Full wwPDB EM Validation Report ⓘ

Oct 26, 2026 – 02:33 PM EDT

PDB ID	:	9O5Y / pdb_00009o5y
EMDB ID	:	EMD-70153
Title	:	VAR2CSA in complex with V2C.015 Fab
Authors	:	Raghavan, S.S.R.; Ward, A.B.
Deposited on	:	2025-04-10
Resolution	:	3.50 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:

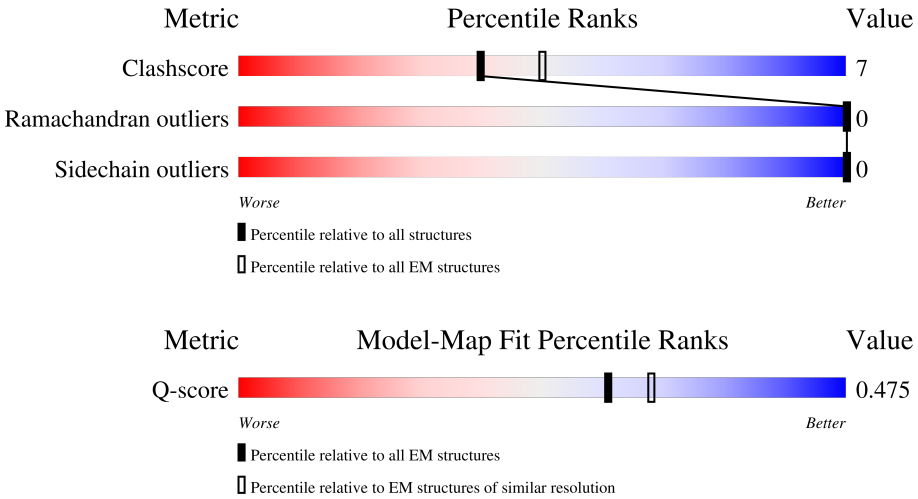
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.50 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	13950 (3.00 - 4.00)

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	H	122	77% 23%
2	L	112	10% 74% 26%
3	A	2683	10% 88%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4360 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 V2C.015 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	122	Total	C	N	O	S	0	0
			965	608	167	184	6		

- Molecule 2 is a protein called V2C.015 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	112	Total	C	N	O	S	0	0
			866	550	140	173	3		

- Molecule 3 is a protein called Erythrocyte membrane protein 1, PfEMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	311	Total	C	N	O	S	0	0
			2529	1596	434	482	17		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A024V5I6
A	-18	LYS	-	expression tag	UNP A0A024V5I6
A	-17	LEU	-	expression tag	UNP A0A024V5I6
A	-16	CYS	-	expression tag	UNP A0A024V5I6
A	-15	ILE	-	expression tag	UNP A0A024V5I6
A	-14	LEU	-	expression tag	UNP A0A024V5I6
A	-13	LEU	-	expression tag	UNP A0A024V5I6
A	-12	ALA	-	expression tag	UNP A0A024V5I6
A	-11	VAL	-	expression tag	UNP A0A024V5I6
A	-10	VAL	-	expression tag	UNP A0A024V5I6
A	-9	ALA	-	expression tag	UNP A0A024V5I6
A	-8	PHE	-	expression tag	UNP A0A024V5I6
A	-7	VAL	-	expression tag	UNP A0A024V5I6
A	-6	GLY	-	expression tag	UNP A0A024V5I6
A	-5	LEU	-	expression tag	UNP A0A024V5I6

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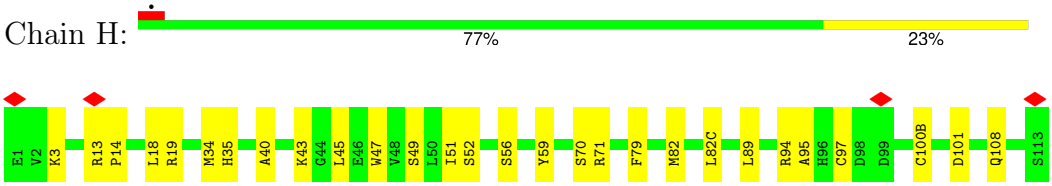
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP A0A024V5I6
A	-3	LEU	-	expression tag	UNP A0A024V5I6
A	-2	GLY	-	expression tag	UNP A0A024V5I6
A	-1	GLY	-	expression tag	UNP A0A024V5I6
A	0	THR	-	expression tag	UNP A0A024V5I6
A	2510	GLY	GLU	conflict	UNP A0A024V5I6
A	2630	GLY	-	expression tag	UNP A0A024V5I6
A	2631	SER	-	expression tag	UNP A0A024V5I6
A	2632	GLU	-	expression tag	UNP A0A024V5I6
A	2633	ASN	-	expression tag	UNP A0A024V5I6
A	2634	LEU	-	expression tag	UNP A0A024V5I6
A	2635	TYR	-	expression tag	UNP A0A024V5I6
A	2636	PHE	-	expression tag	UNP A0A024V5I6
A	2637	GLN	-	expression tag	UNP A0A024V5I6
A	2638	SER	-	expression tag	UNP A0A024V5I6
A	2639	ALA	-	expression tag	UNP A0A024V5I6
A	2640	SER	-	expression tag	UNP A0A024V5I6
A	2641	GLY	-	expression tag	UNP A0A024V5I6
A	2642	LEU	-	expression tag	UNP A0A024V5I6
A	2643	ASN	-	expression tag	UNP A0A024V5I6
A	2644	ASP	-	expression tag	UNP A0A024V5I6
A	2645	ILE	-	expression tag	UNP A0A024V5I6
A	2646	PHE	-	expression tag	UNP A0A024V5I6
A	2647	GLU	-	expression tag	UNP A0A024V5I6
A	2648	ALA	-	expression tag	UNP A0A024V5I6
A	2649	GLN	-	expression tag	UNP A0A024V5I6
A	2650	LYS	-	expression tag	UNP A0A024V5I6
A	2651	ILE	-	expression tag	UNP A0A024V5I6
A	2652	GLU	-	expression tag	UNP A0A024V5I6
A	2653	TRP	-	expression tag	UNP A0A024V5I6
A	2654	HIS	-	expression tag	UNP A0A024V5I6
A	2655	GLU	-	expression tag	UNP A0A024V5I6
A	2656	HIS	-	expression tag	UNP A0A024V5I6
A	2657	HIS	-	expression tag	UNP A0A024V5I6
A	2658	HIS	-	expression tag	UNP A0A024V5I6
A	2659	HIS	-	expression tag	UNP A0A024V5I6
A	2660	HIS	-	expression tag	UNP A0A024V5I6
A	2661	HIS	-	expression tag	UNP A0A024V5I6
A	2662	HIS	-	expression tag	UNP A0A024V5I6
A	2663	HIS	-	expression tag	UNP A0A024V5I6

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.

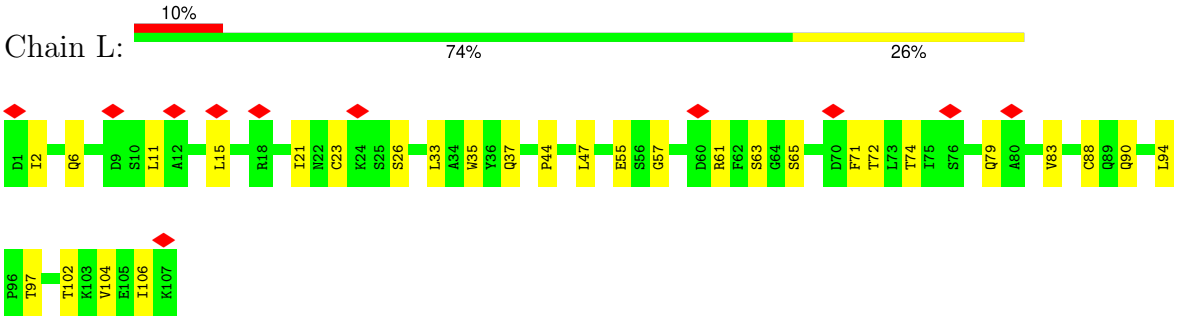
• Molecule 1: V2C.015 Heavy chain

Chain H:



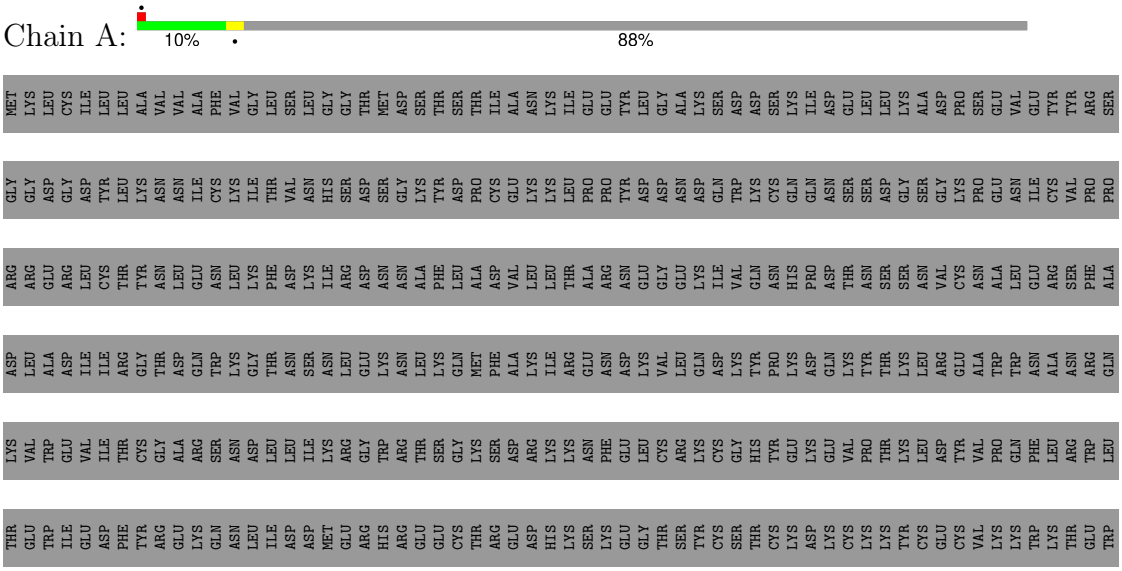
• Molecule 2: V2C.015 Light chain

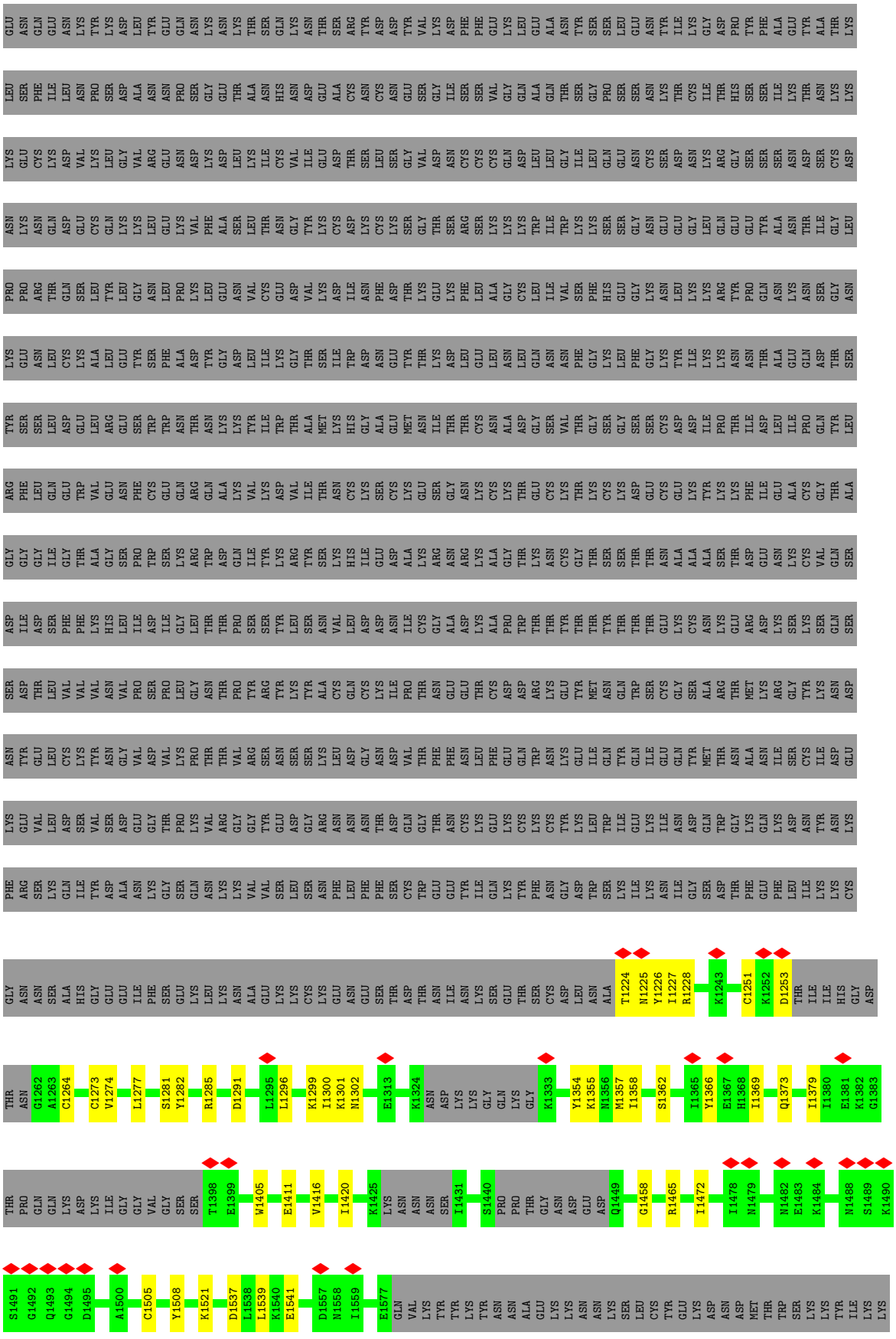
Chain L:

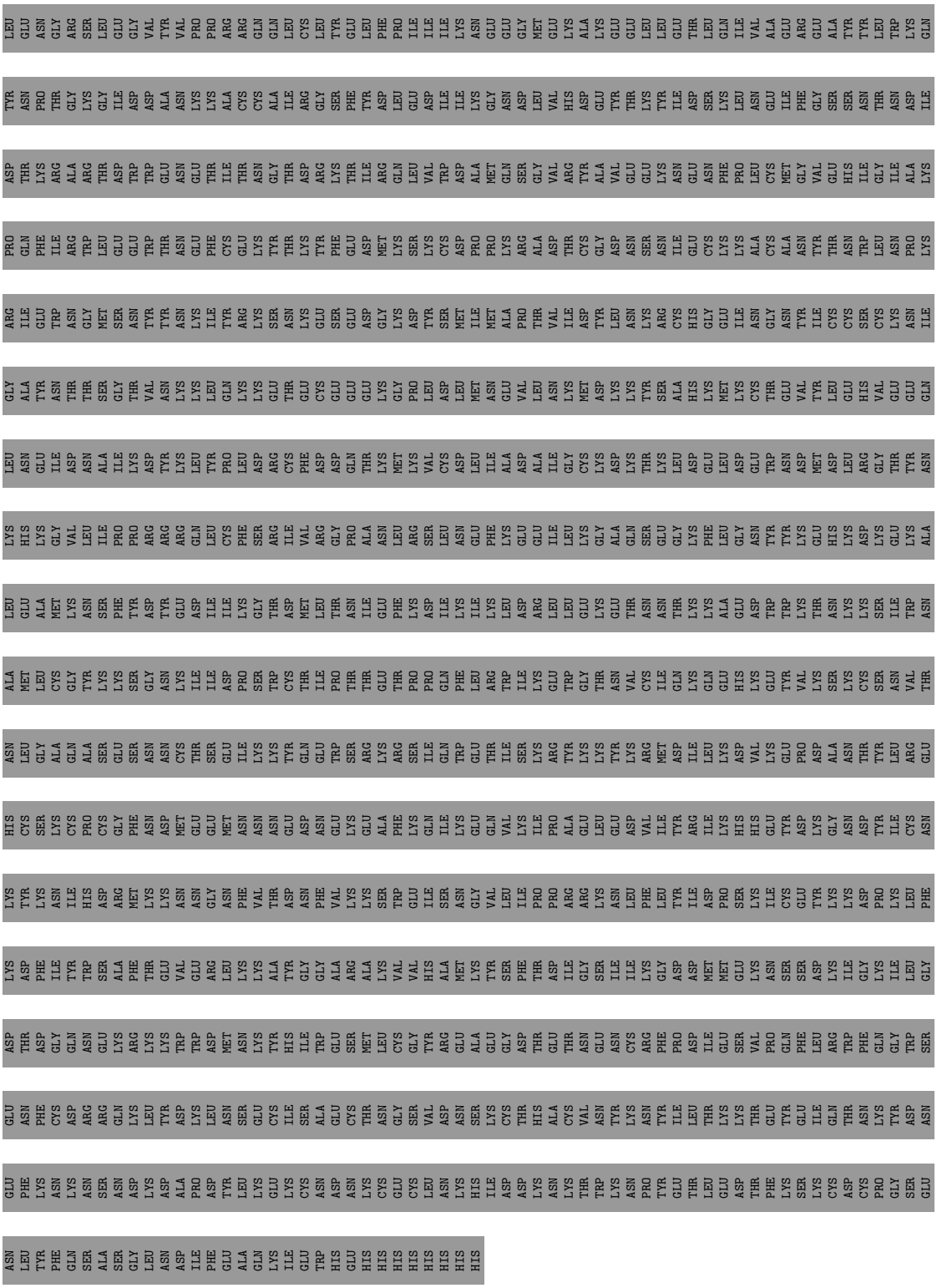


• Molecule 3: Erythrocyte membrane protein 1, PfEMP1

Chain A:




GLU ASN GLN GLU ASN LYS TYR LYS ASP LEU TYR GLU GLN ASN LYS ASN LYS THR SER GLN LYS ASN THR SER ARG TYR ASP ASP TYR VAL LYS ASP PHE PHE GLU GLY LYS LEU GLU ALA ASN TYR SER SER LEU GLU ASN TYR ILE LYS GLY ASP PRO TYR PHE ALA GLU TYR ALA THR LYS
LEU SER PHE ILE LEU ASN PRO SER ASP ALA ASN ASN PRO SER GLY GLU THR ALA ASN HIS ASN ASP GLU ALA CYS ASN CYS ASN GLU SER GLY THR CYS ILE THR HIS SER SER SER ILE LYS THR ASN LYS LYS
LYS GLU CYS LYS ASP VAL LYS LEU GLY VAL ARG GLU ASN ASP LYS ASP LEU LYS ILE CYS VAL ILE GLU ASP LEU GLY ILE LEU GLN GLU ASN CYS CYS GLN ASP LEU LEU GLY ILE LEU GLN GLU ASN CYS SER ASP ASN LYS ARG GLY SER SER SER ILE LYS ASN ASP SER CYS ASP
ASN LYS ASN GLN ASP GLU CYS GLN LYS LYS LYS SER GLY THR SER LEU THR ASN GLY TYR LYS CYS ASP LYS CYS LYS SER GLY THR SER LYS LYS SER SER GLU GLY GLN GLY LEU GLN ILE TRP ILE LYS LYS ARG GLY TYR ALA ASN THR ILE GLY LEU
PRO PRO ARG THR GLN SER LEU TYR LEU GLY ASN LEU PRO LYS LEU GLU ASN VAL CYS GLU ASP VAL LYS ASP ILE ASN PHE ASP THR LYS GLU LYS ASP ASN LEU LYS LYS ARG TYR PRO GLN ASN LEU LYS ALA GLY CYS LEU ILE VAL SER PHE HIS GLU GLY LYS ASN GLU GLU GLY LEU GLN ARG GLU GLU TYR PRO GLN ASN LYS SER GLY ASN
LYS GLU ASN LEU CYS LYS ALA LEU GLU TYR LEU ILE LYS GLY THR SER ILE TRP ASP ASP LEU LEU ASN LEU GLN ASN ASN PHE GLY LYS LEU PHE GLY LYS TYR THR LYS ASP LEU GLU LEU ASN LEU GLN GLN ASP THR SER
TYR SER SER LEU ASP GLU LEU ARG GLU HIS GLY ALA GLU MET MET ASN ILE THR THR GLY SER GLY SER SER CYS ASP ASP ILE PRO THR ILE ASP LEU LEU ILE PRO GLN TYR LEU
ARG PHE LEU GLN GLU TRP VAL GLU ASN PHE CYS GLU GLN ARG GLN ALA LYS VAL LYS ASP VAL ILE THR ASN CYS LYS SER CYS LYS GLU SER GLY ASN LYS CYS LYS LYS THR GLU CYS LYS THR THR LYS CYS LYS ASP GLU CYS LYS TYR ILE GLU ALA CYS GLY ARG LYS
GLY GLY GLY ILE GLY THR ALA GLY SER PRO TRP SER LYS ARG TRP ASP GLN ILE TYR LYS LYS ARG TYR SER LYS HIS ILE GLU ASP ALA LYS ARG ASN ARG LYS ALA GLY THR LYS ASN CYS GLY THR SER SER THR THR ASN ALA ALA ALA SER THR ASP GLU ASN LYS ALA GLN
ASP ILE ASP SER PHE PHE LYS HIS LEU ILE ASP ILE GLY LEU THR THR PRO SER SER TYR LEU SER ASN VAL LEU ASP ASP ASN ILE CYS GLY ALA ASP LYS ALA PRO TRP THR THR TYR THR THR THR THR THR THR GLU LYS CYS ASN LYS ASP GLU ARG ASP LYS SER LYS SER GLN SER
SER ASP THR LEU VAL VAL ASN VAL PRO SER PRO LEU GLY ASN THR PRO TYR ARG TYR LYS TYR SER ALA CYS GLN CYS LYS ILE PRO PRO THR ASN GLU GLU GLU THR CYS ASP ASP ARG LYS GLU TYR MET ASN GLN TRP SER CYS GLY SER ALA ARG THR MET LYS ARG GLY TYR LYS ASN ASP
ASN TYR GLU LEU CYS LYS TYR ASN GLY VAL ASP VAL LYS PRO THR THR VAL ARG SER ASN SER SER LYS LEU ASP GLY ASN ASP VAL THR PHE PHE ASN LEU PHE GLU GLN TRP ASN LYS GLU ILE GLN TYR THR GLN ILE GLU GLN TYR MET THR ASN ALA ASN ILE SER LYS ILE
LYS GLU VAL LEU ASP SER VAL ARG GLY ASN ASN ASN THR ASP GLN GLY THR ASN CYS LYS LYS CYS CYS LYS CYS TYR LYS LEU TRP ILE GLU LYS ILE ASN ASP GLN GLY SER ASP THR PHE GLU PHE LEU ILE LYS LYS ASN
PHE ARG SER LYS GLN ILE TYR ALA ASN VAL SER LEU PHE PHE SER CYS TRP GLU GLU ILE GLN TYR LYS ILE ILE ASN LYS SER GLU THR SER CYS ASP LEU ASN ALA T1224 N1225 Y1226 I1227 R1228 K1243 C1251 K1252 D1253 THR ILE ILE HIS GLY ASP
THR ASN G1262 A1263 C1264 C1273 V1274 L1277 S1281 Y1282 R1285 D1291 L1295 L1296 K1299 I1300 K1301 N1302 E1313 K1324 ASN ASP LYS LYS GLY GLN LYS GLY K1333 Y1354 K1355 N1356 M1357 I1358 S1362 I1365 Y1366 E1367 H1368 I1369 Q1373 I1379 I1380 E1381 K1382 G1383
THR PRO GLN GLN LYS ASP LYS ILE GLY GLY VAL GLY SER T1398 E1399 W1405 E1411 V1416 I1420 K1425 LYS ASN ASN ASN SER I1431 S1440 PRO PRO THR GLY ASN ASP GLU ASP Q1449 G1458 R1465 I1472 I1478 N1479 N1482 E1483 K1484 N1488 S1489 K1490
S1491 G1492 Q1493 G1494 D1495 A1500 C1505 Y1508 K1521 D1537 L1538 L1539 K1540 E1541 D1557 N1558 I1559 E1577 GLN VAL LYS TYR TYR LYS TYR ASN ASN ALA GLU LYS LYS ASN ASN LYS SER LEU CYS TYR GLU LYS ASP ASN ASP MET THR TRP SER LYS LYS TYR ILE LYS LYS


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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	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	H	0.20	0/989	0.38	0/1339
2	L	0.18	0/887	0.38	0/1205
3	A	0.19	0/2577	0.33	0/3447
All	All	0.19	0/4453	0.35	0/5991

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	H	965	0	911	19	0
2	L	866	0	838	21	0
3	A	2529	0	2467	25	0
All	All	4360	0	4216	61	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 7.

All (61) 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:A:1362:SER:OG	3:A:1373:GLN:NE2	2.25	0.69

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Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100(B):CYS:H	3:A:1281:SER:HB3	1.59	0.68
1:H:82:MET:HB3	1:H:82(C):LEU:HD21	1.77	0.67
2:L:6:GLN:HE22	2:L:88:CYS:H	1.44	0.65
2:L:55:GLU:HG3	2:L:57:GLY:H	1.63	0.63
3:A:1227:ILE:HD11	3:A:1302:ASN:HB3	1.79	0.63
2:L:11:LEU:HB2	2:L:104:VAL:HG12	1.82	0.62
3:A:1366:TYR:HB2	3:A:1369:ILE:HG22	1.84	0.60
3:A:1251:CYS:HB3	3:A:1264:CYS:HA	1.83	0.59
3:A:1273:CYS:O	3:A:1354:TYR:OH	2.20	0.59
3:A:1301:LYS:NZ	3:A:1411:GLU:OE2	2.28	0.59
1:H:35:HIS:HE1	1:H:95:ALA:HB2	1.68	0.58
1:H:45:LEU:HD11	2:L:44:PRO:HG2	1.87	0.57
1:H:51:ILE:HG23	1:H:71:ARG:HH21	1.70	0.57
3:A:1281:SER:O	3:A:1285:ARG:NH2	2.38	0.57
3:A:1226:TYR:OH	3:A:1228:ARG:NH2	2.39	0.56
2:L:6:GLN:NE2	2:L:88:CYS:H	2.03	0.56
1:H:13:ARG:HE	1:H:14:PRO:HD2	1.71	0.55
1:H:97:CYS:HA	1:H:100(B):CYS:HA	1.88	0.55
1:H:94:ARG:NH2	1:H:101:ASP:OD2	2.40	0.55
2:L:65:SER:OG	2:L:72:THR:OG1	2.24	0.55
1:H:18:LEU:HD12	1:H:19:ARG:H	1.72	0.54
2:L:94:LEU:H	3:A:1282:TYR:HB3	1.73	0.54
2:L:90:GLN:HE21	2:L:97:THR:H	1.56	0.51
2:L:63:SER:OG	2:L:74:THR:OG1	2.29	0.51
1:H:89:LEU:HD13	1:H:108:GLN:HG2	1.92	0.50
1:H:49:SER:HA	1:H:59:TYR:HA	1.93	0.50
1:H:70:SER:HB3	1:H:79:PHE:HB2	1.93	0.50
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.94	0.50
2:L:83:VAL:HA	2:L:104:VAL:HG23	1.94	0.49
3:A:1224:THR:OG1	3:A:1225:ASN:N	2.44	0.49
3:A:1300:ILE:HG12	3:A:1358:ILE:HD11	1.95	0.48
2:L:21:ILE:HD11	2:L:102:THR:HG21	1.97	0.47
3:A:1282:TYR:HB2	3:A:1285:ARG:HH22	1.78	0.47
2:L:15:LEU:HD21	2:L:106:ILE:HD13	1.96	0.47
3:A:1291:ASP:OD2	3:A:1299:LYS:NZ	2.49	0.46
3:A:1296:LEU:HD13	3:A:1379:ILE:HD13	1.97	0.46
1:H:40:ALA:HB3	1:H:43:LYS:HD3	1.97	0.46
1:H:52:SER:OG	1:H:56:SER:OG	2.32	0.45
3:A:1521:LYS:HE3	3:A:1521:LYS:HB3	1.68	0.45
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.52	0.45
3:A:1253:ASP:OD1	3:A:1521:LYS:NZ	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1274:VAL:HG22	3:A:1277:LEU:HB2	1.99	0.45
1:H:34:MET:HE3	1:H:34:MET:HB3	1.85	0.44
3:A:1458:GLY:HA3	3:A:1539:LEU:HD22	2.00	0.44
2:L:2:ILE:HG23	2:L:26:SER:HB3	1.99	0.44
2:L:6:GLN:NE2	2:L:88:CYS:SG	2.86	0.44
1:H:35:HIS:CE1	1:H:95:ALA:HB2	2.50	0.43
1:H:18:LEU:HB3	1:H:82:MET:HG3	2.01	0.43
3:A:1354:TYR:HD1	3:A:1357:MET:HE2	1.84	0.43
3:A:1416:VAL:O	3:A:1420:ILE:HG13	2.19	0.43
2:L:23:CYS:HB3	2:L:71:PHE:HB2	1.99	0.42
1:H:47:TRP:CH2	2:L:94:LEU:HD22	2.55	0.42
3:A:1355:LYS:HG3	3:A:1405:TRP:CE2	2.54	0.42
2:L:61:ARG:NE	2:L:79:GLN:HE22	2.17	0.41
2:L:23:CYS:SG	2:L:33:LEU:HD11	2.61	0.41
1:H:3:LYS:HE3	1:H:3:LYS:HB3	1.76	0.41
2:L:11:LEU:HD21	2:L:21:ILE:HD13	2.02	0.41
3:A:1465:ARG:HG3	3:A:1508:TYR:OH	2.21	0.41
3:A:1472:ILE:HD11	3:A:1505:CYS:SG	2.61	0.40
3:A:1537:ASP:O	3:A:1541:GLU:HG2	2.21	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	H	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
2	L	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
3	A	299/2683 (11%)	291 (97%)	8 (3%)	0	100	100
All	All	529/2917 (18%)	506 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	H	104/104 (100%)	104 (100%)	0	100	100
2	L	97/97 (100%)	97 (100%)	0	100	100
3	A	275/2429 (11%)	275 (100%)	0	100	100
All	All	476/2630 (18%)	476 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	6	GLN
2	L	90	GLN
3	A	1348	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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.

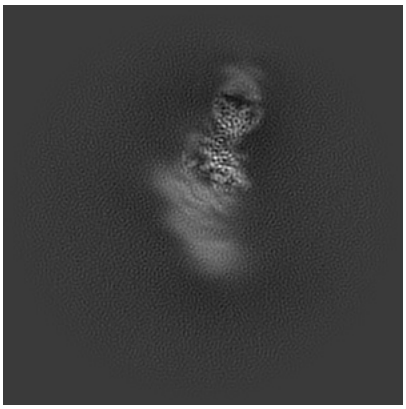
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70153. These allow visual inspection of the internal detail of the map and identification of artifacts.

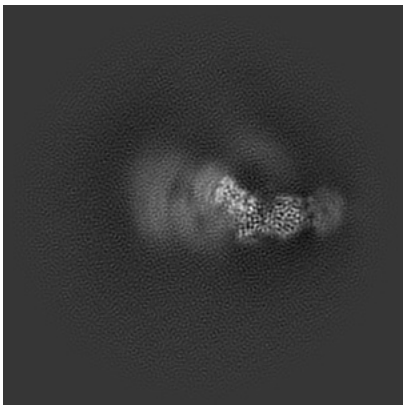
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

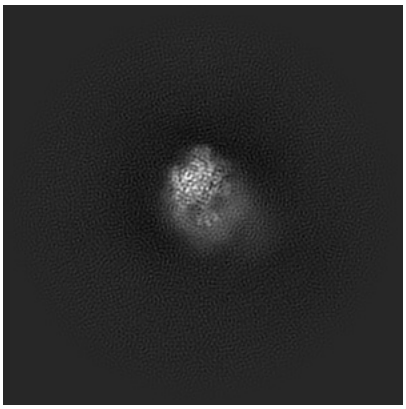
6.1.1 Primary map



X

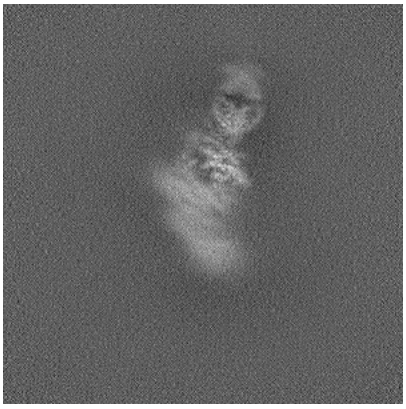


Y

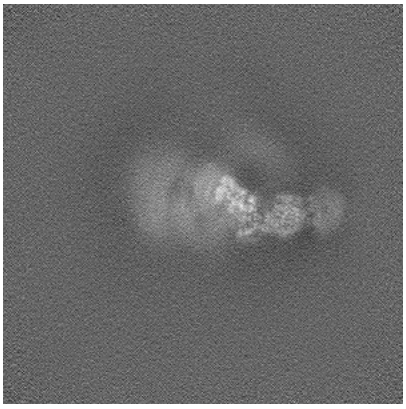


Z

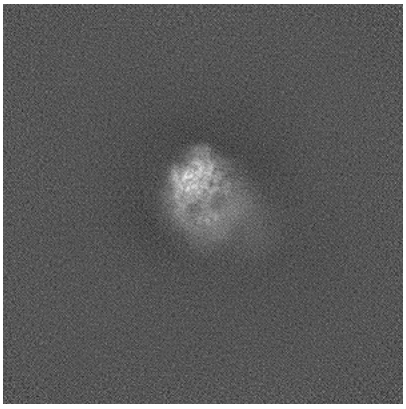
6.1.2 Raw map



X



Y

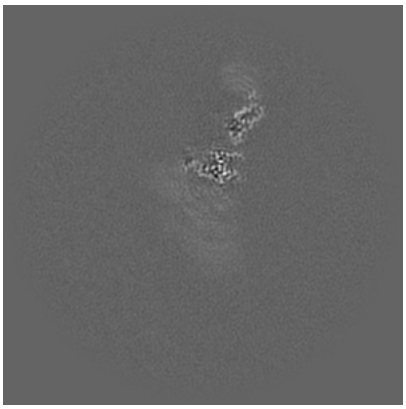


Z

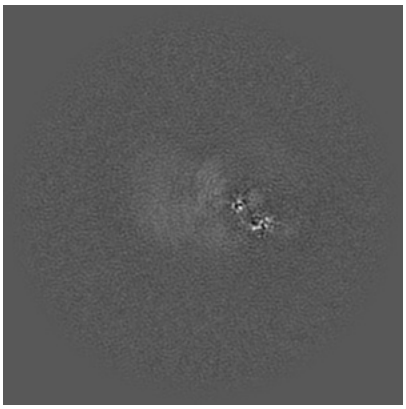
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

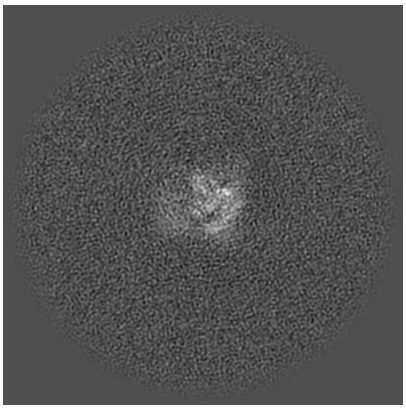
6.2.1 Primary map



X Index: 256

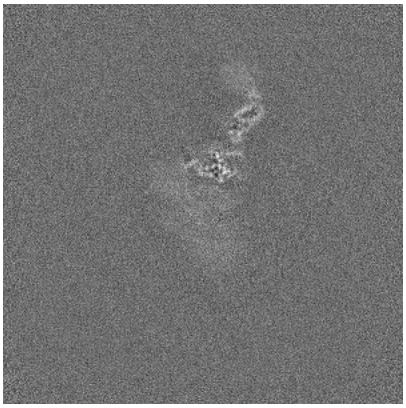


Y Index: 256

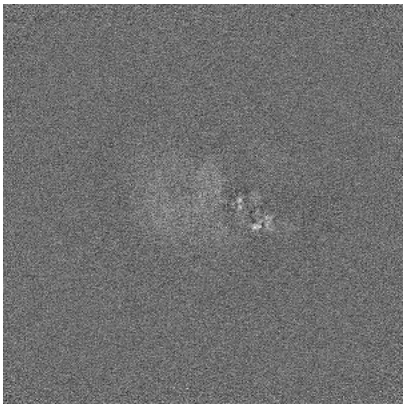


Z Index: 256

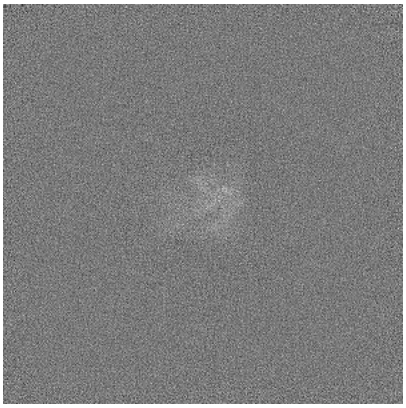
6.2.2 Raw map



X Index: 256



Y Index: 256

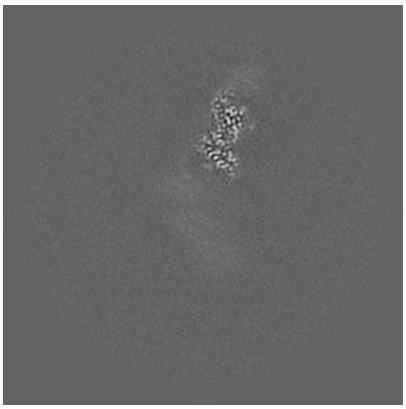


Z Index: 256

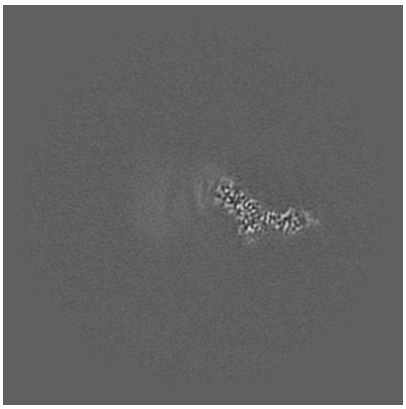
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

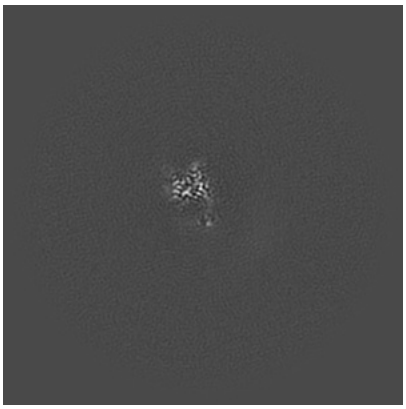
6.3.1 Primary map



X Index: 235

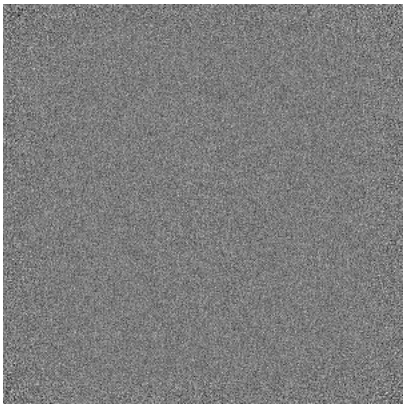


Y Index: 278

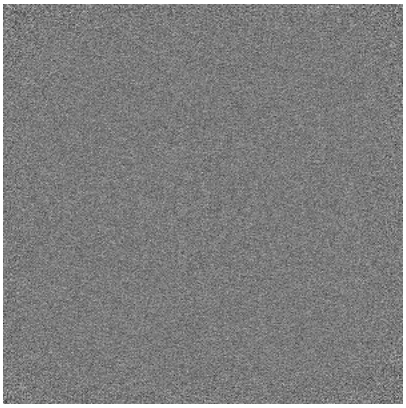


Z Index: 316

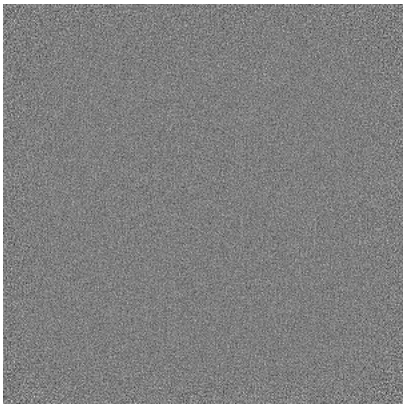
6.3.2 Raw map



X Index: 0



Y Index: 0

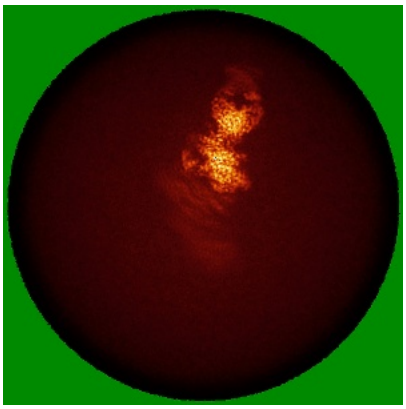


Z Index: 511

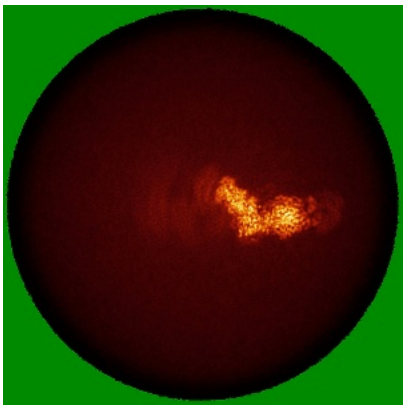
The images above show the largest variance slices of the map in three orthogonal directions.

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

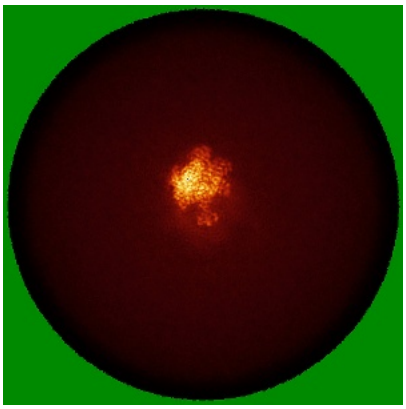
6.4.1 Primary map



X

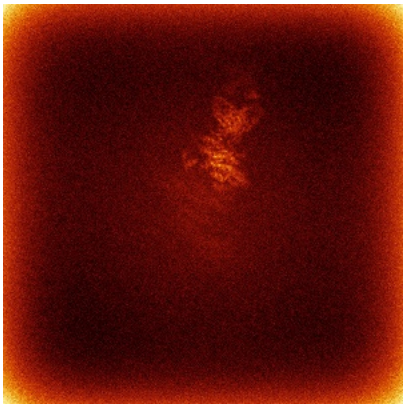


Y

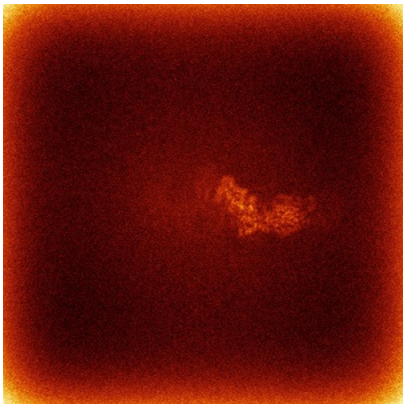


Z

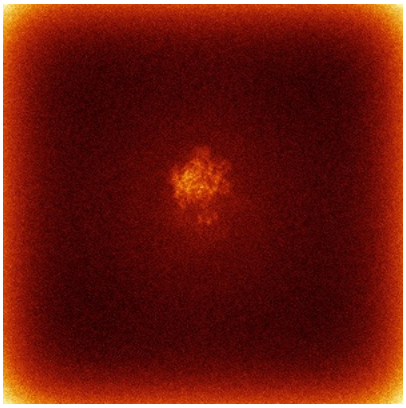
6.4.2 Raw map



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 0.05. 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.

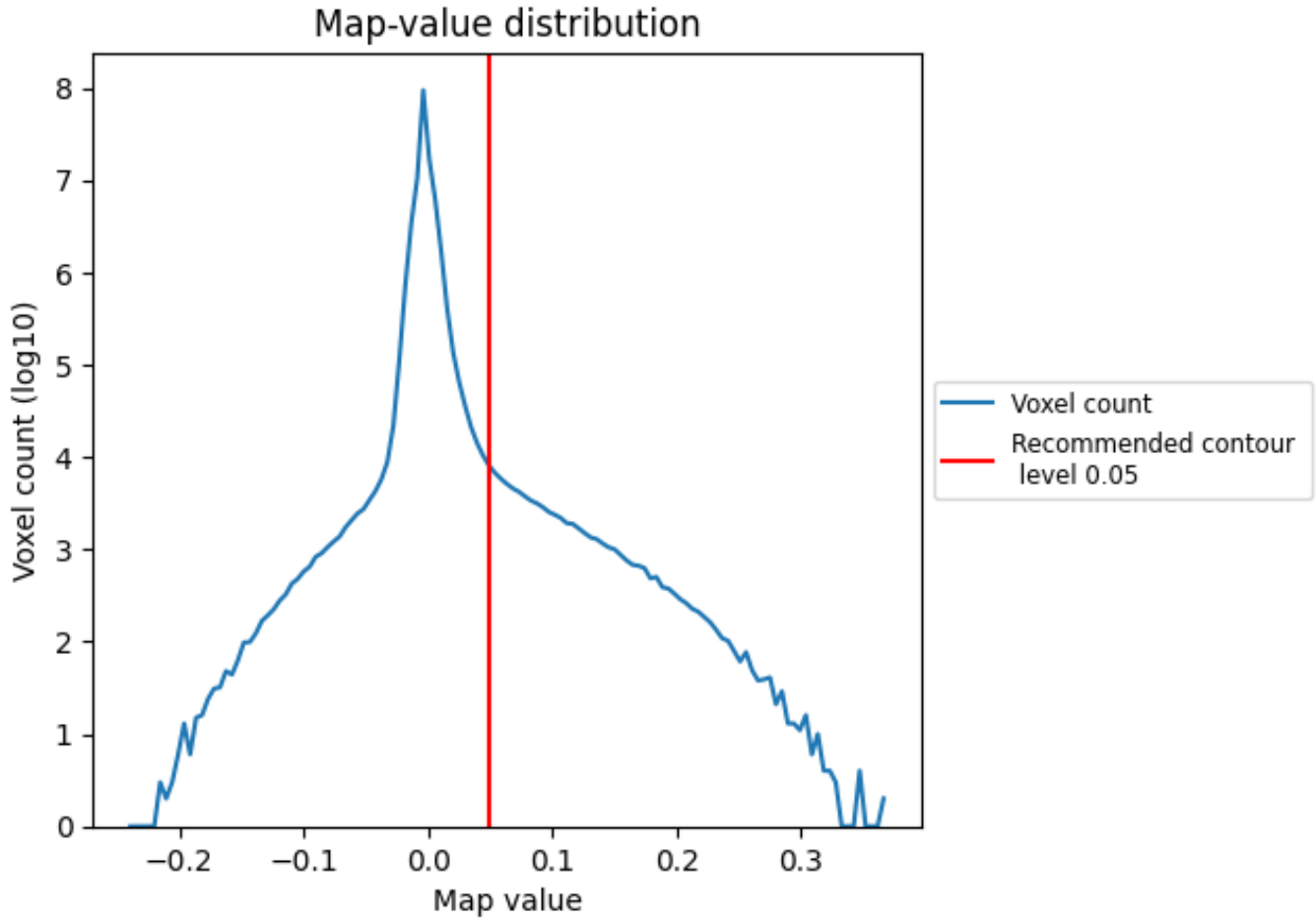
6.6 Mask visualisation (i)

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

7 Map analysis

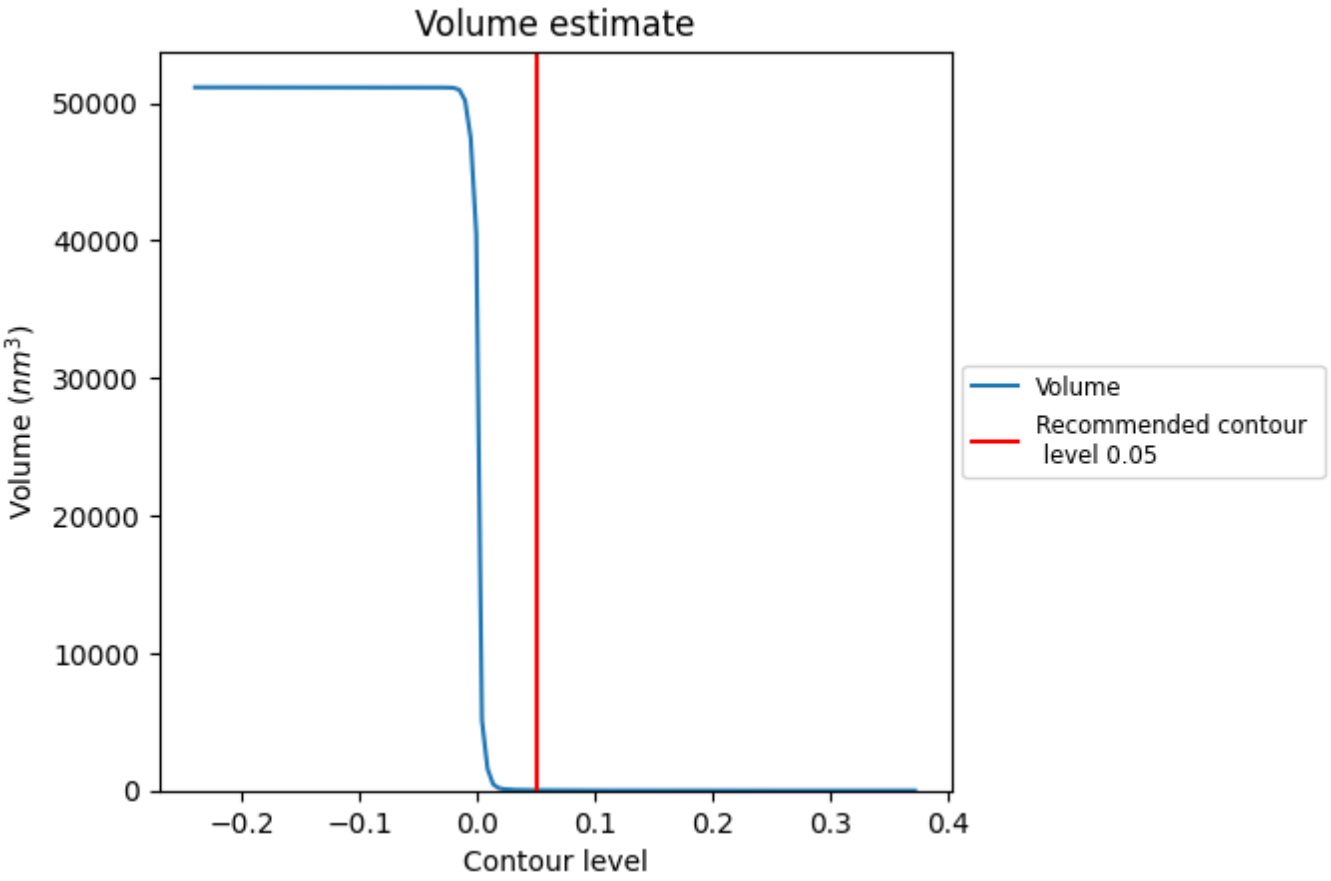
This section contains the results of statistical analysis of the map.

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.

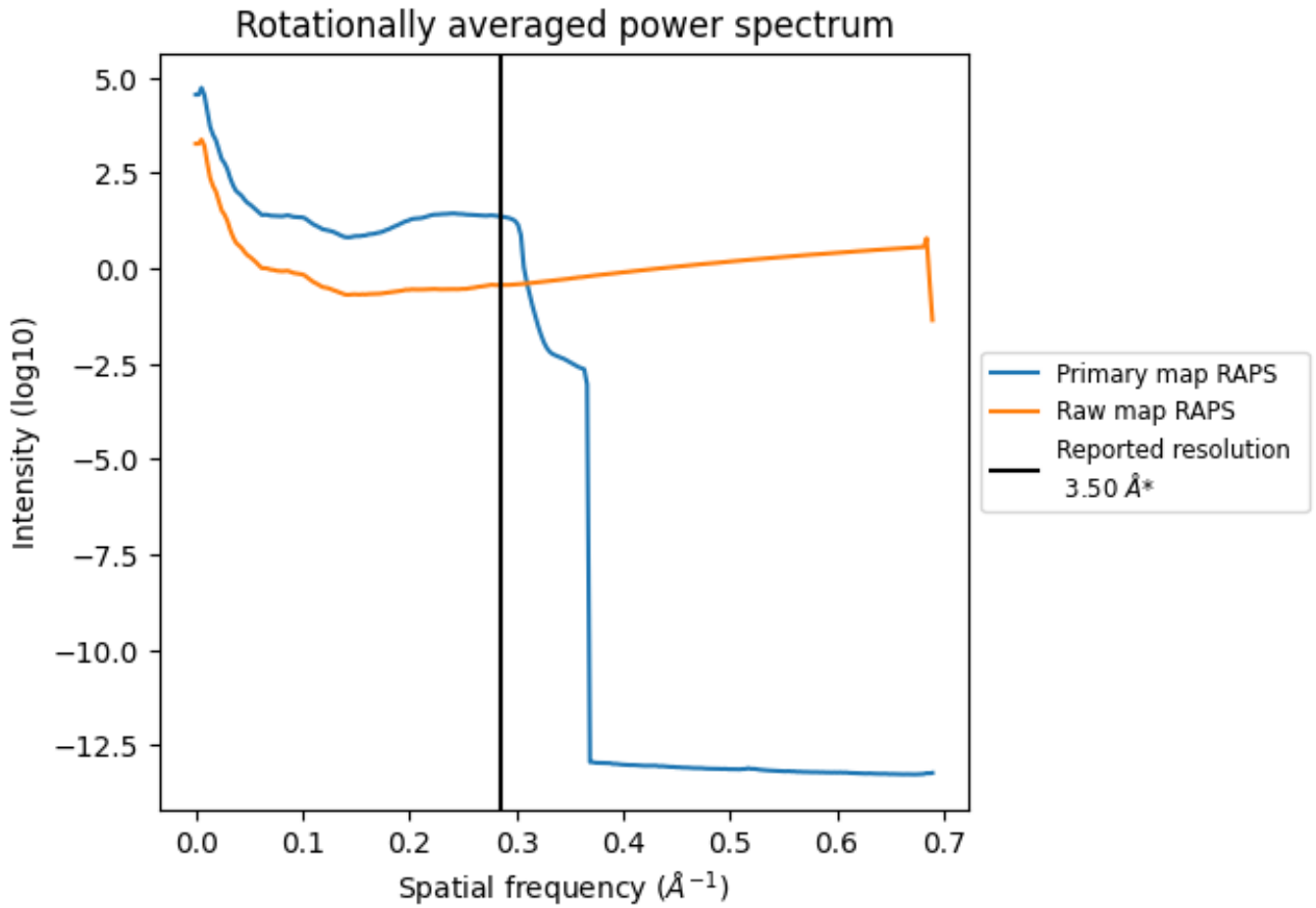
7.2 Volume estimate



The volume at the recommended contour level is 28 nm^3; this corresponds to an approximate mass of 26 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)

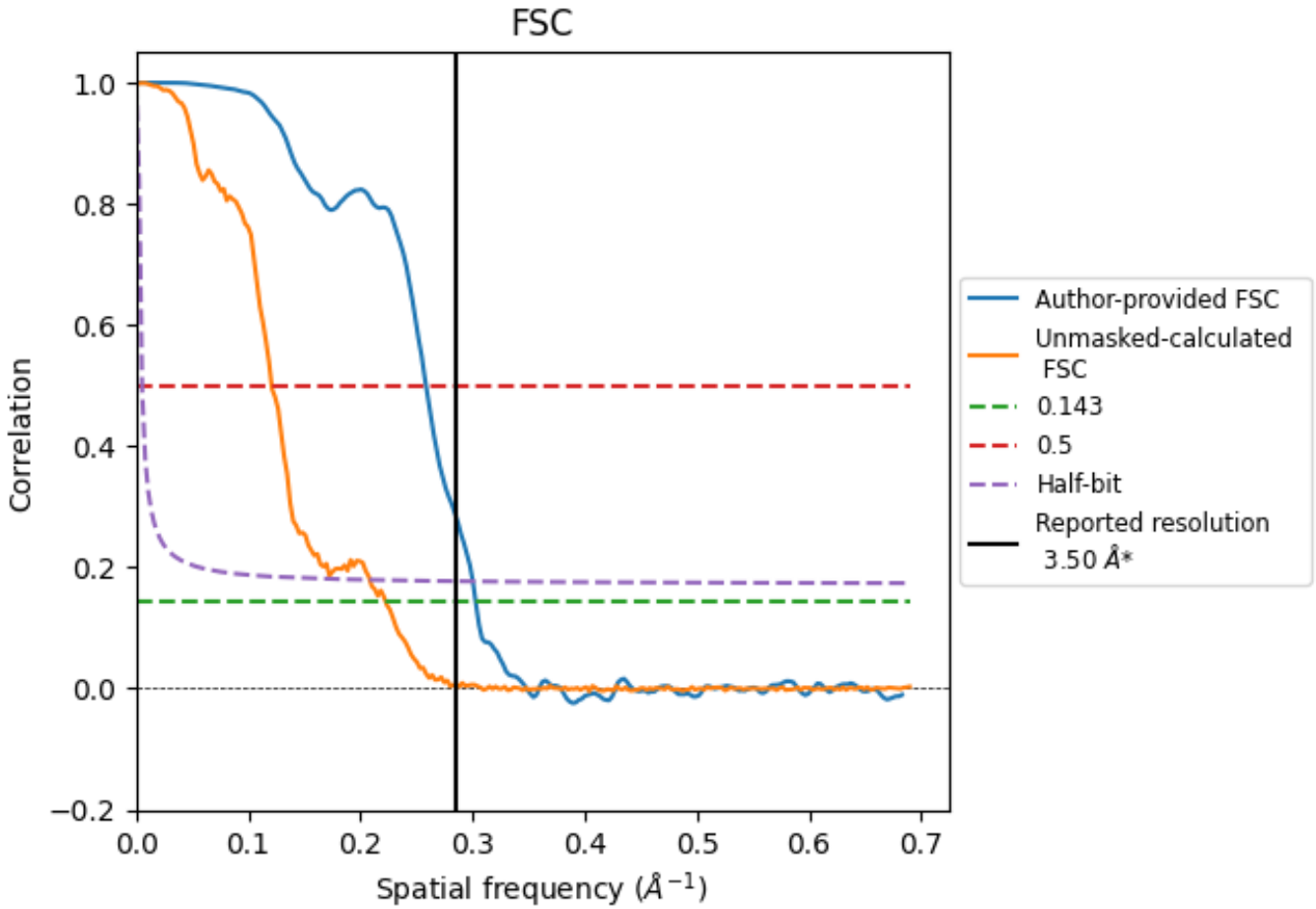


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.30	3.87	3.33
Unmasked-calculated*	4.49	8.27	4.80

*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 4.49 differs from the reported value 3.5 by more than 10 %

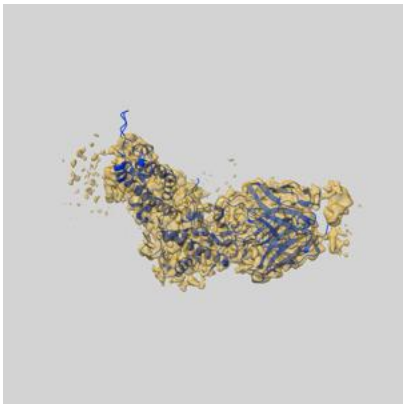
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70153 and PDB model 9O5Y. Per-residue inclusion information can be found in section 3 on page 5.

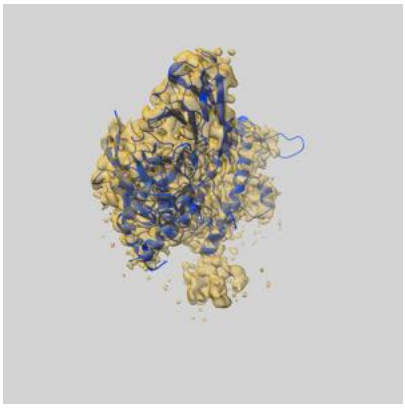
9.1 Map-model overlay



X



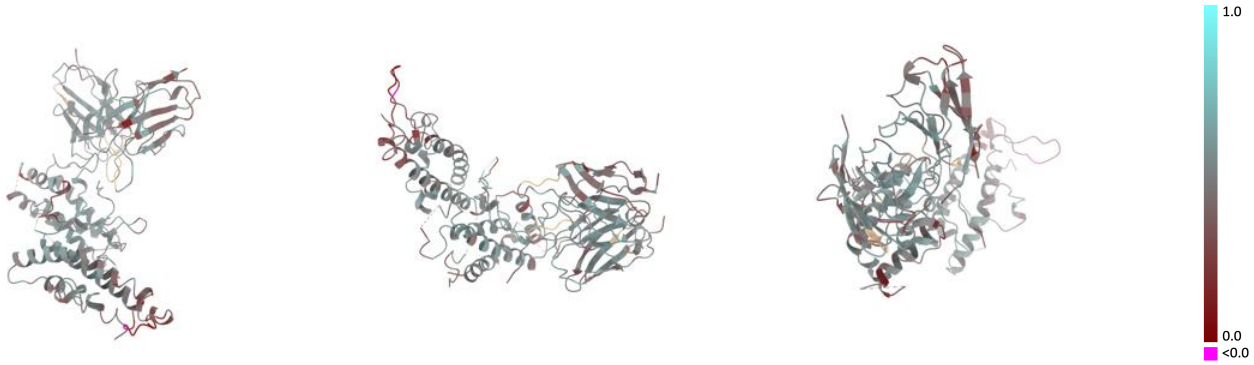
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

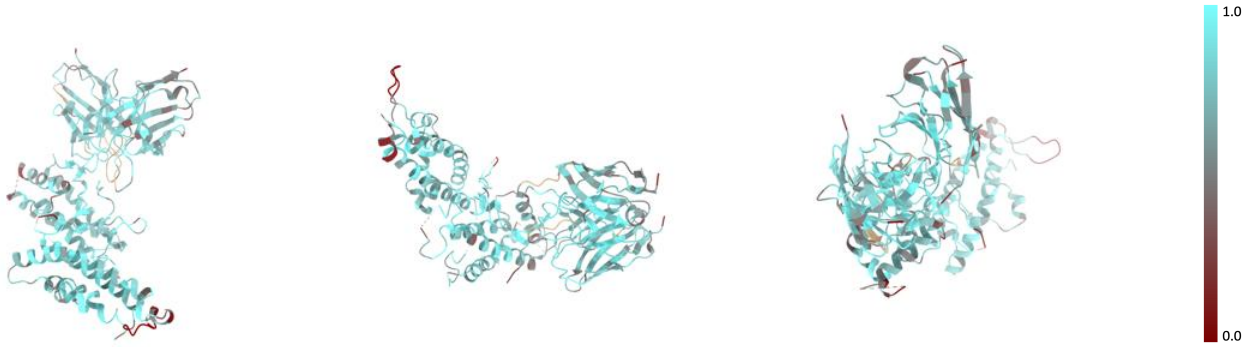
9.2 Q-score mapped to coordinate model (i)



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.

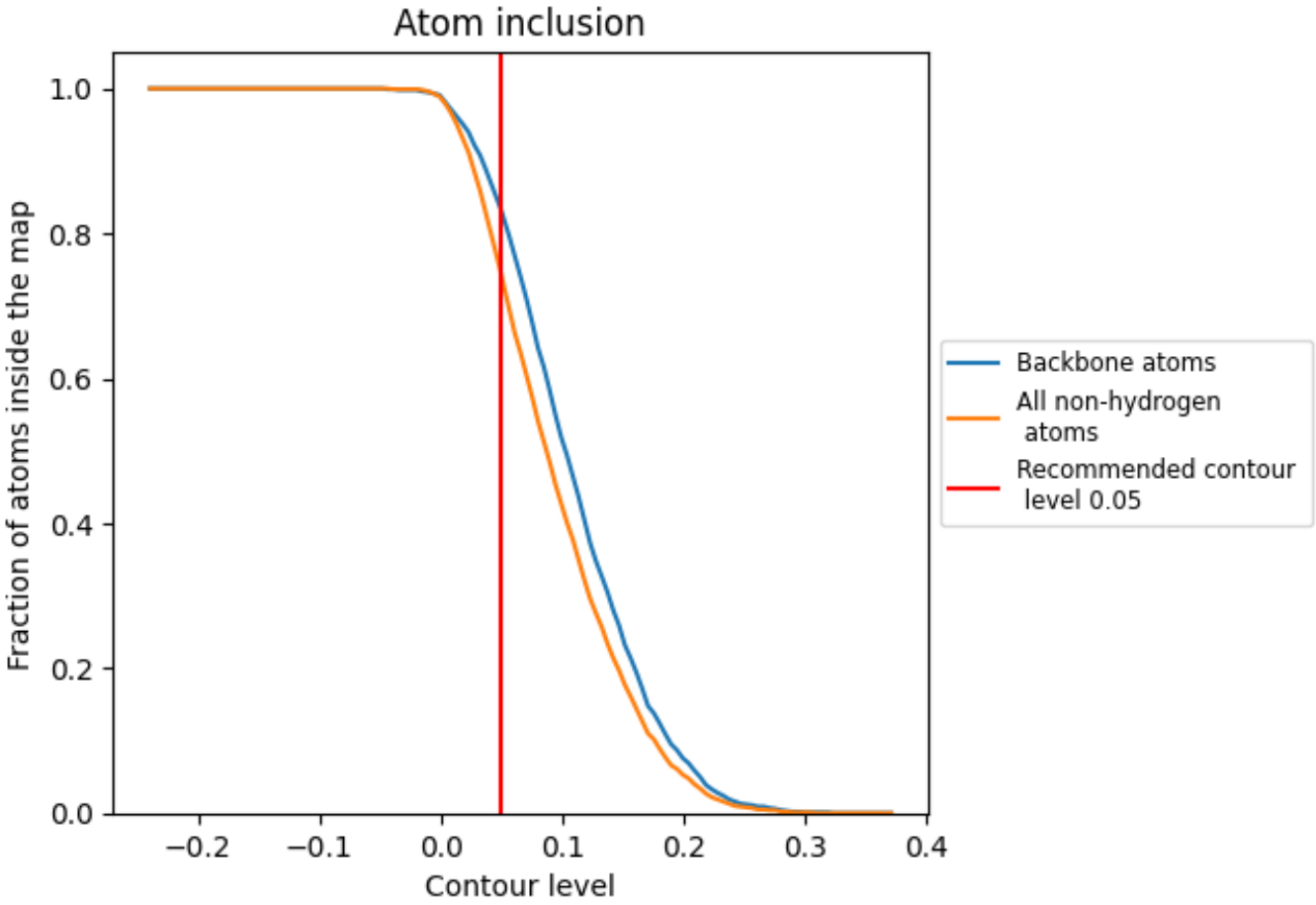
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 74% 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 (0.05) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7440	0.4750
A	0.7450	0.4670
H	0.7700	0.5010
L	0.7160	0.4700