



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:56 AM UTC

PDB ID : 7BUB / pdb_00007bub
EMDB ID : EMD-30194
Title : Cryo-EM structure of Dengue virus serotype 2 complexed with Fab SIgN-3C at pH 6.5
Authors : Zhang, S.; Chew, S.V.; Lim, X.N.; Ng, T.S.; Kostyuchenko, V.A.; Lok, S.M.
Deposited on : 2020-04-06
Resolution : 4.20 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

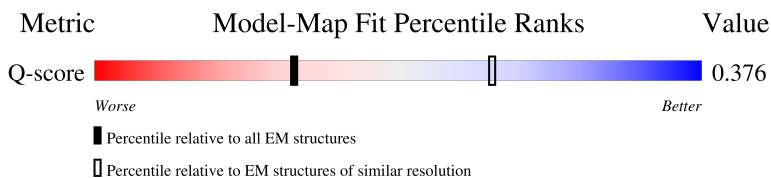
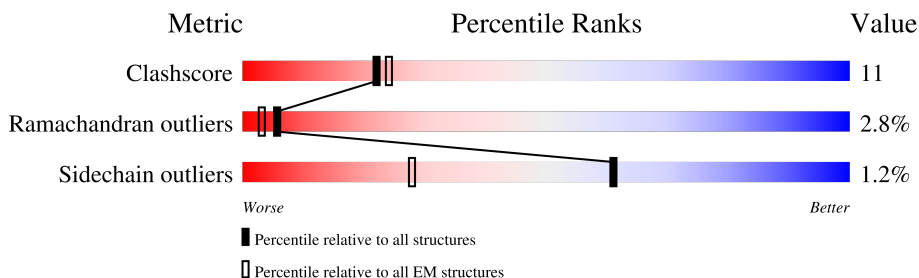
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	G	132	27% (red), 67% (green), 28% (yellow), 5% (orange)
1	H	132	24% (red), 64% (green), 31% (yellow), 5% (orange)
2	I	107	29% (red), 70% (green), 25% (yellow), . . (orange)
2	L	107	33% (red), 66% (green), 33% (yellow), . (orange)

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Mol	Chain	Length	Quality of chain
3	A	495	<p>21% 72% 24%</p>
3	B	495	<p>21% 75% 21%</p>
3	C	495	<p>20% 75% 22%</p>
4	D	72	<p>40% 81% 19%</p>
4	E	72	<p>29% 92% 8%</p>
4	F	72	<p>39% 86% 14%</p>
5	J	2	<p>50% 50% 50%</p>
5	K	2	<p>50% 50% 50%</p>
5	M	2	<p>100% 50% 50%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16389 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 SIgN-3C Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	132	Total	C	N	O	S	0	0
			994	620	176	193	5		
1	H	132	Total	C	N	O	S	0	0
			994	620	176	193	5		

- Molecule 2 is a protein called SIgN-3C Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	107	Total	C	N	O	S	0	0
			834	526	139	167	2		
2	L	107	Total	C	N	O	S	0	0
			834	526	139	167	2		

- Molecule 3 is a protein called Dengue virus serotype2 E protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	495	Total	C	N	O	S	0	0
			3644	2352	644	619	29		
3	A	495	Total	C	N	O	S	0	0
			3650	2356	645	619	30		
3	C	495	Total	C	N	O	S	0	0
			3638	2351	641	616	30		

- Molecule 4 is a protein called Dengue virus serotype 2 M protein.

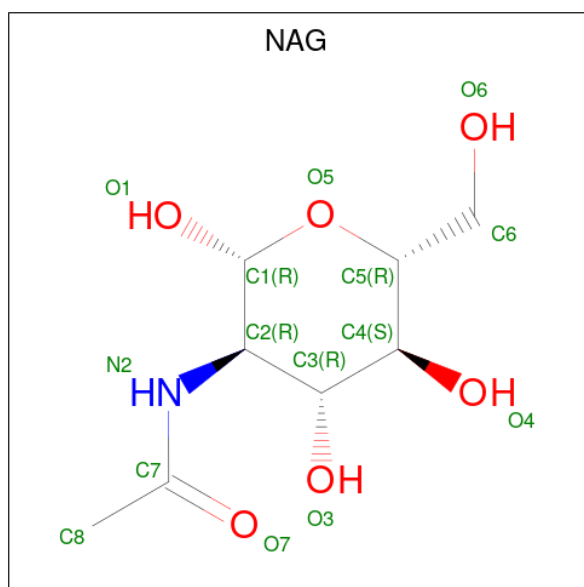
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	72	Total	C	N	O	S	0	0
			559	371	96	89	3		
4	D	72	Total	C	N	O	S	0	0
			560	372	96	89	3		
4	F	72	Total	C	N	O	S	0	0
			556	370	94	89	3		

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



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

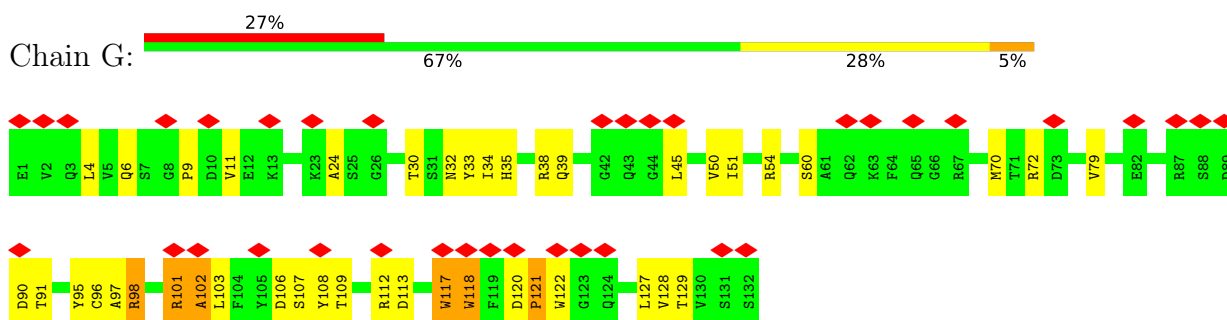


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	C	1	14	8	1	5	0

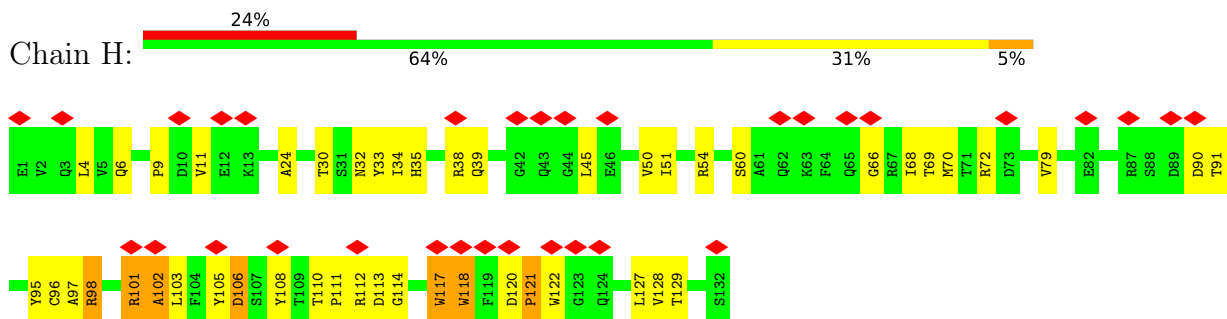
3 Residue-property plots [i](#)

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

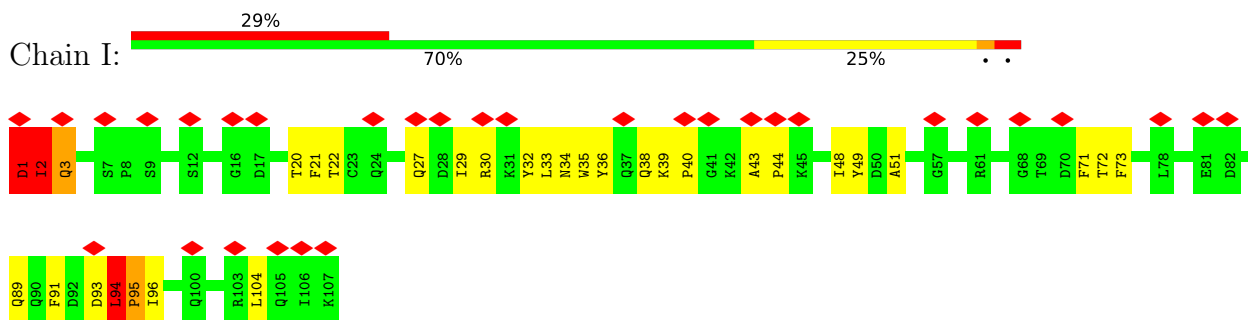
- Molecule 1: SIgN-3C Fab heavy chain



- Molecule 1: SIgN-3C Fab heavy chain

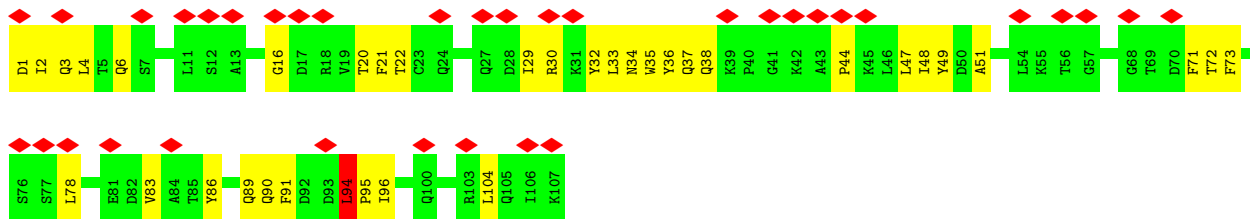


- Molecule 2: SIgN-3C Fab light chain

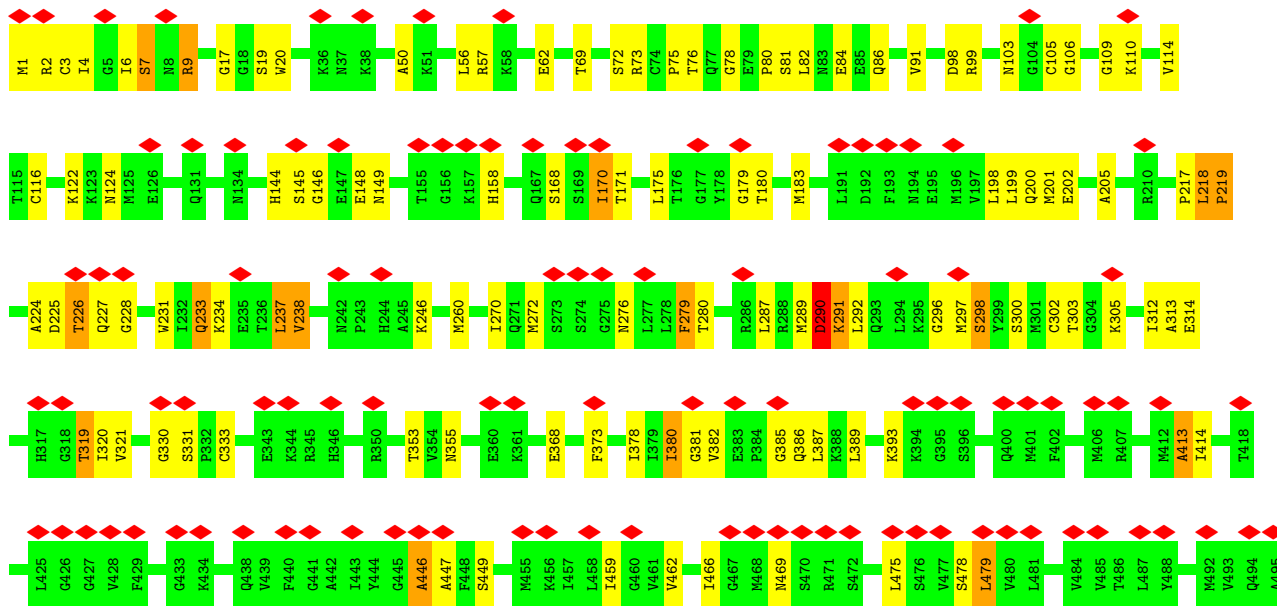
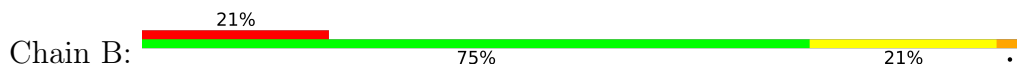


- Molecule 2: SIgN-3C Fab light chain

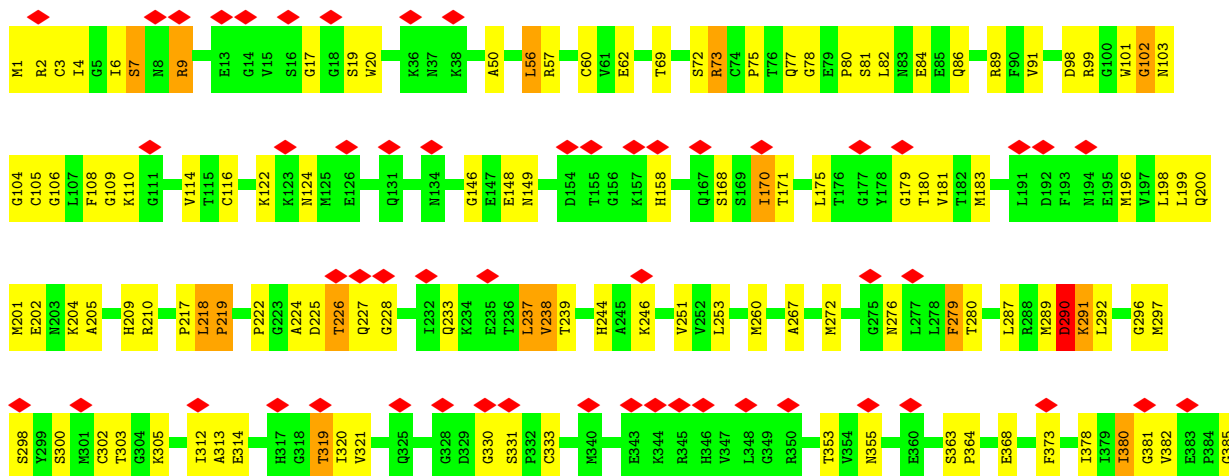


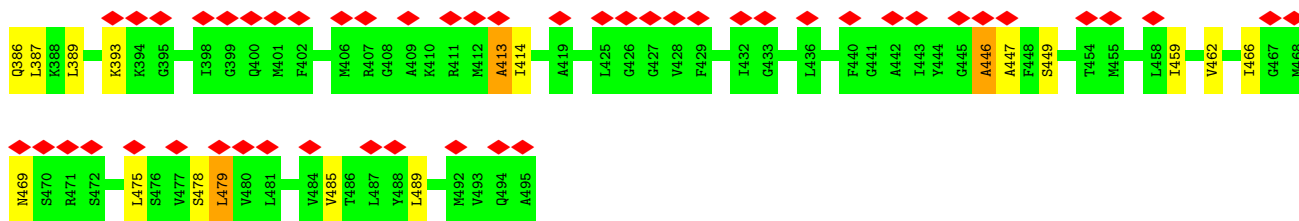


• Molecule 3: Dengue virus serotype2 E protein

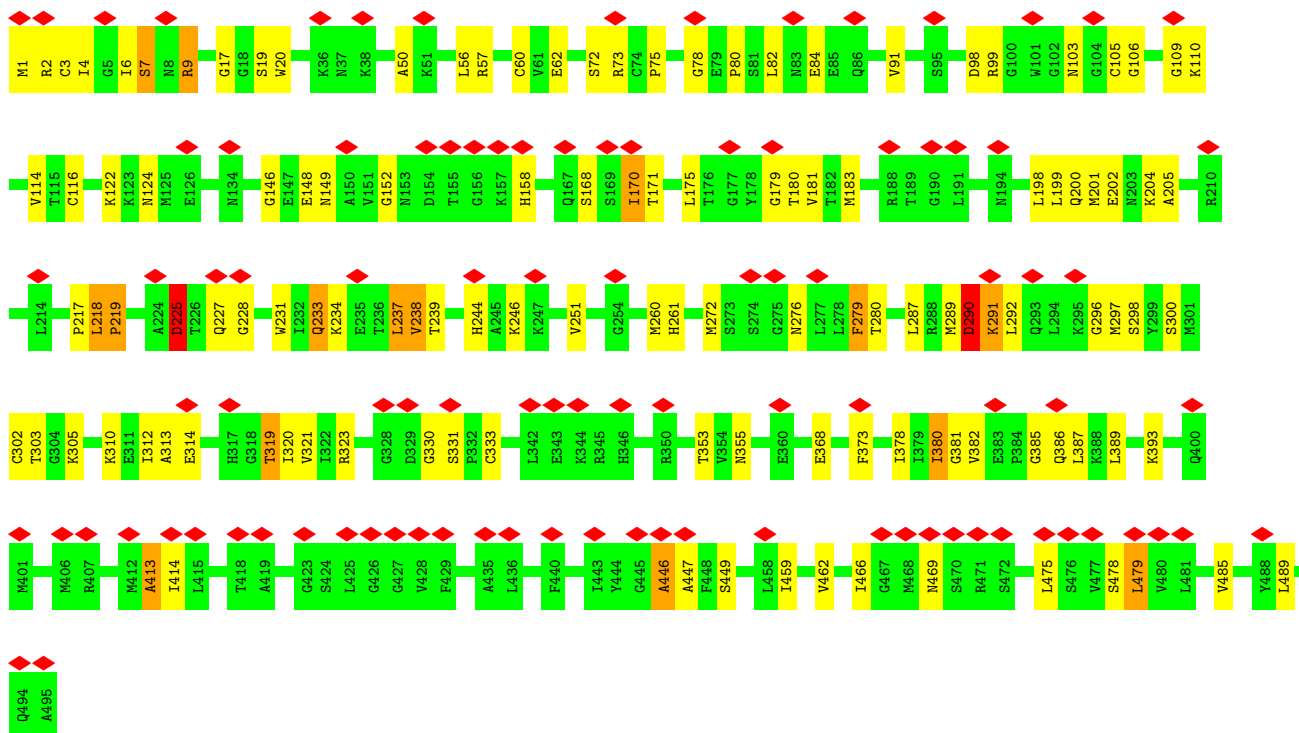
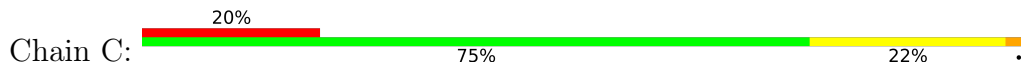


• Molecule 3: Dengue virus serotype2 E protein

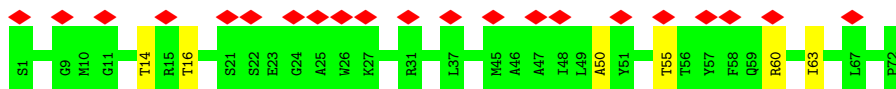
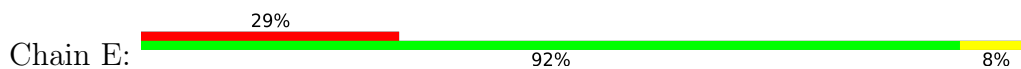




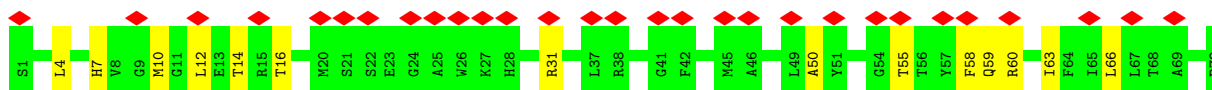
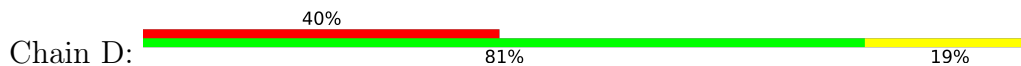
• Molecule 3: Dengue virus serotype2 E protein



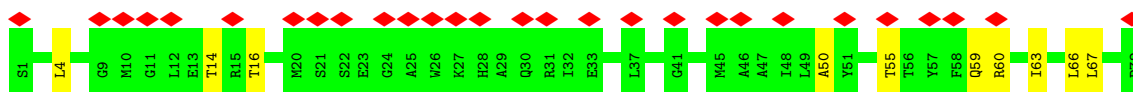
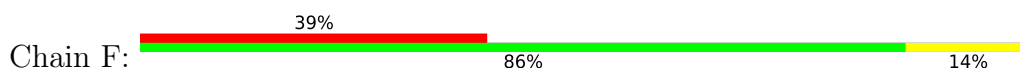
• Molecule 4: Dengue virus serotype 2 M protein



• Molecule 4: Dengue virus serotype 2 M protein



• Molecule 4: Dengue virus serotype 2 M protein



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	16.593	Depositor
Minimum map value	-8.891	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.8	Depositor
Map size (Å)	720.80005, 720.80005, 720.80005	wwPDB
Map dimensions	424, 424, 424	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7000002, 1.7000002, 1.7000002	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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.44	1/1019 (0.1%)	1.01	6/1381 (0.4%)
1	H	0.43	1/1019 (0.1%)	0.87	5/1381 (0.4%)
2	I	0.37	0/852	0.77	3/1154 (0.3%)
2	L	0.37	0/852	0.69	1/1154 (0.1%)
3	A	0.41	0/3726	1.04	17/5040 (0.3%)
3	B	0.41	0/3720	1.04	16/5032 (0.3%)
3	C	0.41	0/3714	1.03	17/5022 (0.3%)
4	D	0.34	0/576	0.79	0/787
4	E	0.34	0/575	0.80	0/786
4	F	0.34	0/572	0.79	0/782
All	All	0.40	2/16625 (0.0%)	0.97	65/22519 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	3
1	H	0	2
2	I	0	2
2	L	0	2
3	A	0	16
3	B	0	16
3	C	0	18
All	All	0	59

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	120	ASP	C-N	5.52	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	120	ASP	C-N	5.46	1.38	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	106	ASP	N-CA-C	11.76	124.77	110.19
1	G	98	ARG	N-CA-C	10.82	126.09	108.34
1	G	102	ALA	N-CA-C	-10.69	92.90	109.25
1	H	102	ALA	N-CA-C	-10.65	92.95	109.25
3	A	102	GLY	N-CA-C	-8.12	103.09	112.50
1	H	106	ASP	N-CA-C	8.08	128.02	110.80
3	A	246	LYS	CA-C-N	7.12	131.91	121.31
3	A	246	LYS	C-N-CA	7.12	131.91	121.31
1	H	101	ARG	N-CA-C	7.01	125.73	110.80
1	G	101	ARG	N-CA-C	6.99	125.69	110.80
3	B	246	LYS	CA-C-N	6.90	132.33	121.56
3	B	246	LYS	C-N-CA	6.90	132.33	121.56
3	C	246	LYS	CA-C-N	6.88	132.29	121.56
3	C	246	LYS	C-N-CA	6.88	132.29	121.56
3	B	279	PHE	CA-C-N	6.78	134.49	121.54
3	B	279	PHE	C-N-CA	6.78	134.49	121.54
3	A	279	PHE	CA-C-N	6.77	134.47	121.54
3	A	279	PHE	C-N-CA	6.77	134.47	121.54
3	C	279	PHE	CA-C-N	6.77	134.47	121.54
3	C	279	PHE	C-N-CA	6.77	134.47	121.54
3	B	7	SER	CA-C-N	6.60	134.14	121.54
3	B	7	SER	C-N-CA	6.60	134.14	121.54
3	A	7	SER	CA-C-N	6.56	134.07	121.54
3	A	7	SER	C-N-CA	6.56	134.07	121.54
3	C	7	SER	CA-C-N	6.54	134.03	121.54
3	C	7	SER	C-N-CA	6.54	134.03	121.54
2	I	1	ASP	CA-C-N	6.37	133.43	121.97
2	I	1	ASP	C-N-CA	6.37	133.43	121.97
1	G	107	SER	CA-C-N	-5.90	112.60	122.64
1	G	107	SER	C-N-CA	-5.90	112.60	122.64
3	B	17	GLY	N-CA-C	-5.72	107.09	115.72
3	C	17	GLY	N-CA-C	-5.70	107.11	115.72
3	A	17	GLY	N-CA-C	-5.69	107.13	115.72
3	A	6	ILE	CA-C-N	5.67	132.38	121.54
3	A	6	ILE	C-N-CA	5.67	132.38	121.54
3	C	6	ILE	CA-C-N	5.67	132.38	121.54
3	C	6	ILE	C-N-CA	5.67	132.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6	ILE	CA-C-N	5.67	132.37	121.54
3	B	6	ILE	C-N-CA	5.67	132.37	121.54
1	H	105	TYR	CA-C-N	5.57	132.17	121.54
1	H	105	TYR	C-N-CA	5.57	132.17	121.54
3	B	219	PRO	CA-C-N	5.52	129.53	121.31
3	B	219	PRO	C-N-CA	5.52	129.53	121.31
3	B	319	THR	CA-C-N	5.52	128.10	120.49
3	B	319	THR	C-N-CA	5.52	128.10	120.49
3	C	319	THR	CA-C-N	5.51	128.10	120.49
3	C	319	THR	C-N-CA	5.51	128.10	120.49
3	A	319	THR	CA-C-N	5.50	128.08	120.49
3	A	319	THR	C-N-CA	5.50	128.08	120.49
3	A	219	PRO	CA-C-N	5.49	129.49	121.31
3	A	219	PRO	C-N-CA	5.49	129.49	121.31
3	C	219	PRO	CA-C-N	5.48	129.48	121.31
3	C	219	PRO	C-N-CA	5.48	129.48	121.31
3	B	330	GLY	N-CA-C	5.37	119.14	112.64
3	B	280	THR	CA-C-N	5.35	131.35	121.67
3	B	280	THR	C-N-CA	5.35	131.35	121.67
3	C	280	THR	CA-C-N	5.34	131.34	121.67
3	C	280	THR	C-N-CA	5.34	131.34	121.67
3	C	330	GLY	N-CA-C	5.32	119.08	112.64
3	A	330	GLY	N-CA-C	5.32	119.07	112.64
2	I	94	LEU	N-CA-C	5.30	121.53	109.81
3	A	280	THR	CA-C-N	5.29	131.25	121.67
3	A	280	THR	C-N-CA	5.29	131.25	121.67
2	L	94	LEU	N-CA-C	5.29	121.50	109.81
3	C	225	ASP	N-CA-C	5.04	116.46	111.07

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	148	GLU	Peptide
3	A	149	ASN	Peptide
3	A	168	SER	Peptide
3	A	218	LEU	Peptide
3	A	237	LEU	Peptide
3	A	279	PHE	Peptide
3	A	290	ASP	Peptide
3	A	297	MET	Peptide
3	A	331	SER	Peptide

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Mol	Chain	Res	Type	Group
3	A	353	THR	Peptide
3	A	385	GLY	Peptide
3	A	413	ALA	Peptide
3	A	446	ALA	Peptide
3	A	56	LEU	Peptide
3	A	7	SER	Peptide
3	A	9	ARG	Peptide
3	B	148	GLU	Peptide
3	B	149	ASN	Peptide
3	B	168	SER	Peptide
3	B	218	LEU	Peptide
3	B	237	LEU	Peptide
3	B	279	PHE	Peptide
3	B	290	ASP	Peptide
3	B	297	MET	Peptide
3	B	331	SER	Peptide
3	B	353	THR	Peptide
3	B	385	GLY	Peptide
3	B	413	ALA	Peptide
3	B	446	ALA	Peptide
3	B	56	LEU	Peptide
3	B	7	SER	Peptide
3	B	9	ARG	Peptide
3	C	148	GLU	Peptide
3	C	149	ASN	Peptide
3	C	168	SER	Peptide
3	C	218	LEU	Peptide
3	C	225	ASP	Peptide
3	C	227	GLN	Peptide
3	C	237	LEU	Peptide
3	C	279	PHE	Peptide
3	C	290	ASP	Peptide
3	C	297	MET	Peptide
3	C	331	SER	Peptide
3	C	353	THR	Peptide
3	C	385	GLY	Peptide
3	C	413	ALA	Peptide
3	C	446	ALA	Peptide
3	C	56	LEU	Peptide
3	C	7	SER	Peptide
3	C	9	ARG	Peptide
1	G	112	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	G	117	TRP	Peptide
1	G	121	PRO	Peptide
1	H	117	TRP	Peptide
1	H	121	PRO	Peptide
2	I	29	ILE	Peptide
2	I	94	LEU	Peptide
2	L	29	ILE	Peptide
2	L	94	LEU	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	994	0	941	56	0
1	H	994	0	941	61	0
2	I	834	0	814	26	0
2	L	834	0	814	22	0
3	A	3650	0	3714	103	0
3	B	3644	0	3708	75	0
3	C	3638	0	3703	69	0
4	D	560	0	579	14	0
4	E	559	0	577	3	0
4	F	556	0	572	9	0
5	J	28	0	25	0	0
5	K	28	0	25	0	0
5	M	28	0	25	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
All	All	16389	0	16477	377	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 11.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:ALA:HB3	1:H:118:TRP:CD2	1.46	1.51
1:H:97:ALA:CB	1:H:118:TRP:CG	2.01	1.43
1:H:97:ALA:CB	1:H:118:TRP:CD2	2.01	1.43
1:H:97:ALA:HB3	1:H:118:TRP:CG	1.50	1.41
1:H:98:ARG:O	1:H:118:TRP:CZ3	1.75	1.39
1:G:60:SER:HB3	3:A:226:THR:CG2	1.51	1.37
1:H:97:ALA:HB1	1:H:118:TRP:CE3	1.65	1.31
1:H:97:ALA:HB2	1:H:118:TRP:CB	1.62	1.28
3:B:226:THR:CG2	1:H:60:SER:HB3	1.65	1.25
1:G:98:ARG:CG	1:G:121:PRO:HG3	1.70	1.21
3:B:226:THR:HG21	1:H:60:SER:CB	1.78	1.13
1:G:60:SER:CB	3:A:226:THR:HG21	1.78	1.12
1:H:98:ARG:O	1:H:118:TRP:CH2	2.03	1.09
1:G:98:ARG:HG2	1:G:121:PRO:CG	1.82	1.07
3:A:73:ARG:HG2	3:A:78:GLY:HA3	1.31	1.07
1:G:60:SER:HB3	3:A:226:THR:HG21	1.28	1.05
1:G:60:SER:CB	3:A:226:THR:CG2	2.34	1.04
1:H:97:ALA:CB	1:H:118:TRP:HB3	1.88	1.02
1:G:60:SER:HB3	3:A:226:THR:HG22	1.41	1.00
1:G:60:SER:N	3:A:226:THR:HG21	1.78	0.99
3:B:226:THR:HG21	1:H:60:SER:HB3	0.96	0.96
1:H:98:ARG:O	1:H:118:TRP:HZ3	1.38	0.96
3:A:73:ARG:HG2	3:A:78:GLY:CA	1.96	0.95
1:H:97:ALA:CB	1:H:118:TRP:CB	2.33	0.94
1:H:97:ALA:CB	1:H:118:TRP:CE3	2.36	0.94
1:G:98:ARG:HG2	1:G:121:PRO:HG3	0.94	0.94
1:H:97:ALA:HB2	1:H:118:TRP:HB3	0.95	0.94
1:G:60:SER:CA	3:A:226:THR:HG21	1.98	0.92
1:G:32:ASN:HD21	1:G:98:ARG:HH21	1.03	0.92
1:G:97:ALA:HB3	1:G:118:TRP:CD2	2.04	0.92
3:A:73:ARG:H	3:A:80:PRO:HG3	1.45	0.82
1:H:112:ARG:O	2:L:32:TYR:HE1	1.62	0.82
3:A:73:ARG:CG	3:A:78:GLY:HA3	2.11	0.80
1:G:32:ASN:HD21	1:G:98:ARG:NH2	1.79	0.79
3:B:86:GLN:HE22	3:A:89:ARG:HH21	1.29	0.79
1:G:98:ARG:CD	1:G:121:PRO:HG3	2.14	0.77
1:H:97:ALA:HB3	1:H:118:TRP:CE2	2.14	0.77
3:B:86:GLN:NE2	3:A:89:ARG:HH21	1.85	0.75
3:B:475:LEU:O	3:B:479:LEU:HB3	1.88	0.73
3:A:73:ARG:HG2	3:A:78:GLY:C	2.13	0.73
1:H:97:ALA:HB3	1:H:118:TRP:CD1	2.21	0.73
3:C:475:LEU:O	3:C:479:LEU:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:475:LEU:O	3:A:479:LEU:HB3	1.88	0.72
1:H:98:ARG:C	1:H:118:TRP:CH2	2.67	0.71
1:G:97:ALA:HB3	1:G:118:TRP:CE3	2.26	0.71
3:B:86:GLN:NE2	3:A:89:ARG:NH2	2.38	0.71
3:A:244:HIS:HB3	4:F:16:THR:HG22	1.72	0.70
1:H:6:GLN:NE2	1:H:96:CYS:SG	2.65	0.70
1:H:98:ARG:HG3	1:H:121:PRO:CG	2.21	0.70
3:A:69:THR:HG22	1:H:72:ARG:HH12	1.58	0.69
3:A:200:GLN:NE2	3:A:272:MET:SD	2.66	0.69
3:C:200:GLN:NE2	3:C:272:MET:SD	2.66	0.69
3:C:73:ARG:HG2	3:C:78:GLY:HA3	1.75	0.68
3:B:200:GLN:NE2	3:B:272:MET:SD	2.66	0.68
3:B:73:ARG:HG2	3:B:78:GLY:HA3	1.75	0.68
3:A:105:CYS:SG	3:A:106:GLY:N	2.69	0.66
3:B:86:GLN:HE22	3:A:89:ARG:NH2	1.93	0.66
1:H:98:ARG:HG3	1:H:121:PRO:HG2	1.77	0.66
3:A:196:MET:HE1	4:D:12:LEU:HG	1.76	0.66
3:C:105:CYS:SG	3:C:106:GLY:N	2.69	0.66
2:I:1:ASP:OD1	2:I:1:ASP:N	2.29	0.66
3:B:105:CYS:SG	3:B:106:GLY:N	2.69	0.65
1:G:117:TRP:N	2:I:36:TYR:OH	2.31	0.64
3:B:76:THR:O	3:A:210:ARG:NH1	2.30	0.64
3:B:224:ALA:HB3	3:A:81:SER:HB3	1.80	0.64
1:G:60:SER:CA	3:A:226:THR:CG2	2.71	0.64
2:L:32:TYR:HB3	2:L:91:PHE:HB3	1.80	0.64
2:I:32:TYR:HB3	2:I:91:PHE:HB3	1.80	0.64
3:A:101:TRP:NE1	3:C:310:LYS:NZ	2.46	0.64
3:A:171:THR:HB	3:A:183:MET:O	1.97	0.64
4:D:55:THR:HA	4:D:60:ARG:HE	1.62	0.64
1:G:97:ALA:CB	1:G:118:TRP:CE3	2.80	0.64
4:E:55:THR:HA	4:E:60:ARG:HE	1.62	0.64
3:A:225:ASP:O	3:A:227:GLN:N	2.31	0.63
3:C:171:THR:HB	3:C:183:MET:O	1.97	0.63
3:B:305:LYS:H	3:B:386:GLN:HG3	1.64	0.63
3:B:171:THR:HB	3:B:183:MET:O	1.97	0.63
1:G:102:ALA:O	1:G:103:LEU:C	2.42	0.63
3:C:82:LEU:HD23	3:C:84:GLU:H	1.64	0.63
3:B:82:LEU:HD23	3:B:84:GLU:H	1.64	0.62
3:B:227:GLN:HA	1:H:66:GLY:HA2	1.80	0.62
3:A:305:LYS:H	3:A:386:GLN:HG3	1.64	0.62
3:C:305:LYS:H	3:C:386:GLN:HG3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4:ILE:HD13	3:A:9:ARG:HH22	1.65	0.62
1:G:33:TYR:OH	1:G:102:ALA:HB3	2.00	0.62
3:A:82:LEU:HD23	3:A:84:GLU:H	1.64	0.62
4:F:55:THR:HA	4:F:60:ARG:HE	1.62	0.61
1:H:33:TYR:OH	1:H:102:ALA:HB3	2.00	0.61
1:H:98:ARG:HE	1:H:121:PRO:HG3	1.65	0.61
3:B:4:ILE:HD13	3:B:9:ARG:HH22	1.65	0.61
3:B:78:GLY:HA2	3:A:56:LEU:HD13	1.82	0.61
3:C:4:ILE:HD13	3:C:9:ARG:HH22	1.65	0.61
3:B:228:GLY:O	3:A:86:GLN:NE2	2.34	0.61
2:L:3:GLN:HA	2:L:3:GLN:OE1	2.00	0.60
3:A:20:TRP:HA	3:A:287:LEU:O	2.01	0.60
1:H:102:ALA:O	1:H:103:LEU:C	2.42	0.60
3:B:78:GLY:H	3:A:56:LEU:HD22	1.66	0.60
3:C:20:TRP:HA	3:C:287:LEU:O	2.01	0.59
3:B:2:ARG:HH22	3:B:158:HIS:HB2	1.67	0.59
3:A:381:GLY:HA3	3:A:386:GLN:HB2	1.84	0.59
3:C:2:ARG:HH22	3:C:158:HIS:HB2	1.67	0.59
3:C:381:GLY:HA3	3:C:386:GLN:HB2	1.84	0.59
3:A:2:ARG:HH22	3:A:158:HIS:HB2	1.67	0.59
3:A:101:TRP:CD1	3:C:310:LYS:HZ1	2.21	0.59
3:B:3:CYS:O	3:B:9:ARG:NH2	2.36	0.58
1:G:97:ALA:HB3	1:G:118:TRP:CG	2.37	0.58
1:H:11:VAL:HG22	1:H:129:THR:HB	1.85	0.58
3:B:20:TRP:HA	3:B:287:LEU:O	2.01	0.58
1:G:32:ASN:ND2	1:G:98:ARG:HH21	1.87	0.58
1:G:97:ALA:HB2	1:G:118:TRP:HB3	1.84	0.58
3:B:381:GLY:HA3	3:B:386:GLN:HB2	1.84	0.58
3:A:3:CYS:O	3:A:9:ARG:NH2	2.36	0.58
3:A:101:TRP:NE1	3:C:310:LYS:HZ3	2.02	0.58
3:C:3:CYS:O	3:C:9:ARG:NH2	2.36	0.58
1:G:35:HIS:O	1:G:96:CYS:HA	2.03	0.58
3:B:199:LEU:O	3:B:205:ALA:HA	2.04	0.57
1:G:11:VAL:HG22	1:G:129:THR:HB	1.85	0.57
1:H:117:TRP:N	2:L:36:TYR:OH	2.37	0.57
2:I:38:GLN:HA	2:I:44:PRO:HB3	1.86	0.57
2:L:33:LEU:HB3	2:L:51:ALA:HB2	1.86	0.57
2:L:38:GLN:HA	2:L:44:PRO:HB3	1.86	0.57
3:C:199:LEU:O	3:C:205:ALA:HA	2.04	0.56
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.87	0.56
1:H:98:ARG:HG3	1:H:121:PRO:HG3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:34:ASN:HD22	2:L:49:TYR:HA	1.70	0.56
2:I:33:LEU:HB3	2:I:51:ALA:HB2	1.86	0.56
2:I:34:ASN:HD22	2:I:49:TYR:HA	1.70	0.56
3:A:199:LEU:O	3:A:205:ALA:HA	2.04	0.56
3:B:227:GLN:CG	1:H:68:ILE:O	2.54	0.56
3:B:81:SER:HB3	3:A:224:ALA:HB3	1.86	0.56
3:A:204:LYS:HE2	3:C:251:VAL:HG13	1.88	0.55
1:G:32:ASN:ND2	1:G:98:ARG:HE	2.05	0.55
1:G:39:GLN:HB2	1:G:45:LEU:HD23	1.87	0.55
3:B:99:ARG:HA	3:B:103:ASN:HD22	1.72	0.55
1:H:112:ARG:O	2:L:32:TYR:CE1	2.51	0.55
3:A:101:TRP:HD1	3:A:108:PHE:CZ	2.24	0.55
2:I:2:ILE:HD11	2:I:93:ASP:HB2	1.88	0.55
3:C:378:ILE:HG23	3:C:389:LEU:HB2	1.88	0.55
1:G:60:SER:N	3:A:226:THR:CG2	2.61	0.55
3:B:226:THR:HG21	1:H:60:SER:CA	2.36	0.55
3:A:99:ARG:HA	3:A:103:ASN:HD22	1.72	0.55
3:B:99:ARG:HH11	3:B:105:CYS:HB3	1.72	0.54
3:B:378:ILE:HG23	3:B:389:LEU:HB2	1.88	0.54
1:G:109:THR:HA	2:I:91:PHE:HE2	1.73	0.54
3:B:227:GLN:HG3	1:H:68:ILE:O	2.07	0.54
3:C:99:ARG:HH11	3:C:105:CYS:HB3	1.73	0.54
2:I:3:GLN:OE1	2:I:3:GLN:HA	1.98	0.54
3:C:99:ARG:HA	3:C:103:ASN:HD22	1.72	0.54
3:C:302:CYS:SG	3:C:303:THR:N	2.81	0.54
3:A:378:ILE:HG23	3:A:389:LEU:HB2	1.88	0.54
1:H:98:ARG:C	1:H:118:TRP:CZ3	2.76	0.53
3:A:99:ARG:HH11	3:A:105:CYS:HB3	1.72	0.53
3:B:302:CYS:SG	3:B:303:THR:N	2.81	0.53
1:H:33:TYR:O	1:H:98:ARG:HA	2.08	0.53
3:B:175:LEU:HB2	3:B:179:GLY:HA3	1.91	0.53
3:A:302:CYS:SG	3:A:303:THR:N	2.81	0.52
1:H:110:THR:N	1:H:111:PRO:CD	2.73	0.52
3:B:225:ASP:O	3:B:227:GLN:N	2.42	0.52
3:B:19:SER:HB3	3:B:289:MET:H	1.74	0.52
3:A:19:SER:HB3	3:A:289:MET:H	1.74	0.52
3:A:62:GLU:HB3	3:A:122:LYS:HB2	1.92	0.52
2:L:20:THR:HA	2:L:73:PHE:O	2.10	0.52
3:A:102:GLY:HA3	3:C:152:GLY:HA3	1.92	0.52
3:C:175:LEU:HB2	3:C:179:GLY:HA3	1.91	0.52
3:A:175:LEU:HB2	3:A:179:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:SER:HB3	3:C:289:MET:H	1.74	0.52
3:C:62:GLU:HB3	3:C:122:LYS:HB2	1.92	0.51
3:C:180:THR:HB	3:C:291:LYS:HB3	1.93	0.51
2:I:20:THR:HA	2:I:73:PHE:O	2.10	0.51
3:B:180:THR:HB	3:B:291:LYS:HB3	1.93	0.51
2:L:21:PHE:HZ	2:L:104:LEU:HD11	1.76	0.51
1:G:98:ARG:HG3	1:G:98:ARG:O	2.10	0.51
3:A:50:ALA:HB3	3:A:276:ASN:HD22	1.76	0.51
3:B:466:ILE:HD12	3:B:469:ASN:HD22	1.76	0.51
3:C:466:ILE:HD12	3:C:469:ASN:HD22	1.76	0.51
3:B:50:ALA:HB3	3:B:276:ASN:HD22	1.76	0.51
3:C:50:ALA:HB3	3:C:276:ASN:HD22	1.76	0.51
3:C:310:LYS:HD2	3:C:323:ARG:HB2	1.93	0.50
3:A:180:THR:HB	3:A:291:LYS:HB3	1.93	0.50
1:H:97:ALA:HB1	1:H:118:TRP:HE3	1.56	0.50
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.93	0.50
2:I:21:PHE:HZ	2:I:104:LEU:HD11	1.76	0.50
2:I:35:TRP:HB2	2:I:48:ILE:HB	1.93	0.50
1:G:117:TRP:CD1	2:I:89:GLN:HE22	2.29	0.50
3:C:181:VAL:HG22	3:C:292:LEU:HD11	1.93	0.50
3:A:321:VAL:HG12	3:A:368:GLU:HB3	1.93	0.50
3:B:300:SER:HG	3:B:333:CYS:HG	1.59	0.50
3:A:466:ILE:HD12	3:A:469:ASN:HD22	1.76	0.50
2:I:1:ASP:N	2:I:95:PRO:CG	2.75	0.50
3:A:181:VAL:HG22	3:A:292:LEU:HD11	1.93	0.50
1:H:35:HIS:O	1:H:96:CYS:HA	2.11	0.50
1:G:117:TRP:HA	1:G:118:TRP:CD2	2.46	0.50
1:G:32:ASN:N	1:G:101:ARG:HE	2.10	0.49
3:B:62:GLU:HB3	3:B:122:LYS:HB2	1.92	0.49
2:I:2:ILE:CG2	2:I:27:GLN:CG	2.90	0.49
3:B:321:VAL:HG12	3:B:368:GLU:HB3	1.93	0.49
3:A:227:GLN:O	3:A:227:GLN:HG2	2.12	0.49
3:B:226:THR:O	1:H:66:GLY:N	2.45	0.49
2:I:1:ASP:H2	2:I:95:PRO:CG	2.26	0.49
3:B:171:THR:CB	3:B:183:MET:O	2.60	0.49
3:A:101:TRP:HD1	3:A:108:PHE:CE2	2.30	0.49
3:C:321:VAL:HG12	3:C:368:GLU:HB3	1.93	0.49
3:B:1:MET:HE1	3:B:146:GLY:H	1.78	0.49
3:B:300:SER:OG	3:B:333:CYS:SG	2.71	0.49
4:D:66:LEU:HD23	4:F:66:LEU:HB3	1.94	0.49
3:C:1:MET:HE1	3:C:146:GLY:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:TRP:HA	1:H:118:TRP:CD2	2.47	0.49
2:I:94:LEU:HA	2:I:96:ILE:HG13	1.95	0.49
1:G:4:LEU:HD12	1:G:122:TRP:HA	1.95	0.48
1:G:32:ASN:ND2	1:G:98:ARG:NH2	2.54	0.48
1:H:32:ASN:N	1:H:101:ARG:HE	2.10	0.48
2:L:94:LEU:HA	2:L:96:ILE:HG13	1.95	0.48
3:C:300:SER:OG	3:C:333:CYS:SG	2.71	0.48
3:A:251:VAL:HG13	3:C:204:LYS:HE2	1.93	0.48
3:A:171:THR:CB	3:A:183:MET:O	2.60	0.48
4:E:14:THR:HG23	4:E:16:THR:H	1.79	0.48
4:D:4:LEU:HD21	4:F:4:LEU:HD21	1.96	0.48
3:C:171:THR:CB	3:C:183:MET:O	2.60	0.48
3:A:300:SER:OG	3:A:333:CYS:SG	2.71	0.48
1:H:30:THR:HB	1:H:54:ARG:HB2	1.95	0.48
3:C:446:ALA:O	3:C:449:SER:N	2.47	0.48
1:G:122:TRP:HZ2	2:I:43:ALA:HA	1.79	0.47
3:A:267:ALA:HB2	4:D:7:HIS:CD2	2.48	0.47
4:F:14:THR:HG23	4:F:16:THR:H	1.79	0.47
3:B:233:GLN:HB3	3:B:234:LYS:H	1.49	0.47
3:A:1:MET:HE1	3:A:146:GLY:H	1.78	0.47
3:B:446:ALA:O	3:B:449:SER:N	2.47	0.47
1:G:30:THR:HB	1:G:54:ARG:HB2	1.96	0.47
1:H:4:LEU:HD12	1:H:122:TRP:HA	1.95	0.47
1:H:117:TRP:CD1	2:L:89:GLN:HE22	2.32	0.47
3:C:310:LYS:HD2	3:C:323:ARG:CB	2.45	0.47
1:H:4:LEU:HD23	1:H:24:ALA:HA	1.97	0.47
1:G:91:THR:HG23	1:G:129:THR:HA	1.97	0.47
3:A:446:ALA:O	3:A:449:SER:N	2.47	0.47
1:H:6:GLN:HE22	1:H:95:TYR:HA	1.79	0.47
1:G:6:GLN:NE2	1:G:96:CYS:SG	2.87	0.46
1:G:91:THR:HA	1:G:128:VAL:O	2.16	0.46
1:G:6:GLN:HE22	1:G:95:TYR:HA	1.79	0.46
2:I:1:ASP:N	2:I:95:PRO:HG3	2.30	0.46
3:C:198:LEU:HB3	3:C:200:GLN:HE22	1.81	0.46
4:D:14:THR:HG23	4:D:16:THR:H	1.79	0.46
1:H:98:ARG:HE	1:H:121:PRO:CG	2.27	0.46
3:A:201:MET:HB2	3:A:260:MET:HE1	1.98	0.46
1:H:54:ARG:H	1:H:101:ARG:HH22	1.64	0.46
1:G:54:ARG:H	1:G:101:ARG:HH22	1.64	0.46
1:H:91:THR:HA	1:H:128:VAL:O	2.16	0.46
1:G:38:ARG:HH22	1:G:90:ASP:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:ASP:O	1:H:114:GLY:C	2.58	0.46
1:G:4:LEU:HD23	1:G:24:ALA:HA	1.97	0.46
2:I:43:ALA:HA	2:I:44:PRO:HD3	1.78	0.46
4:E:50:ALA:HA	4:E:63:ILE:HD11	1.98	0.46
3:A:198:LEU:HB3	3:A:200:GLN:HE22	1.81	0.46
4:D:50:ALA:HA	4:D:63:ILE:HD11	1.98	0.46
3:B:201:MET:HB2	3:B:260:MET:HE1	1.98	0.45
3:A:253:LEU:O	3:C:261:HIS:ND1	2.49	0.45
3:C:170:ILE:C	3:C:183:MET:O	2.59	0.45
1:H:38:ARG:HH22	1:H:90:ASP:HA	1.81	0.45
3:B:198:LEU:HB3	3:B:200:GLN:HE22	1.81	0.45
3:A:73:ARG:HE	3:A:78:GLY:HA3	1.82	0.45
4:F:50:ALA:HA	4:F:63:ILE:HD11	1.98	0.45
2:I:21:PHE:O	2:I:72:THR:HA	2.16	0.45
3:B:170:ILE:C	3:B:183:MET:O	2.59	0.45
3:C:233:GLN:HB3	3:C:234:LYS:H	1.49	0.45
2:L:21:PHE:O	2:L:72:THR:HA	2.15	0.45
3:A:170:ILE:C	3:A:183:MET:O	2.59	0.45
2:L:2:ILE:HG23	2:L:2:ILE:O	2.16	0.45
1:H:91:THR:HG23	1:H:129:THR:HA	1.98	0.45
3:B:314:GLU:HA	3:B:320:ILE:HG22	1.99	0.45
4:D:16:THR:HG22	3:C:244:HIS:HB3	1.98	0.44
3:C:310:LYS:CB	3:C:323:ARG:HB3	2.47	0.44
3:B:231:TRP:HB2	3:B:234:LYS:HE3	1.99	0.44
2:L:2:ILE:HG12	2:L:90:GLN:OE1	2.17	0.44
3:B:72:SER:OG	3:B:99:ARG:NH2	2.51	0.44
3:A:225:ASP:O	3:A:228:GLY:N	2.51	0.44
3:C:72:SER:OG	3:C:99:ARG:NH2	2.51	0.44
3:A:209:HIS:NE2	4:D:10:MET:SD	2.84	0.44
3:C:201:MET:HB2	3:C:260:MET:HE1	1.98	0.44
3:C:314:GLU:HA	3:C:320:ILE:HG22	1.99	0.44
3:C:231:TRP:HB2	3:C:234:LYS:HE3	1.99	0.44
1:G:98:ARG:CD	1:G:121:PRO:CG	2.93	0.44
3:C:459:ILE:HA	3:C:462:VAL:HG12	1.99	0.44
3:A:314:GLU:HA	3:A:320:ILE:HG22	2.00	0.44
1:H:34:ILE:HG13	1:H:79:VAL:HG21	2.00	0.44
3:A:72:SER:OG	3:A:99:ARG:NH2	2.51	0.43
3:A:73:ARG:HG3	3:A:77:GLN:O	2.18	0.43
3:A:209:HIS:CD2	4:D:10:MET:HB3	2.53	0.43
3:C:98:ASP:HA	3:C:110:LYS:HA	2.00	0.43
3:C:310:LYS:HZ2	3:C:321:VAL:HG23	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:TYR:CE2	1:G:101:ARG:HA	2.53	0.43
3:B:98:ASP:HA	3:B:110:LYS:HA	2.00	0.43
3:A:80:PRO:HB2	3:A:114:VAL:HG13	2.01	0.43
3:B:459:ILE:HA	3:B:462:VAL:HG12	1.99	0.43
3:A:75:PRO:HG3	3:A:99:ARG:HB2	2.00	0.43
3:A:75:PRO:HB3	3:A:109:GLY:HA3	2.00	0.43
3:A:459:ILE:HA	3:A:462:VAL:HG12	1.99	0.43
1:G:97:ALA:HB1	1:G:98:ARG:H	1.67	0.43
1:G:102:ALA:CB	1:G:108:TYR:CD2	3.01	0.43
3:A:98:ASP:HA	3:A:110:LYS:HA	2.00	0.43
3:B:80:PRO:HB2	3:B:114:VAL:HG13	2.01	0.43
3:C:75:PRO:HB3	3:C:109:GLY:HA3	2.00	0.43
1:H:33:TYR:CE2	1:H:101:ARG:HA	2.53	0.43
1:G:34:ILE:HG13	1:G:79:VAL:HG21	2.00	0.43
3:B:175:LEU:HD12	3:B:179:GLY:HA3	2.01	0.43
3:C:175:LEU:HD12	3:C:179:GLY:HA3	2.01	0.43
3:A:73:ARG:N	3:A:80:PRO:HG3	2.24	0.42
2:I:39:LYS:HA	2:I:40:PRO:HD3	1.91	0.42
1:H:102:ALA:CB	1:H:108:TYR:CD2	3.01	0.42
3:B:75:PRO:HB3	3:B:109:GLY:HA3	2.00	0.42
3:A:73:ARG:CG	3:A:77:GLN:O	2.67	0.42
4:D:59:GLN:HE21	4:F:59:GLN:HE21	1.67	0.42
3:C:75:PRO:HG3	3:C:99:ARG:HB2	2.00	0.42
3:B:75:PRO:HG3	3:B:99:ARG:HB2	2.00	0.42
1:G:117:TRP:HB3	2:I:89:GLN:OE1	2.20	0.42
3:B:227:GLN:NE2	1:H:69:THR:OG1	2.53	0.42
4:D:66:LEU:HD21	4:F:67:LEU:HD12	2.01	0.42
2:I:2:ILE:CG2	2:I:27:GLN:HB2	2.50	0.42
3:A:296:GLY:O	3:A:355:ASN:ND2	2.53	0.42
3:A:175:LEU:HD12	3:A:179:GLY:HA3	2.00	0.42
3:B:296:GLY:O	3:B:355:ASN:ND2	2.53	0.42
3:A:73:ARG:NE	3:A:78:GLY:HA3	2.35	0.42
3:C:80:PRO:HB2	3:C:114:VAL:HG13	2.01	0.42
1:G:72:ARG:HH12	3:B:69:THR:HG22	1.84	0.42
3:A:201:MET:HG3	3:A:202:GLU:H	1.85	0.42
3:A:290:ASP:O	3:A:292:LEU:N	2.53	0.42
3:C:201:MET:HG3	3:C:202:GLU:H	1.85	0.42
1:G:98:ARG:O	1:G:118:TRP:HZ3	2.02	0.41
3:B:290:ASP:O	3:B:292:LEU:N	2.53	0.41
3:A:312:ILE:HG13	3:A:313:ALA:H	1.85	0.41
3:A:373:PHE:O	3:A:393:LYS:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:PRO:HB3	1:G:127:LEU:HB3	2.02	0.41
1:G:98:ARG:O	1:G:118:TRP:CZ3	2.73	0.41
3:A:101:TRP:C	3:A:104:GLY:H	2.29	0.41
1:G:51:ILE:HD12	1:G:70:MET:HB3	2.02	0.41
3:B:81:SER:HB2	3:A:222:PRO:HB2	2.02	0.41
3:B:201:MET:HG3	3:B:202:GLU:H	1.85	0.41
3:B:380:ILE:HD11	3:B:387:LEU:HB3	2.02	0.41
3:A:363:SER:HA	3:A:364:PRO:HD3	1.87	0.41
3:C:290:ASP:O	3:C:292:LEU:N	2.53	0.41
3:C:312:ILE:HG13	3:C:313:ALA:H	1.86	0.41
3:A:380:ILE:HD11	3:A:387:LEU:HB3	2.02	0.41
1:G:60:SER:C	3:A:226:THR:HG23	2.45	0.41
3:B:144:HIS:HB3	3:B:145:SER:H	1.70	0.41
3:B:312:ILE:HG13	3:B:313:ALA:H	1.86	0.41
3:C:225:ASP:O	3:C:228:GLY:N	2.35	0.41
3:C:380:ILE:HD11	3:C:387:LEU:HB3	2.03	0.41
1:H:51:ILE:HD12	1:H:70:MET:HB3	2.02	0.41
3:A:91:VAL:O	3:A:116:CYS:HA	2.20	0.41
3:C:296:GLY:O	3:C:355:ASN:ND2	2.53	0.41
1:H:9:PRO:HB3	1:H:127:LEU:HB3	2.01	0.41
2:I:2:ILE:HG23	2:I:27:GLN:HG3	2.02	0.41
3:B:91:VAL:O	3:B:116:CYS:HA	2.20	0.41
3:A:122:LYS:O	3:A:124:ASN:ND2	2.54	0.41
3:C:99:ARG:HB3	3:C:105:CYS:SG	2.61	0.41
3:C:373:PHE:O	3:C:393:LYS:O	2.38	0.41
3:B:122:LYS:O	3:B:124:ASN:ND2	2.54	0.41
3:B:373:PHE:O	3:B:393:LYS:O	2.38	0.41
3:C:485:VAL:O	3:C:489:LEU:HB2	2.21	0.41
3:B:270:ILE:HD12	3:B:270:ILE:HA	1.89	0.40
3:B:298:SER:O	3:B:298:SER:OG	2.33	0.40
3:A:101:TRP:CD1	3:C:310:LYS:NZ	2.88	0.40
3:A:239:THR:O	3:A:251:VAL:HB	2.21	0.40
4:D:31:ARG:NH1	4:F:4:LEU:HD22	2.36	0.40
3:C:73:ARG:H	3:C:80:PRO:HG3	1.86	0.40
3:C:239:THR:O	3:C:251:VAL:HB	2.21	0.40
2:L:6:GLN:NE2	2:L:86:TYR:O	2.44	0.40
2:L:37:GLN:HB3	2:L:47:LEU:HD11	2.02	0.40
3:A:462:VAL:HG23	4:D:58:PHE:CZ	2.55	0.40
3:A:485:VAL:O	3:A:489:LEU:HB2	2.21	0.40
3:C:91:VAL:O	3:C:116:CYS:HA	2.20	0.40
2:I:22:THR:HA	2:I:71:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:60:CYS:HA	3:A:124:ASN:HD22	1.87	0.40
2:L:22:THR:HA	2:L:71:PHE:O	2.21	0.40
2:L:16:GLY:N	2:L:78:LEU:O	2.50	0.40
2:L:21:PHE:HB2	2:L:73:PHE:HB3	2.04	0.40
3:C:60:CYS:HA	3:C:124:ASN:HD22	1.87	0.40
3:C:122:LYS:O	3:C:124:ASN:ND2	2.54	0.40
2:L:4:LEU:HD22	2:L:90:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	130/132 (98%)	110 (85%)	18 (14%)	2 (2%)	8	38
1	H	130/132 (98%)	110 (85%)	18 (14%)	2 (2%)	8	38
2	I	105/107 (98%)	94 (90%)	8 (8%)	3 (3%)	3	24
2	L	105/107 (98%)	94 (90%)	9 (9%)	2 (2%)	6	32
3	A	493/495 (100%)	365 (74%)	110 (22%)	18 (4%)	2	20
3	B	493/495 (100%)	365 (74%)	111 (22%)	17 (3%)	3	21
3	C	493/495 (100%)	368 (75%)	109 (22%)	16 (3%)	3	22
4	D	70/72 (97%)	60 (86%)	10 (14%)	0	100	100
4	E	70/72 (97%)	60 (86%)	10 (14%)	0	100	100
4	F	70/72 (97%)	60 (86%)	10 (14%)	0	100	100
All	All	2159/2179 (99%)	1686 (78%)	413 (19%)	60 (3%)	6	25

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	291	LYS
3	B	478	SER
3	A	226	THR
3	A	291	LYS
3	A	478	SER
3	C	291	LYS
3	C	478	SER
1	H	106	ASP
3	B	57	ARG
3	B	226	THR
3	B	298	SER
3	A	57	ARG
3	A	298	SER
3	C	57	ARG
3	C	298	SER
3	B	233	GLN
3	B	290	ASP
3	A	73	ARG
3	A	233	GLN
3	A	290	ASP
3	C	233	GLN
3	C	290	ASP
1	G	113	ASP
2	I	30	ARG
3	B	319	THR
3	B	413	ALA
3	B	447	ALA
3	B	479	LEU
3	A	319	THR
3	A	413	ALA
3	A	447	ALA
3	A	479	LEU
3	C	217	PRO
3	C	319	THR
3	C	413	ALA
3	C	447	ALA
3	C	479	LEU
2	L	30	ARG
1	G	118	TRP
2	I	2	ILE
3	B	217	PRO
3	B	238	VAL
3	A	217	PRO

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Mol	Chain	Res	Type
3	A	238	VAL
3	C	238	VAL
1	H	118	TRP
2	I	95	PRO
2	L	95	PRO
3	B	170	ILE
3	A	170	ILE
3	C	170	ILE
3	B	218	LEU
3	B	414	ILE
3	A	218	LEU
3	A	414	ILE
3	C	218	LEU
3	C	414	ILE
3	B	219	PRO
3	A	219	PRO
3	C	219	PRO

5.3.2 Protein sidechains [i](#)

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	G	105/109 (96%)	104 (99%)	1 (1%)	68	75
1	H	105/109 (96%)	103 (98%)	2 (2%)	50	66
2	I	94/94 (100%)	91 (97%)	3 (3%)	34	56
2	L	94/94 (100%)	92 (98%)	2 (2%)	47	65
3	A	369/419 (88%)	365 (99%)	4 (1%)	65	73
3	B	369/419 (88%)	365 (99%)	4 (1%)	65	73
3	C	368/419 (88%)	364 (99%)	4 (1%)	65	73
4	D	56/60 (93%)	56 (100%)	0	100	100
4	E	56/60 (93%)	56 (100%)	0	100	100
4	F	55/60 (92%)	55 (100%)	0	100	100
All	All	1671/1843 (91%)	1651 (99%)	20 (1%)	61	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	50	VAL
2	I	1	ASP
2	I	2	ILE
2	I	3	GLN
3	B	237	LEU
3	B	238	VAL
3	B	380	ILE
3	B	382	VAL
3	A	237	LEU
3	A	238	VAL
3	A	380	ILE
3	A	382	VAL
3	C	237	LEU
3	C	238	VAL
3	C	380	ILE
3	C	382	VAL
1	H	50	VAL
1	H	98	ARG
2	L	1	ASP
2	L	83	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	6	GLN
1	G	32	ASN
2	I	34	ASN
3	B	86	GLN
3	B	103	ASN
3	B	124	ASN
3	B	200	GLN
3	B	227	GLN
3	B	316	GLN
3	B	400	GLN
3	B	469	ASN
3	A	103	ASN
3	A	124	ASN
3	A	200	GLN
3	A	282	HIS
3	A	316	GLN
3	A	400	GLN

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Mol	Chain	Res	Type
3	A	469	ASN
4	D	59	GLN
3	C	103	ASN
3	C	124	ASN
3	C	200	GLN
3	C	400	GLN
3	C	469	ASN
1	H	6	GLN
2	L	34	ASN
2	L	37	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	J	1	3,5	14,14,15	0.44	0	17,19,21	1.07	1 (5%)
5	NAG	J	2	5	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	K	1	3,5	14,14,15	0.64	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	K	2	5	14,14,15	0.36	0	17,19,21	0.48	0
5	NAG	M	1	3,5	14,14,15	0.30	0	17,19,21	1.10	1 (5%)
5	NAG	M	2	5	14,14,15	0.23	0	17,19,21	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	4/6/23/26	0/1/1/1
5	NAG	K	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	3/6/23/26	0/1/1/1
5	NAG	M	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	1	NAG	C1-C2	2.15	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1	NAG	C1-O5-C5	4.16	117.76	112.19
5	J	1	NAG	C1-O5-C5	3.72	117.17	112.19
5	K	1	NAG	C1-O5-C5	3.36	116.69	112.19

There are no chirality outliers.

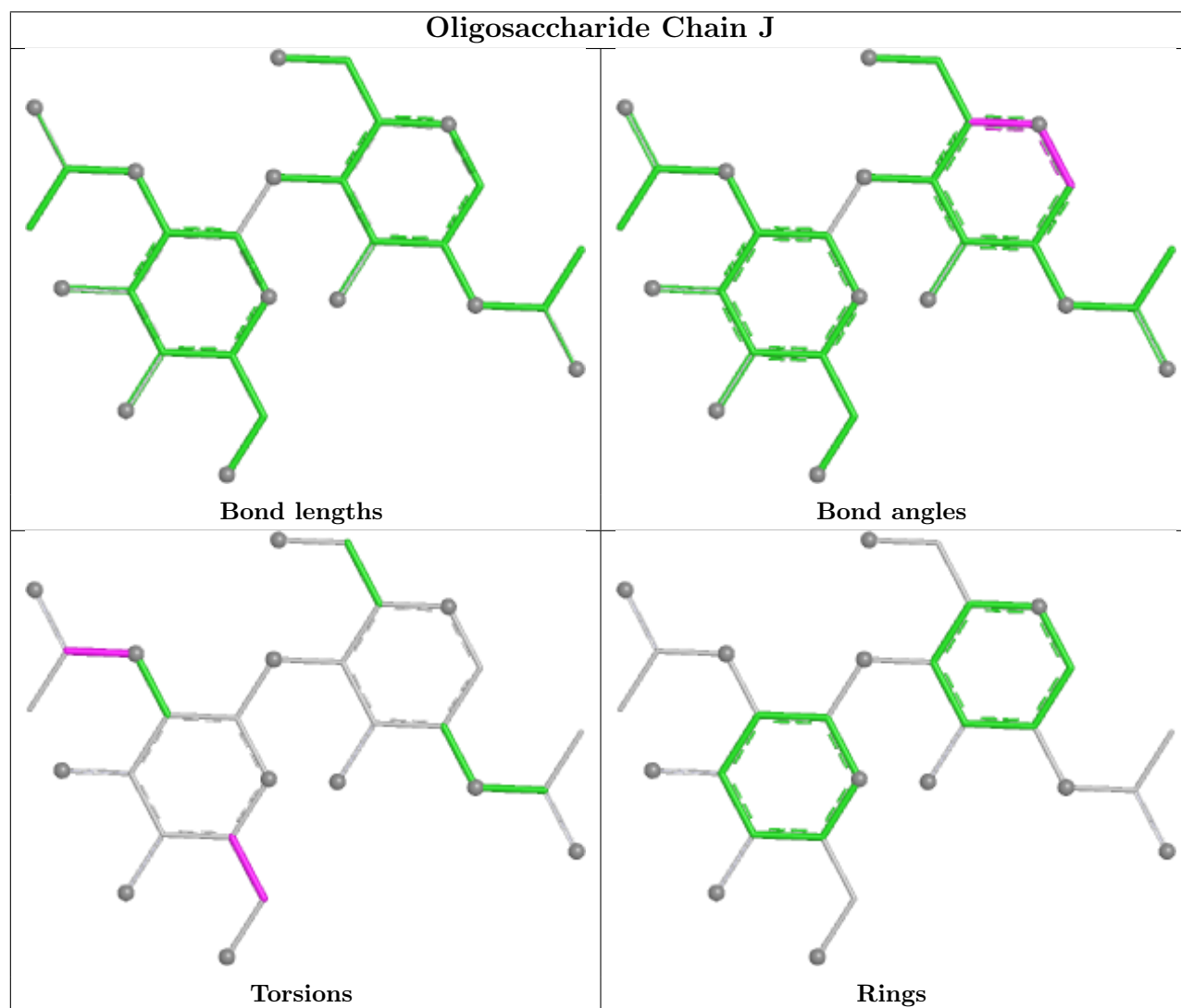
All (11) torsion outliers are listed below:

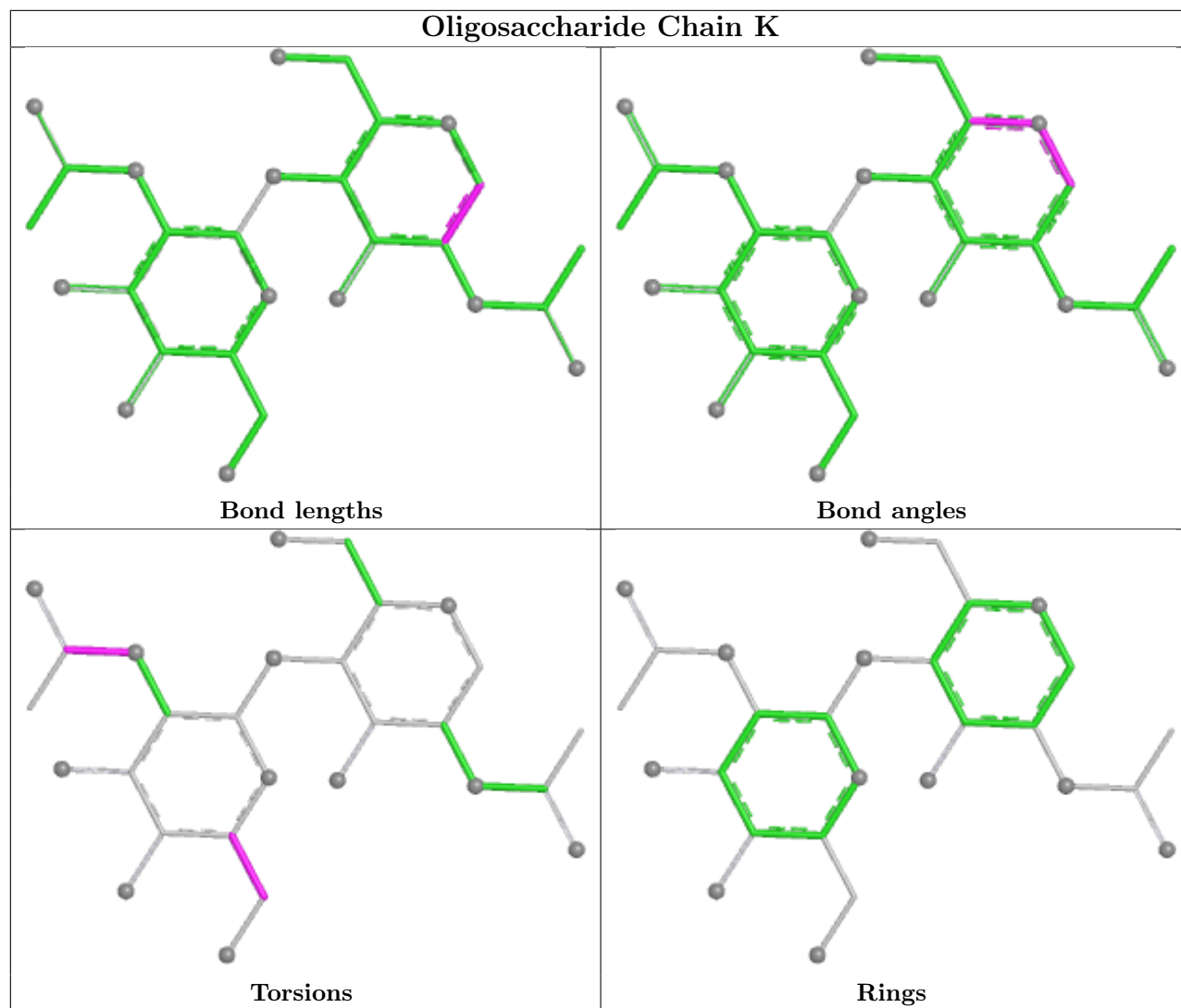
Mol	Chain	Res	Type	Atoms
5	J	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	K	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6

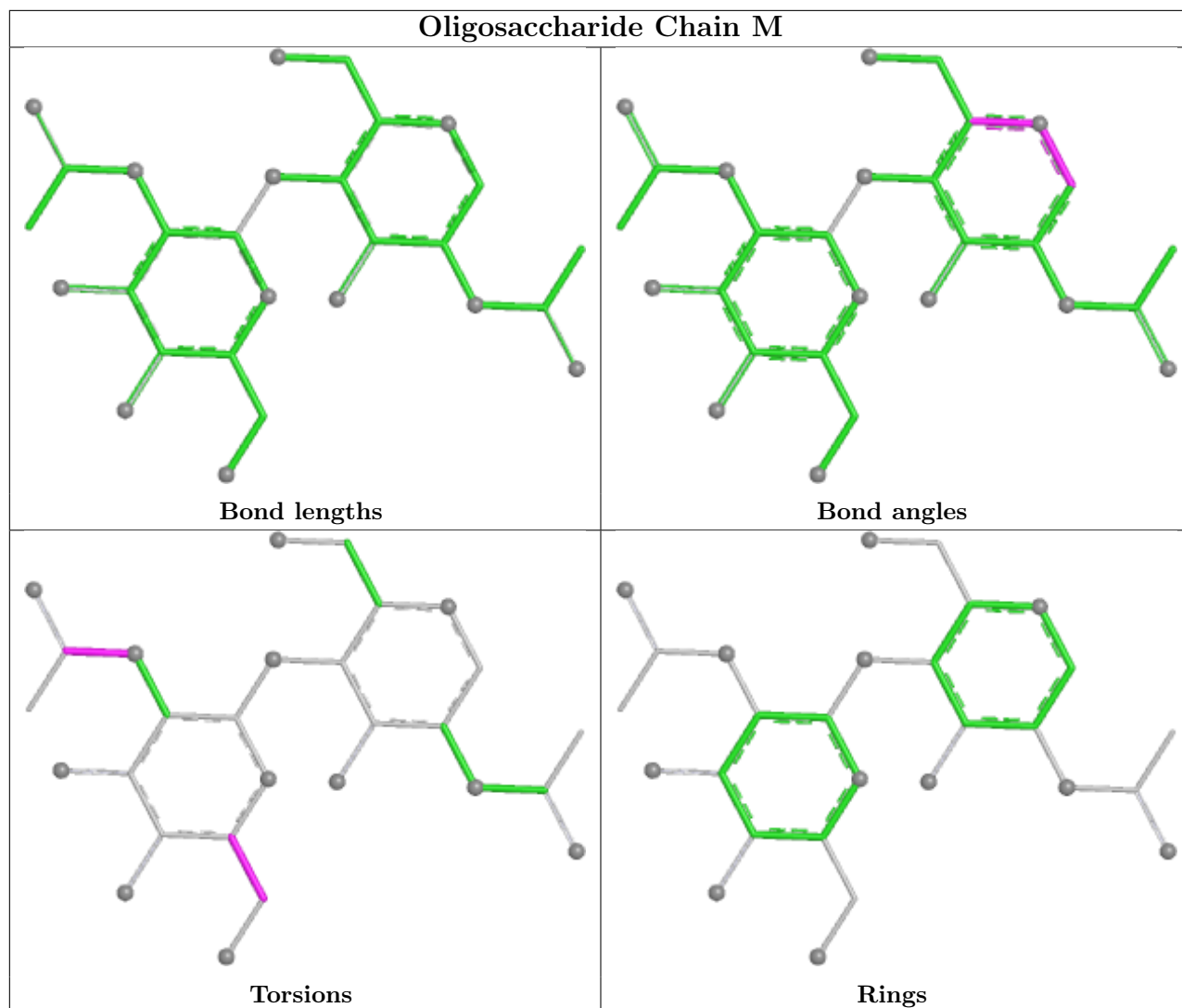
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	501	3	14,14,15	0.47	0	17,19,21	0.57	0
6	NAG	B	501	3	14,14,15	0.24	0	17,19,21	0.65	1 (5%)
6	NAG	A	501	3	14,14,15	0.35	0	17,19,21	0.60	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	501	3	-	4/6/23/26	0/1/1/1
6	NAG	B	501	3	-	2/6/23/26	0/1/1/1
6	NAG	A	501	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	NAG	C1-O5-C5	2.25	115.20	112.19
6	A	501	NAG	C1-O5-C5	2.05	114.94	112.19

There are no chirality outliers.

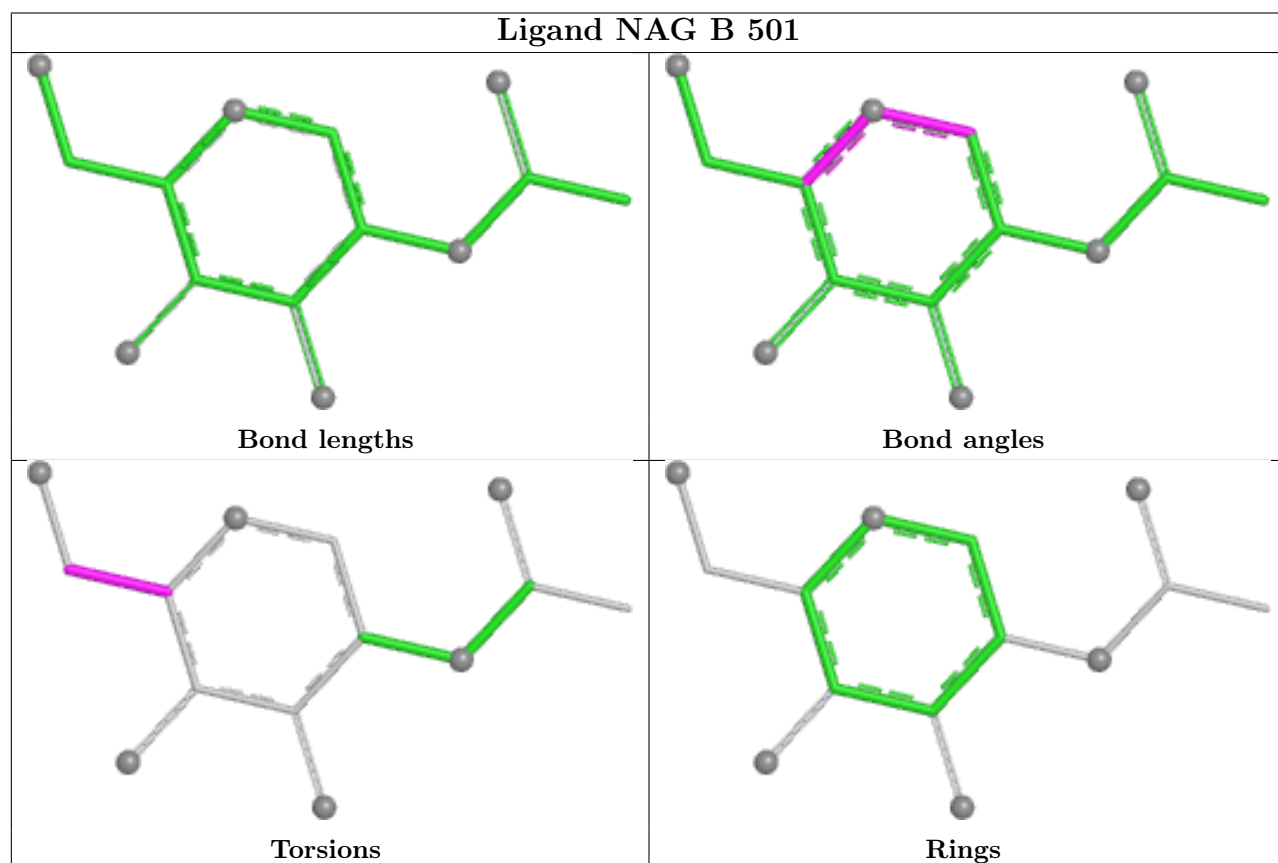
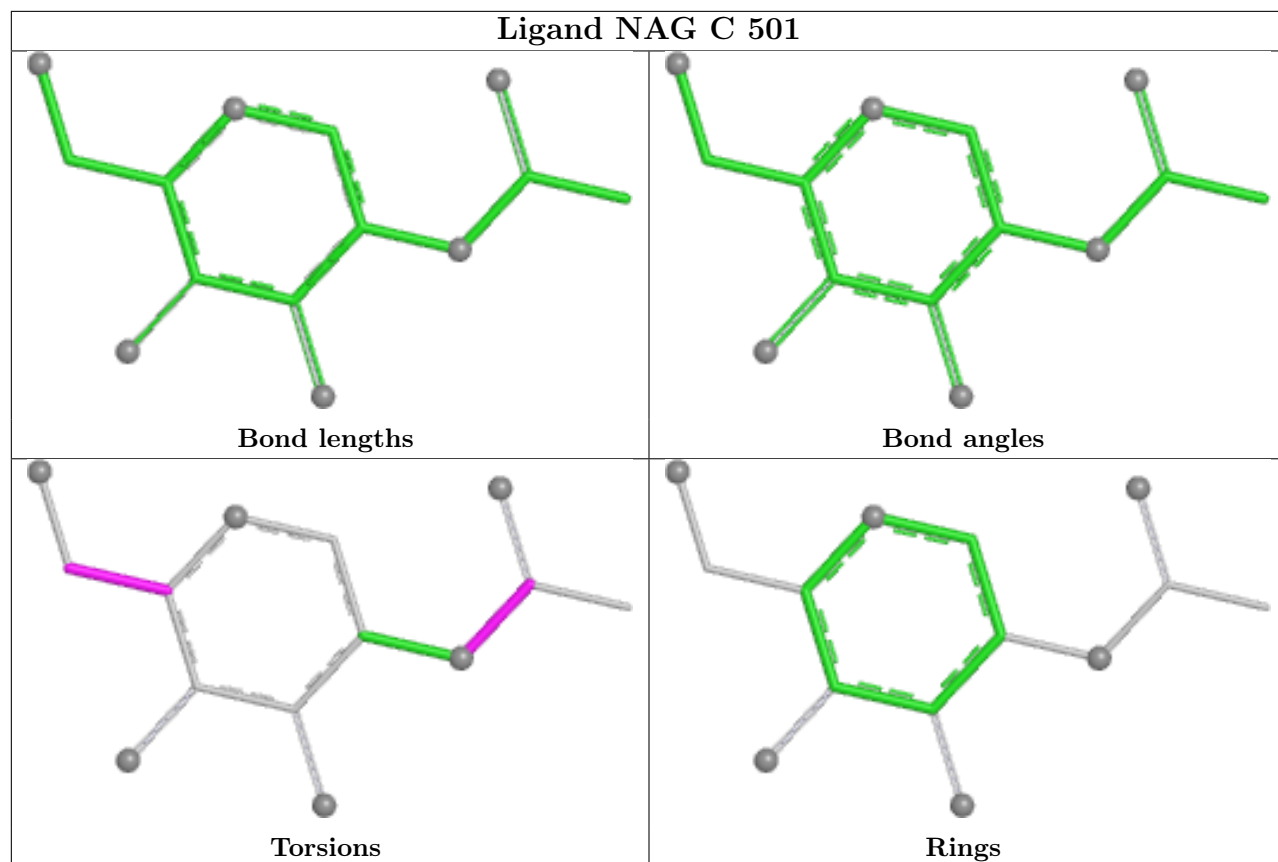
All (6) torsion outliers are listed below:

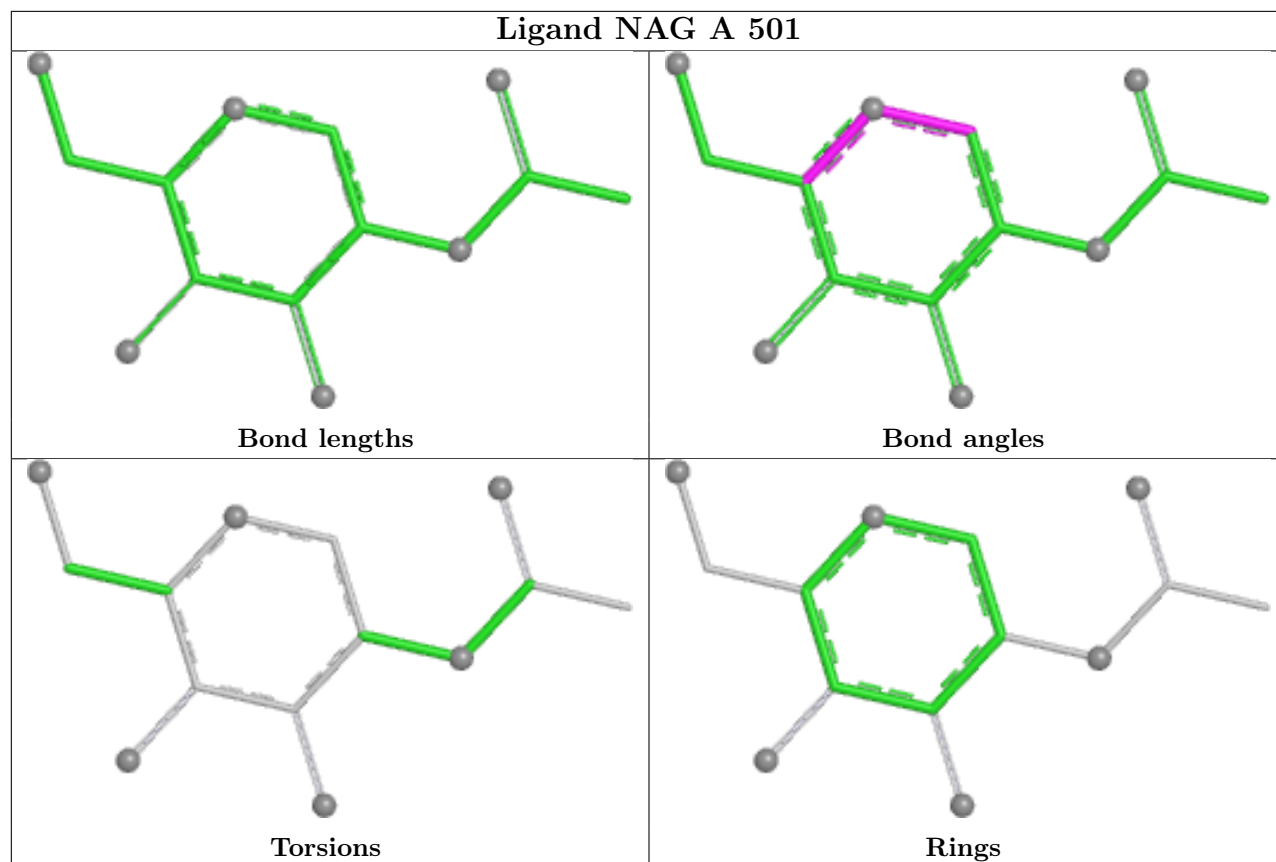
Mol	Chain	Res	Type	Atoms
6	B	501	NAG	O5-C5-C6-O6
6	B	501	NAG	C4-C5-C6-O6
6	C	501	NAG	O5-C5-C6-O6
6	C	501	NAG	C4-C5-C6-O6
6	C	501	NAG	C8-C7-N2-C2
6	C	501	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 [\(i\)](#)

There are no chain breaks in this entry.

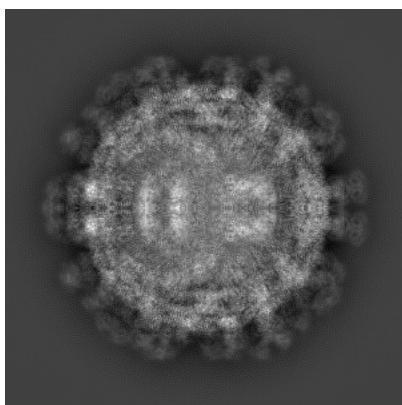
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30194. These allow visual inspection of the internal detail of the map and identification of artifacts.

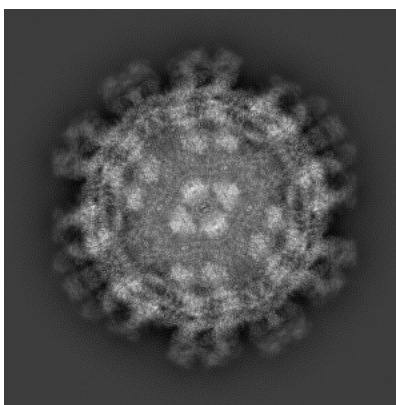
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

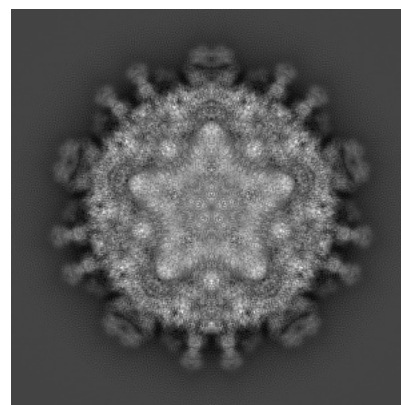
6.1.1 Primary map



X



Y

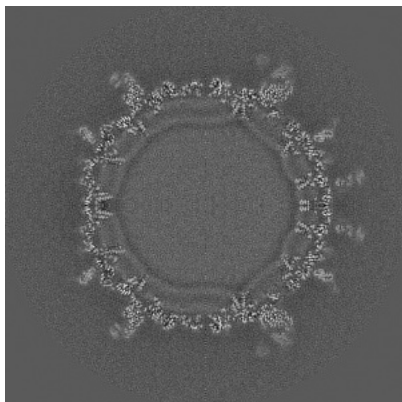


Z

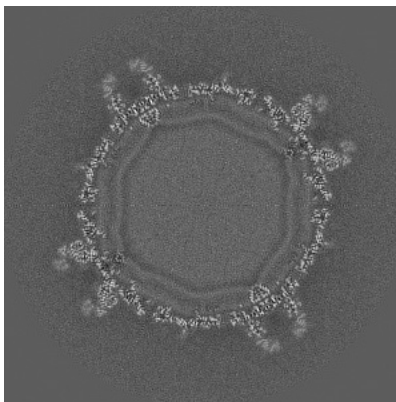
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

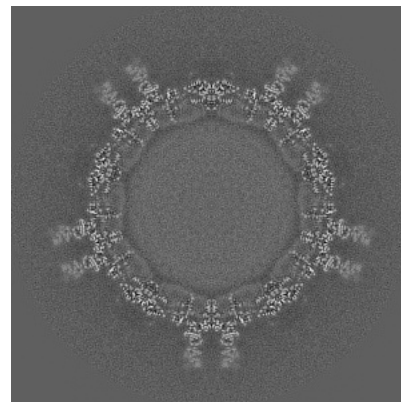
6.2.1 Primary map



X Index: 212



Y Index: 212

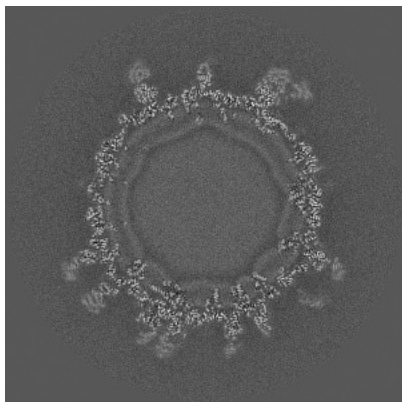


Z Index: 212

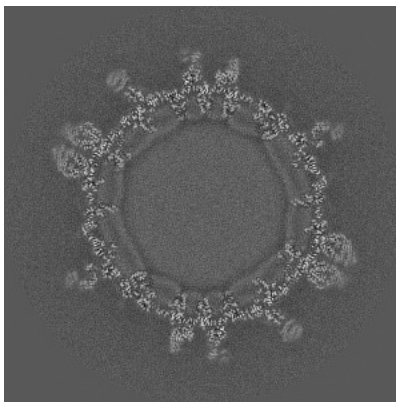
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

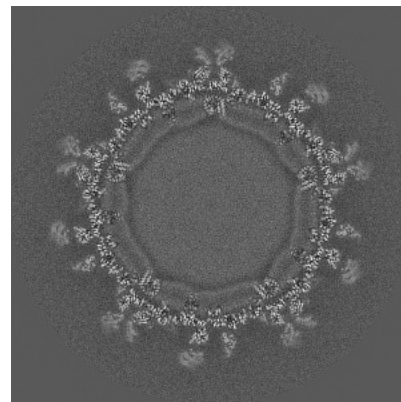
6.3.1 Primary map



X Index: 257



Y Index: 240

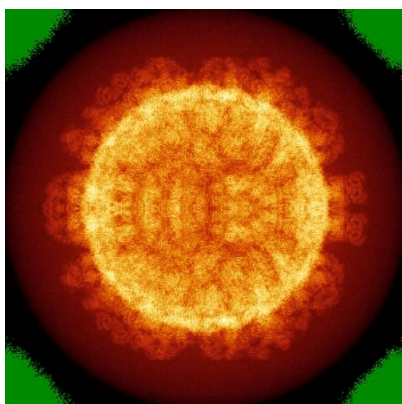


Z Index: 192

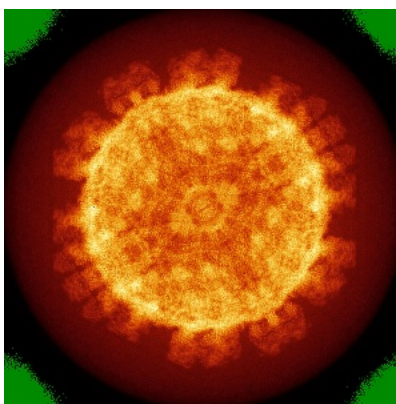
The images above show the largest variance slices of the map in three orthogonal directions.

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

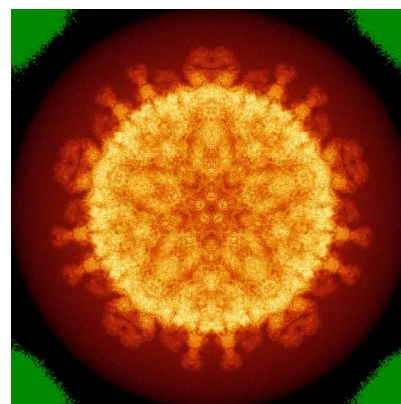
6.4.1 Primary map



X



Y

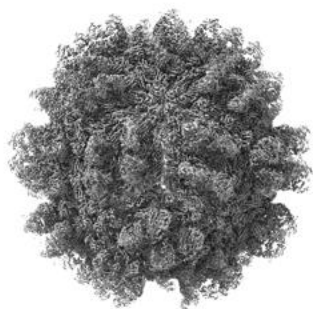


Z

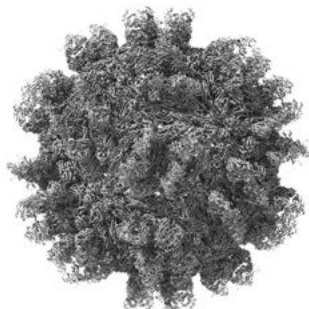
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

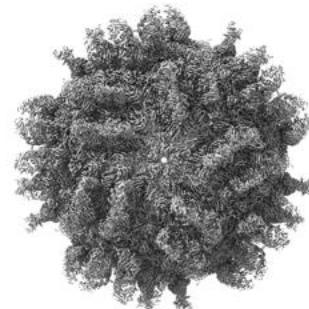
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

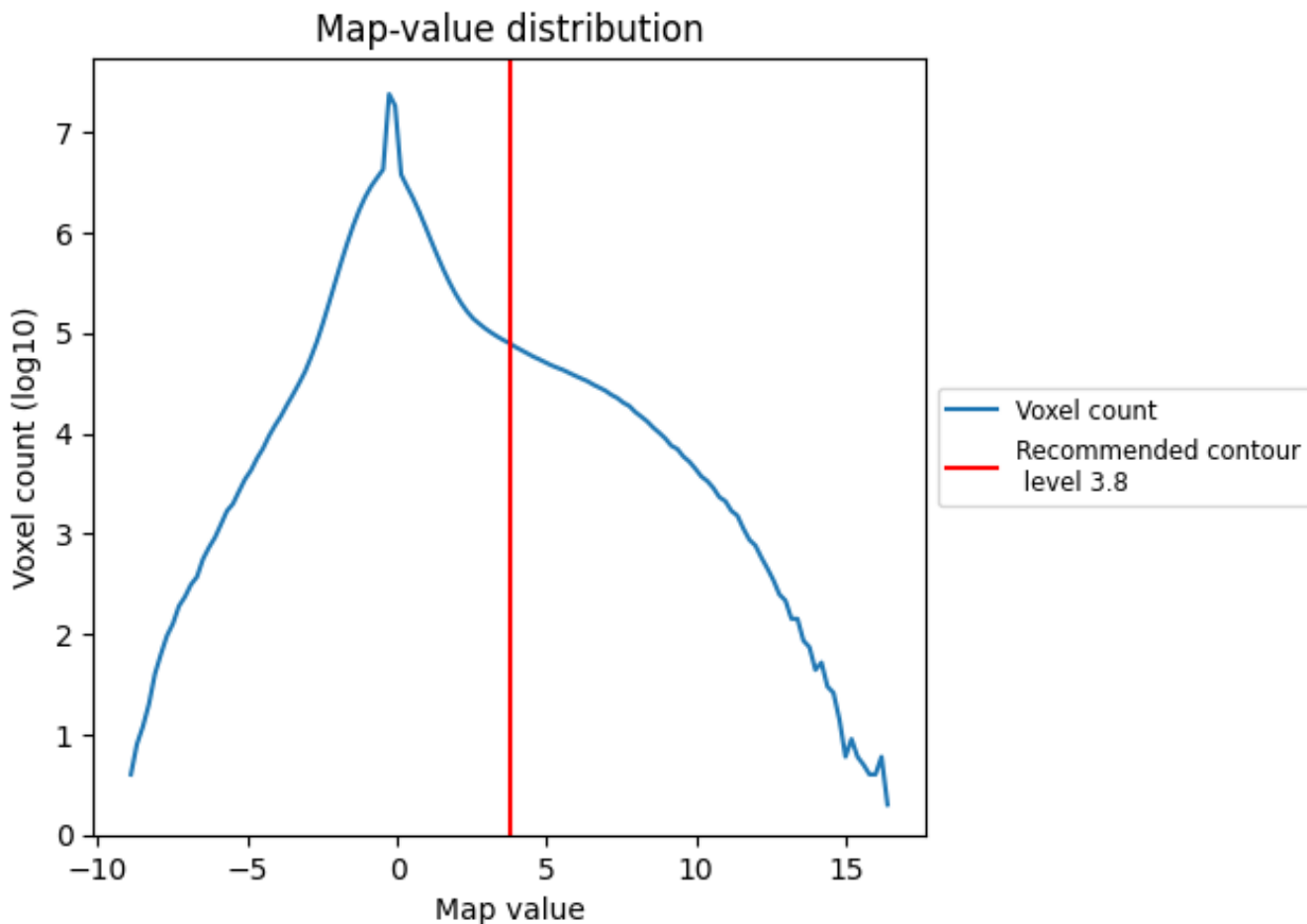
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

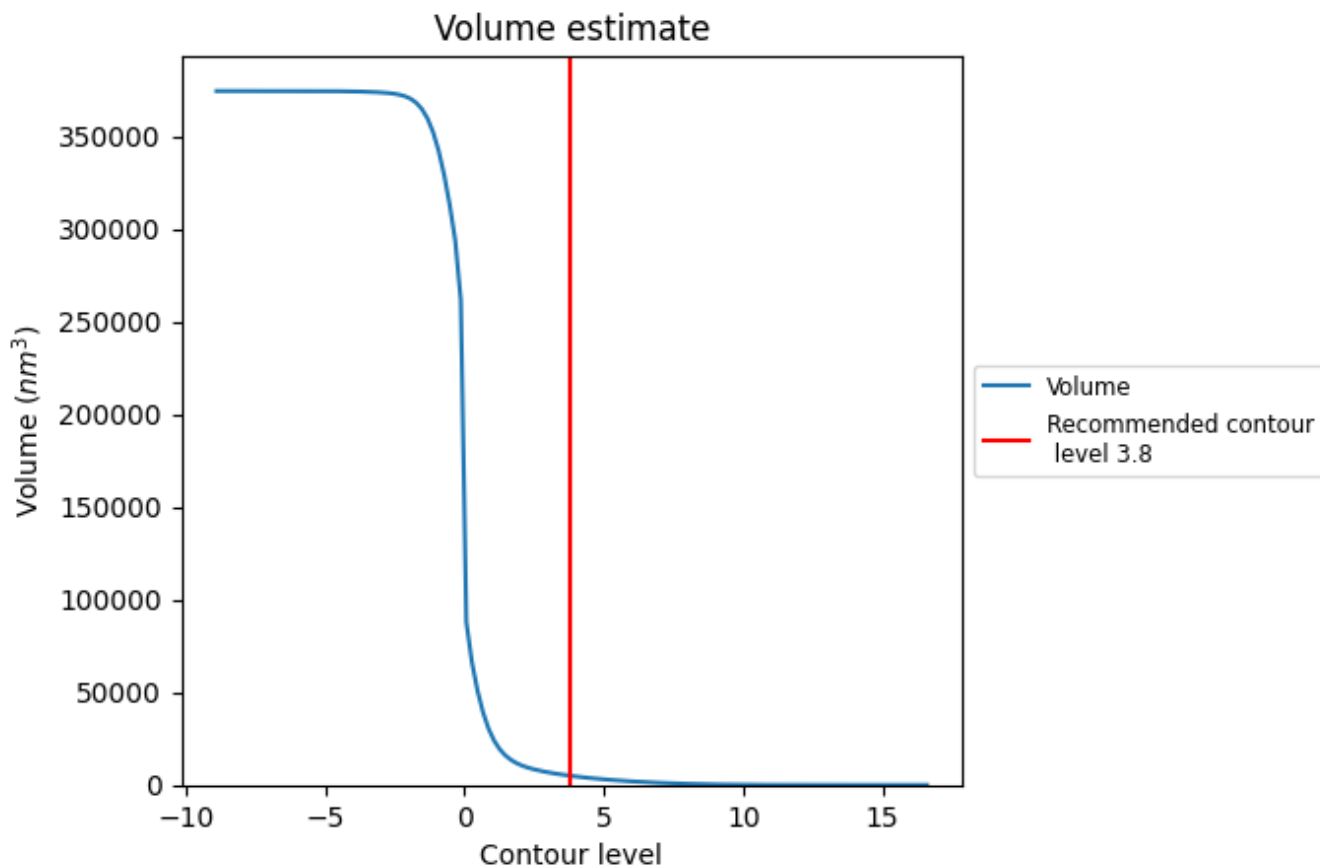
This section contains the results of statistical analysis of the map.

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.

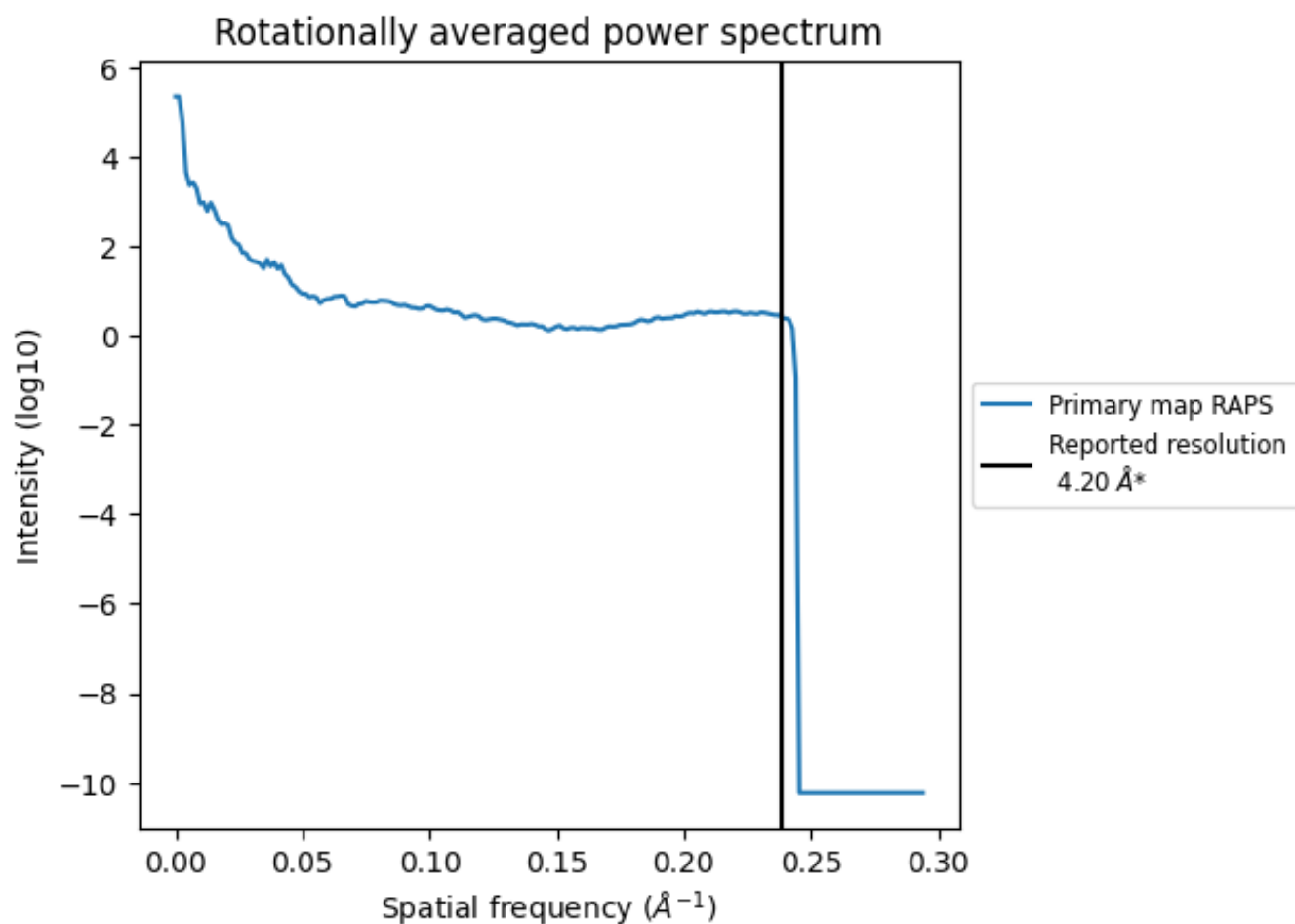
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4940 nm³; this corresponds to an approximate mass of 4463 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 [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation

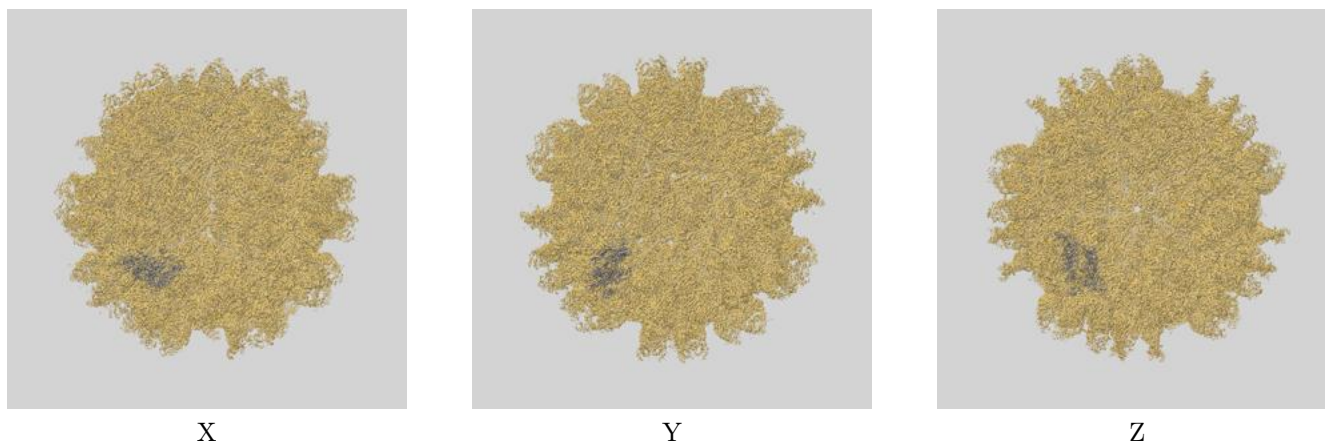
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

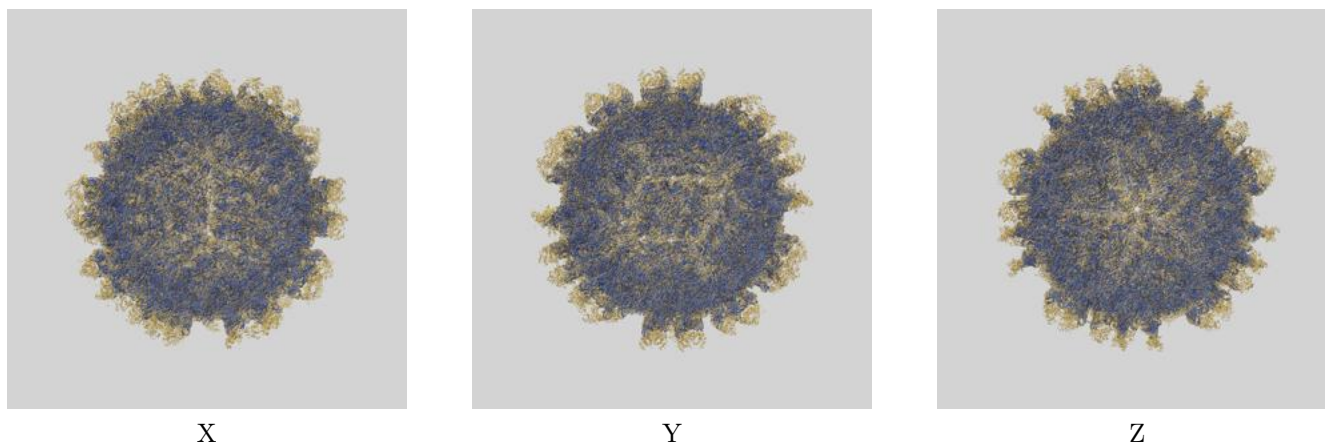
This section contains information regarding the fit between EMDB map EMD-30194 and PDB model 7BUB. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

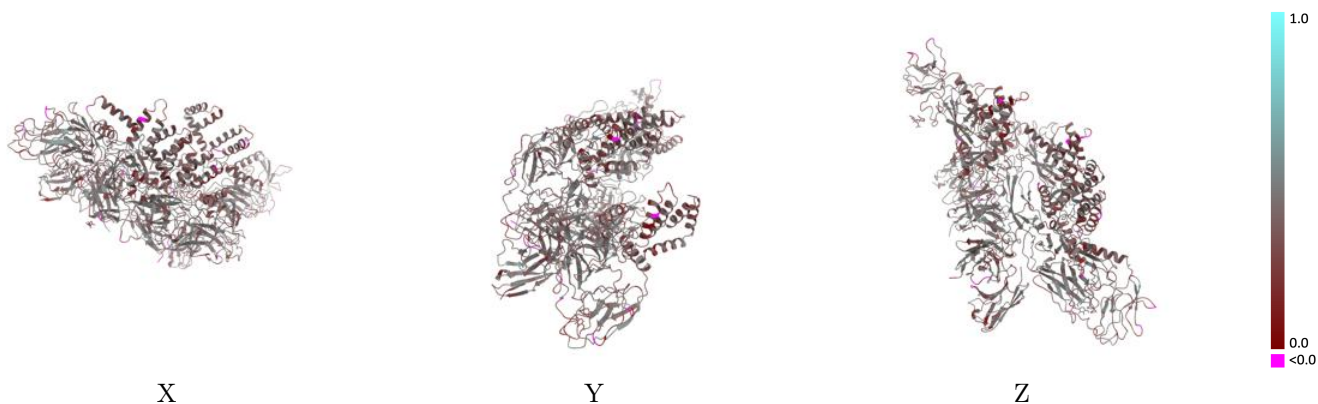


9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 3.8 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](#)

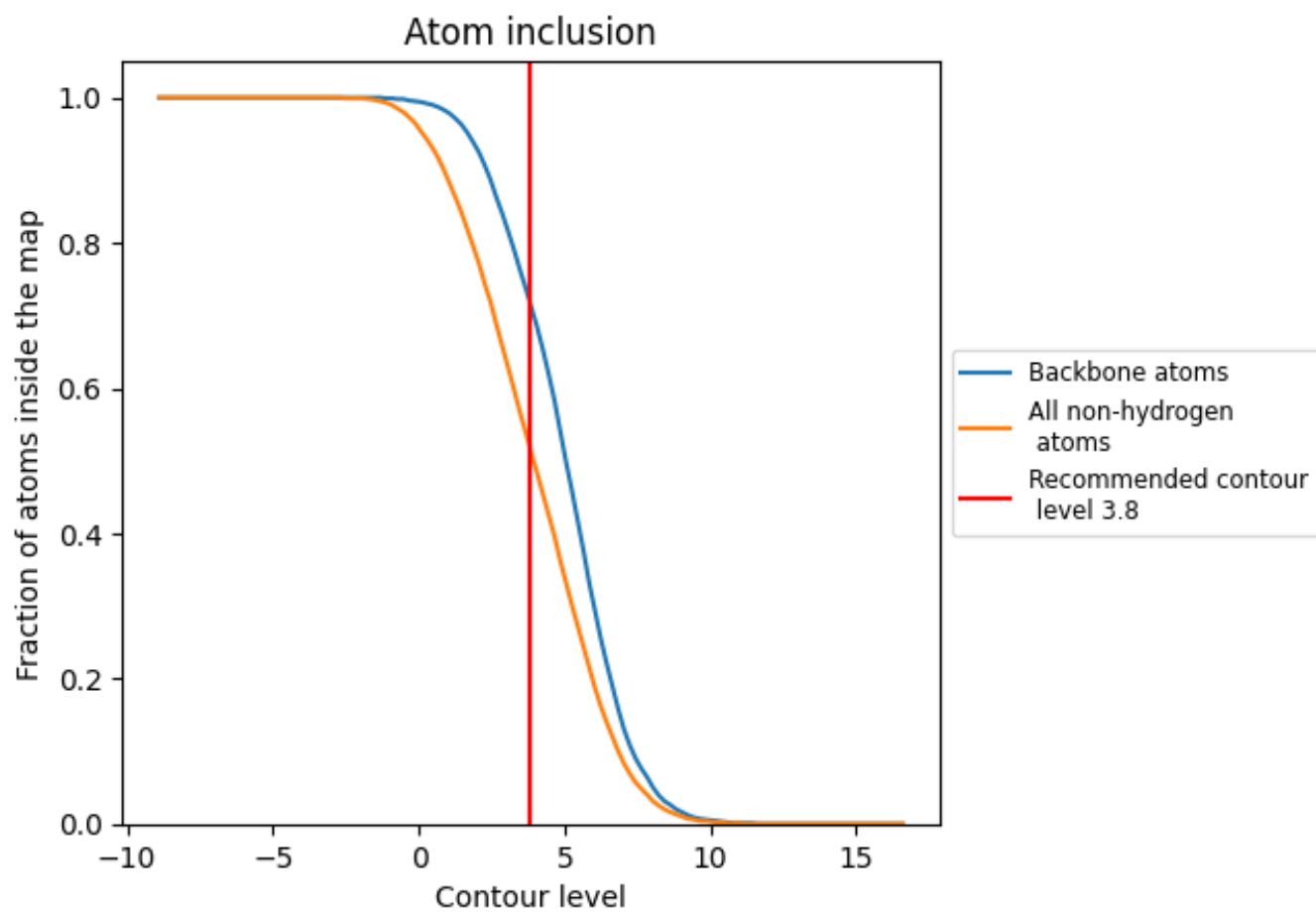


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.





























9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (3.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5200	 0.3760
A	 0.5380	 0.3870
B	 0.5430	 0.3770
C	 0.5370	 0.3770
D	 0.4500	 0.3620
E	 0.4620	 0.3490
F	 0.4510	 0.3650
G	 0.5000	 0.3600
H	 0.5080	 0.3670
I	 0.4830	 0.3730
J	 0.2860	 0.2980
K	 0.2140	 0.4630
L	 0.4940	 0.3870
M	 0.1790	 0.3560

