



Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 01:51 PM EST

PDB ID : 9NJL / pdb_00009njl
EMDB ID : EMD-49486
Title : MARV GP in complex with MARV16 Fab
Authors : Addetia, A.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veesler, D.
Deposited on : 2025-02-27
Resolution : 2.60 Å(reported)

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 : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

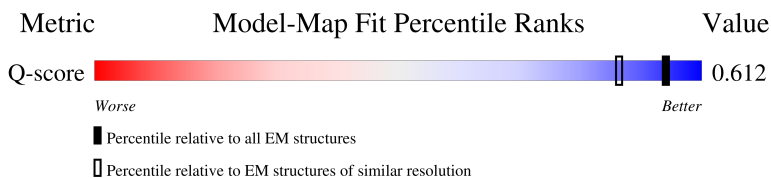
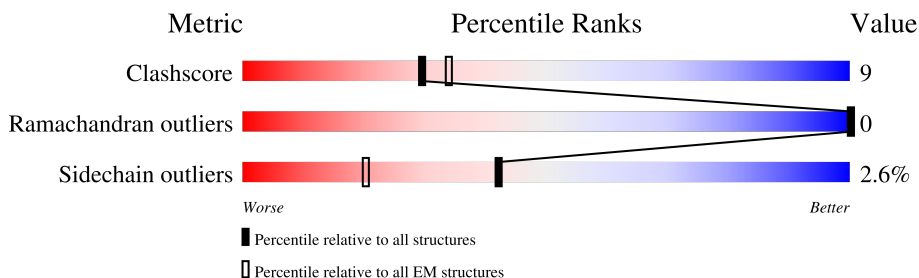
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

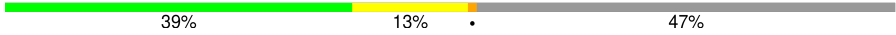
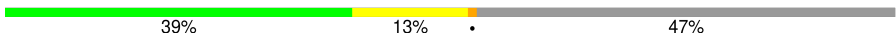


The reported resolution of this entry is 2.60 Å.

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	8728 (2.10 - 3.10)

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	H	223	
1	I	223	
1	J	223	
2	L	214	

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Mol	Chain	Length	Quality of chain
2	N	214	
2	P	214	
3	A	266	
3	C	266	
3	E	266	
4	B	211	
4	D	211	
4	F	211	
5	G	3	
5	M	3	
5	Q	3	
6	K	6	
6	O	6	
6	R	6	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11307 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 MARV16 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	119	Total	C	N	O	S	0	0
			891	568	156	163	4		
1	I	119	Total	C	N	O	S	0	0
			891	568	156	163	4		
1	J	119	Total	C	N	O	S	0	0
			891	568	156	163	4		

- Molecule 2 is a protein called MARV16 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	107	Total	C	N	O	S	0	0
			755	490	125	137	3		
2	N	107	Total	C	N	O	S	0	0
			755	490	125	137	3		
2	P	107	Total	C	N	O	S	0	0
			755	490	125	137	3		

- Molecule 3 is a protein called Envelope glycoprotein GP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	172	Total	C	N	O	S	0	0
			1282	816	227	233	6		
3	C	172	Total	C	N	O	S	0	0
			1282	816	227	233	6		
3	E	172	Total	C	N	O	S	0	0
			1282	816	227	233	6		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	GLN	-	expression tag	UNP P35253
A	258	HIS	-	expression tag	UNP P35253
A	259	LEU	-	expression tag	UNP P35253

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Chain	Residue	Modelled	Actual	Comment	Reference
A	260	VAL	-	expression tag	UNP P35253
A	261	TYR	-	expression tag	UNP P35253
A	262	PHE	-	expression tag	UNP P35253
A	263	ARG	-	expression tag	UNP P35253
A	264	ARG	-	expression tag	UNP P35253
A	265	LYS	-	expression tag	UNP P35253
A	266	ARG	-	expression tag	UNP P35253
C	257	GLN	-	expression tag	UNP P35253
C	258	HIS	-	expression tag	UNP P35253
C	259	LEU	-	expression tag	UNP P35253
C	260	VAL	-	expression tag	UNP P35253
C	261	TYR	-	expression tag	UNP P35253
C	262	PHE	-	expression tag	UNP P35253
C	263	ARG	-	expression tag	UNP P35253
C	264	ARG	-	expression tag	UNP P35253
C	265	LYS	-	expression tag	UNP P35253
C	266	ARG	-	expression tag	UNP P35253
E	257	GLN	-	expression tag	UNP P35253
E	258	HIS	-	expression tag	UNP P35253
E	259	LEU	-	expression tag	UNP P35253
E	260	VAL	-	expression tag	UNP P35253
E	261	TYR	-	expression tag	UNP P35253
E	262	PHE	-	expression tag	UNP P35253
E	263	ARG	-	expression tag	UNP P35253
E	264	ARG	-	expression tag	UNP P35253
E	265	LYS	-	expression tag	UNP P35253
E	266	ARG	-	expression tag	UNP P35253

- Molecule 4 is a protein called Envelope glycoprotein GP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	87	Total	C	N	O	S	0	0
			670	431	118	119	2		
4	D	87	Total	C	N	O	S	0	0
			670	431	118	119	2		
4	F	87	Total	C	N	O	S	0	0
			670	431	118	119	2		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	439	ALA	TRP	engineered mutation	UNP P35253

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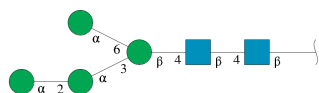
Chain	Residue	Modelled	Actual	Comment	Reference
B	445	GLY	PHE	engineered mutation	UNP P35253
B	447	ASN	PHE	engineered mutation	UNP P35253
B	589	ILE	HIS	engineered mutation	UNP P35253
B	638	SER	-	expression tag	UNP P35253
B	639	HIS	-	expression tag	UNP P35253
B	640	HIS	-	expression tag	UNP P35253
B	641	HIS	-	expression tag	UNP P35253
B	642	HIS	-	expression tag	UNP P35253
B	643	HIS	-	expression tag	UNP P35253
B	644	HIS	-	expression tag	UNP P35253
B	645	HIS	-	expression tag	UNP P35253
B	646	HIS	-	expression tag	UNP P35253
D	439	ALA	TRP	engineered mutation	UNP P35253
D	445	GLY	PHE	engineered mutation	UNP P35253
D	447	ASN	PHE	engineered mutation	UNP P35253
D	589	ILE	HIS	engineered mutation	UNP P35253
D	638	SER	-	expression tag	UNP P35253
D	639	HIS	-	expression tag	UNP P35253
D	640	HIS	-	expression tag	UNP P35253
D	641	HIS	-	expression tag	UNP P35253
D	642	HIS	-	expression tag	UNP P35253
D	643	HIS	-	expression tag	UNP P35253
D	644	HIS	-	expression tag	UNP P35253
D	645	HIS	-	expression tag	UNP P35253
D	646	HIS	-	expression tag	UNP P35253
F	439	ALA	TRP	engineered mutation	UNP P35253
F	445	GLY	PHE	engineered mutation	UNP P35253
F	447	ASN	PHE	engineered mutation	UNP P35253
F	589	ILE	HIS	engineered mutation	UNP P35253
F	638	SER	-	expression tag	UNP P35253
F	639	HIS	-	expression tag	UNP P35253
F	640	HIS	-	expression tag	UNP P35253
F	641	HIS	-	expression tag	UNP P35253
F	642	HIS	-	expression tag	UNP P35253
F	643	HIS	-	expression tag	UNP P35253
F	644	HIS	-	expression tag	UNP P35253
F	645	HIS	-	expression tag	UNP P35253
F	646	HIS	-	expression tag	UNP P35253

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



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

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	6	Total	C	N	O	0	0
			72	40	2	30		
6	O	6	Total	C	N	O	0	0
			72	40	2	30		
6	R	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	H	1	Total	O	0
			1	1	
8	L	1	Total	O	0
			1	1	
8	A	14	Total	O	0
			14	14	

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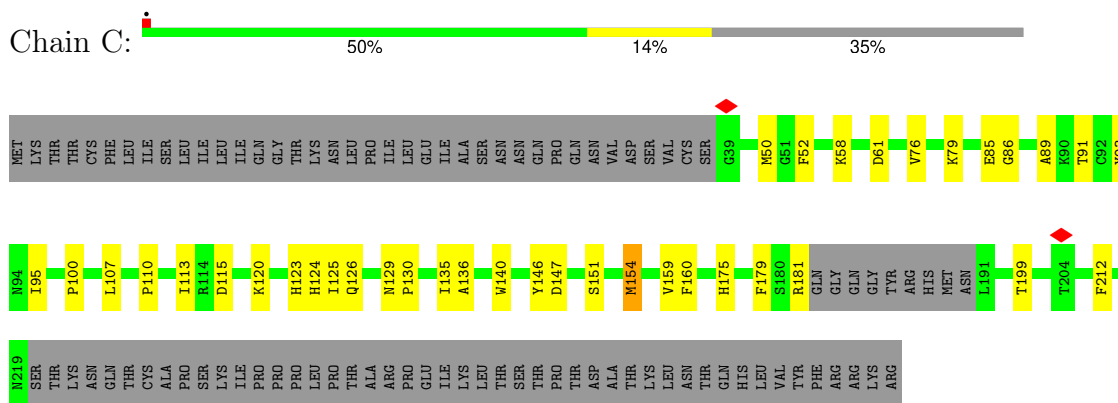
Mol	Chain	Residues	Atoms		AltConf
8	B	2	Total 2	O 2	0
8	I	1	Total 1	O 1	0
8	N	1	Total 1	O 1	0
8	C	14	Total 14	O 14	0
8	D	2	Total 2	O 2	0
8	J	1	Total 1	O 1	0
8	P	1	Total 1	O 1	0
8	E	14	Total 14	O 14	0
8	F	2	Total 2	O 2	0

HIS	ASN	D1
GLN	PHE	
GLY	TYR	M4
LEU	PRO	
SER	ARG	D17
SER	GLU	R18
PRO	ALA	
VAL	LYS	I21
THR	VAL	C22
LYS	GLN	T23
SER	TRP	
PHE	LYS	Q27
ASN	VAL	
ARG	ASP	W35
GLY	ASN	Y36
GLU	ALA	Q37
CYS	LEU	
	GLN	L47
	SER	
	GLY	R61
	ASN	
	SER	L73
	GLN	
	GLU	L89
	SER	Q90
	VAL	S91
	THR	
	GLU	F98
	GLN	
	ASP	K107
	SER	ARG
	LYS	THR
	ASP	VAL
	SER	ALA
	THR	ALA
	TYR	PRO
	LEU	SER
	SER	VAL
	LEU	PHE
	SER	ILE
	THR	PHE
	LEU	PRO
	THR	PRO
	LEU	SER
	SER	ASP
	LYS	GLU
	ALA	GLN
	ASP	LEU
	TYR	LYS
	GLU	SER
	LYS	GLY
	HIS	THR
	LYS	ALA
	VAL	SER
	TYR	VAL
	ALA	VAL
	CYS	CYS
	GLU	LEU
	GLU	LEU
	THR	ASN

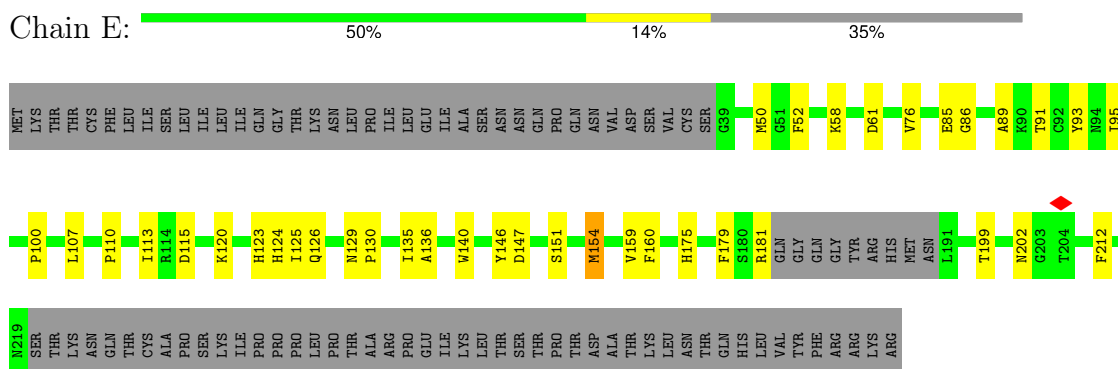
Residue	Position	Conservation Score	Conservation Grade
SER	91	0.00	Low
PRO	92	0.00	Low
VAL	93	0.00	Low
THR	94	0.00	Low
LYS	95	0.00	Low
SER	96	0.00	Low
PHE	97	0.00	Low
ARG	98	0.00	Low
GLY	99	0.00	Low
GLY	100	0.00	Low
CYS	101	0.00	Low
GLU	102	0.00	Low
ALA	103	0.00	Low
VAL	104	0.00	Low
THR	105	0.00	Low
LYS	106	0.00	Low
TRP	107	0.00	Low
ASP	108	0.00	Low
GLN	109	0.00	Low
VAL	110	0.00	Low
GLY	111	0.00	Low
ASN	112	0.00	Low
GLN	113	0.00	Low
GLU	114	0.00	Low
SER	115	0.00	Low
VAL	116	0.00	Low
THR	117	0.00	Low
GLY	118	0.00	Low
ASN	119	0.00	Low
GLU	120	0.00	Low
ASP	121	0.00	Low
GLN	122	0.00	Low
ASP	123	0.00	Low
LYS	124	0.00	Low
ALA	125	0.00	Low
ASP	126	0.00	Low
THR	127	0.00	Low
LEU	128	0.00	Low
THR	129	0.00	Low
LEU	130	0.00	Low
SER	131	0.00	Low
LYS	132	0.00	Low
ALA	133	0.00	Low
THR	134	0.00	Low
GLY	135	0.00	Low
THR	136	0.00	Low
ALA	137	0.00	Low
SER	138	0.00	Low
VAL	139	0.00	Low
VAL	140	0.00	Low
CYS	141	0.00	Low
LEU	142	0.00	Low
ASN	143	0.00	Low
THR	144	0.00	Low
GLN	145	0.00	Low
GLY	146	0.00	Low
THR	147	0.00	Low
ASN	148	0.00	Low
GLN	149	0.00	Low
SER	150	0.00	Low
THR	151	0.00	Low
VAL	152	0.00	Low
ASP	153	0.00	Low
GLY	154	0.00	Low
GLU	155	0.00	Low
ASN	156	0.00	Low
THR	157	0.00	Low
GLY	158	0.00	Low
THR	159	0.00	Low
LEU	160	0.00	Low
THR	161	0.00	Low
LEU	162	0.00	Low
SER	163	0.00	Low
ASP	164	0.00	Low
LYS	165	0.00	Low
ALA	166	0.00	Low
ASP	167	0.00	Low
THR	168	0.00	Low
GLU	169	0.00	Low
LYS	170	0.00	Low
HIS	171	0.00	Low
LYS	172	0.00	Low
VAL	173	0.00	Low
THR	174	0.00	Low
VAL	175	0.00	Low
ALA	176	0.00	Low
VAL	177	0.00	Low
CYS	178	0.00	Low
GLU	179	0.00	Low
VAL	180	0.00	Low
THR	181	0.00	Low
HIS	182	0.00	Low
GLN	183	0.00	Low
GLY	184	0.00	Low
LEU	185	0.00	Low
SER	186	0.00	Low
THR	187	0.00	Low
PRO	188	0.00	Low
ALA	189	0.00	Low
ALA	190	0.00	Low
PRO	191	0.00	Low
SER	192	0.00	Low
SER	193	0.00	Low
VAL	194	0.00	Low
PHE	195	0.00	Low
THR	196	0.00	Low
ILE	197	0.00	Low
PHE	198	0.00	Low
PRO	199	0.00	Low
PRO	200	0.00	Low
SER	201	0.00	Low
ASP	202	0.00	Low
GLU	203	0.00	Low
GLN	204	0.00	Low
ARG	205	0.00	Low
THR	206	0.00	Low
VAL	207	0.00	Low
ALA	208	0.00	Low

GLN	PHE	D1
GLY	TYR	
LEU	PRO	M4
SER	ARG	
SER	GLU	D17
PRO	ALA	R18
VAL	LYS	
THR	VAL	I21
LYS	GLN	T22
SER	TRP	C23
PHE	LYS	
ASN	VAL	Q27
ARG	ASP	
GLY	ASN	W35
GLU	ALA	Y36
CYS	LEU	Q37
	GLN	
	SER	L47
	GLY	
	ASN	R61
	SER	
	GLN	L73
	GLU	
	SER	L89
	VAL	Q90
	THR	
	GLU	F98
	ASP	
	GLN	K107
	SER	ARG
	LYS	THR
	ASP	VAL
	SER	ALA
	THR	ALA
	TYR	PRO
	SER	SER
	LEU	VAL
	SER	PHE
	THR	ILE
	LEU	PHE
	LEU	PRO
	THR	PRO
	LEU	SER
	SER	ASP
	LYS	GLN
	ALA	LEU
	ASP	LEU
	TYR	LYS
	GLU	SER
	LYS	GLY
	HIS	THR
	LYS	ALA
	VAL	SER
	TYR	VAL
	ALA	VAL
	CYS	CYS
	GLU	LEU
	VAL	LEU
	THR	ASN
	HIS	ASN

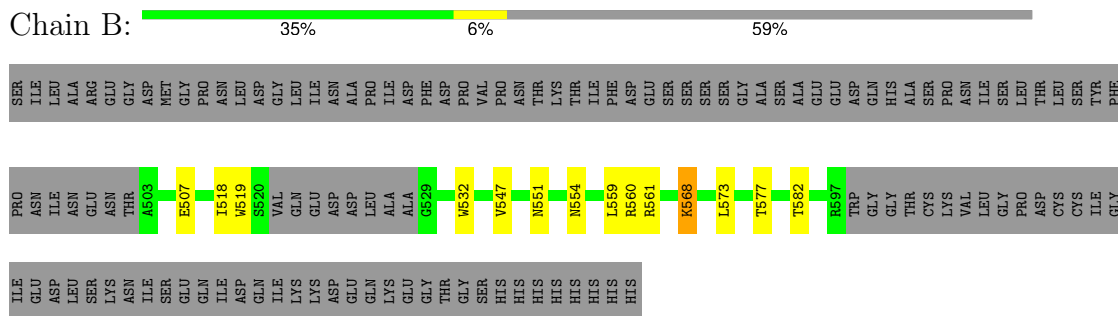
Protein	Residue	Score	Rank	Category
Protein 1	THR	P100	1	High
	ASN	L107	2	High
	GLN	P110	3	High
	THR	I113	4	High
	CYS	R114	5	High
	ALA	D115	6	High
	LEU	K120	7	High
	LEU	H123	8	High
	PRO	H124	9	High
	PRO	I125	10	High
Protein 2	THR	Q126	11	High
	ALA	N129	12	High
	ARG	P130	13	High
	PRO	I135	14	High
	GLU	A136	15	High
	LEU	W140	16	High
	LEU	Y146	17	High
	THR	D147	18	High
	THR	S151	19	High
	ASP	M154	20	High
Protein 3	ALA	V159	21	High
	THR	F160	22	High
	LYS	H175	23	High
	ASN	F179	24	High
	THR	S180	25	High
	GLN	R181	26	High
	LEU	GLN	27	High
	THR	GLY	28	High
	THR	GLN	29	High
	THR	GLY	30	High
Protein 4	THR	TVR	31	High
	ARG	ARG	32	High
	ARG	HIS	33	High
	LYS	MET	34	High
	ARG	ASN	35	High
	THR	L191	36	High
	THR	T199	37	High
	THR	T204	38	High
	THR	F212	39	High
	THR	N219	40	High
Protein 5	THR	G39	41	High
	THR	M50	42	High
	THR	G51	43	High
	THR	F52	44	High
	THR	K53	45	High
	THR	D61	46	High
	THR	V76	47	High
	THR	E85	48	High
	THR	G86	49	High
	THR	A89	50	High
Protein 6	THR	K90	51	High
	THR	T91	52	High
	THR	G92	53	High
	THR	Y93	54	High
	THR	N94	55	High
	THR	G39	56	High
	THR	M50	57	High
	THR	G51	58	High
	THR	F52	59	High
	THR	K53	60	High



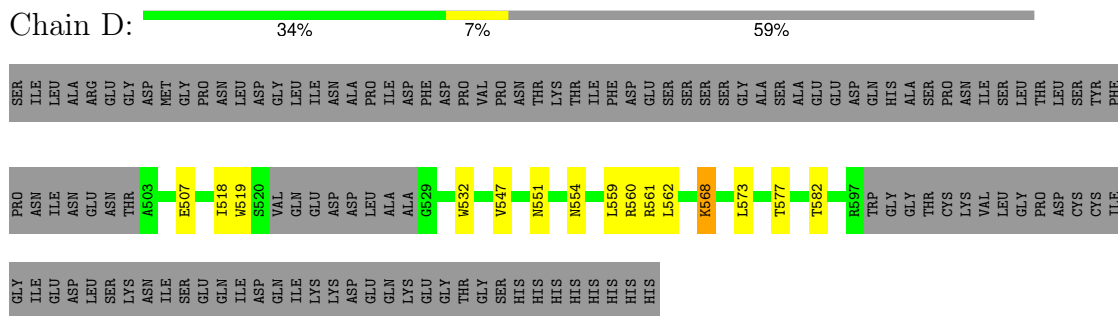
- Molecule 3: Envelope glycoprotein GP1



- Molecule 4: Envelope glycoprotein GP2

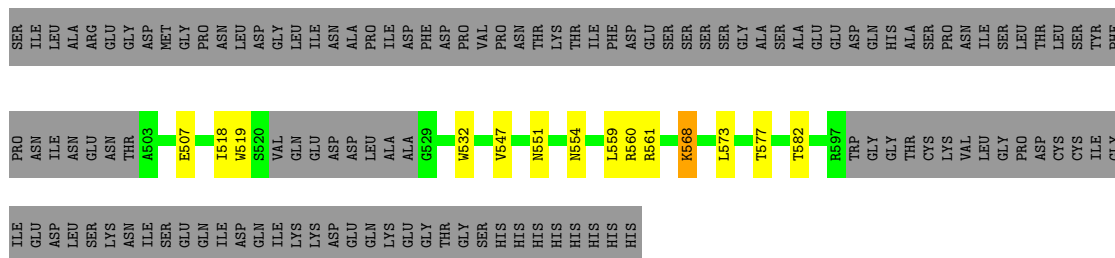


- Molecule 4: Envelope glycoprotein GP2



- Molecule 4: Envelope glycoprotein GP2

Chain F: 



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

Chain G: 




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

Chain M: 




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

Chain Q: 

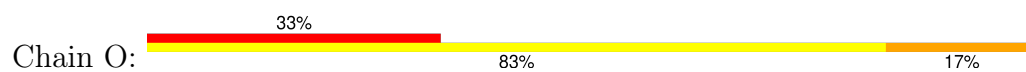


- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

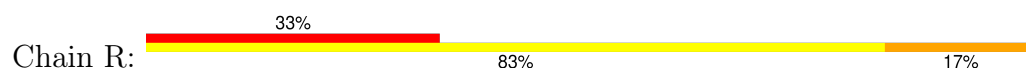
Chain K: 



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	368509	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.749	Depositor
Minimum map value	-3.549	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.829, 0.829, 0.829	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: MAN, NAG, BMA

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	H	0.22	0/911	0.52	0/1242
1	I	0.22	0/911	0.52	0/1242
1	J	0.22	0/911	0.52	0/1242
2	L	0.26	0/772	0.68	0/1056
2	N	0.26	0/772	0.67	0/1056
2	P	0.26	0/772	0.68	0/1056
3	A	0.19	0/1314	0.53	0/1787
3	C	0.19	0/1314	0.53	0/1787
3	E	0.19	0/1314	0.53	0/1787
4	B	0.22	0/680	0.66	0/923
4	D	0.22	0/680	0.66	0/923
4	F	0.22	0/680	0.66	0/923
All	All	0.22	0/11031	0.59	0/15024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	891	0	817	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	891	0	817	24	0
1	J	891	0	817	24	0
2	L	755	0	694	10	0
2	N	755	0	694	7	0
2	P	755	0	694	9	0
3	A	1282	0	1176	29	0
3	C	1282	0	1176	31	0
3	E	1282	0	1176	30	0
4	B	670	0	655	12	0
4	D	670	0	655	13	0
4	F	670	0	655	12	0
5	G	39	0	34	1	0
5	M	39	0	34	1	0
5	Q	39	0	34	1	0
6	K	72	0	61	1	0
6	O	72	0	61	1	0
6	R	72	0	61	1	0
7	A	42	0	39	0	0
7	C	42	0	39	0	0
7	E	42	0	39	0	0
8	A	14	0	0	2	0
8	B	2	0	0	0	0
8	C	14	0	0	2	0
8	D	2	0	0	0	0
8	E	14	0	0	2	0
8	F	2	0	0	0	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0
8	J	1	0	0	0	0
8	L	1	0	0	0	0
8	N	1	0	0	0	0
8	P	1	0	0	0	0
All	All	11307	0	10428	196	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 9.

All (196) 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:J:51:ILE:HD11	1:J:55:GLU:HG2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:ILE:HD11	1:H:55:GLU:HG2	1.65	0.79
1:I:51:ILE:HD11	1:I:55:GLU:HG2	1.65	0.78
2:N:37:GLN:HB2	2:N:47:LEU:HD11	1.69	0.74
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.69	0.73
2:P:37:GLN:HB2	2:P:47:LEU:HD11	1.69	0.73
3:C:85:GLU:HG3	4:D:518:ILE:HD12	1.73	0.71
3:E:85:GLU:HG3	4:F:518:ILE:HD12	1.73	0.70
3:C:95:ILE:HG12	3:C:125:ILE:HB	1.74	0.69
3:E:95:ILE:HG12	3:E:125:ILE:HB	1.74	0.69
3:A:95:ILE:HG12	3:A:125:ILE:HB	1.74	0.69
3:A:85:GLU:HG3	4:B:518:ILE:HD12	1.73	0.69
1:I:91:THR:HG23	1:I:117:THR:HA	1.76	0.67
1:I:83:LEU:HB3	1:I:86:LEU:HD21	1.78	0.66
1:J:83:LEU:HB3	1:J:86:LEU:HD21	1.78	0.66
1:J:91:THR:HG23	1:J:117:THR:HA	1.76	0.66
1:H:91:THR:HG23	1:H:117:THR:HA	1.76	0.65
1:H:83:LEU:HB3	1:H:86:LEU:HD21	1.78	0.64
1:I:12:VAL:HG21	1:I:18:LEU:HB2	1.80	0.64
1:J:12:VAL:HG21	1:J:18:LEU:HB2	1.80	0.63
1:H:12:VAL:HG21	1:H:18:LEU:HB2	1.80	0.61
1:I:3:GLN:HE21	1:I:5:VAL:HG22	1.66	0.60
1:H:3:GLN:HE21	1:H:5:VAL:HG22	1.66	0.60
1:J:3:GLN:HE21	1:J:5:VAL:HG22	1.66	0.59
3:E:52:PHE:CZ	4:F:559:LEU:HB3	2.40	0.56
3:A:52:PHE:CZ	4:B:559:LEU:HB3	2.40	0.56
3:C:52:PHE:CZ	4:D:559:LEU:HB3	2.40	0.56
1:J:34:MET:HB3	1:J:79:LEU:HD22	1.87	0.56
1:I:34:MET:HB3	1:I:79:LEU:HD22	1.87	0.55
1:H:34:MET:HB3	1:H:79:LEU:HD22	1.87	0.55
3:A:126:GLN:O	3:A:199:THR:HA	2.09	0.53
3:C:126:GLN:O	3:C:199:THR:HA	2.09	0.53
3:A:129:ASN:CG	3:A:130:PRO:HD2	2.34	0.53
3:E:129:ASN:CG	3:E:130:PRO:HD2	2.34	0.53
8:A:401:HOH:O	4:B:560:ARG:HD3	2.09	0.53
8:C:401:HOH:O	4:D:560:ARG:HD3	2.08	0.53
3:E:126:GLN:O	3:E:199:THR:HA	2.09	0.53
1:J:99:ARG:HG3	1:J:107:LEU:HD23	1.91	0.53
1:I:99:ARG:HG3	1:I:107:LEU:HD23	1.91	0.52
3:C:129:ASN:CG	3:C:130:PRO:HD2	2.34	0.52
1:J:67:ARG:O	1:J:84:ASN:HB2	2.10	0.52
1:H:67:ARG:O	1:H:84:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:401:HOH:O	4:F:560:ARG:HD3	2.09	0.52
3:C:91:THR:HG23	3:C:123:HIS:CD2	2.45	0.52
3:A:91:THR:HG23	3:A:123:HIS:CD2	2.45	0.52
3:A:146:TYR:CE1	3:A:160:PHE:HB3	2.45	0.51
2:P:4:MET:HE3	2:P:90:GLN:HG2	1.93	0.51
1:H:99:ARG:HG3	1:H:107:LEU:HD23	1.91	0.51
3:E:91:THR:HG23	3:E:123:HIS:HD2	1.76	0.51
3:E:110:PRO:HD2	3:E:113:ILE:HG13	1.93	0.51
1:H:28:THR:HG22	4:B:507:GLU:CD	2.36	0.51
3:E:146:TYR:CE1	3:E:160:PHE:HB3	2.45	0.51
2:L:4:MET:HE3	2:L:90:GLN:HG2	1.92	0.51
1:J:28:THR:HG22	4:F:507:GLU:CD	2.36	0.51
3:C:110:PRO:HD2	3:C:113:ILE:HG13	1.93	0.51
3:C:146:TYR:CE1	3:C:160:PHE:HB3	2.45	0.51
1:I:67:ARG:O	1:I:84:ASN:HB2	2.10	0.51
3:C:91:THR:HG23	3:C:123:HIS:HD2	1.76	0.51
3:E:91:THR:HG23	3:E:123:HIS:CD2	2.45	0.51
1:H:18:LEU:HD12	1:H:19:ARG:N	2.27	0.50
1:I:28:THR:HG22	4:D:507:GLU:CD	2.36	0.50
3:A:110:PRO:HD2	3:A:113:ILE:HG13	1.93	0.50
1:I:18:LEU:HD12	1:I:19:ARG:N	2.27	0.50
2:N:4:MET:HE3	2:N:90:GLN:HG2	1.93	0.50
1:J:18:LEU:HD12	1:J:19:ARG:N	2.27	0.50
3:E:124:HIS:HE1	5:Q:1:NAG:O7	1.95	0.50
3:A:91:THR:HG23	3:A:123:HIS:HD2	1.76	0.49
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.48	0.49
3:A:124:HIS:HE1	5:G:1:NAG:O7	1.95	0.49
3:A:175:HIS:HD2	3:A:179:PHE:CD1	2.31	0.49
3:A:95:ILE:HD13	3:A:212:PHE:CE2	2.48	0.49
1:I:97:VAL:HG11	1:I:107:LEU:HB3	1.95	0.49
1:H:97:VAL:HG11	1:H:107:LEU:HB3	1.95	0.49
3:C:50:MET:HG2	3:C:85:GLU:OE2	2.13	0.49
3:C:95:ILE:HD13	3:C:212:PHE:CE2	2.48	0.49
2:N:23:CYS:HB2	2:N:35:TRP:CH2	2.48	0.48
3:E:95:ILE:HD13	3:E:212:PHE:CE2	2.48	0.48
3:C:175:HIS:HD2	3:C:179:PHE:CD1	2.31	0.48
2:P:23:CYS:HB2	2:P:35:TRP:CH2	2.48	0.48
1:H:51:ILE:HD13	1:H:71:SER:HA	1.95	0.48
3:E:175:HIS:HD2	3:E:179:PHE:CD1	2.31	0.48
3:A:50:MET:HG2	3:A:85:GLU:OE2	2.13	0.48
3:C:124:HIS:HE1	5:M:1:NAG:O7	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:50:MET:HG2	3:E:85:GLU:OE2	2.13	0.48
3:E:76:VAL:O	3:E:135:ILE:HD11	2.14	0.48
3:E:85:GLU:HB2	4:F:519:TRP:O	2.13	0.48
1:H:18:LEU:HD21	1:H:116:VAL:HG22	1.95	0.48
3:C:85:GLU:HB2	4:D:519:TRP:O	2.13	0.48
3:A:85:GLU:HB2	4:B:519:TRP:O	2.13	0.47
1:J:18:LEU:HD21	1:J:116:VAL:HG22	1.95	0.47
3:A:76:VAL:O	3:A:135:ILE:HD11	2.14	0.47
1:I:18:LEU:HD21	1:I:116:VAL:HG22	1.95	0.47
1:I:51:ILE:HD13	1:I:71:SER:HA	1.95	0.47
3:C:76:VAL:O	3:C:135:ILE:HD11	2.14	0.47
3:E:86:GLY:HA3	4:F:519:TRP:CZ2	2.50	0.47
3:C:181:ARG:HD3	4:D:547:VAL:HG22	1.97	0.47
1:H:28:THR:HG22	4:B:507:GLU:OE2	2.15	0.47
3:A:86:GLY:HA3	4:B:519:TRP:CZ2	2.50	0.47
3:C:86:GLY:HA3	4:D:519:TRP:CZ2	2.50	0.47
1:J:97:VAL:HG11	1:J:107:LEU:HB3	1.95	0.47
1:J:51:ILE:HD13	1:J:71:SER:HA	1.95	0.47
2:P:73:LEU:HD12	2:P:73:LEU:HA	1.77	0.47
1:J:28:THR:HG22	4:F:507:GLU:OE2	2.15	0.47
3:A:181:ARG:HD3	4:B:547:VAL:HG22	1.96	0.47
4:D:573:LEU:O	4:D:577:THR:HG23	2.15	0.47
4:B:573:LEU:O	4:B:577:THR:HG23	2.15	0.46
1:I:28:THR:HG22	4:D:507:GLU:OE2	2.15	0.46
3:E:181:ARG:HD3	4:F:547:VAL:HG22	1.97	0.46
3:A:136:ALA:HB1	3:A:154:MET:HE3	1.98	0.46
1:H:86:LEU:HA	1:H:86:LEU:HD23	1.66	0.46
4:F:573:LEU:O	4:F:577:THR:HG23	2.15	0.46
1:H:36:TRP:CG	1:H:81:LEU:HD22	2.51	0.46
3:E:136:ALA:HB1	3:E:154:MET:HE3	1.98	0.46
1:I:36:TRP:CG	1:I:81:LEU:HD22	2.51	0.46
3:C:136:ALA:HB1	3:C:154:MET:HE3	1.98	0.45
1:J:36:TRP:CG	1:J:81:LEU:HD22	2.51	0.45
2:L:4:MET:HE3	2:L:90:GLN:HB3	1.99	0.45
3:A:95:ILE:HD13	3:A:212:PHE:HE2	1.81	0.45
2:N:4:MET:HE3	2:N:90:GLN:HB3	1.99	0.45
3:E:95:ILE:HD13	3:E:212:PHE:HE2	1.81	0.44
1:J:86:LEU:HD23	1:J:86:LEU:HA	1.66	0.44
3:E:140:TRP:CE2	6:R:2:NAG:H5	2.52	0.44
3:E:61:ASP:O	3:E:91:THR:HG21	2.18	0.44
3:A:61:ASP:O	3:A:91:THR:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:551:ASN:ND2	4:D:554:ASN:HA	2.32	0.44
3:A:140:TRP:CE2	6:K:2:NAG:H5	2.52	0.44
4:B:551:ASN:ND2	4:B:554:ASN:HA	2.32	0.44
3:C:115:ASP:O	3:C:147:ASP:HB2	2.18	0.44
3:C:140:TRP:CE2	6:O:2:NAG:H5	2.52	0.44
3:A:89:ALA:HB1	8:A:405:HOH:O	2.18	0.44
3:A:115:ASP:O	3:A:147:ASP:HB2	2.18	0.44
2:P:4:MET:HE3	2:P:90:GLN:HB3	1.99	0.44
1:J:51:ILE:HG12	1:J:72:ARG:HD2	2.00	0.44
1:J:22:CYS:HB3	1:J:79:LEU:HB3	2.00	0.43
1:I:22:CYS:HB3	1:I:79:LEU:HB3	2.00	0.43
3:C:61:ASP:OD1	3:C:61:ASP:N	2.50	0.43
3:E:115:ASP:O	3:E:147:ASP:HB2	2.18	0.43
3:E:89:ALA:HB1	8:E:405:HOH:O	2.18	0.43
3:C:95:ILE:HD13	3:C:212:PHE:HE2	1.81	0.43
4:F:551:ASN:ND2	4:F:554:ASN:HA	2.32	0.43
3:C:107:LEU:HD11	3:C:135:ILE:HG21	2.01	0.43
1:H:22:CYS:HB3	1:H:79:LEU:HB3	2.00	0.43
1:H:51:ILE:HG12	1:H:72:ARG:HD2	2.00	0.43
1:I:13:LYS:HD3	1:I:13:LYS:HA	1.89	0.43
3:C:89:ALA:HB1	8:C:405:HOH:O	2.18	0.43
3:A:107:LEU:HD11	3:A:135:ILE:HG21	2.01	0.43
3:C:79:LYS:HD3	3:C:79:LYS:HA	1.80	0.43
1:I:51:ILE:HG12	1:I:72:ARG:HD2	2.00	0.42
1:J:53:SER:HB2	3:E:58:LYS:HE2	2.01	0.42
3:C:61:ASP:O	3:C:91:THR:HG21	2.18	0.42
1:J:8:GLY:O	1:J:18:LEU:HD11	2.19	0.42
1:H:8:GLY:O	1:H:18:LEU:HD11	2.19	0.42
3:A:100:PRO:HD3	3:A:129:ASN:O	2.20	0.42
2:N:21:ILE:HB	2:N:73:LEU:HB3	2.01	0.42
3:C:100:PRO:HD3	3:C:129:ASN:O	2.20	0.42
1:H:53:SER:HB2	3:A:58:LYS:HE2	2.01	0.42
2:L:21:ILE:HB	2:L:73:LEU:HB3	2.01	0.42
1:I:38:ARG:HB3	1:I:94:TYR:CD2	2.55	0.42
3:A:89:ALA:O	3:A:120:LYS:HD2	2.20	0.42
1:I:53:SER:HB2	3:C:58:LYS:HE2	2.01	0.42
1:H:38:ARG:HB3	1:H:94:TYR:CD2	2.55	0.41
1:I:8:GLY:O	1:I:18:LEU:HD11	2.19	0.41
1:J:38:ARG:HB3	1:J:94:TYR:CD2	2.55	0.41
1:J:68:PHE:CD1	1:J:83:LEU:HA	2.55	0.41
3:E:100:PRO:HD3	3:E:129:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:17:ASP:OD1	2:L:18:ARG:N	2.53	0.41
3:E:89:ALA:O	3:E:120:LYS:HD2	2.20	0.41
3:A:115:ASP:HB3	3:A:159:VAL:HB	2.02	0.41
4:B:568:LYS:HE3	4:F:532:TRP:CD1	2.55	0.41
3:E:107:LEU:HD11	3:E:135:ILE:HG21	2.01	0.41
4:B:532:TRP:CD1	4:D:568:LYS:HE3	2.55	0.41
1:H:35:ASN:HD21	1:H:99:ARG:HB2	1.85	0.41
1:H:68:PHE:CD1	1:H:83:LEU:HA	2.56	0.41
3:A:93:TYR:HB2	3:A:160:PHE:CE1	2.56	0.41
1:I:105:ASP:O	2:N:91:SER:HB2	2.21	0.41
2:L:73:LEU:HA	2:L:73:LEU:HD12	1.77	0.41
3:C:89:ALA:O	3:C:120:LYS:HD2	2.20	0.41
3:C:115:ASP:HB3	3:C:159:VAL:HB	2.02	0.41
1:J:35:ASN:HD21	1:J:99:ARG:HB2	1.85	0.41
2:P:21:ILE:HB	2:P:73:LEU:HB3	2.01	0.41
2:P:89:LEU:HB2	2:P:98:PHE:CD1	2.56	0.41
3:E:93:TYR:HB2	3:E:160:PHE:CE1	2.56	0.41
1:I:35:ASN:HD21	1:I:99:ARG:HB2	1.85	0.41
2:P:17:ASP:OD1	2:P:18:ARG:N	2.53	0.41
3:E:202:ASN:OD1	3:E:202:ASN:N	2.51	0.41
2:L:89:LEU:HB2	2:L:98:PHE:CD1	2.56	0.40
2:N:89:LEU:HB2	2:N:98:PHE:CD1	2.56	0.40
1:H:105:ASP:O	2:L:91:SER:HB2	2.21	0.40
1:I:68:PHE:CD1	1:I:83:LEU:HA	2.55	0.40
3:E:115:ASP:HB3	3:E:159:VAL:HB	2.02	0.40
1:J:38:ARG:HA	1:J:93:VAL:O	2.22	0.40
2:L:61:ARG:H	2:L:61:ARG:HG2	1.65	0.40
3:C:93:TYR:HB2	3:C:160:PHE:CE1	2.56	0.40
4:D:532:TRP:CD1	4:F:568:LYS:HE3	2.55	0.40
4:D:562:LEU:HD12	4:D:562:LEU:HA	1.85	0.40
2:P:61:ARG:H	2:P:61:ARG:HG2	1.66	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	H	117/223 (52%)	114 (97%)	3 (3%)	0	100	100
1	I	117/223 (52%)	114 (97%)	3 (3%)	0	100	100
1	J	117/223 (52%)	114 (97%)	3 (3%)	0	100	100
2	L	105/214 (49%)	95 (90%)	10 (10%)	0	100	100
2	N	105/214 (49%)	95 (90%)	10 (10%)	0	100	100
2	P	105/214 (49%)	95 (90%)	10 (10%)	0	100	100
3	A	168/266 (63%)	163 (97%)	5 (3%)	0	100	100
3	C	168/266 (63%)	163 (97%)	5 (3%)	0	100	100
3	E	168/266 (63%)	163 (97%)	5 (3%)	0	100	100
4	B	83/211 (39%)	79 (95%)	4 (5%)	0	100	100
4	D	83/211 (39%)	79 (95%)	4 (5%)	0	100	100
4	F	83/211 (39%)	79 (95%)	4 (5%)	0	100	100
All	All	1419/2742 (52%)	1353 (95%)	66 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	H	84/192 (44%)	81 (96%)	3 (4%)	30	56
1	I	84/192 (44%)	81 (96%)	3 (4%)	30	56
1	J	84/192 (44%)	81 (96%)	3 (4%)	30	56
2	L	67/187 (36%)	66 (98%)	1 (2%)	60	81
2	N	67/187 (36%)	66 (98%)	1 (2%)	60	81
2	P	67/187 (36%)	66 (98%)	1 (2%)	60	81
3	A	122/234 (52%)	120 (98%)	2 (2%)	58	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	122/234 (52%)	120 (98%)	2 (2%)	58	79
3	E	122/234 (52%)	120 (98%)	2 (2%)	58	79
4	B	67/183 (37%)	64 (96%)	3 (4%)	23	47
4	D	67/183 (37%)	64 (96%)	3 (4%)	23	47
4	F	67/183 (37%)	64 (96%)	3 (4%)	23	47
All	All	1020/2388 (43%)	993 (97%)	27 (3%)	42	67

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	12	VAL
1	H	28	THR
2	L	27	GLN
3	A	151	SER
3	A	154	MET
4	B	561	ARG
4	B	568	LYS
4	B	582	THR
1	I	3	GLN
1	I	12	VAL
1	I	28	THR
2	N	27	GLN
3	C	151	SER
3	C	154	MET
4	D	561	ARG
4	D	568	LYS
4	D	582	THR
1	J	3	GLN
1	J	12	VAL
1	J	28	THR
2	P	27	GLN
3	E	151	SER
3	E	154	MET
4	F	561	ARG
4	F	568	LYS
4	F	582	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	101	ASN
1	H	103	ASN
2	L	27	GLN
2	L	34	ASN
3	A	57	GLN
3	A	126	GLN
3	A	131	HIS
3	A	175	HIS
4	B	565	GLN
4	B	587	ASN
1	I	3	GLN
1	I	101	ASN
1	I	103	ASN
2	N	27	GLN
2	N	34	ASN
3	C	57	GLN
3	C	126	GLN
3	C	131	HIS
3	C	175	HIS
4	D	565	GLN
4	D	587	ASN
1	J	3	GLN
1	J	101	ASN
1	J	103	ASN
2	P	27	GLN
2	P	34	ASN
3	E	57	GLN
3	E	126	GLN
3	E	131	HIS
3	E	175	HIS
4	F	565	GLN
4	F	587	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

27 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	1	5,3	14,14,15	0.74	0	17,19,21	1.12	1 (5%)
5	NAG	G	2	5	14,14,15	0.72	0	17,19,21	0.86	1 (5%)
5	BMA	G	3	5	11,11,12	0.80	0	15,15,17	1.84	1 (6%)
6	NAG	K	1	4,6	14,14,15	0.78	0	17,19,21	1.18	2 (11%)
6	NAG	K	2	6	14,14,15	0.74	0	17,19,21	0.95	1 (5%)
6	BMA	K	3	6	11,11,12	0.83	0	15,15,17	1.64	1 (6%)
6	MAN	K	4	6	11,11,12	0.64	0	15,15,17	1.09	1 (6%)
6	MAN	K	5	6	11,11,12	0.72	0	15,15,17	1.07	1 (6%)
6	MAN	K	6	6	11,11,12	0.69	0	15,15,17	1.22	1 (6%)
5	NAG	M	1	5,3	14,14,15	0.73	0	17,19,21	1.12	1 (5%)
5	NAG	M	2	5	14,14,15	0.71	0	17,19,21	0.86	1 (5%)
5	BMA	M	3	5	11,11,12	0.78	0	15,15,17	1.84	1 (6%)
6	NAG	O	1	4,6	14,14,15	0.77	0	17,19,21	1.17	2 (11%)
6	NAG	O	2	6	14,14,15	0.75	0	17,19,21	0.95	1 (5%)
6	BMA	O	3	6	11,11,12	0.83	0	15,15,17	1.64	1 (6%)
6	MAN	O	4	6	11,11,12	0.65	0	15,15,17	1.08	1 (6%)
6	MAN	O	5	6	11,11,12	0.72	0	15,15,17	1.06	1 (6%)
6	MAN	O	6	6	11,11,12	0.69	0	15,15,17	1.22	1 (6%)
5	NAG	Q	1	5,3	14,14,15	0.73	0	17,19,21	1.11	1 (5%)
5	NAG	Q	2	5	14,14,15	0.72	0	17,19,21	0.86	1 (5%)
5	BMA	Q	3	5	11,11,12	0.81	0	15,15,17	1.85	1 (6%)
6	NAG	R	1	4,6	14,14,15	0.79	0	17,19,21	1.18	2 (11%)
6	NAG	R	2	6	14,14,15	0.73	0	17,19,21	0.94	1 (5%)
6	BMA	R	3	6	11,11,12	0.84	0	15,15,17	1.64	1 (6%)
6	MAN	R	4	6	11,11,12	0.64	0	15,15,17	1.08	1 (6%)
6	MAN	R	5	6	11,11,12	0.72	0	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	R	6	6	11,11,12	0.70	0	15,15,17	1.22	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
6	NAG	K	1	4,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	2/2/19/22	0/1/1/1
6	MAN	K	5	6	-	1/2/19/22	0/1/1/1
6	MAN	K	6	6	-	0/2/19/22	0/1/1/1
5	NAG	M	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
6	NAG	O	1	4,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	2/2/19/22	0/1/1/1
6	MAN	O	4	6	-	2/2/19/22	0/1/1/1
6	MAN	O	5	6	-	1/2/19/22	0/1/1/1
6	MAN	O	6	6	-	0/2/19/22	0/1/1/1
5	NAG	Q	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	0/2/19/22	0/1/1/1
6	NAG	R	1	4,6	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	2/2/19/22	0/1/1/1
6	MAN	R	5	6	-	1/2/19/22	0/1/1/1
6	MAN	R	6	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	3	BMA	C1-O5-C5	6.18	120.47	112.19
5	M	3	BMA	C1-O5-C5	6.17	120.46	112.19
5	G	3	BMA	C1-O5-C5	6.14	120.42	112.19
6	R	3	BMA	C1-O5-C5	5.38	119.39	112.19
6	K	3	BMA	C1-O5-C5	5.37	119.39	112.19
6	O	3	BMA	C1-O5-C5	5.35	119.35	112.19
6	K	6	MAN	C1-O5-C5	3.81	117.29	112.19
6	R	6	MAN	C1-O5-C5	3.80	117.28	112.19
6	O	6	MAN	C1-O5-C5	3.79	117.26	112.19
6	K	4	MAN	C1-O5-C5	3.23	116.51	112.19
6	O	4	MAN	C1-O5-C5	3.22	116.50	112.19
6	R	4	MAN	C1-O5-C5	3.22	116.50	112.19
6	R	1	NAG	C1-O5-C5	3.17	116.43	112.19
6	K	5	MAN	C1-O5-C5	3.15	116.41	112.19
6	K	1	NAG	C1-O5-C5	3.14	116.39	112.19
6	R	5	MAN	C1-O5-C5	3.14	116.39	112.19
6	O	5	MAN	C1-O5-C5	3.12	116.37	112.19
6	O	1	NAG	C1-O5-C5	3.11	116.36	112.19
6	K	2	NAG	C1-O5-C5	3.07	116.30	112.19
6	O	2	NAG	C1-O5-C5	3.07	116.30	112.19
6	R	2	NAG	C1-O5-C5	3.02	116.23	112.19
5	G	1	NAG	C1-O5-C5	2.72	115.83	112.19
5	M	1	NAG	C1-O5-C5	2.70	115.80	112.19
5	Q	1	NAG	C1-O5-C5	2.69	115.79	112.19
6	K	1	NAG	O5-C1-C2	-2.64	107.21	111.29
6	R	1	NAG	O5-C1-C2	-2.63	107.22	111.29
6	O	1	NAG	O5-C1-C2	-2.63	107.23	111.29
5	M	2	NAG	C1-O5-C5	2.48	115.51	112.19
5	G	2	NAG	C1-O5-C5	2.47	115.49	112.19
5	Q	2	NAG	C1-O5-C5	2.46	115.48	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	4	MAN	O5-C5-C6-O6
6	O	4	MAN	O5-C5-C6-O6
6	R	4	MAN	O5-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
6	O	3	BMA	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
6	K	5	MAN	O5-C5-C6-O6
6	O	5	MAN	O5-C5-C6-O6

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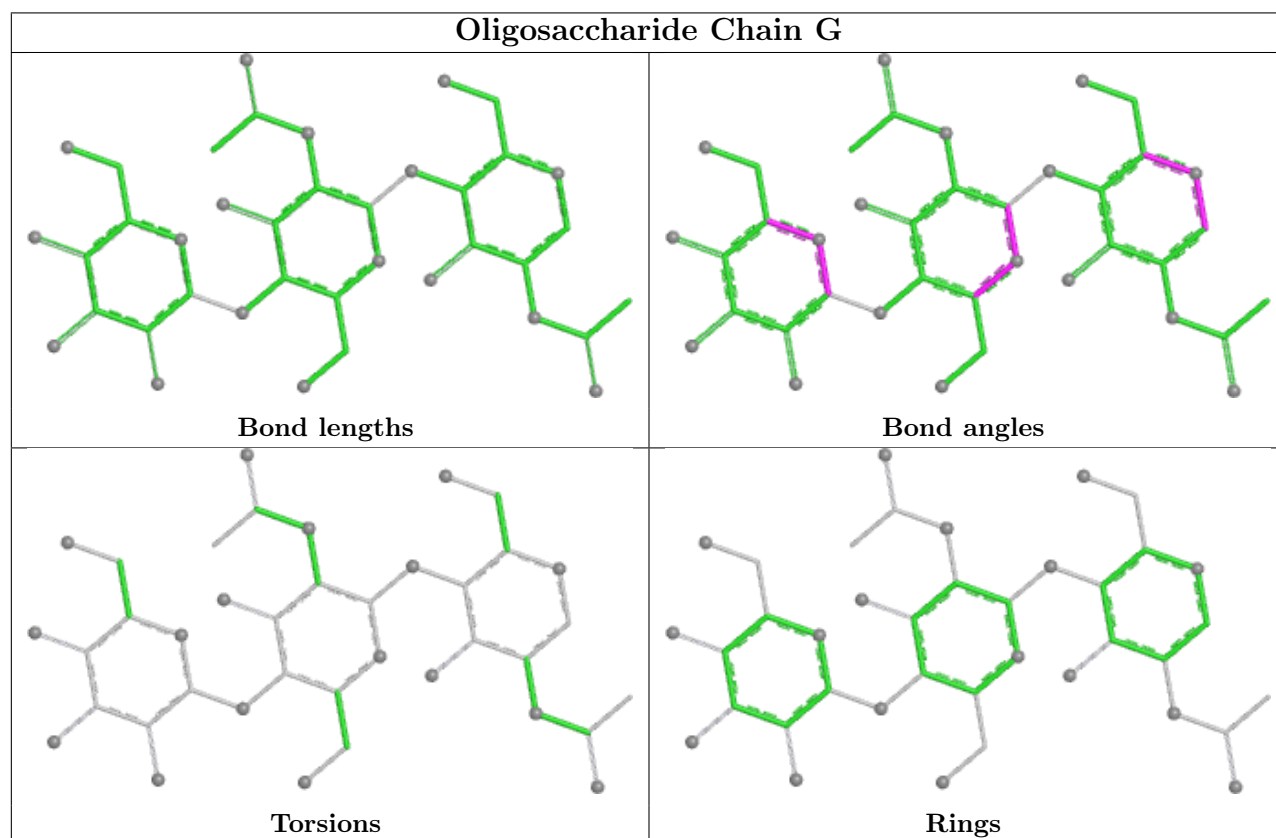
Mol	Chain	Res	Type	Atoms
6	R	5	MAN	O5-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6
6	O	3	BMA	C4-C5-C6-O6
6	R	3	BMA	C4-C5-C6-O6
6	R	4	MAN	C4-C5-C6-O6
6	K	4	MAN	C4-C5-C6-O6
6	O	4	MAN	C4-C5-C6-O6

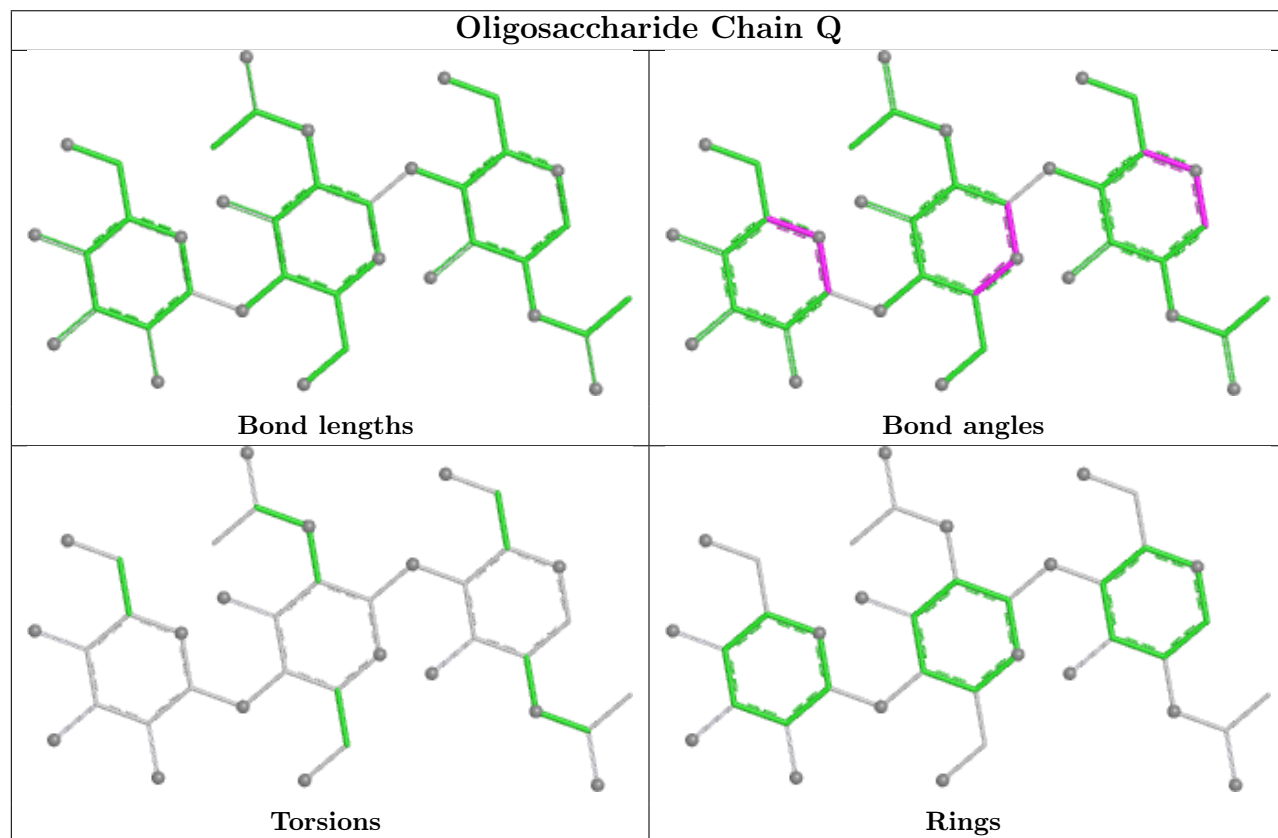
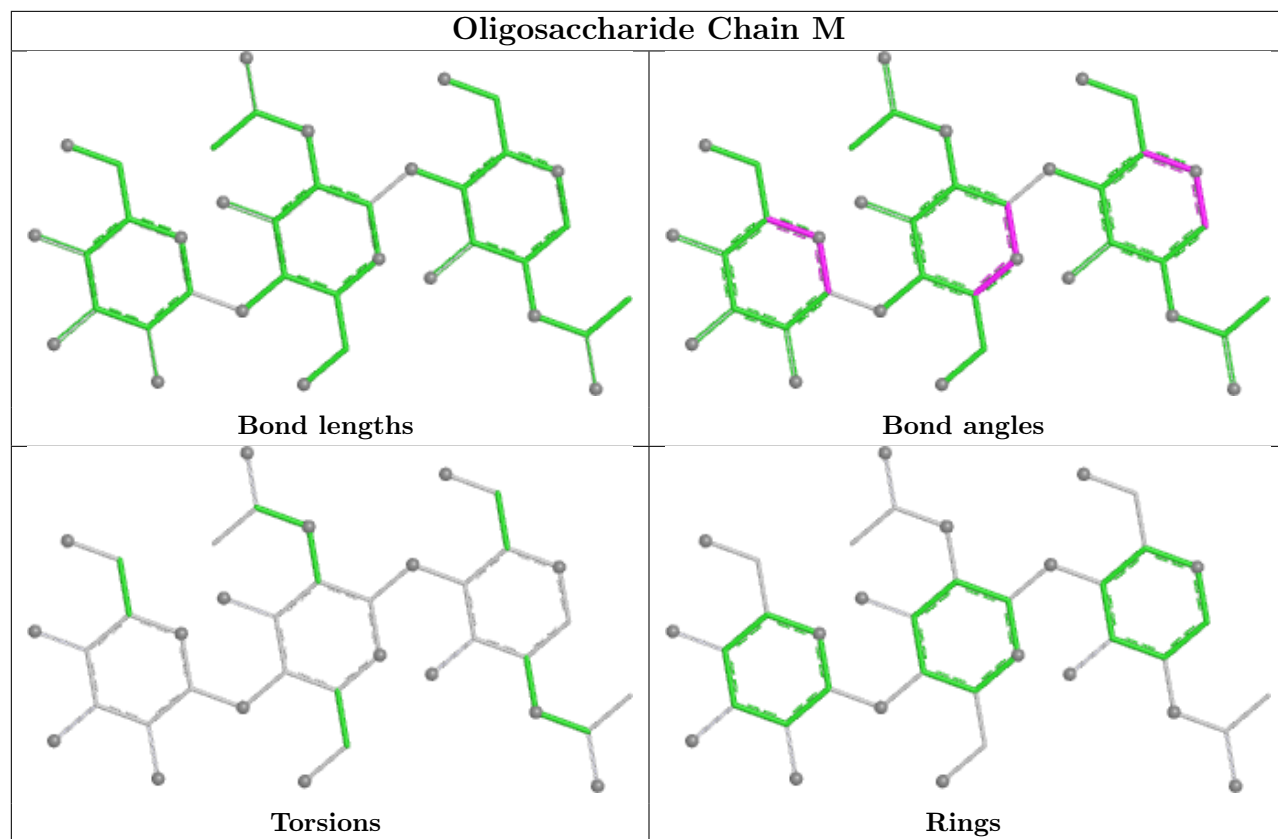
There are no ring outliers.

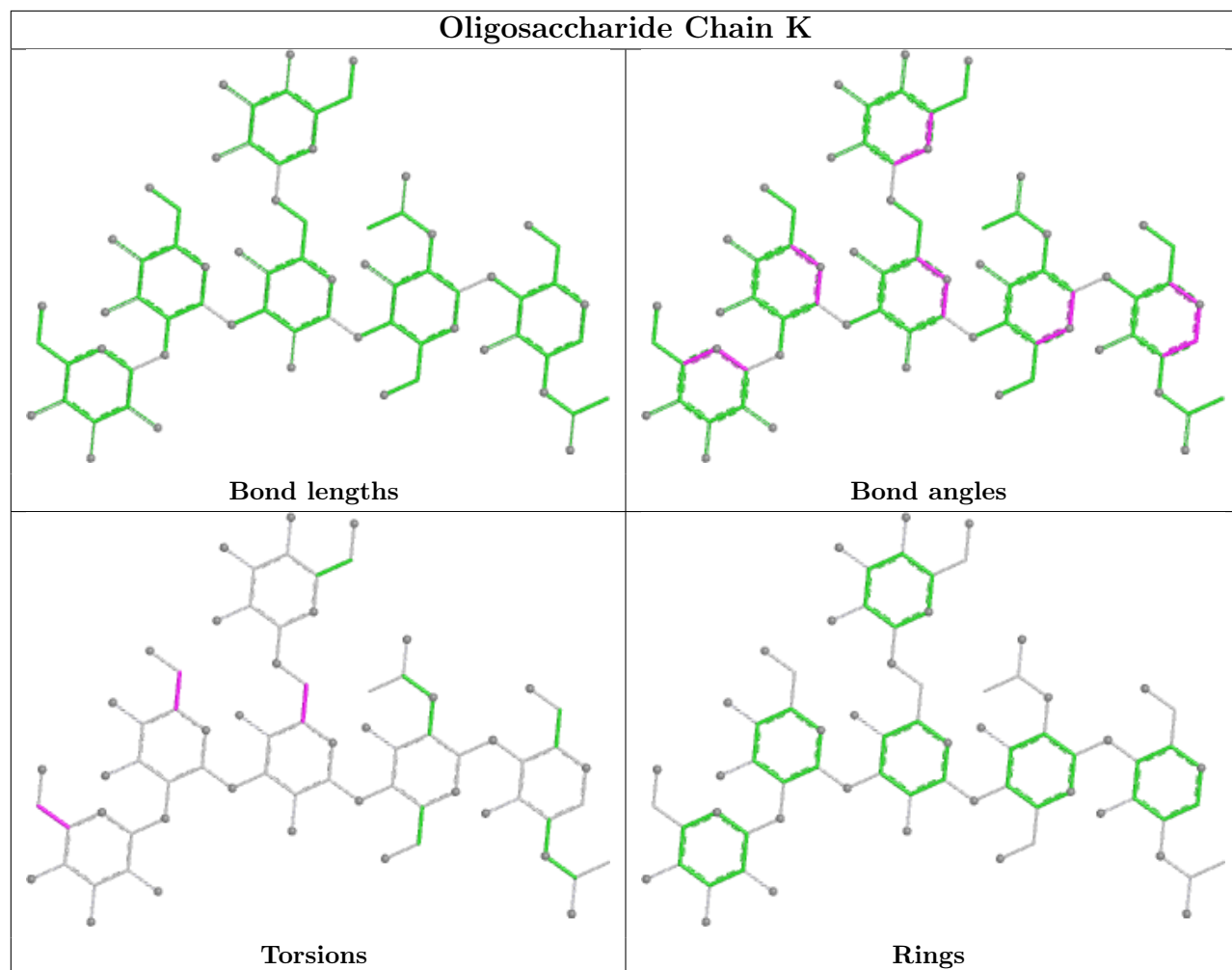
6 monomers are involved in 6 short contacts:

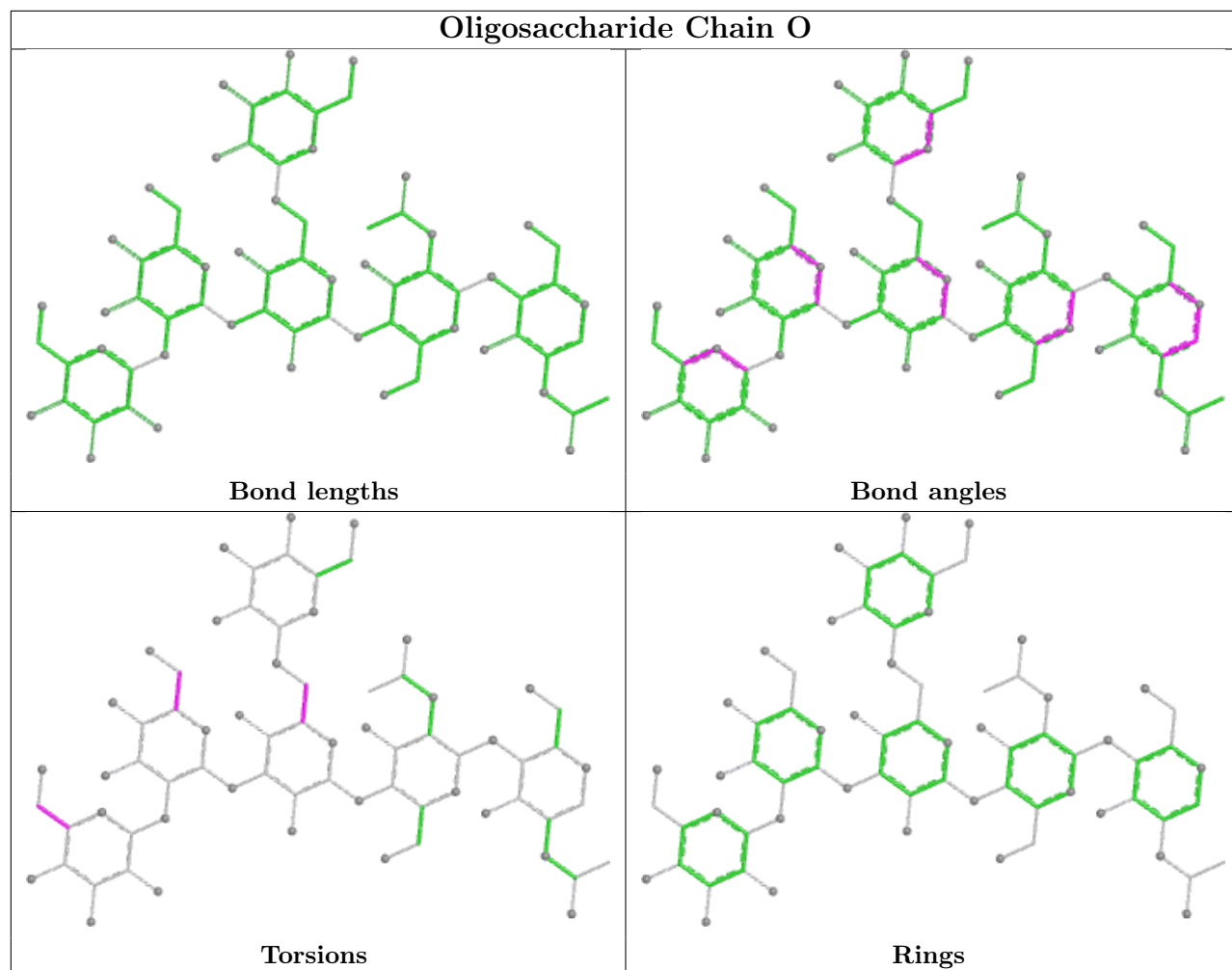
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	1	NAG	1	0
5	M	1	NAG	1	0
6	R	2	NAG	1	0
6	O	2	NAG	1	0
6	K	2	NAG	1	0
5	G	1	NAG	1	0

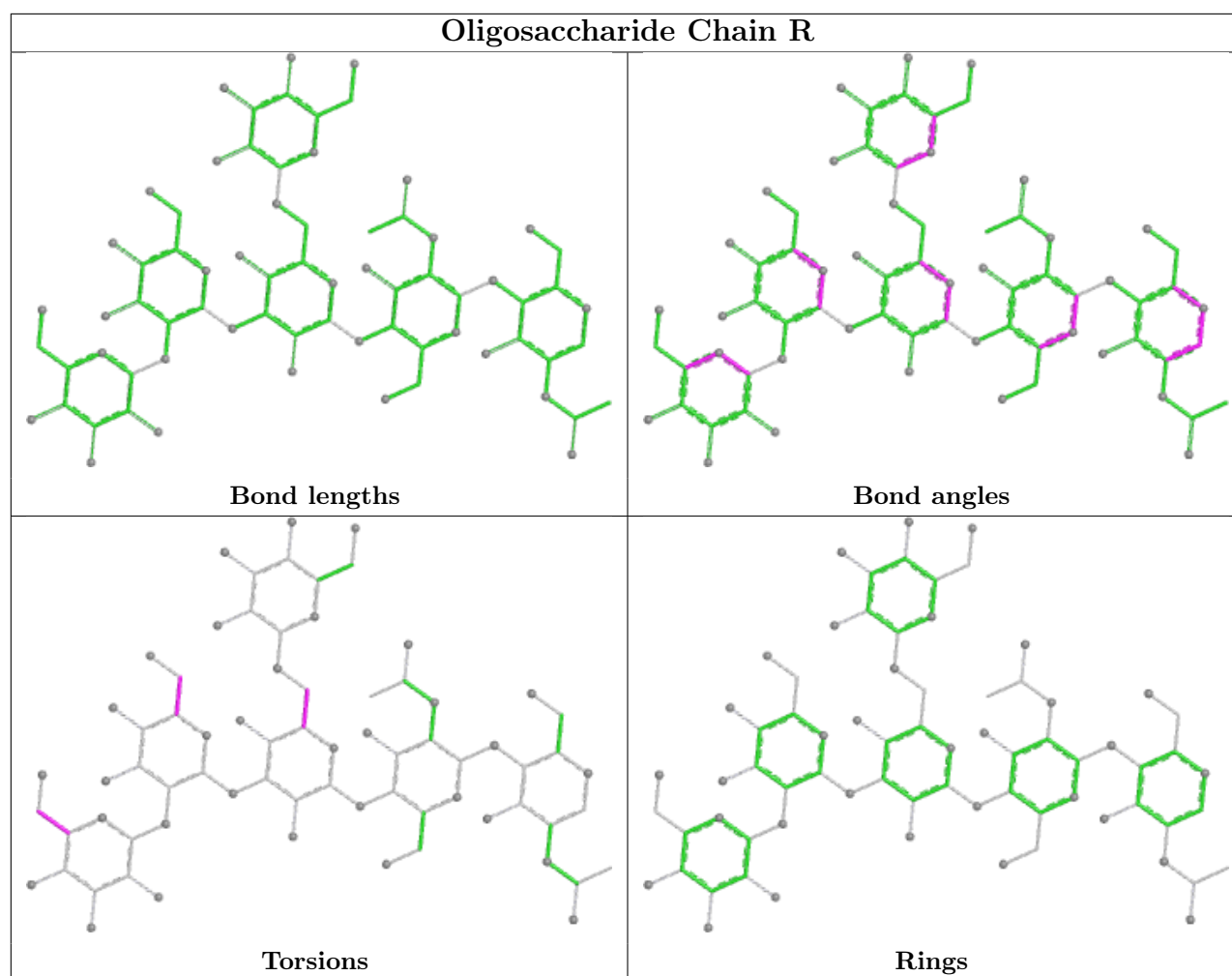
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

9 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
7	NAG	E	302	3	14,14,15	0.71	0	17,19,21	0.86	0
7	NAG	A	303	3	14,14,15	0.63	0	17,19,21	0.94	1 (5%)
7	NAG	A	302	3	14,14,15	0.71	0	17,19,21	0.86	0
7	NAG	C	303	3	14,14,15	0.64	0	17,19,21	0.94	1 (5%)
7	NAG	C	301	3	14,14,15	0.71	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	302	3	14,14,15	0.72	0	17,19,21	0.86	0
7	NAG	E	303	3	14,14,15	0.63	0	17,19,21	0.95	1 (5%)
7	NAG	A	301	3	14,14,15	0.71	0	17,19,21	0.79	0
7	NAG	E	301	3	14,14,15	0.72	0	17,19,21	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	302	3	-	2/6/23/26	0/1/1/1
7	NAG	A	303	3	-	0/6/23/26	0/1/1/1
7	NAG	A	302	3	-	2/6/23/26	0/1/1/1
7	NAG	C	303	3	-	0/6/23/26	0/1/1/1
7	NAG	C	301	3	-	0/6/23/26	0/1/1/1
7	NAG	C	302	3	-	2/6/23/26	0/1/1/1
7	NAG	E	303	3	-	0/6/23/26	0/1/1/1
7	NAG	A	301	3	-	0/6/23/26	0/1/1/1
7	NAG	E	301	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	303	NAG	O5-C1-C2	-2.04	108.13	111.29
7	E	303	NAG	O5-C1-C2	-2.03	108.14	111.29
7	C	303	NAG	O5-C1-C2	-2.03	108.15	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	302	NAG	C8-C7-N2-C2
7	A	302	NAG	O7-C7-N2-C2
7	C	302	NAG	C8-C7-N2-C2
7	C	302	NAG	O7-C7-N2-C2
7	E	302	NAG	C8-C7-N2-C2
7	E	302	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

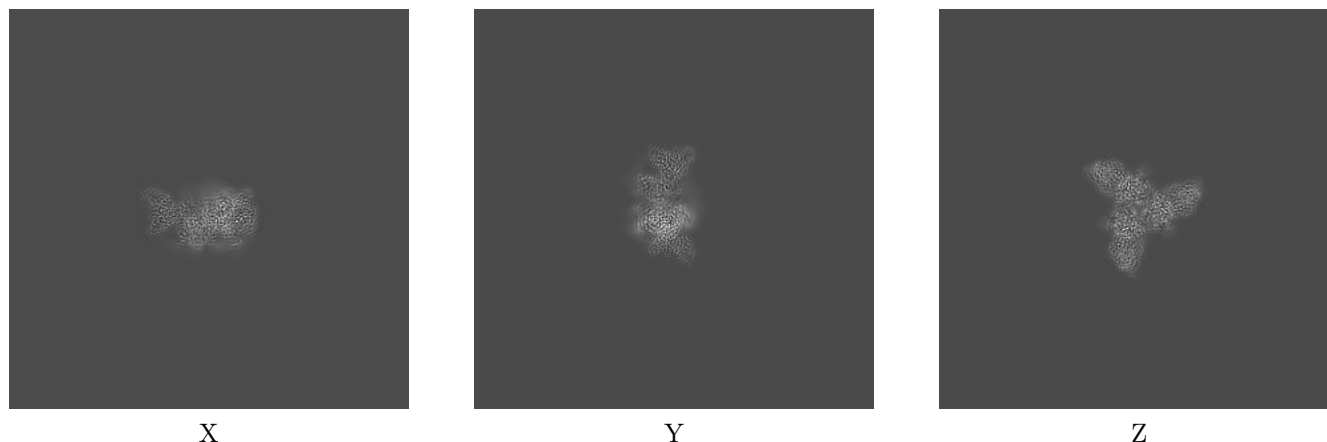
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49486. These allow visual inspection of the internal detail of the map and identification of artifacts.

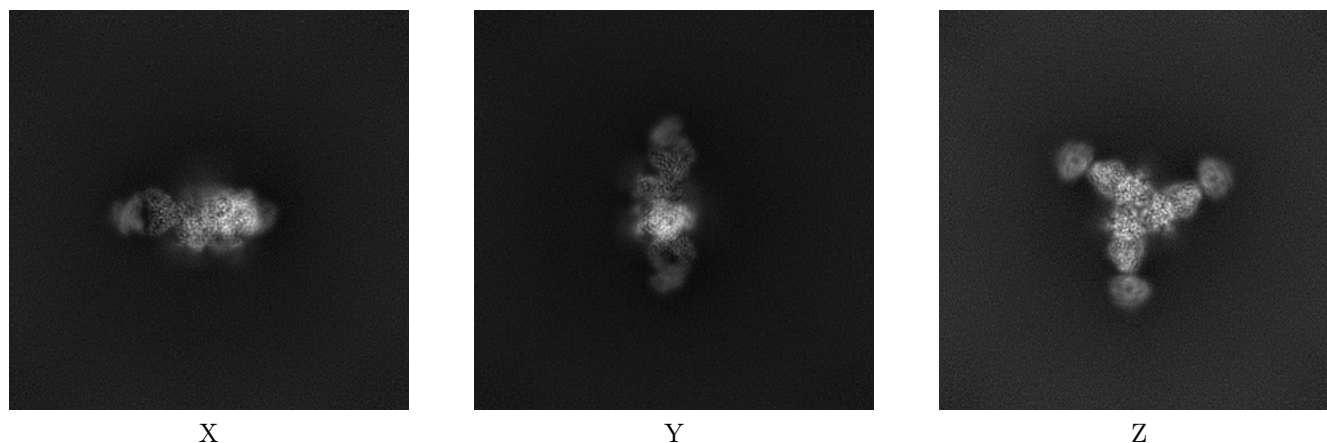
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



6.1.2 Raw map



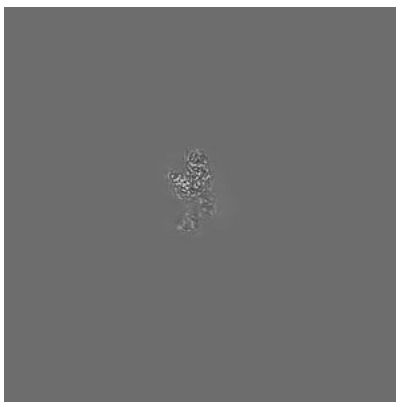
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

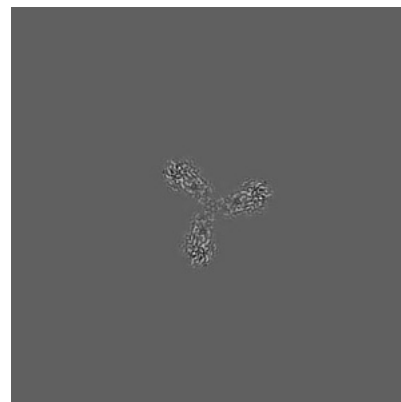
6.2.1 Primary map



X Index: 256

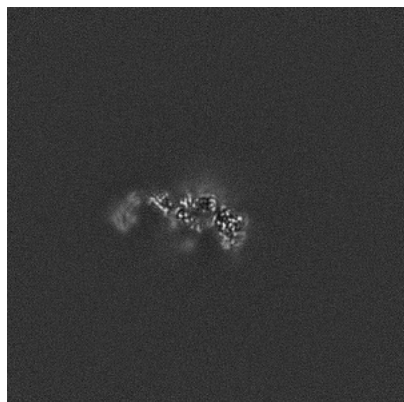


Y Index: 256

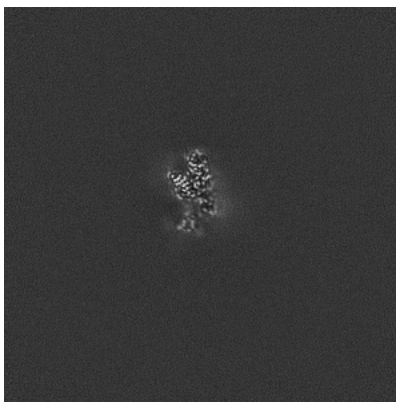


Z Index: 256

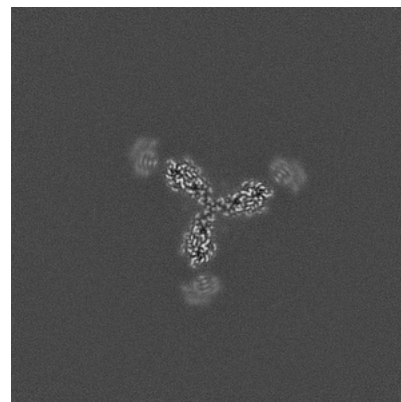
6.2.2 Raw map



X Index: 256



Y Index: 256

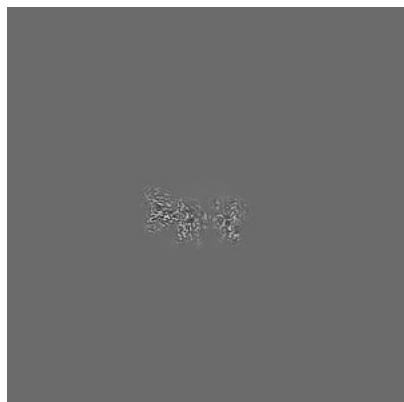


Z Index: 256

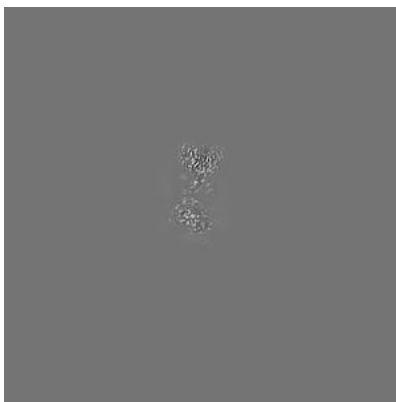
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

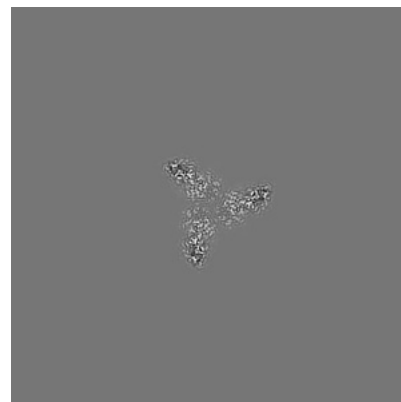
6.3.1 Primary map



X Index: 239

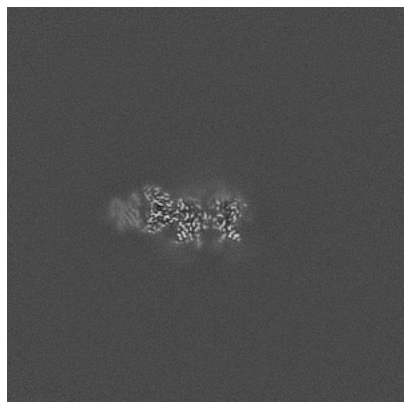


Y Index: 273

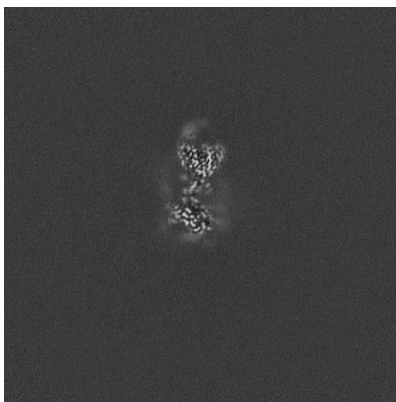


Z Index: 244

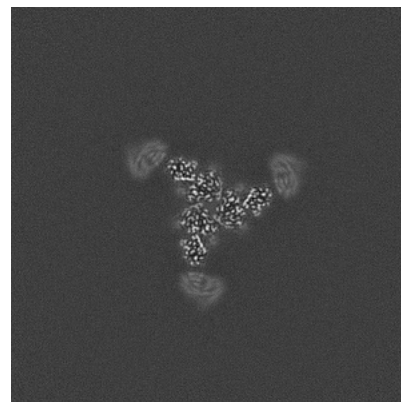
6.3.2 Raw map



X Index: 239



Y Index: 274

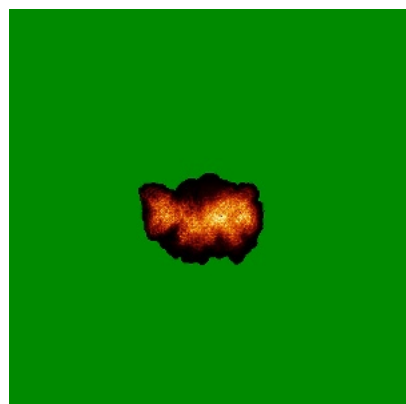


Z Index: 240

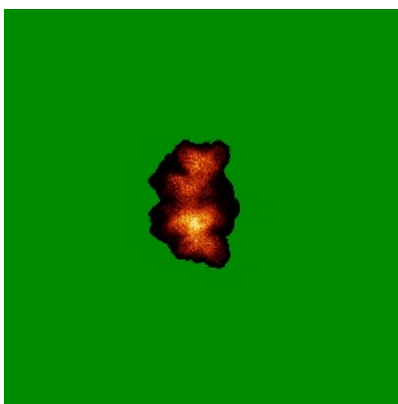
The images above show the largest variance slices of the map in three orthogonal directions.

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

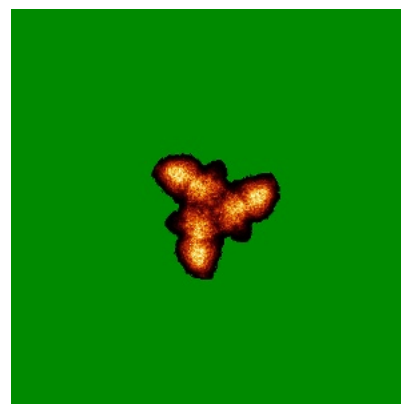
6.4.1 Primary map



X

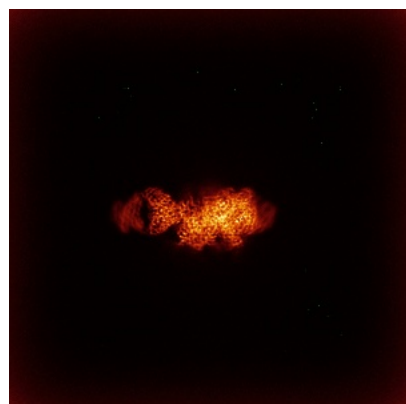


Y

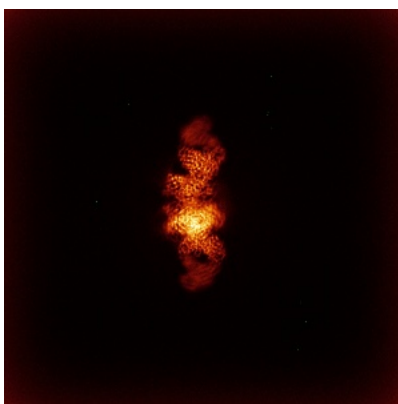


Z

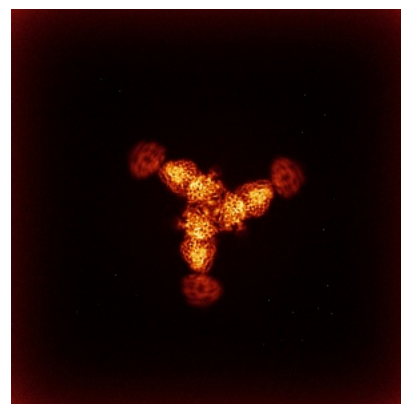
6.4.2 Raw map



X



Y

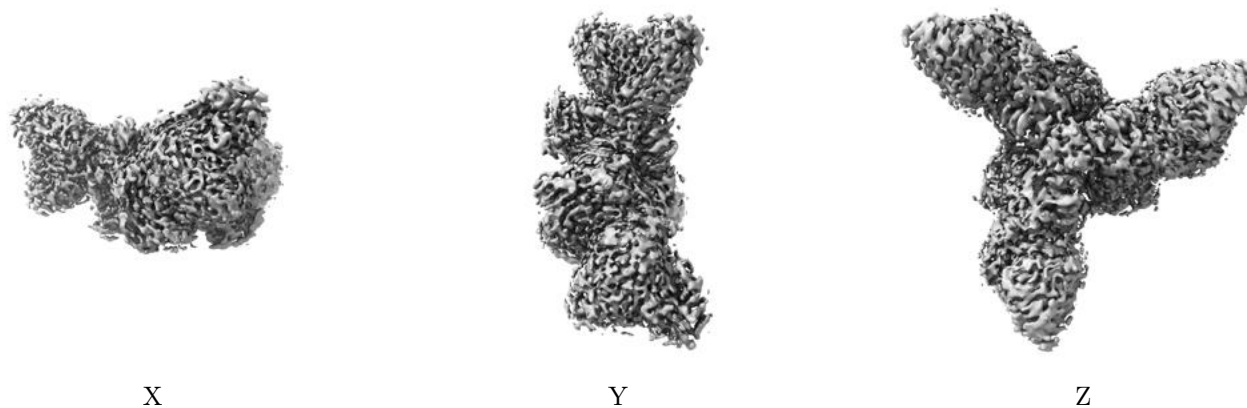


Z

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.

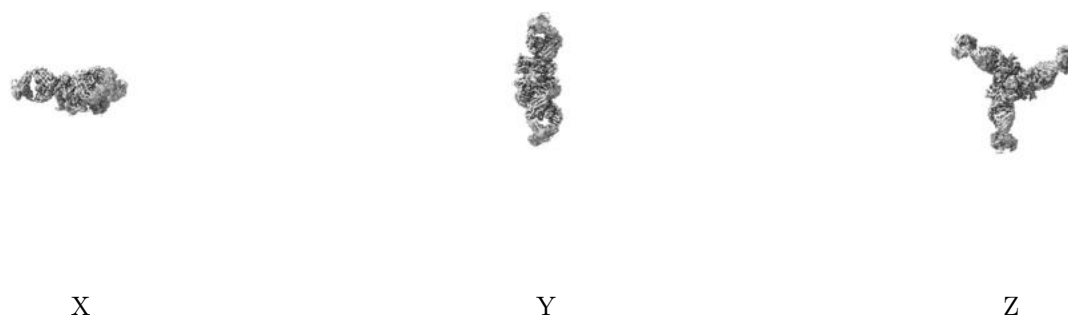
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

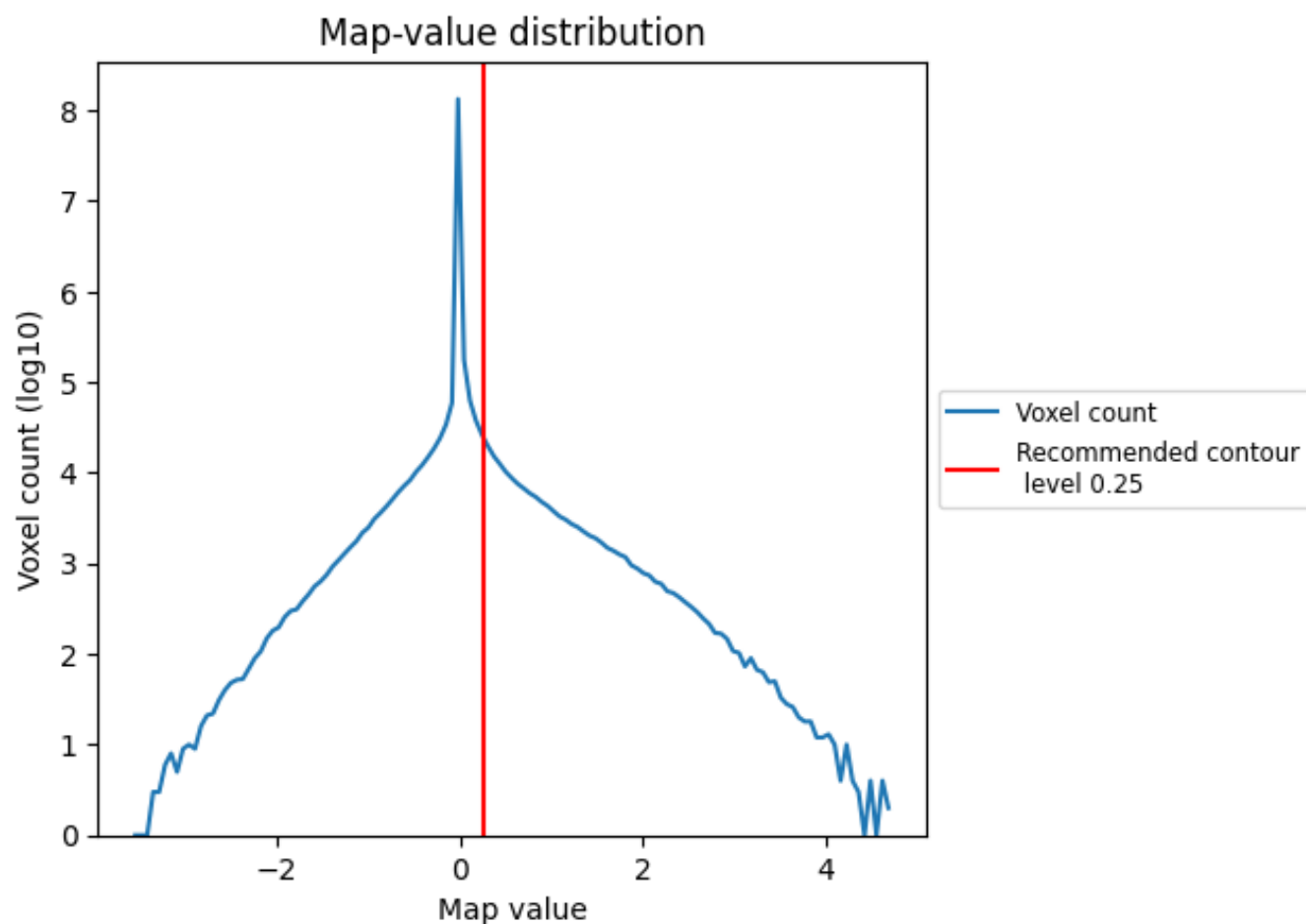
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

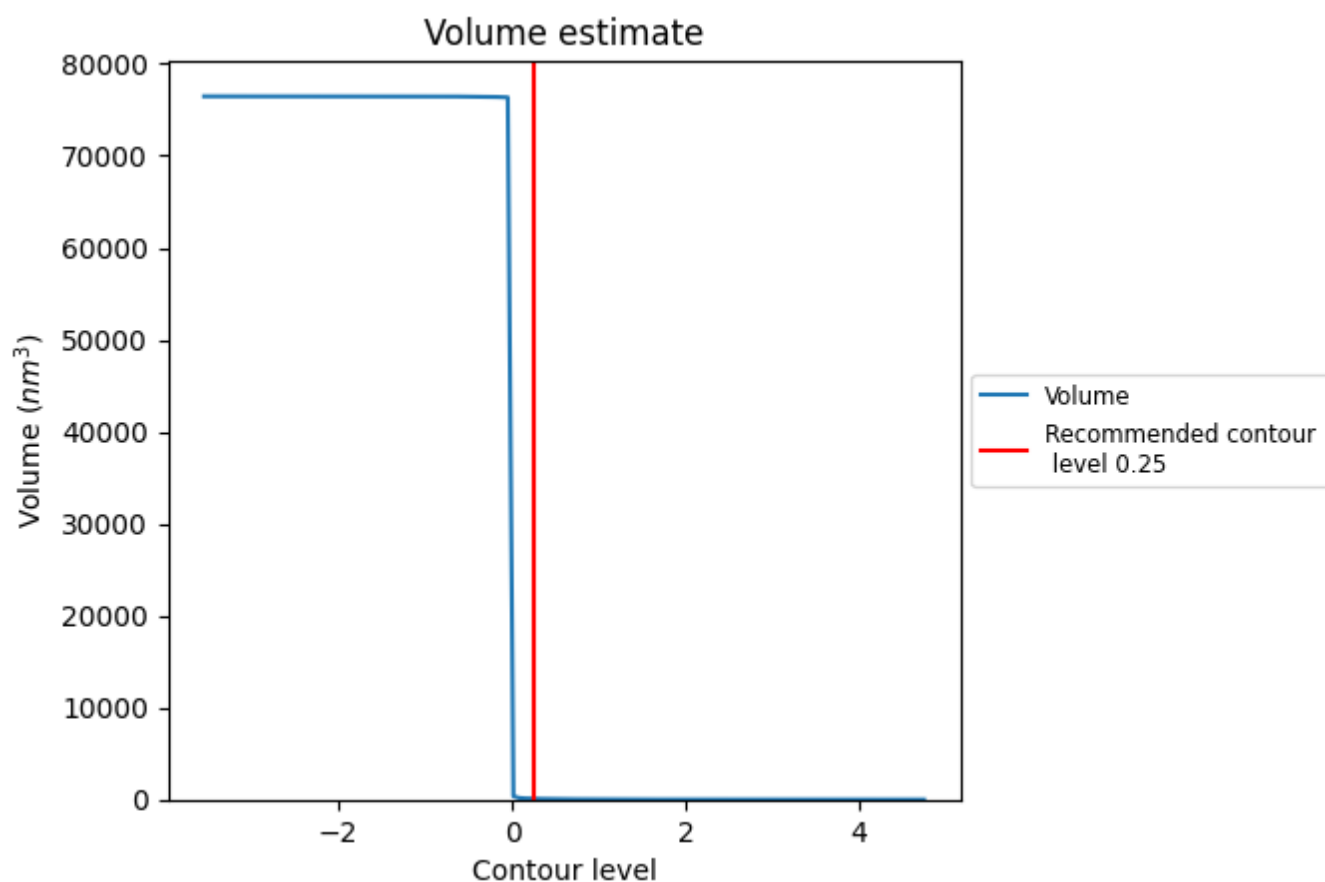
This section contains the results of statistical analysis of the map.

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.

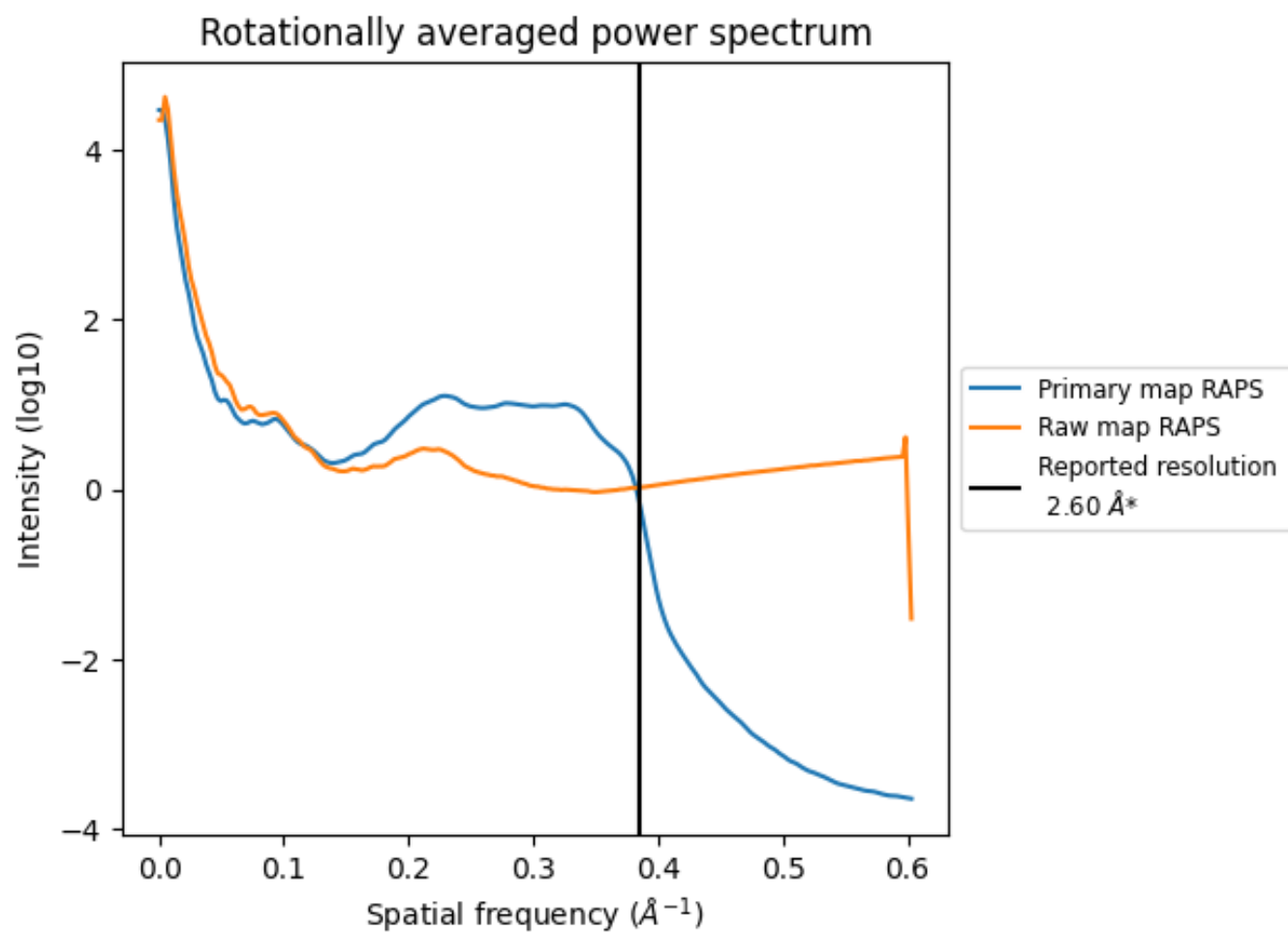
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 92 nm³; this corresponds to an approximate mass of 83 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 ⓘ

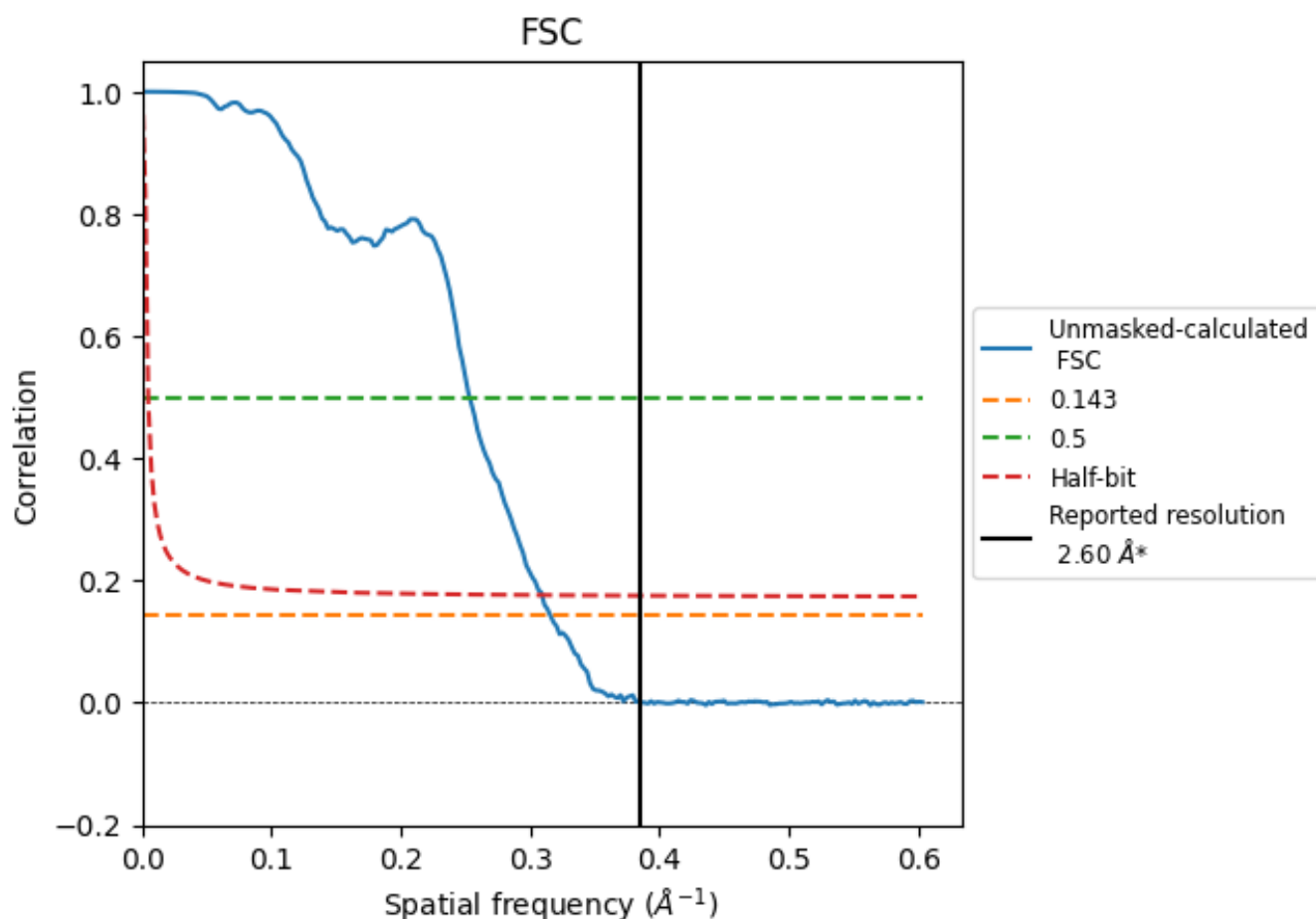


*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

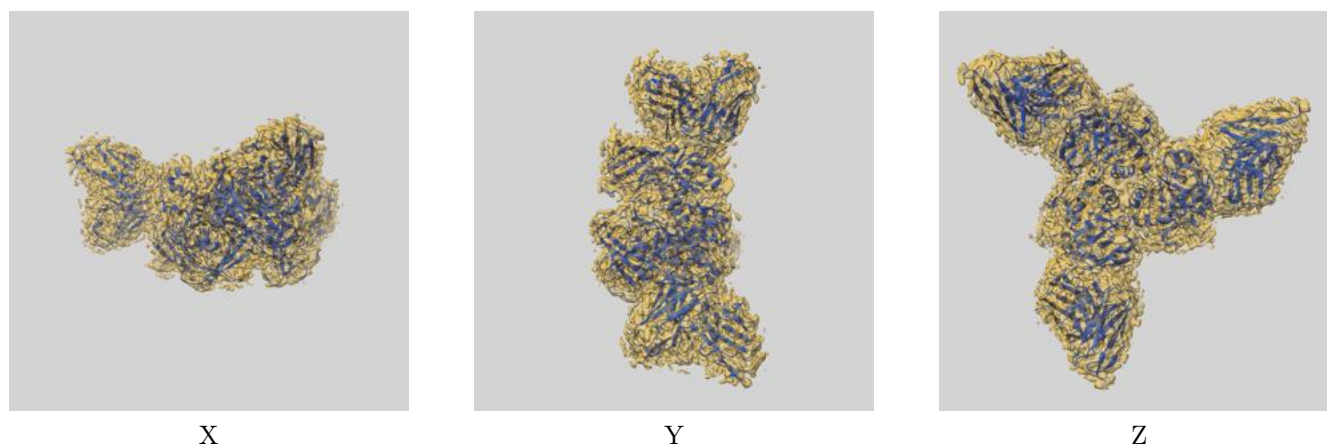
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	3.95	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

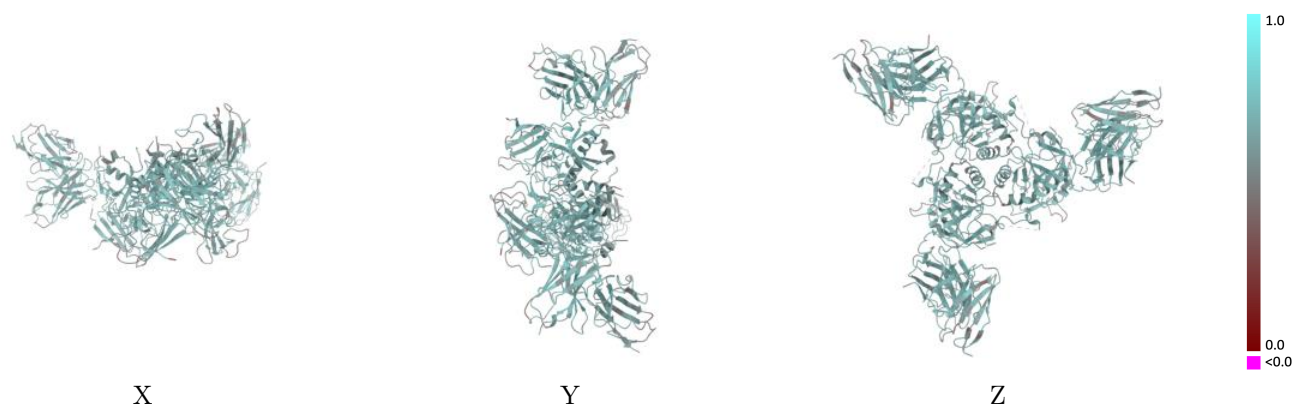
This section contains information regarding the fit between EMDB map EMD-49486 and PDB model 9NJJ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



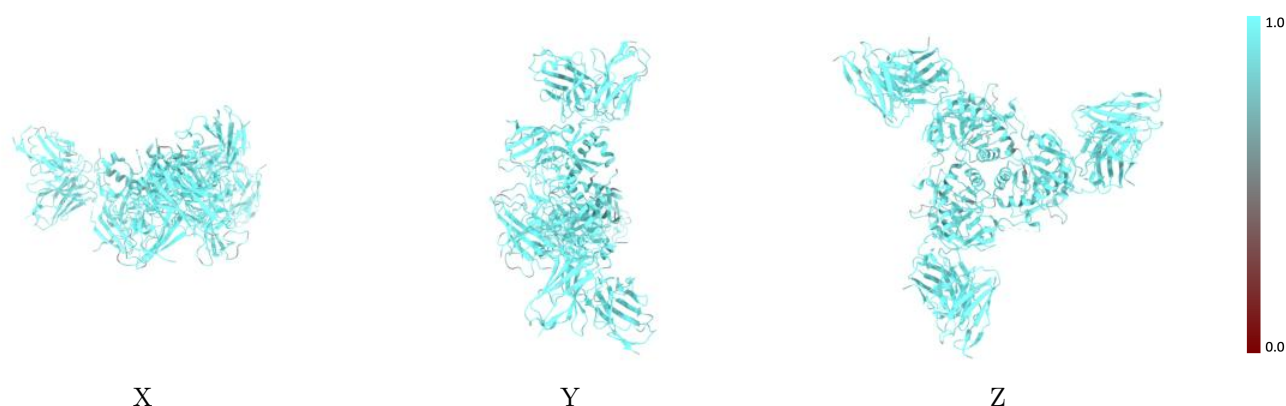
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



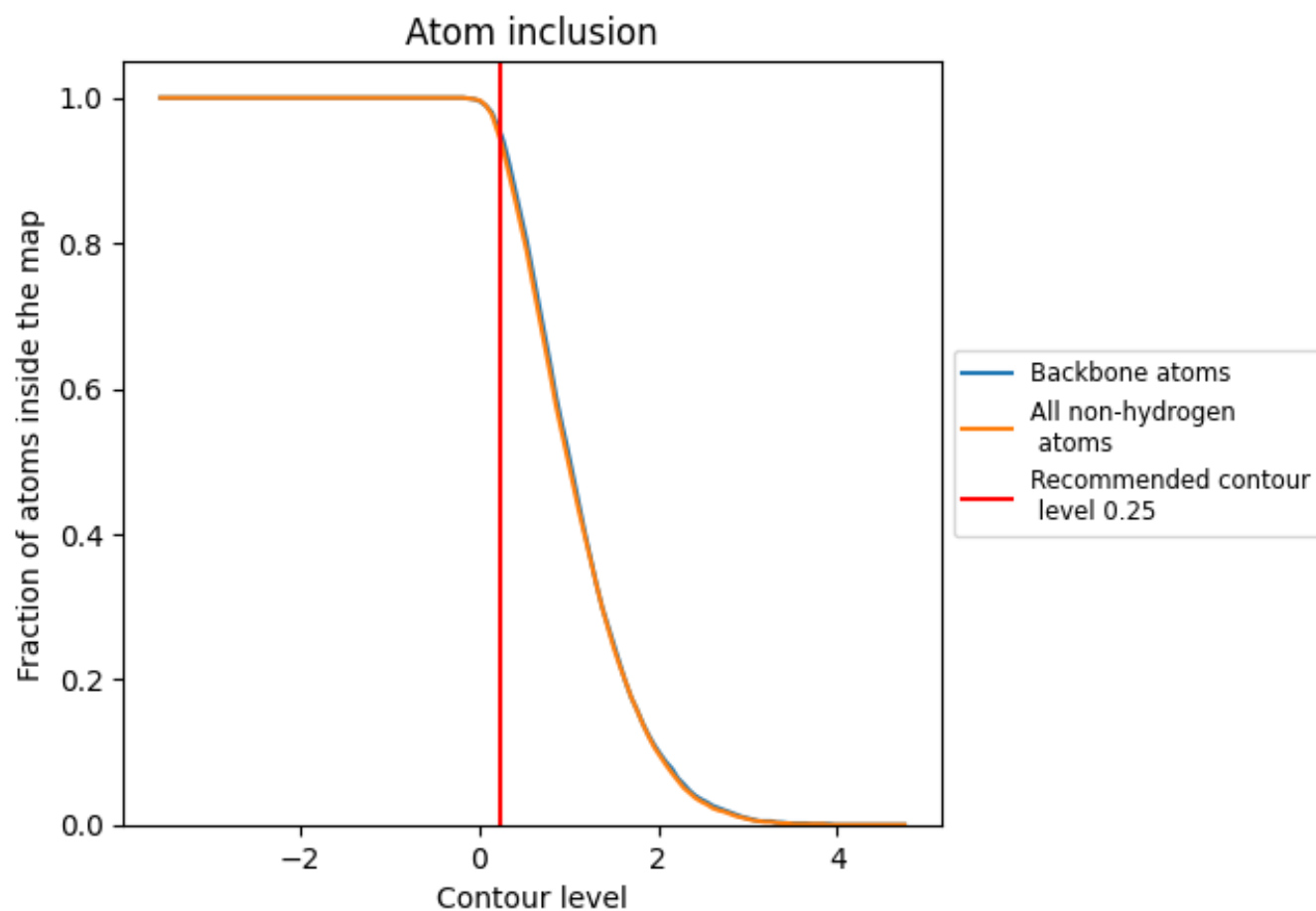
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.6120
A	 0.9350	 0.6180
B	 0.9660	 0.6240
C	 0.9340	 0.6140
D	 0.9680	 0.6240
E	 0.9350	 0.6140
F	 0.9650	 0.6250
G	 0.5640	 0.4760
H	 0.9680	 0.6310
I	 0.9670	 0.6310
J	 0.9680	 0.6290
K	 0.7080	 0.4860
L	 0.9370	 0.5930
M	 0.5640	 0.4580
N	 0.9410	 0.5920
O	 0.6940	 0.4870
P	 0.9380	 0.5890
Q	 0.5640	 0.4770
R	 0.7080	 0.4820

