



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:16 PM UTC

PDB ID : 8DYW / pdb_00008dyw
EMDB ID : EMD-27784
Title : Cryo-EM structure of 239 Fab in complex with recombinant shortened Plasmodium falciparum circumsporozoite protein (rsCSP)
Authors : Martin, G.M.; Ward, A.B.
Deposited on : 2022-08-05
Resolution : 3.72 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
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

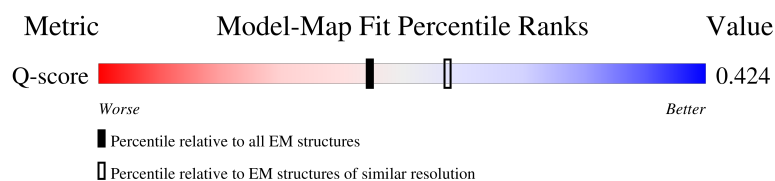
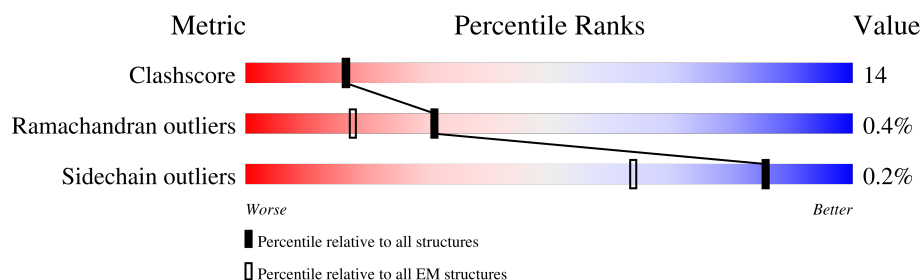
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.72 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	10474 (3.22 - 4.22)

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	I	278	
2	B	215	
2	D	215	
2	F	215	

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Mol	Chain	Length	Quality of chain
2	L	215	 39%11%50%
2	N	215	 41%9%50%
2	P	215	 40%11%50%
2	R	215	 36%13%50%
2	T	215	 32%18%50%
2	V	215	 32%19%50%
2	X	215	 33%16%50%
3	A	450	 18%9%73%
3	C	450	 18%9%73%
3	E	450	 19%7%73%
3	H	450	 20%7%73%
3	M	450	 18%8%73%
3	O	450	 18%9%73%
3	Q	450	 17%9%73%
3	S	450	 16%11%73%
3	U	450	 16%11%73%
3	W	450	 12%14%13%73%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18494 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 Circumsporozoite protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	I	80	Total	C	N	O	0	0
			564	324	117	123		

- Molecule 2 is a protein called 239 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	B	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	D	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	F	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	N	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	P	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	R	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	T	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	V	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	X	108	Total	C	N	O	S	0	0
			833	521	143	166	3		

- Molecule 3 is a protein called 239 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	121	Total	C	N	O	S	0	0
			960	604	174	178	4		
3	A	121	Total	C	N	O	S	0	0
			960	604	174	178	4		

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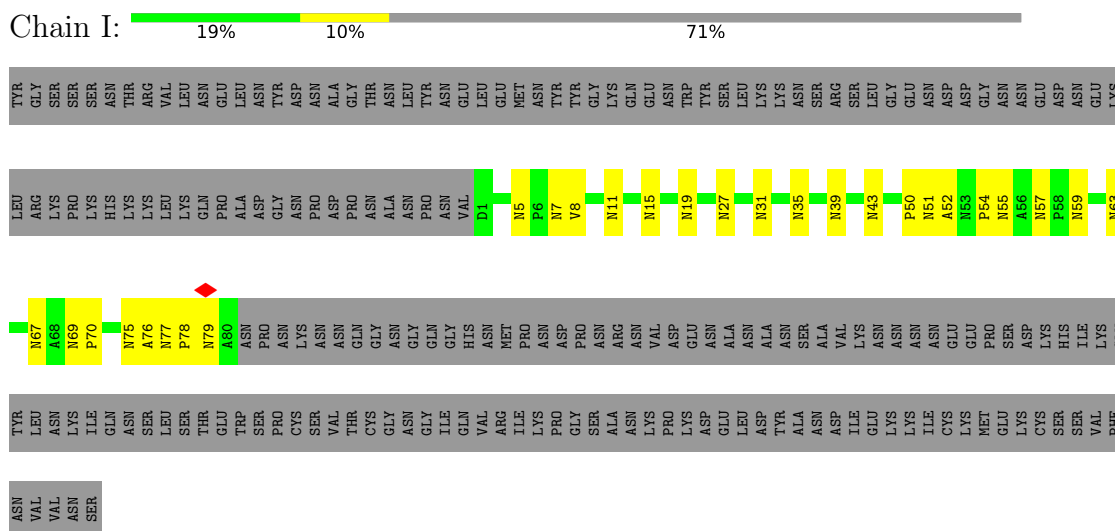
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	E	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	M	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	O	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	Q	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	S	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	U	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	W	121	Total 960	C 604	N 174	O 178	S 4	0	0

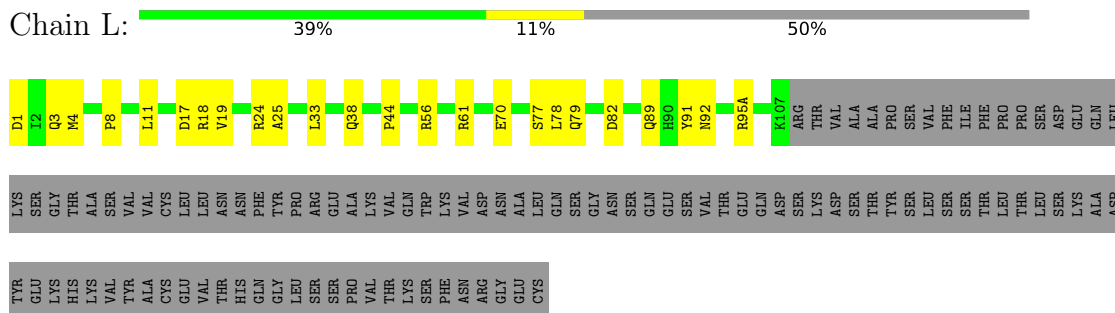
3 Residue-property plots [i](#)

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.

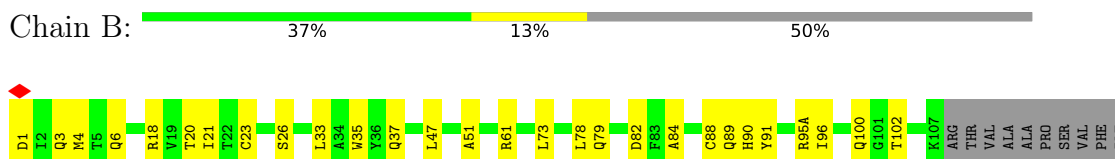
• Molecule 1: Circumsporozoite protein



• Molecule 2: 239 Fab light chain



• Molecule 2: 239 Fab light chain



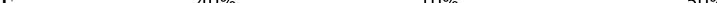
[illegible]

- Molecule 2: 239 Fab light chain

Chain D: 38% 12% 50%

Tyr	Thr	Lys	D1
Leu	Ser	Gly	I2
Lys	Thr	Thr	
His	Lys	Ala	T6
His	Val	Ser	S7
Val	Tyr	Val	P8
		Val	
Ala		Val	L11
Cys	Cys	Leu	
Leu	Val	Leu	R18
Val	Thr	Asn	
Thr	His	Asn	C23
His	Gln	Phe	
Gln	Gly	Thr	S26
Gly	Leu	Pro	Q27
Leu	Ser	Arg	
Ser	Ser	Glu	L33
Pro	Pro	Ala	
Val	Val	Lys	Q38
Thr	Thr	Val	K39
Lys	Lys	Gln	
Ser	Ser	Trp	P44
Phe	Phe	Lys	
Asn	Asn	Val	T65
Arg	Arg	Asp	R66
Gly	Gly	Asn	
Leu	Glu	Ala	F71
Cys		Leu	
		Gln	D81
		Ser	
		Gly	Y91
		Asn	N92
		Ser	
		Ser	
		Gln	R95A
		Glu	
		Ser	Q100
		Val	G101
		Thr	T102
		Glu	
		Gln	I106
		Asp	K107
		Ser	
		Lys	Thr
		Asp	Val
		Ser	Ala
		Thr	Ala
		Tyr	Pro
		Ser	
		Leu	Val
		Ser	Phe
		Ser	Ile
		Thr	Phe
		Leu	Pro
		Thr	
		Leu	Ser
		Lys	Asp
		Ala	Glu
		Ser	Leu

- Molecule 2: 239 Fab light chain

Chain F:  40% 10% 50%

HIS	THR	D1
LYS	ALA	I2
VAL	SER	Q3
TYR	VAL	Q6
ALA	VAL	
CYS	CYS	S26
GLU	LEU	
VAL	LEU	
THR	ASN	Q37
HIS	ASN	Q38
GLN	PHE	K39
GLY	TYR	
LEU	PRO	K42
SER	ARG	
SER	GLU	L46
PRO	ALA	L47
VAL	LYS	
THR	VAL	R56
LYS	GLN	
SER	TRP	R61
PHE	LYS	F62
ASN	VAL	
ARG	ASP	L78
GLY	ASN	
GLU	ALA	D82
CYS	LEU	F93
	GLN	A84
	SER	T85
	GLY	Y86
	ASN	
	SER	H90
	GLN	
	GLU	S95
	SER	R95A
	VAL	
	THR	T102
	GLU	
	GLN	T106
	ASP	K107
	SER	ARG
	LYS	THR
	ASP	VAL
	SER	ALA
	THR	ALA
	TYR	PRO
	SER	SER
	LEU	VAL
	SER	PHE
	SER	ILE
	THR	PHE
	LEU	PRO
	THR	PRO
	LEU	SER
	SER	ASP
	LYS	GLU
	ALA	GLN
	ASP	LEU
	TYR	LYS
	GLU	SER
	LYS	GLY

- Molecule 2: 239 Fab light chain

Chain N: 41% 9% 50%

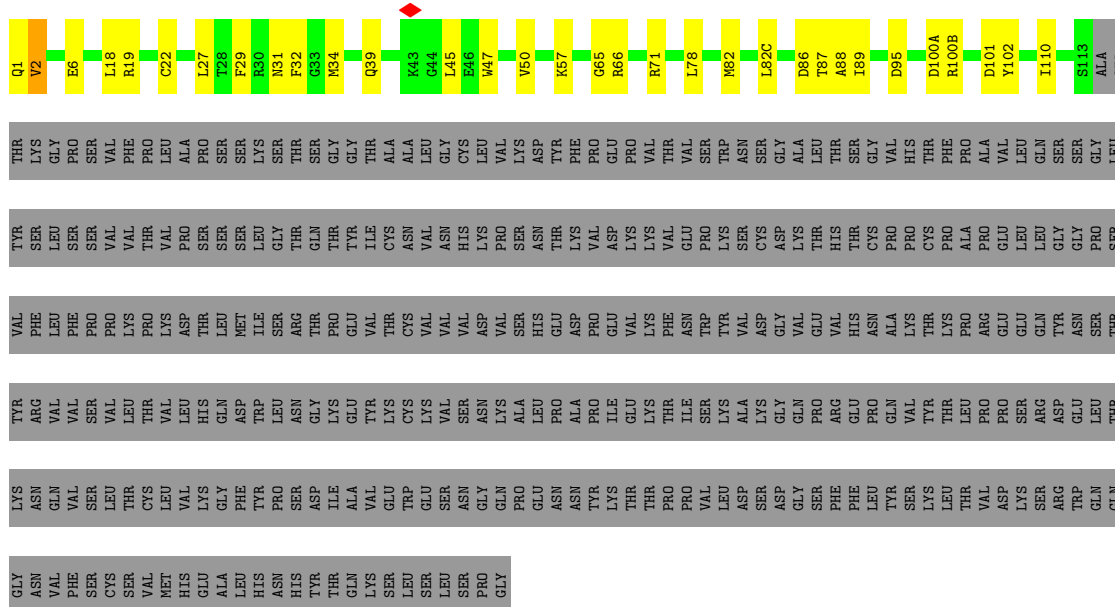
[illegible]

- Molecule 2: 239 Fab light chain

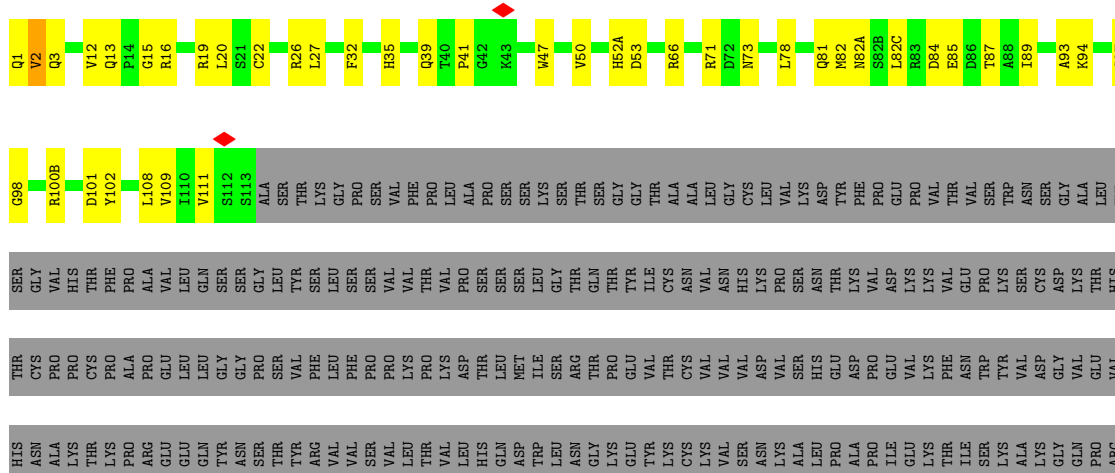
Chain P: 40% 11% 50%

D1	D2	D3	D4	D5	D6	D7	D8	D9	D10	D11	D12	D13	D14	D15	D16	D17	D18	D19	D20	D21	D22	D23	D24	D25	D26	D27	D28	D29	D30	D31	D32	D33	D34	D35	D36	D37	D38	D39	D40	D41	D42	D43	D44	D45	D46	D47	D48	D49	D50	D51	D52	D53	D54	D55	D56	D57	D58	D59	D60	D61	D62	D63	D64	D65	D66	D67	D68	D69	D70	D71	D72	D73	D74	D75	D76	D77	D78	D79	D80	D81	D82	D83	D84	D85	D86	D87	D88	D89	D90	D91	D92	D93	D94	D95	D96	D97	D98	D99	D100	D101	D102	D103	D104	D105	D106	D107	D108	D109	D110	D111	D112	D113	D114	D115	D116	D117	D118	D119	D120	D121	D122	D123	D124	D125	D126	D127	D128	D129	D130	D131	D132	D133	D134	D135	D136	D137	D138	D139	D140	D141	D142	D143	D144	D145	D146	D147	D148	D149	D150	D151	D152	D153	D154	D155	D156	D157	D158	D159	D160	D161	D162	D163	D164	D165	D166	D167	D168	D169	D170	D171	D172	D173	D174	D175	D176	D177	D178	D179	D180	D181	D182	D183	D184	D185	D186	D187	D188	D189	D190	D191	D192	D193	D194	D195	D196	D197	D198	D199	D200	D201	D202	D203	D204	D205	D206	D207	D208	D209	D210	D211	D212	D213	D214	D215	D216	D217	D218	D219	D220	D221	D222	D223	D224	D225	D226	D227	D228	D229	D230	D231	D232	D233	D234	D235	D236	D237	D238	D239	D240	D241	D242	D243	D244	D245	D246	D247	D248	D249	D250	D251	D252	D253	D254	D255	D256	D257	D258	D259	D260	D261	D262	D263	D264	D265	D266	D267	D268	D269	D270	D271	D272	D273	D274	D275	D276	D277	D278	D279	D280	D281	D282	D283	D284	D285	D286	D287	D288	D289	D290	D291	D292	D293	D294	D295	D296	D297	D298	D299	D300	D301	D302	D303	D304	D305	D306	D307	D308	D309	D310	D311	D312	D313	D314	D315	D316	D317	D318	D319	D320	D321	D322	D323	D324	D325	D326	D327	D328	D329	D330	D331	D332	D333	D334	D335	D336	D337	D338	D339	D340	D341	D342	D343	D344	D345	D346	D347	D348	D349	D350	D351	D352	D353	D354	D355	D356	D357	D358	D359	D360	D361	D362	D363	D364	D365	D366	D367	D368	D369	D370	D371	D372	D373	D374	D375	D376	D377	D378	D379	D380	D381	D382	D383	D384	D385	D386	D387	D388	D389	D390	D391	D392	D393	D394	D395	D396	D397	D398	D399	D400	D401	D402	D403	D404	D405	D406	D407	D408	D409	D410	D411	D412	D413	D414	D415	D416	D417	D418	D419	D420	D421	D422	D423	D424	D425	D426	D427	D428	D429	D430	D431	D432	D433	D434	D435	D436	D437	D438	D439	D440	D441	D442	D443	D444	D445	D446	D447	D448	D449	D450	D451	D452	D453	D454	D455	D456	D457	D458	D459	D460	D461	D462	D463	D464	D465	D466	D467	D468	D469	D470	D471	D472	D473	D474	D475	D476	D477	D478	D479	D480	D481	D482	D483	D484	D485	D486	D487	D488	D489	D490	D491	D492	D493	D494	D495	D496	D497	D498	D499	D500	D501	D502	D503	D504	D505	D506	D507	D508	D509	D510	D511	D512	D513	D514	D515	D516	D517	D518	D519	D520	D521	D522	D523	D524	D5
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- Molecule 3: 239 Fab heavy chain



- Molecule 3: 239 Fab heavy chain



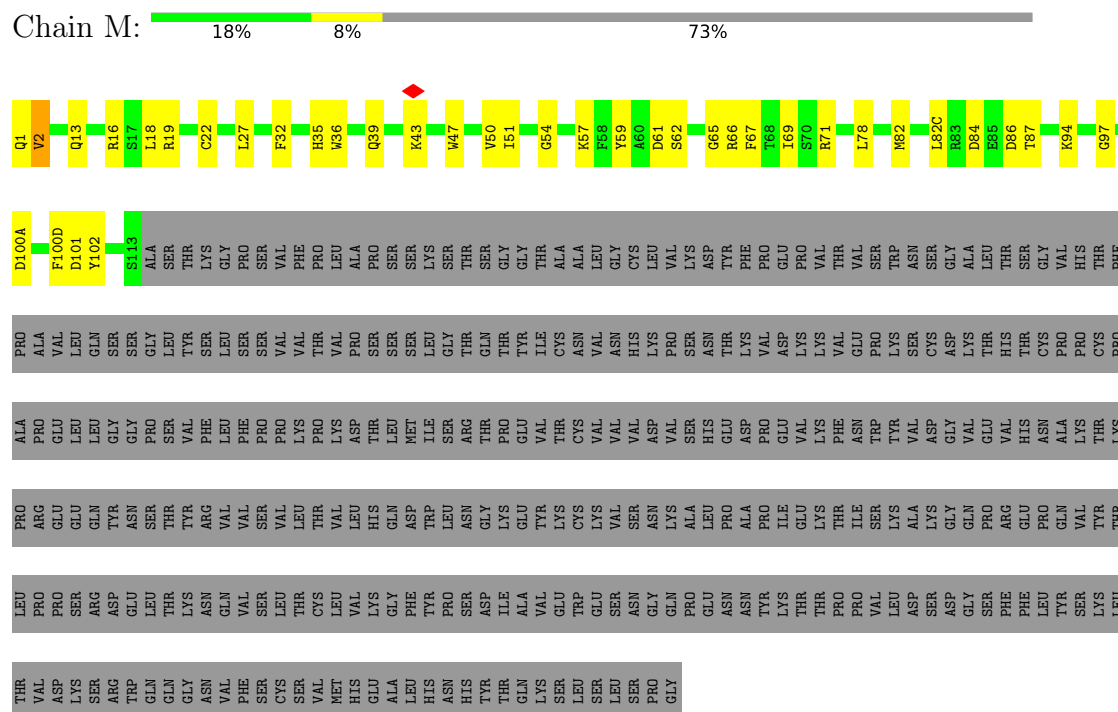
- Molecule 3: 239 Fab heavy chain

[illegible]

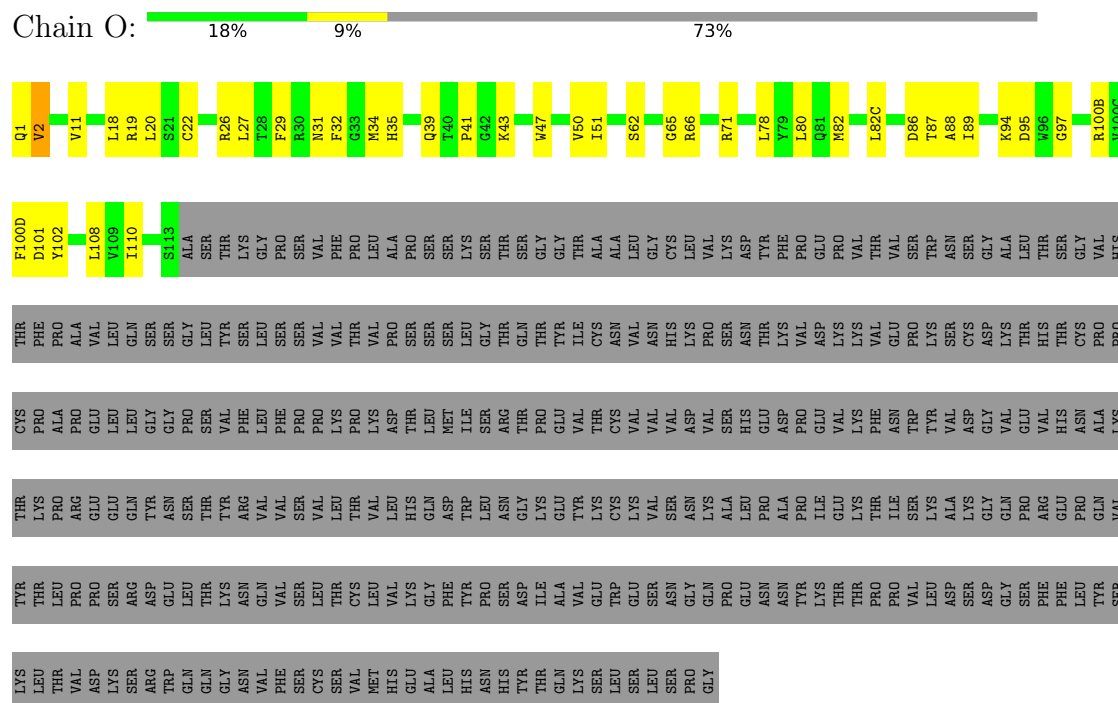
- Molecule 3: 239 Fab heavy chain

[illegible]

- Molecule 3: 239 Fab heavy chain

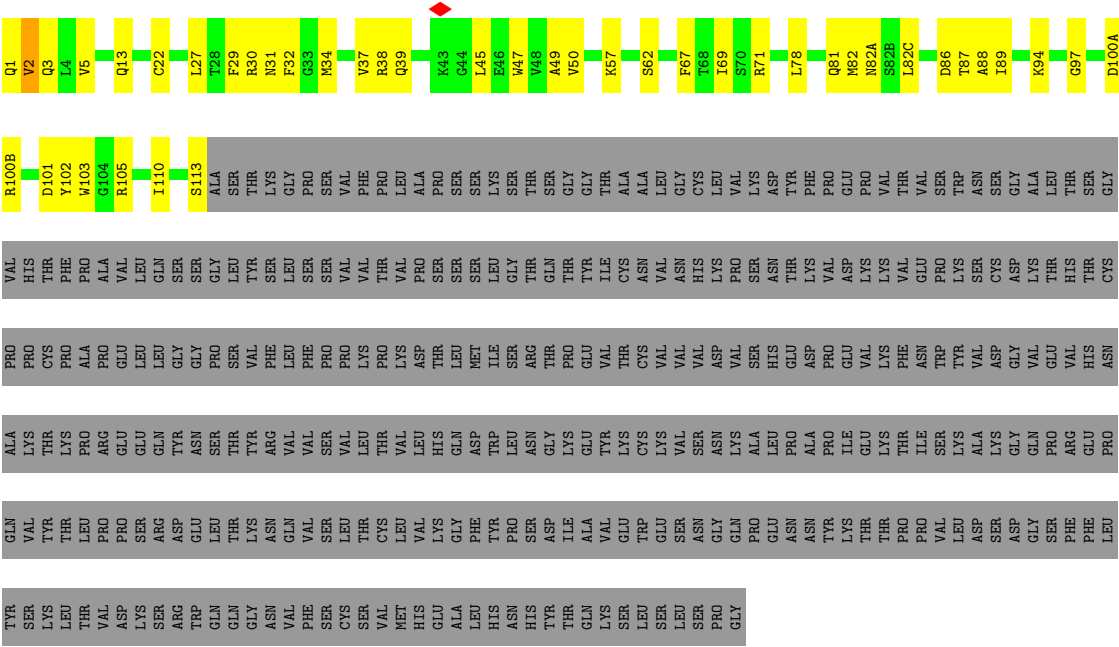


- Molecule 3: 239 Fab heavy chain

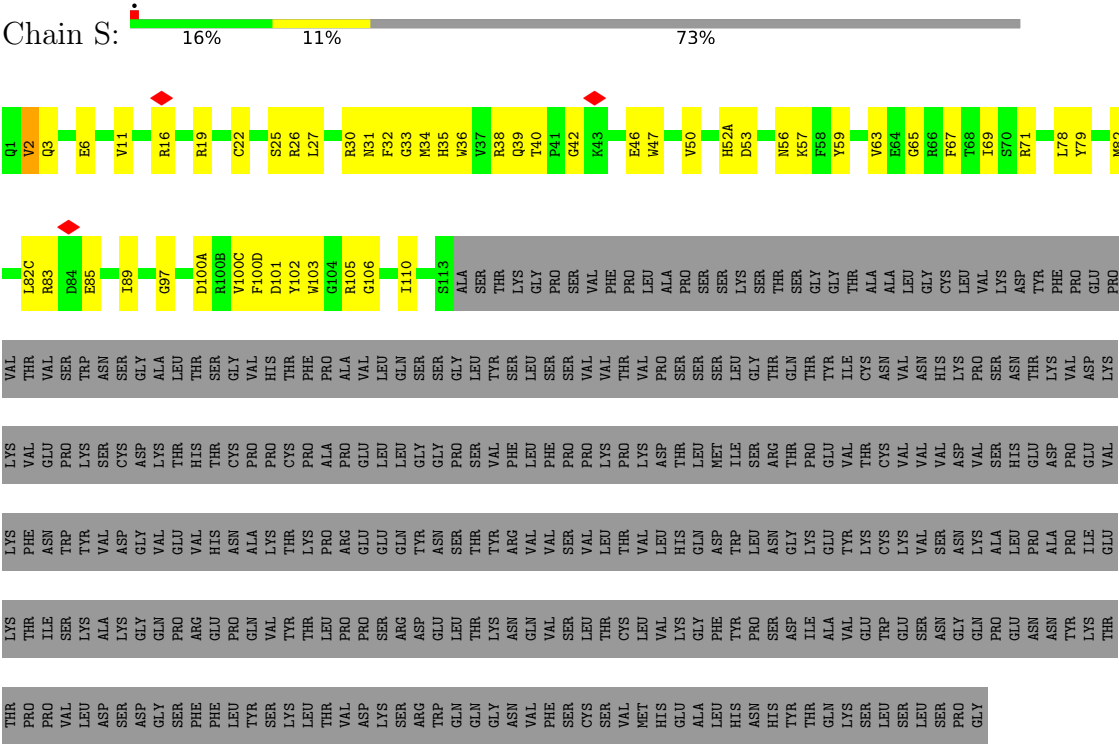


- Molecule 3: 239 Fab heavy chain

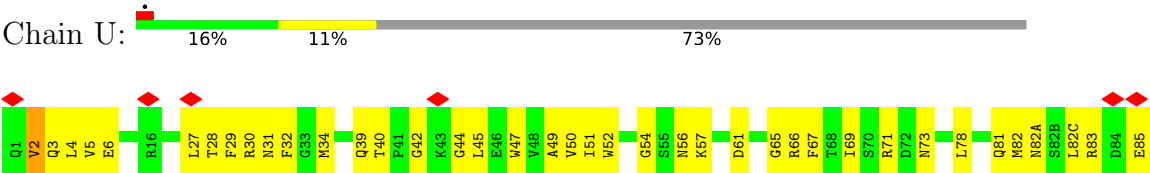




• Molecule 3: 239 Fab heavy chain



• Molecule 3: 239 Fab heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.464	Depositor
Minimum map value	-1.767	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	253.0, 253.0, 253.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	I	0.18	0/583	0.35	0/823
2	B	0.13	0/851	0.39	0/1155
2	D	0.16	0/851	0.43	0/1155
2	F	0.14	0/851	0.44	2/1155 (0.2%)
2	L	0.12	0/851	0.35	0/1155
2	N	0.14	0/851	0.38	0/1155
2	P	0.13	0/851	0.37	0/1155
2	R	0.13	0/851	0.38	0/1155
2	T	0.17	0/851	0.50	0/1155
2	V	0.15	0/851	0.47	0/1155
2	X	0.14	0/851	0.40	0/1155
3	A	0.50	2/983 (0.2%)	0.93	4/1330 (0.3%)
3	C	0.14	0/983	0.42	0/1330
3	E	0.14	0/983	0.36	0/1330
3	H	0.16	0/983	0.44	0/1330
3	M	0.15	0/983	0.39	0/1330
3	O	0.14	0/983	0.36	0/1330
3	Q	0.17	0/983	0.47	0/1330
3	S	0.15	0/983	0.43	0/1330
3	U	0.16	0/983	0.48	0/1330
3	W	0.17	0/983	0.51	0/1330
All	All	0.19	2/18923 (0.0%)	0.46	6/25673 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	41	PRO	CB-CG	-10.93	0.94	1.49
3	A	41	PRO	CG-CD	-9.89	1.17	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	41	PRO	N-CD-CG	-17.55	76.87	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	41	PRO	CA-CB-CG	-16.73	72.71	104.50
3	A	41	PRO	CB-CG-CD	15.23	154.84	106.10
3	A	41	PRO	CA-N-CD	-8.57	100.00	112.00
2	F	38	GLN	CA-C-N	-5.20	112.78	120.68
2	F	38	GLN	C-N-CA	-5.20	112.78	120.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	564	0	484	35	0
2	B	833	0	810	22	0
2	D	833	0	810	18	0
2	F	833	0	810	17	0
2	L	833	0	810	14	0
2	N	833	0	810	13	0
2	P	833	0	810	17	0
2	R	833	0	810	22	0
2	T	833	0	810	29	0
2	V	833	0	810	33	0
2	X	833	0	810	29	0
3	A	960	0	922	30	0
3	C	960	0	922	29	0
3	E	960	0	922	23	0
3	H	960	0	922	21	0
3	M	960	0	922	28	0
3	O	960	0	922	27	0
3	Q	960	0	922	34	0
3	S	960	0	922	44	0
3	U	960	0	922	49	0
3	W	960	0	922	53	0
All	All	18494	0	17804	510	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 14.

All (510) 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:E:82:MET:HB3	3:E:82(C):LEU:HD11	1.58	0.84
2:X:6:GLN:NE2	2:X:88:CYS:SG	2.52	0.82
3:W:33:GLY:HA2	3:W:71:ARG:HH22	1.45	0.82
2:B:6:GLN:HE21	2:B:100:GLN:HG2	1.46	0.80
2:F:3:GLN:HE21	2:F:26:SER:HB3	1.46	0.80
3:S:82:MET:HB3	3:S:82(C):LEU:HD11	1.64	0.79
3:M:51:ILE:HD11	3:M:54:GLY:HA2	1.65	0.78
3:U:6:GLU:OE2	3:U:106:GLY:N	2.14	0.78
2:T:42:LYS:HA	3:S:105:ARG:HH12	1.50	0.77
3:W:89:ILE:HG13	3:W:108:LEU:HD13	1.67	0.76
3:U:6:GLU:N	3:U:6:GLU:OE1	2.17	0.76
3:S:2:VAL:H	3:S:26:ARG:HD3	1.50	0.75
2:T:39:LYS:NZ	2:T:81:ASP:O	2.20	0.75
3:C:87:THR:HG22	3:C:111:VAL:H	1.52	0.74
3:S:85:GLU:N	3:S:85:GLU:OE2	2.21	0.74
3:H:57:LYS:O	3:O:31:ASN:ND2	2.22	0.73
3:U:51:ILE:HD11	3:U:54:GLY:HA2	1.69	0.73
3:Q:82:MET:HB3	3:Q:82(C):LEU:HD11	1.70	0.73
3:S:101:ASP:OD1	3:S:102:TYR:N	2.22	0.73
3:U:31:ASN:ND2	3:W:57:LYS:O	2.23	0.72
2:V:5:THR:O	2:V:24:ARG:N	2.17	0.72
3:A:71:ARG:NH1	3:A:73:ASN:OD1	2.21	0.72
3:M:1:GLN:OE1	3:M:1:GLN:N	2.21	0.72
1:I:75:ASN:ND2	2:X:92:ASN:O	2.23	0.72
2:D:5:THR:HA	2:D:100:GLN:HE22	1.55	0.71
3:U:32:PHE:O	3:U:71:ARG:NH2	2.23	0.71
2:D:6:GLN:NE2	2:D:100:GLN:OE1	2.20	0.71
3:A:32:PHE:O	3:A:71:ARG:NH2	2.24	0.71
3:H:101:ASP:OD1	3:H:102:TYR:N	2.24	0.70
3:Q:81:GLN:NE2	3:Q:82(A):ASN:OD1	2.21	0.70
2:B:3:GLN:HG3	2:B:26:SER:HB3	1.73	0.70
3:Q:32:PHE:O	3:Q:71:ARG:NH2	2.25	0.70
3:C:75:LYS:NZ	3:C:79:TYR:OH	2.25	0.70
3:C:5:VAL:HG22	3:C:105:ARG:HH12	1.57	0.69
2:V:6:GLN:HA	2:V:23:CYS:HA	1.75	0.69
3:E:31:ASN:ND2	3:M:57:LYS:O	2.26	0.69
3:O:66:ARG:NH2	3:O:86:ASP:OD2	2.24	0.69
2:P:22:THR:HG22	2:P:72:THR:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:31:ASN:ND2	3:Q:57:LYS:O	2.25	0.68
3:O:101:ASP:OD1	3:O:102:TYR:N	2.26	0.68
3:C:31:ASN:ND2	3:E:57:LYS:O	2.27	0.68
3:H:82:MET:HB3	3:H:82(C):LEU:HD11	1.73	0.68
2:T:91:TYR:CE1	3:S:100(A):ASP:HA	2.29	0.68
3:U:96:TRP:O	2:X:95(A):ARG:NH2	2.27	0.68
3:O:32:PHE:O	3:O:71:ARG:NH2	2.27	0.67
3:U:29:PHE:O	3:U:71:ARG:NH2	2.24	0.67
2:B:18:ARG:HH22	2:B:20:THR:HG23	1.60	0.67
3:C:22:CYS:HB3	3:C:78:LEU:HB3	1.77	0.66
2:X:82:ASP:O	2:X:86:TYR:OH	2.12	0.66
2:R:1:ASP:OD2	2:R:95(A):ARG:NH1	2.29	0.66
2:X:85:THR:HG22	2:X:103:ARG:HG2	1.78	0.65
1:I:5:ASN:ND2	3:A:98:GLY:O	2.30	0.65
2:P:1:ASP:OD1	2:P:95(A):ARG:NH1	2.30	0.65
2:V:41:GLY:O	3:U:105:ARG:NH1	2.30	0.65
3:E:32:PHE:O	3:E:71:ARG:NH2	2.29	0.65
2:B:1:ASP:OD1	2:B:95(A):ARG:NH1	2.29	0.64
2:X:90:HIS:HD2	2:X:92:ASN:H	1.45	0.64
2:V:29:VAL:HG13	2:V:92:ASN:HB2	1.80	0.64
3:A:101:ASP:OD1	3:A:102:TYR:N	2.30	0.64
2:F:39:LYS:HG2	2:F:84:ALA:HB2	1.79	0.64
3:W:34:MET:HG2	3:W:71:ARG:NH2	2.11	0.64
3:M:22:CYS:HB3	3:M:78:LEU:HB3	1.79	0.64
3:U:83:ARG:HH11	3:U:85:GLU:HG3	1.62	0.64
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.30	0.63
2:B:4:MET:HE1	2:B:90:HIS:HB3	1.79	0.63
2:B:6:GLN:OE1	2:B:102:THR:OG1	2.13	0.63
2:B:6:GLN:HA	2:B:23:CYS:HA	1.79	0.63
2:X:33:LEU:HD21	2:X:88:CYS:HB2	1.79	0.63
3:A:87:THR:HG22	3:A:111:VAL:H	1.64	0.63
3:W:39:GLN:HE21	3:W:43:LYS:HA	1.63	0.63
3:W:94:LYS:HZ1	3:W:102:TYR:HD2	1.46	0.63
3:A:13:GLN:N	3:A:13:GLN:OE1	2.30	0.63
2:P:3:GLN:OE1	2:P:3:GLN:N	2.28	0.63
3:W:91:TYR:HB3	3:W:103:TRP:HZ3	1.64	0.62
3:C:101:ASP:OD2	3:C:102:TYR:N	2.32	0.62
2:X:46:LEU:HD22	3:W:101:ASP:HA	1.81	0.62
3:W:3:GLN:HE21	3:W:105:ARG:HD2	1.64	0.62
2:L:61:ARG:NE	2:L:82:ASP:OD1	2.32	0.62
2:D:39:LYS:NZ	2:D:81:ASP:O	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:23:ALA:HA	3:W:77:THR:HA	1.81	0.61
2:N:4:MET:HE1	2:N:90:HIS:HB3	1.83	0.61
2:X:6:GLN:HE22	2:X:88:CYS:H	1.48	0.61
3:E:89:ILE:HG12	3:E:108:LEU:HD13	1.81	0.61
2:R:61:ARG:NE	2:R:82:ASP:OD1	2.30	0.61
3:E:2:VAL:HG23	3:M:65:GLY:HA3	1.83	0.60
3:M:66:ARG:NH2	3:M:86:ASP:OD2	2.34	0.60
3:C:32:PHE:O	3:C:71:ARG:NH2	2.32	0.60
3:M:101:ASP:OD1	3:M:102:TYR:N	2.35	0.60
2:R:37:GLN:HB3	2:R:47:LEU:HD21	1.83	0.60
3:A:84:ASP:OD1	3:A:85:GLU:N	2.35	0.60
2:V:24:ARG:HH21	2:V:71:PHE:H	1.48	0.60
3:A:3:GLN:OE1	3:A:3:GLN:N	2.35	0.60
2:F:37:GLN:HB3	2:F:47:LEU:HD21	1.84	0.60
2:P:33:LEU:HD21	2:P:88:CYS:HB2	1.84	0.60
3:S:11:VAL:HG22	3:S:110:ILE:HB	1.84	0.60
1:I:27:ASN:ND2	2:N:92:ASN:O	2.36	0.59
2:V:46:LEU:HD22	3:U:101:ASP:HA	1.83	0.59
2:N:106:ILE:HD12	2:N:106:ILE:H	1.68	0.59
2:V:29:VAL:HG11	2:V:90:HIS:HB2	1.85	0.59
3:W:103:TRP:O	3:W:105:ARG:NH2	2.33	0.59
3:S:32:PHE:O	3:S:71:ARG:NH2	2.35	0.59
2:B:33:LEU:HB3	2:B:51:ALA:HB2	1.85	0.59
3:C:2:VAL:HG23	3:E:65:GLY:HA3	1.85	0.59
3:S:3:GLN:N	3:S:3:GLN:OE1	2.31	0.59
3:H:32:PHE:O	3:H:71:ARG:NH2	2.35	0.59
1:I:11:ASN:ND2	2:D:92:ASN:O	2.36	0.59
1:I:77:ASN:OD1	1:I:79:ASN:ND2	2.35	0.59
2:V:82:ASP:O	2:V:86:TYR:OH	2.20	0.59
3:U:66:ARG:HG3	3:U:67:PHE:CD1	2.38	0.58
1:I:67:ASN:ND2	2:V:92:ASN:O	2.35	0.58
3:M:32:PHE:O	3:M:71:ARG:NH2	2.36	0.58
3:S:67:PHE:CE1	3:S:82:MET:HG2	2.38	0.58
3:W:6:GLU:HG3	3:W:22:CYS:SG	2.43	0.58
2:P:4:MET:HE2	2:P:90:HIS:HB3	1.83	0.58
1:I:19:ASN:ND2	2:F:95:SER:O	2.34	0.58
2:F:39:LYS:HB2	2:F:42:LYS:HZ3	1.68	0.58
2:F:61:ARG:NE	2:F:82:ASP:OD1	2.37	0.58
3:O:27:LEU:HD11	3:O:94:LYS:HE2	1.85	0.58
2:T:91:TYR:HE1	3:S:100(A):ASP:HA	1.65	0.58
3:E:101:ASP:OD1	3:E:102:TYR:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:27:LEU:HD11	3:M:94:LYS:HE2	1.86	0.57
3:S:83:ARG:HG3	3:S:85:GLU:OE2	2.04	0.57
2:V:39:LYS:HG3	2:V:42:LYS:HB3	1.86	0.57
3:H:29:PHE:HE1	3:H:34:MET:HE2	1.69	0.57
2:R:6:GLN:OE1	2:R:102:THR:OG1	2.17	0.57
1:I:59:ASN:ND2	2:T:92:ASN:O	2.35	0.57
2:D:38:GLN:HB2	2:D:44:PRO:HB3	1.85	0.57
3:W:68:THR:HB	3:W:81:GLN:HG3	1.85	0.57
2:D:27:GLN:N	2:D:27:GLN:OE1	2.37	0.57
3:U:39:GLN:HB3	3:U:89:ILE:HG23	1.87	0.57
3:W:101:ASP:OD1	3:W:102:TYR:N	2.34	0.57
2:T:2:ILE:HD12	2:T:90:HIS:CE1	2.40	0.57
2:T:18:ARG:HH21	2:T:76:GLY:HA2	1.70	0.57
2:X:21:ILE:HG12	2:X:73:LEU:HB3	1.86	0.57
3:O:51:ILE:HD13	3:O:71:ARG:HB3	1.87	0.56
3:M:2:VAL:HG23	3:O:65:GLY:HA3	1.88	0.56
2:T:85:THR:HG22	2:T:103:ARG:HG2	1.88	0.56
2:X:35:TRP:HD1	2:X:48:ILE:HB	1.70	0.56
3:Q:49:ALA:HB1	3:Q:69:ILE:HD13	1.87	0.56
3:U:101:ASP:OD1	3:U:102:TYR:N	2.36	0.56
2:T:4:MET:HA	2:T:4:MET:HE2	1.85	0.56
3:Q:30:ARG:NE	3:S:56:ASN:OD1	2.39	0.56
2:X:1:ASP:OD1	2:X:95(A):ARG:NH1	2.39	0.56
3:W:6:GLU:CD	3:W:106:GLY:H	2.14	0.56
3:O:22:CYS:HB3	3:O:78:LEU:HB3	1.88	0.56
3:Q:3:GLN:N	3:Q:3:GLN:OE1	2.39	0.56
2:T:2:ILE:HG12	2:T:27:GLN:HE22	1.72	0.55
2:V:58:VAL:HG13	2:V:62:PHE:HD1	1.70	0.55
3:E:38:ARG:NH2	3:E:46:GLU:OE1	2.36	0.55
3:W:51:ILE:HG23	3:W:71:ARG:HH21	1.71	0.55
3:A:27:LEU:HD11	3:A:94:LYS:HG3	1.87	0.55
3:A:39:GLN:HB3	3:A:89:ILE:HG23	1.89	0.54
2:N:33:LEU:HB2	2:N:51:ALA:HB2	1.89	0.54
3:Q:47:TRP:HZ2	3:Q:50:VAL:HG12	1.72	0.54
2:D:100:GLN:CD	2:D:100:GLN:H	2.15	0.54
2:R:6:GLN:HA	2:R:23:CYS:HA	1.89	0.54
3:Q:101:ASP:OD1	3:Q:102:TYR:N	2.38	0.54
1:I:76:ALA:HB3	3:W:52:TRP:HH2	1.72	0.54
3:A:12:VAL:HG21	3:A:82(C):LEU:HD23	1.89	0.54
2:T:78:LEU:HD21	2:T:83:PHE:CZ	2.43	0.54
2:V:1:ASP:OD1	2:V:95(A):ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1:GLN:OE1	3:O:1:GLN:N	2.35	0.54
3:H:1:GLN:O	3:H:2:VAL:HB	2.08	0.54
3:Q:87:THR:HG23	3:Q:110:ILE:HA	1.88	0.54
3:Q:29:PHE:HE1	3:Q:34:MET:HE2	1.72	0.53
2:L:1:ASP:OD1	2:L:95(A):ARG:NH1	2.41	0.53
3:U:29:PHE:HE2	3:U:71:ARG:HG3	1.73	0.53
3:W:32:PHE:CE2	3:W:94:LYS:HD3	2.43	0.53
2:R:8:PRO:HD2	2:R:21:ILE:HD13	1.90	0.53
3:U:40:THR:HG22	3:U:44:GLY:H	1.72	0.53
3:U:47:TRP:HZ2	3:U:50:VAL:HG12	1.72	0.53
3:U:105:ARG:O	3:U:105:ARG:NE	2.42	0.53
1:I:51:ASN:HB3	3:Q:100(B):ARG:HG3	1.91	0.53
3:H:6:GLU:OE2	3:H:6:GLU:N	2.42	0.53
2:T:38:GLN:HB2	2:T:44:PRO:HB3	1.90	0.53
3:W:72:ASP:HB3	3:W:79:TYR:HE2	1.74	0.53
3:E:35:HIS:HB2	3:E:93:ALA:HB3	1.91	0.53
2:X:2:ILE:O	2:X:97:THR:OG1	2.23	0.53
2:L:56:ARG:NH1	3:Q:62:SER:HA	2.24	0.53
3:C:18:LEU:HD12	3:C:19:ARG:H	1.74	0.53
3:U:82:MET:HG2	3:U:82(C):LEU:HD21	1.91	0.53
1:I:43:ASN:ND2	2:L:92:ASN:O	2.41	0.53
2:B:18:ARG:NH2	2:B:20:THR:HG23	2.24	0.53
2:T:1:ASP:OD1	2:T:95(A):ARG:NH1	2.40	0.53
3:U:6:GLU:HG2	3:U:107:THR:OG1	2.09	0.52
1:I:63:ASN:ND2	3:S:97:GLY:HA2	2.25	0.52
3:O:41:PRO:O	3:O:43:LYS:NZ	2.41	0.52
2:V:24:ARG:NH2	2:V:71:PHE:H	2.07	0.52
3:S:36:TRP:HE1	3:S:78:LEU:HD11	1.74	0.52
3:W:35:HIS:CD2	3:W:47:TRP:HE1	2.27	0.52
3:A:2:VAL:HG23	3:C:65:GLY:HA3	1.91	0.52
2:R:21:ILE:HD11	2:R:102:THR:HG21	1.92	0.52
3:O:47:TRP:HZ2	3:O:50:VAL:HG12	1.75	0.52
3:S:22:CYS:HB3	3:S:78:LEU:HB3	1.91	0.52
3:U:40:THR:HG23	3:U:42:GLY:H	1.75	0.52
3:W:81:GLN:HE22	3:W:82(A):ASN:ND2	2.08	0.52
2:T:6:GLN:O	2:T:100:GLN:NE2	2.43	0.52
1:I:77:ASN:ND2	3:W:98:GLY:O	2.43	0.52
3:C:38:ARG:NH1	3:C:46:GLU:OE1	2.43	0.52
3:E:2:VAL:HG13	3:E:27:LEU:HD12	1.91	0.51
2:X:6:GLN:NE2	2:X:99:GLY:HA3	2.26	0.51
3:A:20:LEU:HD12	3:A:82:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2:ILE:HB	2:X:90:HIS:CE1	2.45	0.51
3:W:95:ASP:OD1	3:W:96:TRP:N	2.44	0.51
2:B:91:TYR:HB2	3:A:100(B):ARG:HB2	1.93	0.51
3:W:95:ASP:OD1	3:W:97:GLY:N	2.32	0.51
2:X:33:LEU:HD23	2:X:34:ALA:N	2.26	0.51
1:I:15:ASN:ND2	3:C:97:GLY:HA2	2.25	0.51
3:S:105:ARG:HA	3:S:105:ARG:NE	2.25	0.51
2:P:33:LEU:HD23	2:P:34:ALA:H	1.76	0.51
3:Q:38:ARG:NH1	3:Q:86:ASP:OD1	2.44	0.51
3:H:65:GLY:HA3	3:O:2:VAL:HG23	1.92	0.51
2:N:6:GLN:O	2:N:100:GLN:NE2	2.42	0.51
2:R:18:ARG:NH1	2:R:20:THR:HG23	2.26	0.51
3:U:2:VAL:HG23	3:W:65:GLY:HA3	1.92	0.51
3:U:34:MET:HB3	3:U:78:LEU:HD22	1.92	0.51
2:X:35:TRP:CD1	2:X:48:ILE:HB	2.45	0.51
2:T:37:GLN:HB3	2:T:47:LEU:HD11	1.92	0.51
3:U:89:ILE:HD13	3:U:108:LEU:HB2	1.93	0.51
3:S:34:MET:HG2	3:S:71:ARG:NH2	2.26	0.50
3:S:47:TRP:HZ2	3:S:50:VAL:HG12	1.76	0.50
3:C:95:ASP:OD2	3:C:100(B):ARG:NE	2.32	0.50
2:P:7:SER:O	2:P:22:THR:OG1	2.28	0.50
3:O:11:VAL:HG12	3:O:110:ILE:HB	1.93	0.50
3:H:39:GLN:HB3	3:H:89:ILE:HG23	1.93	0.50
2:B:21:ILE:HG13	2:B:73:LEU:HB2	1.94	0.50
2:D:6:GLN:OE1	2:D:102:THR:OG1	2.17	0.50
3:Q:29:PHE:CE1	3:Q:34:MET:HE2	2.45	0.50
3:W:61:ASP:OD1	3:W:62:SER:N	2.43	0.50
3:A:35:HIS:HB2	3:A:93:ALA:HB3	1.94	0.50
3:E:1:GLN:NE2	3:E:1:GLN:N	2.59	0.50
3:S:6:GLU:CD	3:S:106:GLY:H	2.20	0.50
2:V:66:GLY:HA3	2:V:71:PHE:HA	1.92	0.50
3:U:56:ASN:OD1	3:U:57:LYS:N	2.45	0.50
3:S:2:VAL:HG13	3:S:27:LEU:HD12	1.92	0.50
1:I:79:ASN:ND2	3:W:97:GLY:HA2	2.27	0.50
1:I:50:PRO:HD2	2:R:94:TYR:HA	1.93	0.49
3:A:22:CYS:HB3	3:A:78:LEU:HB3	1.94	0.49
2:R:91:TYR:CE2	3:Q:100(A):ASP:HA	2.47	0.49
3:Q:5:VAL:HG13	3:Q:105:ARG:HH21	1.76	0.49
3:S:78:LEU:HD12	3:S:79:TYR:N	2.27	0.49
3:E:66:ARG:NH2	3:E:86:ASP:OD2	2.45	0.49
2:R:33:LEU:HD23	2:R:89:GLN:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:36:TYR:HB3	2:V:44:PRO:HB2	1.93	0.49
2:B:6:GLN:HB3	2:B:88:CYS:SG	2.53	0.49
2:T:46:LEU:HD13	3:S:100(C):VAL:HG21	1.93	0.49
3:W:37:VAL:HB	3:W:103:TRP:HH2	1.77	0.49
3:C:38:ARG:HD3	3:C:90:TYR:CZ	2.48	0.49
2:T:26:SER:OG	2:T:27:GLN:OE1	2.21	0.49
3:U:29:PHE:CE2	3:U:71:ARG:HG3	2.48	0.49
3:M:82:MET:HB2	3:M:82(C):LEU:HD11	1.95	0.49
2:T:79:GLN:HG3	2:T:81:ASP:H	1.77	0.49
3:A:1:GLN:HE21	3:A:1:GLN:H1	1.59	0.48
2:T:27:GLN:OE1	2:T:27:GLN:N	2.45	0.48
3:W:93:ALA:HB1	3:W:100(D):PHE:CD2	2.48	0.48
3:C:82:MET:HB3	3:C:82(C):LEU:HD21	1.94	0.48
3:S:38:ARG:HB3	3:S:46:GLU:HG3	1.93	0.48
3:M:39:GLN:HE21	3:M:43:LYS:HE3	1.78	0.48
2:V:77:SER:O	2:V:79:GLN:NE2	2.47	0.48
1:I:35:ASN:ND2	2:P:92:ASN:O	2.44	0.48
2:V:18:ARG:HD2	2:V:75:ILE:O	2.14	0.48
2:F:1:ASP:OD1	2:F:95(A):ARG:NH1	2.47	0.48
3:M:16:ARG:O	3:M:82(C):LEU:HD13	2.13	0.48
3:M:84:ASP:O	3:M:87:THR:HG22	2.14	0.48
3:W:3:GLN:NE2	3:W:105:ARG:HD2	2.26	0.48
3:H:2:VAL:HG22	3:H:27:LEU:HB2	1.96	0.48
3:Q:1:GLN:O	3:Q:2:VAL:HB	2.13	0.48
3:S:31:ASN:ND2	3:U:57:LYS:O	2.46	0.48
1:I:75:ASN:O	3:W:100(B):ARG:NH1	2.39	0.48
3:C:18:LEU:HD12	3:C:19:ARG:N	2.29	0.48
1:I:76:ALA:HB3	3:W:52:TRP:CH2	2.47	0.48
2:B:37:GLN:HB3	2:B:47:LEU:HD21	1.95	0.48
3:U:3:GLN:OE1	3:U:5:VAL:HG23	2.14	0.48
2:R:75:ILE:HD11	2:R:86:TYR:HE1	1.78	0.47
3:U:27:LEU:HD11	3:U:94:LYS:HG3	1.95	0.47
3:S:52(A):HIS:ND1	3:S:53:ASP:OD2	2.47	0.47
3:U:83:ARG:HH11	3:U:83:ARG:HG3	1.79	0.47
1:I:51:ASN:ND2	2:R:95:SER:O	2.47	0.47
3:O:87:THR:HG23	3:O:110:ILE:HA	1.96	0.47
3:U:51:ILE:HD12	3:U:52:TRP:H	1.80	0.47
1:I:69:ASN:ND2	3:U:98:GLY:O	2.47	0.47
2:N:91:TYR:CE2	3:M:100(A):ASP:HA	2.49	0.47
3:Q:2:VAL:HG23	3:S:65:GLY:HA3	1.96	0.47
2:B:100:GLN:OE1	2:B:100:GLN:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:HIS:HB2	3:C:93:ALA:HB3	1.96	0.47
2:F:56:ARG:NH1	3:M:62:SER:HA	2.30	0.47
3:E:1:GLN:N	3:E:26:ARG:HE	2.11	0.47
3:M:2:VAL:HG13	3:M:27:LEU:HD12	1.97	0.47
2:V:24:ARG:HG2	2:V:24:ARG:HH11	1.79	0.47
2:V:41:GLY:C	3:U:105:ARG:HH12	2.22	0.47
3:W:27:LEU:HD11	3:W:94:LYS:HE2	1.95	0.47
2:D:55:TYR:OH	2:D:56:ARG:NH2	2.48	0.47
3:E:1:GLN:NE2	3:E:1:GLN:H3	2.13	0.47
2:X:15:VAL:HA	2:X:78:LEU:HD22	1.95	0.47
2:L:38:GLN:HB2	2:L:44:PRO:HB3	1.97	0.47
2:N:56:ARG:NH1	3:O:62:SER:HA	2.29	0.47
3:M:67:PHE:CZ	3:M:82:MET:HG2	2.50	0.47
3:Q:13:GLN:HE22	3:Q:113:SER:HB3	1.79	0.47
2:F:6:GLN:OE1	2:F:102:THR:N	2.48	0.47
2:P:4:MET:HE1	2:P:25:ALA:HB2	1.96	0.47
3:C:1:GLN:O	3:C:2:VAL:HB	2.15	0.47
2:N:61:ARG:NE	2:N:82:ASP:OD1	2.33	0.47
3:U:40:THR:HG23	3:U:42:GLY:N	2.30	0.47
2:L:77:SER:O	2:L:79:GLN:NE2	2.48	0.46
2:L:91:TYR:CE2	3:H:100(A):ASP:HA	2.50	0.46
2:T:24:ARG:NE	2:T:70:GLU:OE1	2.48	0.46
1:I:77:ASN:HD22	3:W:99:ALA:HA	1.80	0.46
2:P:47:LEU:HA	2:P:58:VAL:HG21	1.97	0.46
2:V:42:LYS:HZ2	2:V:43:ALA:HB3	1.79	0.46
2:D:6:GLN:NE2	2:D:101:GLY:H	2.14	0.46
3:U:28:THR:HG21	3:W:57:LYS:O	2.16	0.46
1:I:31:ASN:ND2	3:M:97:GLY:HA2	2.29	0.46
3:C:27:LEU:HD11	3:C:94:LYS:HG3	1.98	0.46
2:R:95(A):ARG:HB3	3:Q:47:TRP:HZ3	1.79	0.46
3:Q:22:CYS:HB3	3:Q:78:LEU:HB3	1.98	0.46
3:W:83:ARG:NH2	3:W:85:GLU:OE2	2.41	0.46
3:S:25:SER:O	3:S:26:ARG:HG2	2.15	0.46
2:F:37:GLN:HB2	2:F:86:TYR:CE2	2.50	0.46
3:S:16:ARG:O	3:S:82(C):LEU:HD13	2.16	0.46
3:H:47:TRP:HZ2	3:H:50:VAL:HG12	1.80	0.46
3:O:20:LEU:HD12	3:O:80:LEU:HD22	1.98	0.46
3:Q:67:PHE:CE1	3:Q:82:MET:HG2	2.51	0.46
2:B:61:ARG:NE	2:B:82:ASP:OD2	2.49	0.45
3:O:35:HIS:HE2	3:O:95:ASP:HB2	1.81	0.45
3:Q:27:LEU:HD11	3:Q:94:LYS:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1:GLN:H1	3:A:1:GLN:NE2	2.14	0.45
3:C:108:LEU:HD12	3:C:109:VAL:N	2.31	0.45
2:F:2:ILE:HD12	2:F:90:HIS:CE1	2.51	0.45
2:N:36:TYR:HE1	2:N:46:LEU:HD13	1.81	0.45
3:W:60:ALA:HB3	3:W:63:VAL:HG22	1.97	0.45
3:A:108:LEU:HD12	3:A:109:VAL:N	2.32	0.45
3:O:1:GLN:H3	3:O:26:ARG:HE	1.63	0.45
2:V:34:ALA:N	2:V:89:GLN:O	2.46	0.45
2:X:90:HIS:CD2	2:X:92:ASN:H	2.29	0.45
3:A:12:VAL:HA	3:A:16:ARG:NH2	2.32	0.45
2:F:78:LEU:HD12	2:F:78:LEU:HA	1.84	0.45
2:V:33:LEU:HD12	2:V:89:GLN:O	2.17	0.45
1:I:52:ALA:O	1:I:54:PRO:HD3	2.17	0.45
2:P:33:LEU:HD23	2:P:34:ALA:N	2.31	0.45
3:U:51:ILE:HB	3:U:69:ILE:HD12	1.98	0.45
3:H:18:LEU:HD12	3:H:19:ARG:H	1.82	0.45
2:B:35:TRP:CD1	2:B:73:LEU:HD21	2.52	0.45
3:Q:39:GLN:HB2	3:Q:45:LEU:HD23	1.99	0.45
2:L:19:VAL:HG22	2:L:78:LEU:HD11	1.98	0.45
3:A:53:ASP:OD1	3:A:53:ASP:C	2.60	0.45
2:D:18:ARG:HG3	2:D:18:ARG:HH11	1.81	0.45
2:T:33:LEU:HD22	2:T:71:PHE:CG	2.52	0.45
3:U:81:GLN:CD	3:U:82(A):ASN:HD21	2.25	0.45
2:X:98:PHE:CD1	3:W:45:LEU:HB2	2.52	0.45
1:I:7:ASN:ND2	3:A:97:GLY:HA2	2.32	0.45
1:I:55:ASN:ND2	3:Q:97:GLY:HA2	2.32	0.45
2:X:87:TYR:HD2	2:X:98:PHE:CD1	2.35	0.45
2:X:89:GLN:HB2	2:X:98:PHE:CE2	2.51	0.45
2:N:47:LEU:HA	2:N:58:VAL:HG21	1.98	0.44
2:T:43:ALA:H	3:S:105:ARG:HH22	1.64	0.44
3:W:4:LEU:HD22	3:W:22:CYS:SG	2.57	0.44
3:H:29:PHE:CE1	3:H:34:MET:HE2	2.51	0.44
1:I:19:ASN:HB3	3:E:100(B):ARG:HG3	1.99	0.44
1:I:35:ASN:ND2	2:P:95:SER:O	2.50	0.44
2:L:24:ARG:NH2	2:L:70:GLU:OE1	2.50	0.44
2:D:2:ILE:HG23	2:D:26:SER:OG	2.17	0.44
3:S:39:GLN:HB3	3:S:89:ILE:HG23	2.00	0.44
3:S:40:THR:HG23	3:S:42:GLY:H	1.82	0.44
3:H:22:CYS:HB3	3:H:78:LEU:HB3	1.98	0.44
3:Q:39:GLN:HB3	3:Q:89:ILE:HG23	2.00	0.44
3:H:95:ASP:OD2	3:H:100(B):ARG:NE	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:LEU:HD12	2:F:62:PHE:CD2	2.52	0.44
3:E:87:THR:HG23	3:E:110:ILE:HA	1.98	0.44
3:S:59:TYR:HE2	3:S:69:ILE:HG23	1.83	0.44
1:I:78:PRO:HB2	3:W:33:GLY:HA3	1.99	0.44
3:O:29:PHE:CE1	3:O:34:MET:HE2	2.52	0.44
2:B:61:ARG:NH2	2:B:82:ASP:OD1	2.51	0.44
3:S:26:ARG:NE	3:U:65:GLY:O	2.49	0.44
2:L:33:LEU:HD23	2:L:89:GLN:O	2.17	0.44
3:H:39:GLN:O	3:H:88:ALA:HB1	2.18	0.44
2:R:55:TYR:CG	2:R:56:ARG:N	2.85	0.44
2:T:21:ILE:HD12	2:T:86:TYR:HD2	1.83	0.44
2:B:33:LEU:HD12	2:B:89:GLN:O	2.18	0.43
2:D:1:ASP:OD1	2:D:95(A):ARG:NH1	2.42	0.43
3:W:39:GLN:HB2	3:W:45:LEU:HD13	2.00	0.43
2:P:6:GLN:HA	2:P:23:CYS:HA	2.00	0.43
2:X:38:GLN:HB2	2:X:44:PRO:HB3	1.99	0.43
3:C:12:VAL:O	3:C:111:VAL:HA	2.18	0.43
2:V:24:ARG:HH21	2:V:70:GLU:HA	1.84	0.43
3:U:78:LEU:HD23	3:U:92:CYS:SG	2.58	0.43
2:P:98:PHE:HZ	3:O:100(D):PHE:HE2	1.66	0.43
3:C:39:GLN:HB3	3:C:89:ILE:CG2	2.49	0.43
2:F:47:LEU:HD12	2:F:62:PHE:HD2	1.83	0.43
2:R:100:GLN:CD	2:R:100:GLN:H	2.25	0.43
3:Q:39:GLN:O	3:Q:88:ALA:HB1	2.19	0.43
3:S:63:VAL:HB	3:S:67:PHE:CD2	2.54	0.43
2:V:2:ILE:HB	2:V:90:HIS:CE1	2.53	0.43
2:V:37:GLN:HE21	2:V:45:ASN:HB2	1.84	0.43
1:I:78:PRO:HA	3:W:52:TRP:CE3	2.53	0.43
1:I:39:ASN:ND2	3:O:97:GLY:HA2	2.32	0.43
2:F:106:ILE:HD12	2:F:106:ILE:H	1.83	0.43
2:R:80:PRO:HA	2:R:83:PHE:HE2	1.83	0.43
3:W:38:ARG:HH12	3:W:86:ASP:C	2.27	0.43
2:R:38:GLN:HE21	2:R:87:TYR:HE1	1.67	0.43
2:X:66:GLY:HA3	2:X:71:PHE:HA	2.01	0.43
2:P:47:LEU:O	2:P:48:ILE:HD13	2.18	0.43
3:S:33:GLY:HA2	3:S:71:ARG:HH22	1.82	0.43
2:D:6:GLN:HA	2:D:23:CYS:HA	2.00	0.42
2:N:3:GLN:HG3	2:N:26:SER:HB3	2.01	0.42
3:O:18:LEU:HD23	3:O:19:ARG:N	2.34	0.42
2:T:75:ILE:HD13	2:T:75:ILE:HA	1.79	0.42
2:V:47:LEU:HD23	2:V:62:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:35:HIS:CD2	3:W:50:VAL:HB	2.54	0.42
3:A:2:VAL:H	3:A:26:ARG:HD3	1.84	0.42
3:S:35:HIS:CG	3:S:100(D):PHE:HE1	2.37	0.42
3:C:47:TRP:HZ2	3:C:50:VAL:HG12	1.84	0.42
3:O:82:MET:HB2	3:O:82(C):LEU:HD11	2.00	0.42
3:Q:2:VAL:HG22	3:Q:27:LEU:HB2	2.00	0.42
2:T:43:ALA:H	3:S:105:ARG:NH2	2.17	0.42
2:L:18:ARG:NH1	2:L:18:ARG:HB3	2.34	0.42
3:A:47:TRP:HZ2	3:A:50:VAL:HG12	1.84	0.42
2:D:106:ILE:HD12	2:D:107:LYS:H	1.84	0.42
3:O:39:GLN:O	3:O:88:ALA:HB1	2.20	0.42
2:D:33:LEU:HD22	2:D:71:PHE:CG	2.54	0.42
3:C:82(C):LEU:HB3	3:C:111:VAL:HG21	2.02	0.42
2:N:98:PHE:HZ	3:M:100(D):PHE:HE2	1.67	0.42
2:L:17:ASP:OD1	2:L:18:ARG:N	2.50	0.42
2:V:20:THR:HG22	2:V:74:THR:HG23	2.01	0.42
2:X:17:ASP:OD1	2:X:18:ARG:N	2.51	0.42
3:W:66:ARG:HG3	3:W:67:PHE:CD1	2.55	0.42
2:B:35:TRP:CH2	2:B:88:CYS:HB3	2.55	0.42
3:E:75:LYS:HE3	3:E:77:THR:HG21	2.00	0.42
2:B:37:GLN:HG3	2:B:84:ALA:HB3	2.02	0.42
2:F:37:GLN:HB2	2:F:86:TYR:HE2	1.85	0.42
3:M:13:GLN:OE1	3:M:16:ARG:NE	2.53	0.42
3:S:19:ARG:HD2	3:S:79:TYR:HD1	1.84	0.42
2:X:48:ILE:HD13	2:X:54:LEU:HA	2.02	0.42
1:I:8:VAL:HG22	3:A:52(A):HIS:CG	2.55	0.42
3:M:18:LEU:HD12	3:M:19:ARG:H	1.85	0.42
3:U:82:MET:HG3	3:U:82(C):LEU:HD11	2.01	0.42
3:C:2:VAL:HG11	3:C:27:LEU:HD12	2.02	0.41
3:E:6:GLU:HB2	3:E:107:THR:OG1	2.19	0.41
3:M:35:HIS:CG	3:M:100(D):PHE:HE1	2.38	0.41
3:U:4:LEU:HD11	3:U:34:MET:HE1	2.02	0.41
3:W:94:LYS:NZ	3:W:102:TYR:HD2	2.17	0.41
3:M:47:TRP:HZ2	3:M:50:VAL:HG12	1.86	0.41
3:M:51:ILE:HD13	3:M:57:LYS:HG2	2.02	0.41
3:Q:27:LEU:HD11	3:Q:94:LYS:HE2	2.02	0.41
2:V:24:ARG:HG2	2:V:24:ARG:NH1	2.35	0.41
3:U:49:ALA:HB1	3:U:69:ILE:HD13	2.02	0.41
3:H:45:LEU:HD23	3:H:45:LEU:HA	1.80	0.41
2:T:47:LEU:HD23	2:T:62:PHE:CD1	2.55	0.41
2:L:4:MET:HE1	2:L:25:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:PRO:HG2	2:D:11:LEU:HB2	2.02	0.41
3:M:61:ASP:OD2	3:M:62:SER:N	2.53	0.41
2:P:24:ARG:HG3	2:P:24:ARG:HH11	1.84	0.41
3:U:61:ASP:OD2	3:U:61:ASP:N	2.52	0.41
2:B:78:LEU:HD12	2:B:79:GLN:N	2.35	0.41
3:A:19:ARG:HE	3:A:81:GLN:HB2	1.86	0.41
3:A:66:ARG:HB3	3:A:82(A):ASN:O	2.19	0.41
3:C:39:GLN:O	3:C:88:ALA:HB1	2.21	0.41
3:E:39:GLN:O	3:E:88:ALA:HB1	2.19	0.41
2:X:87:TYR:CE2	3:W:45:LEU:HD23	2.55	0.41
3:O:89:ILE:HG12	3:O:108:LEU:HD13	2.02	0.41
3:Q:31:ASN:ND2	3:S:57:LYS:O	2.53	0.41
2:L:8:PRO:HG2	2:L:11:LEU:HB2	2.02	0.41
3:S:30:ARG:H	3:S:30:ARG:HG2	1.72	0.41
3:U:29:PHE:HE1	3:U:34:MET:HE2	1.86	0.41
3:U:30:ARG:HB2	3:U:73:ASN:CG	2.45	0.41
3:U:96:TRP:CD1	3:U:96:TRP:C	2.98	0.41
3:W:47:TRP:HZ2	3:W:50:VAL:HG12	1.85	0.41
2:B:96:ILE:HD12	3:A:47:TRP:CD2	2.55	0.41
3:E:47:TRP:HZ2	3:E:50:VAL:HG12	1.85	0.41
2:R:89:GLN:HG3	2:R:98:PHE:CZ	2.56	0.41
3:Q:37:VAL:HG11	3:Q:103:TRP:CH2	2.56	0.41
3:S:40:THR:HG23	3:S:42:GLY:N	2.35	0.41
2:V:6:GLN:HB3	2:V:88:CYS:SG	2.60	0.41
2:V:44:PRO:HG3	3:U:45:LEU:HD11	2.02	0.41
3:E:35:HIS:CG	3:E:100(D):PHE:HE1	2.39	0.41
3:M:59:TYR:CE2	3:M:69:ILE:HG22	2.56	0.41
2:R:4:MET:HE2	2:R:4:MET:HA	2.03	0.41
2:R:83:PHE:CE1	2:R:106:ILE:HG13	2.56	0.41
3:Q:30:ARG:CZ	3:Q:30:ARG:HB3	2.51	0.41
3:S:34:MET:HE3	3:S:34:MET:HB3	1.93	0.41
3:U:4:LEU:HD23	3:U:4:LEU:HA	1.89	0.41
3:U:82:MET:HE3	3:U:82:MET:HB2	1.66	0.41
3:C:45:LEU:HD23	3:C:45:LEU:HA	1.78	0.41
2:R:38:GLN:HE22	3:Q:39:GLN:HE22	1.69	0.41
2:T:38:GLN:HE21	2:T:87:TYR:HE1	1.69	0.41
2:V:2:ILE:HG13	2:V:27:GLN:OE1	2.20	0.41
3:W:96:TRP:N	3:W:100(C):VAL:O	2.54	0.41
2:D:91:TYR:CE2	3:C:100(A):ASP:HA	2.55	0.40
3:C:27:LEU:HD23	3:C:28:THR:C	2.46	0.40
2:P:10:THR:O	2:P:11:LEU:HD23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:73:LEU:HD12	2:X:73:LEU:HA	1.93	0.40
1:I:70:PRO:HB2	3:U:52:TRP:HA	2.02	0.40
3:A:15:GLY:N	3:A:82(C):LEU:O	2.42	0.40
2:F:46:LEU:C	2:F:47:LEU:HD22	2.47	0.40
3:W:29:PHE:HZ	3:W:78:LEU:HB2	1.86	0.40
3:W:82(C):LEU:HA	3:W:82(C):LEU:HD22	1.89	0.40
1:I:57:ASN:HD21	2:T:93:SER:HB3	1.87	0.40
1:I:75:ASN:ND2	2:X:95:SER:O	2.50	0.40
3:H:87:THR:HG23	3:H:110:ILE:HA	2.03	0.40
3:E:27:LEU:HD11	3:E:94:LYS:HE2	2.02	0.40
3:S:100(D):PHE:HB2	3:S:103:TRP:NE1	2.36	0.40
3:W:82(C):LEU:HD12	3:W:111:VAL:HG21	2.03	0.40
2:N:39:LYS:HE3	2:N:39:LYS:HB2	1.90	0.40
3:M:36:TRP:HD1	3:M:69:ILE:HD12	1.85	0.40
3:O:95:ASP:OD2	3:O:100(B):ARG:NE	2.36	0.40
2:V:103:ARG:HD2	2:V:104:LEU:N	2.35	0.40
3:A:52(A):HIS:CE1	3:A:53:ASP:HB3	2.56	0.40
3:O:29:PHE:HE1	3:O:34:MET:HE2	1.86	0.40
2:T:11:LEU:HD11	2:T:19:VAL:HG23	2.03	0.40
2:V:42:LYS:HA	2:V:42:LYS:HD2	1.92	0.40
3:W:91:TYR:HB3	3:W:103:TRP:CZ3	2.49	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	I	78/278 (28%)	67 (86%)	11 (14%)	0	100	100
2	B	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
2	D	106/215 (49%)	102 (96%)	4 (4%)	0	100	100
2	F	106/215 (49%)	103 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
2	N	106/215 (49%)	102 (96%)	4 (4%)	0	100	100
2	P	106/215 (49%)	102 (96%)	4 (4%)	0	100	100
2	R	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
2	T	106/215 (49%)	99 (93%)	7 (7%)	0	100	100
2	V	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
2	X	106/215 (49%)	100 (94%)	6 (6%)	0	100	100
3	A	119/450 (26%)	114 (96%)	4 (3%)	1 (1%)	16	47
3	C	119/450 (26%)	112 (94%)	6 (5%)	1 (1%)	16	47
3	E	119/450 (26%)	117 (98%)	1 (1%)	1 (1%)	16	47
3	H	119/450 (26%)	116 (98%)	2 (2%)	1 (1%)	16	47
3	M	119/450 (26%)	116 (98%)	2 (2%)	1 (1%)	16	47
3	O	119/450 (26%)	117 (98%)	1 (1%)	1 (1%)	16	47
3	Q	119/450 (26%)	114 (96%)	4 (3%)	1 (1%)	16	47
3	S	119/450 (26%)	114 (96%)	4 (3%)	1 (1%)	16	47
3	U	119/450 (26%)	112 (94%)	6 (5%)	1 (1%)	16	47
3	W	119/450 (26%)	114 (96%)	4 (3%)	1 (1%)	16	47
All	All	2328/6928 (34%)	2233 (96%)	85 (4%)	10 (0%)	31	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	2	VAL
3	H	2	VAL
3	C	2	VAL
3	O	2	VAL
3	A	2	VAL
3	E	2	VAL
3	M	2	VAL
3	S	2	VAL
3	U	2	VAL
3	W	2	VAL

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	I	62/240 (26%)	62 (100%)	0	100	100
2	B	93/189 (49%)	93 (100%)	0	100	100
2	D	93/189 (49%)	93 (100%)	0	100	100
2	F	93/189 (49%)	92 (99%)	1 (1%)	65	73
2	L	93/189 (49%)	92 (99%)	1 (1%)	65	73
2	N	93/189 (49%)	93 (100%)	0	100	100
2	P	93/189 (49%)	93 (100%)	0	100	100
2	R	93/189 (49%)	92 (99%)	1 (1%)	65	73
2	T	93/189 (49%)	93 (100%)	0	100	100
2	V	93/189 (49%)	93 (100%)	0	100	100
2	X	93/189 (49%)	92 (99%)	1 (1%)	65	73
3	A	101/399 (25%)	101 (100%)	0	100	100
3	C	101/399 (25%)	101 (100%)	0	100	100
3	E	101/399 (25%)	100 (99%)	1 (1%)	68	74
3	H	101/399 (25%)	101 (100%)	0	100	100
3	M	101/399 (25%)	101 (100%)	0	100	100
3	O	101/399 (25%)	101 (100%)	0	100	100
3	Q	101/399 (25%)	101 (100%)	0	100	100
3	S	101/399 (25%)	101 (100%)	0	100	100
3	U	101/399 (25%)	101 (100%)	0	100	100
3	W	101/399 (25%)	101 (100%)	0	100	100
All	All	2002/6120 (33%)	1997 (100%)	5 (0%)	85	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	3	GLN

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Mol	Chain	Res	Type
2	F	78	LEU
3	E	1	GLN
2	R	33	LEU
2	X	50	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	39	ASN
1	I	55	ASN
2	L	79	GLN
3	A	1	GLN
3	A	52(A)	HIS
2	F	3	GLN
2	F	37	GLN
2	F	50	GLN
2	N	37	GLN
2	N	38	GLN
2	N	50	GLN
3	M	82(A)	ASN
3	S	13	GLN
2	V	37	GLN
3	U	82(A)	ASN
2	X	38	GLN
2	X	50	GLN
2	X	90	HIS
3	W	3	GLN
3	W	35	HIS
3	W	39	GLN
3	W	82(A)	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

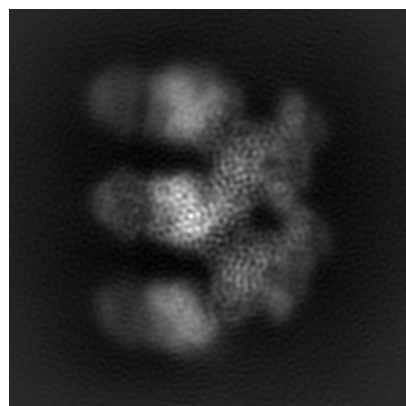
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27784. These allow visual inspection of the internal detail of the map and identification of artifacts.

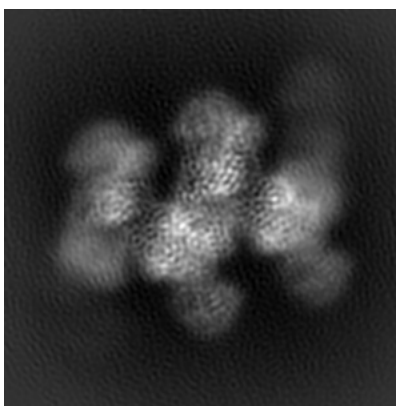
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

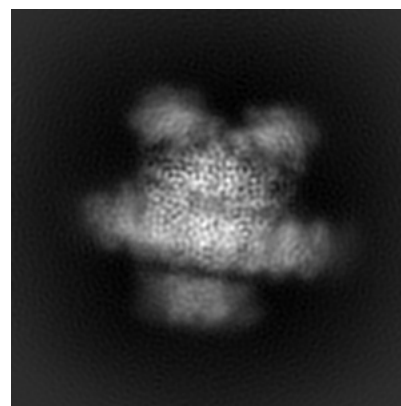
6.1.1 Primary map



X

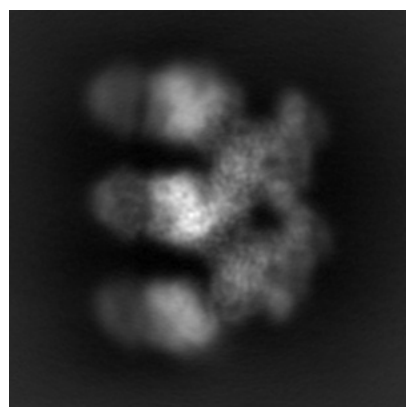


Y

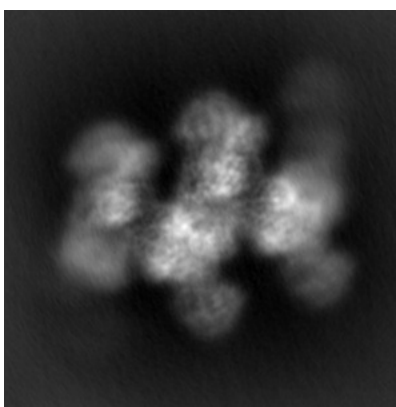


Z

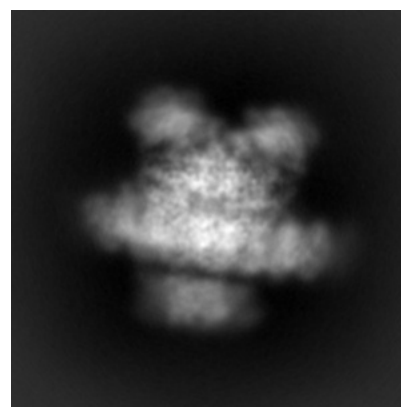
6.1.2 Raw map



X



Y

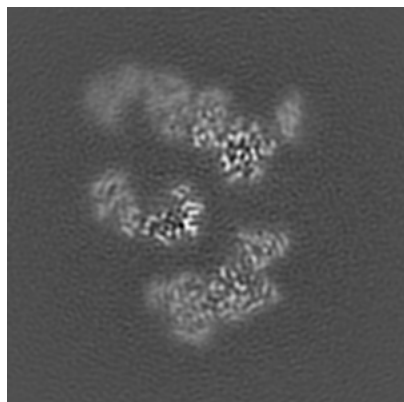


Z

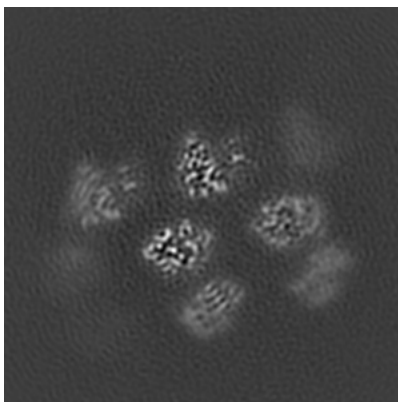
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

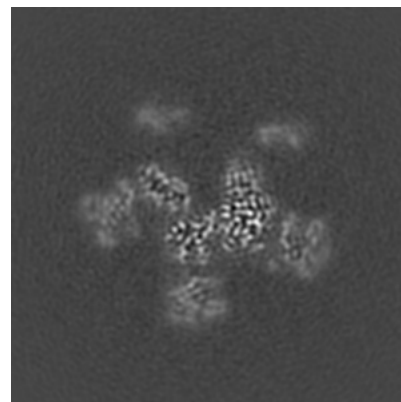
6.2.1 Primary map



X Index: 110

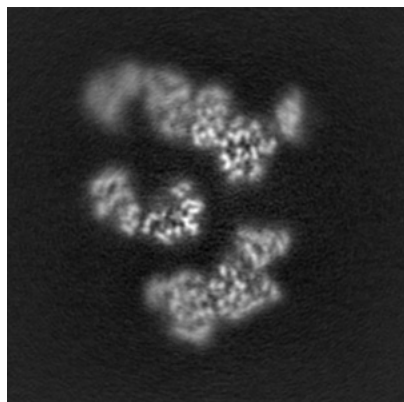


Y Index: 110

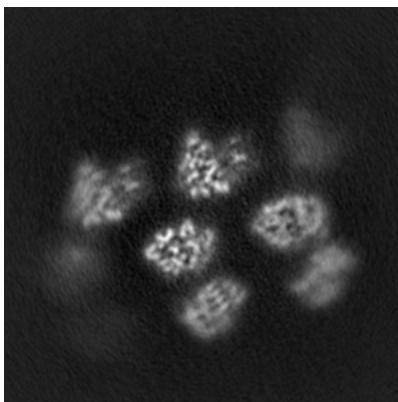


Z Index: 110

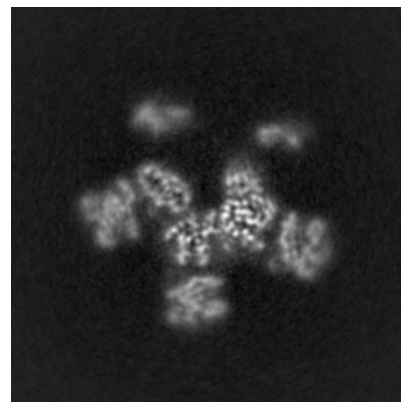
6.2.2 Raw map



X Index: 110



Y Index: 110

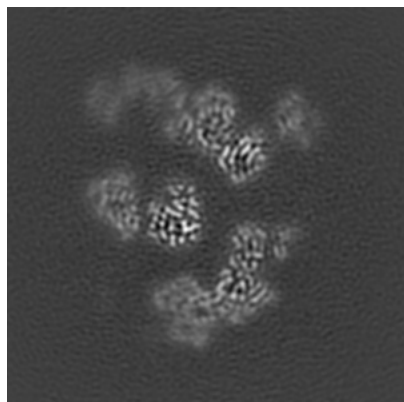


Z Index: 110

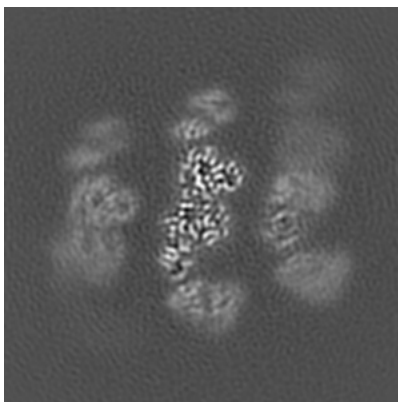
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

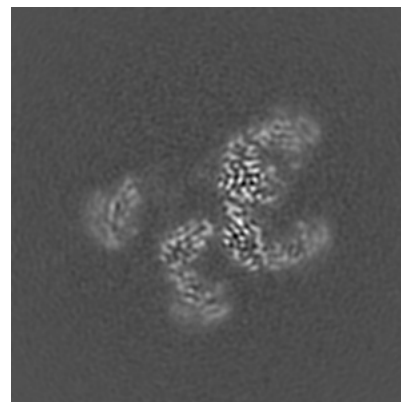
6.3.1 Primary map



X Index: 106

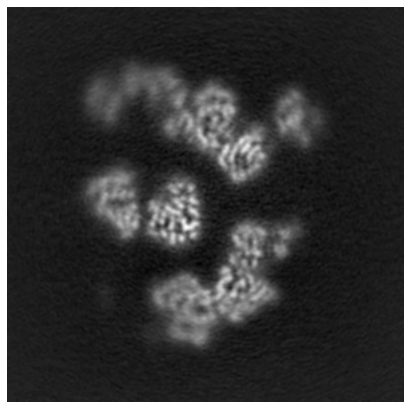


Y Index: 99

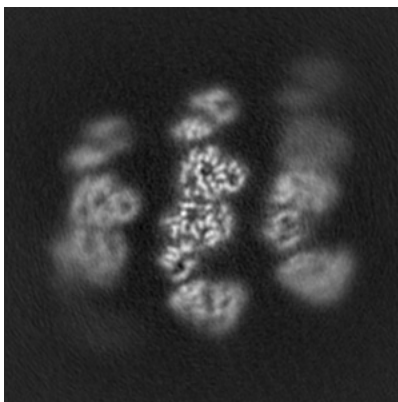


Z Index: 120

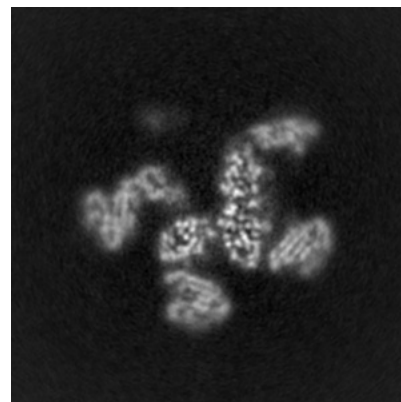
6.3.2 Raw map



X Index: 106



Y Index: 99

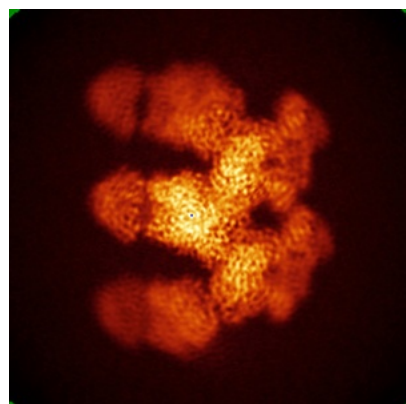


Z Index: 116

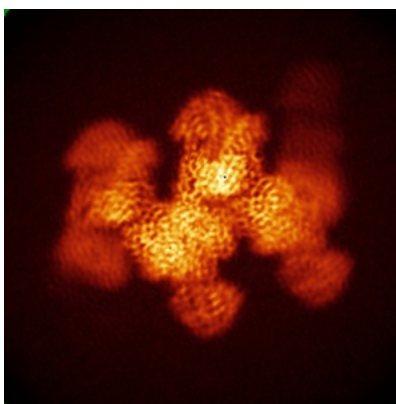
The images above show the largest variance slices of the map in three orthogonal directions.

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

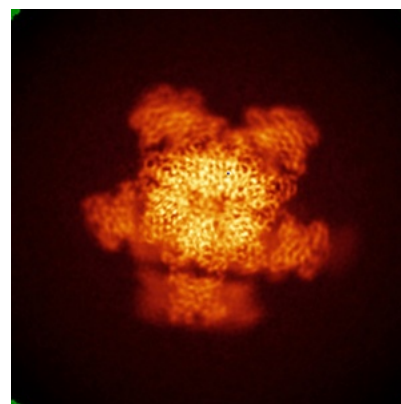
6.4.1 Primary map



X

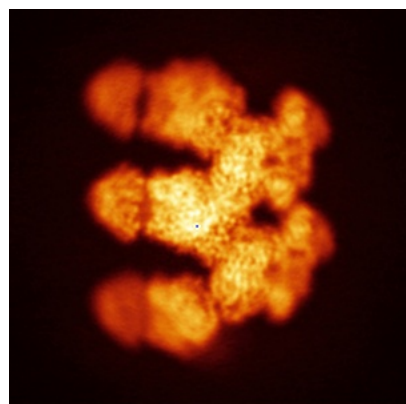


Y

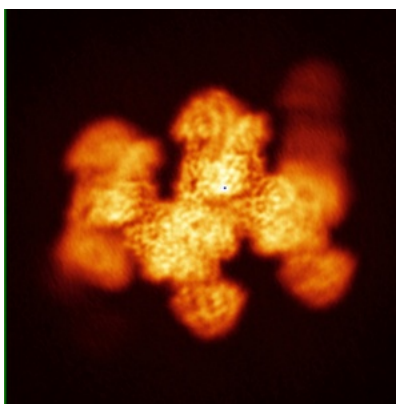


Z

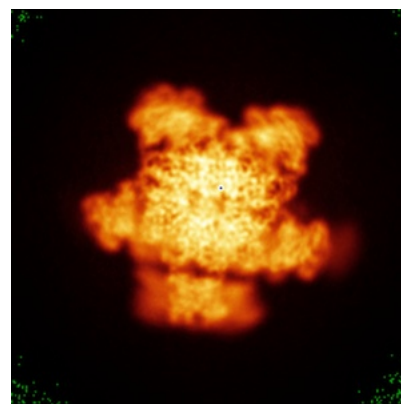
6.4.2 Raw map



X



Y

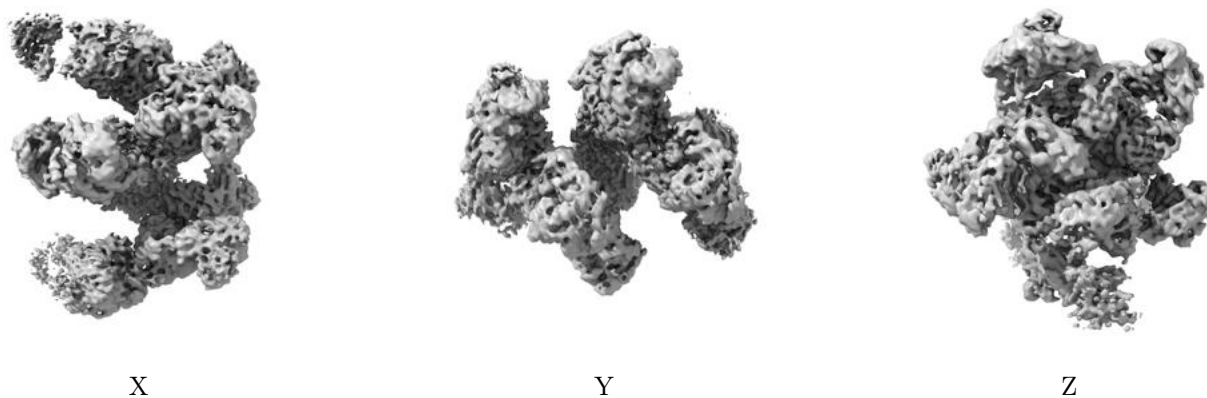


Z

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.

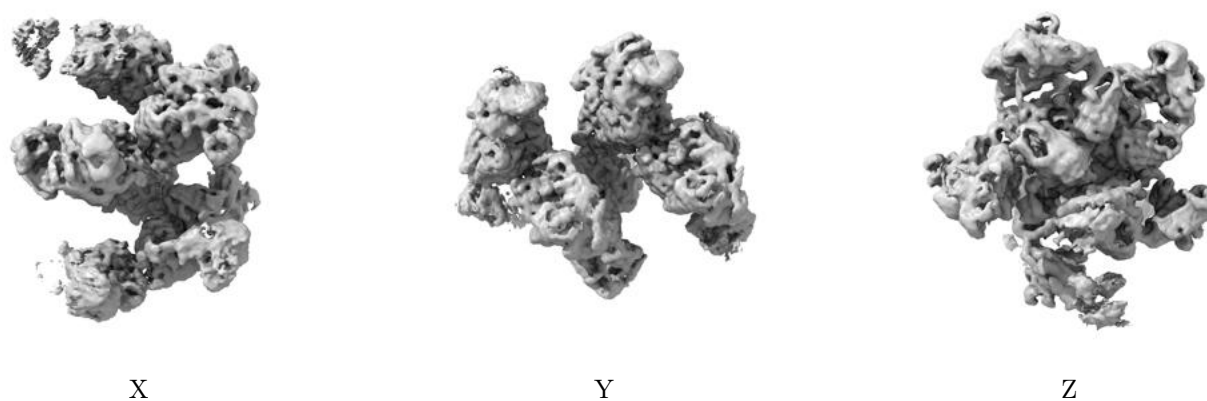
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

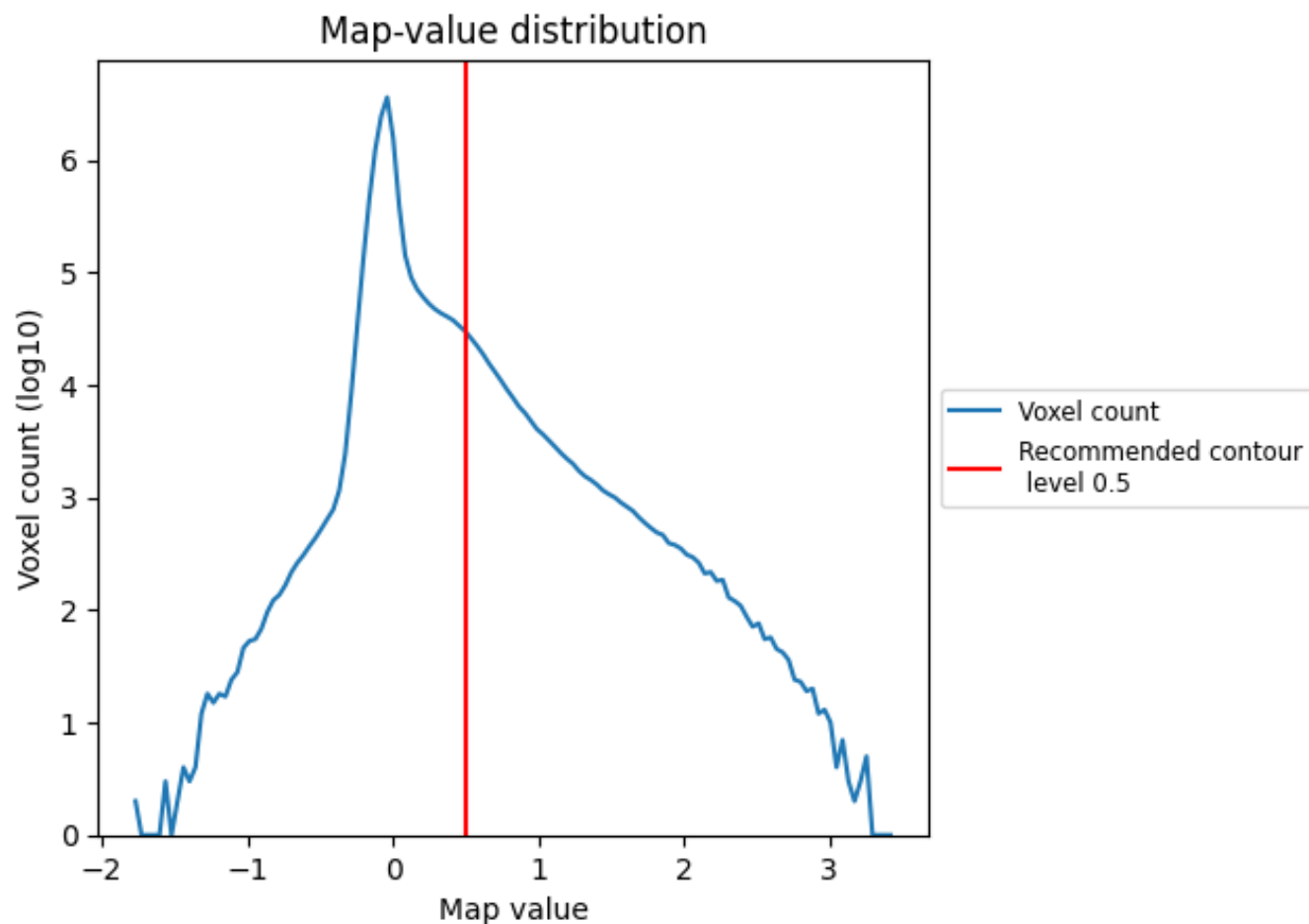
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

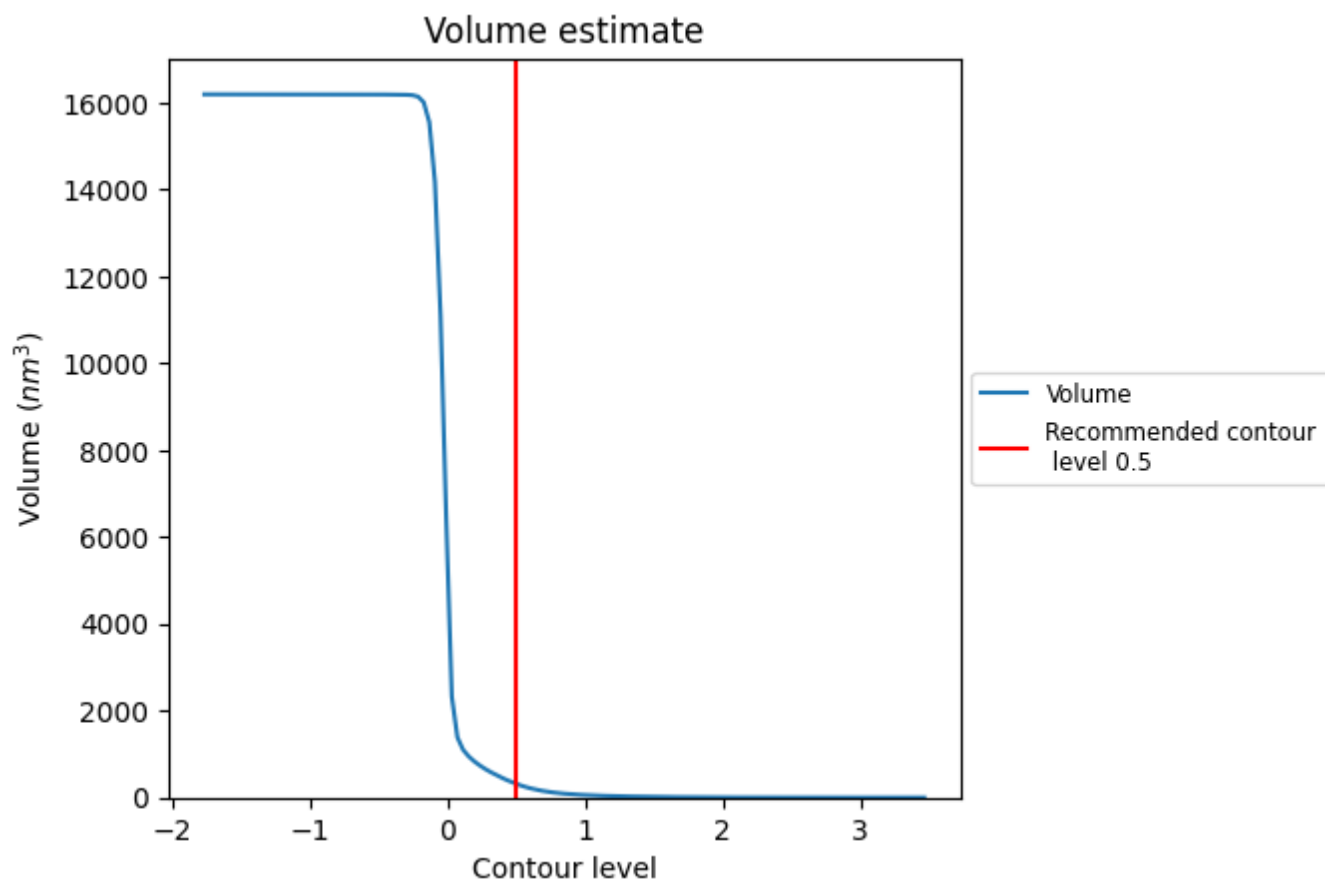
This section contains the results of statistical analysis of the map.

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.

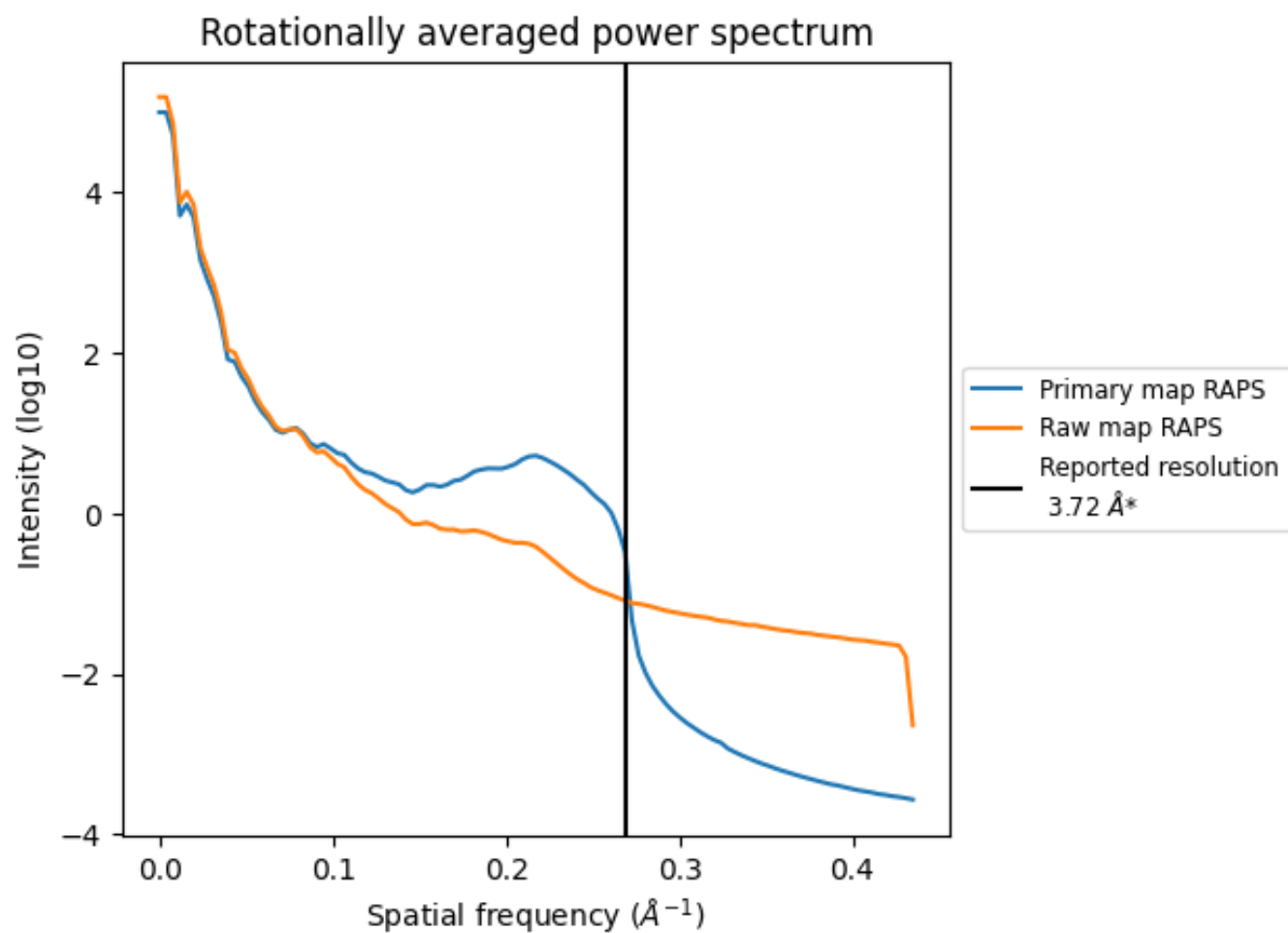
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 316 nm³; this corresponds to an approximate mass of 286 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

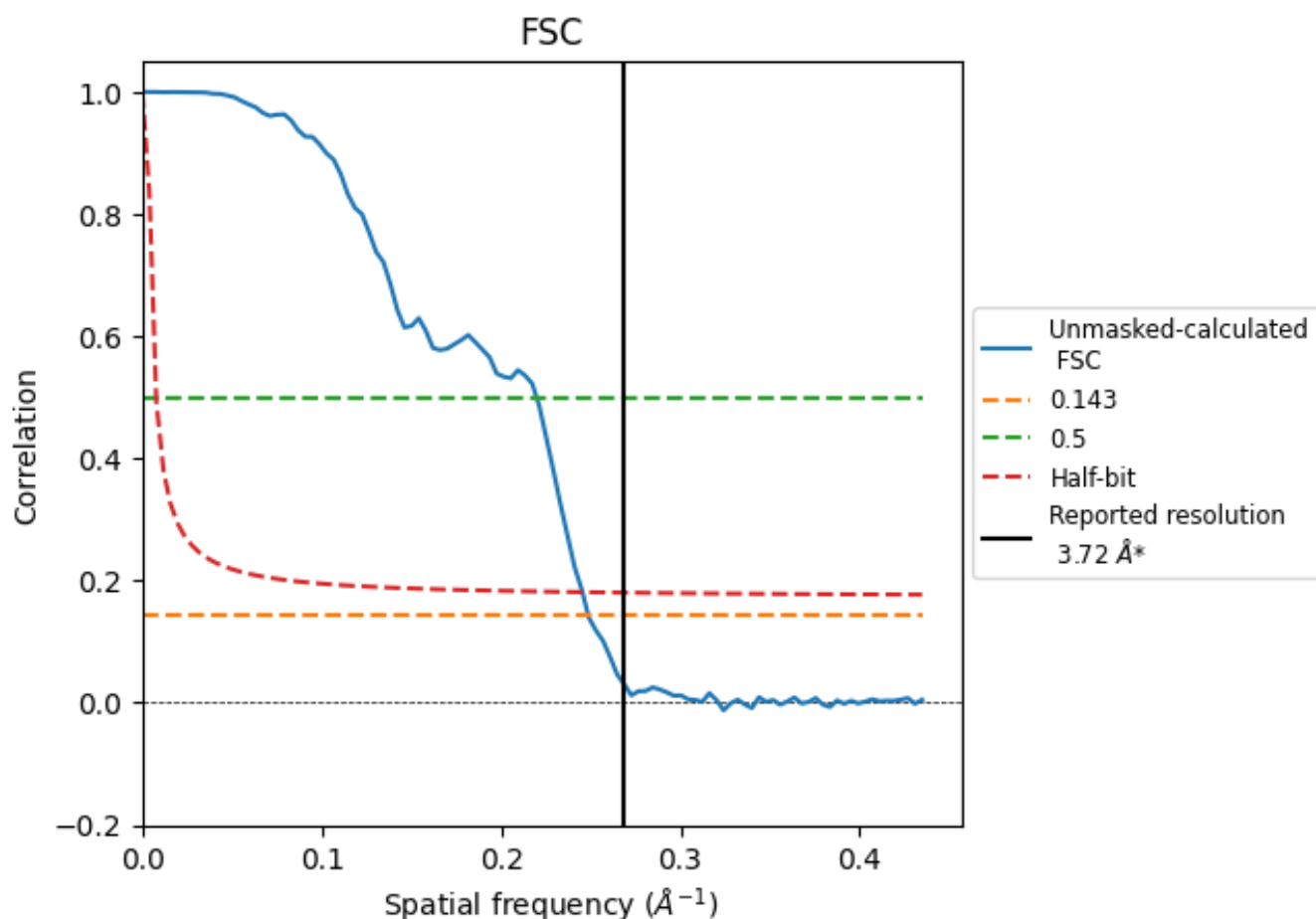


*Reported resolution corresponds to spatial frequency of 0.269 Å⁻¹

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 $0.269 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

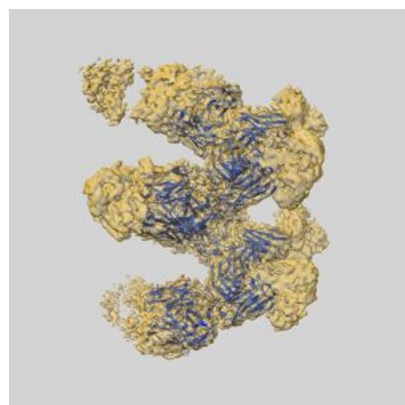
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	4.55	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

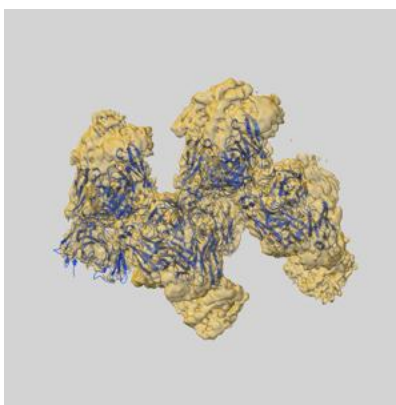
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27784 and PDB model 8DYW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

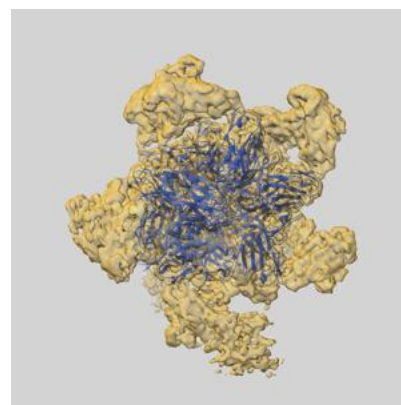
9.1 Map-model overlay [i](#)



X



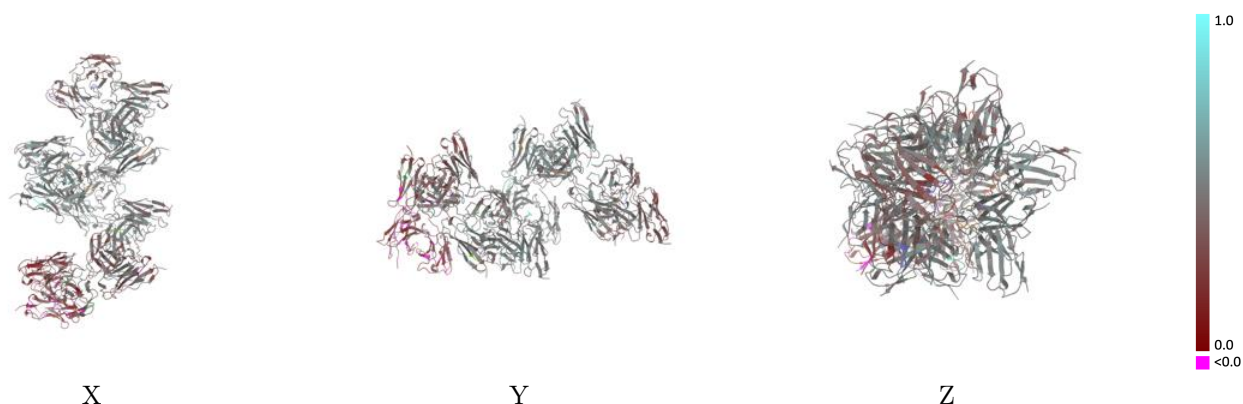
Y



Z

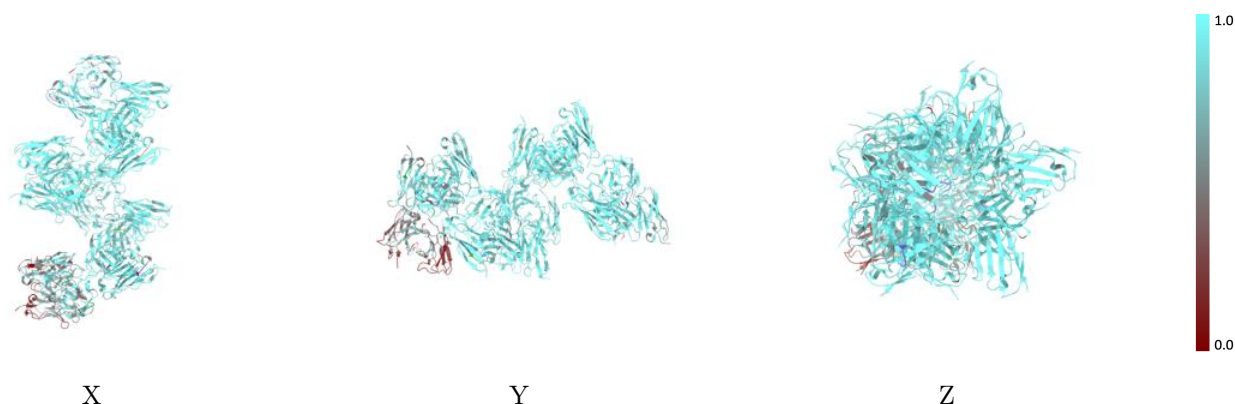
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



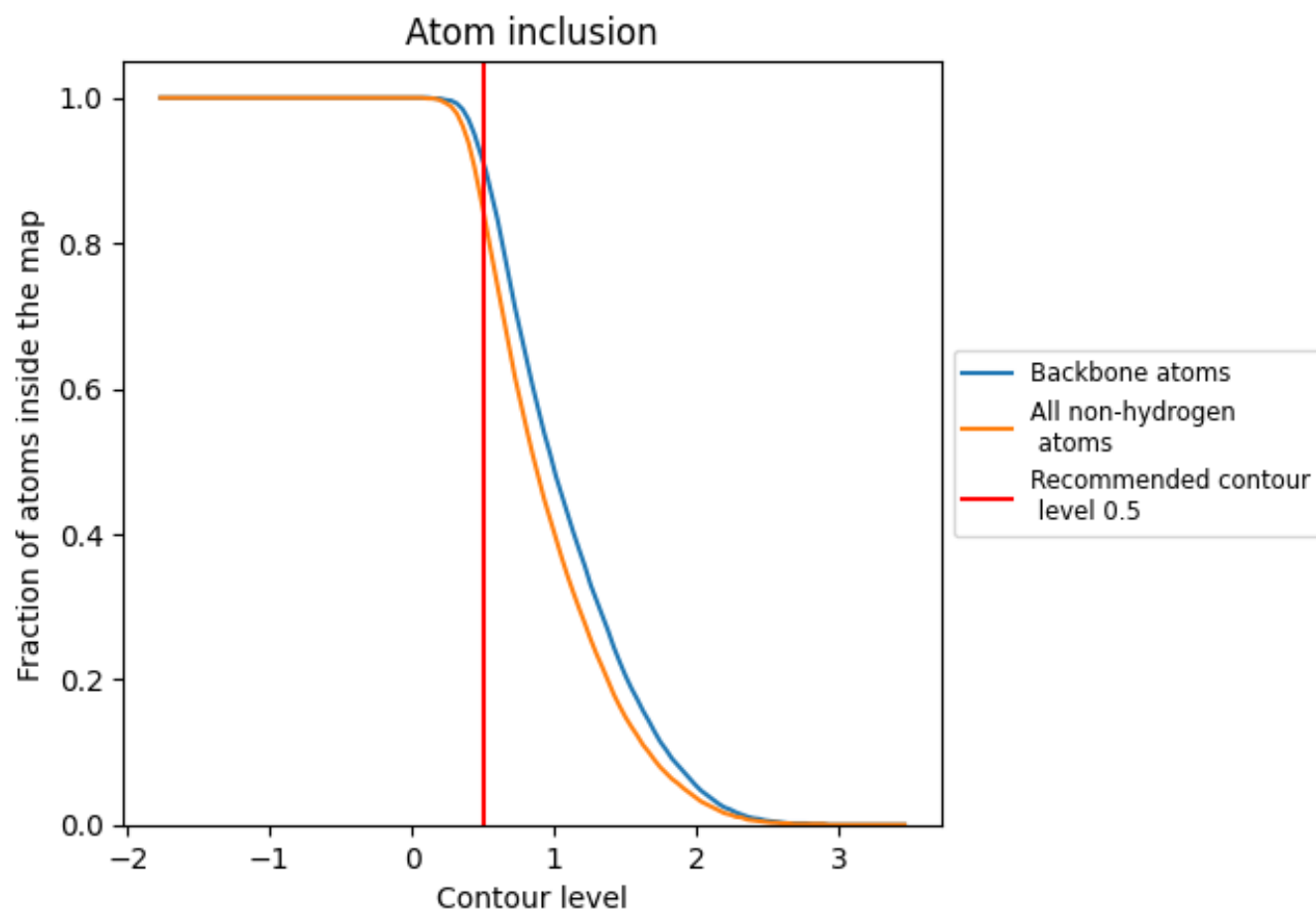
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.4240
A	 0.8780	 0.4100
B	 0.8320	 0.3790
C	 0.9290	 0.4680
D	 0.9130	 0.4580
E	 0.9420	 0.5000
F	 0.9220	 0.4900
H	 0.9270	 0.4980
I	 0.9450	 0.4320
L	 0.9320	 0.4820
M	 0.9510	 0.5050
N	 0.9410	 0.5020
O	 0.9510	 0.5040
P	 0.9410	 0.4910
Q	 0.9070	 0.4630
R	 0.9000	 0.4520
S	 0.8740	 0.4140
T	 0.8720	 0.4120
U	 0.7740	 0.3240
V	 0.7590	 0.3270
W	 0.4200	 0.1930
X	 0.3030	 0.1930

