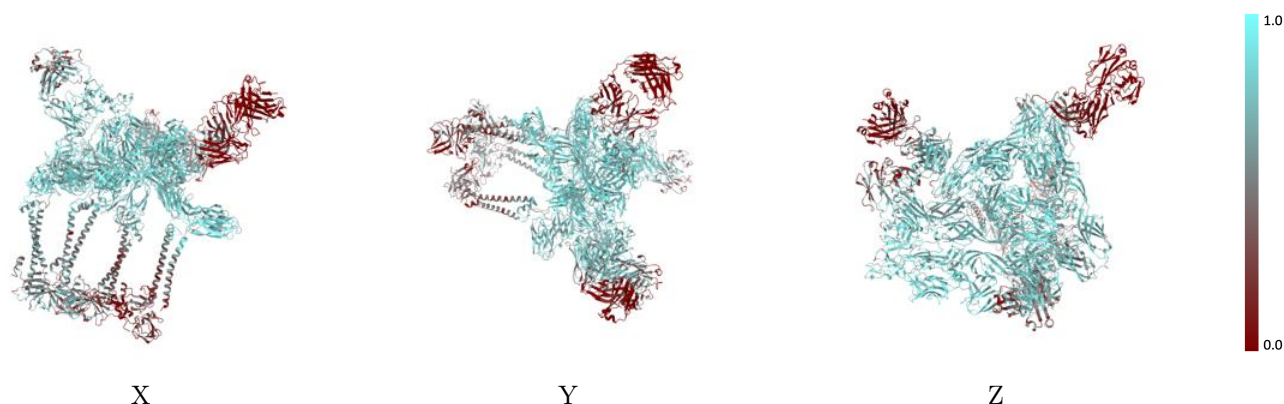
The images above show the 3D surface view of the map at the recommended contour level 0.135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



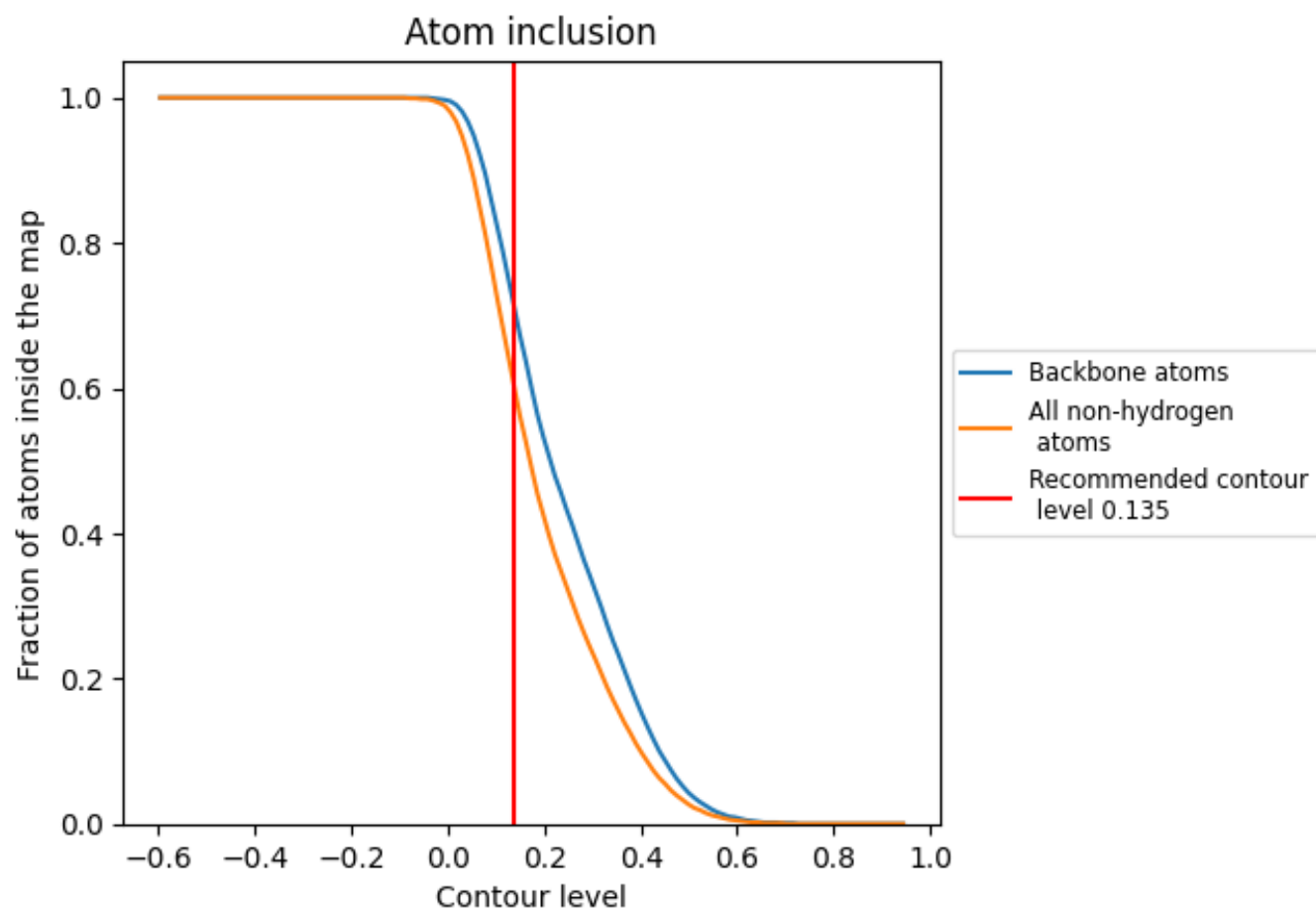
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.135).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (0.135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6100	 0.3880
A	 0.7750	 0.4800
B	 0.7370	 0.4400
C	 0.7430	 0.4480
D	 0.7680	 0.4570
E	 0.7170	 0.4250
F	 0.7210	 0.4260
G	 0.7240	 0.4300
H	 0.7520	 0.4410
I	 0.2040	 0.2520
J	 0.4650	 0.3540
K	 0.3040	 0.3210
L	 0.4710	 0.3810
M	 0.4090	 0.2800
N	 0.3910	 0.2660
O	 0.0560	 0.1670
P	 0.0840	 0.1590
Q	 0.6200	 0.3840
R	 0.6280	 0.3710
S	 0.6610	 0.3960
T	 0.6250	 0.3680
U	 0.4790	 0.4400
V	 0.4290	 0.3320
W	 0.6050	 0.4210
X	 0.4900	 0.4000
Y	 0.4480	 0.3480

