



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 12:07 PM EDT

PDB ID : 9PZC / pdb_00009pzc
EMDB ID : EMD-72061
Title : HCMV trimer in complex with G1L (II), G1L (A), B5L, C4K, B1K, A7K, A12K, and C5K Fabs
Authors : Goldsmith, J.A.; McLellan, J.S.
Deposited on : 2025-08-09
Resolution : 3.20 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

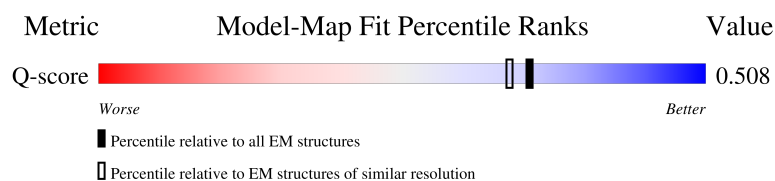
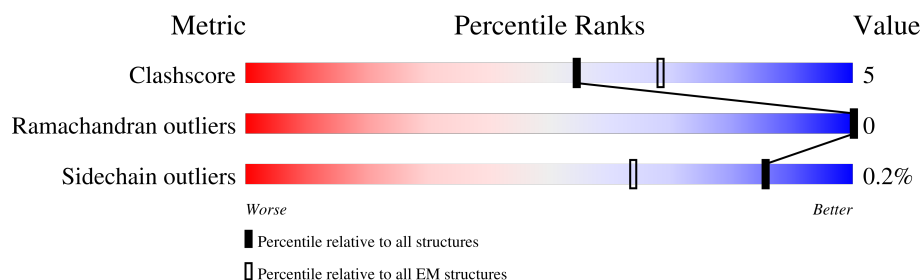
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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




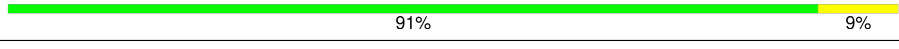
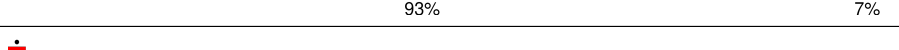
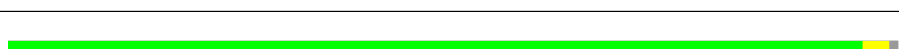
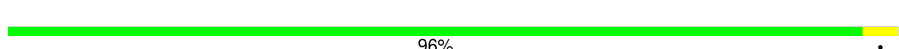
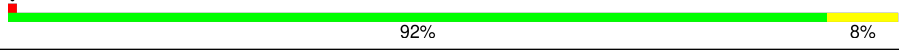

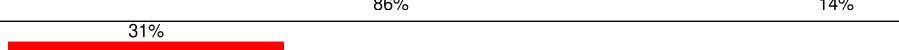




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	743	 24% 77% 11% 12%
2	B	268	 24% 76% 9% 14%
3	C	110	 82% 18%
4	D	125	 86% 14%

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Mol	Chain	Length	Quality of chain
5	E	119	
6	F	108	
7	G	116	
8	H	123	
9	I	108	
10	J	107	
11	K	121	
12	L	110	
13	M	106	
14	N	123	
15	O	119	
16	P	108	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 19396 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	655	Total	C	N	O	S	0	0
			5256	3357	894	979	26		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	THR	ALA	conflict	UNP Q69155

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	230	Total	C	N	O	S	0	0
			1819	1160	317	334	8		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	MET	-	expression tag	UNP Q8JP80
B	12	SER	-	expression tag	UNP Q8JP80
B	13	VAL	-	expression tag	UNP Q8JP80
B	14	PRO	-	expression tag	UNP Q8JP80
B	15	THR	-	expression tag	UNP Q8JP80
B	16	GLN	-	expression tag	UNP Q8JP80
B	17	VAL	-	expression tag	UNP Q8JP80
B	18	LEU	-	expression tag	UNP Q8JP80
B	19	GLY	-	expression tag	UNP Q8JP80
B	20	LEU	-	expression tag	UNP Q8JP80
B	21	LEU	-	expression tag	UNP Q8JP80
B	22	LEU	-	expression tag	UNP Q8JP80
B	23	LEU	-	expression tag	UNP Q8JP80
B	24	TRP	-	expression tag	UNP Q8JP80
B	25	LEU	-	expression tag	UNP Q8JP80
B	26	THR	-	expression tag	UNP Q8JP80

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	ASP	-	expression tag	UNP Q8JP80
B	28	ALA	-	expression tag	UNP Q8JP80
B	29	ARG	-	expression tag	UNP Q8JP80
B	30	CYS	-	expression tag	UNP Q8JP80
B	41	GLU	LYS	conflict	UNP Q8JP80
B	77	ARG	GLY	conflict	UNP Q8JP80

- Molecule 3 is a protein called Immunoglobulin lambda variable 1-51.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	110	Total	C	N	O	S	0	0
			812	507	136	167	2		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	LEU	VAL	conflict	UNP P01701
C	18	ARG	LYS	conflict	UNP P01701
C	24	THR	SER	conflict	UNP P01701
C	27	THR	SER	conflict	UNP P01701
C	29	VAL	GLY	conflict	UNP P01701
C	38	HIS	GLN	conflict	UNP P01701
C	52	VAL	ASN	conflict	UNP P01701
C	59	SER	PRO	conflict	UNP P01701
C	70	THR	SER	conflict	UNP P01701
C	74	THR	GLY	conflict	UNP P01701
C	84	SER	ALA	conflict	UNP P01701
C	95B	LEU	-	expression tag	UNP P01701
C	96	GLY	-	expression tag	UNP P01701
C	97	VAL	-	expression tag	UNP P01701
C	98	PHE	-	expression tag	UNP P01701
C	99	GLY	-	expression tag	UNP P01701
C	100	GLY	-	expression tag	UNP P01701
C	101	GLY	-	expression tag	UNP P01701
C	102	THR	-	expression tag	UNP P01701
C	103	LYS	-	expression tag	UNP P01701
C	104	VAL	-	expression tag	UNP P01701
C	105	THR	-	expression tag	UNP P01701
C	106	VAL	-	expression tag	UNP P01701
C	106A	LEU	-	expression tag	UNP P01701

- Molecule 4 is a protein called G1L Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	125	Total	C	N	O	S	0	0
			969	620	170	173	6		

- Molecule 5 is a protein called Immunoglobulin heavy variable 1-46.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	119	Total	C	N	O	S	0	0
			929	579	165	179	6		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	18	MET	VAL	conflict	UNP P01743
E	31	ASN	SER	conflict	UNP P01743
E	34	LEU	MET	conflict	UNP P01743
E	50	LEU	ILE	conflict	UNP P01743
E	52	ASP	ASN	conflict	UNP P01743
E	56	ASN	SER	conflict	UNP P01743
E	58	ASN	SER	conflict	UNP P01743
E	73	ARG	THR	conflict	UNP P01743
E	84	PRO	SER	conflict	UNP P01743
E	88	THR	ALA	conflict	UNP P01743
E	95	GLY	-	expression tag	UNP P01743
E	96	GLY	-	expression tag	UNP P01743
E	97	TYR	-	expression tag	UNP P01743
E	98	ASN	-	expression tag	UNP P01743
E	99	SER	-	expression tag	UNP P01743
E	100	ARG	-	expression tag	UNP P01743
E	100A	LEU	-	expression tag	UNP P01743
E	100B	ARG	-	expression tag	UNP P01743
E	100C	LEU	-	expression tag	UNP P01743
E	101	ASP	-	expression tag	UNP P01743
E	102	SER	-	expression tag	UNP P01743
E	103	TRP	-	expression tag	UNP P01743
E	104	GLY	-	expression tag	UNP P01743
E	105	GLN	-	expression tag	UNP P01743
E	106	GLY	-	expression tag	UNP P01743
E	107	THR	-	expression tag	UNP P01743
E	108	LEU	-	expression tag	UNP P01743
E	109	VAL	-	expression tag	UNP P01743
E	110	THR	-	expression tag	UNP P01743
E	111	VAL	-	expression tag	UNP P01743
E	112	SER	-	expression tag	UNP P01743

- Molecule 6 is a protein called Immunoglobulin kappa variable 3-20.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	108	Total	C	N	O	S	0	0
			814	510	137	165	2		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	40	SER	PRO	conflict	UNP P01619
F	66	ALA	GLY	conflict	UNP P01619
F	85	LEU	VAL	conflict	UNP P01619
F	96	LEU	-	expression tag	UNP P01619
F	97	THR	-	expression tag	UNP P01619
F	98	PHE	-	expression tag	UNP P01619
F	99	GLY	-	expression tag	UNP P01619
F	100	GLY	-	expression tag	UNP P01619
F	101	GLY	-	expression tag	UNP P01619
F	102	THR	-	expression tag	UNP P01619
F	103	LYS	-	expression tag	UNP P01619
F	104	VAL	-	expression tag	UNP P01619
F	105	GLU	-	expression tag	UNP P01619
F	106	ILE	-	expression tag	UNP P01619
F	107	LYS	-	expression tag	UNP P01619

- Molecule 7 is a protein called A12K Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	116	Total	C	N	O	S	0	0
			913	581	156	171	5		

- Molecule 8 is a protein called Immunoglobulin heavy variable 4-34.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S	0	0
			967	612	172	181	2		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	15	TRP	SER	conflict	UNP P06331
H	29	ILE	PHE	conflict	UNP P06331
H	30	ASN	SER	conflict	UNP P06331
H	31	GLU	GLY	conflict	UNP P06331

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Chain	Residue	Modelled	Actual	Comment	Reference
H	43	GLY	LYS	conflict	UNP P06331
H	67	ILE	VAL	conflict	UNP P06331
H	69	THR	ILE	conflict	UNP P06331
H	81	ARG	LYS	conflict	UNP P06331
H	84	VAL	ALA	conflict	UNP P06331
H	95	GLY	-	expression tag	UNP P06331
H	96	HIS	-	expression tag	UNP P06331
H	97	ARG	-	expression tag	UNP P06331
H	98	LYS	-	expression tag	UNP P06331
H	99	GLY	-	expression tag	UNP P06331
H	100	ALA	-	expression tag	UNP P06331
H	100A	ARG	-	expression tag	UNP P06331
H	100B	ILE	-	expression tag	UNP P06331
H	100C	SER	-	expression tag	UNP P06331
H	100D	GLY	-	expression tag	UNP P06331
H	100E	ARG	-	expression tag	UNP P06331
H	100F	ASN	-	expression tag	UNP P06331
H	100G	TRP	-	expression tag	UNP P06331
H	100H	PHE	-	expression tag	UNP P06331
H	101	ASP	-	expression tag	UNP P06331
H	102	PRO	-	expression tag	UNP P06331
H	103	TRP	-	expression tag	UNP P06331
H	104	GLY	-	expression tag	UNP P06331
H	105	GLN	-	expression tag	UNP P06331
H	106	GLY	-	expression tag	UNP P06331
H	107	SER	-	expression tag	UNP P06331
H	108	LEU	-	expression tag	UNP P06331
H	109	VAL	-	expression tag	UNP P06331
H	110	THR	-	expression tag	UNP P06331
H	111	VAL	-	expression tag	UNP P06331
H	112	SER	-	expression tag	UNP P06331

- Molecule 9 is a protein called A12K Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	107	Total	C	N	O	S	0	0
			815	514	140	158	3		

- Molecule 10 is a protein called Immunoglobulin kappa variable 1-39.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	107	Total	C	N	O	S	0	0
			821	513	139	166	3		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	31	THR	SER	conflict	UNP P01597
J	37	ARG	GLN	conflict	UNP P01597
J	45	SER	LYS	conflict	UNP P01597
J	51	ILE	ALA	conflict	UNP P01597
J	56	THR	SER	conflict	UNP P01597
J	76	ASN	SER	conflict	UNP P01597
J	77	ASN	SER	conflict	UNP P01597
J	92	PHE	TYR	conflict	UNP P01597
J	96	ARG	-	expression tag	UNP P01597
J	97	THR	-	expression tag	UNP P01597
J	98	PHE	-	expression tag	UNP P01597
J	99	GLY	-	expression tag	UNP P01597
J	100	GLN	-	expression tag	UNP P01597
J	101	GLY	-	expression tag	UNP P01597
J	102	THR	-	expression tag	UNP P01597
J	103	LYS	-	expression tag	UNP P01597
J	104	VAL	-	expression tag	UNP P01597
J	105	GLU	-	expression tag	UNP P01597
J	106	ILE	-	expression tag	UNP P01597
J	107	LYS	-	expression tag	UNP P01597

- Molecule 11 is a protein called Immunoglobulin heavy variable 4-39.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	121	Total	C	N	O	S	0	0
			941	600	152	186	3		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	2	VAL	LEU	conflict	UNP P01824
K	27	ALA	GLY	conflict	UNP P01824
K	33	GLY	SER	conflict	UNP P01824
K	40	SER	PRO	conflict	UNP P01824
K	50	THR	SER	conflict	UNP P01824
K	75	ASN	LYS	conflict	UNP P01824
K	80	MET	LEU	conflict	UNP P01824

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Chain	Residue	Modelled	Actual	Comment	Reference
K	93	VAL	ALA	conflict	UNP P01824
K	95	ARG	-	expression tag	UNP P01824
K	96	VAL	-	expression tag	UNP P01824
K	97	THR	-	expression tag	UNP P01824
K	98	TYR	-	expression tag	UNP P01824
K	99	THR	-	expression tag	UNP P01824
K	100	LYS	-	expression tag	UNP P01824
K	100A	THR	-	expression tag	UNP P01824
K	100B	TRP	-	expression tag	UNP P01824
K	100C	ALA	-	expression tag	UNP P01824
K	100D	PHE	-	expression tag	UNP P01824
K	101	ASP	-	expression tag	UNP P01824
K	102	TYR	-	expression tag	UNP P01824
K	103	TRP	-	expression tag	UNP P01824
K	104	GLY	-	expression tag	UNP P01824
K	105	GLN	-	expression tag	UNP P01824
K	106	GLY	-	expression tag	UNP P01824
K	107	THR	-	expression tag	UNP P01824
K	108	LEU	-	expression tag	UNP P01824
K	109	VAL	-	expression tag	UNP P01824
K	110	THR	-	expression tag	UNP P01824
K	111	VAL	-	expression tag	UNP P01824
K	112	SER	-	expression tag	UNP P01824

- Molecule 12 is a protein called B5L Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	108	Total	C	N	O	S	0	0
			795	494	134	165	2		

- Molecule 13 is a protein called C5K Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	106	Total	C	N	O	S	0	0
			832	526	137	165	4		

- Molecule 14 is a protein called Immunoglobulin heavy variable 1-46.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	121	Total	C	N	O	S	0	0
			920	574	163	178	5		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	27	ASP	TYR	conflict	UNP P01743
N	29	LEU	PHE	conflict	UNP P01743
N	30	ARG	THR	conflict	UNP P01743
N	31	ARG	SER	conflict	UNP P01743
N	34	ILE	MET	conflict	UNP P01743
N	58	THR	SER	conflict	UNP P01743
N	68	SER	THR	conflict	UNP P01743
N	82A	ARG	SER	conflict	UNP P01743
N	85	ASP	GLU	conflict	UNP P01743
N	95	GLY	-	expression tag	UNP P01743
N	96	GLY	-	expression tag	UNP P01743
N	97	PRO	-	expression tag	UNP P01743
N	98	THR	-	expression tag	UNP P01743
N	99	VAL	-	expression tag	UNP P01743
N	100	VAL	-	expression tag	UNP P01743
N	100A	VAL	-	expression tag	UNP P01743
N	100B	VAL	-	expression tag	UNP P01743
N	100C	ALA	-	expression tag	UNP P01743
N	100D	ALA	-	expression tag	UNP P01743
N	100E	THR	-	expression tag	UNP P01743
N	100F	PRO	-	expression tag	UNP P01743
N	100G	PHE	-	expression tag	UNP P01743
N	101	ASP	-	expression tag	UNP P01743
N	102	ASP	-	expression tag	UNP P01743
N	103	TRP	-	expression tag	UNP P01743
N	104	GLY	-	expression tag	UNP P01743
N	105	GLN	-	expression tag	UNP P01743
N	106	GLY	-	expression tag	UNP P01743
N	107	THR	-	expression tag	UNP P01743
N	108	LEU	-	expression tag	UNP P01743
N	109	VAL	-	expression tag	UNP P01743
N	110	THR	-	expression tag	UNP P01743
N	111	VAL	-	expression tag	UNP P01743
N	112	SER	-	expression tag	UNP P01743

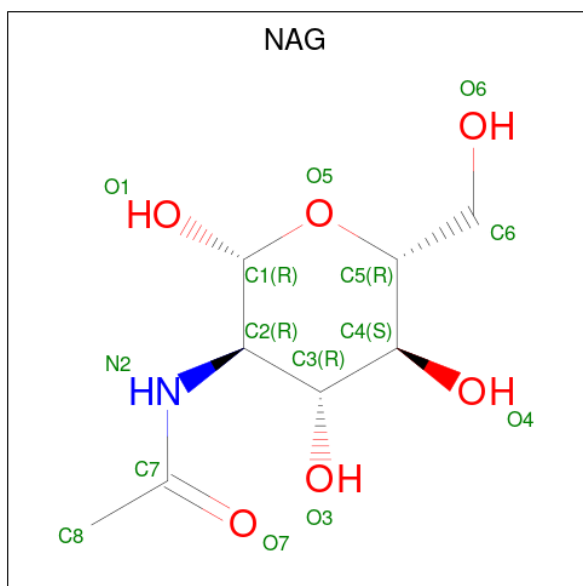
- Molecule 15 is a protein called C4K Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	119	Total	C	N	O	S	0	0
			926	580	165	177	4		

- Molecule 16 is a protein called C4K Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	108	Total	C	N	O	S	0	0
			825	518	146	159	2		

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

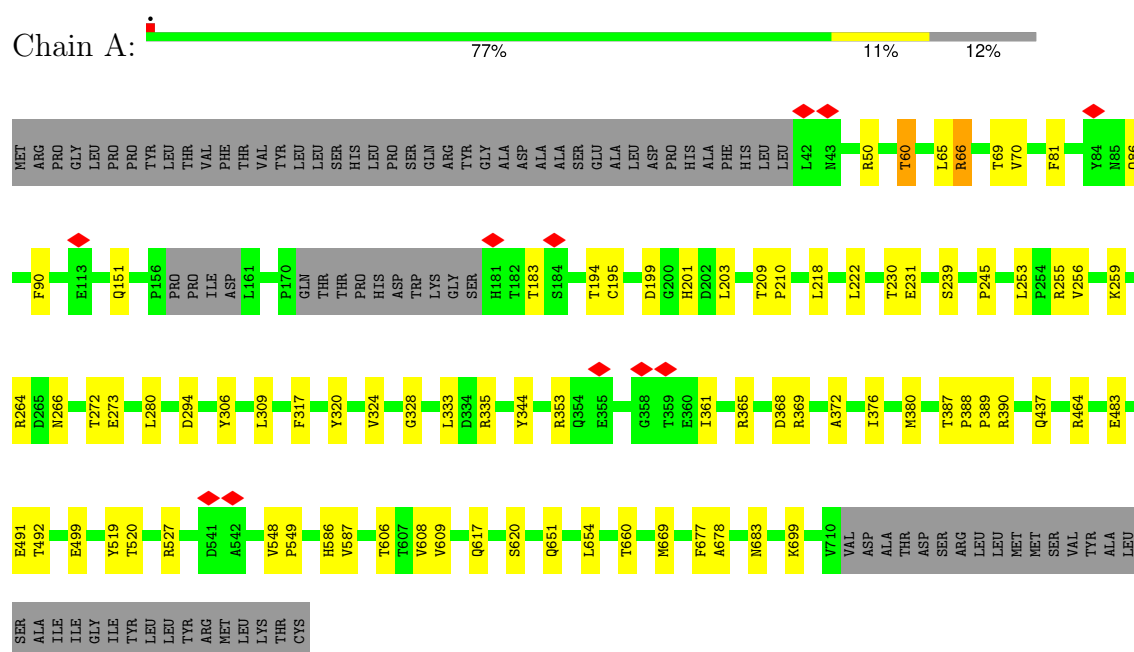


Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	B	1	Total	C	N	O	0
			14	8	1	5	

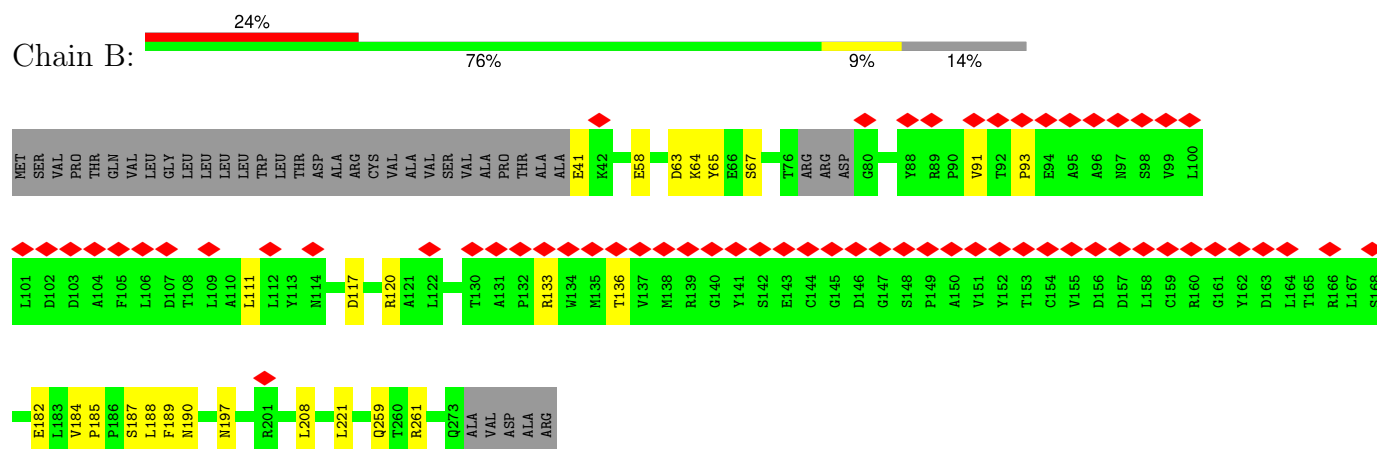
3 Residue-property plots

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: Envelope glycoprotein H

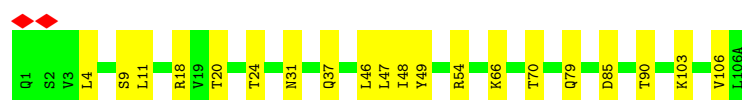


• Molecule 2: Envelope glycoprotein L




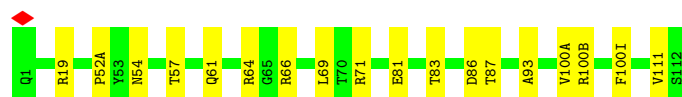
• Molecule 3: Immunoglobulin lambda variable 1-51

Chain C:  82% 18%



- Molecule 4: G1L Fab heavy chain

Chain D:  86% 14%



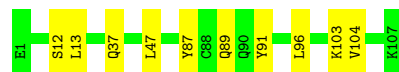
- Molecule 5: Immunoglobulin heavy variable 1-46

Chain E:  90% 10%



- Molecule 6: Immunoglobulin kappa variable 3-20

Chain F:  91% 9%




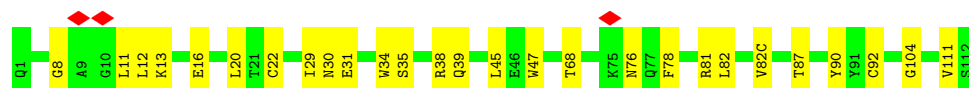
- Molecule 7: A12K Fab heavy chain

Chain G:  93% 7%



- Molecule 8: Immunoglobulin heavy variable 4-34

Chain H:  78% 22%



- Molecule 9: A12K Fab light chain

Chain I:  96% ..



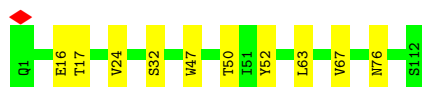
- Molecule 10: Immunoglobulin kappa variable 1-39

Chain J:  96% .




- Molecule 11: Immunoglobulin heavy variable 4-39

Chain K:  92% 8% .




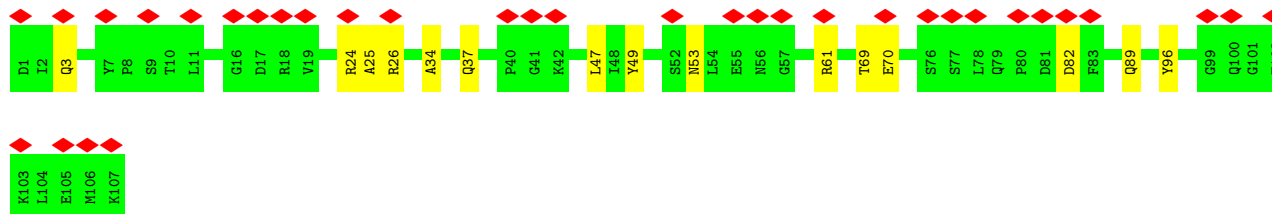
- Molecule 12: B5L Fab light chain

Chain L:  89% 9% .




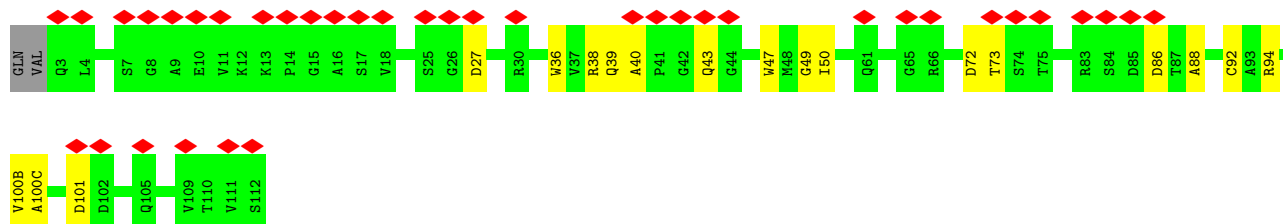
- Molecule 13: C5K Fab light chain

Chain M:  32% 86% 14% .




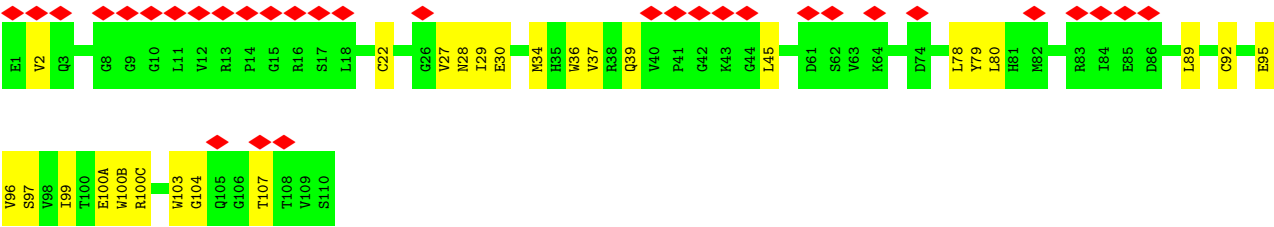
- Molecule 14: Immunoglobulin heavy variable 1-46

Chain N:  31% 84% 15% .

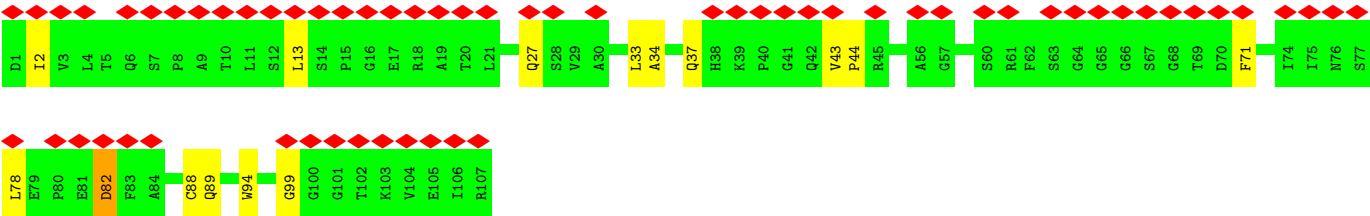
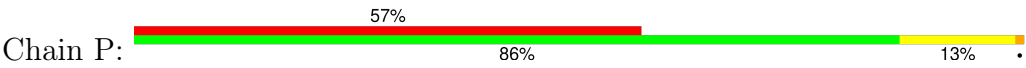


- Molecule 15: C4K Fab heavy chain

Chain O:  27% 78% 22% .



● Molecule 16: C4K Fab light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.684	Depositor
Minimum map value	-0.286	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	376.0, 376.0, 376.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.94, 0.94, 0.94	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/5376	0.43	0/7321
2	B	0.14	0/1863	0.35	0/2543
3	C	0.15	0/829	0.32	0/1131
4	D	0.16	0/995	0.28	0/1348
5	E	0.16	0/949	0.31	0/1283
6	F	0.15	0/831	0.33	0/1125
7	G	0.15	0/935	0.32	0/1262
8	H	0.16	0/995	0.36	0/1355
9	I	0.15	0/836	0.35	0/1135
10	J	0.14	0/838	0.30	0/1136
11	K	0.15	0/966	0.29	0/1318
12	L	0.15	0/813	0.31	0/1106
13	M	0.15	0/852	0.35	0/1152
14	N	0.14	0/939	0.31	0/1274
15	O	0.16	0/945	0.38	0/1281
16	P	0.16	0/845	0.40	0/1146
All	All	0.19	0/19807	0.36	0/26916

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5256	0	5208	56	0
2	B	1819	0	1813	18	0
3	C	812	0	797	11	0
4	D	969	0	951	10	0
5	E	929	0	904	8	0
6	F	814	0	796	7	0
7	G	913	0	897	5	0
8	H	967	0	930	18	0
9	I	815	0	796	2	0
10	J	821	0	804	2	0
11	K	941	0	911	5	0
12	L	795	0	756	6	0
13	M	832	0	803	10	0
14	N	920	0	904	12	0
15	O	926	0	908	26	0
16	P	825	0	804	12	0
17	A	28	0	26	0	0
17	B	14	0	13	0	0
All	All	19396	0	19021	197	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 5.

All (197) 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:C:46:LEU:HD21	3:C:49:TYR:HB3	1.56	0.88
1:A:272:THR:HG22	1:A:273:GLU:H	1.50	0.77
13:M:34:ALA:HB3	13:M:89:GLN:HE21	1.50	0.76
1:A:256:VAL:O	1:A:264:ARG:NH2	2.20	0.75
1:A:328:GLY:O	4:D:54:ASN:ND2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HD3	1:A:70:VAL:HG22	1.71	0.73
14:N:47:TRP:HZ2	14:N:50:ILE:HG23	1.53	0.72
2:B:58:GLU:HA	15:O:99:ILE:HD11	1.72	0.71
15:O:29:ILE:HG21	15:O:34:MET:CE	2.21	0.71
1:A:365:ARG:NH2	1:A:368:ASP:OD2	2.25	0.70
12:L:38:GLN:NE2	12:L:42:LYS:O	2.25	0.69
1:A:464:ARG:NH2	1:A:499:GLU:OE2	2.26	0.68
11:K:32:SER:O	11:K:52:TYR:OH	2.10	0.68
1:A:464:ARG:NH1	1:A:519:TYR:O	2.28	0.67
3:C:85:ASP:OD1	3:C:103:LYS:NZ	2.23	0.67
14:N:47:TRP:CZ2	14:N:50:ILE:HG23	2.30	0.67
1:A:491:GLU:OE2	1:A:519:TYR:OH	2.14	0.66
1:A:677:PHE:O	1:A:683:ASN:ND2	2.29	0.66
15:O:29:ILE:HG21	15:O:34:MET:HE3	1.78	0.64
4:D:61:GLN:OE1	4:D:64:ARG:NH1	2.31	0.64
3:C:31:ASN:O	3:C:66:LYS:NZ	2.31	0.64
2:B:91:VAL:HG22	2:B:93:PRO:HD2	1.80	0.64
1:A:651:GLN:HB2	1:A:699:LYS:HD3	1.81	0.63
12:L:54:ARG:NH1	12:L:62:PHE:O	2.31	0.62
15:O:34:MET:SD	15:O:78:LEU:HB2	2.40	0.62
7:G:52:SER:O	7:G:71:ARG:NH1	2.32	0.62
11:K:24:VAL:O	11:K:76:ASN:ND2	2.32	0.62
1:A:203:LEU:HD12	1:A:280:LEU:HD23	1.81	0.62
1:A:587:VAL:HG13	1:A:617:GLN:HE21	1.65	0.62
8:H:39:GLN:HB2	8:H:45:LEU:HD23	1.81	0.61
6:F:37:GLN:HB2	6:F:47:LEU:HD11	1.83	0.60
8:H:8:GLY:HA3	8:H:20:LEU:HD23	1.84	0.60
1:A:654:LEU:HB2	1:A:669:MET:HE3	1.82	0.60
11:K:47:TRP:HE1	11:K:50:THR:HG23	1.67	0.59
15:O:29:ILE:HG22	15:O:29:ILE:O	2.03	0.59
4:D:66:ARG:NH2	4:D:86:ASP:OD2	2.36	0.58
5:E:87:THR:HG23	5:E:110:THR:HA	1.85	0.58
15:O:89:LEU:HD12	15:O:107:THR:O	2.03	0.58
14:N:40:ALA:HB3	14:N:43:GLN:HB2	1.86	0.57
1:A:499:GLU:OE1	1:A:520:THR:OG1	2.22	0.57
4:D:87:THR:HB	4:D:111:VAL:HG12	1.86	0.57
8:H:82:LEU:HD23	8:H:82(C):VAL:HG22	1.86	0.56
1:A:309:LEU:HD23	1:A:369:ARG:HD2	1.87	0.56
8:H:92:CYS:O	8:H:104:GLY:N	2.38	0.56
4:D:83:THR:O	4:D:111:VAL:HG11	2.06	0.55
8:H:82:LEU:CD2	8:H:82(C):VAL:HG22	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ASP:OD1	2:B:64:LYS:N	2.39	0.55
13:M:24:ARG:CZ	13:M:70:GLU:OE2	2.54	0.55
1:A:60:THR:HG21	1:A:90:PHE:HA	1.87	0.55
16:P:43:VAL:HG13	16:P:44:PRO:C	2.32	0.55
16:P:88:CYS:O	16:P:99:GLY:N	2.39	0.54
1:A:317:PHE:CD2	1:A:376:ILE:HD12	2.43	0.54
3:C:4:LEU:HD11	3:C:90:THR:HG22	1.90	0.54
15:O:29:ILE:HG21	15:O:34:MET:HE2	1.89	0.54
8:H:30:ASN:O	8:H:30:ASN:ND2	2.41	0.53
1:A:201:HIS:O	1:A:259:LYS:NZ	2.41	0.53
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.89	0.53
1:A:230:THR:HG22	1:A:231:GLU:H	1.73	0.53
4:D:19:ARG:HG3	4:D:81:GLU:HB2	1.90	0.53
10:J:33:LEU:HD13	10:J:71:PHE:CD1	2.44	0.53
2:B:117:ASP:OD2	2:B:120:ARG:NH1	2.41	0.53
13:M:61:ARG:NH1	13:M:82:ASP:OD2	2.42	0.53
13:M:96:TYR:OH	14:N:100(C):ALA:O	2.27	0.52
16:P:43:VAL:HG13	16:P:44:PRO:O	2.09	0.52
11:K:63:LEU:O	11:K:67:VAL:HG12	2.09	0.52
1:A:65:LEU:HD22	1:A:86:GLN:HG2	1.91	0.51
3:C:9:SER:O	3:C:11:LEU:HD12	2.11	0.51
1:A:272:THR:HG22	1:A:273:GLU:N	2.22	0.51
2:B:184:VAL:CG2	2:B:188:LEU:HB2	2.41	0.51
1:A:492:THR:HG23	1:A:527:ARG:HG2	1.94	0.50
1:A:194:THR:HA	1:A:210:PRO:HA	1.93	0.50
1:A:606:THR:HG23	1:A:606:THR:O	2.10	0.50
1:A:387:THR:HG22	1:A:388:PRO:HD2	1.92	0.50
15:O:34:MET:SD	15:O:78:LEU:HD22	2.51	0.50
12:L:61:ARG:NH1	12:L:82:ASP:OD2	2.34	0.50
8:H:30:ASN:O	8:H:30:ASN:CG	2.55	0.49
1:A:209:THR:CG2	1:A:255:ARG:HH12	2.26	0.49
14:N:38:ARG:NH2	14:N:86:ASP:OD1	2.42	0.49
15:O:22:CYS:O	15:O:78:LEU:N	2.44	0.49
2:B:182:GLU:HB2	2:B:190:ASN:HB2	1.95	0.49
10:J:24:ARG:NE	10:J:70:ASP:OD2	2.39	0.49
1:A:586:HIS:O	1:A:620:SER:N	2.38	0.48
1:A:199:ASP:N	1:A:199:ASP:OD1	2.46	0.48
8:H:35:SER:OG	8:H:47:TRP:NE1	2.45	0.48
1:A:66:ARG:HH11	1:A:70:VAL:HG11	1.78	0.48
5:E:100(A):LEU:HB3	6:F:96:LEU:HD13	1.95	0.48
15:O:36:TRP:CG	15:O:80:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:25:ALA:O	13:M:69:THR:OG1	2.31	0.48
15:O:34:MET:SD	15:O:78:LEU:HD13	2.54	0.48
16:P:82:ASP:N	16:P:82:ASP:OD1	2.47	0.48
15:O:100(A):GLU:HG3	15:O:100(B):TRP:CD1	2.49	0.48
1:A:66:ARG:HE	1:A:70:VAL:HG21	1.78	0.47
1:A:294:ASP:OD2	1:A:335:ARG:NH1	2.43	0.47
8:H:87:THR:HB	8:H:111:VAL:HG22	1.96	0.47
12:L:47:ILE:HG22	12:L:48:ILE:HG12	1.96	0.47
15:O:103:TRP:HB2	16:P:43:VAL:HG22	1.95	0.47
8:H:29:ILE:HD12	8:H:76:ASN:HA	1.97	0.47
2:B:67:SER:HB2	14:N:100(B):VAL:HG21	1.95	0.47
1:A:437:GLN:NE2	1:A:483:GLU:OE2	2.42	0.47
12:L:48:ILE:HG22	12:L:50:ASP:O	2.15	0.47
4:D:93:ALA:HB1	4:D:100(I):PHE:HB3	1.98	0.46
5:E:43:GLN:O	6:F:87:TYR:OH	2.20	0.46
7:G:82:MET:HB3	7:G:82(C):LEU:HD21	1.97	0.46
14:N:27:ASP:OD2	14:N:94:ARG:NE	2.48	0.46
16:P:13:LEU:HD23	16:P:78:LEU:HD22	1.98	0.46
4:D:100(A):VAL:HG23	4:D:100(B):ARG:H	1.80	0.46
15:O:28:ASN:ND2	15:O:30:GLU:OE1	2.48	0.46
3:C:85:ASP:OD1	3:C:103:LYS:CE	2.63	0.46
5:E:30:THR:HG21	5:E:73:ARG:CZ	2.46	0.46
2:B:65:TYR:O	2:B:67:SER:N	2.50	0.45
8:H:82(C):VAL:HG12	8:H:111:VAL:HG11	1.97	0.45
3:C:48:ILE:HD13	3:C:54:ARG:HG2	1.98	0.45
15:O:95:GLU:OE2	15:O:100(C):ARG:HA	2.15	0.45
1:A:548:VAL:CG2	1:A:549:PRO:HD3	2.47	0.45
15:O:28:ASN:OD1	15:O:30:GLU:OE1	2.34	0.45
15:O:37:VAL:HG11	15:O:103:TRP:CZ3	2.52	0.45
2:B:189:PHE:HE2	2:B:221:LEU:HD23	1.81	0.45
8:H:13:LYS:N	8:H:16:GLU:OE1	2.38	0.44
14:N:36:TRP:CZ3	14:N:92:CYS:HB3	2.52	0.44
1:A:81:PHE:HB2	2:B:184:VAL:HG12	1.99	0.44
1:A:230:THR:HG22	1:A:231:GLU:N	2.30	0.44
8:H:22:CYS:HB3	8:H:78:PHE:HB2	1.98	0.44
16:P:33:LEU:HD22	16:P:71:PHE:CG	2.52	0.44
16:P:33:LEU:HD22	16:P:71:PHE:CD1	2.52	0.44
13:M:3:GLN:HB3	13:M:26:ARG:HG3	2.00	0.44
1:A:151:GLN:O	1:A:365:ARG:NH1	2.50	0.44
15:O:28:ASN:OD1	15:O:30:GLU:CD	2.61	0.44
8:H:68:THR:HB	8:H:81:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:78:LEU:HG	15:O:79:TYR:N	2.33	0.44
5:E:82(C):LEU:HD23	5:E:111:VAL:HG22	2.00	0.44
14:N:72:ASP:OD1	14:N:73:THR:N	2.51	0.44
1:A:266:ASN:ND2	2:B:259:GLN:OE1	2.50	0.43
1:A:388:PRO:O	1:A:390:ARG:N	2.50	0.43
2:B:111:LEU:O	2:B:197:ASN:ND2	2.51	0.43
1:A:372:ALA:O	1:A:376:ILE:HG12	2.18	0.43
2:B:184:VAL:HG22	2:B:188:LEU:HB2	1.99	0.43
1:A:669:MET:HE2	1:A:678:ALA:HB3	1.99	0.43
1:A:222:LEU:H	1:A:222:LEU:HD23	1.84	0.43
7:G:20:LEU:HG	7:G:82:MET:HE2	2.00	0.43
15:O:95:GLU:HG3	15:O:96:VAL:H	1.84	0.43
1:A:253:LEU:O	1:A:253:LEU:HG	2.19	0.43
5:E:13:LYS:HG3	5:E:14:PRO:HD2	2.01	0.43
6:F:89:GLN:NE2	6:F:96:LEU:HD11	2.33	0.43
13:M:37:GLN:HB3	13:M:47:LEU:HD11	2.00	0.43
1:A:218:LEU:O	1:A:387:THR:OG1	2.37	0.43
1:A:231:GLU:O	1:A:353:ARG:NH2	2.35	0.43
1:A:608:VAL:HG12	1:A:609:VAL:N	2.34	0.43
2:B:41:GLU:N	2:B:41:GLU:OE1	2.52	0.43
7:G:28:THR:HG23	7:G:28:THR:O	2.19	0.43
7:G:40:SER:HB3	7:G:88:ALA:HB2	2.01	0.43
8:H:34:TRP:CG	8:H:78:PHE:CZ	3.07	0.43
2:B:133:ARG:O	2:B:136:THR:OG1	2.34	0.42
13:M:3:GLN:HB3	13:M:26:ARG:CD	2.49	0.42
15:O:39:GLN:HB2	15:O:45:LEU:HD23	2.01	0.42
13:M:49:TYR:CZ	13:M:53:ASN:HB3	2.54	0.42
6:F:89:GLN:HE22	6:F:91:TYR:HB3	1.85	0.42
8:H:38:ARG:HD3	8:H:90:TYR:CZ	2.54	0.42
1:A:218:LEU:HD22	1:A:333:LEU:HD23	2.01	0.42
9:I:24:ARG:HG3	9:I:70:GLU:HG2	2.02	0.42
8:H:11:LEU:C	8:H:12:LEU:HD12	2.45	0.42
1:A:183:THR:N	1:A:361:ILE:O	2.43	0.41
11:K:16:GLU:HG3	11:K:17:THR:H	1.85	0.41
12:L:50:ASP:O	12:L:51:VAL:C	2.63	0.41
15:O:96:VAL:HG12	15:O:97:SER:H	1.84	0.41
4:D:52(A):PRO:HA	4:D:71:ARG:HD3	2.02	0.41
15:O:99:ILE:HD12	16:P:94:TRP:CE2	2.56	0.41
1:A:608:VAL:HG21	1:A:660:THR:HG22	2.02	0.41
6:F:103:LYS:NZ	6:F:104:VAL:O	2.51	0.41
8:H:29:ILE:O	8:H:31:GLU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:81:GLU:OE1	9:I:81:GLU:N	2.50	0.41
14:N:39:GLN:O	14:N:88:ALA:HB1	2.20	0.41
1:A:387:THR:HG22	1:A:389:PRO:HD2	2.02	0.41
2:B:208:LEU:HD12	2:B:208:LEU:O	2.19	0.41
2:B:261:ARG:NE	5:E:52:ASP:OD2	2.53	0.41
4:D:57:THR:HG21	4:D:69:LEU:HB2	2.03	0.41
1:A:317:PHE:CZ	1:A:376:ILE:HG23	2.56	0.41
1:A:320:TYR:O	1:A:324:VAL:HG13	2.20	0.41
13:M:34:ALA:HB3	13:M:89:GLN:NE2	2.26	0.41
15:O:92:CYS:O	15:O:104:GLY:N	2.54	0.41
16:P:34:ALA:O	16:P:89:GLN:N	2.51	0.41
16:P:37:GLN:O	16:P:44:PRO:HB2	2.21	0.41
1:A:317:PHE:CE2	1:A:376:ILE:HD12	2.55	0.41
1:A:344:TYR:CD2	1:A:380:MET:HE2	2.56	0.41
3:C:18:ARG:HH12	3:C:20:THR:CG2	2.34	0.41
3:C:79:GLN:O	3:C:106:VAL:HG21	2.21	0.41
15:O:2:VAL:HG13	15:O:27:VAL:HB	2.02	0.41
1:A:272:THR:HG21	1:A:306:TYR:HE2	1.86	0.41
2:B:185:PRO:O	2:B:187:SER:N	2.45	0.40
14:N:94:ARG:NH2	14:N:101:ASP:OD2	2.47	0.40
6:F:12:SER:C	6:F:13:LEU:HD12	2.46	0.40
14:N:47:TRP:CZ2	14:N:49:GLY:HA2	2.56	0.40
1:A:239:SER:HB2	1:A:245:PRO:HB3	2.03	0.40
3:C:24:THR:HG23	3:C:70:THR:HG22	2.03	0.40
15:O:29:ILE:O	15:O:29:ILE:CG2	2.68	0.40
16:P:2:ILE:HG12	16:P:27:GLN:HB2	2.02	0.40
1:A:548:VAL:HG23	1:A:549:PRO:HD3	2.03	0.40
5:E:30:THR:HB	5:E:53:SER:HB3	2.02	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	649/743 (87%)	630 (97%)	19 (3%)	0	100	100
2	B	226/268 (84%)	223 (99%)	3 (1%)	0	100	100
3	C	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
4	D	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
5	E	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
6	F	106/108 (98%)	101 (95%)	5 (5%)	0	100	100
7	G	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
8	H	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
9	I	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
10	J	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
11	K	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
12	L	106/110 (96%)	102 (96%)	4 (4%)	0	100	100
13	M	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
14	N	119/123 (97%)	114 (96%)	5 (4%)	0	100	100
15	O	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
16	P	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
All	All	2445/2614 (94%)	2361 (97%)	84 (3%)	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	594/670 (89%)	591 (100%)	3 (0%)	81	85
2	B	200/230 (87%)	200 (100%)	0	100	100
3	C	93/93 (100%)	93 (100%)	0	100	100
4	D	99/99 (100%)	99 (100%)	0	100	100
5	E	100/100 (100%)	100 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	89/89 (100%)	89 (100%)	0	100	100
7	G	100/100 (100%)	100 (100%)	0	100	100
8	H	103/103 (100%)	103 (100%)	0	100	100
9	I	90/91 (99%)	90 (100%)	0	100	100
10	J	94/94 (100%)	94 (100%)	0	100	100
11	K	105/105 (100%)	105 (100%)	0	100	100
12	L	88/90 (98%)	88 (100%)	0	100	100
13	M	91/91 (100%)	91 (100%)	0	100	100
14	N	99/101 (98%)	99 (100%)	0	100	100
15	O	101/101 (100%)	101 (100%)	0	100	100
16	P	87/87 (100%)	86 (99%)	1 (1%)	65	79
All	All	2133/2244 (95%)	2129 (100%)	4 (0%)	85	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	69	THR
1	A	195	CYS
16	P	82	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	252	HIS
1	A	331	GLN
1	A	475	HIS
1	A	617	GLN
1	A	693	HIS
2	B	177	HIS
2	B	267	HIS
2	B	273	GLN
3	C	30	ASN
3	C	31	ASN
3	C	37	GLN
5	E	58	ASN

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Mol	Chain	Res	Type
5	E	98	ASN
7	G	6	GLN
7	G	39	GLN
8	H	76	ASN
9	I	38	GLN
10	J	3	GLN
10	J	38	GLN
11	K	39	GLN
12	L	79	GLN
13	M	89	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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	$\# Z > 2$
17	NAG	A	801	1	14,14,15	0.38	0	17,19,21	0.44	0
17	NAG	A	802	1	14,14,15	0.38	0	17,19,21	0.49	0
17	NAG	B	301	2	14,14,15	0.70	0	17,19,21	0.82	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
17	NAG	A	801	1	-	2/6/23/26	0/1/1/1
17	NAG	A	802	1	-	2/6/23/26	0/1/1/1
17	NAG	B	301	2	-	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.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	801	NAG	C8-C7-N2-C2
17	A	801	NAG	O7-C7-N2-C2
17	A	802	NAG	C8-C7-N2-C2
17	A	802	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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.

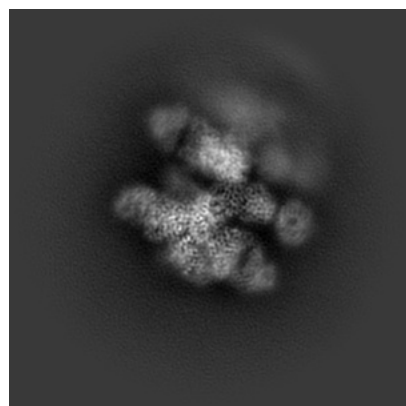
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72061. These allow visual inspection of the internal detail of the map and identification of artifacts.

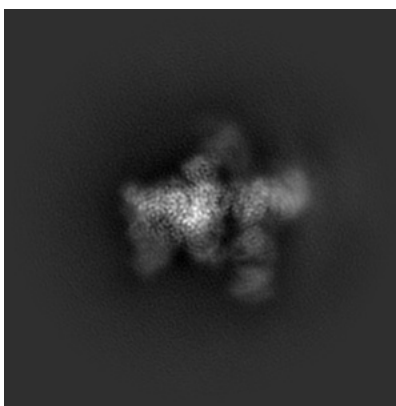
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

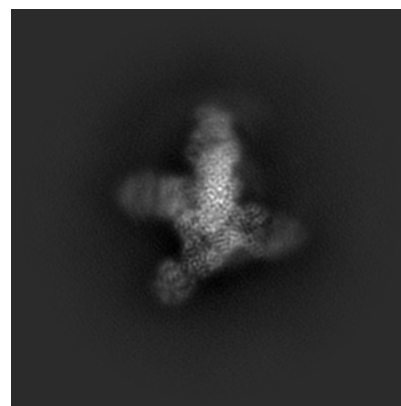
6.1.1 Primary map



X

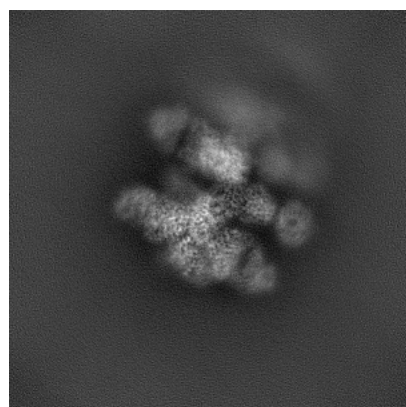


Y

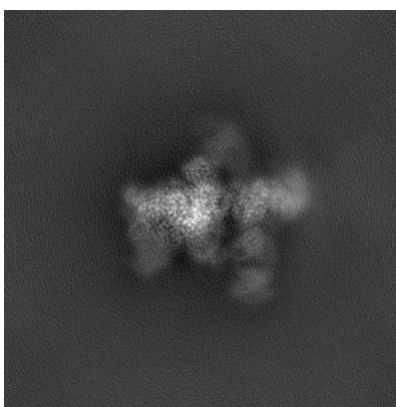


Z

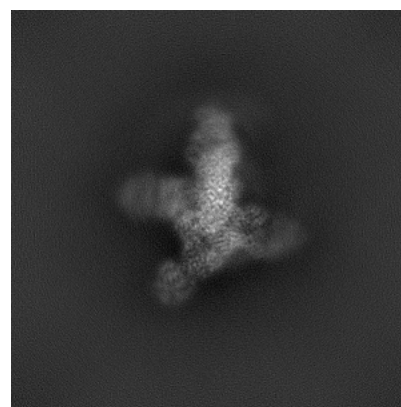
6.1.2 Raw map



X



Y

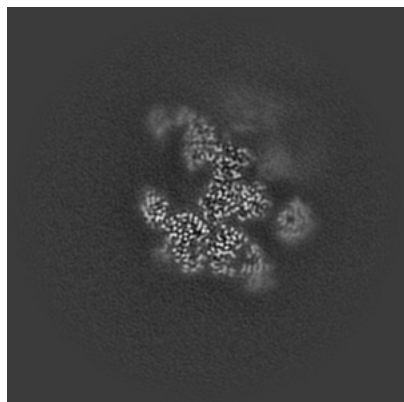


Z

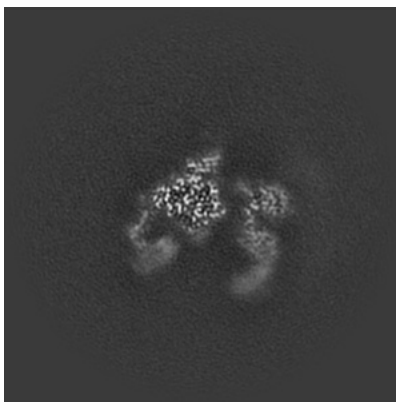
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

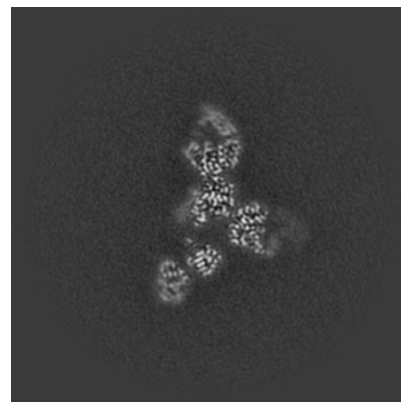
6.2.1 Primary map



X Index: 200

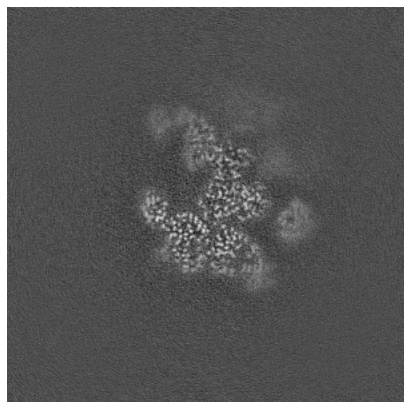


Y Index: 200

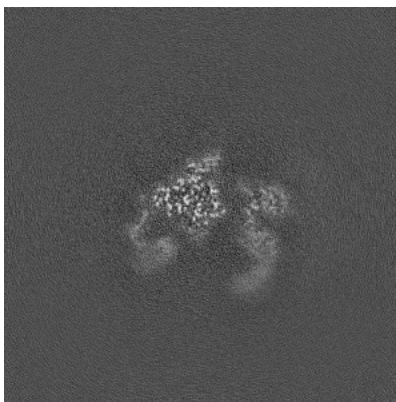


Z Index: 200

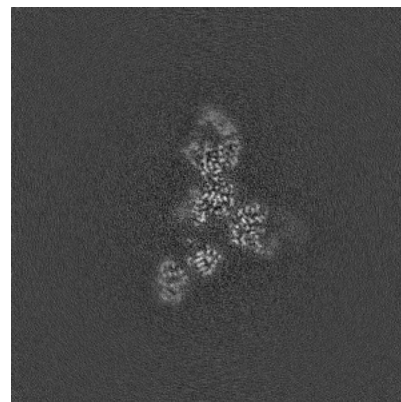
6.2.2 Raw map



X Index: 200



Y Index: 200

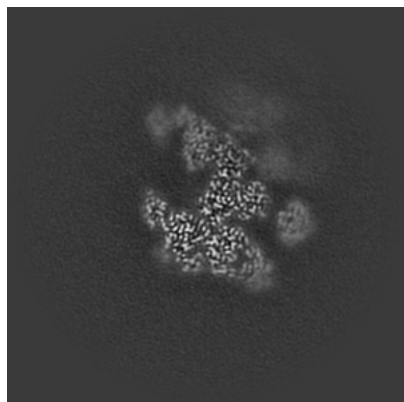


Z Index: 200

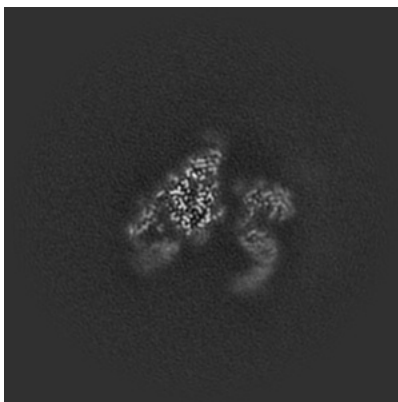
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

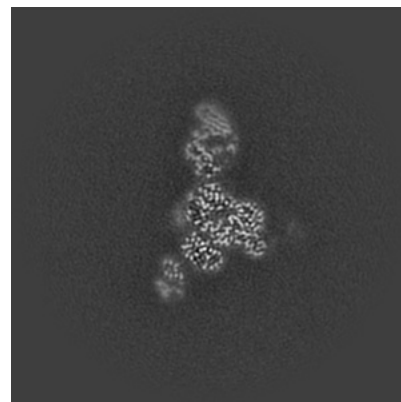
6.3.1 Primary map



X Index: 202

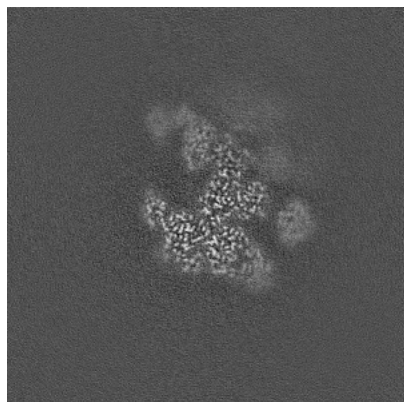


Y Index: 197

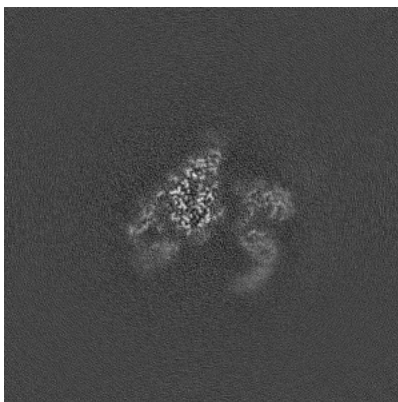


Z Index: 192

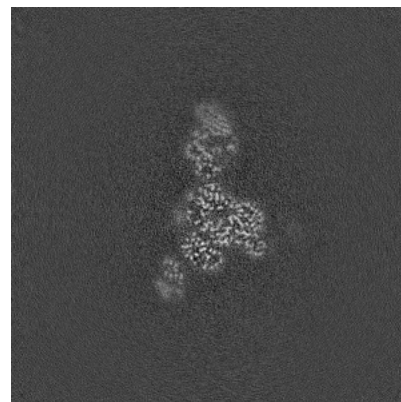
6.3.2 Raw map



X Index: 202



Y Index: 197

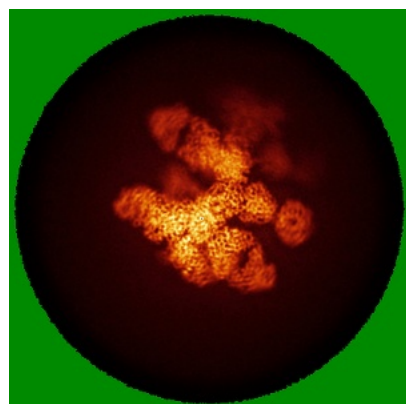


Z Index: 192

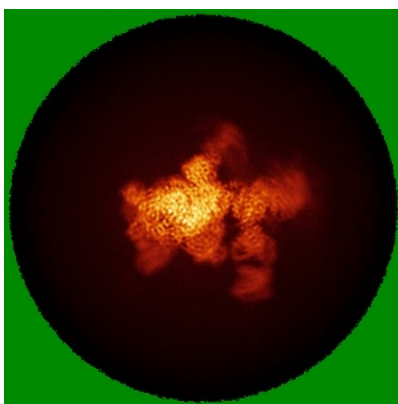
The images above show the largest variance slices of the map in three orthogonal directions.

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

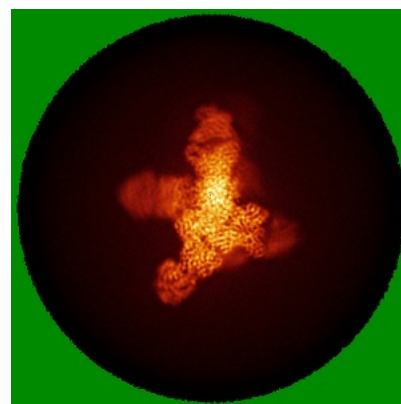
6.4.1 Primary map



X

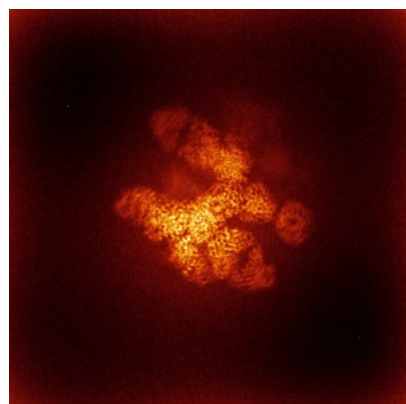


Y

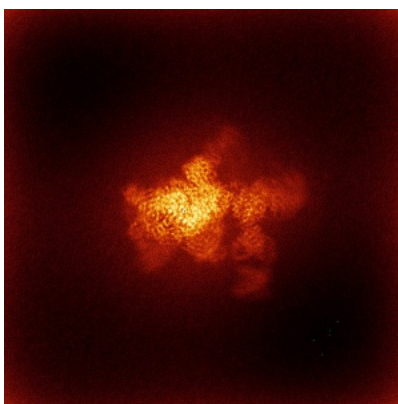


Z

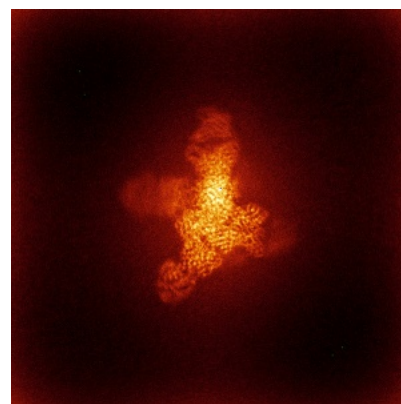
6.4.2 Raw map



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.

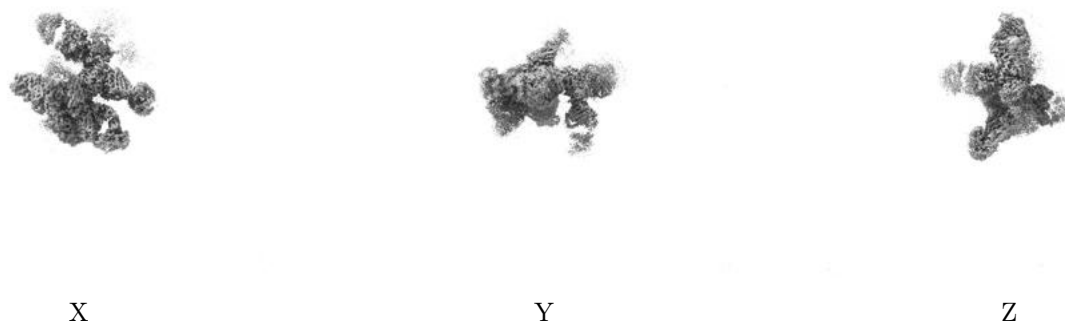
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

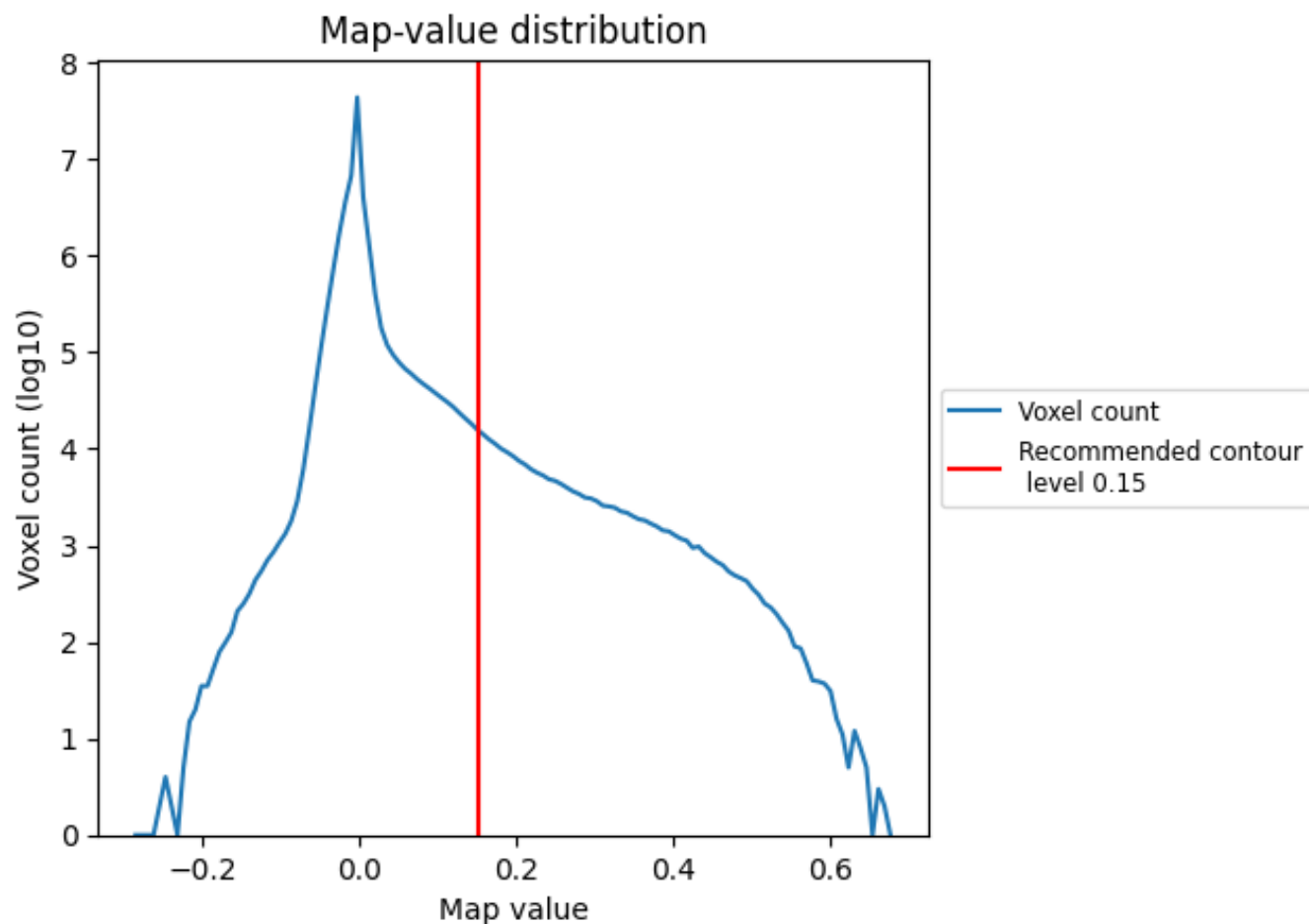
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

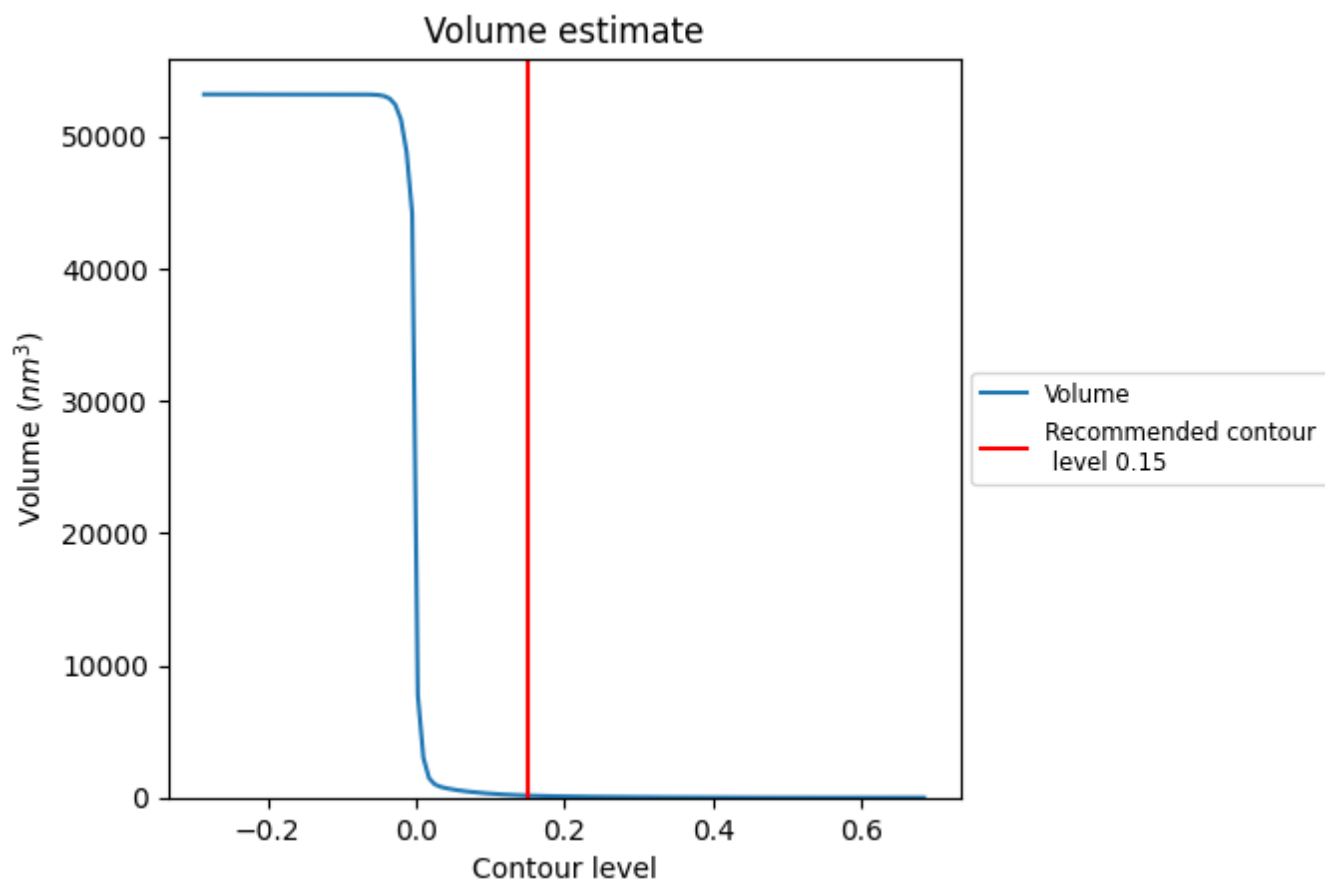
This section contains the results of statistical analysis of the map.

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.

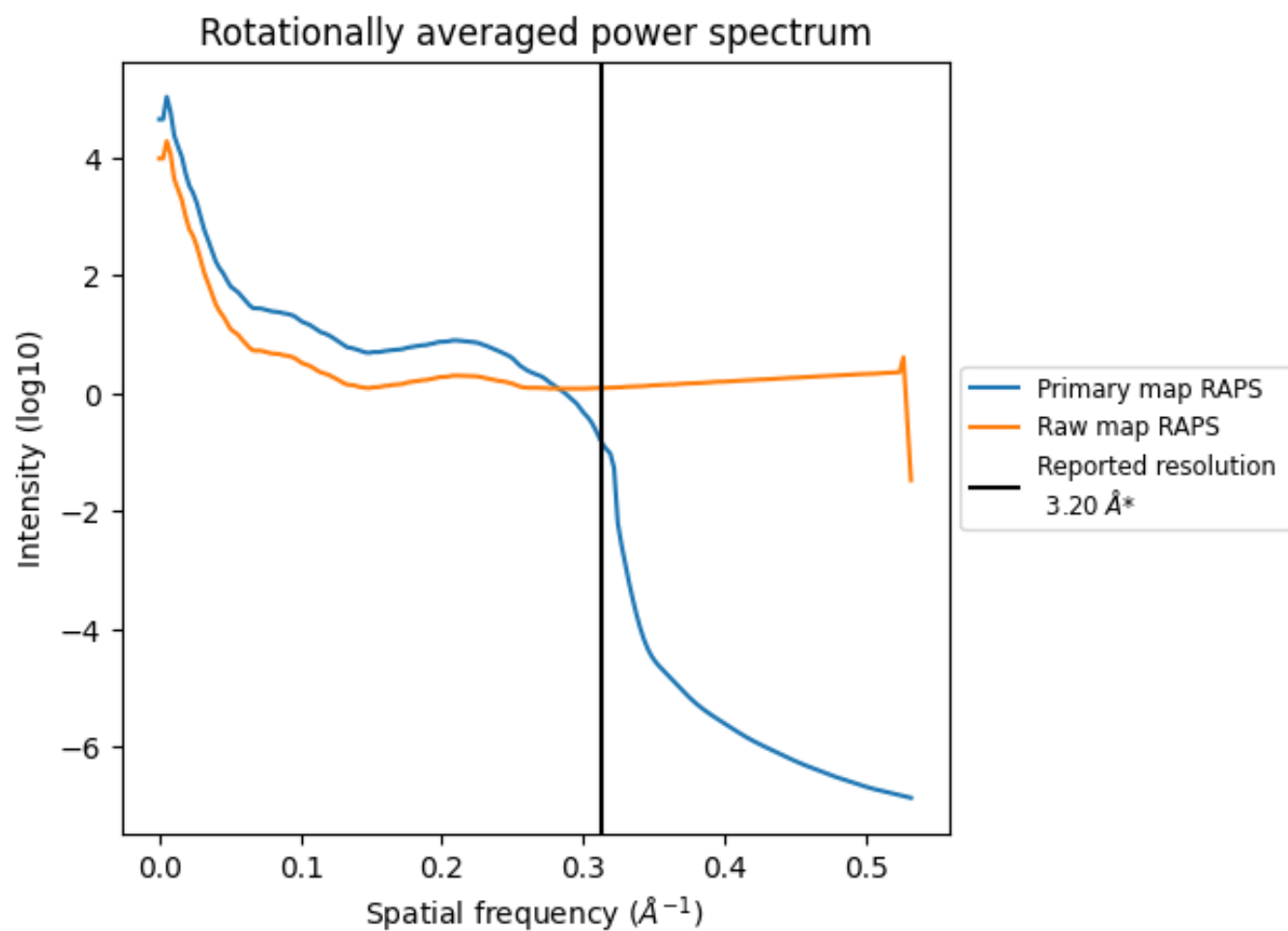
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm^3 ; this corresponds to an approximate mass of 137 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

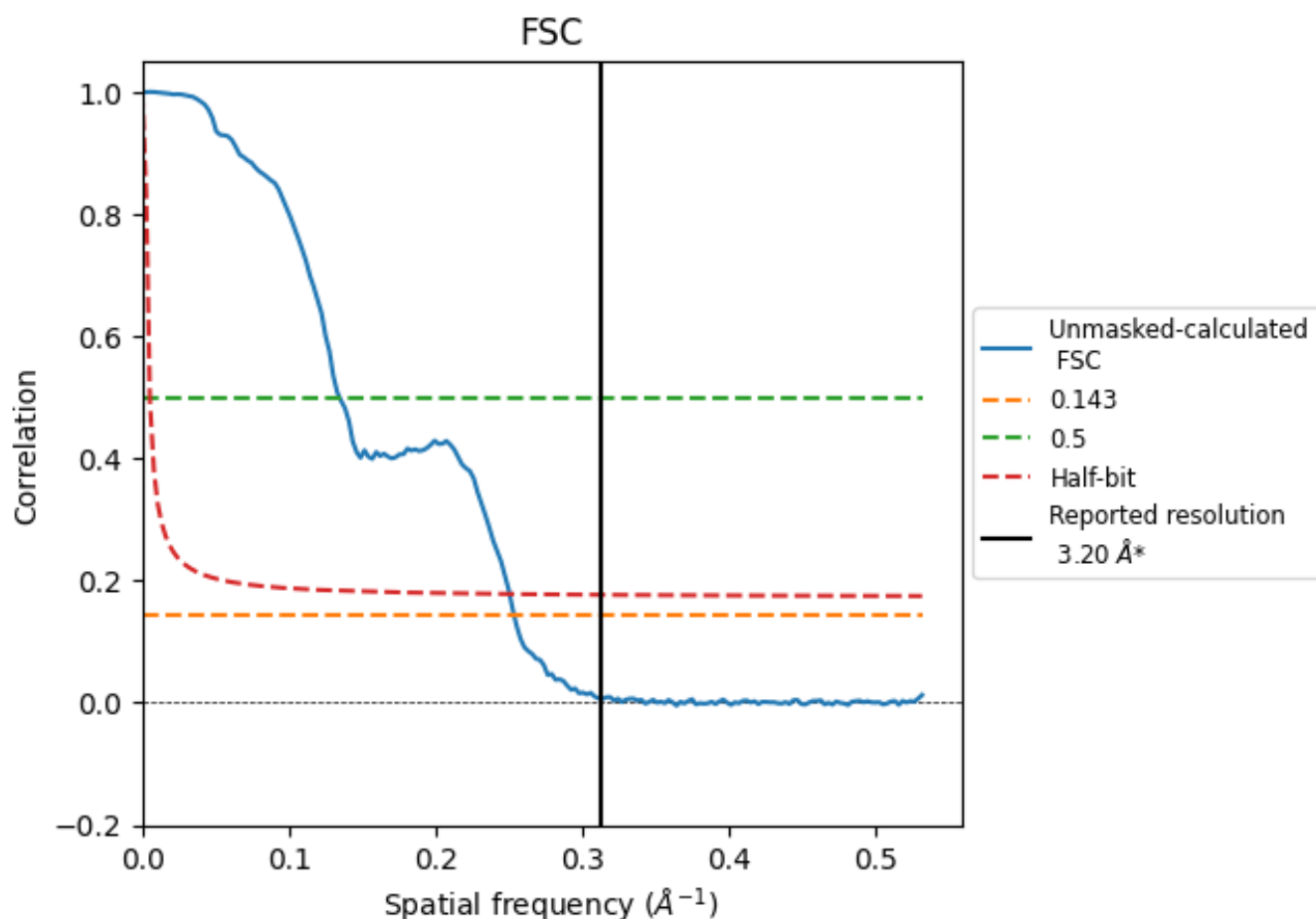


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

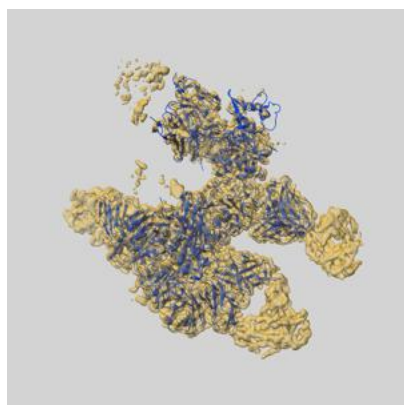
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	7.43	3.99

*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 3.94 differs from the reported value 3.2 by more than 10 %

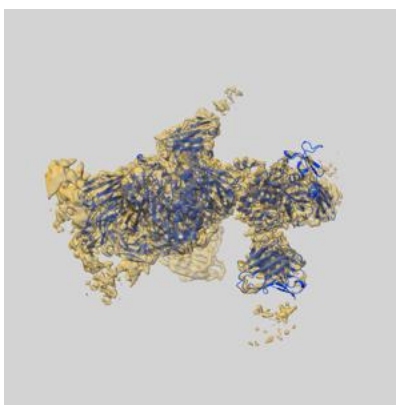
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72061 and PDB model 9PZC. Per-residue inclusion information can be found in section [3](#) on page [13](#).

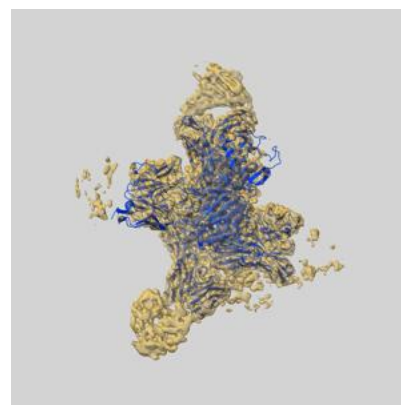
9.1 Map-model overlay [i](#)



X



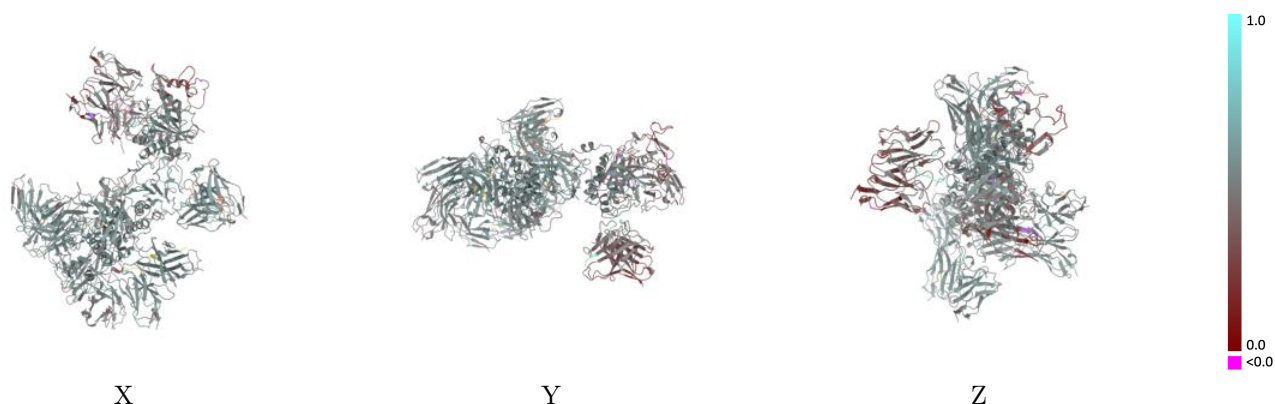
Y



Z

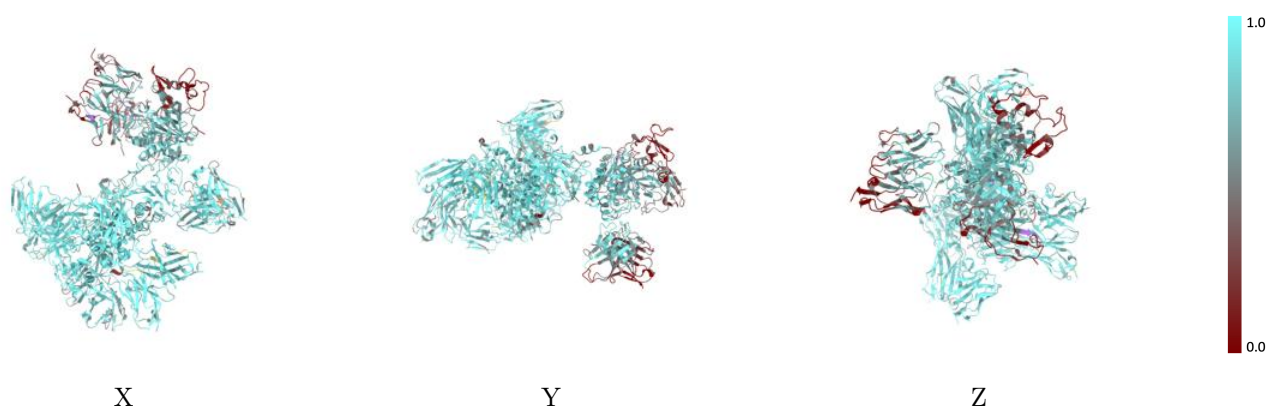
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



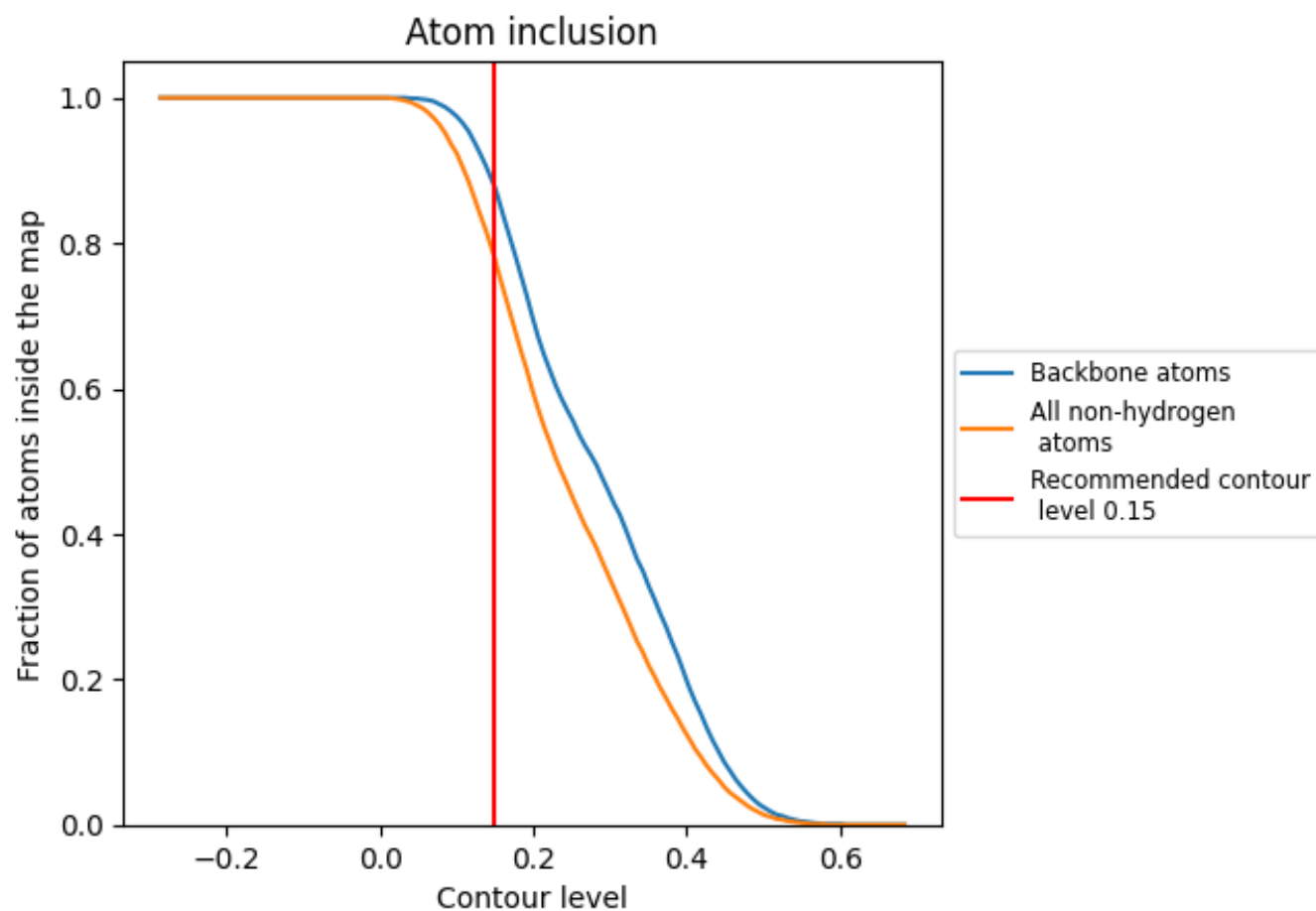
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.5080
A	 0.8740	 0.5430
B	 0.6050	 0.4730
C	 0.8570	 0.5260
D	 0.8700	 0.5320
E	 0.8140	 0.5340
F	 0.8090	 0.5260
G	 0.9050	 0.5540
H	 0.8220	 0.5050
I	 0.8860	 0.5400
J	 0.8930	 0.5420
K	 0.8870	 0.5510
L	 0.8950	 0.5440
M	 0.5340	 0.4370
N	 0.5540	 0.4290
O	 0.5640	 0.3940
P	 0.3830	 0.3560

