



## Full wwPDB EM Validation Report ⓘ

Sep 15, 2025 – 10:15 AM EDT

PDB ID : 9P99 / pdb\_00009p99  
EMDB ID : EMD-71403  
Title : CryoEM structure of integrin alphaEbeta7 bound to E-cadherin  
Authors : Hollis, J.A.; Campbell, M.G.  
Deposited on : 2025-06-24  
Resolution : 3.37 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.45.1

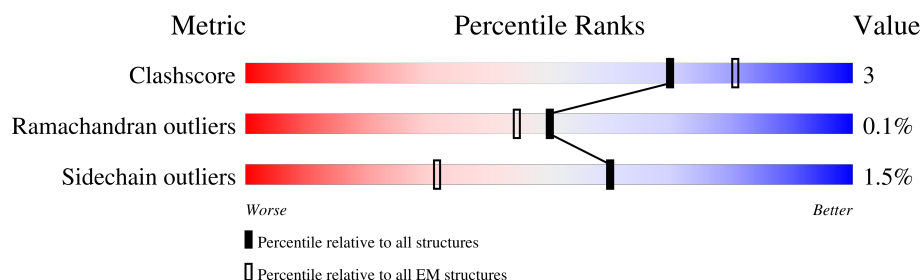
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.37 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  $\geq 3$ , 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	1176	<div> <div>10%</div> <div>59%</div> <div>6%</div> <div>35%</div> </div>
2	B	776	<div> <div>18%</div> <div>44%</div> <div>•</div> <div>51%</div> </div>
3	C	331	<div> <div>•</div> <div>28%</div> <div>•</div> <div>69%</div> </div>
4	D	3	<div> <div>100%</div> <div>33%</div> <div>67%</div> </div>
4	E	3	<div> <div>33%</div> <div>100%</div> </div>
5	F	2	<div> <div>100%</div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19367 atoms, of which 9577 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 Integrin alpha-E.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	768	Total	C	H	N	O	S	0	0
			11652	3706	5766	1026	1122	32		

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1106	GLY	-	expression tag	UNP P38570
A	1107	THR	-	expression tag	UNP P38570
A	1108	GLY	-	expression tag	UNP P38570
A	1109	GLY	-	expression tag	UNP P38570
A	1110	LEU	-	expression tag	UNP P38570
A	1111	GLU	-	expression tag	UNP P38570
A	1112	VAL	-	expression tag	UNP P38570
A	1113	LEU	-	expression tag	UNP P38570
A	1114	PHE	-	expression tag	UNP P38570
A	1115	GLN	-	expression tag	UNP P38570
A	1116	GLY	-	expression tag	UNP P38570
A	1117	PRO	-	expression tag	UNP P38570
A	1118	GLY	-	expression tag	UNP P38570
A	1119	GLU	-	expression tag	UNP P38570
A	1120	ASN	-	expression tag	UNP P38570
A	1121	ALA	-	expression tag	UNP P38570
A	1122	GLN	-	expression tag	UNP P38570
A	1123	CYS	-	expression tag	UNP P38570
A	1124	GLU	-	expression tag	UNP P38570
A	1125	LYS	-	expression tag	UNP P38570
A	1126	GLU	-	expression tag	UNP P38570
A	1127	LEU	-	expression tag	UNP P38570
A	1128	GLN	-	expression tag	UNP P38570
A	1129	ALA	-	expression tag	UNP P38570
A	1130	LEU	-	expression tag	UNP P38570
A	1131	GLU	-	expression tag	UNP P38570
A	1132	LYS	-	expression tag	UNP P38570
A	1133	GLU	-	expression tag	UNP P38570

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1134	ASN	-	expression tag	UNP P38570
A	1135	ALA	-	expression tag	UNP P38570
A	1136	GLN	-	expression tag	UNP P38570
A	1137	LEU	-	expression tag	UNP P38570
A	1138	GLU	-	expression tag	UNP P38570
A	1139	TRP	-	expression tag	UNP P38570
A	1140	GLU	-	expression tag	UNP P38570
A	1141	LEU	-	expression tag	UNP P38570
A	1142	GLN	-	expression tag	UNP P38570
A	1143	ALA	-	expression tag	UNP P38570
A	1144	LEU	-	expression tag	UNP P38570
A	1145	GLU	-	expression tag	UNP P38570
A	1146	LYS	-	expression tag	UNP P38570
A	1147	GLU	-	expression tag	UNP P38570
A	1148	LEU	-	expression tag	UNP P38570
A	1149	ALA	-	expression tag	UNP P38570
A	1150	GLN	-	expression tag	UNP P38570
A	1151	TRP	-	expression tag	UNP P38570
A	1152	SER	-	expression tag	UNP P38570
A	1153	HIS	-	expression tag	UNP P38570
A	1154	PRO	-	expression tag	UNP P38570
A	1155	GLN	-	expression tag	UNP P38570
A	1156	PHE	-	expression tag	UNP P38570
A	1157	GLU	-	expression tag	UNP P38570
A	1158	LYS	-	expression tag	UNP P38570

- Molecule 2 is a protein called Integrin beta-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	379	Total	C	H	N	O	S	0	0
			5819	1839	2876	525	566	13		

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	705	ASP	-	expression tag	UNP P26010
B	706	THR	-	expression tag	UNP P26010
B	707	SER	-	expression tag	UNP P26010
B	708	GLY	-	expression tag	UNP P26010
B	709	LEU	-	expression tag	UNP P26010
B	710	GLU	-	expression tag	UNP P26010
B	711	VAL	-	expression tag	UNP P26010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	712	LEU	-	expression tag	UNP P26010
B	713	PHE	-	expression tag	UNP P26010
B	714	GLN	-	expression tag	UNP P26010
B	715	GLY	-	expression tag	UNP P26010
B	716	PRO	-	expression tag	UNP P26010
B	717	GLY	-	expression tag	UNP P26010
B	718	LYS	-	expression tag	UNP P26010
B	719	ASN	-	expression tag	UNP P26010
B	720	ALA	-	expression tag	UNP P26010
B	721	GLN	-	expression tag	UNP P26010
B	722	CYS	-	expression tag	UNP P26010
B	723	LYS	-	expression tag	UNP P26010
B	724	LYS	-	expression tag	UNP P26010
B	725	LYS	-	expression tag	UNP P26010
B	726	LEU	-	expression tag	UNP P26010
B	727	GLN	-	expression tag	UNP P26010
B	728	ALA	-	expression tag	UNP P26010
B	729	LEU	-	expression tag	UNP P26010
B	730	LYS	-	expression tag	UNP P26010
B	731	LYS	-	expression tag	UNP P26010
B	732	LYS	-	expression tag	UNP P26010
B	733	ASN	-	expression tag	UNP P26010
B	734	ALA	-	expression tag	UNP P26010
B	735	GLN	-	expression tag	UNP P26010
B	736	LEU	-	expression tag	UNP P26010
B	737	LYS	-	expression tag	UNP P26010
B	738	TRP	-	expression tag	UNP P26010
B	739	LYS	-	expression tag	UNP P26010
B	740	LEU	-	expression tag	UNP P26010
B	741	GLN	-	expression tag	UNP P26010
B	742	ALA	-	expression tag	UNP P26010
B	743	LEU	-	expression tag	UNP P26010
B	744	LYS	-	expression tag	UNP P26010
B	745	LYS	-	expression tag	UNP P26010
B	746	LYS	-	expression tag	UNP P26010
B	747	LEU	-	expression tag	UNP P26010
B	748	ALA	-	expression tag	UNP P26010
B	749	GLN	-	expression tag	UNP P26010
B	750	GLY	-	expression tag	UNP P26010
B	751	GLY	-	expression tag	UNP P26010
B	752	HIS	-	expression tag	UNP P26010
B	753	HIS	-	expression tag	UNP P26010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	754	HIS	-	expression tag	UNP P26010
B	755	HIS	-	expression tag	UNP P26010
B	756	HIS	-	expression tag	UNP P26010
B	757	HIS	-	expression tag	UNP P26010

- Molecule 3 is a protein called Cadherin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	103	Total	C	H	N	O	S	0	0
			1598	512	792	132	160	2		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-113	MET	-	initiating methionine	UNP P12830
C	-112	ALA	-	expression tag	UNP P12830
C	-111	SER	-	expression tag	UNP P12830
C	-110	MET	-	expression tag	UNP P12830
C	-109	HIS	-	expression tag	UNP P12830
C	-108	HIS	-	expression tag	UNP P12830
C	-107	HIS	-	expression tag	UNP P12830
C	-106	HIS	-	expression tag	UNP P12830
C	-105	HIS	-	expression tag	UNP P12830
C	-104	HIS	-	expression tag	UNP P12830
C	-103	GLY	-	expression tag	UNP P12830
C	-102	SER	-	expression tag	UNP P12830
C	-101	SER	-	expression tag	UNP P12830
C	-100	MET	-	expression tag	UNP P12830
C	-99	ALA	-	expression tag	UNP P12830
C	-98	SER	-	expression tag	UNP P12830
C	-97	MET	-	expression tag	UNP P12830
C	-96	SER	-	expression tag	UNP P12830
C	-95	ASP	-	expression tag	UNP P12830
C	-94	SER	-	expression tag	UNP P12830
C	-93	GLU	-	expression tag	UNP P12830
C	-92	VAL	-	expression tag	UNP P12830
C	-91	ASN	-	expression tag	UNP P12830
C	-90	GLN	-	expression tag	UNP P12830
C	-89	GLU	-	expression tag	UNP P12830
C	-88	ALA	-	expression tag	UNP P12830
C	-87	LYS	-	expression tag	UNP P12830
C	-86	PRO	-	expression tag	UNP P12830

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-85	GLU	-	expression tag	UNP P12830
C	-84	VAL	-	expression tag	UNP P12830
C	-83	LYS	-	expression tag	UNP P12830
C	-82	PRO	-	expression tag	UNP P12830
C	-81	GLU	-	expression tag	UNP P12830
C	-80	VAL	-	expression tag	UNP P12830
C	-79	LYS	-	expression tag	UNP P12830
C	-78	PRO	-	expression tag	UNP P12830
C	-77	GLU	-	expression tag	UNP P12830
C	-76	THR	-	expression tag	UNP P12830
C	-75	HIS	-	expression tag	UNP P12830
C	-74	ILE	-	expression tag	UNP P12830
C	-73	ASN	-	expression tag	UNP P12830
C	-72	LEU	-	expression tag	UNP P12830
C	-71	LYS	-	expression tag	UNP P12830
C	-70	VAL	-	expression tag	UNP P12830
C	-69	SER	-	expression tag	UNP P12830
C	-68	ASP	-	expression tag	UNP P12830
C	-67	GLY	-	expression tag	UNP P12830
C	-66	SER	-	expression tag	UNP P12830
C	-65	SER	-	expression tag	UNP P12830
C	-64	GLU	-	expression tag	UNP P12830
C	-63	ILE	-	expression tag	UNP P12830
C	-62	PHE	-	expression tag	UNP P12830
C	-61	PHE	-	expression tag	UNP P12830
C	-60	LYS	-	expression tag	UNP P12830
C	-59	ILE	-	expression tag	UNP P12830
C	-58	LYS	-	expression tag	UNP P12830
C	-57	LYS	-	expression tag	UNP P12830
C	-56	THR	-	expression tag	UNP P12830
C	-55	THR	-	expression tag	UNP P12830
C	-54	PRO	-	expression tag	UNP P12830
C	-53	LEU	-	expression tag	UNP P12830
C	-52	ARG	-	expression tag	UNP P12830
C	-51	ARG	-	expression tag	UNP P12830
C	-50	LEU	-	expression tag	UNP P12830
C	-49	MET	-	expression tag	UNP P12830
C	-48	GLU	-	expression tag	UNP P12830
C	-47	ALA	-	expression tag	UNP P12830
C	-46	PHE	-	expression tag	UNP P12830
C	-45	ALA	-	expression tag	UNP P12830
C	-44	LYS	-	expression tag	UNP P12830

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-43	ARG	-	expression tag	UNP P12830
C	-42	GLN	-	expression tag	UNP P12830
C	-41	GLY	-	expression tag	UNP P12830
C	-40	LYS	-	expression tag	UNP P12830
C	-39	GLU	-	expression tag	UNP P12830
C	-38	MET	-	expression tag	UNP P12830
C	-37	ASP	-	expression tag	UNP P12830
C	-36	SER	-	expression tag	UNP P12830
C	-35	LEU	-	expression tag	UNP P12830
C	-34	ARG	-	expression tag	UNP P12830
C	-33	PHE	-	expression tag	UNP P12830
C	-32	LEU	-	expression tag	UNP P12830
C	-31	TYR	-	expression tag	UNP P12830
C	-30	ASP	-	expression tag	UNP P12830
C	-29	GLY	-	expression tag	UNP P12830
C	-28	ILE	-	expression tag	UNP P12830
C	-27	ARG	-	expression tag	UNP P12830
C	-26	ILE	-	expression tag	UNP P12830
C	-25	GLN	-	expression tag	UNP P12830
C	-24	ALA	-	expression tag	UNP P12830
C	-23	ASP	-	expression tag	UNP P12830
C	-22	GLN	-	expression tag	UNP P12830
C	-21	THR	-	expression tag	UNP P12830
C	-20	PRO	-	expression tag	UNP P12830
C	-19	GLU	-	expression tag	UNP P12830
C	-18	ASP	-	expression tag	UNP P12830
C	-17	LEU	-	expression tag	UNP P12830
C	-16	ASP	-	expression tag	UNP P12830
C	-15	MET	-	expression tag	UNP P12830
C	-14	GLU	-	expression tag	UNP P12830
C	-13	ASP	-	expression tag	UNP P12830
C	-12	ASN	-	expression tag	UNP P12830
C	-11	ASP	-	expression tag	UNP P12830
C	-10	ILE	-	expression tag	UNP P12830
C	-9	ILE	-	expression tag	UNP P12830
C	-8	GLU	-	expression tag	UNP P12830
C	-7	ALA	-	expression tag	UNP P12830
C	-6	HIS	-	expression tag	UNP P12830
C	-5	ARG	-	expression tag	UNP P12830
C	-4	GLU	-	expression tag	UNP P12830
C	-3	GLN	-	expression tag	UNP P12830
C	-2	ILE	-	expression tag	UNP P12830

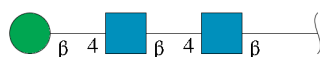
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P12830
C	0	GLY	-	expression tag	UNP P12830

- Molecule 4 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
4	D	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
4	E	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	B	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	3	Total	Ca	0
			3	3	

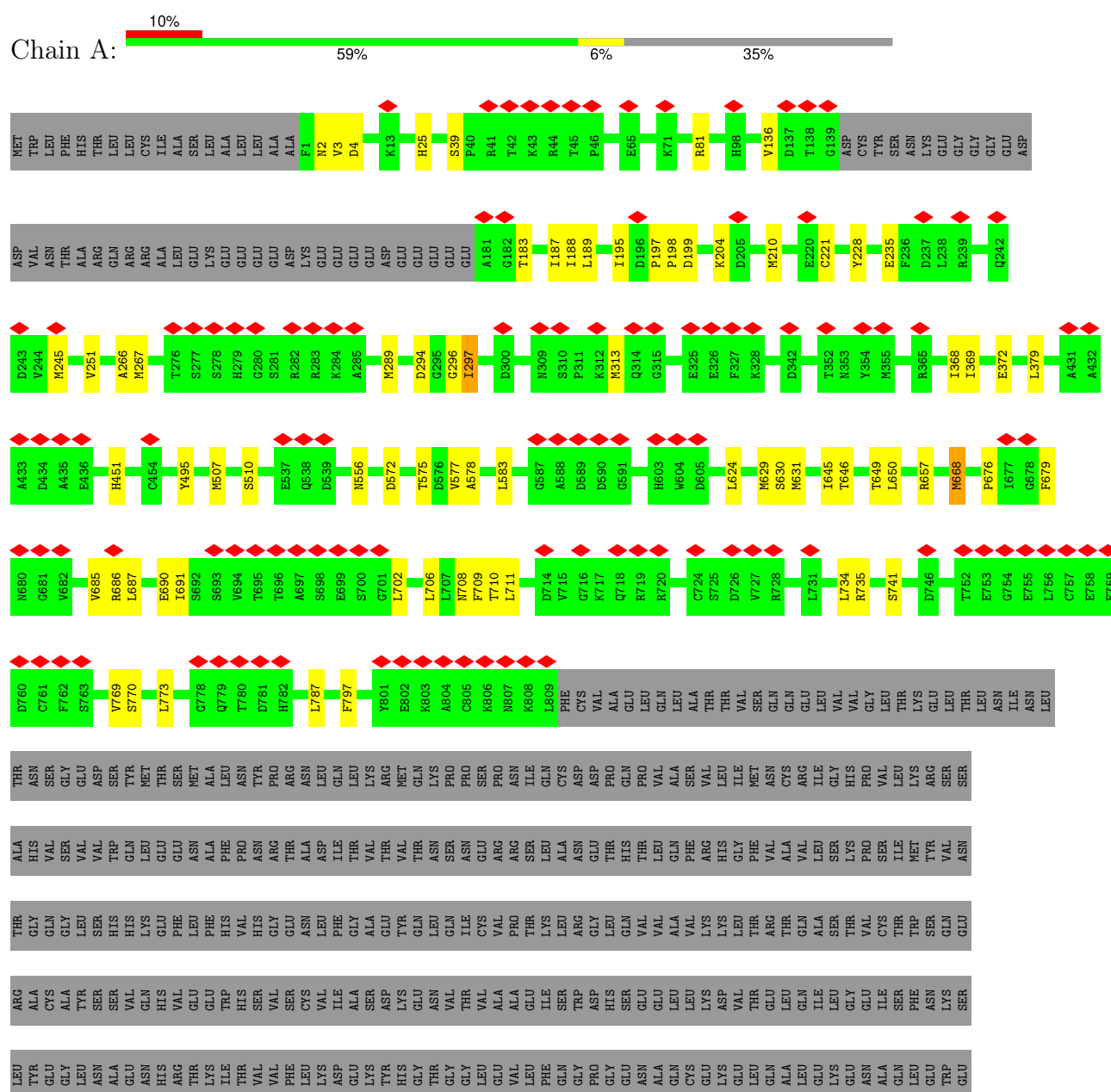
- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Mn	0
			1	1	
8	B	3	Total	Mn	0
			3	3	

### 3 Residue-property plots

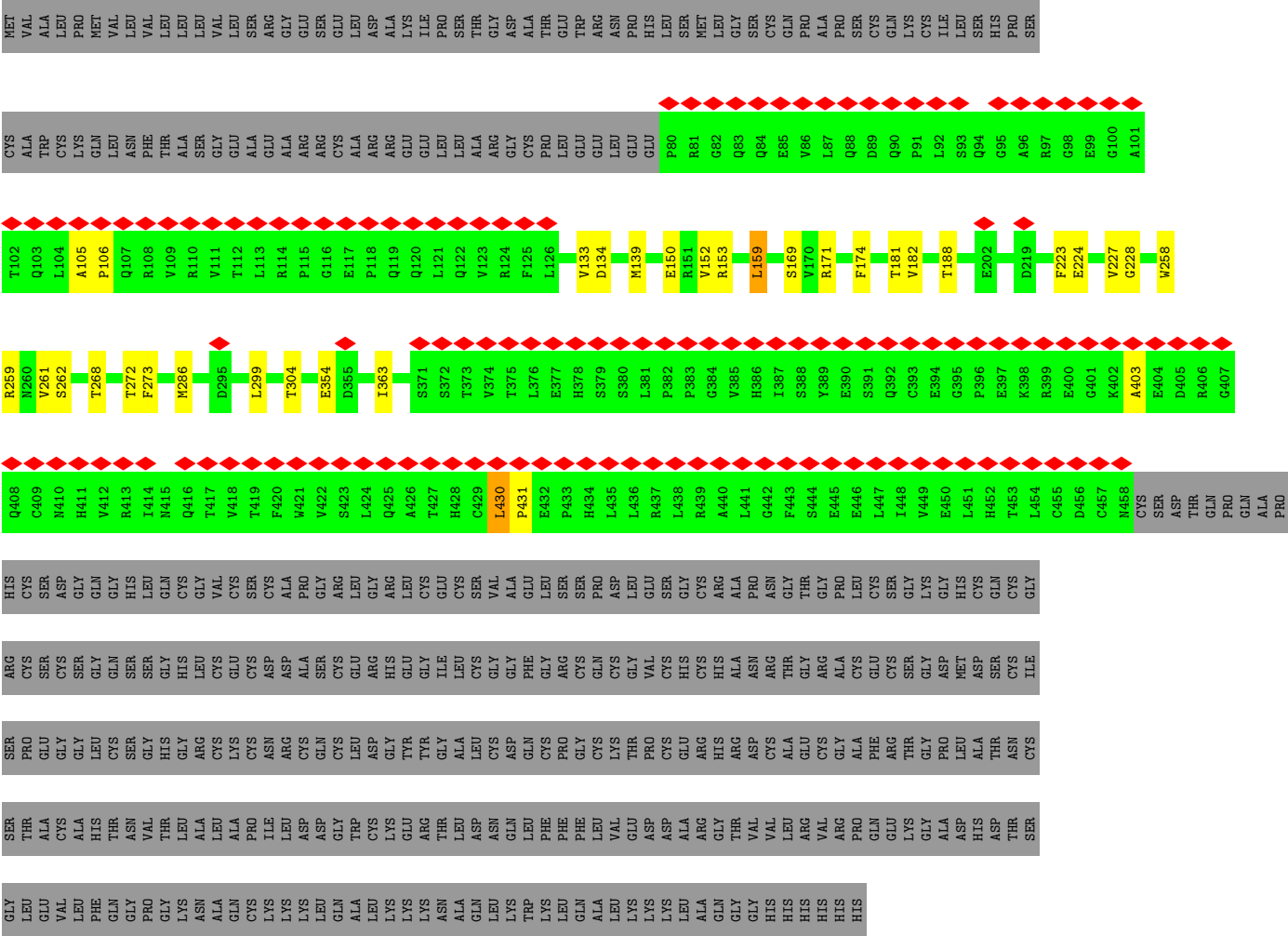
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Integrin alpha-E

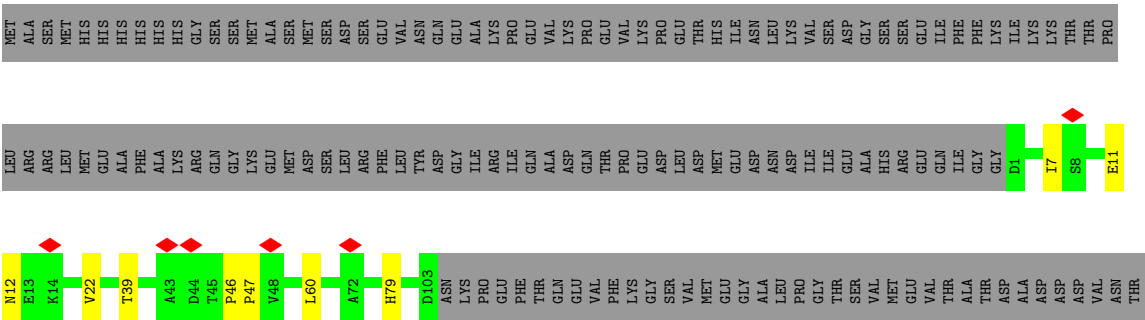


LEU  
GLN  
ALA  
LEU  
LEU  
GLY  
LYS  
GLU  
LEU  
GLN  
TRP  
SER  
HIS  
PRO  
GLN  
PHE  
GLU  
LYS

● Molecule 2: Integrin beta-7



● Molecule 3: Cadherin-1



TYR ASN ALA ILE THR THR SER GLN ASP PRO GLU PRO LYS ASN MET PHE THR ILE ASN ARG ASN THR GLY VAL ILE SER VAL VAL THR THR GLY LEU ASP ARG GLU SER PHE PRO THR THR LEU VAL VAL GLN ALA ASP LEU GLY GLY LEU

SER THR THR ALA THR ALA VAL ILE THR VAL THR ASP THR ASP ASN ASN

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



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	487193	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.721	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	408.408, 408.408, 408.408	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.122, 1.122, 1.122	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, CA, NAG, MN

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	0.25	0/6010	0.39	0/8148
2	B	0.22	0/3006	0.40	1/4081 (0.0%)
3	C	0.25	0/825	0.43	0/1125
All	All	0.24	0/9841	0.40	1/13354 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	ALA	CB-CA-C	-5.08	110.74	116.63

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	5886	5766	5762	39	0
2	B	2943	2876	2874	24	0
3	C	806	792	794	4	0
4	D	39	37	34	0	0
4	E	39	37	34	0	0
5	F	28	27	25	0	0
6	A	28	28	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	14	13	1	0
7	A	3	0	0	0	0
8	A	1	0	0	0	0
8	B	3	0	0	0	0
All	All	9790	9577	9562	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (66) 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)
2:B:159:LEU:HD12	2:B:363:ILE:HD13	1.74	0.70
2:B:159:LEU:CD1	2:B:363:ILE:HD13	2.28	0.64
1:A:188:ILE:HD12	1:A:289:MET:HE3	1.79	0.64
2:B:152:VAL:CG1	2:B:268:THR:HG21	2.32	0.60
2:B:258:TRP:O	6:B:801:NAG:H83	2.05	0.55
2:B:224:GLU:HA	2:B:224:GLU:OE2	2.06	0.55
2:B:261:VAL:HG13	2:B:262:SER:N	2.22	0.54
1:A:629:MET:HE1	1:A:650:LEU:HD13	1.88	0.54
2:B:261:VAL:HG13	2:B:262:SER:H	1.72	0.53
1:A:572:ASP:C	1:A:572:ASP:OD2	2.52	0.52
1:A:650:LEU:HD21	2:B:286:MET:SD	2.50	0.52
1:A:187:ILE:HD11	1:A:210:MET:HE3	1.92	0.52
1:A:734:LEU:C	1:A:735:ARG:HD2	2.35	0.52
1:A:228:TYR:CB	1:A:266:ALA:HB2	2.40	0.51
1:A:624:LEU:HD22	1:A:649:THR:HG21	1.92	0.51
2:B:272:THR:HG22	2:B:273:PHE:N	2.26	0.51
2:B:152:VAL:HG11	2:B:268:THR:HG21	1.92	0.50
2:B:354:GLU:N	2:B:354:GLU:OE1	2.43	0.50
1:A:708:ASN:OD1	1:A:708:ASN:C	2.54	0.50
1:A:235:GLU:HA	1:A:235:GLU:OE1	2.12	0.50
2:B:150:GLU:HA	2:B:150:GLU:OE1	2.11	0.50
2:B:139:MET:HE3	2:B:174:PHE:CD1	2.47	0.49
1:A:706:LEU:O	1:A:773:LEU:HD12	2.12	0.49
1:A:668:MET:HE3	1:A:797:PHE:CD2	2.48	0.49
2:B:182:VAL:CG1	2:B:304:THR:HG23	2.43	0.49
1:A:296:GLY:O	1:A:297:ILE:C	2.56	0.48
1:A:369:ILE:HG21	1:A:379:LEU:HD11	1.95	0.48
1:A:25:HIS:HA	1:A:81:ARG:HD2	1.95	0.47
2:B:153:ARG:HD3	2:B:228:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:ILE:CD1	1:A:702:LEU:HD22	2.45	0.47
2:B:105:ALA:HB1	2:B:106:PRO:HD2	1.95	0.47
2:B:152:VAL:HG12	2:B:268:THR:HG21	1.97	0.47
3:C:7:ILE:HD11	3:C:60:LEU:CD2	2.45	0.47
1:A:687:LEU:HD21	1:A:769:VAL:HG11	1.97	0.46
1:A:577:VAL:HG12	1:A:578:ALA:N	2.30	0.46
1:A:556:ASN:O	1:A:583:LEU:HB3	2.16	0.45
1:A:195:ILE:HG23	1:A:199:ASP:HB2	1.99	0.44
2:B:430:LEU:HB3	2:B:431:PRO:CD	2.48	0.43
3:C:46:PRO:HA	3:C:47:PRO:C	2.42	0.43
1:A:690:GLU:HA	1:A:741:SER:O	2.18	0.43
2:B:188:THR:O	2:B:188:THR:HG22	2.18	0.43
1:A:267:MET:HE3	1:A:313:MET:HE1	1.99	0.43
1:A:294:ASP:OD1	1:A:294:ASP:C	2.61	0.43
1:A:204:LYS:HE3	1:A:251:VAL:O	2.18	0.43
1:A:507:MET:HE3	1:A:575:THR:OG1	2.18	0.43
1:A:630:SER:C	1:A:631:MET:HG2	2.42	0.43
2:B:169:SER:O	2:B:169:SER:OG	2.36	0.43
1:A:4:ASP:HB3	1:A:657:ARG:HG2	2.01	0.43
1:A:685:VAL:HG12	1:A:686:ARG:N	2.34	0.42
2:B:223:PHE:O	2:B:227:VAL:HG12	2.20	0.42
2:B:139:MET:HE3	2:B:174:PHE:CE1	2.55	0.42
1:A:197:PRO:N	1:A:198:PRO:CD	2.83	0.42
1:A:709:PHE:HA	1:A:770:SER:O	2.19	0.42
1:A:645:ILE:HG22	1:A:646:THR:N	2.35	0.41
1:A:136:VAL:O	1:A:136:VAL:HG13	2.18	0.41
3:C:11:GLU:HG3	3:C:12:ASN:HB2	2.02	0.41
1:A:183:THR:CG2	1:A:221:CYS:SG	3.09	0.41
1:A:188:ILE:HD12	1:A:289:MET:CE	2.48	0.41
1:A:3:VAL:HG22	1:A:645:ILE:CD1	2.51	0.41
3:C:39:THR:HG21	3:C:79:HIS:CD2	2.55	0.41
1:A:676:PRO:HD2	1:A:679:PHE:CG	2.56	0.41
2:B:171:ARG:HD2	2:B:259:ARG:NE	2.36	0.41
1:A:668:MET:HE3	1:A:797:PHE:CE2	2.56	0.40
1:A:267:MET:HG2	1:A:289:MET:HE1	2.03	0.40
2:B:133:VAL:HG12	2:B:134:ASP:N	2.36	0.40
1:A:451:HIS:O	1:A:510:SER:HA	2.22	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	764/1176 (65%)	736 (96%)	28 (4%)	0	100	100
2	B	377/776 (49%)	353 (94%)	23 (6%)	1 (0%)	37	66
3	C	101/331 (30%)	90 (89%)	11 (11%)	0	100	100
All	All	1242/2283 (54%)	1179 (95%)	62 (5%)	1 (0%)	50	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	430	LEU

### 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	636/996 (64%)	624 (98%)	12 (2%)	52	72
2	B	328/651 (50%)	325 (99%)	3 (1%)	75	86
3	C	92/290 (32%)	91 (99%)	1 (1%)	70	82
All	All	1056/1937 (54%)	1040 (98%)	16 (2%)	60	77

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	39	SER

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Mol	Chain	Res	Type
1	A	189	LEU
1	A	245	MET
1	A	297	ILE
1	A	368	ILE
1	A	372	GLU
1	A	495	TYR
1	A	668	MET
1	A	710	THR
1	A	711	LEU
1	A	787	LEU
2	B	159	LEU
2	B	181	THR
2	B	299	LEU
3	C	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	522	HIS
1	A	807	ASN
2	B	230	GLN
2	B	386	HIS
3	C	79	HIS
3	C	102	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 ⓘ

8 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
4	NAG	D	1	1,4	14,14,15	0.72	0	17,19,21	0.87	0
4	NAG	D	2	4	14,14,15	0.67	0	17,19,21	1.15	1 (5%)
4	BMA	D	3	4	11,11,12	0.83	0	15,15,17	2.87	6 (40%)
4	NAG	E	1	1,4	14,14,15	0.85	1 (7%)	17,19,21	1.03	1 (5%)
4	NAG	E	2	4	14,14,15	0.77	0	17,19,21	1.08	1 (5%)
4	BMA	E	3	4	11,11,12	0.86	0	15,15,17	2.63	5 (33%)
5	NAG	F	1	5,1	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
5	NAG	F	2	5	14,14,15	0.73	0	17,19,21	0.94	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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	O5-C1	-2.02	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C1-O5-C5	9.16	124.46	112.19
4	E	3	BMA	C1-O5-C5	8.13	123.09	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	BMA	C3-C4-C5	3.42	116.42	110.23
4	D	3	BMA	C3-C4-C5	3.34	116.29	110.23
4	E	2	NAG	O5-C1-C2	-3.12	106.46	111.29
4	E	3	BMA	C2-C3-C4	2.87	115.90	110.86
4	D	3	BMA	C2-C3-C4	2.83	115.84	110.86
5	F	1	NAG	O5-C1-C2	-2.73	107.06	111.29
4	D	2	NAG	O4-C4-C5	2.64	115.84	109.32
4	E	1	NAG	C2-N2-C7	2.54	126.31	122.90
4	E	3	BMA	O4-C4-C3	-2.14	105.34	110.38
4	D	3	BMA	O4-C4-C3	-2.12	105.38	110.38
4	E	3	BMA	O3-C3-C2	-2.09	105.80	110.05
4	D	3	BMA	O3-C3-C2	-2.06	105.85	110.05
4	D	3	BMA	O5-C5-C4	2.05	115.82	110.83

There are no chirality outliers.

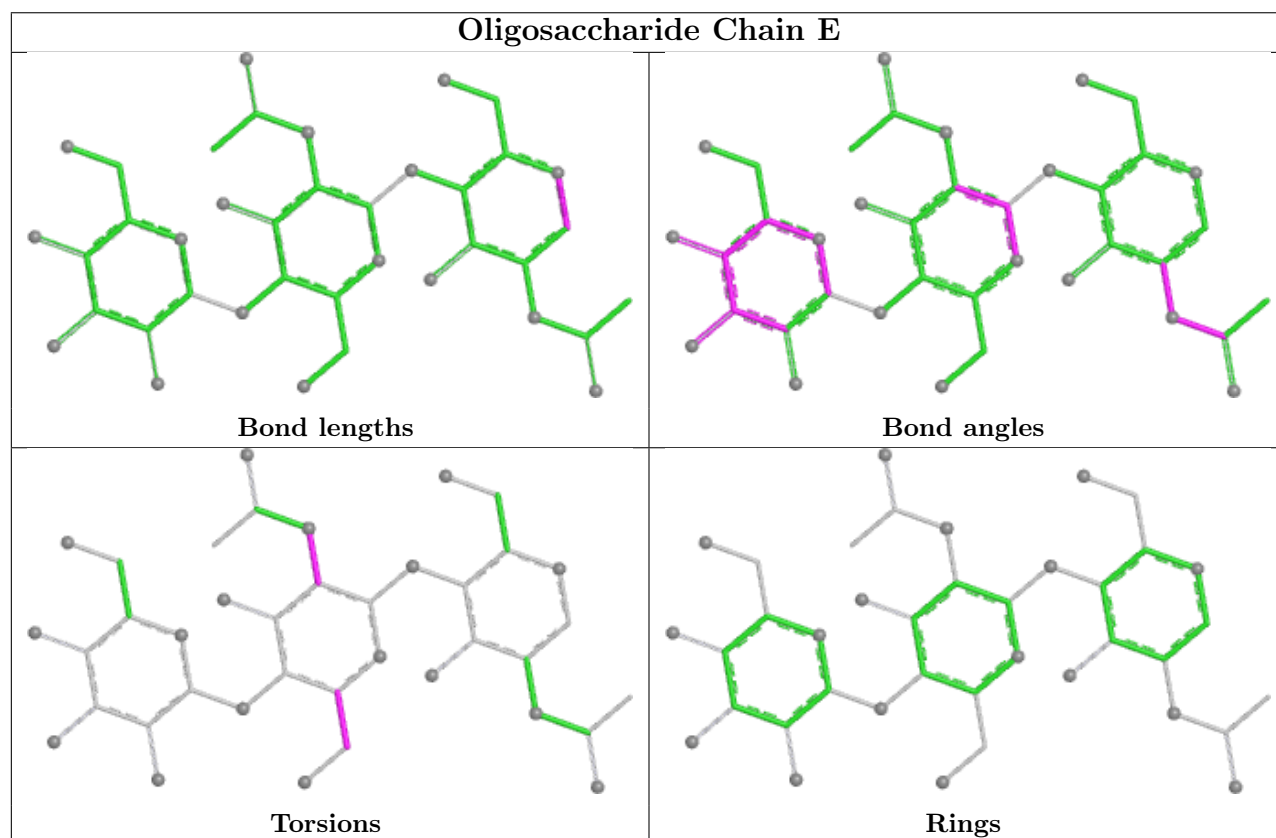
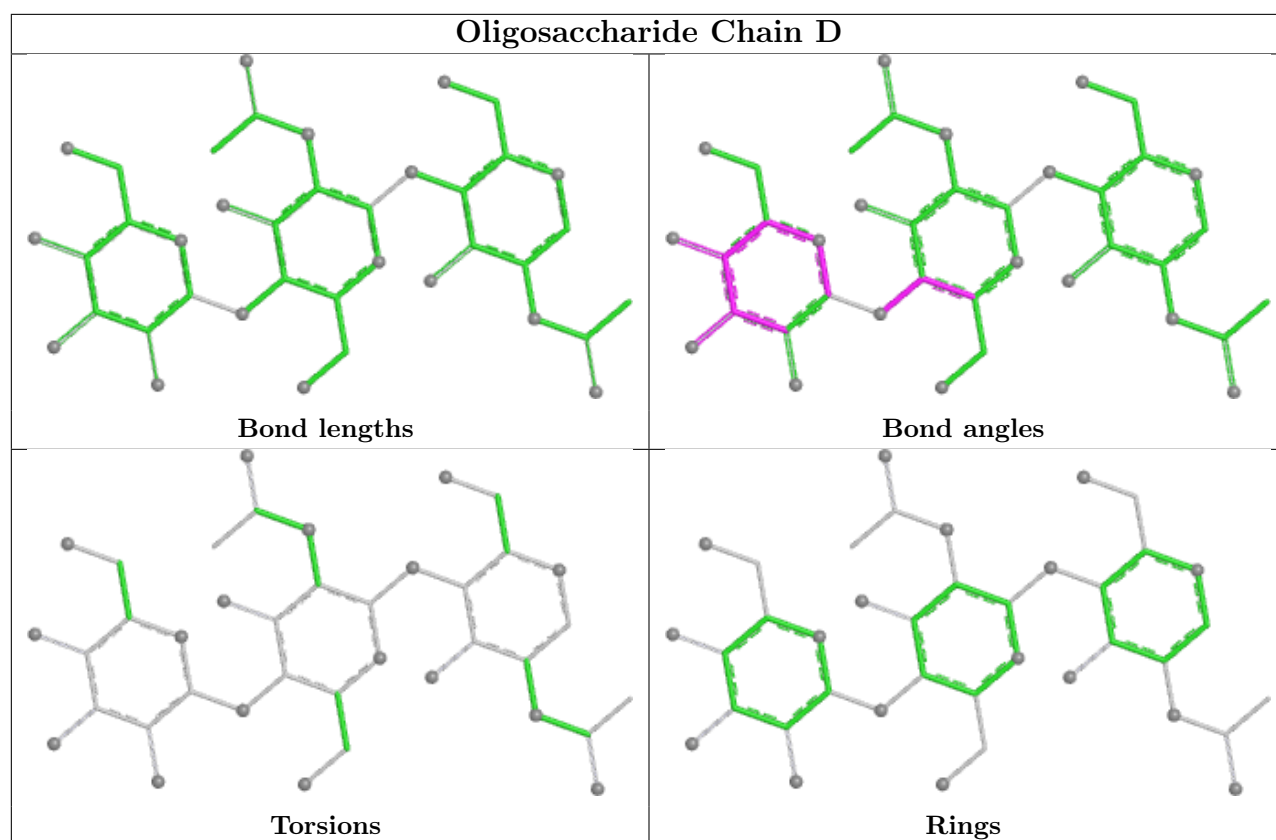
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
5	F	2	NAG	C3-C2-N2-C7
5	F	2	NAG	C1-C2-N2-C7

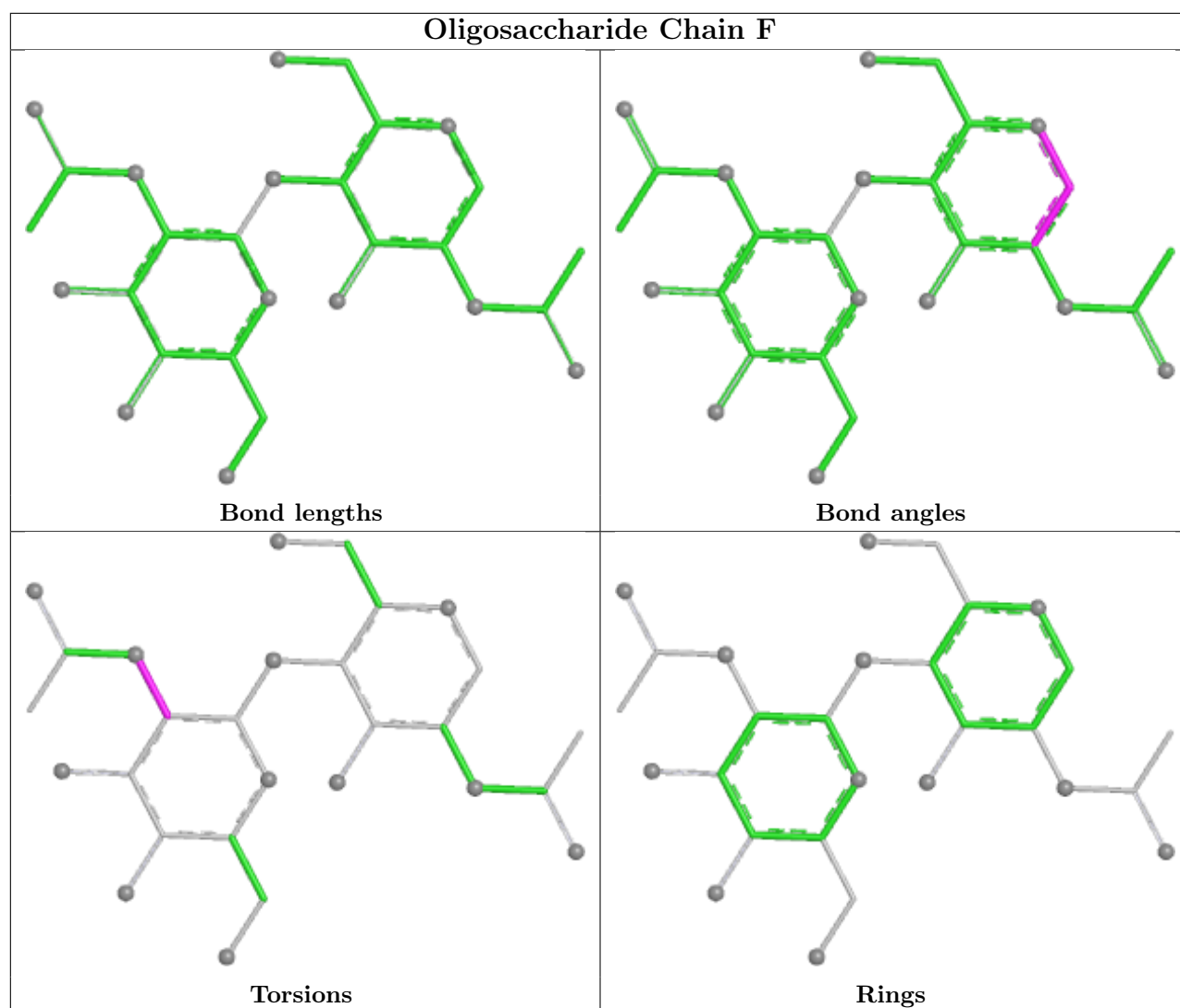
There are no ring outliers.

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](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

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	A	1201	1	14,14,15	0.73	0	17,19,21	0.98	0
6	NAG	A	1202	1	14,14,15	0.69	0	17,19,21	1.11	1 (5%)
6	NAG	B	801	2	14,14,15	0.72	0	17,19,21	1.07	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1202	1	-	1/6/23/26	0/1/1/1
6	NAG	B	801	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	801	NAG	C1-O5-C5	2.81	115.96	112.19
6	A	1202	NAG	C2-N2-C7	2.57	126.34	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1201	NAG	C1-C2-N2-C7
6	A	1202	NAG	C1-C2-N2-C7
6	B	801	NAG	C3-C2-N2-C7
6	B	801	NAG	C1-C2-N2-C7
6	A	1201	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	801	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.

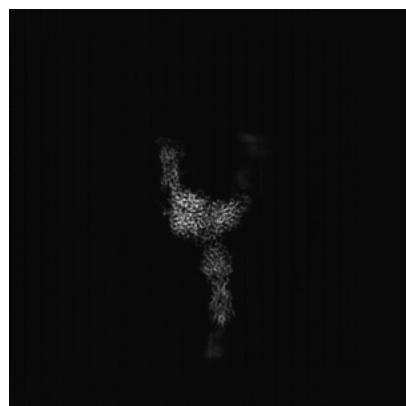
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71403. These allow visual inspection of the internal detail of the map and identification of artifacts.

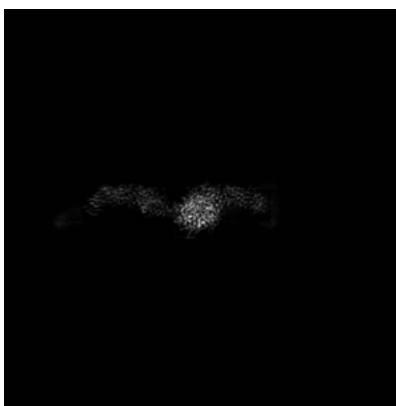
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

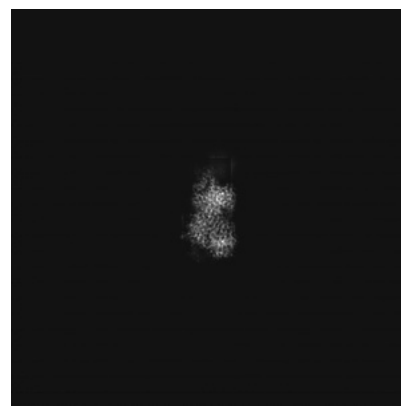
#### 6.1.1 Primary map



X

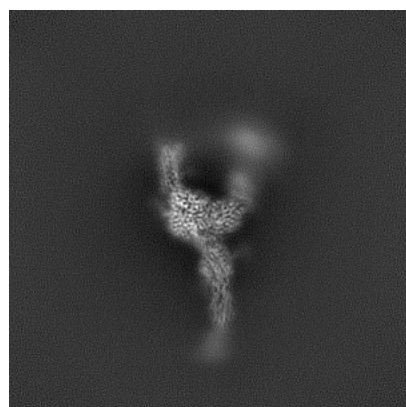


Y

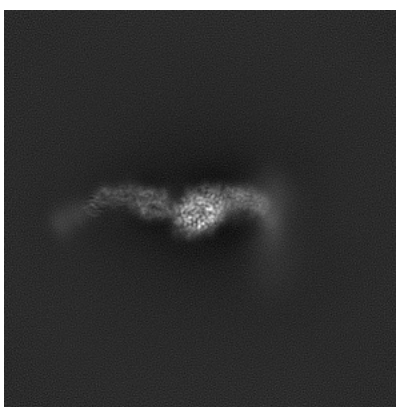


Z

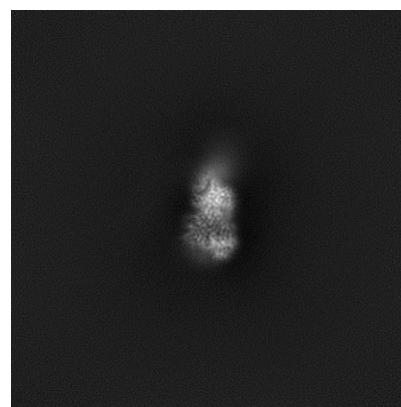
#### 6.1.2 Raw map



X



Y

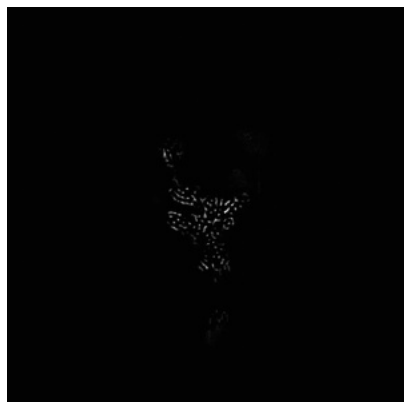


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 182

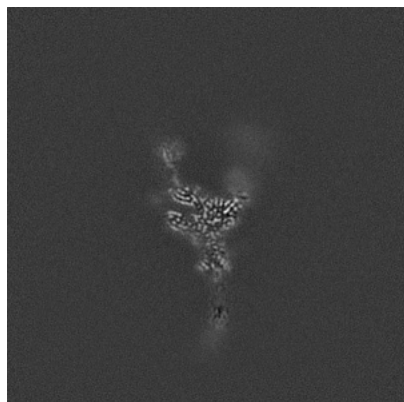


Y Index: 182

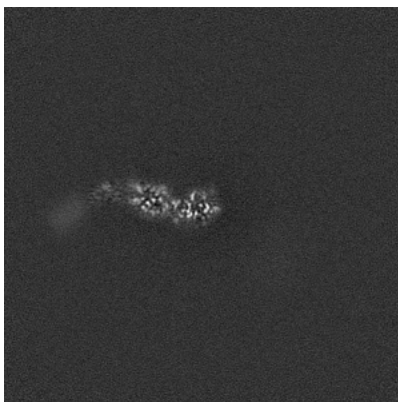


Z Index: 182

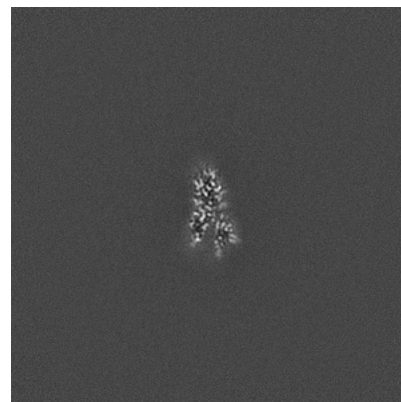
### 6.2.2 Raw map



X Index: 182



Y Index: 182



Z Index: 182

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: 183

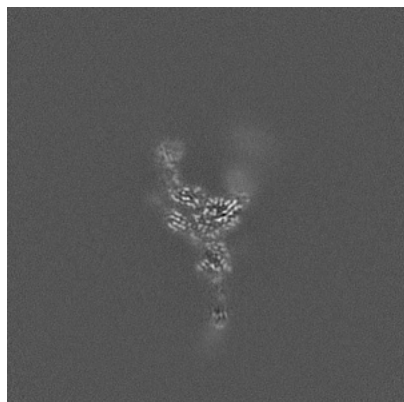


Y Index: 194

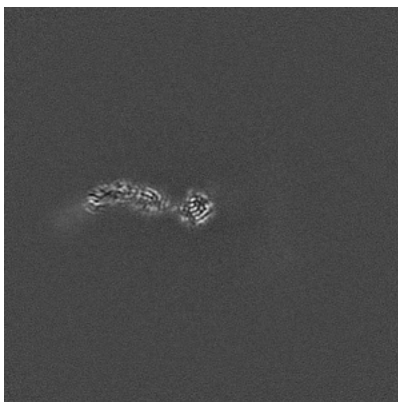


Z Index: 177

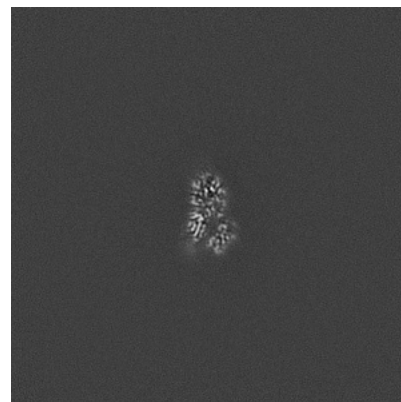
### 6.3.2 Raw map



X Index: 183



Y Index: 194

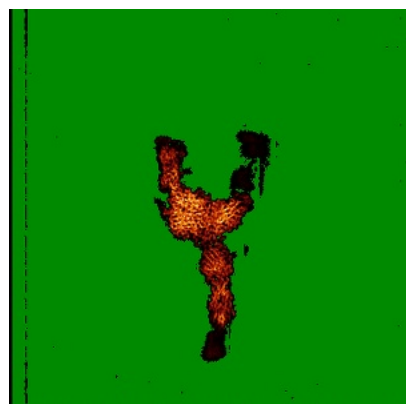


Z Index: 177

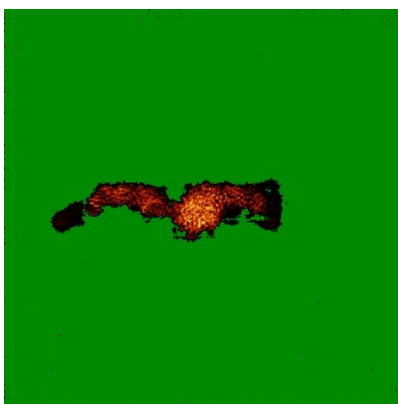
The images above show the largest variance slices of the map in three orthogonal directions.

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

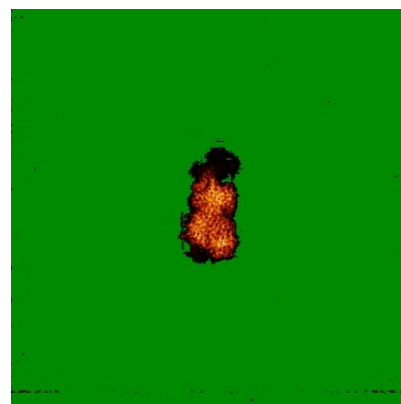
### 6.4.1 Primary map



X

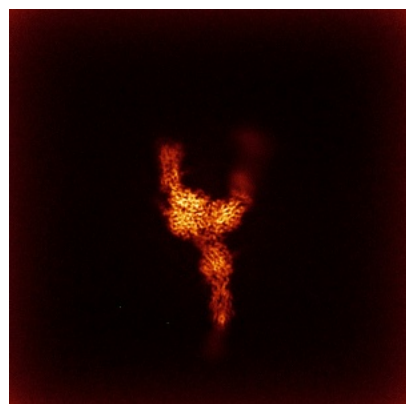


Y

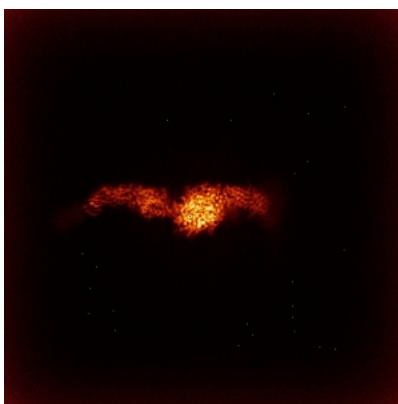


Z

### 6.4.2 Raw map



X



Y

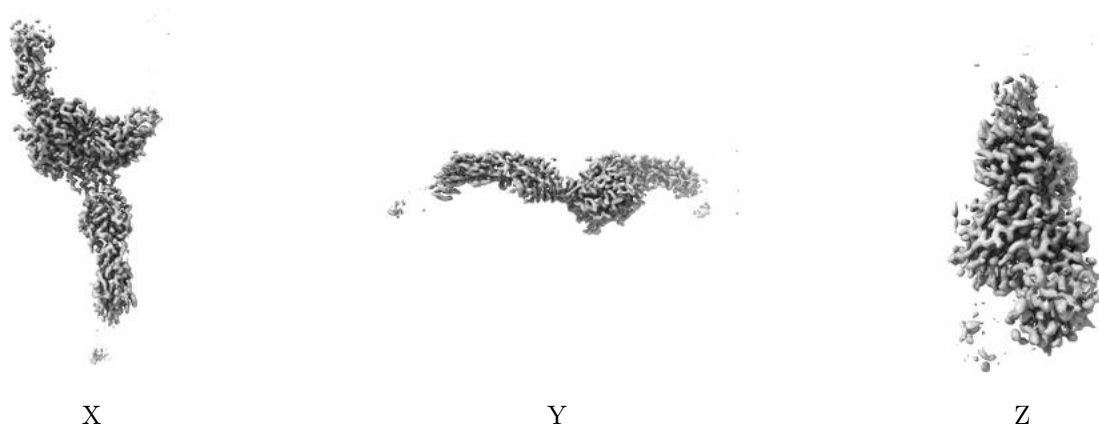


Z

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 0.1. 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](#)

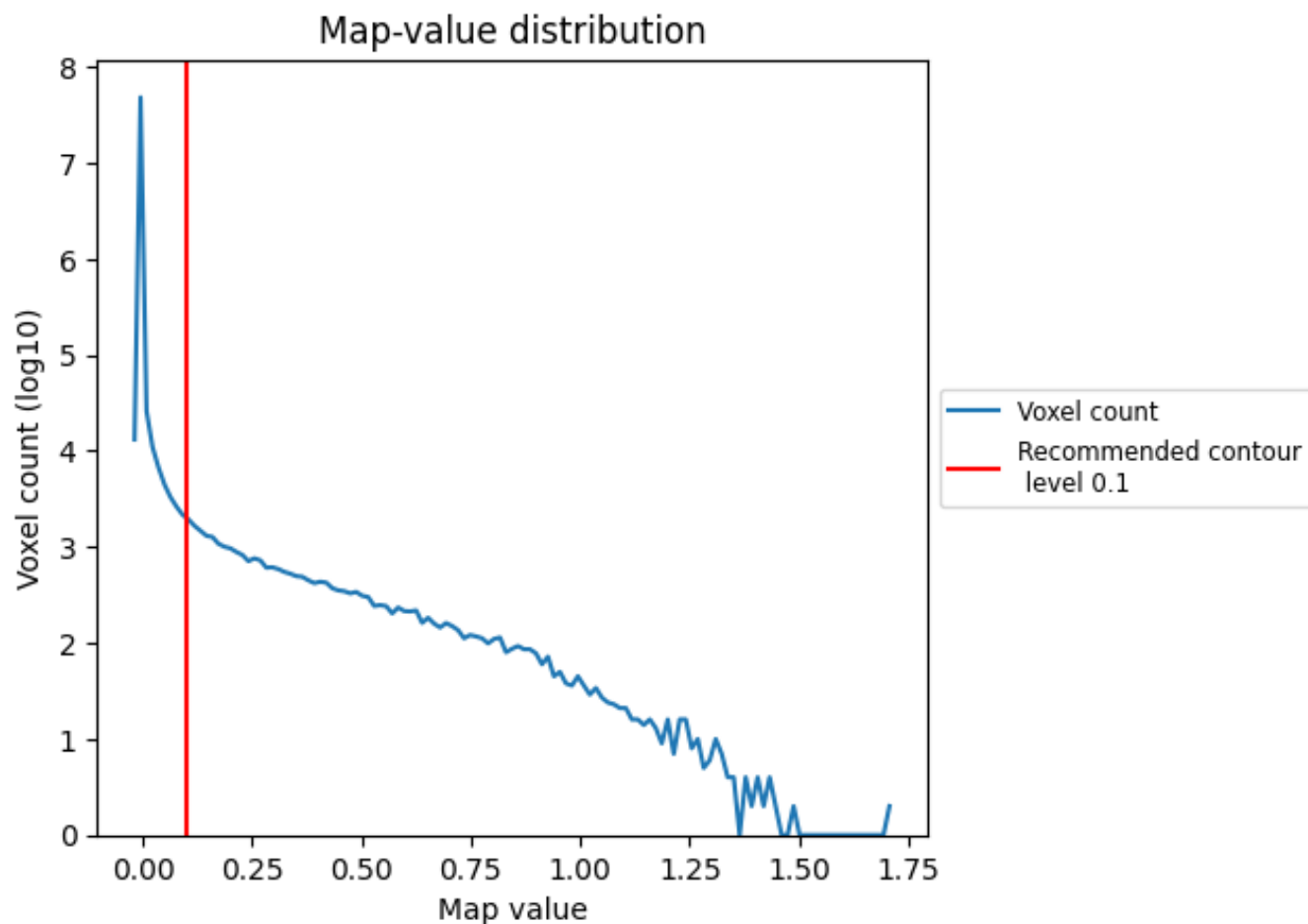
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

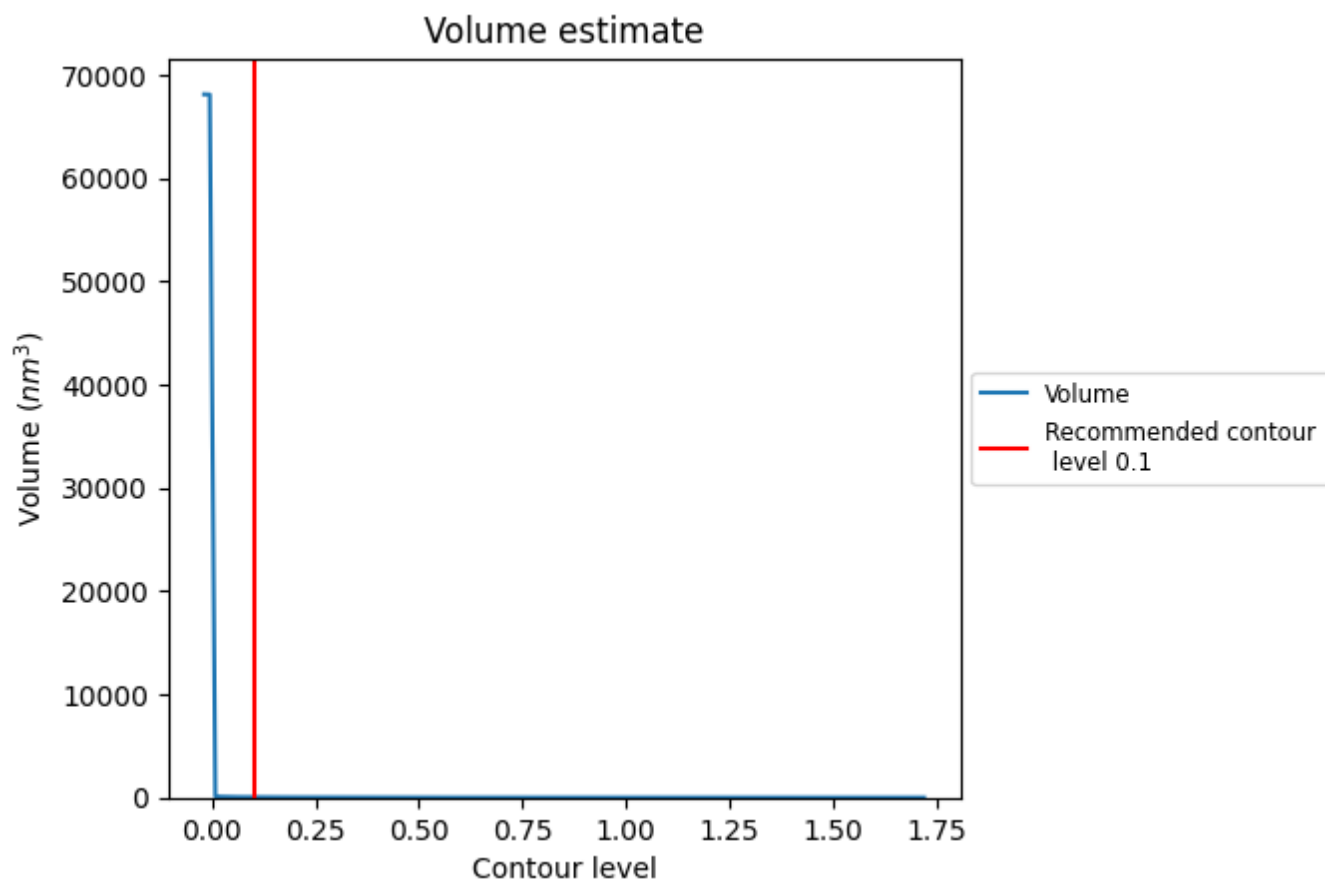
This section contains the results of statistical analysis of the map.

### 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.

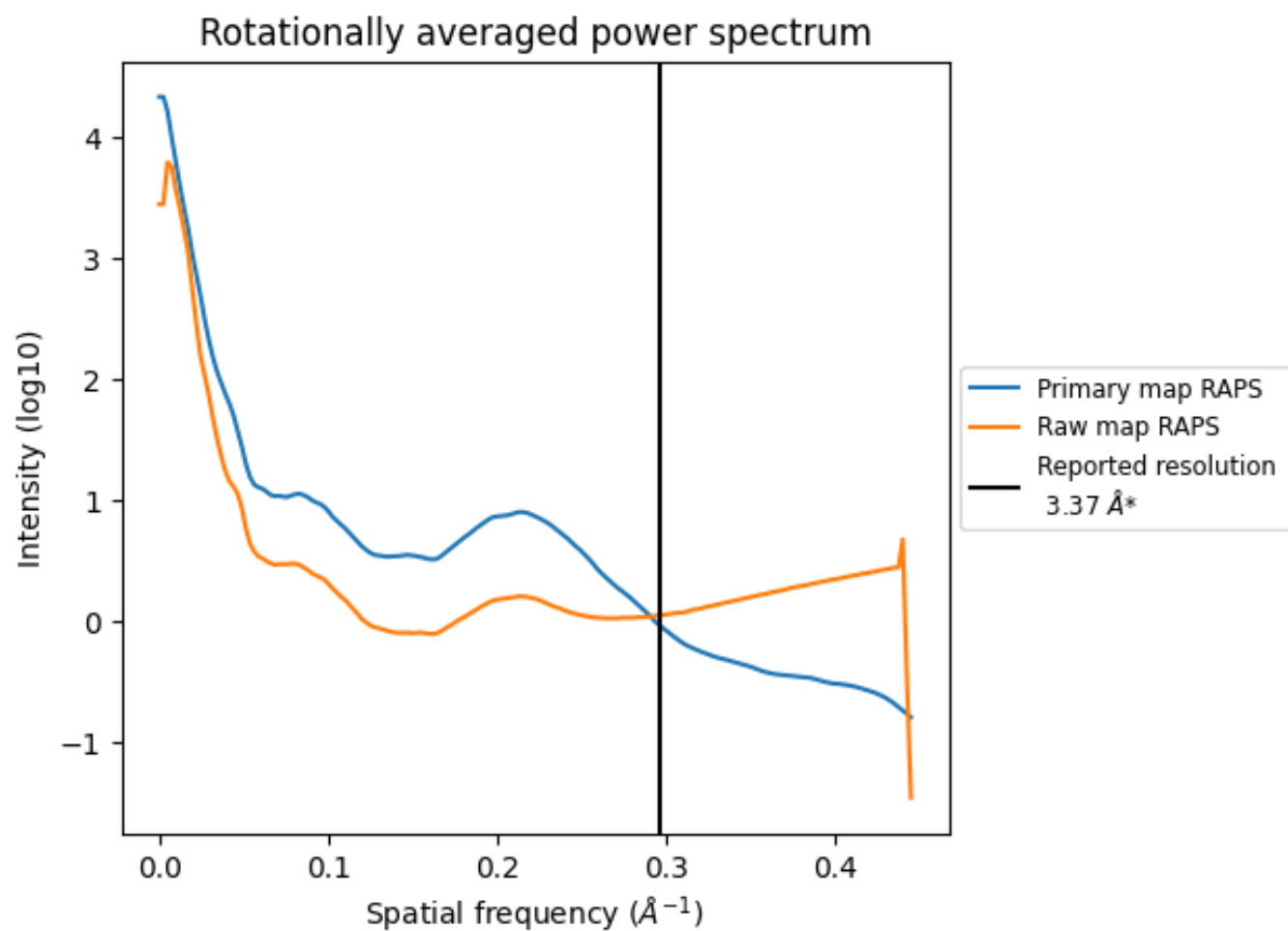
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm<sup>3</sup>; this corresponds to an approximate mass of 36 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 ⓘ

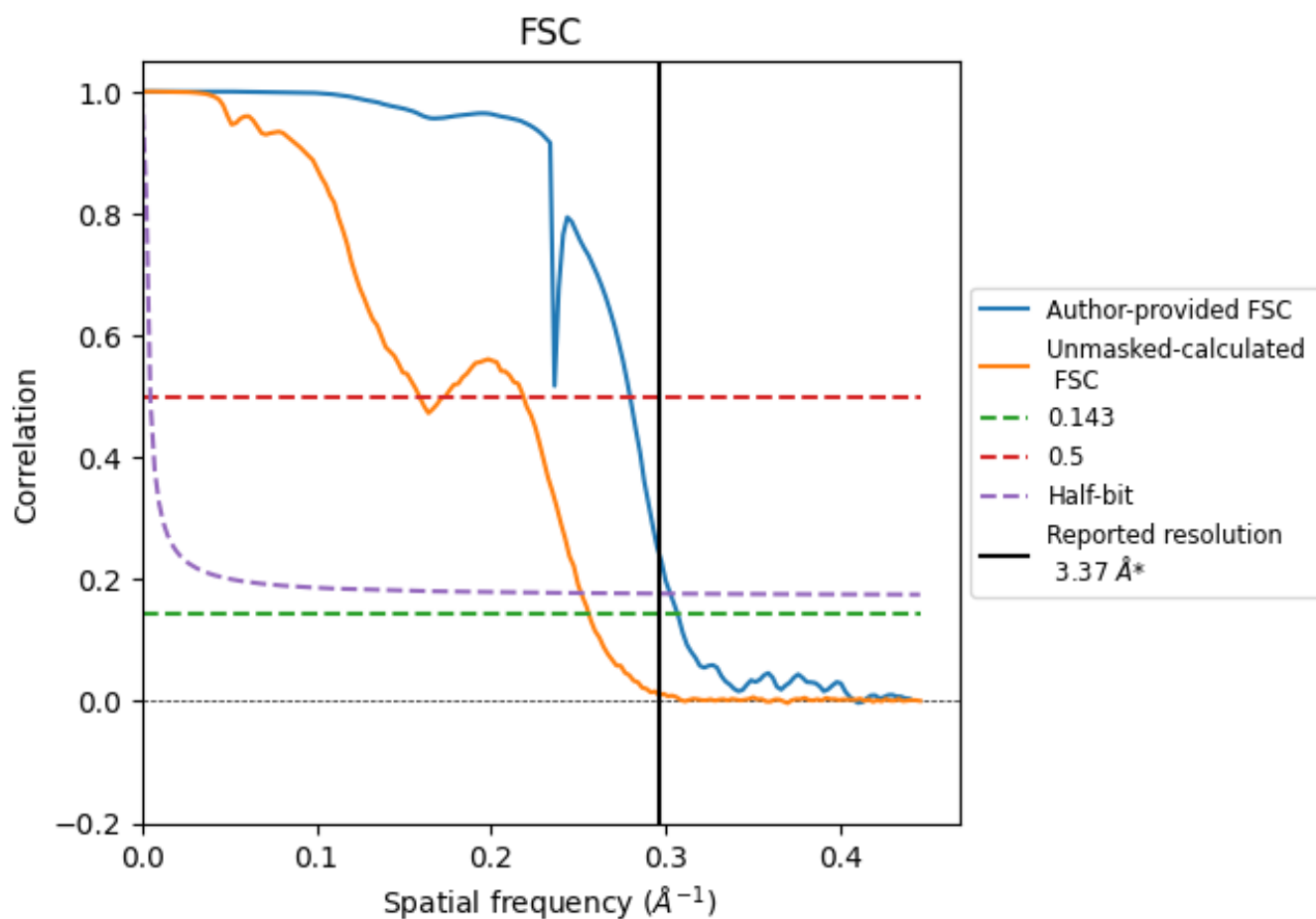


\*Reported resolution corresponds to spatial frequency of  $0.297 \text{ \AA}^{-1}$

## 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 0.297  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

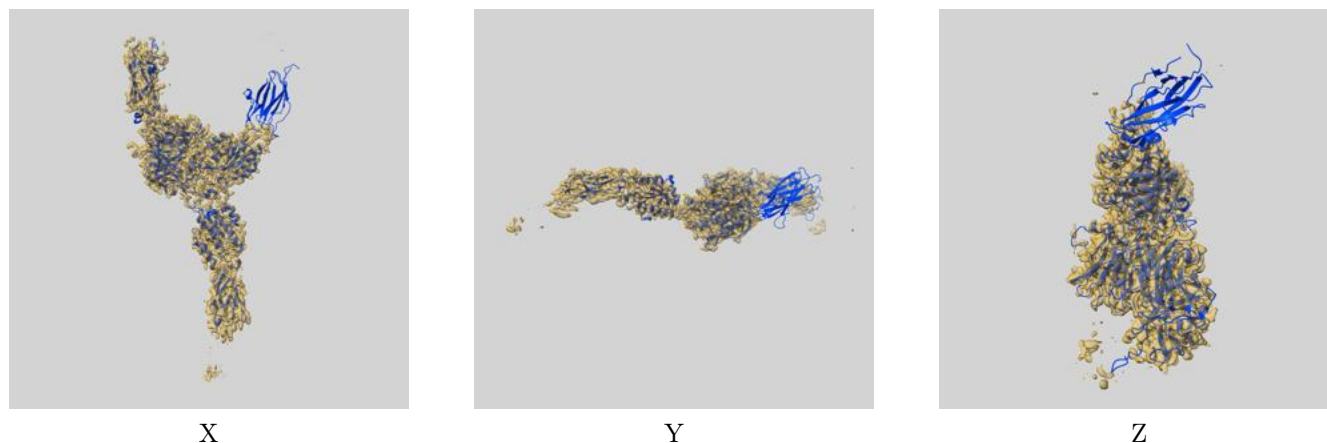
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	3.26	3.58	3.30
Unmasked-calculated*	3.91	6.29	3.98

\*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 3.91 differs from the reported value 3.37 by more than 10 %

## 9 Map-model fit [i](#)

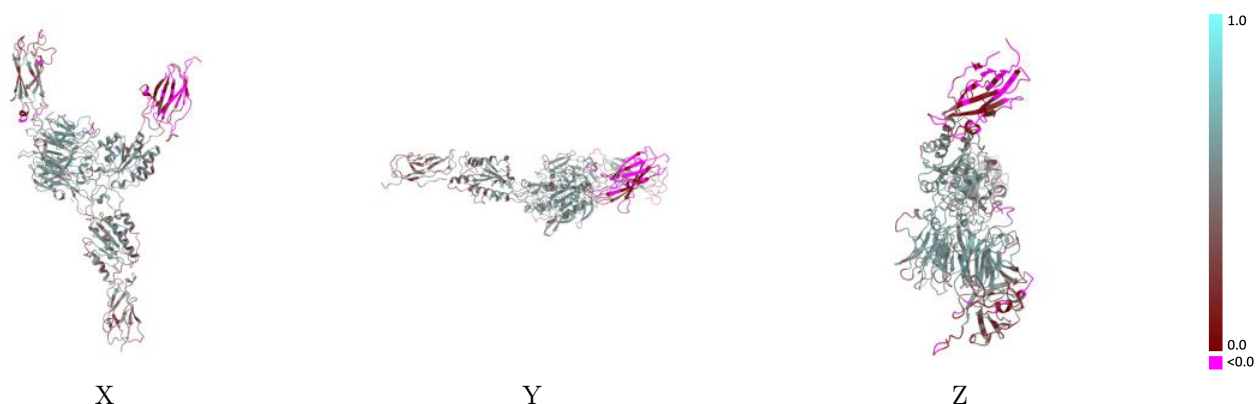
This section contains information regarding the fit between EMDB map EMD-71403 and PDB model 9P99. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



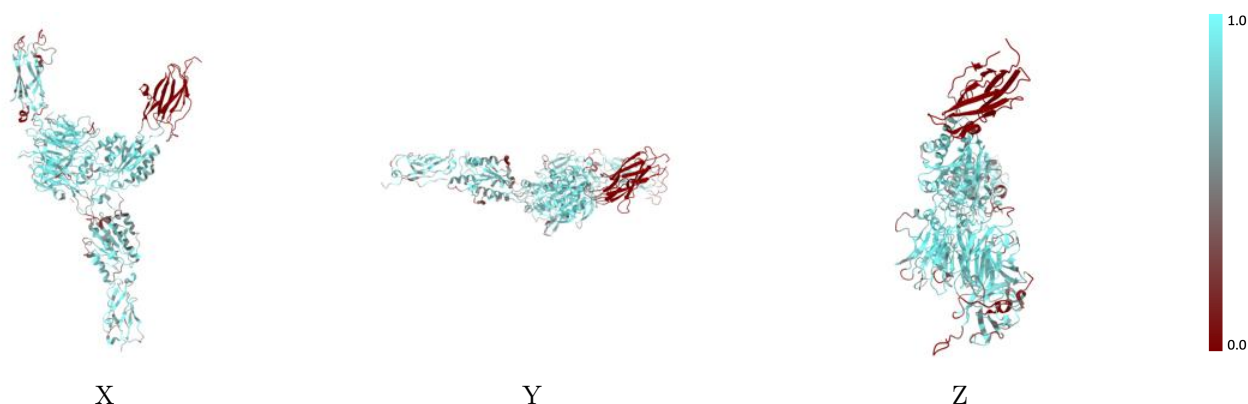
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

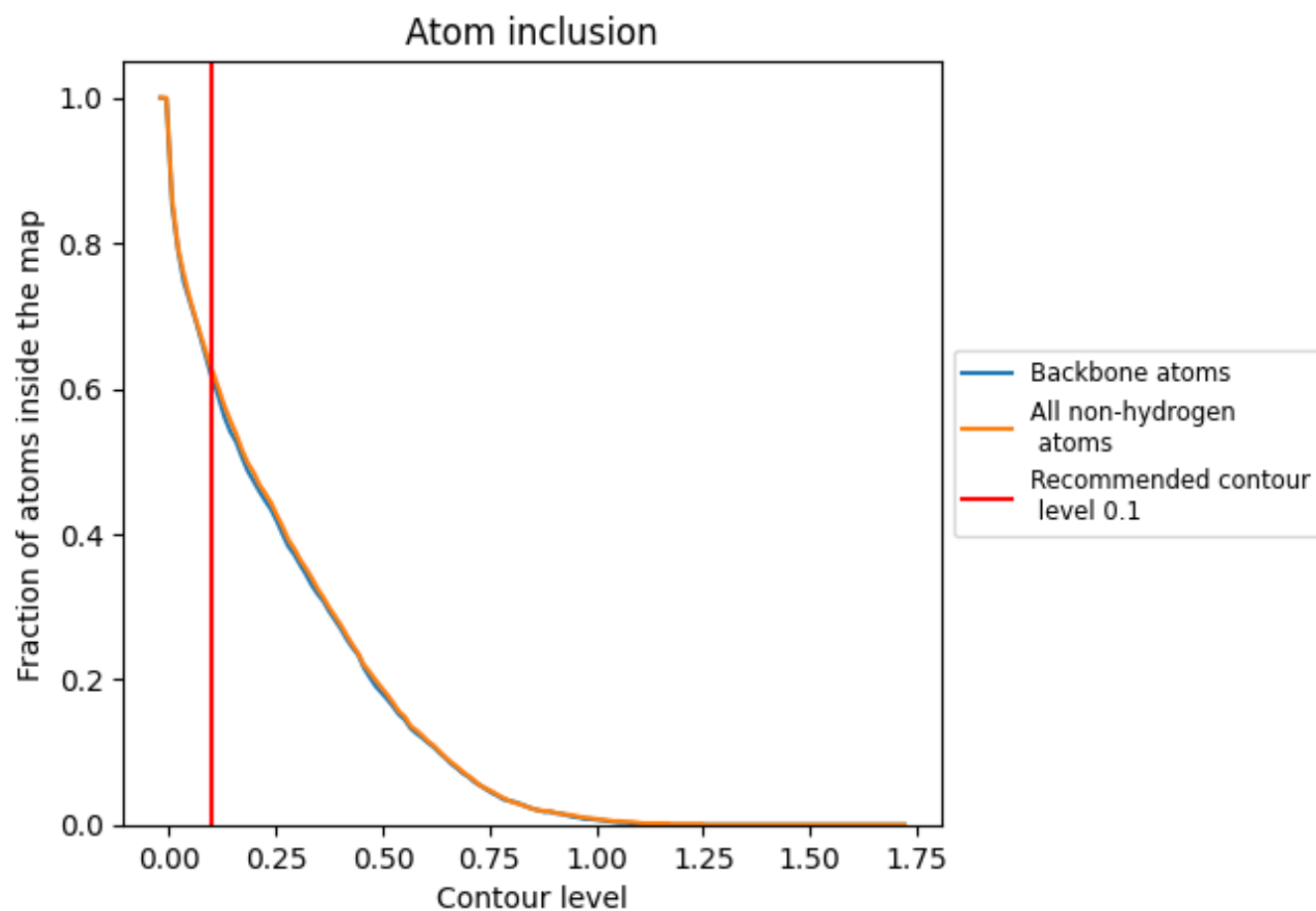
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.1).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 63% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6260	<div></div> 0.4110
A	<div></div> 0.6940	<div></div> 0.4560
B	<div></div> 0.5180	<div></div> 0.3380
C	<div></div> 0.6760	<div></div> 0.3600
D	<div></div> 0.1280	<div></div> 0.2930
E	<div></div> 0.5130	<div></div> 0.3820
F	<div></div> 0.1790	<div></div> 0.2610

1.0

0.0

<0.0