



Full wwPDB EM Validation Report ⓘ

Oct 19, 2024 – 08:17 AM EDT

PDB ID : 8DPL
EMDB ID : EMD-27637
Title : Structure of EBOV GP lacking the mucin-like domain with 2.1.1D5 scFv and 6D6 scFv bound
Authors : Yu, X.; Saphire, E.O.
Deposited on : 2022-07-15
Resolution : 2.53 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

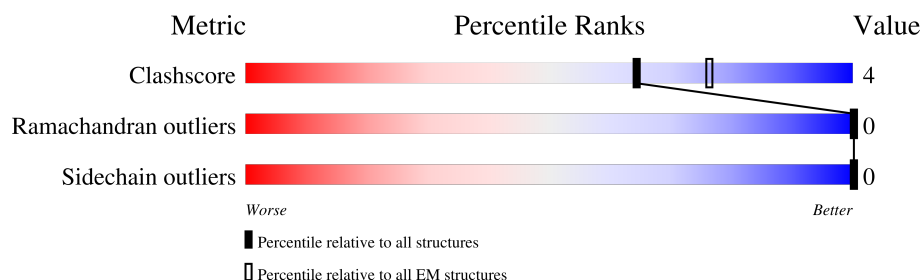
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 Å.

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













Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	120	
1	F	120	
1	K	120	
2	B	112	
2	G	112	
2	L	112	
3	C	243	
3	H	243	

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Mol	Chain	Length	Quality of chain
3	O	243	 82% 9% 9%
4	D	280	 55% 8% 38%
4	I	280	 55% 8% 38%
4	M	280	 56% 6% 38%
5	E	136	 61% 10% 29%
5	J	136	 60% 10% 29%
5	N	136	 61% 10% 29%
6	P	6	 50% 50%
6	Q	6	 50% 50%
6	R	6	 50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16872 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 2.1.1D5 heavy chain variable domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	119	Total	C	N	O	S	0	0
			909	574	157	174	4		
1	A	119	Total	C	N	O	S	0	0
			909	574	157	174	4		
1	K	119	Total	C	N	O	S	0	0
			909	574	157	174	4		

- Molecule 2 is a protein called 2.1.1D5 light chain variable domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	111	Total	C	N	O	S	0	0
			817	510	137	168	2		
2	B	111	Total	C	N	O	S	0	0
			817	510	137	168	2		
2	L	111	Total	C	N	O	S	0	0
			817	510	137	168	2		

- Molecule 3 is a protein called 6D6 single-chain variable fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	221	Total	C	N	O	S	0	0
			1709	1082	284	336	7		
3	C	221	Total	C	N	O	S	0	0
			1709	1082	284	336	7		
3	O	221	Total	C	N	O	S	0	0
			1709	1082	284	336	7		

- Molecule 4 is a protein called Glycoprotein GP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	174	Total	C	N	O	S	0	0
			1344	855	231	253	5		

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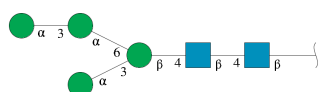
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	174	Total	C	N	O	S	0	0
			1344	855	231	253	5		
4	M	174	Total	C	N	O	S	0	0
			1344	855	231	253	5		

- Molecule 5 is a protein called Glycoprotein GP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	96	Total	C	N	O	S	0	0
			759	486	133	137	3		
5	E	96	Total	C	N	O	S	0	0
			759	486	133	137	3		
5	N	96	Total	C	N	O	S	0	0
			759	486	133	137	3		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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	P	6	Total	C	N	O	0	0
			72	40	2	30		
6	Q	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 (three-letter code: NAG) (formula: C₈H₁₅NO₆).

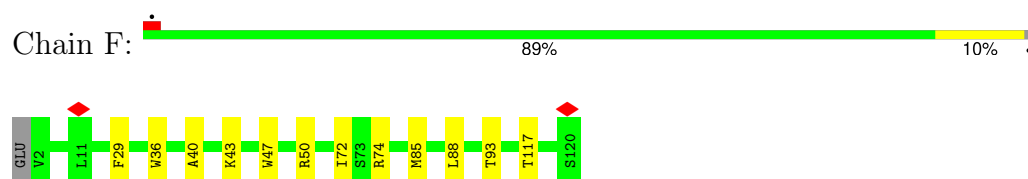


Mol	Chain	Residues	Atoms				AltConf
7	I	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	
7	M	1	Total	C	N	O	0
			14	8	1	5	

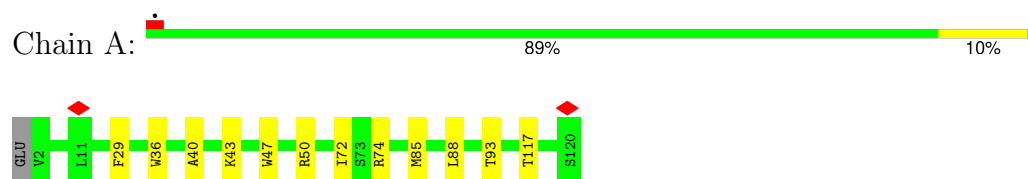
3 Residue-property plots [i](#)

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.

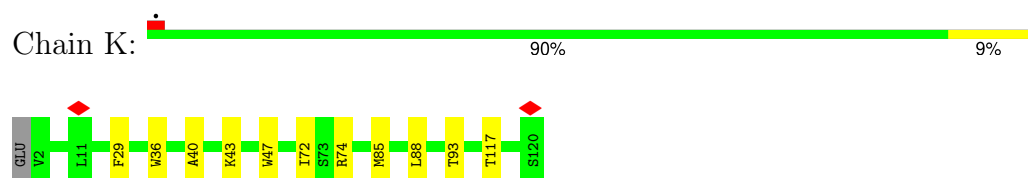
- Molecule 1: 2.1.1D5 heavy chain variable domain



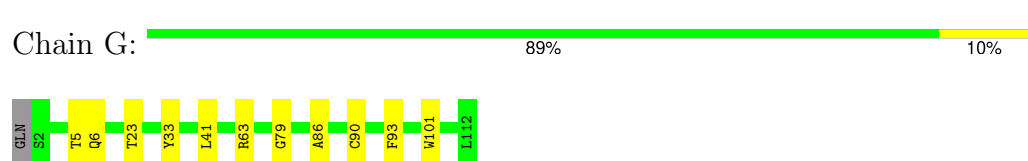
- Molecule 1: 2.1.1D5 heavy chain variable domain



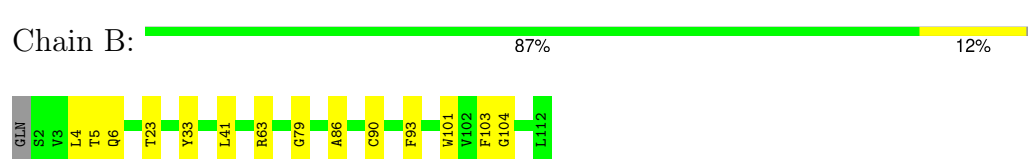
- Molecule 1: 2.1.1D5 heavy chain variable domain




- Molecule 2: 2.1.1D5 light chain variable domain



- Molecule 2: 2.1.1D5 light chain variable domain




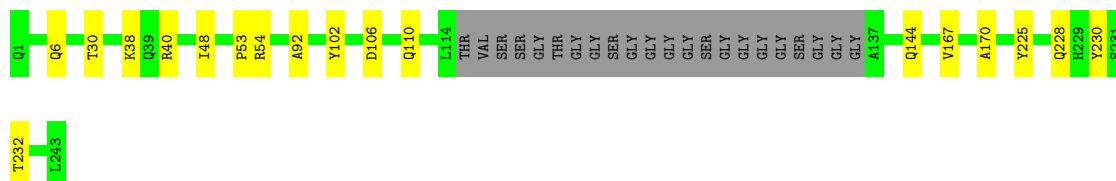
- Molecule 2: 2.1.1D5 light chain variable domain

Chain L:  88% 12%




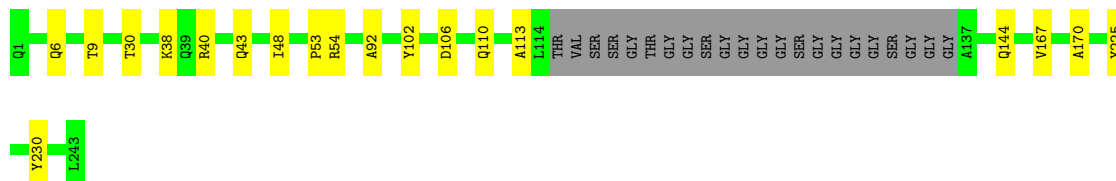
- Molecule 3: 6D6 single-chain variable fragment

Chain H:  84% 7% 9%




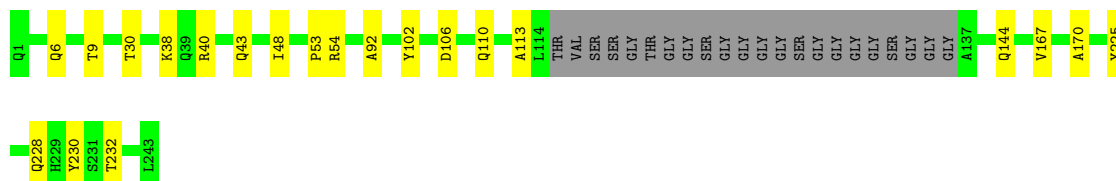
- Molecule 3: 6D6 single-chain variable fragment

Chain C:  83% 8% 9%



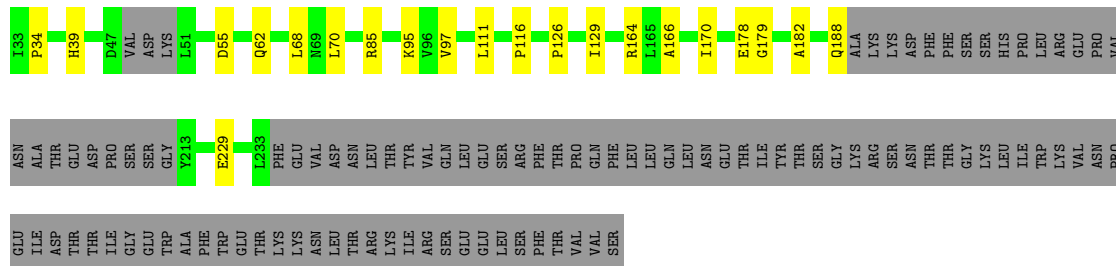
- Molecule 3: 6D6 single-chain variable fragment

Chain O:  82% 9% 9%



- Molecule 4: Glycoprotein GP1

Chain I:  55% 8% 38%



- Molecule 4: Glycoprotein GP1

GLU	ASN	I33
ILE	ALA	P34
ASP	THR	
THR	GLU	D47
THR	ASP	V47
ILE	PRO	ASP
GLY	SER	LYS
GLU	SER	L51
TRP	GLY	
ALA	Y213	Q62
PHE		
TRP	E229	L68
GLU		H69
THR	L233	L70
LYS	PHE	
LYS	GLU	R85
ASN	VAL	
LEU	ASP	K95
THR	ASN	Y96
ARG	LEU	V97
LYS	THR	
ILE	TYR	E106
ARG	VAL	
SER	GLN	L111
GLU	LEU	
GLU	GLU	P116
LEU	SER	
LEU	ARG	P126
PHE	PHE	
THR	THR	I129
VAL	PRO	
VAL	GLN	R136
SER	PHE	
	LEU	R164
	LEU	I165
	GLN	A166
	LEU	
	ASN	I170
	GLU	
	THR	E178
	ILE	G179
	TYR	
	THR	A182
	SER	
	GLY	Q188
	LYS	ALA
	ARG	LYS
	SER	LYS
	ASN	ASP
	THR	PHE
	THR	PHE
	GLY	SER
	LYS	SER
	LEU	HIS
	ILE	PRO
	TRP	LEU
	LYS	ARG
	VAL	GLU
	ASN	PRO
	PRO	VAL

Position	Sequence	Score	Label
1	GLY	SER	I33
2	GLU	GLY	P34
3	TRP	GLY	D47
4	ALA	Y213	VAL
5	PHE		ASP
6	TRP	E229	L51
7	GLU		L51
8	THR	L233	Q62
9	LYS	PHE	L68
10	LYS	GLU	H69
11	ASN	VAL	L70
12	LEU	ASP	R85
13	ARG	ASN	Y97
14	LYS	THR	L111
15	THR	LEU	P126
16	ILE	SER	T129
17	ARG	ARG	R134
18	GLU	PHE	R164
19	GLU	LEU	L165
20	GLU	LEU	A166
21	ASN	ASN	I170
22	GLU	GLU	E178
23	THR	THR	G179
24	ILE	TYR	A182
25	TYR	SER	Q188
26	SER	GLY	ALA
27	LYS	LYS	LYS
28	ARG	ARG	ASP
29	SER	SER	PHE
30	ASN	ASN	PHE
31	THR	THR	SER
32	THR	GLY	SER
33	LYS	LYS	THR
34	LEU	LEU	PRO
35	ILE	ILE	LEU
36	TRP	TRP	ARG
37	LYS	LYS	GLU
38	VAL	VAL	PRO
39	ASN	ASN	VAL
40	THR	THR	ASP
41	GLU	GLU	THR
42	ILE	ILE	GLU
43	THR	THR	THR
44	THR	THR	ASP
45	THR	THR	THR

HIS	GLU
ASP	A503
PHE	
VAL	H516
ASP	
LYS	L529
THR	
LEU	I532
PRO	
ASP	L547
	Q551
	D552
	G553
	L558
	R559
	Q560
	L561
	A562
	N563
	E564
	T565
	L573
	R574
	A575
	L584
	G598
GLY	
THR	CYS
CYS	HIS
HIS	ILE
ILE	LEU
LEU	PRO
PRO	ASP
ASP	CYS
CYS	ILE
ILE	GLU
GLU	PRO
PRO	HIS
HIS	ASP
ASP	TRP
TRP	THR
THR	LYS
LYS	ASN
ASN	ILE
ILE	THR
THR	ASP
ASP	LYS
LYS	ILE
ILE	ASP
ASP	GLN
GLN	ILE
ILE	ILE

PHE	GLU
VAL	AS03
ASP	AS03
LYS	AS16
THR	AS16
LEU	AS27
PRO	AS28
ASP	AS29
	AS30
	AS30
	AS47
	AS47
	AS51
	AS52
	AS53
	AS53
	AS58
	AS58
	AS62
	AS62
	AS66
	AS66
	AS73
	AS74
	AS75
	AS75
	AS84
	AS84
	AS98
	AS98
GLY	GLY
THR	THR
CYS	CYS
HIS	HIS
ILE	ILE
LEU	LEU
GLY	GLY
PRO	PRO
ASP	ASP
CYS	CYS
CYS	CYS
ILE	ILE
GLU	GLU
PRO	PRO
HIS	HIS
ASP	ASP
THR	THR
THR	THR
LYS	LYS
ASN	ASN
ILE	ILE
THR	THR
ASP	ASP
LYS	LYS
ILE	ILE
ASP	ASP
GLN	GLN
ILE	ILE
ILE	ILE
THR	THR
ASP	ASP

GLU	AS03	HS16	LS29	ES45	GS46	LS47	QS51	DS52	GS53	LS58	FS59	QS60	LS61	AS62	NF63	ES64	TS65	AS75	IS84	GS98	GLY	THR	CYS	CYS	HIS	ILE	ILE	LEU	GLY	PRO	ASP	ASP	CYS	CYS	ILE	ILE	GLU	PRO	HIS	ASP	TRP	THR	THR	LYS	ASP	LYS	ILE	ASP	GLN	ILE	ILE	ILE	HIS	ASP
-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PHE
VAL
ASP
LYS
THR
LEU
PRO
ASP

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

Chain P:  50% 50%

MAG1
MAG2
EM13
MAN4
MAN5
MAN6

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

Chain Q:  50% 50%

MAG1
MAG2
EM13
MAN4
MAN5
MAN6

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

Chain R:  50% 50%

MAG1
MAG2
EM13
MAN4
MAN5
MAN6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	610008	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.565	Depositor
Minimum map value	-0.501	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.24	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98999995, 0.98999995, 0.98999995	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, BMA, 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	A	0.24	0/929	0.43	0/1259
1	F	0.24	0/929	0.43	0/1259
1	K	0.24	0/929	0.43	0/1259
2	B	0.24	0/836	0.42	0/1139
2	G	0.24	0/836	0.42	0/1139
2	L	0.25	0/836	0.42	0/1139
3	C	0.25	0/1753	0.43	0/2380
3	H	0.25	0/1753	0.43	0/2380
3	O	0.25	0/1753	0.43	0/2380
4	D	0.25	0/1376	0.43	0/1868
4	I	0.25	0/1376	0.43	0/1868
4	M	0.25	0/1376	0.43	0/1868
5	E	0.23	0/777	0.38	0/1058
5	J	0.23	0/777	0.38	0/1058
5	N	0.23	0/777	0.38	0/1058
All	All	0.24	0/17013	0.42	0/23112

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	A	909	0	886	8	0
1	F	909	0	886	7	0
1	K	909	0	886	6	0
2	B	817	0	779	8	0
2	G	817	0	779	6	0
2	L	817	0	779	7	0
3	C	1709	0	1631	14	0
3	H	1709	0	1631	12	0
3	O	1709	0	1631	15	0
4	D	1344	0	1301	15	0
4	I	1344	0	1301	15	0
4	M	1344	0	1301	14	0
5	E	759	0	744	10	0
5	J	759	0	744	11	0
5	N	759	0	744	10	0
6	P	72	0	61	0	0
6	Q	72	0	61	0	0
6	R	72	0	61	0	0
7	D	14	0	13	1	0
7	I	14	0	13	1	0
7	M	14	0	13	1	0
All	All	16872	0	16245	129	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 4.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:40:ARG:HD2	3:O:92:ALA:HB2	1.74	0.70
3:H:40:ARG:HD2	3:H:92:ALA:HB2	1.74	0.68
3:C:40:ARG:HD2	3:C:92:ALA:HB2	1.74	0.68
4:D:229:GLU:HG2	7:D:401:NAG:H82	1.75	0.67
1:A:29:PHE:O	1:A:74:ARG:NH2	2.31	0.64
2:G:6:GLN:NE2	2:G:90:CYS:SG	2.71	0.64
1:K:29:PHE:O	1:K:74:ARG:NH2	2.31	0.63
2:L:6:GLN:NE2	2:L:90:CYS:SG	2.72	0.63
1:F:29:PHE:O	1:F:74:ARG:NH2	2.31	0.63
2:B:6:GLN:NE2	2:B:90:CYS:SG	2.72	0.63
4:D:126:PRO:HD2	4:D:129:ILE:HD12	1.81	0.62
4:M:126:PRO:HD2	4:M:129:ILE:HD12	1.81	0.62
4:I:68:LEU:HD11	5:J:558:LEU:HG	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:LEU:HD11	5:E:558:LEU:HG	1.82	0.62
4:I:62:GLN:OE1	4:I:188:GLN:NE2	2.33	0.62
4:D:62:GLN:OE1	4:D:188:GLN:NE2	2.33	0.61
4:I:126:PRO:HD2	4:I:129:ILE:HD12	1.81	0.61
3:O:170:ALA:HB3	3:O:230:TYR:HB2	1.83	0.60
4:M:229:GLU:HG2	7:M:401:NAG:H82	1.83	0.59
4:I:34:PRO:HD2	5:J:565:THR:HG23	1.84	0.58
4:D:34:PRO:HD2	5:E:565:THR:HG23	1.84	0.58
4:M:68:LEU:HD11	5:N:558:LEU:HG	1.84	0.58
3:C:170:ALA:HB3	3:C:230:TYR:HB2	1.86	0.58
2:L:41:LEU:HD23	2:L:86:ALA:HB2	1.86	0.58
4:M:62:GLN:OE1	4:M:188:GLN:NE2	2.33	0.57
3:O:6:GLN:H	3:O:110:GLN:HE22	1.52	0.57
3:H:6:GLN:H	3:H:110:GLN:HE22	1.53	0.57
3:H:170:ALA:HB3	3:H:230:TYR:HB2	1.87	0.57
4:D:164:ARG:NH2	5:N:575:ALA:O	2.37	0.56
2:G:41:LEU:HD23	2:G:86:ALA:HB2	1.86	0.56
4:I:164:ARG:NH2	5:E:575:ALA:O	2.38	0.56
4:M:34:PRO:HD2	5:N:565:THR:HG23	1.86	0.56
5:J:575:ALA:O	4:M:164:ARG:NH2	2.38	0.55
2:B:41:LEU:HD23	2:B:86:ALA:HB2	1.87	0.55
3:C:6:GLN:H	3:C:110:GLN:HE22	1.53	0.55
4:D:70:LEU:HG	4:D:179:GLY:HA2	1.89	0.54
3:C:30:THR:HA	3:C:53:PRO:HB2	1.89	0.53
3:O:38:LYS:HB2	3:O:48:ILE:HD11	1.90	0.53
3:C:38:LYS:HB2	3:C:48:ILE:HD11	1.90	0.53
3:H:38:LYS:HB2	3:H:48:ILE:HD11	1.89	0.53
3:O:30:THR:HA	3:O:53:PRO:HB2	1.91	0.53
4:M:85:ARG:NH1	4:M:178:GLU:OE2	2.42	0.53
4:I:85:ARG:NH1	4:I:178:GLU:OE2	2.41	0.52
3:H:30:THR:HA	3:H:53:PRO:HB2	1.91	0.52
3:H:106:ASP:N	3:H:106:ASP:OD1	2.40	0.52
3:O:167:VAL:HG12	3:O:230:TYR:HB3	1.92	0.51
4:I:70:LEU:HG	4:I:179:GLY:HA2	1.92	0.51
4:M:70:LEU:HG	4:M:179:GLY:HA2	1.92	0.51
4:I:97:VAL:HG12	4:I:166:ALA:HB3	1.92	0.51
3:C:6:GLN:H	3:C:110:GLN:NE2	2.09	0.51
3:O:6:GLN:H	3:O:110:GLN:NE2	2.09	0.51
4:D:85:ARG:NH1	4:D:178:GLU:OE2	2.43	0.50
2:L:63:ARG:NH1	2:L:79:GLY:O	2.44	0.49
3:C:167:VAL:HG12	3:C:230:TYR:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:GLN:H	3:H:110:GLN:NE2	2.09	0.49
3:H:167:VAL:HG12	3:H:230:TYR:HB3	1.94	0.49
2:B:63:ARG:NH1	2:B:79:GLY:O	2.45	0.49
2:G:63:ARG:NH1	2:G:79:GLY:O	2.46	0.49
1:A:93:THR:HG23	1:A:117:THR:HA	1.94	0.49
4:D:97:VAL:HG12	4:D:166:ALA:HB3	1.93	0.49
2:B:5:THR:HB	2:B:23:THR:HB	1.95	0.48
3:C:106:ASP:N	3:C:106:ASP:OD1	2.43	0.48
1:K:93:THR:HG23	1:K:117:THR:HA	1.95	0.48
1:F:93:THR:HG23	1:F:117:THR:HA	1.95	0.48
2:G:5:THR:HB	2:G:23:THR:HB	1.95	0.48
4:M:97:VAL:HG12	4:M:166:ALA:HB3	1.95	0.48
5:N:551:GLN:HG2	5:N:553:GLY:H	1.79	0.48
3:H:228:GLN:NE2	3:H:232:THR:OG1	2.36	0.48
4:I:111:LEU:HD12	4:I:170:ILE:HG21	1.96	0.48
1:A:40:ALA:HB3	1:A:43:LYS:HB2	1.96	0.48
5:J:551:GLN:HG2	5:J:553:GLY:H	1.79	0.48
1:K:85:MET:HB3	1:K:88:LEU:HD21	1.96	0.47
5:E:551:GLN:HG2	5:E:553:GLY:H	1.79	0.47
1:F:85:MET:HB3	1:F:88:LEU:HD21	1.96	0.47
3:O:144:GLN:HE22	3:O:225:TYR:HA	1.80	0.47
1:F:40:ALA:HB3	1:F:43:LYS:HB2	1.96	0.47
1:K:40:ALA:HB3	1:K:43:LYS:HB2	1.96	0.47
1:F:36:TRP:HD1	1:F:72:ILE:HD12	1.80	0.47
1:A:36:TRP:HD1	1:A:72:ILE:HD12	1.80	0.46
1:A:85:MET:HB3	1:A:88:LEU:HD21	1.96	0.46
2:L:5:THR:HB	2:L:23:THR:HB	1.96	0.46
1:K:36:TRP:HD1	1:K:72:ILE:HD12	1.81	0.45
3:C:144:GLN:HE22	3:C:225:TYR:HA	1.81	0.45
3:C:102:TYR:HB3	5:J:529:LEU:HD13	1.98	0.45
1:K:47:TRP:CG	2:L:101:TRP:HB2	2.52	0.45
3:O:106:ASP:N	3:O:106:ASP:OD1	2.40	0.45
3:H:144:GLN:HE22	3:H:225:TYR:HA	1.82	0.44
2:B:33:TYR:CD1	2:B:93:PHE:HB2	2.53	0.44
3:O:228:GLN:NE2	3:O:232:THR:OG1	2.37	0.44
5:N:560:GLN:NE2	5:N:564:GLU:OE2	2.51	0.44
3:O:102:TYR:HB3	5:E:529:LEU:HD13	1.99	0.44
3:H:54:ARG:NH1	4:I:34:PRO:HG3	2.33	0.43
3:O:54:ARG:NH1	4:M:34:PRO:HG3	2.32	0.43
1:F:47:TRP:CG	2:G:101:TRP:HB2	2.53	0.43
2:L:33:TYR:CD1	2:L:93:PHE:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:102:TYR:HB3	5:N:529:LEU:HD13	2.00	0.43
1:A:47:TRP:CG	2:B:101:TRP:HB2	2.53	0.43
5:E:584:ILE:H	5:E:584:ILE:HD12	1.84	0.43
5:J:584:ILE:H	5:J:584:ILE:HD12	1.84	0.43
5:N:584:ILE:H	5:N:584:ILE:HD12	1.84	0.43
1:A:50:ARG:NH2	4:D:116:PRO:O	2.52	0.42
2:G:33:TYR:CD1	2:G:93:PHE:HB2	2.54	0.42
4:D:182:ALA:HB2	5:E:562:ALA:HB2	2.01	0.42
3:C:54:ARG:NH1	4:D:34:PRO:HG3	2.34	0.42
4:I:182:ALA:HB2	5:J:562:ALA:HB2	2.01	0.42
4:M:111:LEU:HD12	4:M:170:ILE:HG21	2.02	0.42
4:M:182:ALA:HB2	5:N:562:ALA:HB2	2.02	0.42
1:F:50:ARG:NH2	4:I:116:PRO:O	2.52	0.42
2:L:4:LEU:HB2	2:L:104:GLY:HA2	2.02	0.42
4:I:95:LYS:NZ	5:J:573:LEU:O	2.44	0.42
5:E:527:ILE:HD11	5:E:530:ALA:HB3	2.00	0.42
5:E:516:HIS:CE1	5:E:547:LEU:HD13	2.55	0.42
2:B:4:LEU:HB2	2:B:104:GLY:HA2	2.02	0.41
5:N:516:HIS:CE1	5:N:547:LEU:HD13	2.55	0.41
5:J:560:GLN:NE2	5:J:564:GLU:OE2	2.54	0.41
5:J:516:HIS:CE1	5:J:547:LEU:HD13	2.56	0.41
4:D:95:LYS:NZ	5:E:573:LEU:O	2.46	0.41
3:C:40:ARG:HB2	3:C:43:GLN:HB2	2.03	0.41
3:O:9:THR:HG23	3:O:113:ALA:HB3	2.03	0.41
4:I:39:HIS:NE2	4:I:55:ASP:OD1	2.35	0.41
4:M:134:ARG:NH1	5:N:545:GLU:OE2	2.54	0.41
3:O:40:ARG:HB2	3:O:43:GLN:HB2	2.03	0.41
4:D:111:LEU:HD12	4:D:170:ILE:HG21	2.03	0.41
4:I:229:GLU:HG2	7:I:401:NAG:H82	2.03	0.40
4:D:106:GLU:HA	4:D:136:ARG:HB3	2.02	0.40
1:A:47:TRP:HB2	2:B:103:PHE:HE2	1.87	0.40
3:C:102:TYR:CE1	5:J:532:ILE:HD11	2.57	0.40
3:O:54:ARG:HH12	4:M:34:PRO:HG3	1.86	0.40
3:C:9:THR:HG23	3:C:113:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
1	F	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
1	K	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
2	B	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
2	G	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
2	L	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
3	C	217/243 (89%)	207 (95%)	10 (5%)	0	100	100
3	H	217/243 (89%)	206 (95%)	11 (5%)	0	100	100
3	O	217/243 (89%)	206 (95%)	11 (5%)	0	100	100
4	D	168/280 (60%)	165 (98%)	3 (2%)	0	100	100
4	I	168/280 (60%)	165 (98%)	3 (2%)	0	100	100
4	M	168/280 (60%)	165 (98%)	3 (2%)	0	100	100
5	E	94/136 (69%)	93 (99%)	1 (1%)	0	100	100
5	J	94/136 (69%)	93 (99%)	1 (1%)	0	100	100
5	N	94/136 (69%)	93 (99%)	1 (1%)	0	100	100
All	All	2115/2673 (79%)	2062 (98%)	53 (2%)	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	A	96/97 (99%)	96 (100%)	0	100	100
1	F	96/97 (99%)	96 (100%)	0	100	100
1	K	96/97 (99%)	96 (100%)	0	100	100
2	B	90/91 (99%)	90 (100%)	0	100	100
2	G	90/91 (99%)	90 (100%)	0	100	100
2	L	90/91 (99%)	90 (100%)	0	100	100
3	C	186/195 (95%)	186 (100%)	0	100	100
3	H	186/195 (95%)	186 (100%)	0	100	100
3	O	186/195 (95%)	186 (100%)	0	100	100
4	D	143/242 (59%)	143 (100%)	0	100	100
4	I	143/242 (59%)	143 (100%)	0	100	100
4	M	143/242 (59%)	143 (100%)	0	100	100
5	E	77/115 (67%)	77 (100%)	0	100	100
5	J	77/115 (67%)	77 (100%)	0	100	100
5	N	77/115 (67%)	77 (100%)	0	100	100
All	All	1776/2220 (80%)	1776 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	P	1	6,5	14,14,15	0.26	0	17,19,21	0.46	0
6	NAG	P	2	6	14,14,15	0.27	0	17,19,21	0.45	0
6	BMA	P	3	6	11,11,12	0.55	0	15,15,17	0.73	0
6	MAN	P	4	6	11,11,12	0.59	0	15,15,17	1.04	2 (13%)
6	MAN	P	5	6	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
6	MAN	P	6	6	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
6	NAG	Q	1	6,5	14,14,15	0.25	0	17,19,21	0.45	0
6	NAG	Q	2	6	14,14,15	0.28	0	17,19,21	0.45	0
6	BMA	Q	3	6	11,11,12	0.55	0	15,15,17	0.74	0
6	MAN	Q	4	6	11,11,12	0.60	0	15,15,17	1.03	2 (13%)
6	MAN	Q	5	6	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
6	MAN	Q	6	6	11,11,12	0.60	0	15,15,17	1.03	2 (13%)
6	NAG	R	1	6,5	14,14,15	0.24	0	17,19,21	0.46	0
6	NAG	R	2	6	14,14,15	0.28	0	17,19,21	0.44	0
6	BMA	R	3	6	11,11,12	0.57	0	15,15,17	0.74	0
6	MAN	R	4	6	11,11,12	0.59	0	15,15,17	1.04	2 (13%)
6	MAN	R	5	6	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
6	MAN	R	6	6	11,11,12	0.61	0	15,15,17	1.04	2 (13%)

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	P	1	6,5	-	3/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	MAN	P	4	6	-	0/2/19/22	0/1/1/1
6	MAN	P	5	6	-	0/2/19/22	0/1/1/1
6	MAN	P	6	6	-	0/2/19/22	0/1/1/1
6	NAG	Q	1	6,5	-	3/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	6	MAN	C1-O5-C5	2.72	115.84	112.19
6	Q	6	MAN	C1-O5-C5	2.69	115.80	112.19
6	P	6	MAN	C1-O5-C5	2.68	115.78	112.19
6	P	4	MAN	C1-O5-C5	2.61	115.69	112.19
6	Q	4	MAN	C1-O5-C5	2.61	115.69	112.19
6	R	4	MAN	C1-O5-C5	2.59	115.65	112.19
6	Q	5	MAN	C1-O5-C5	2.45	115.47	112.19
6	R	5	MAN	C1-O5-C5	2.44	115.45	112.19
6	P	5	MAN	C1-O5-C5	2.40	115.40	112.19
6	R	4	MAN	O2-C2-C3	-2.30	105.39	110.15
6	P	4	MAN	O2-C2-C3	-2.29	105.40	110.15
6	Q	4	MAN	O2-C2-C3	-2.29	105.41	110.15
6	R	6	MAN	O2-C2-C3	-2.19	105.62	110.15
6	R	5	MAN	O2-C2-C3	-2.17	105.66	110.15
6	Q	6	MAN	O2-C2-C3	-2.17	105.66	110.15
6	P	6	MAN	O2-C2-C3	-2.17	105.67	110.15
6	Q	5	MAN	O2-C2-C3	-2.14	105.73	110.15
6	P	5	MAN	O2-C2-C3	-2.11	105.79	110.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	1	NAG	C8-C7-N2-C2
6	P	1	NAG	O7-C7-N2-C2

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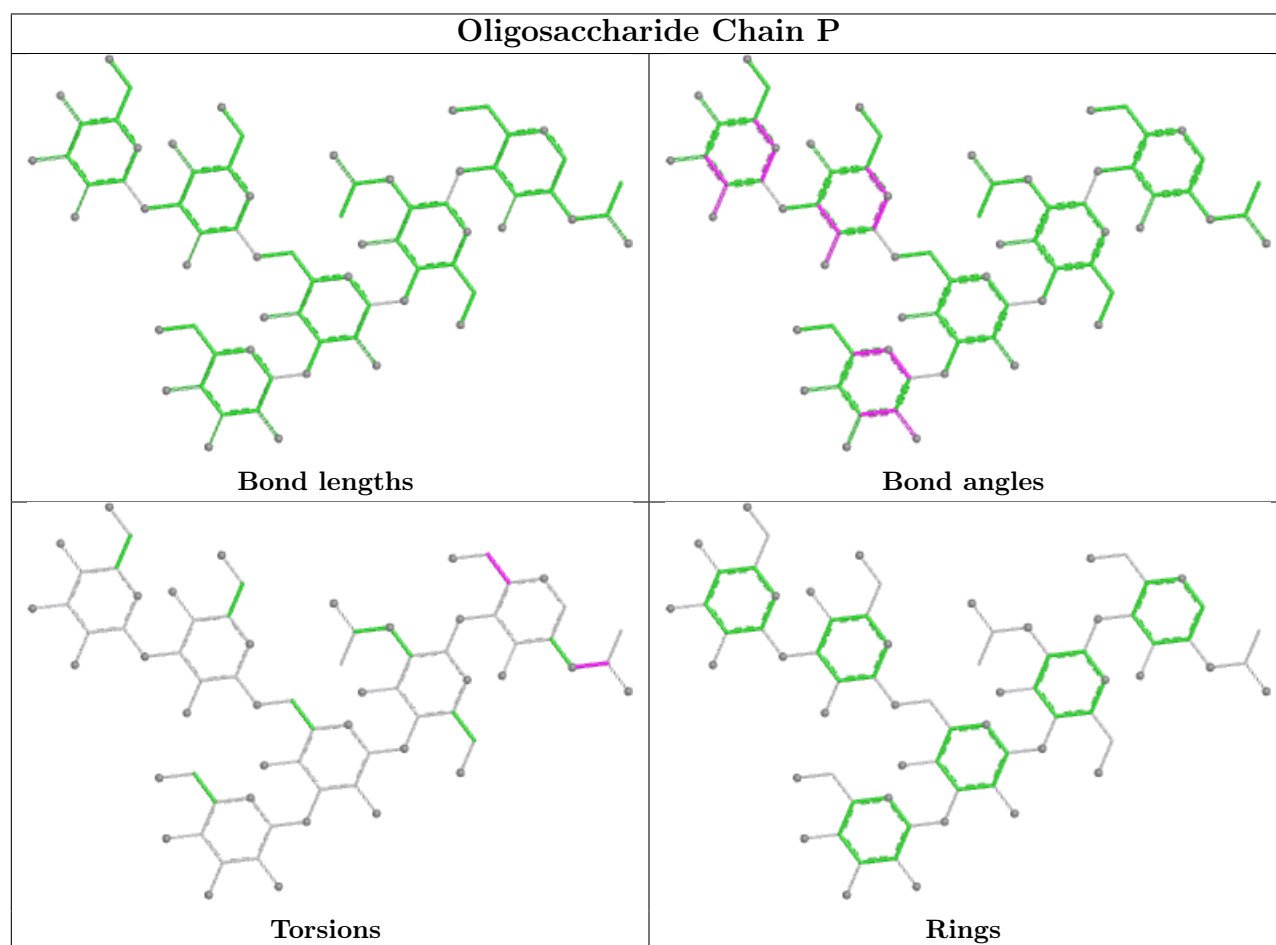
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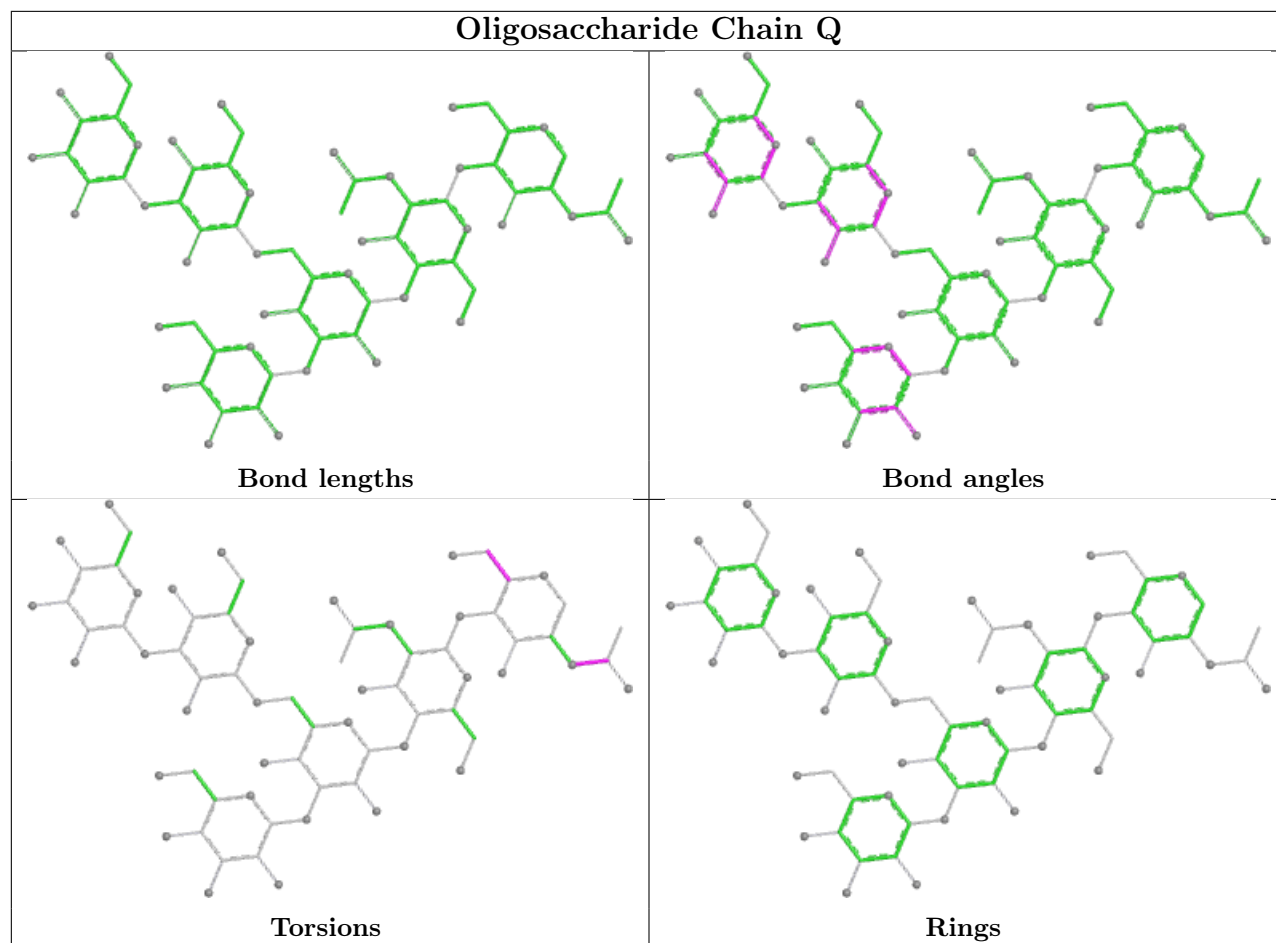
Mol	Chain	Res	Type	Atoms
6	Q	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
6	Q	1	NAG	C4-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6

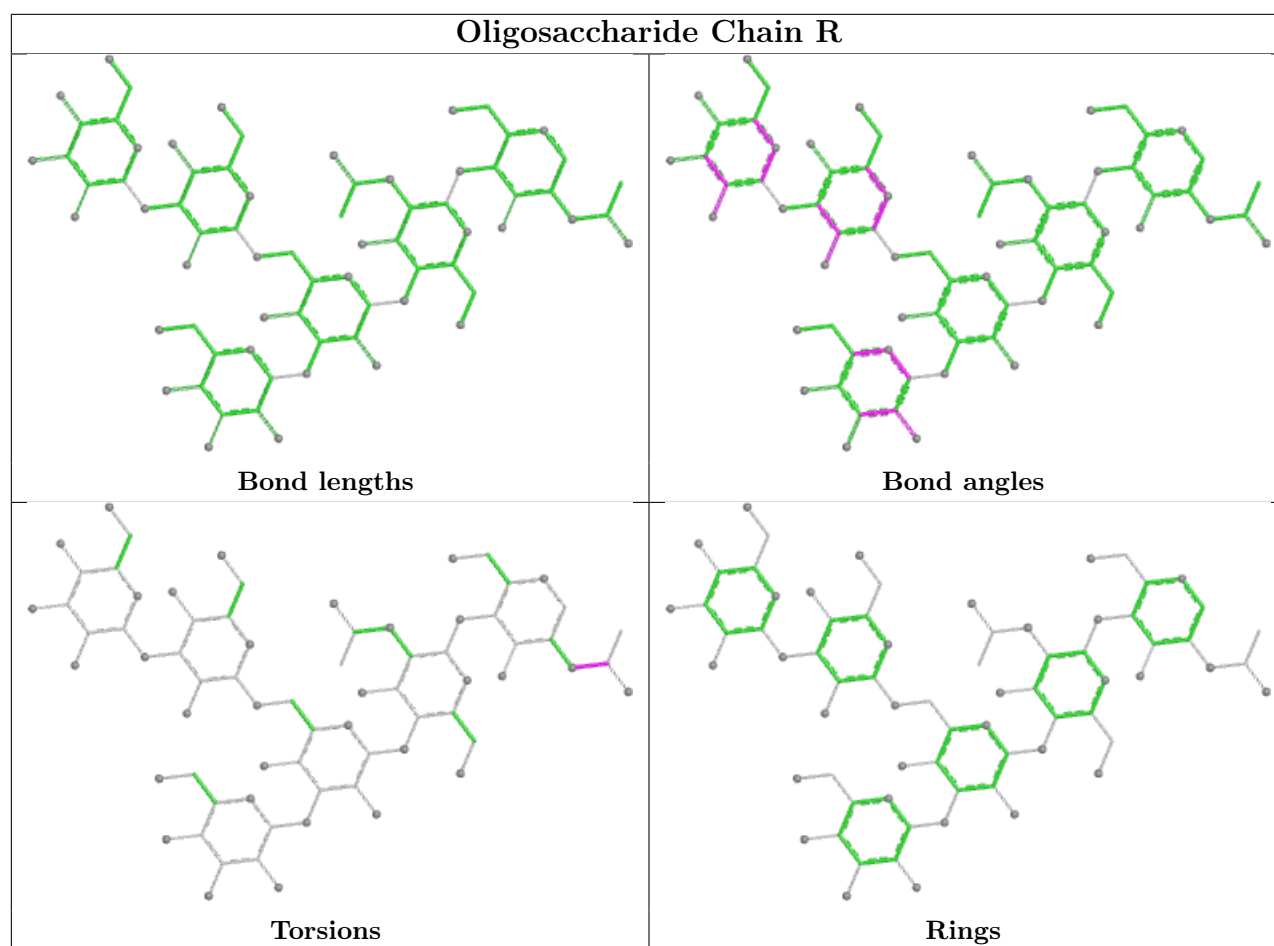
There are no ring outliers.

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	$\# Z > 2$
7	NAG	M	401	4	14,14,15	0.29	0	17,19,21	0.46	0
7	NAG	I	401	4	14,14,15	0.27	0	17,19,21	0.56	0
7	NAG	D	401	4	14,14,15	0.26	0	17,19,21	0.47	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	M	401	4	-	0/6/23/26	0/1/1/1
7	NAG	I	401	4	-	0/6/23/26	0/1/1/1
7	NAG	D	401	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	401	NAG	1	0
7	I	401	NAG	1	0
7	D	401	NAG	1	0

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.

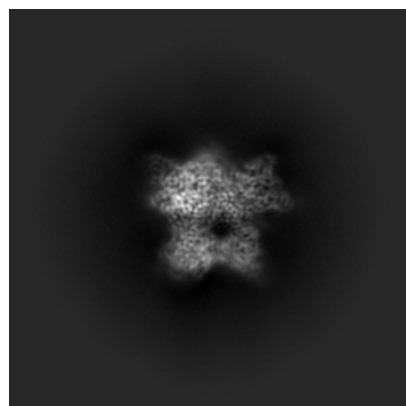
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27637. These allow visual inspection of the internal detail of the map and identification of artifacts.

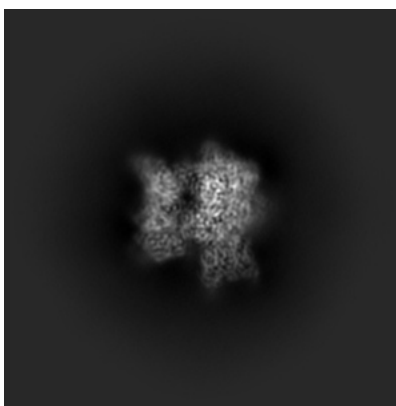
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

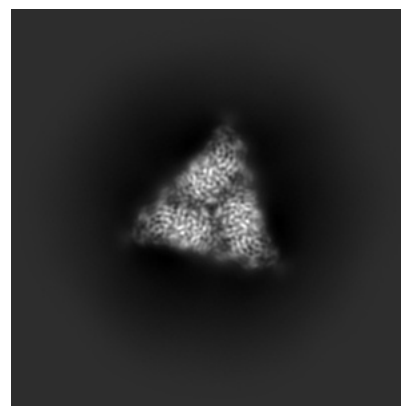
6.1.1 Primary map



X

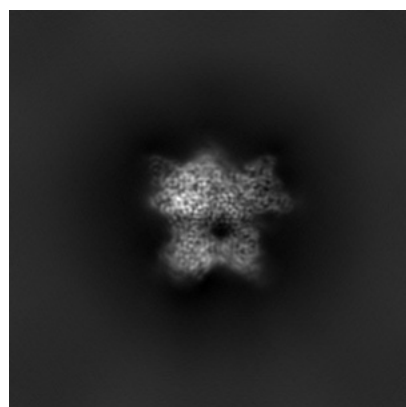


Y

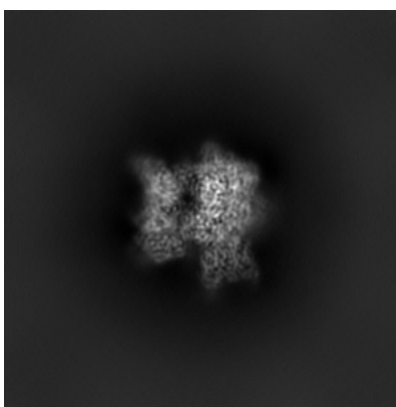


Z

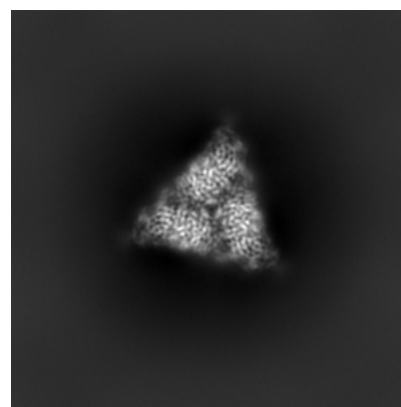
6.1.2 Raw map



X



Y

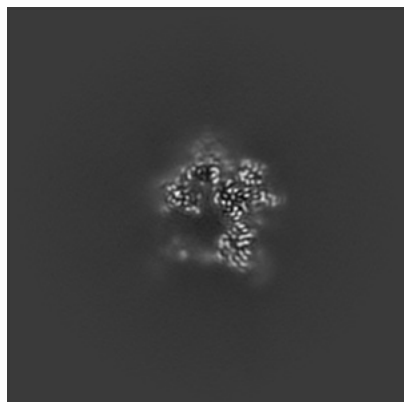


Z

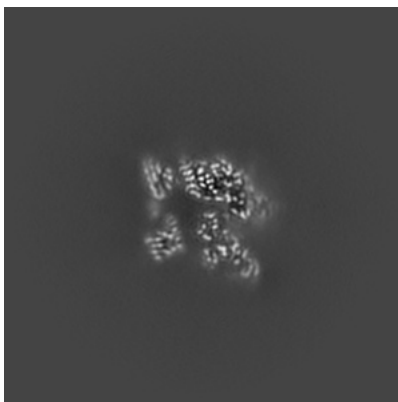
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

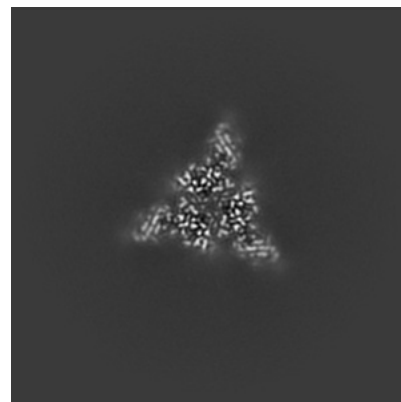
6.2.1 Primary map



X Index: 160

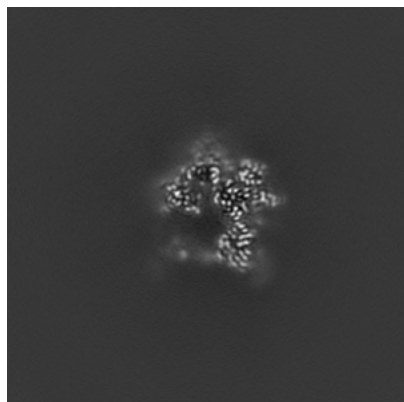


Y Index: 160

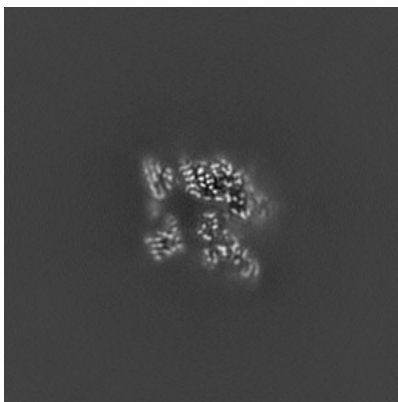


Z Index: 160

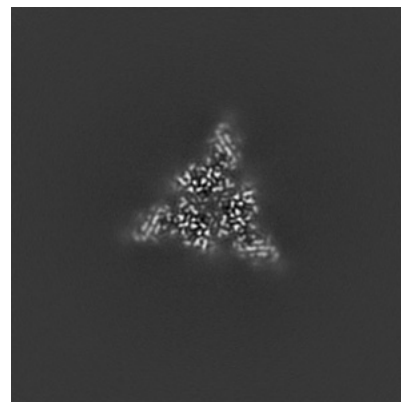
6.2.2 Raw map



X Index: 160



Y Index: 160

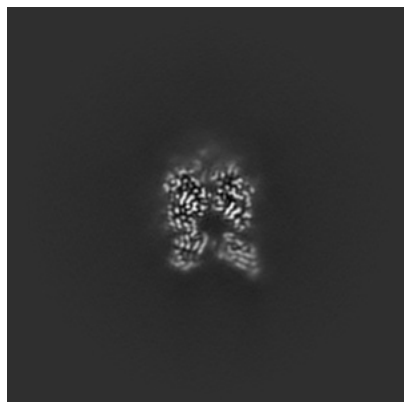


Z Index: 160

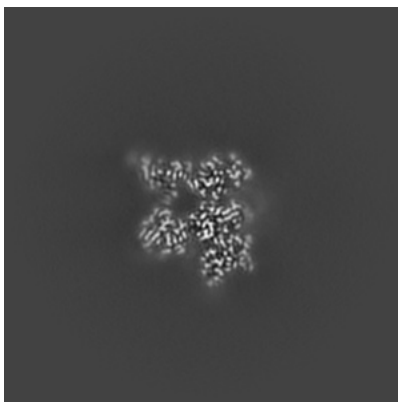
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

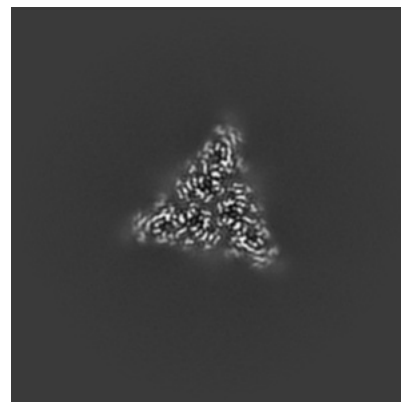
6.3.1 Primary map



X Index: 146

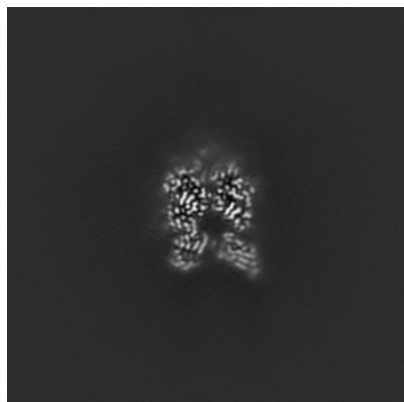


Y Index: 145

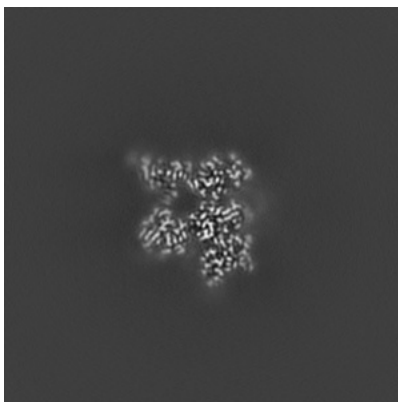


Z Index: 170

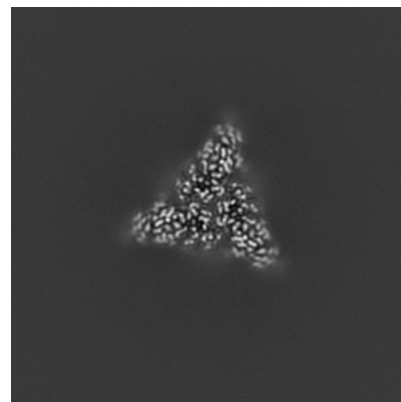
6.3.2 Raw map



X Index: 146



Y Index: 145

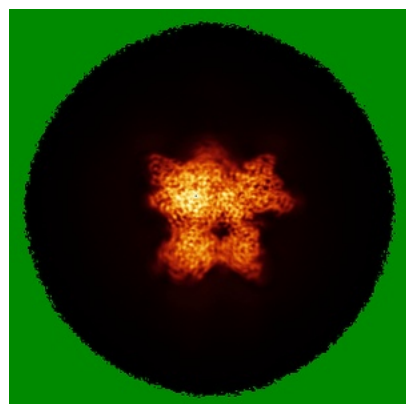


Z Index: 169

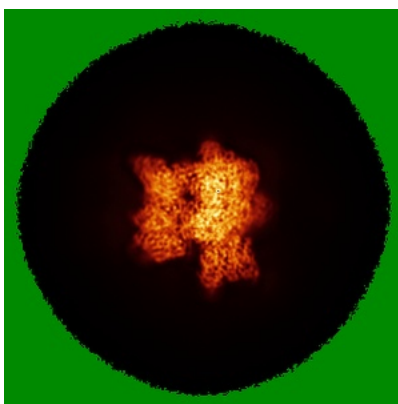
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

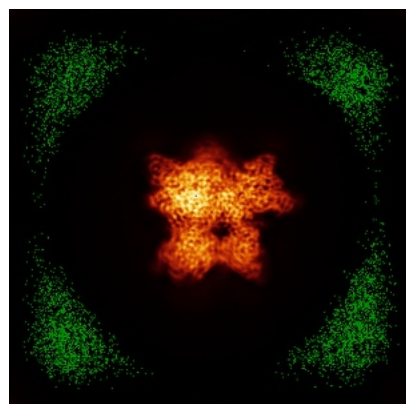


Y

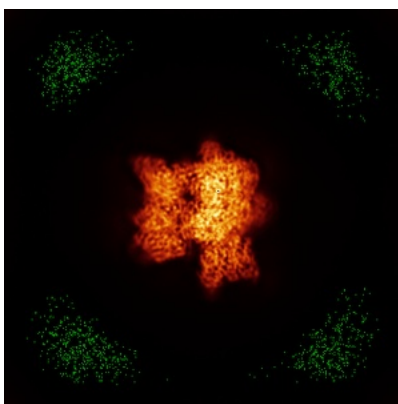


Z

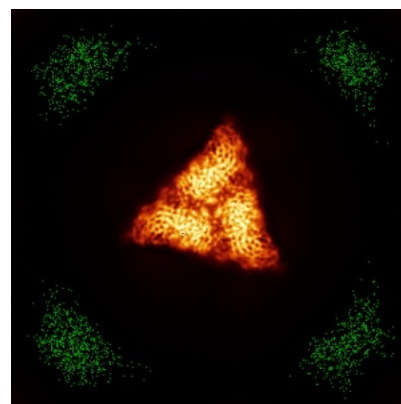
6.4.2 Raw map



X



Y

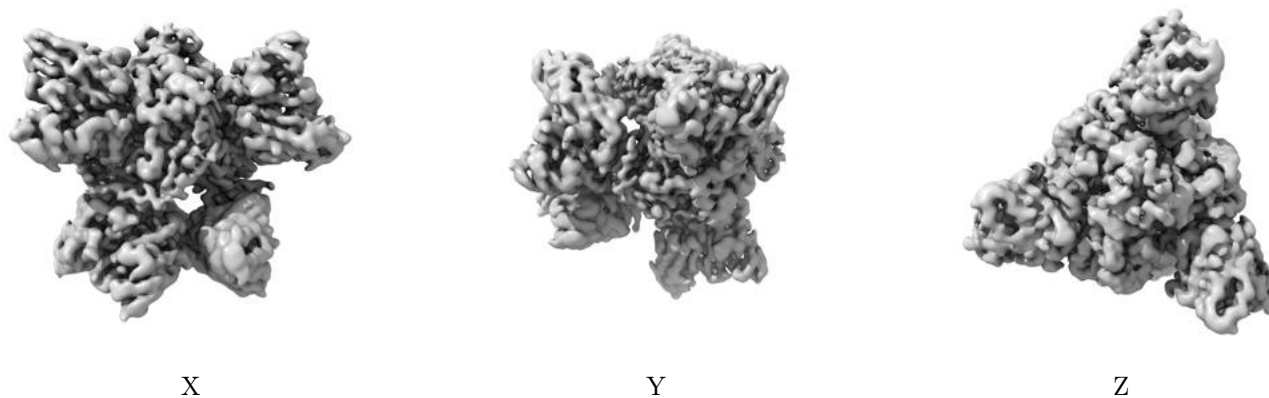


Z

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.

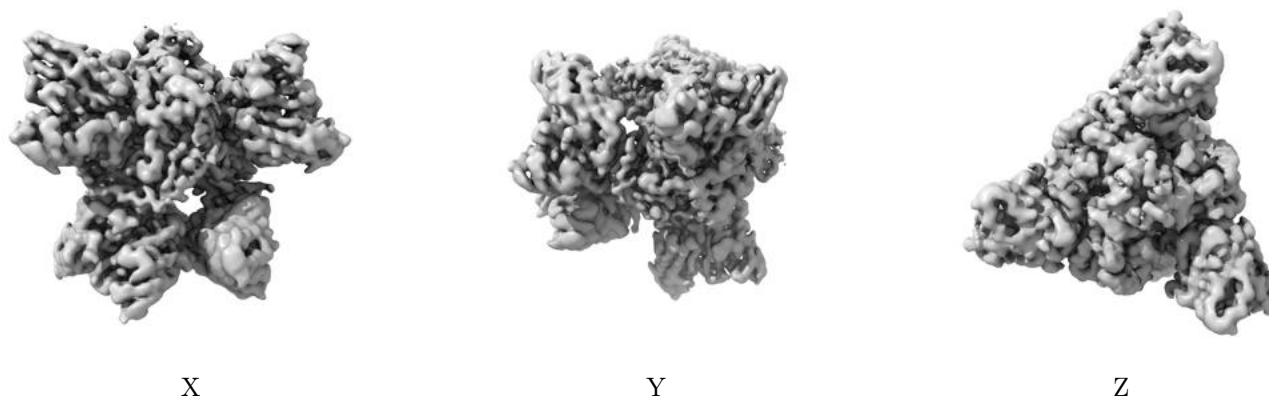
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. 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.

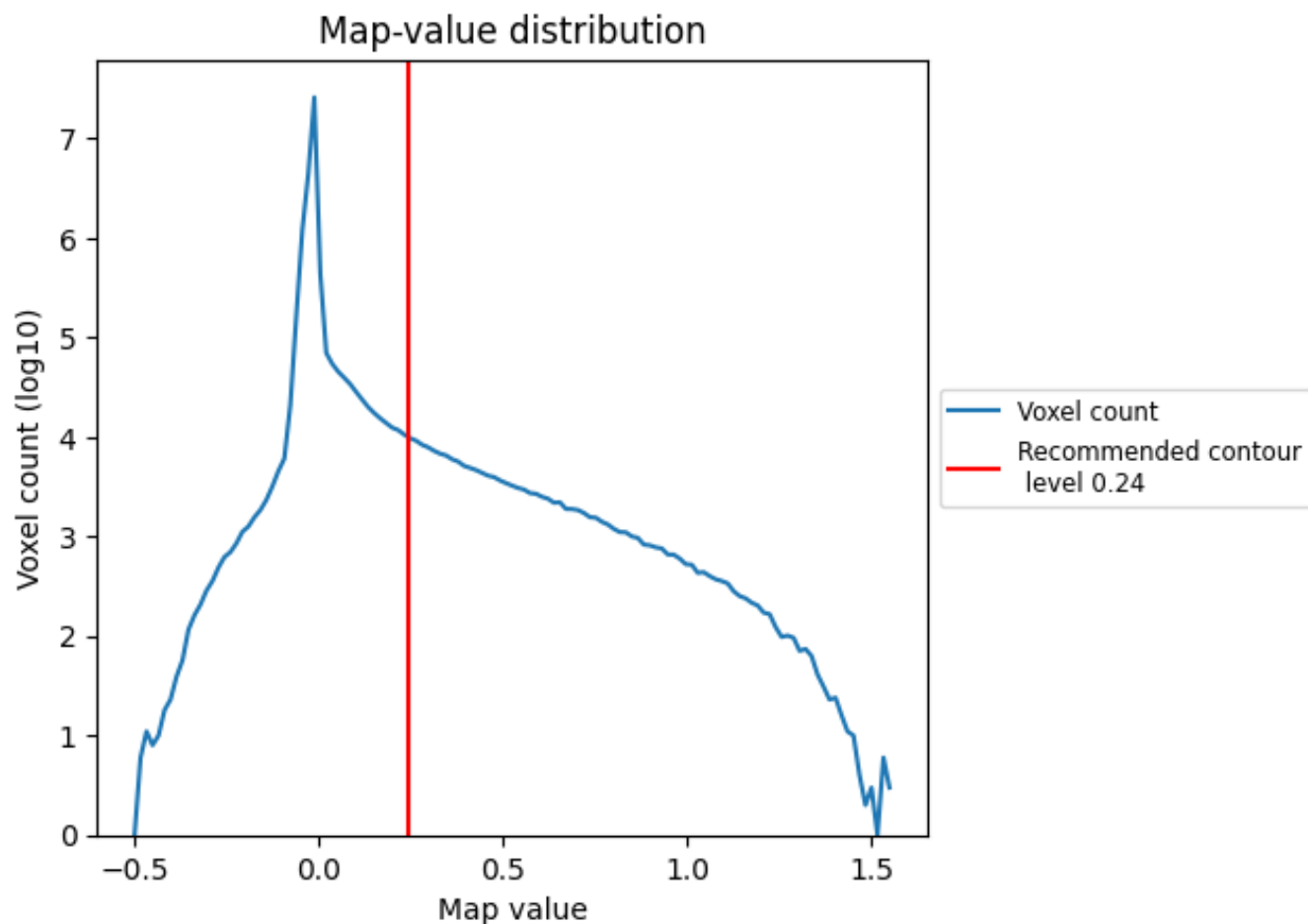
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

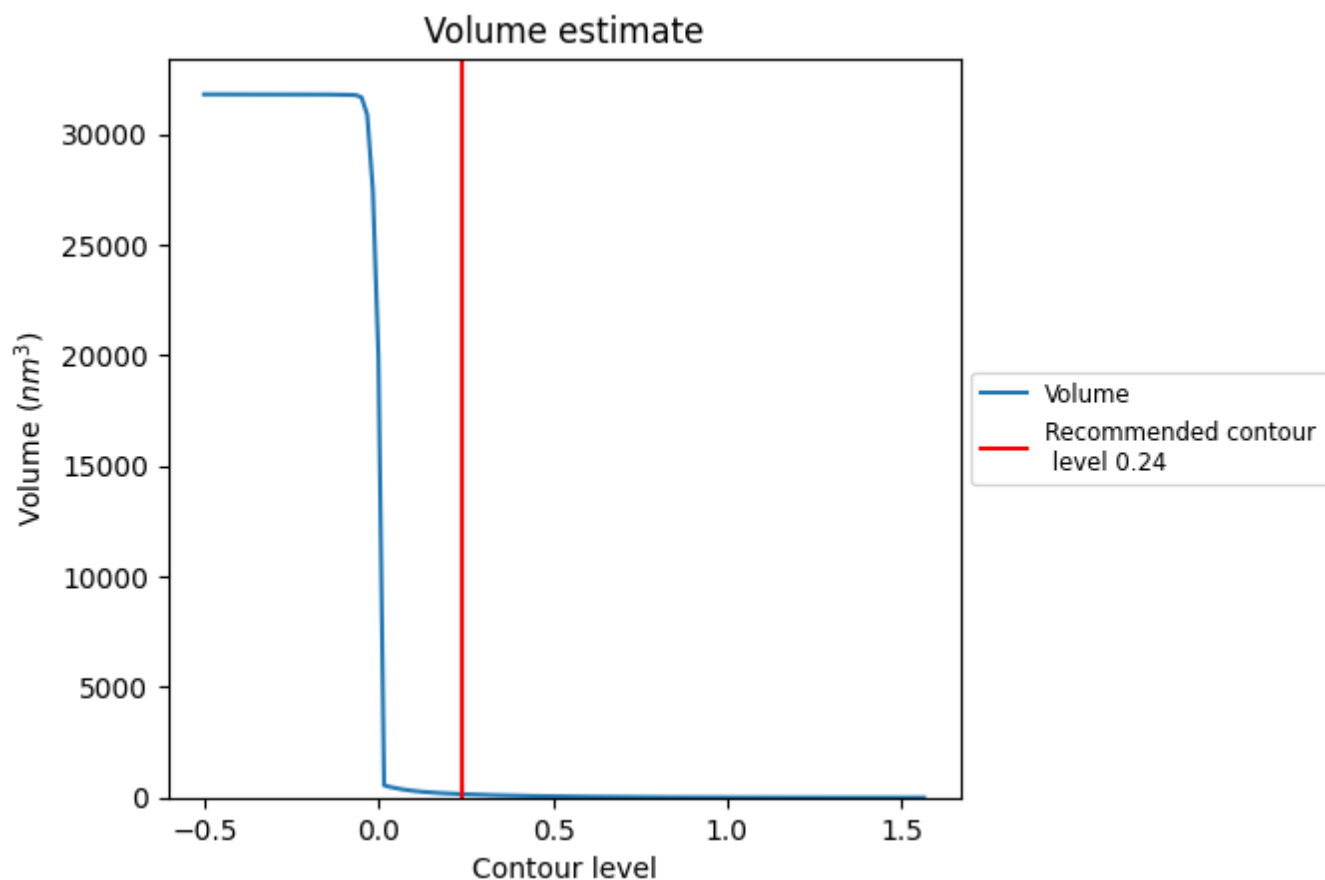
This section contains the results of statistical analysis of the map.

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.

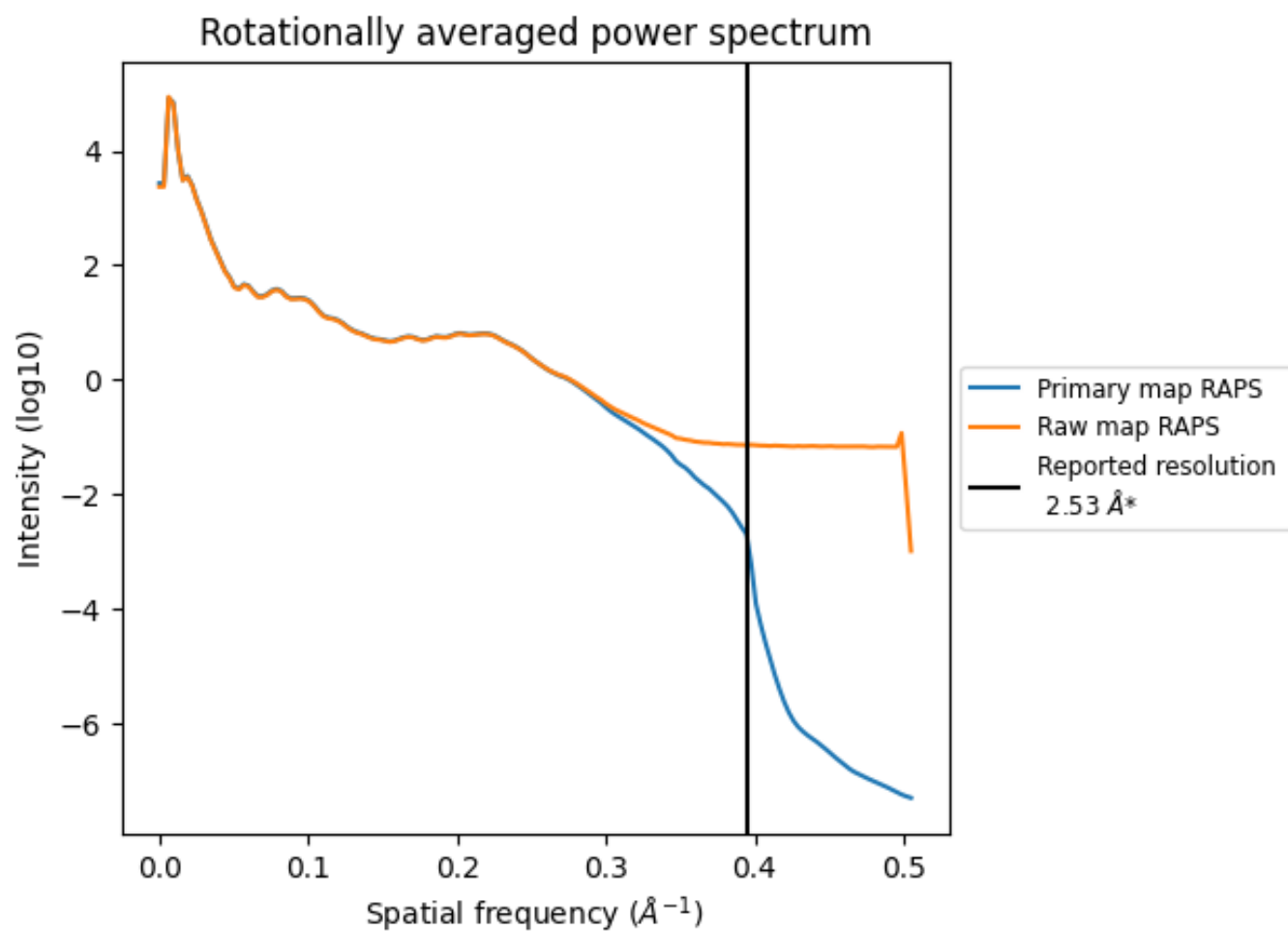
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm^3 ; this corresponds to an approximate mass of 140 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 ⓘ

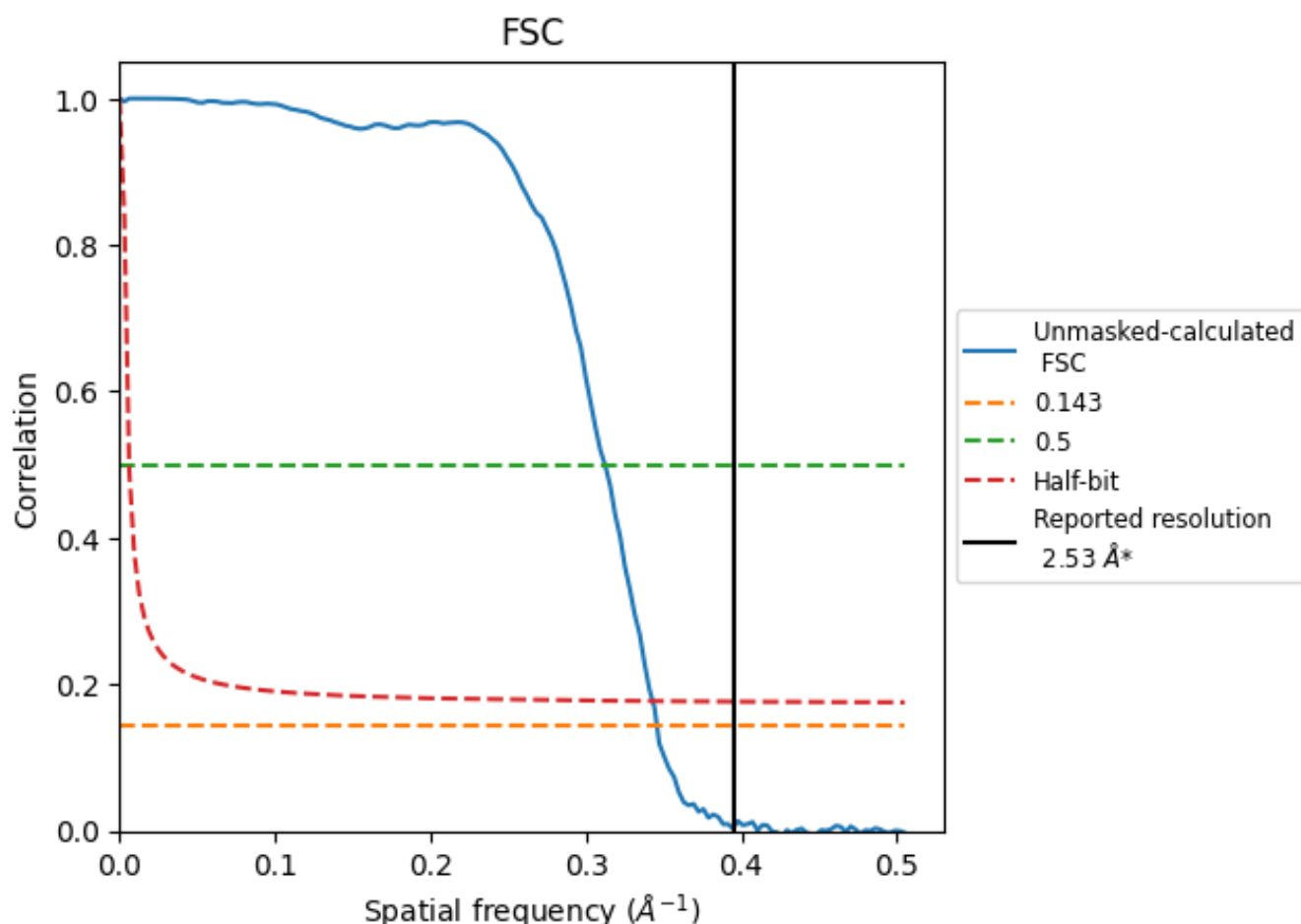


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

8.2 Resolution estimates [i](#)

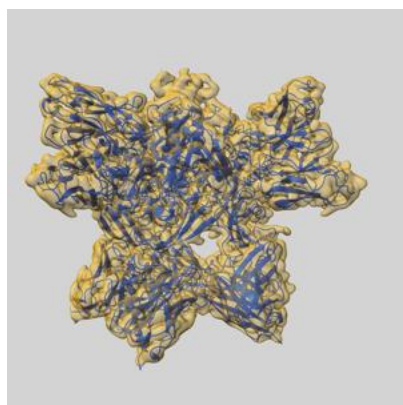
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.89	3.20	2.92

*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 2.89 differs from the reported value 2.53 by more than 10 %

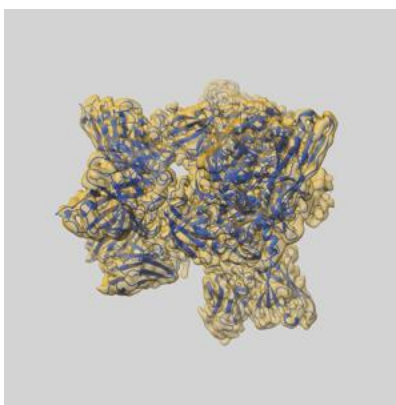
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27637 and PDB model 8DPL. Per-residue inclusion information can be found in section [3](#) on page [7](#).

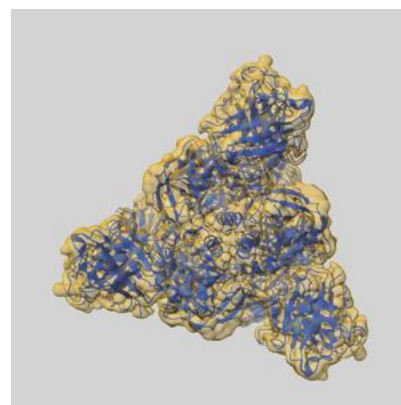
9.1 Map-model overlay [i](#)



X



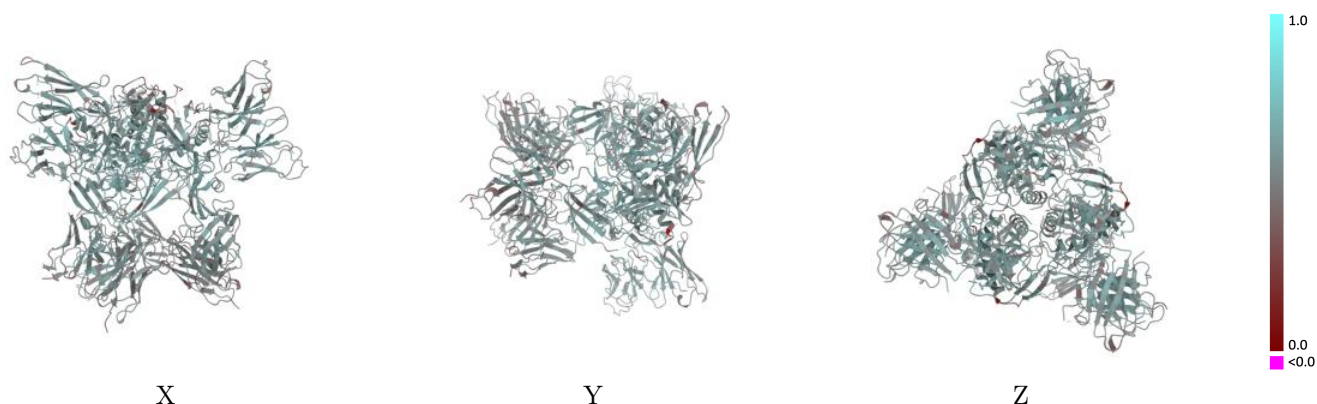
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24 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](#)



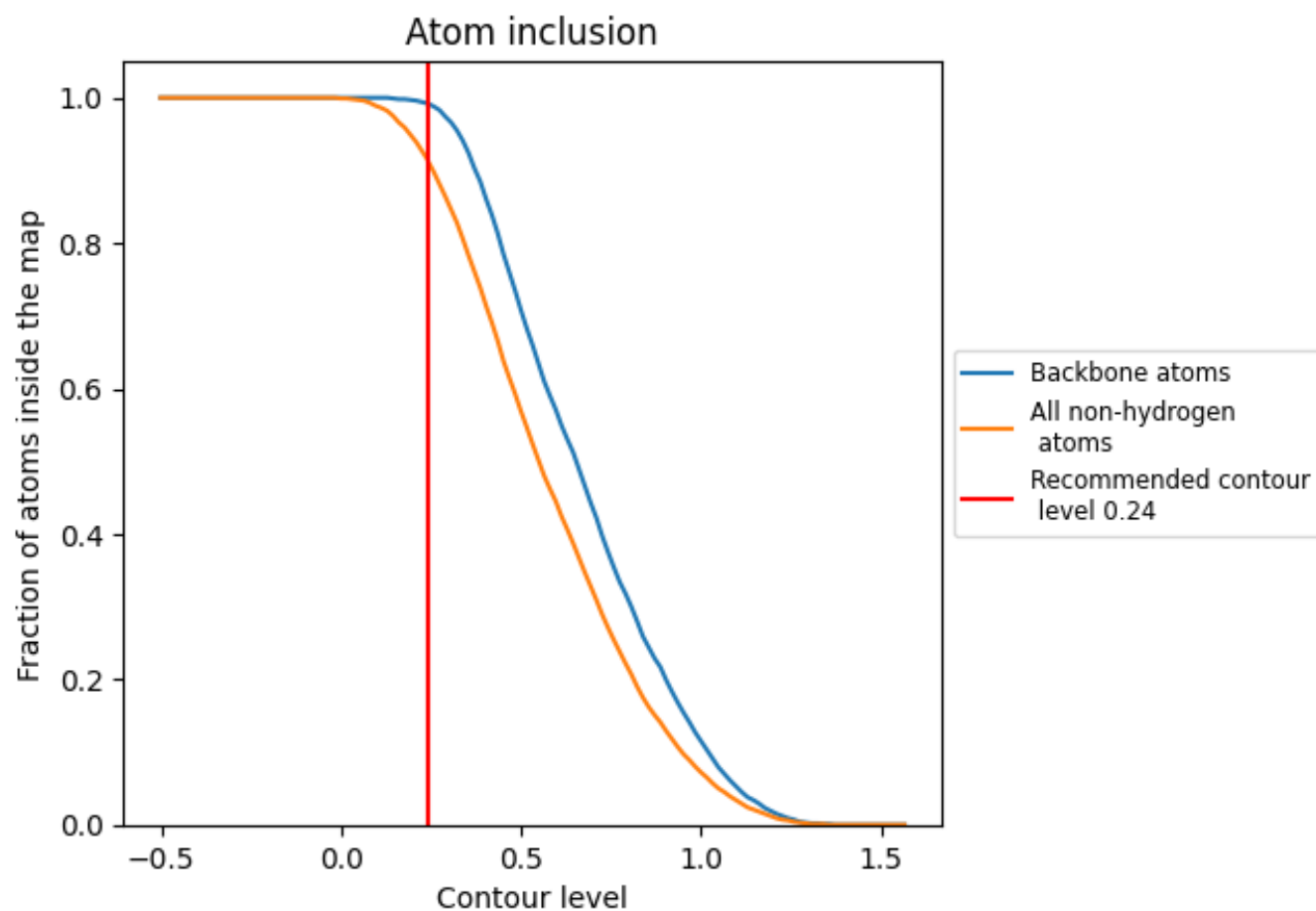
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9150	 0.5360
A	 0.8920	 0.5000
B	 0.9140	 0.5120
C	 0.9030	 0.5400
D	 0.9290	 0.5640
E	 0.9420	 0.5490
F	 0.8890	 0.4980
G	 0.9130	 0.5110
H	 0.9060	 0.5390
I	 0.9270	 0.5630
J	 0.9450	 0.5490
K	 0.8860	 0.5000
L	 0.9090	 0.5100
M	 0.9290	 0.5650
N	 0.9410	 0.5490
O	 0.9000	 0.5400
P	 0.9860	 0.5680
Q	 0.9860	 0.5650
R	 0.9860	 0.5690

