Full wwPDB EM Validation Report

Jul 16, 2024 – 04:20 PM JST

PDB ID	:	8W4F
EMDB ID	:	EMD-36904
Title	:	SARS-CoV-2 spike protein in complex with a trivalent nanobody
Authors	:	Jiang, X.Y.; Qian, J.Q.; Zhu, H.X.; Qin, Q.; Huang, Q.
Deposited on	:	2023-08-24
Resolution	:	4.20 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:

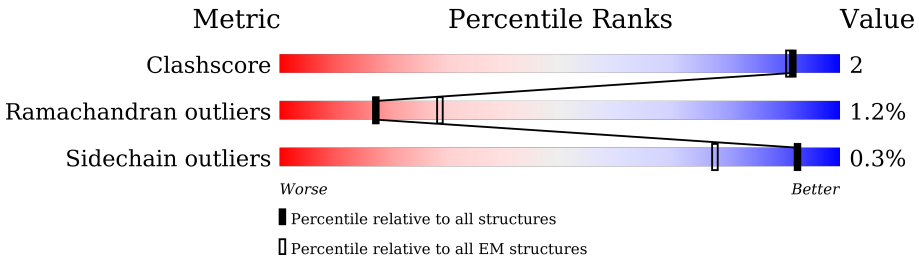
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1120	31% 92% 7%
1	B	1120	30% 92% 8%
1	C	1120	36% 92% 8%
2	D	197	65% 83% 15%
2	E	197	71% 86% 14%
2	F	197	67% 91% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 60429 atoms, of which 29841 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1120	Total	C	H	N	O	S	0	0
			17237	5560	8509	1460	1669	39		
1	B	1120	Total	C	H	N	O	S	0	0
			17237	5560	8509	1460	1669	39		
1	C	1120	Total	C	H	N	O	S	0	0
			17237	5560	8509	1460	1669	39		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	683	ALA	ARG	engineered mutation	UNP P0DTC2
A	685	ALA	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	683	ALA	ARG	engineered mutation	UNP P0DTC2
B	685	ALA	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	683	ALA	ARG	engineered mutation	UNP P0DTC2
C	685	ALA	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Tribody.

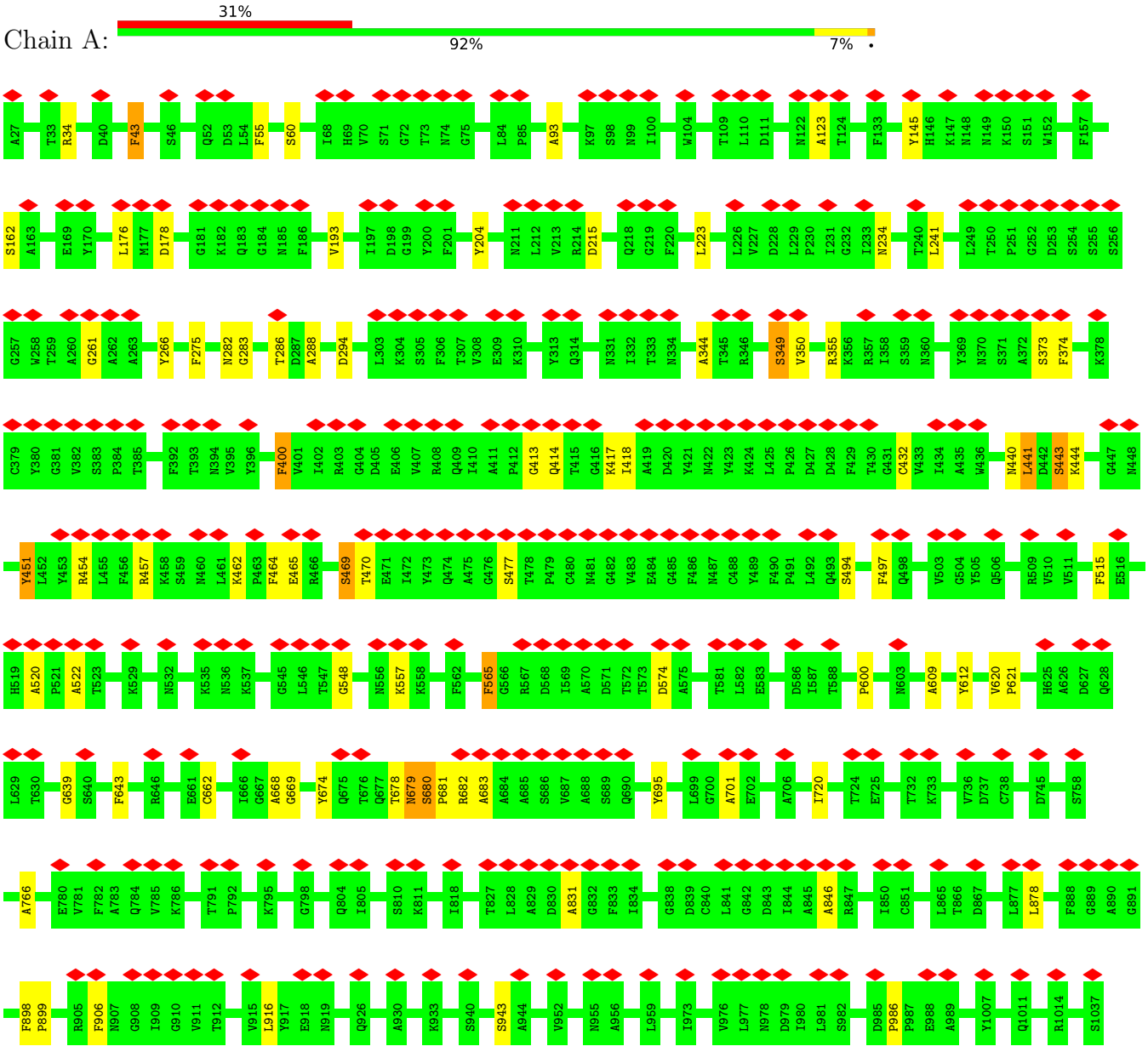
Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	197	Total	C	H	N	O	S	0	0
			2906	917	1438	259	286	6		
2	E	197	Total	C	H	N	O	S	0	0
			2906	917	1438	259	286	6		
2	F	197	Total	C	H	N	O	S	0	0
			2906	917	1438	259	286	6		

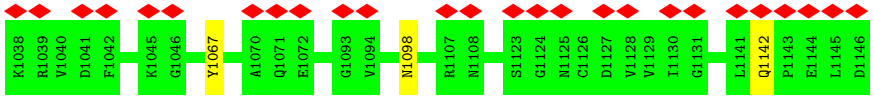
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

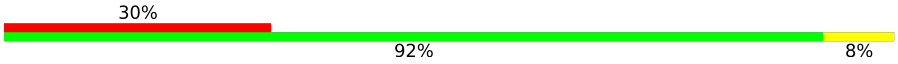
Chain A:

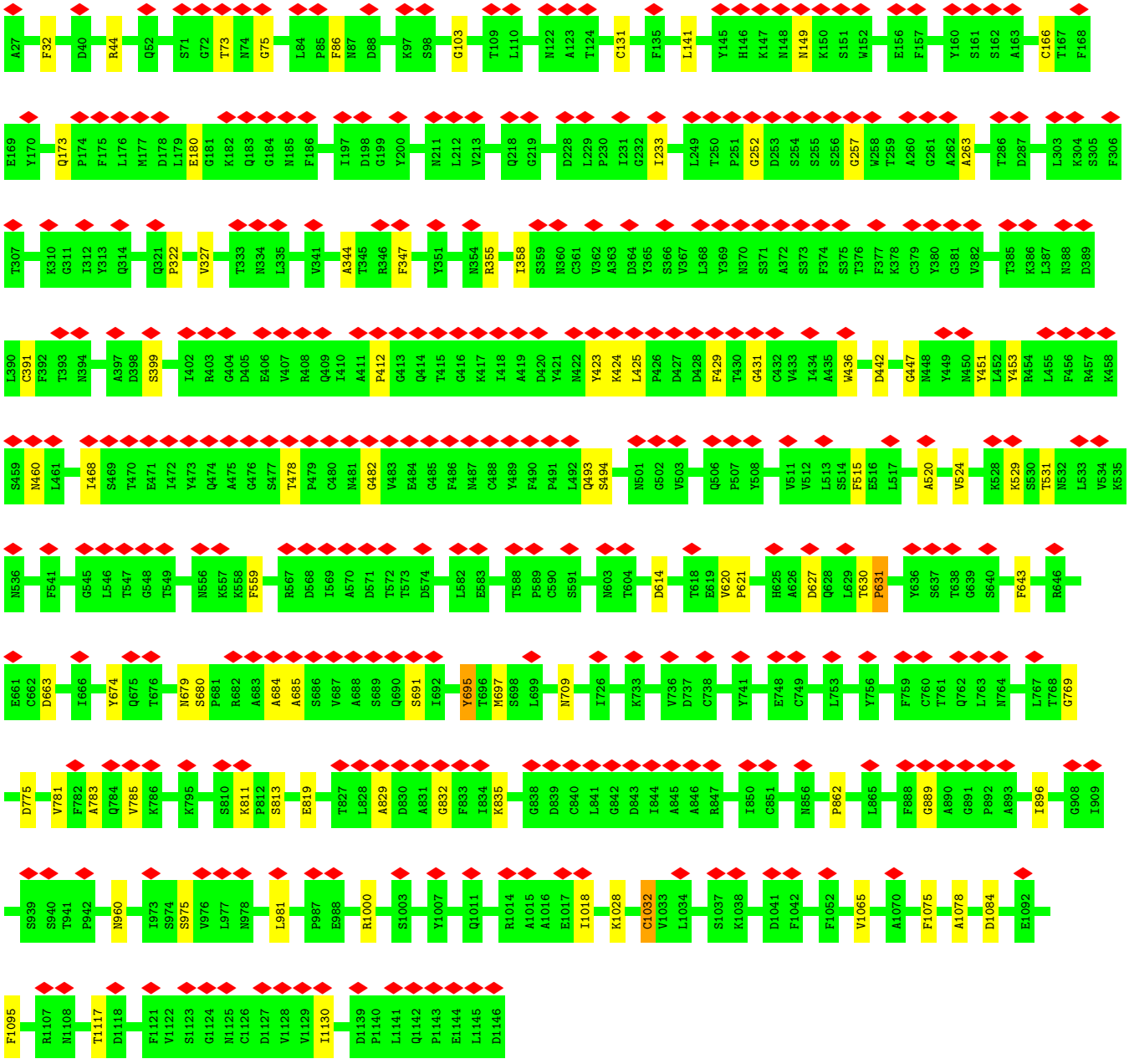




• Molecule 1: Spike glycoprotein

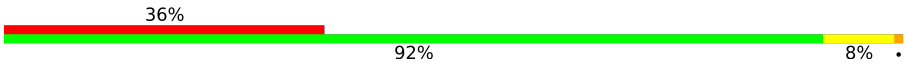
Chain B:

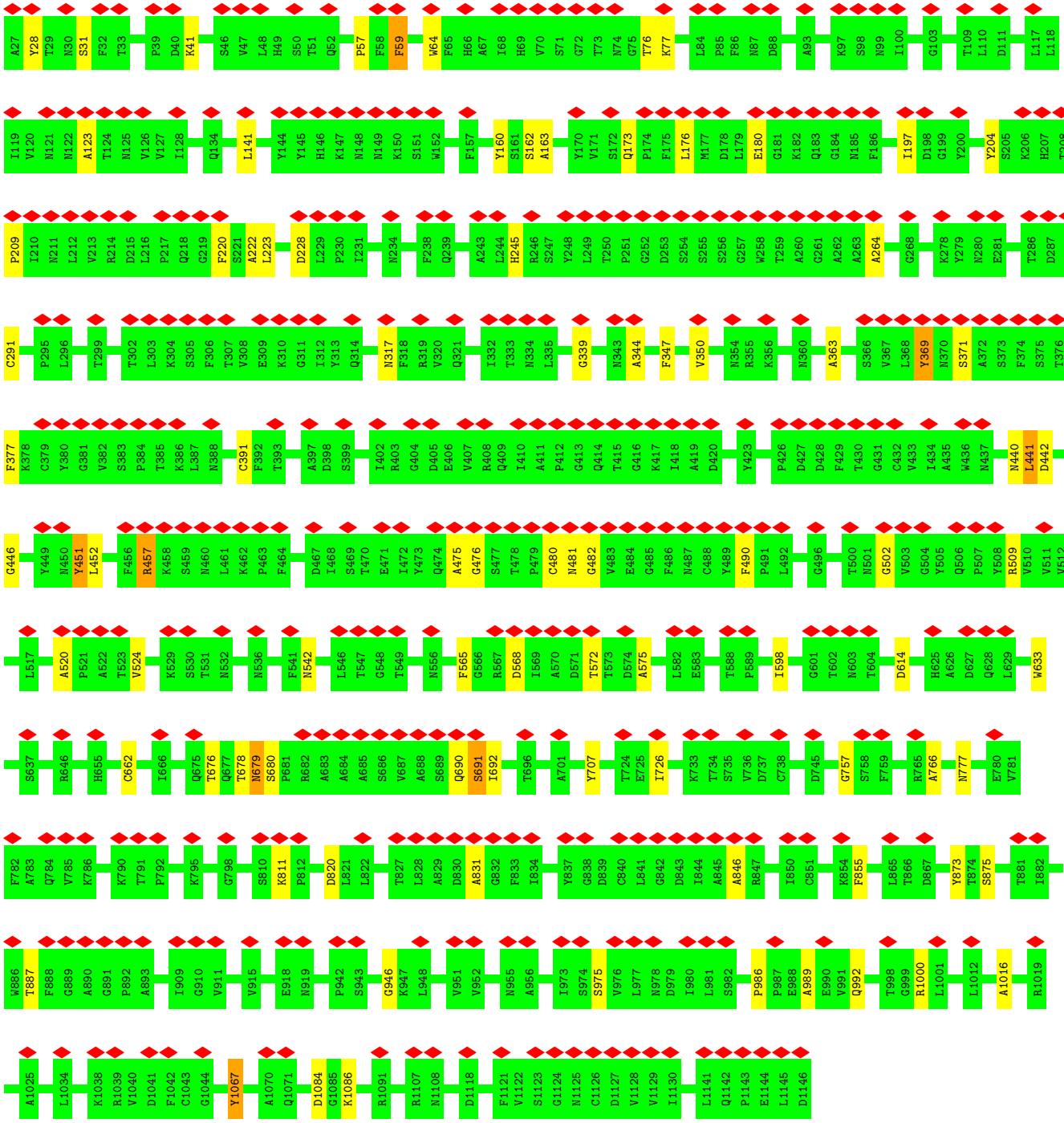




• Molecule 1: Spike glycoprotein

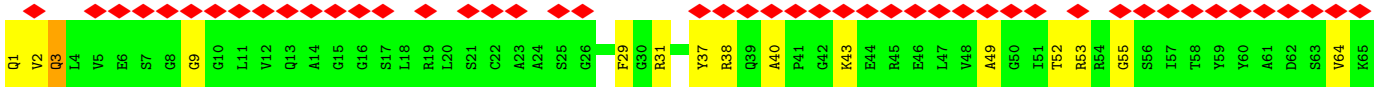
Chain C:

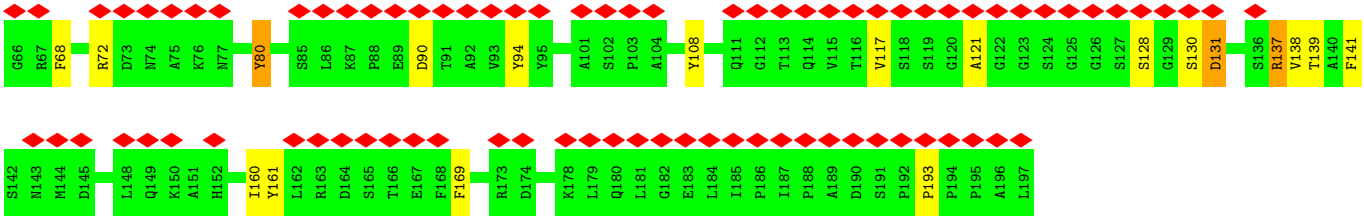




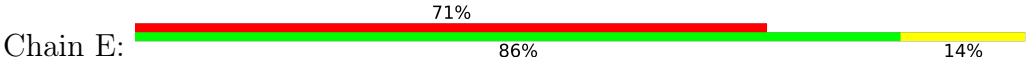
• Molecule 2: Tribody

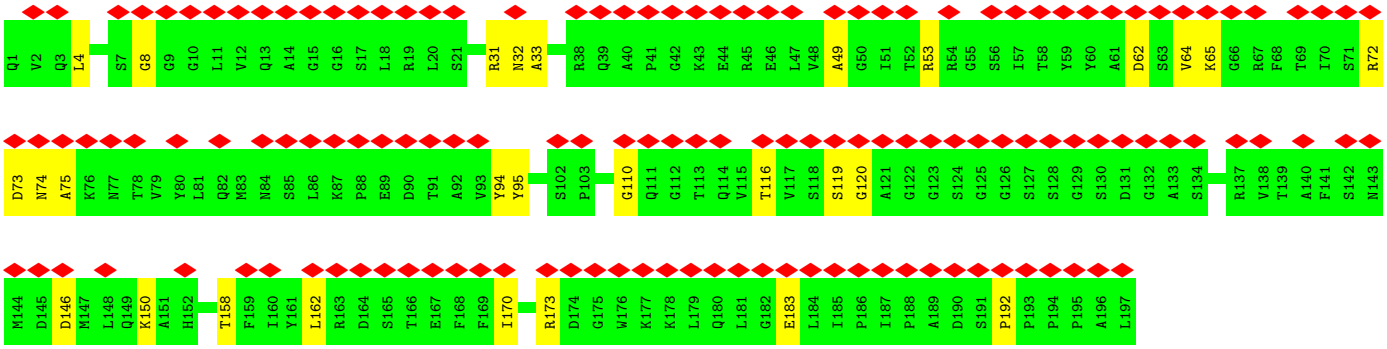
Chain D:



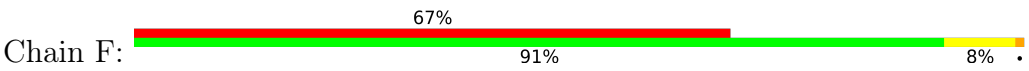


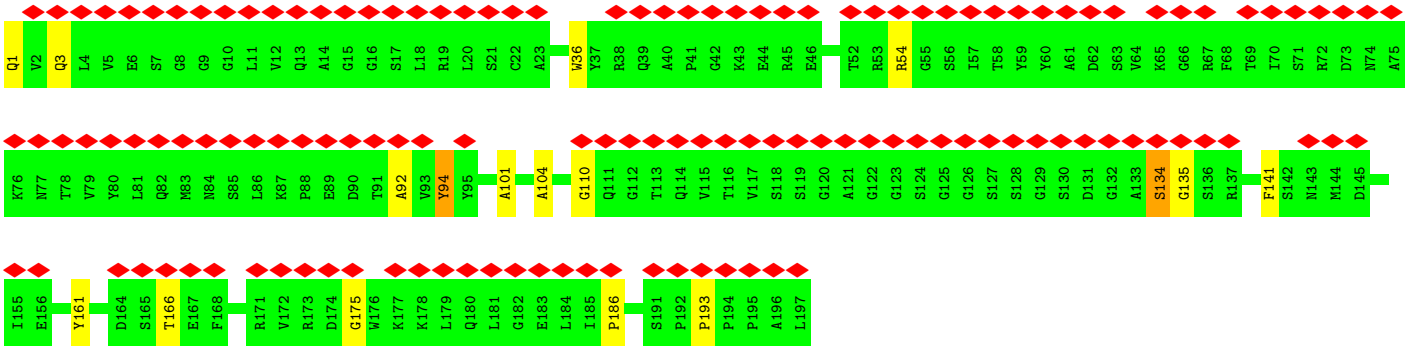
• Molecule 2: Tribody





• Molecule 2: Tribody





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	262855	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.175	Depositor
Minimum map value	-0.506	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.116	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	401.92, 401.92, 401.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.57, 1.57, 1.57	Depositor

5 Model quality

5.1 Standard geometry

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	1.27	14/8937 (0.2%)	1.31	46/12174 (0.4%)
1	B	1.28	18/8937 (0.2%)	1.32	49/12174 (0.4%)
1	C	1.26	13/8937 (0.1%)	1.31	45/12174 (0.4%)
2	D	1.36	6/1499 (0.4%)	1.54	14/2029 (0.7%)
2	E	1.39	4/1499 (0.3%)	1.39	10/2029 (0.5%)
2	F	1.40	6/1499 (0.4%)	1.38	8/2029 (0.4%)
All	All	1.29	61/31308 (0.2%)	1.33	172/42609 (0.4%)

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	3
1	B	0	2
1	C	0	3
2	D	0	2
2	F	0	1
All	All	0	11

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	161	TYR	CZ-OH	7.08	1.49	1.37
2	D	94	TYR	CG-CD2	6.82	1.48	1.39
1	B	257	GLY	CA-C	-6.69	1.41	1.51
1	C	946	GLY	N-CA	-6.27	1.36	1.46
1	B	832	GLY	N-CA	-6.23	1.36	1.46
1	A	283	GLY	N-CA	-6.05	1.36	1.46
1	B	559	PHE	N-CA	-6.04	1.34	1.46
1	A	261	GLY	CA-C	-5.96	1.42	1.51
1	A	674	TYR	CG-CD2	5.90	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1098	ASN	C-N	5.90	1.43	1.33
1	B	44	ARG	N-CA	-5.89	1.34	1.46
1	B	819	GLU	CD-OE1	5.83	1.32	1.25
2	F	36	TRP	CD2-CE2	5.75	1.48	1.41
1	C	509	ARG	NE-CZ	5.72	1.40	1.33
2	F	175	GLY	CA-C	-5.71	1.42	1.51
2	D	80	TYR	CE2-CZ	5.71	1.46	1.38
2	D	9	GLY	CA-C	-5.71	1.42	1.51
1	A	831	ALA	C-N	5.66	1.43	1.33
1	A	282	ASN	C-N	5.65	1.43	1.33
1	C	542	ASN	N-CA	-5.63	1.35	1.46
1	A	34	ARG	NE-CZ	5.62	1.40	1.33
1	B	1018	ILE	CA-C	-5.62	1.38	1.52
2	F	141	PHE	CG-CD1	5.61	1.47	1.38
1	A	215	ASP	CA-C	-5.59	1.38	1.52
1	C	160	TYR	CG-CD2	5.58	1.46	1.39
1	C	875	SER	N-CA	-5.56	1.35	1.46
1	A	600	PRO	N-CD	5.54	1.55	1.47
1	C	451	TYR	CG-CD2	5.53	1.46	1.39
1	B	431	GLY	CA-C	-5.50	1.43	1.51
2	F	1	GLN	N-CA	5.43	1.57	1.46
2	E	72	ARG	CZ-NH2	5.38	1.40	1.33
1	A	413	GLY	N-CA	-5.38	1.38	1.46
1	B	436	TRP	CE3-CZ3	5.35	1.47	1.38
2	E	8	GLY	CA-C	-5.33	1.43	1.51
1	A	60	SER	CA-C	-5.33	1.39	1.52
1	C	757	GLY	CA-C	-5.32	1.43	1.51
1	B	643	PHE	CE1-CZ	5.31	1.47	1.37
2	E	158	THR	N-CA	-5.30	1.35	1.46
1	A	669	GLY	CA-C	-5.29	1.43	1.51
2	E	72	ARG	CD-NE	5.27	1.55	1.46
1	C	992	GLN	N-CA	-5.27	1.35	1.46
1	B	1000	ARG	CD-NE	5.26	1.55	1.46
1	A	639	GLY	C-N	5.26	1.46	1.34
1	C	777	ASN	CB-CG	5.23	1.63	1.51
2	F	186	PRO	N-CA	-5.22	1.38	1.47
1	B	166	CYS	CA-C	-5.20	1.39	1.52
1	C	339	GLY	CA-C	-5.19	1.43	1.51
1	B	684	ALA	CA-CB	5.19	1.63	1.52
1	C	482	GLY	N-CA	-5.19	1.38	1.46
2	D	37	TYR	CG-CD1	5.17	1.45	1.39
1	C	707	TYR	CB-CG	5.13	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	CYS	CB-SG	5.10	1.91	1.82
1	B	103	GLY	CA-C	-5.09	1.43	1.51
1	B	252	GLY	N-CA	-5.09	1.38	1.46
1	B	769	GLY	N-CA	-5.07	1.38	1.46
1	C	565	PHE	CE2-CZ	5.06	1.47	1.37
1	A	241	LEU	CA-C	-5.06	1.39	1.52
2	D	94	TYR	CD2-CE2	5.04	1.47	1.39
1	B	447	GLY	CA-C	-5.04	1.43	1.51
2	F	110	GLY	CA-C	-5.03	1.43	1.51
1	B	889	GLY	CA-C	-5.03	1.43	1.51

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	695	TYR	CB-CG-CD2	13.00	128.80	121.00
2	D	161	TYR	CB-CG-CD2	12.78	128.67	121.00
1	B	423	TYR	CB-CG-CD1	-12.73	113.36	121.00
2	D	37	TYR	CB-CG-CD2	-11.63	114.02	121.00
1	A	497	PHE	CB-CG-CD2	11.58	128.90	120.80
1	C	1067	TYR	CB-CG-CD2	11.05	127.63	121.00
1	C	123	ALA	N-CA-CB	10.85	125.29	110.10
2	D	37	TYR	CG-CD1-CE1	-10.55	112.86	121.30
1	A	497	PHE	CB-CG-CD1	-10.10	113.73	120.80
1	C	457	ARG	NE-CZ-NH2	10.09	125.35	120.30
1	C	1067	TYR	CB-CG-CD1	-10.06	114.97	121.00
2	D	161	TYR	CB-CG-CD1	-10.00	115.00	121.00
1	B	1000	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	C	509	ARG	NE-CZ-NH2	-9.65	115.48	120.30
2	E	95	TYR	CB-CG-CD2	-9.06	115.56	121.00
1	B	451	TYR	CB-CG-CD1	-8.90	115.66	121.00
1	A	565	PHE	CB-CG-CD2	8.69	126.89	120.80
1	B	674	TYR	CB-CG-CD2	8.56	126.14	121.00
1	A	204	TYR	CB-CG-CD1	8.44	126.07	121.00
1	A	400	PHE	CB-CG-CD2	-8.10	115.13	120.80
2	F	104	ALA	N-CA-CB	8.03	121.34	110.10
2	D	37	TYR	CD1-CE1-CZ	7.96	126.97	119.80
1	C	160	TYR	CB-CG-CD2	7.90	125.74	121.00
2	E	94	TYR	CB-CG-CD1	-7.88	116.27	121.00
1	A	565	PHE	CB-CG-CD1	-7.75	115.37	120.80
1	C	369	TYR	CB-CG-CD2	-7.75	116.35	121.00
2	D	94	TYR	CB-CG-CD1	-7.68	116.39	121.00
1	A	288	ALA	CB-CA-C	-7.64	98.64	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	674	TYR	CG-CD1-CE1	7.51	127.31	121.30
2	D	121	ALA	N-CA-CB	7.36	120.40	110.10
1	C	347	PHE	CB-CG-CD2	-7.22	115.75	120.80
1	A	344	ALA	N-CA-CB	7.11	120.05	110.10
1	A	520	ALA	N-CA-CB	7.05	119.97	110.10
1	B	424	LYS	N-CA-C	-7.04	91.98	111.00
1	A	609	ALA	N-CA-CB	7.04	119.95	110.10
2	E	49	ALA	CB-CA-C	-7.01	99.58	110.10
1	B	1095	PHE	CB-CG-CD1	-6.97	115.92	120.80
2	E	49	ALA	N-CA-CB	6.94	119.82	110.10
1	A	674	TYR	CG-CD2-CE2	-6.93	115.75	121.30
1	B	442	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	C	831	ALA	CB-CA-C	-6.91	99.74	110.10
1	A	123	ALA	CB-CA-C	6.87	120.40	110.10
1	A	288	ALA	N-CA-CB	6.86	119.70	110.10
1	B	1000	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	C	633	TRP	CD2-CE3-CZ3	6.75	127.57	118.80
1	B	695	TYR	CZ-CE2-CD2	-6.67	113.80	119.80
1	A	145	TYR	CG-CD2-CE2	6.65	126.62	121.30
2	D	55	GLY	N-CA-C	-6.64	96.50	113.10
1	A	1067	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	B	442	ASP	CB-CG-OD1	6.62	124.25	118.30
1	C	28	TYR	CB-CG-CD1	-6.59	117.05	121.00
1	A	204	TYR	CB-CG-CD2	-6.58	117.06	121.00
2	F	161	TYR	CG-CD1-CE1	-6.54	116.07	121.30
1	B	451	TYR	CB-CG-CD2	6.52	124.91	121.00
1	B	775	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	683	ALA	N-CA-CB	6.41	119.07	110.10
1	C	457	ARG	NH1-CZ-NH2	-6.37	112.39	119.40
1	C	855	PHE	CB-CG-CD2	-6.33	116.37	120.80
1	C	633	TRP	CG-CD2-CE3	6.32	139.59	133.90
1	C	766	ALA	N-CA-CB	6.19	118.77	110.10
1	A	400	PHE	CB-CG-CD1	6.15	125.11	120.80
2	D	193	PRO	CA-C-N	6.15	134.32	117.10
2	E	192	PRO	CA-C-N	6.15	134.32	117.10
1	C	264	ALA	N-CA-CB	6.09	118.63	110.10
1	B	423	TYR	CB-CG-CD2	6.08	124.65	121.00
2	F	101	ALA	N-CA-CB	6.08	118.61	110.10
1	A	294	ASP	CB-CG-OD1	-6.07	112.83	118.30
1	B	1078	ALA	N-CA-CB	6.05	118.57	110.10
1	A	355	ARG	N-CA-C	-6.02	94.75	111.00
2	E	94	TYR	CB-CG-CD2	5.99	124.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	862	PRO	N-CA-CB	5.98	110.48	103.30
1	B	86	PHE	CB-CG-CD1	-5.97	116.62	120.80
1	C	222	ALA	N-CA-CB	5.93	118.40	110.10
1	C	633	TRP	CB-CA-C	5.93	122.25	110.40
1	A	986	PRO	N-CA-CB	5.92	110.41	103.30
1	C	676	THR	N-CA-CB	5.90	121.52	110.30
1	C	317	ASN	N-CA-C	-5.89	95.11	111.00
1	B	515	PHE	N-CA-C	-5.87	95.15	111.00
1	B	1065	VAL	CG1-CB-CG2	5.86	120.27	110.90
1	A	674	TYR	CZ-CE2-CD2	5.85	125.06	119.80
1	B	695	TYR	CD1-CG-CD2	-5.84	111.48	117.90
1	B	1032	CYS	CB-CA-C	-5.83	98.74	110.40
1	C	855	PHE	N-CA-CB	5.83	121.08	110.60
1	B	829	ALA	N-CA-CB	5.82	118.25	110.10
1	C	59	PHE	CB-CG-CD1	-5.82	116.73	120.80
1	A	701	ALA	N-CA-CB	5.80	118.23	110.10
1	A	548	GLY	N-CA-C	-5.79	98.62	113.10
2	F	141	PHE	CB-CG-CD2	5.79	124.85	120.80
2	F	193	PRO	N-CA-C	5.77	127.10	112.10
1	B	423	TYR	CG-CD1-CE1	-5.77	116.69	121.30
2	F	36	TRP	CB-CG-CD2	-5.76	119.11	126.60
1	A	515	PHE	CB-CG-CD1	-5.75	116.78	120.80
1	A	846	ALA	N-CA-CB	5.74	118.14	110.10
1	B	975	SER	O-C-N	-5.73	113.53	122.70
1	A	451	TYR	CD1-CE1-CZ	5.73	124.95	119.80
1	C	344	ALA	N-CA-CB	5.73	118.12	110.10
1	C	363	ALA	CB-CA-C	-5.71	101.53	110.10
1	A	497	PHE	CA-CB-CG	5.70	127.58	113.90
1	C	855	PHE	CB-CG-CD1	5.68	124.78	120.80
1	B	344	ALA	N-CA-CB	5.68	118.05	110.10
1	A	522	ALA	CB-CA-C	-5.67	101.60	110.10
1	B	1117	THR	C-N-CA	5.66	135.85	121.70
1	B	358	ILE	O-C-N	5.66	131.75	122.70
1	C	502	GLY	N-CA-C	-5.64	98.99	113.10
2	F	94	TYR	CB-CG-CD1	-5.64	117.61	121.00
2	D	128	SER	N-CA-C	-5.64	95.78	111.00
1	B	423	TYR	CB-CA-C	5.63	121.67	110.40
1	A	418	ILE	O-C-N	-5.60	113.74	122.70
1	A	477	SER	N-CA-C	-5.57	95.95	111.00
1	A	668	ALA	N-CA-CB	5.57	117.90	110.10
1	C	692	ILE	N-CA-C	-5.56	95.99	111.00
2	E	75	ALA	CB-CA-C	-5.55	101.77	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	137	ARG	C-N-CA	5.54	135.56	121.70
1	C	1016	ALA	N-CA-CB	5.53	117.85	110.10
1	A	145	TYR	O-C-N	5.53	131.54	122.70
1	C	873	TYR	CG-CD2-CE2	-5.52	116.89	121.30
1	A	906	PHE	CD1-CE1-CZ	-5.49	113.51	120.10
1	C	204	TYR	N-CA-C	-5.49	96.18	111.00
1	A	432	CYS	N-CA-CB	5.49	120.48	110.60
1	A	286	THR	O-C-N	-5.46	113.96	122.70
1	A	266	TYR	N-CA-C	-5.43	96.33	111.00
1	A	943	SER	C-N-CA	5.38	135.16	121.70
1	A	720	ILE	O-C-N	5.38	131.31	122.70
1	C	831	ALA	N-CA-CB	5.36	117.61	110.10
1	B	685	ALA	N-CA-C	5.36	125.47	111.00
1	A	193	VAL	N-CA-C	-5.35	96.56	111.00
1	C	846	ALA	N-CA-CB	5.35	117.58	110.10
1	C	480	CYS	C-N-CA	5.34	135.05	121.70
2	D	94	TYR	CG-CD2-CE2	-5.34	117.03	121.30
1	A	515	PHE	CB-CG-CD2	5.34	124.54	120.80
1	A	1142	GLN	CA-C-N	5.34	132.04	117.10
1	B	86	PHE	N-CA-C	-5.33	96.60	111.00
1	A	162	SER	C-N-CA	5.33	135.03	121.70
1	B	684	ALA	CB-CA-C	-5.31	102.14	110.10
1	C	575	ALA	CB-CA-C	-5.31	102.14	110.10
1	B	775	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	291	CYS	CB-CA-C	-5.26	99.89	110.40
1	C	989	ALA	CB-CA-C	-5.25	102.23	110.10
1	B	478	THR	N-CA-C	-5.24	96.85	111.00
1	B	783	ALA	N-CA-CB	5.24	117.44	110.10
1	B	709	ASN	O-C-N	-5.23	114.33	122.70
1	B	663	ASP	N-CA-C	-5.23	96.88	111.00
1	B	811	LYS	N-CA-C	-5.22	96.91	111.00
1	C	220	PHE	CD1-CE1-CZ	-5.22	113.84	120.10
1	C	59	PHE	CG-CD2-CE2	-5.21	115.07	120.80
1	C	64	TRP	N-CA-C	-5.20	96.95	111.00
2	E	162	LEU	N-CA-CB	5.20	120.80	110.40
1	B	614	ASP	O-C-N	5.19	131.00	122.70
2	D	141	PHE	CB-CG-CD2	5.17	124.42	120.80
1	B	391	CYS	N-CA-CB	5.16	119.89	110.60
1	A	462	LYS	N-CA-C	-5.15	97.10	111.00
1	B	643	PHE	CB-CA-C	5.15	120.69	110.40
1	B	781	VAL	O-C-N	-5.15	114.46	122.70
1	C	160	TYR	CG-CD1-CE1	5.15	125.42	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	475	ALA	N-CA-CB	5.14	117.29	110.10
1	B	515	PHE	CA-C-N	-5.13	105.91	117.20
2	D	1	GLN	O-C-N	-5.13	114.49	122.70
1	B	524	VAL	O-C-N	-5.12	114.50	122.70
1	A	93	ALA	N-CA-CB	5.12	117.26	110.10
2	E	170	ILE	N-CA-C	-5.11	97.20	111.00
1	B	429	PHE	CA-C-O	5.11	130.83	120.10
1	C	1016	ALA	CB-CA-C	-5.11	102.44	110.10
1	B	960	ASN	O-C-N	-5.09	114.56	122.70
2	E	183	GLU	CA-C-O	5.09	130.78	120.10
1	C	565	PHE	CG-CD1-CE1	5.06	126.37	120.80
1	B	263	ALA	N-CA-CB	5.05	117.17	110.10
1	B	697	MET	O-C-N	5.04	130.76	122.70
2	F	92	ALA	C-N-CA	5.04	134.30	121.70
1	C	209	PRO	N-CA-CB	-5.03	97.07	102.60
1	A	766	ALA	CB-CA-C	-5.02	102.57	110.10
1	C	766	ALA	CB-CA-C	-5.02	102.57	110.10
1	B	322	PRO	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	PHE	Sidechain
1	A	565	PHE	Sidechain
1	A	695	TYR	Sidechain
1	B	1075	PHE	Sidechain
1	B	695	TYR	Sidechain
1	C	369	TYR	Sidechain
1	C	476	GLY	Peptide
1	C	59	PHE	Sidechain
2	D	29	PHE	Sidechain
2	D	80	TYR	Sidechain
2	F	94	TYR	Sidechain

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	8728	8509	8506	29	0
1	B	8728	8509	8506	19	0
1	C	8728	8509	8506	27	0
2	D	1468	1438	1438	11	0
2	E	1468	1438	1438	10	0
2	F	1468	1438	1438	2	0
All	All	30588	29841	29832	91	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 2.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:VAL:N	1:A:621:PRO:CD	2.54	0.71
1:C:350:VAL:HG22	1:C:350:VAL:O	1.96	0.64
1:A:469:SER:OG	1:A:470:THR:N	2.31	0.64
2:F:134:SER:OG	2:F:135:GLY:N	2.31	0.63
2:E:116:THR:OG1	2:E:119:SER:OG	2.16	0.62
1:C:41:LYS:NZ	1:C:228:ASP:OD2	2.34	0.60
1:A:682:ARG:O	1:A:682:ARG:HG2	2.03	0.59
1:C:442:ASP:OD2	2:E:150:LYS:NZ	2.37	0.57
1:A:176:LEU:O	1:A:176:LEU:HG	2.05	0.57
2:E:173:ARG:N	2:F:166:THR:OG1	2.39	0.56
2:D:43:LYS:NZ	2:D:90:ASP:OD1	2.38	0.55
1:A:349:SER:OG	1:A:350:VAL:N	2.39	0.54
1:A:878:LEU:C	1:A:878:LEU:HD23	2.28	0.54
1:C:975:SER:O	1:C:1000:ARG:NH2	2.41	0.54
1:C:197:ILE:O	1:C:197:ILE:HG23	2.07	0.53
2:D:2:VAL:O	2:D:3:GLN:CB	2.56	0.53
1:C:678:THR:O	1:C:679:ASN:HB2	2.09	0.53
2:E:31:ARG:O	2:E:32:ASN:C	2.47	0.53
1:A:443:SER:OG	1:A:444:LYS:N	2.41	0.53
1:B:141:LEU:C	1:B:141:LEU:HD12	2.29	0.53
1:B:981:LEU:C	1:B:981:LEU:HD23	2.30	0.53
1:A:620:VAL:H	1:A:621:PRO:CD	2.22	0.52
2:D:52:THR:OG1	2:D:53:ARG:N	2.40	0.52
1:C:568:ASP:N	1:C:572:THR:O	2.42	0.52
1:A:620:VAL:H	1:A:621:PRO:HD3	1.75	0.52
2:E:62:ASP:OD1	2:E:65:LYS:NZ	2.36	0.50
1:B:233:ILE:O	1:C:457:ARG:NH1	2.44	0.50
1:B:627:ASP:OD1	1:B:627:ASP:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:LEU:HD13	1:A:916:LEU:C	2.33	0.49
1:A:678:THR:O	1:A:679:ASN:HB2	2.13	0.49
1:C:141:LEU:HD23	1:C:141:LEU:H	1.77	0.48
1:A:557:LYS:NZ	1:A:574:ASP:OD1	2.46	0.48
2:D:2:VAL:O	2:D:3:GLN:HB3	2.12	0.48
1:B:73:THR:C	1:B:75:GLY:H	2.15	0.48
1:C:141:LEU:HD23	1:C:141:LEU:N	2.28	0.48
2:E:119:SER:OG	2:E:120:GLY:N	2.46	0.48
1:C:690:GLN:O	1:C:691:SER:CB	2.61	0.47
1:C:678:THR:O	1:C:679:ASN:CB	2.61	0.47
2:D:160:ILE:HB	2:D:169:PHE:CZ	2.48	0.47
1:A:43:PHE:CD1	1:A:43:PHE:C	2.86	0.47
1:A:678:THR:O	1:A:679:ASN:CB	2.63	0.47
1:A:620:VAL:N	1:A:621:PRO:HD2	2.28	0.47
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.42	0.47
2:E:64:VAL:HG13	2:E:64:VAL:O	2.13	0.46
1:B:425:LEU:C	1:B:425:LEU:HD23	2.36	0.46
1:A:898:PHE:N	1:A:899:PRO:CD	2.77	0.46
1:A:464:PHE:O	1:A:464:PHE:CD2	2.69	0.46
1:B:425:LEU:O	1:B:425:LEU:CD2	2.64	0.46
1:A:454:ARG:NH1	1:A:465:GLU:OE1	2.49	0.46
1:A:451:TYR:HD2	1:A:494:SER:HG	1.64	0.45
1:C:1084:ASP:OD2	1:C:1086:LYS:NZ	2.46	0.45
1:B:453:TYR:O	1:B:493:GLN:N	2.47	0.45
1:A:223:LEU:HD12	1:A:223:LEU:N	2.31	0.45
1:B:327:VAL:N	1:B:531:THR:OG1	2.49	0.45
1:A:898:PHE:HB3	1:A:899:PRO:HD3	1.99	0.44
1:C:391:CYS:HA	1:C:524:VAL:O	2.18	0.44
1:A:55:PHE:HB2	1:A:275:PHE:CE1	2.52	0.44
1:C:31:SER:OG	1:C:57:PRO:O	2.34	0.44
1:C:452:LEU:HD23	1:C:452:LEU:N	2.32	0.43
1:B:1028:LYS:O	1:B:1032:CYS:N	2.50	0.43
2:E:73:ASP:OD1	2:E:74:ASN:N	2.51	0.43
1:B:835:LYS:NZ	1:C:614:ASP:OD2	2.51	0.43
1:A:440:ASN:O	1:A:441:LEU:HB2	2.18	0.43
1:A:680:SER:HB3	1:A:681:PRO:CD	2.48	0.43
1:C:223:LEU:HD12	1:C:223:LEU:N	2.34	0.42
1:B:630:THR:OG1	1:B:631:PRO:HD2	2.19	0.42
1:B:896:ILE:O	1:B:896:ILE:HG23	2.18	0.42
1:C:598:ILE:N	1:C:598:ILE:HD12	2.34	0.42
2:D:117:VAL:HG12	2:D:117:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:VAL:O	1:B:785:VAL:HG13	2.19	0.42
1:C:887:THR:O	1:C:887:THR:HG22	2.17	0.42
2:E:4:LEU:H	2:E:110:GLY:CA	2.33	0.42
1:C:77:LYS:O	1:C:245:HIS:ND1	2.52	0.42
1:A:43:PHE:C	1:A:43:PHE:HD1	2.23	0.42
1:B:620:VAL:N	1:B:621:PRO:CD	2.83	0.42
2:D:130:SER:O	2:D:131:ASP:CB	2.67	0.41
1:A:234:ASN:ND2	1:B:468:ILE:H	2.18	0.41
1:C:440:ASN:O	1:C:441:LEU:HB2	2.20	0.41
1:C:76:THR:O	1:C:77:LYS:HB2	2.20	0.41
2:D:49:ALA:CB	2:D:68:PHE:H	2.33	0.41
1:B:1130:ILE:HD12	1:B:1130:ILE:N	2.35	0.41
1:C:162:SER:OG	1:C:163:ALA:N	2.49	0.41
1:A:620:VAL:N	1:A:621:PRO:HD3	2.32	0.41
1:B:494:SER:O	2:D:31:ARG:HA	2.21	0.41
1:B:347:PHE:CD2	1:B:399:SER:HB2	2.56	0.41
2:D:64:VAL:HG12	2:D:64:VAL:O	2.21	0.41
2:E:146:ASP:OD1	2:E:146:ASP:O	2.38	0.40
1:C:726:ILE:N	1:C:726:ILE:HD12	2.36	0.40
1:A:176:LEU:C	1:A:178:ASP:H	2.24	0.40
1:A:417:LYS:NZ	1:C:371:SER:O	2.49	0.40
2:D:137:ARG:O	2:D:139:THR:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1118/1120 (100%)	1029 (92%)	79 (7%)	10 (1%)	17	56
1	B	1118/1120 (100%)	1042 (93%)	61 (6%)	15 (1%)	12	48
1	C	1118/1120 (100%)	1043 (93%)	63 (6%)	12 (1%)	14	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	195/197 (99%)	162 (83%)	28 (14%)	5 (3%)	5 35
2	E	195/197 (99%)	180 (92%)	13 (7%)	2 (1%)	15 54
2	F	195/197 (99%)	180 (92%)	12 (6%)	3 (2%)	10 46
All	All	3939/3951 (100%)	3636 (92%)	256 (6%)	47 (1%)	17 50

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	SER
1	A	662	CYS
1	B	691	SER
1	C	180	GLU
2	D	3	GLN
2	D	40	ALA
2	D	131	ASP
2	D	138	VAL
1	A	349	SER
1	A	414	GLN
1	C	691	SER
1	A	374	PHE
1	A	441	LEU
1	A	679	ASN
1	B	180	GLU
1	B	529	LYS
1	B	680	SER
1	C	173	GLN
1	C	446	GLY
1	C	662	CYS
1	C	680	SER
2	E	53	ARG
2	F	134	SER
1	A	373	SER
1	A	443	SER
1	A	680	SER
1	B	32	PHE
1	B	149	ASN
1	B	173	GLN
1	B	460	ASN
1	B	631	PRO
1	B	813	SER
1	B	1084	ASP

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Mol	Chain	Res	Type
1	C	176	LEU
1	C	441	LEU
1	C	481	ASN
1	C	679	ASN
2	D	108	TYR
2	E	33	ALA
2	F	54	ARG
2	F	3	GLN
1	B	679	ASN
1	C	520	ALA
1	C	986	PRO
1	B	482	GLY
1	B	520	ALA
1	B	412	PRO

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	972/972 (100%)	968 (100%)	4 (0%)	91 94
1	B	972/972 (100%)	971 (100%)	1 (0%)	93 97
1	C	972/972 (100%)	968 (100%)	4 (0%)	91 94
2	D	152/152 (100%)	150 (99%)	2 (1%)	69 82
2	E	152/152 (100%)	152 (100%)	0	100 100
2	F	152/152 (100%)	152 (100%)	0	100 100
All	All	3372/3372 (100%)	3361 (100%)	11 (0%)	92 95

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	PHE
1	A	457	ARG
1	A	612	TYR
1	A	643	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	355	ARG
1	C	377	PHE
1	C	451	TYR
1	C	490	PHE
1	C	1067	TYR
2	D	38	ARG
2	D	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	C	556	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

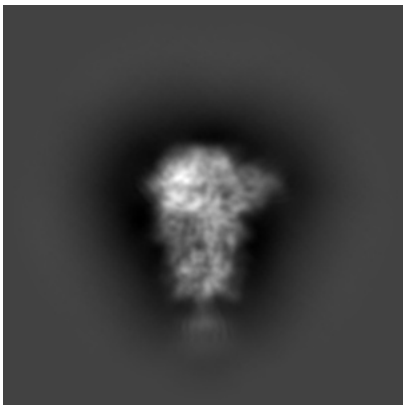
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36904. These allow visual inspection of the internal detail of the map and identification of artifacts.

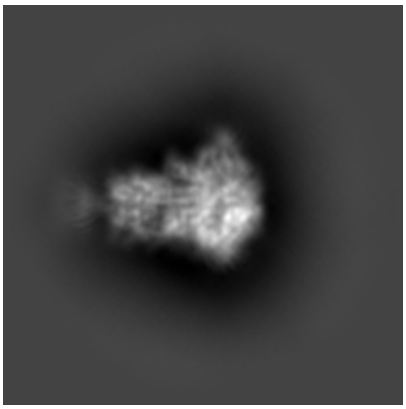
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

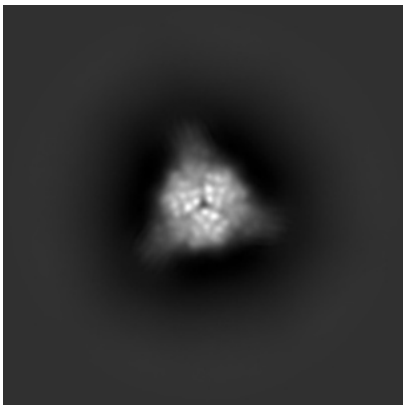
6.1.1 Primary map



X

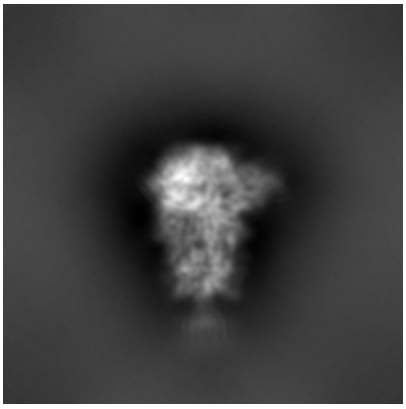


Y

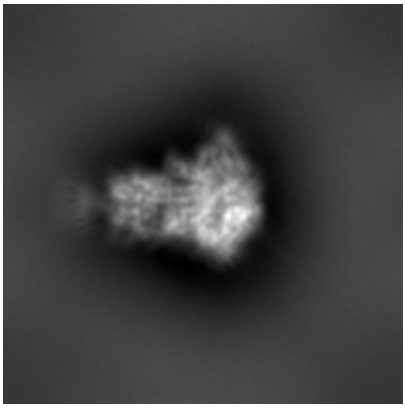


Z

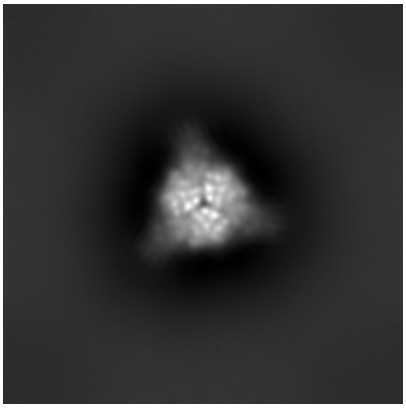
6.1.2 Raw map



X



Y

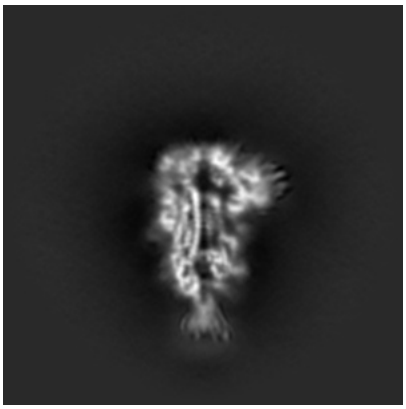


Z

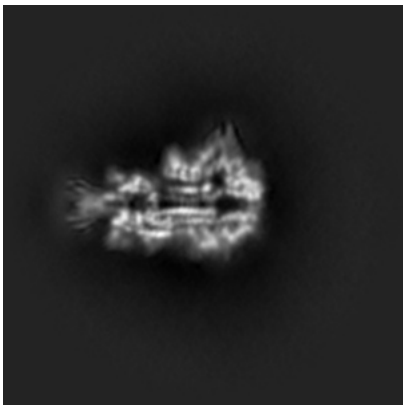
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

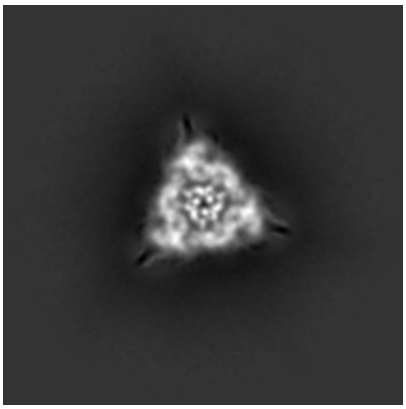
6.2.1 Primary map



X Index: 128

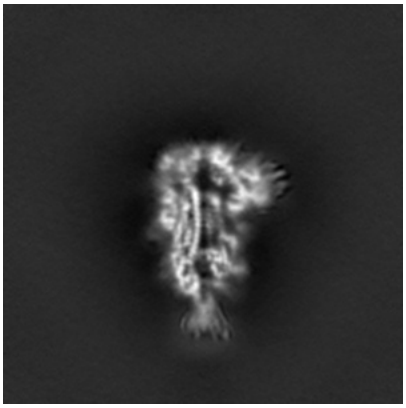


Y Index: 128

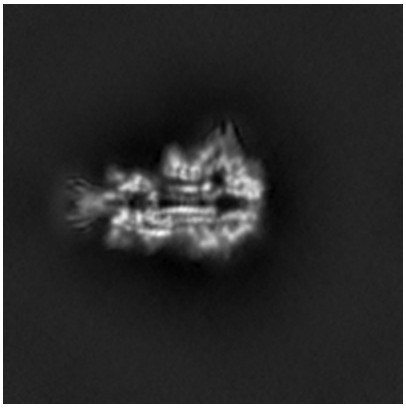


Z Index: 128

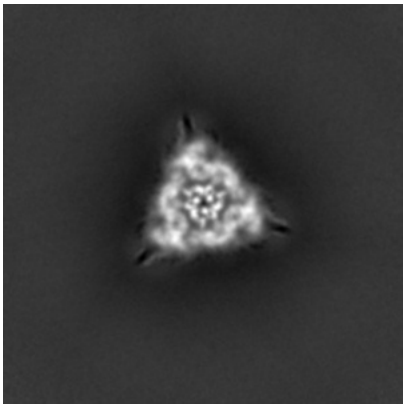
6.2.2 Raw map



X Index: 128



Y Index: 128

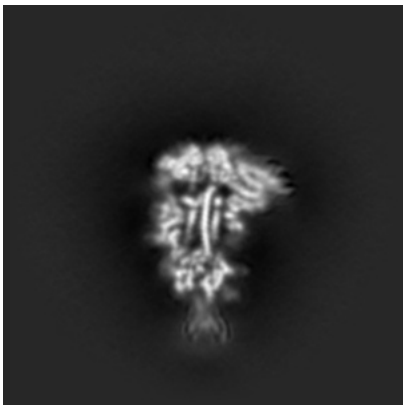


Z Index: 128

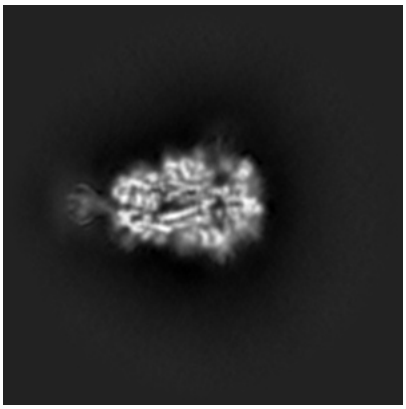
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

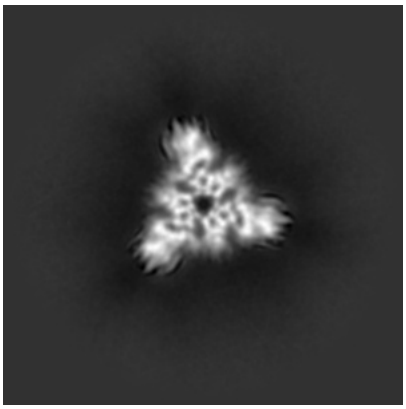
6.3.1 Primary map



X Index: 123

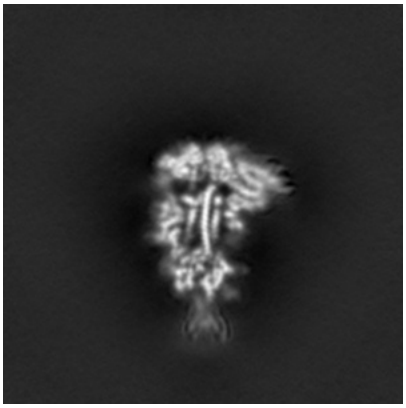


Y Index: 135

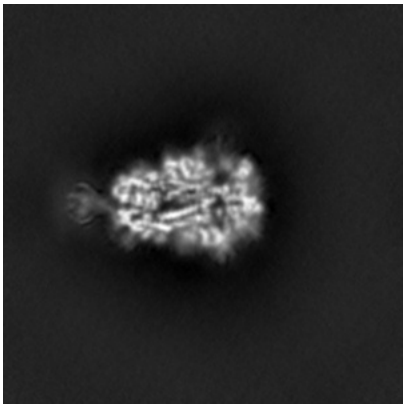


Z Index: 143

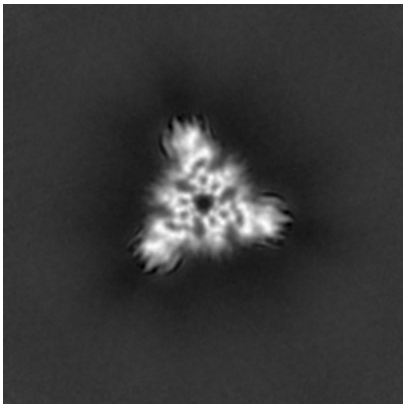
6.3.2 Raw map



X Index: 123



Y Index: 135



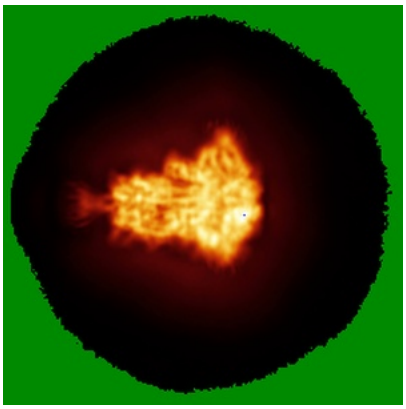
Z Index: 143

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

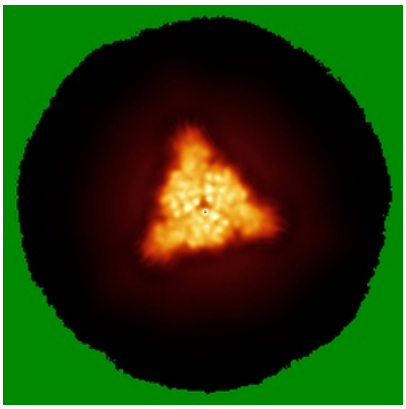
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X

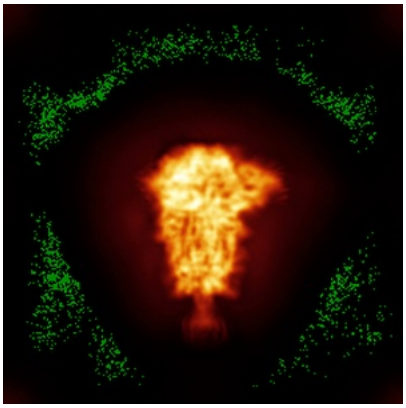


Y

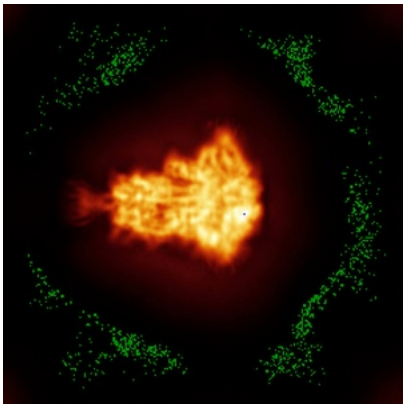


Z

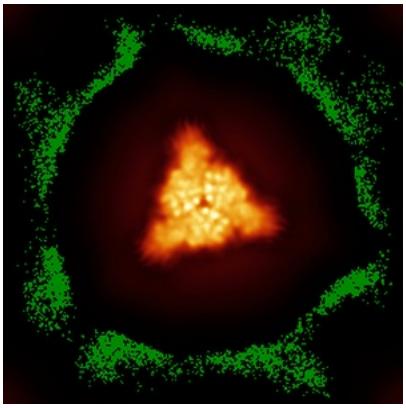
6.4.2 Raw map



X



Y

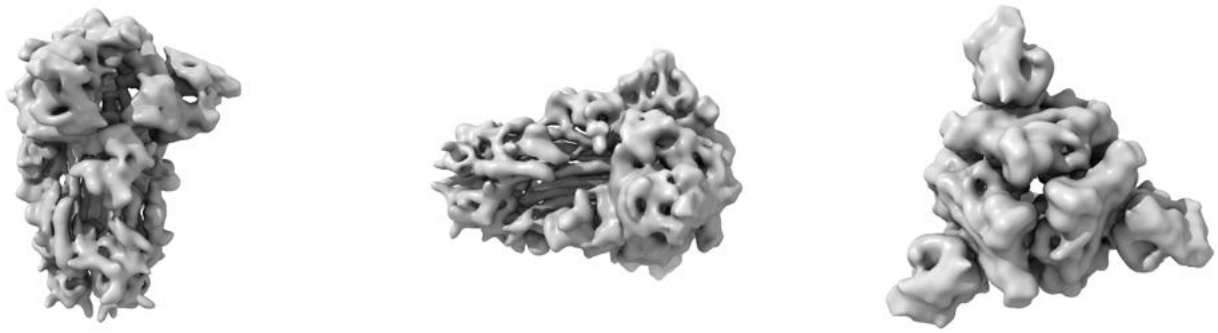


Z

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)

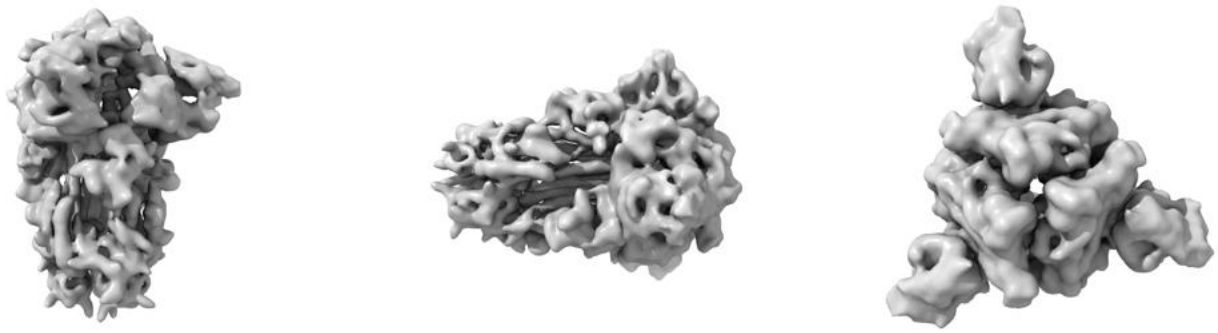
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. 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



X Y Z

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.

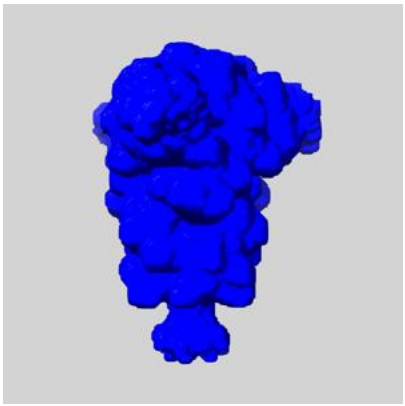
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

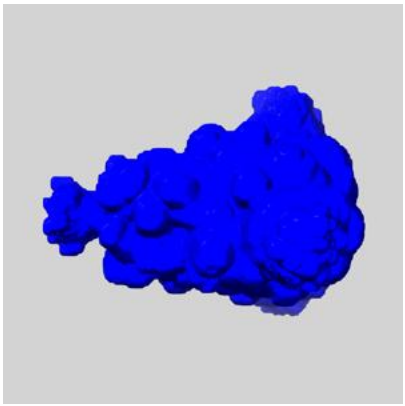
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

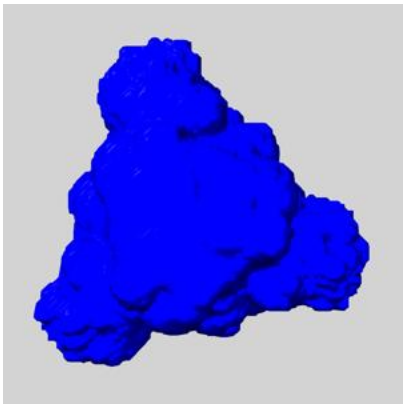
6.6.1 emd_36904_msk_1.map



X



Y

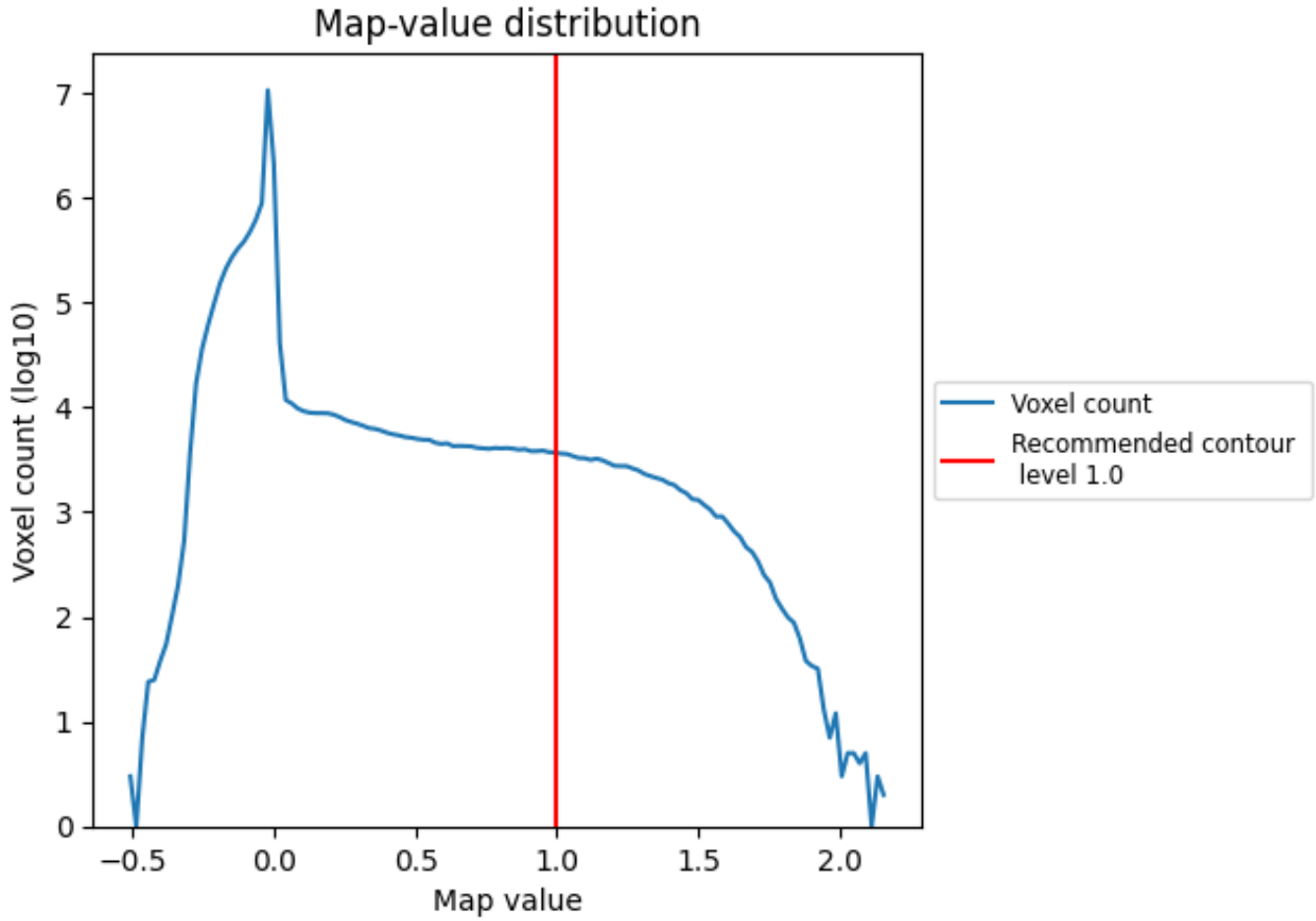


Z

7 Map analysis

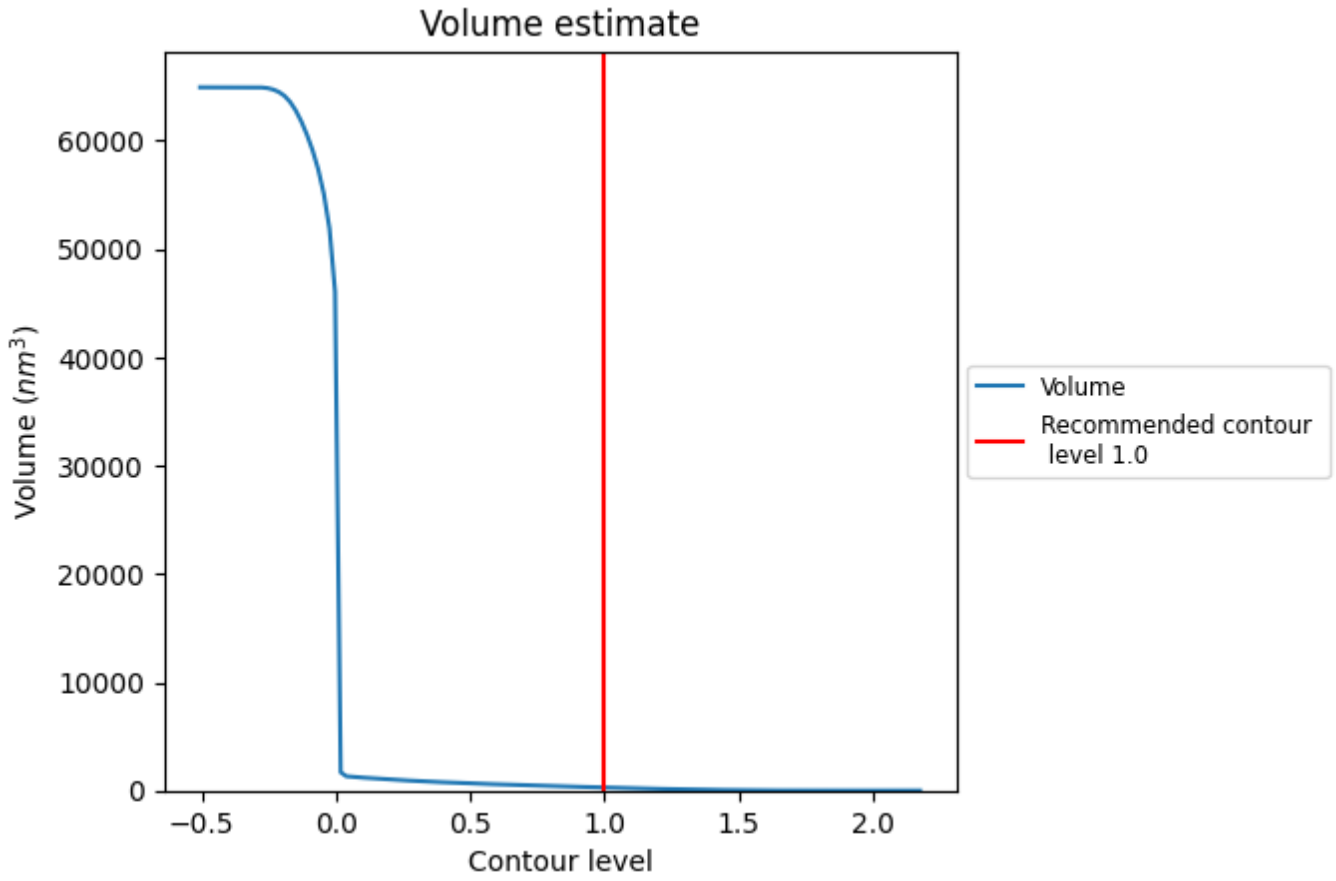
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

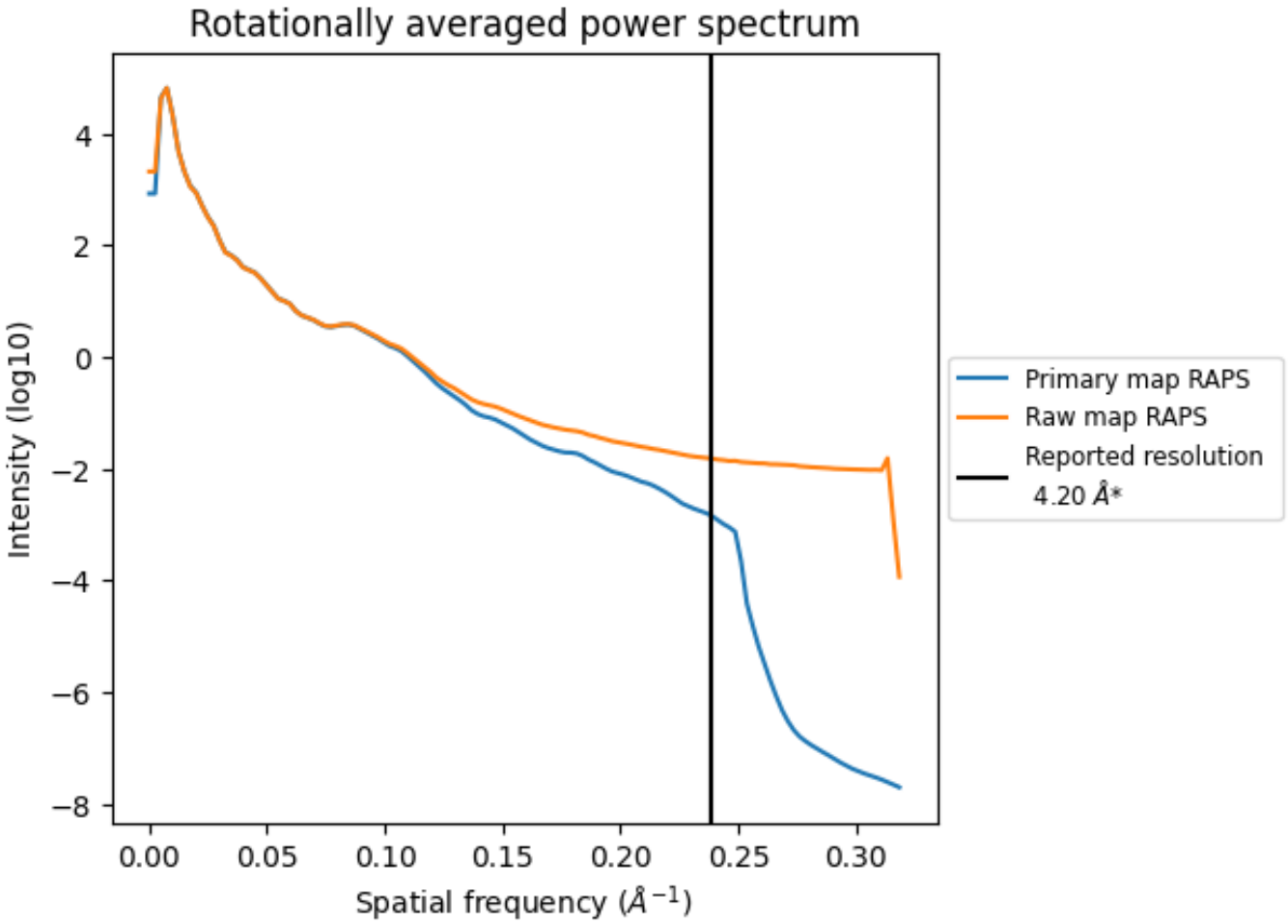
7.2 Volume estimate



The volume at the recommended contour level is 279 nm^3; this corresponds to an approximate mass of 252 kDa.

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

7.3 Rotationally averaged power spectrum (i)

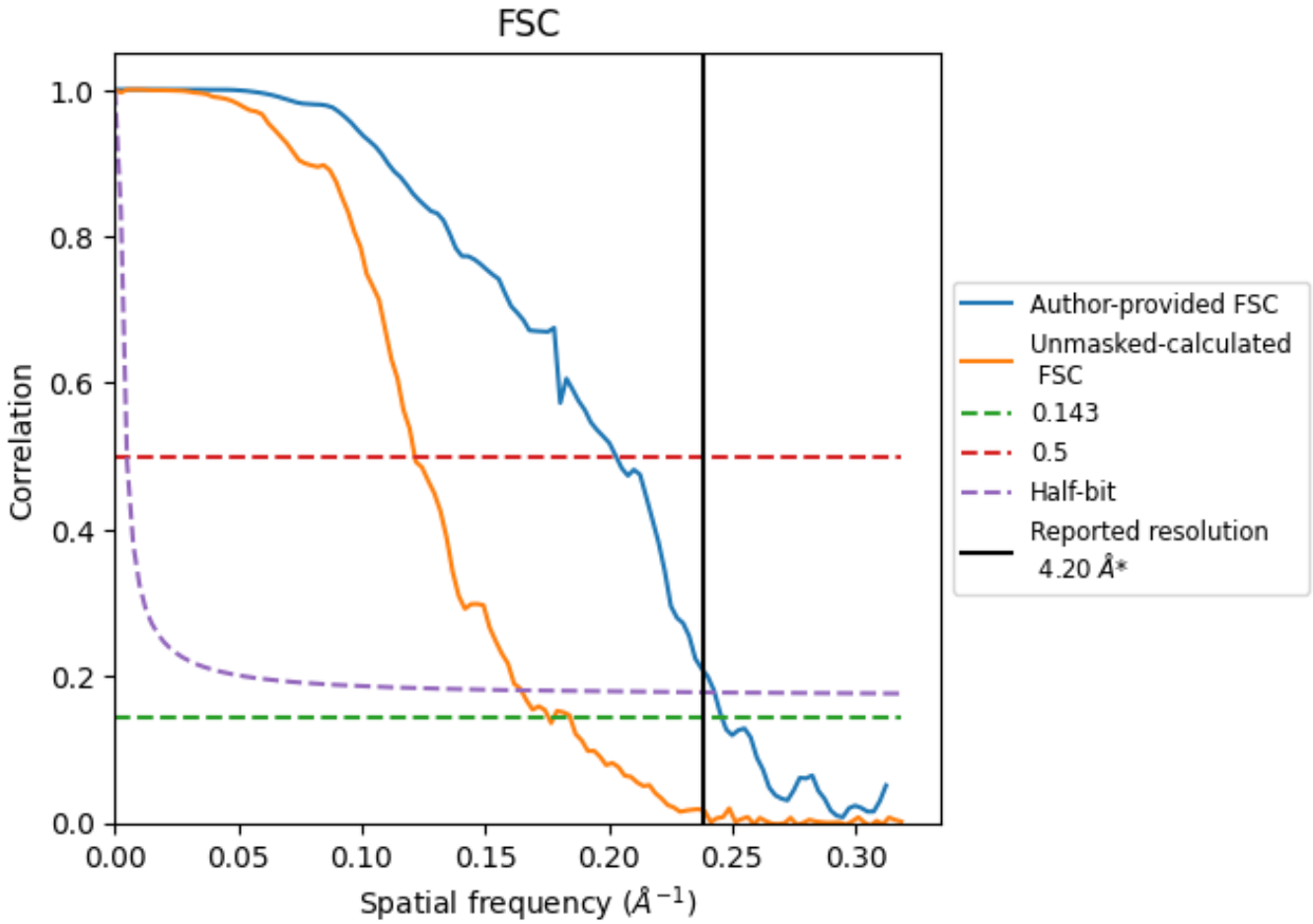


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

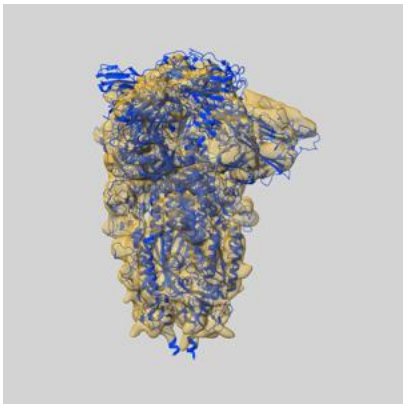
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.07	4.93	4.12
Unmasked-calculated*	5.69	8.23	6.08

*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 5.69 differs from the reported value 4.2 by more than 10 %

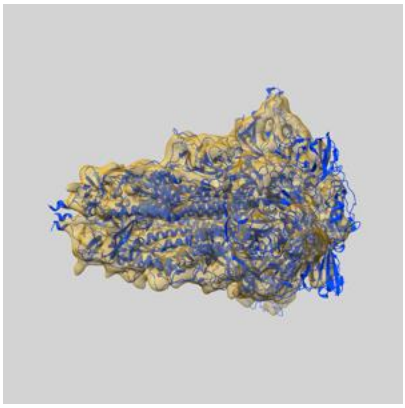
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36904 and PDB model 8W4F. Per-residue inclusion information can be found in section 3 on page 5.

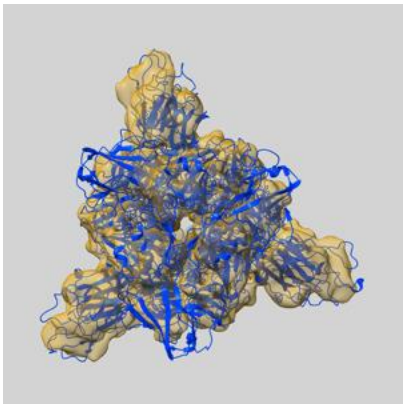
9.1 Map-model overlay



X



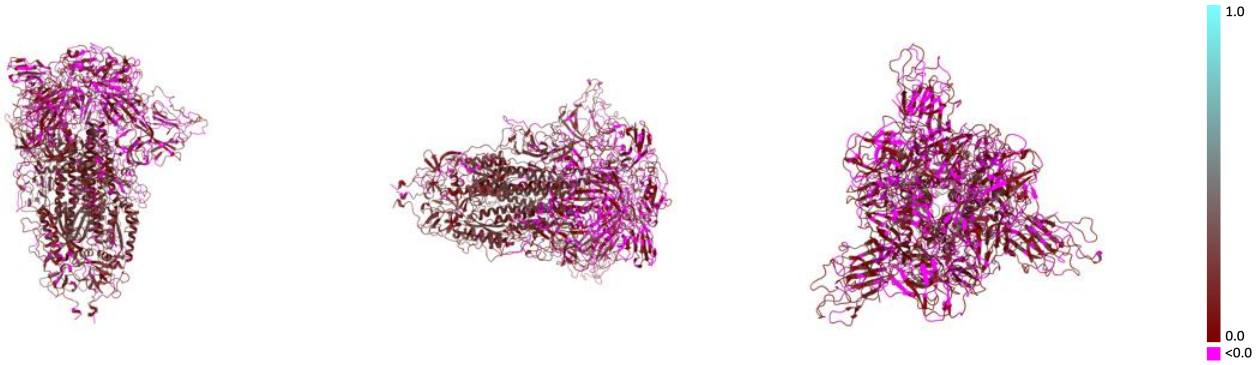
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

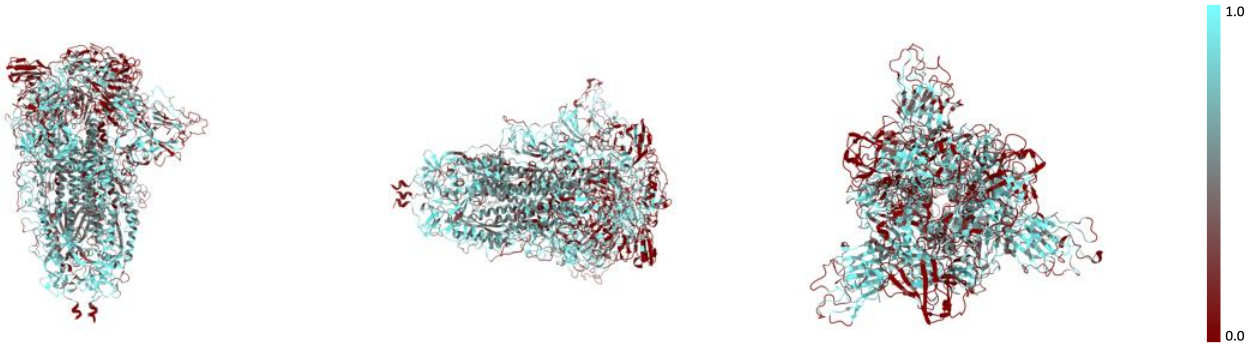
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

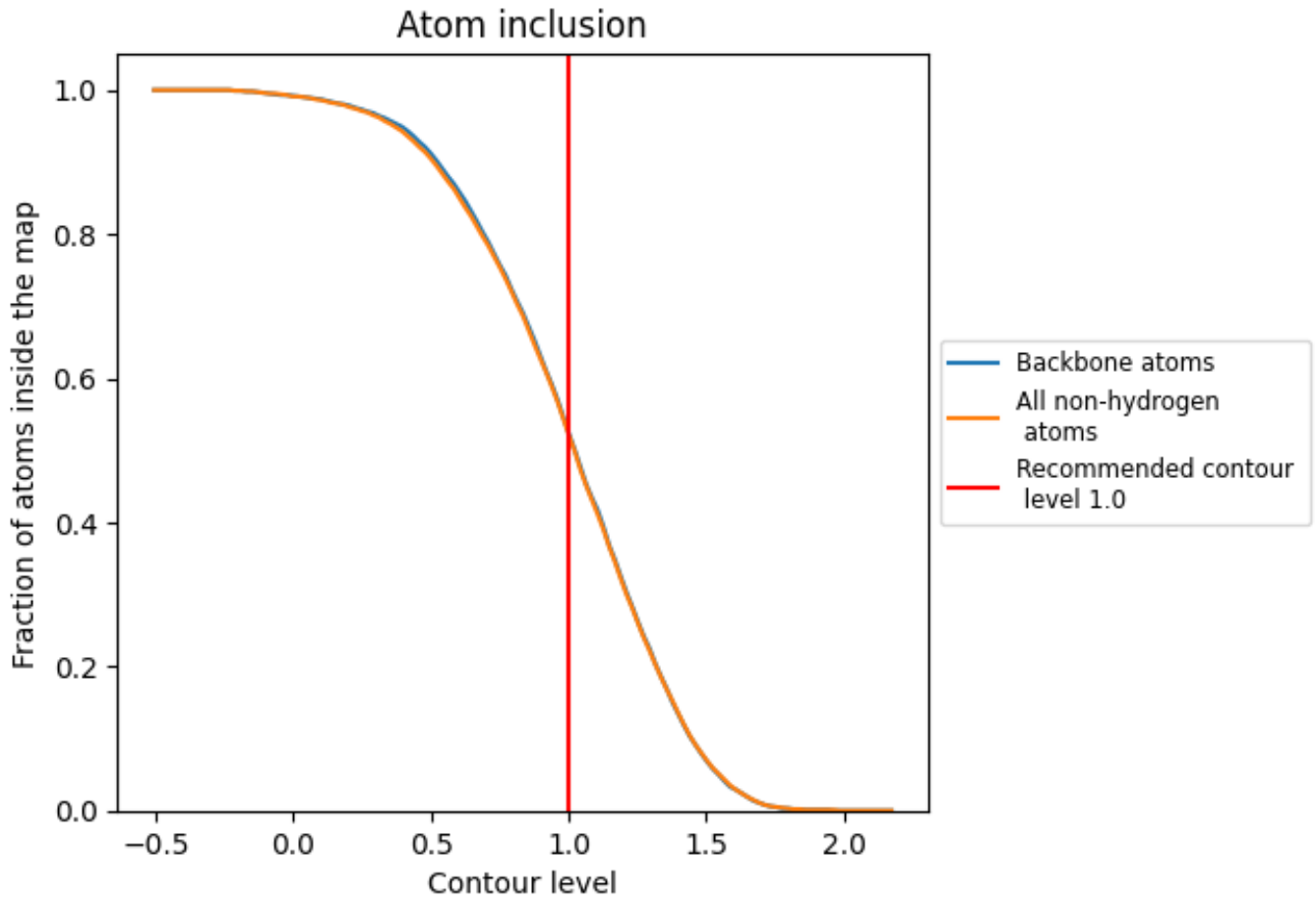
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 52% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5230	0.0930
A	0.5630	0.1030
B	0.5780	0.1200
C	0.5290	0.0870
D	0.3400	0.0320
E	0.2870	0.0230
F	0.2980	0.0340