Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 03:22 PM EDT

PDB ID	:	7SSV
EMDB ID	:	EMD-25414
Title	:	Structure of human Kv1.3 with Fab-ShK fusion
Authors	:	Meyerson, J.R.; Selvakumar, P.; Smider, V.; Huang, R.
Deposited on	:	2021-11-11
Resolution	:	3.39 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 (i) 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 (i)) were used in the production of this report:

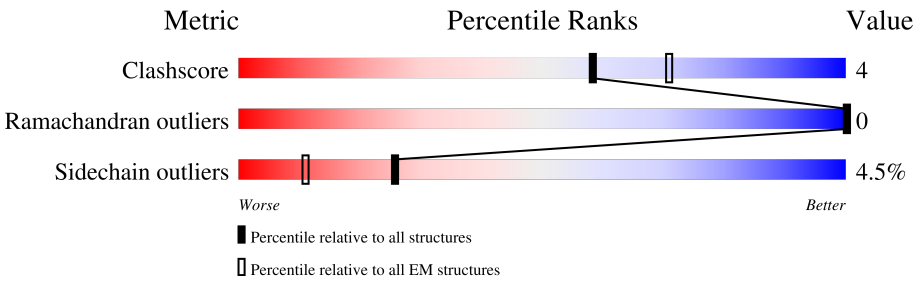
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.39 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	856	34% 6% 59%
1	B	856	35% 6% 59%
1	C	856	35% 6% 59%
1	D	856	36% 5% 59%
2	H	270	82% 91% 5% •
3	L	216	97% 93% 6% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13815 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 Potassium voltage-gated channel subfamily A member 3,Green fluorescent protein fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	350	2844	1872	468	493	11	0	0
1	B	350	2844	1872	468	493	11	0	0
1	C	350	2844	1872	468	493	11	0	0
1	D	350	2844	1872	468	493	11	0	0

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	SER	-	linker	UNP P22001
A	577	LEU	-	linker	UNP P22001
A	578	GLU	-	linker	UNP P22001
A	579	VAL	-	linker	UNP P22001
A	580	LEU	-	linker	UNP P22001
A	581	PHE	-	linker	UNP P22001
A	582	GLN	-	linker	UNP P22001
A	583	GLY	-	linker	UNP P22001
A	584	PRO	-	linker	UNP P22001
A	585	ALA	-	linker	UNP P22001
A	586	ALA	-	linker	UNP P22001
A	587	ALA	-	linker	UNP P22001
A	588	MET	-	linker	UNP P22001
A	589	VAL	-	linker	UNP P22001
A	634	LEU	PHE	conflict	UNP P42212
A	652	LEU	PHE	conflict	UNP P42212
A	653	GLY	SER	conflict	UNP P42212
A	656	LEU	VAL	conflict	UNP P42212
A	660	ALA	SER	conflict	UNP P42212
A	741	THR	MET	conflict	UNP P42212
A	751	ALA	VAL	conflict	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	763	GLY	SER	conflict	UNP P42212
A	791	TYR	THR	conflict	UNP P42212
A	794	LYS	ALA	conflict	UNP P42212
A	819	LEU	HIS	conflict	UNP P42212
A	827	SER	-	expression tag	UNP P42212
A	828	ALA	-	expression tag	UNP P42212
A	829	TRP	-	expression tag	UNP P42212
A	830	SER	-	expression tag	UNP P42212
A	831	HIS	-	expression tag	UNP P42212
A	832	PRO	-	expression tag	UNP P42212
A	833	GLN	-	expression tag	UNP P42212
A	834	PHE	-	expression tag	UNP P42212
A	835	GLU	-	expression tag	UNP P42212
A	836	LYS	-	expression tag	UNP P42212
A	837	GLY	-	expression tag	UNP P42212
A	838	GLY	-	expression tag	UNP P42212
A	839	GLY	-	expression tag	UNP P42212
A	840	SER	-	expression tag	UNP P42212
A	841	GLY	-	expression tag	UNP P42212
A	842	GLY	-	expression tag	UNP P42212
A	843	GLY	-	expression tag	UNP P42212
A	844	SER	-	expression tag	UNP P42212
A	845	GLY	-	expression tag	UNP P42212
A	846	GLY	-	expression tag	UNP P42212
A	847	GLY	-	expression tag	UNP P42212
A	848	SER	-	expression tag	UNP P42212
A	849	TRP	-	expression tag	UNP P42212
A	850	SER	-	expression tag	UNP P42212
A	851	HIS	-	expression tag	UNP P42212
A	852	PRO	-	expression tag	UNP P42212
A	853	GLN	-	expression tag	UNP P42212
A	854	PHE	-	expression tag	UNP P42212
A	855	GLU	-	expression tag	UNP P42212
A	856	LYS	-	expression tag	UNP P42212
B	576	SER	-	linker	UNP P22001
B	577	LEU	-	linker	UNP P22001
B	578	GLU	-	linker	UNP P22001
B	579	VAL	-	linker	UNP P22001
B	580	LEU	-	linker	UNP P22001
B	581	PHE	-	linker	UNP P22001
B	582	GLN	-	linker	UNP P22001
B	583	GLY	-	linker	UNP P22001

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	584	PRO	-	linker	UNP P22001
B	585	ALA	-	linker	UNP P22001
B	586	ALA	-	linker	UNP P22001
B	587	ALA	-	linker	UNP P22001
B	588	MET	-	linker	UNP P22001
B	589	VAL	-	linker	UNP P22001
B	634	LEU	PHE	conflict	UNP P42212
B	652	LEU	PHE	conflict	UNP P42212
B	653	GLY	SER	conflict	UNP P42212
B	656	LEU	VAL	conflict	UNP P42212
B	660	ALA	SER	conflict	UNP P42212
B	741	THR	MET	conflict	UNP P42212
B	751	ALA	VAL	conflict	UNP P42212
B	763	GLY	SER	conflict	UNP P42212
B	791	TYR	THR	conflict	UNP P42212
B	794	LYS	ALA	conflict	UNP P42212
B	819	LEU	HIS	conflict	UNP P42212
B	827	SER	-	expression tag	UNP P42212
B	828	ALA	-	expression tag	UNP P42212
B	829	TRP	-	expression tag	UNP P42212
B	830	SER	-	expression tag	UNP P42212
B	831	HIS	-	expression tag	UNP P42212
B	832	PRO	-	expression tag	UNP P42212
B	833	GLN	-	expression tag	UNP P42212
B	834	PHE	-	expression tag	UNP P42212
B	835	GLU	-	expression tag	UNP P42212
B	836	LYS	-	expression tag	UNP P42212
B	837	GLY	-	expression tag	UNP P42212
B	838	GLY	-	expression tag	UNP P42212
B	839	GLY	-	expression tag	UNP P42212
B	840	SER	-	expression tag	UNP P42212
B	841	GLY	-	expression tag	UNP P42212
B	842	GLY	-	expression tag	UNP P42212
B	843	GLY	-	expression tag	UNP P42212
B	844	SER	-	expression tag	UNP P42212
B	845	GLY	-	expression tag	UNP P42212
B	846	GLY	-	expression tag	UNP P42212
B	847	GLY	-	expression tag	UNP P42212
B	848	SER	-	expression tag	UNP P42212
B	849	TRP	-	expression tag	UNP P42212
B	850	SER	-	expression tag	UNP P42212
B	851	HIS	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	852	PRO	-	expression tag	UNP P42212
B	853	GLN	-	expression tag	UNP P42212
B	854	PHE	-	expression tag	UNP P42212
B	855	GLU	-	expression tag	UNP P42212
B	856	LYS	-	expression tag	UNP P42212
C	576	SER	-	linker	UNP P22001
C	577	LEU	-	linker	UNP P22001
C	578	GLU	-	linker	UNP P22001
C	579	VAL	-	linker	UNP P22001
C	580	LEU	-	linker	UNP P22001
C	581	PHE	-	linker	UNP P22001
C	582	GLN	-	linker	UNP P22001
C	583	GLY	-	linker	UNP P22001
C	584	PRO	-	linker	UNP P22001
C	585	ALA	-	linker	UNP P22001
C	586	ALA	-	linker	UNP P22001
C	587	ALA	-	linker	UNP P22001
C	588	MET	-	linker	UNP P22001
C	589	VAL	-	linker	UNP P22001
C	634	LEU	PHE	conflict	UNP P42212
C	652	LEU	PHE	conflict	UNP P42212
C	653	GLY	SER	conflict	UNP P42212
C	656	LEU	VAL	conflict	UNP P42212
C	660	ALA	SER	conflict	UNP P42212
C	741	THR	MET	conflict	UNP P42212
C	751	ALA	VAL	conflict	UNP P42212
C	763	GLY	SER	conflict	UNP P42212
C	791	TYR	THR	conflict	UNP P42212
C	794	LYS	ALA	conflict	UNP P42212
C	819	LEU	HIS	conflict	UNP P42212
C	827	SER	-	expression tag	UNP P42212
C	828	ALA	-	expression tag	UNP P42212
C	829	TRP	-	expression tag	UNP P42212
C	830	SER	-	expression tag	UNP P42212
C	831	HIS	-	expression tag	UNP P42212
C	832	PRO	-	expression tag	UNP P42212
C	833	GLN	-	expression tag	UNP P42212
C	834	PHE	-	expression tag	UNP P42212
C	835	GLU	-	expression tag	UNP P42212
C	836	LYS	-	expression tag	UNP P42212
C	837	GLY	-	expression tag	UNP P42212
C	838	GLY	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	839	GLY	-	expression tag	UNP P42212
C	840	SER	-	expression tag	UNP P42212
C	841	GLY	-	expression tag	UNP P42212
C	842	GLY	-	expression tag	UNP P42212
C	843	GLY	-	expression tag	UNP P42212
C	844	SER	-	expression tag	UNP P42212
C	845	GLY	-	expression tag	UNP P42212
C	846	GLY	-	expression tag	UNP P42212
C	847	GLY	-	expression tag	UNP P42212
C	848	SER	-	expression tag	UNP P42212
C	849	TRP	-	expression tag	UNP P42212
C	850	SER	-	expression tag	UNP P42212
C	851	HIS	-	expression tag	UNP P42212
C	852	PRO	-	expression tag	UNP P42212
C	853	GLN	-	expression tag	UNP P42212
C	854	PHE	-	expression tag	UNP P42212
C	855	GLU	-	expression tag	UNP P42212
C	856	LYS	-	expression tag	UNP P42212
D	576	SER	-	linker	UNP P22001
D	577	LEU	-	linker	UNP P22001
D	578	GLU	-	linker	UNP P22001
D	579	VAL	-	linker	UNP P22001
D	580	LEU	-	linker	UNP P22001
D	581	PHE	-	linker	UNP P22001
D	582	GLN	-	linker	UNP P22001
D	583	GLY	-	linker	UNP P22001
D	584	PRO	-	linker	UNP P22001
D	585	ALA	-	linker	UNP P22001
D	586	ALA	-	linker	UNP P22001
D	587	ALA	-	linker	UNP P22001
D	588	MET	-	linker	UNP P22001
D	589	VAL	-	linker	UNP P22001
D	634	LEU	PHE	conflict	UNP P42212
D	652	LEU	PHE	conflict	UNP P42212
D	653	GLY	SER	conflict	UNP P42212
D	656	LEU	VAL	conflict	UNP P42212
D	660	ALA	SER	conflict	UNP P42212
D	741	THR	MET	conflict	UNP P42212
D	751	ALA	VAL	conflict	UNP P42212
D	763	GLY	SER	conflict	UNP P42212
D	791	TYR	THR	conflict	UNP P42212
D	794	LYS	ALA	conflict	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	819	LEU	HIS	conflict	UNP P42212
D	827	SER	-	expression tag	UNP P42212
D	828	ALA	-	expression tag	UNP P42212
D	829	TRP	-	expression tag	UNP P42212
D	830	SER	-	expression tag	UNP P42212
D	831	HIS	-	expression tag	UNP P42212
D	832	PRO	-	expression tag	UNP P42212
D	833	GLN	-	expression tag	UNP P42212
D	834	PHE	-	expression tag	UNP P42212
D	835	GLU	-	expression tag	UNP P42212
D	836	LYS	-	expression tag	UNP P42212
D	837	GLY	-	expression tag	UNP P42212
D	838	GLY	-	expression tag	UNP P42212
D	839	GLY	-	expression tag	UNP P42212
D	840	SER	-	expression tag	UNP P42212
D	841	GLY	-	expression tag	UNP P42212
D	842	GLY	-	expression tag	UNP P42212
D	843	GLY	-	expression tag	UNP P42212
D	844	SER	-	expression tag	UNP P42212
D	845	GLY	-	expression tag	UNP P42212
D	846	GLY	-	expression tag	UNP P42212
D	847	GLY	-	expression tag	UNP P42212
D	848	SER	-	expression tag	UNP P42212
D	849	TRP	-	expression tag	UNP P42212
D	850	SER	-	expression tag	UNP P42212
D	851	HIS	-	expression tag	UNP P42212
D	852	PRO	-	expression tag	UNP P42212
D	853	GLN	-	expression tag	UNP P42212
D	854	PHE	-	expression tag	UNP P42212
D	855	GLU	-	expression tag	UNP P42212
D	856	LYS	-	expression tag	UNP P42212

- Molecule 2 is a protein called Fab-ShK fusion, heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	261	1389	829	280	273	7	0	0

- Molecule 3 is a protein called Fab-ShK fusion, light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	L	213	1047	621	213	213	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

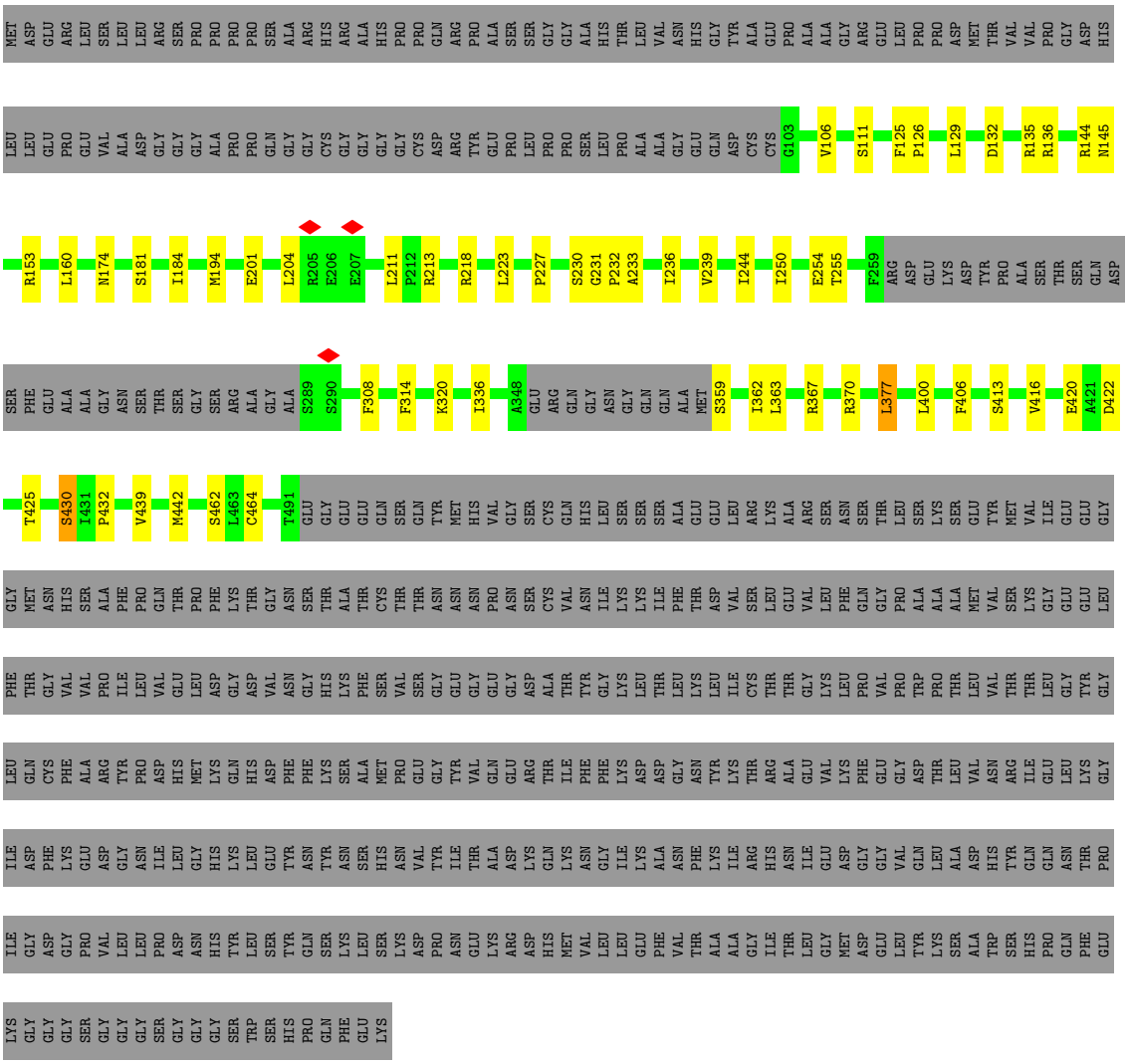
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
4	A	2	2	2	0
			Total	K	
4	C	1	1	1	0

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.

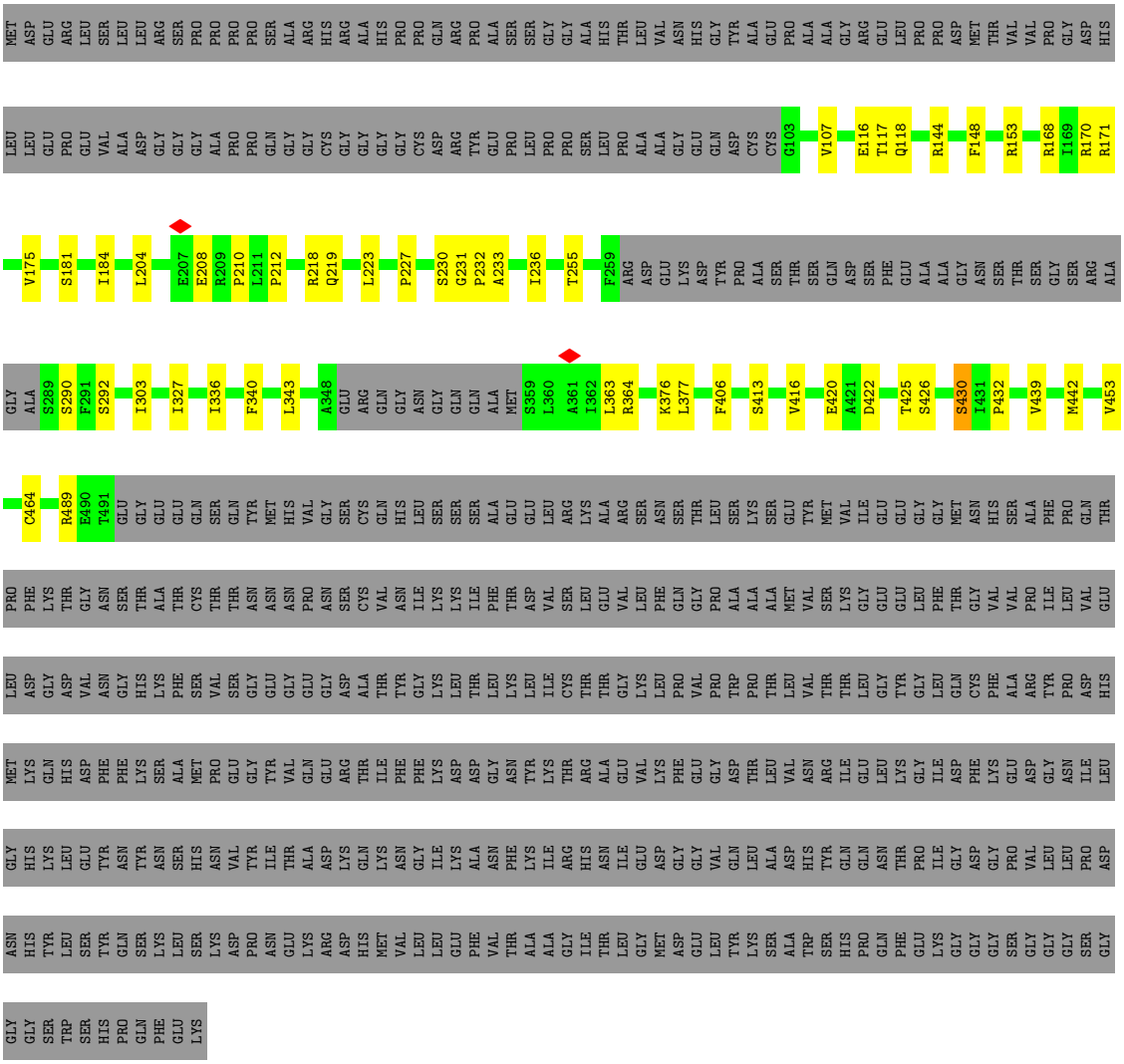
• Molecule 1: Potassium voltage-gated channel subfamily A member 3,Green fluorescent protein fusion

Chain A: 34% 6% 59%



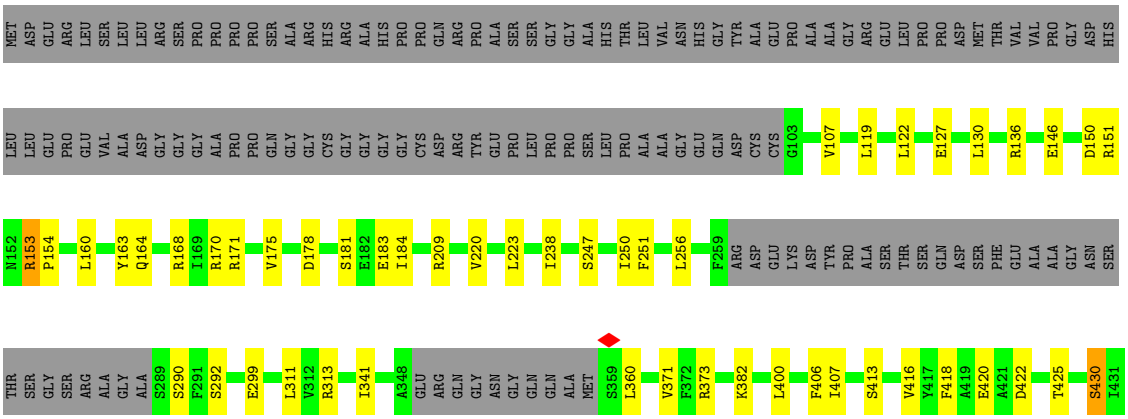
• Molecule 1: Potassium voltage-gated channel subfamily A member 3,Green fluorescent protein fusion

Chain B: 35% 6% 59%



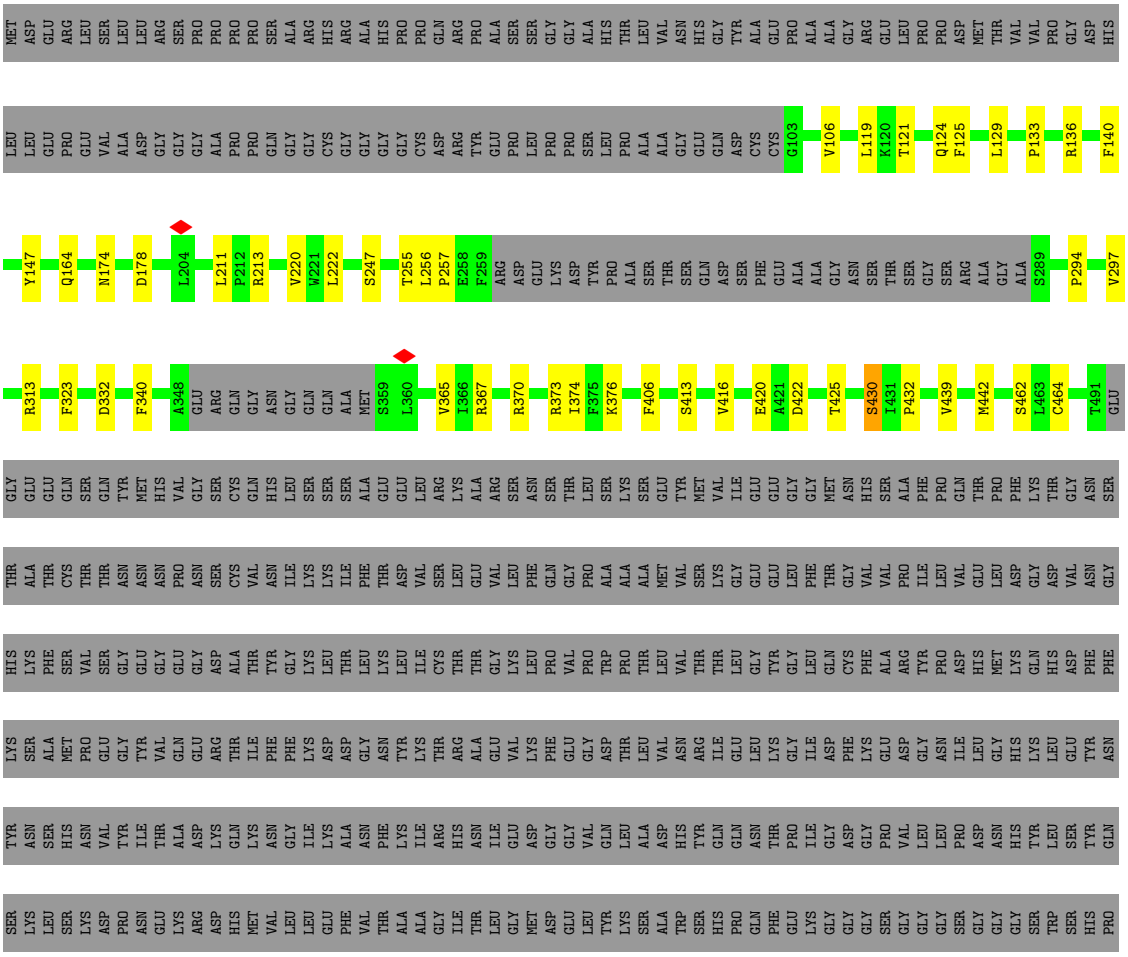
• Molecule 1: Potassium voltage-gated channel subfamily A member 3,Green fluorescent protein fusion

Chain C: 35% 6% 59%



• Molecule 1: Potassium voltage-gated channel subfamily A member 3,Green fluorescent protein fusion

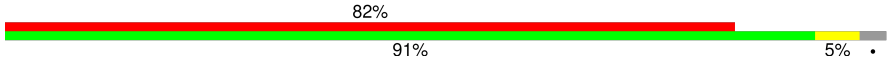
Chain D:



GLN PHE GLU LYS

- Molecule 2: Fab-ShK fusion, heavy chain

Chain H:



Q1 V2 Q3 L4 R5 E6 W7 G8 A9 G10 L11 L12 K13 P14 S15 E16 T17 L18 S19 L20 T21 C22 A23 V24 Y25 G26 G27 S28 F29 S30 D31 K32 Y33 W34 S35 W36 I37 R38 Q39 P40 P41 G42 K43 G44 L45 E46 W47 I48 G49 S50 I51 N52 H53 S54 G55 S56 T57 N58 Y59 N60

P61 S62 L63 K64 S65 R66 V67 T68 I69 S70 V71 D72 T73 S74 K75 N76 Q77 F78 S79 L80 K81 L82 S83 S84 V85 T86 A87 A88 D89 T90 A91 V92 Y93 Y94 C95 T96 S97 V98 H99 Q100 E101 T102 K103 LYS TYR GLN SER R108 F122 M128 L132 R136 C142 SER TYR

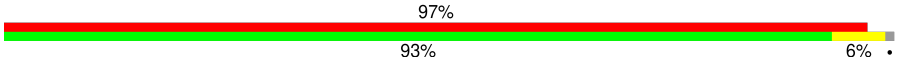
THR TYR N147 Y148 E149 W150 H151 V152 D153 V154 W155 G156 Q157 G158 L159 L160 V161 T162 V163 S164 S165 A166 S167 T168 K169 G170 P171 S172 V173 F174 P175 L176 A177 P178 S179 S180 K181 S182 T183 S184 G185 G186 T187 A188 A189 L190 G191 C192 L193 V194 K195 D196 Y197 F198 P199 E200 P201 V202 T203 V204

S205 W206 N207 S208 G209 A210 L211 T212 S213 G214 V215 H216 T217 F218 P219 A220 V221 L222 Q223 S224 S225 G226 L227 Y228 S229 L230 S231 S232 V233 V234 T235 V236 P237 S238 S239 S240 L241 G242 T243 Q244 T245 Y246 I247 C248 N249 V250 N251 H252 K253 P254 S255 N256 T257 K258 V259 D260 K261 K262 V263 E264

P265 K266 S267 C268 D269 LYS

- Molecule 3: Fab-ShK fusion, light chain

Chain L:



GLN ALA VAL L4 N5 Q6 P7 S8 S9 V10 S11 G12 S13 L14 G15 Q16 K17 V18 T19 I20 S21 C22 S23 G24 S25 S26 S27 N28 I29 G30 N31 N32 Y33 V34 S35 W36 Y37 Q38 Q39 L40 P41 G42 T43 A44 P45 K46 L47 L48 I49 Y50 G51 D52 T53 K54 R55 P56 S57 G58 I59 P60

D61 R62 F63 S64 G65 S66 K67 S68 G69 T70 S71 A72 T73 L74 G75 I76 T77 G78 L79 Q80 T81 G82 D83 E84 A85 D86 Y87 Y88 C89 A90 S91 A92 E93 D94 S97 N98 A99 V100 F101 G102 S103 G104 T105 T106 L107 T108 V109 L110 G111 Q112 P113 K114 A115 A116 P117 S118 V119 T120 L121

F122 P123 P124 S125 S126 E127 E128 L129 Q130 A131 N132 K133 A134 T135 L136 V137 C138 L139 I140 S141 D142 F143 Y144 P145 G146 A147 V148 T149 V150 A151 W152 K153 A154 D155 S156 S157 P158 V159 K160 A161 G162 V163 E164 T165 T166 T167 P168 S169 K170 Q171 S172 N173 N174 K175 Y176 A177 A178 S179 S180 Y181

L182 S183 L184 T185 P186 E187 Q188 W189 K190 S191 H192 R193 S194 Y195 S196 C197 Q198 V199 T200 H201 E202 G203 S204 T205 V206 E207 K208 T209 V210 A211 P212 T213 E214 C215 S216

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90267	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.755	Depositor
Minimum map value	-1.583	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.227	Depositor
Map size (Å)	374.88, 374.88, 374.88	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.852, 0.852, 0.852	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.74	0/2917	0.81	0/3953
1	B	0.83	0/2917	0.85	0/3953
1	C	0.84	0/2917	0.83	0/3953
1	D	0.79	0/2917	0.84	0/3953
2	H	0.48	0/1391	0.70	0/1912
3	L	0.43	0/1046	0.68	0/1452
All	All	0.75	0/14105	0.81	0/19176

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 (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	2844	0	2874	29	0
1	B	2844	0	2874	35	0
1	C	2844	0	2874	28	0
1	D	2844	0	2874	23	0
2	H	1389	0	769	13	0
3	L	1047	0	480	7	0
4	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
All	All	13815	0	12745	119	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 4.

All (119) 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:B:453:VAL:HG11	2:H:122:PHE:CZ	2.12	0.84
3:L:33:TYR:HA	3:L:51:GLY:HA2	1.68	0.75
1:B:453:VAL:HG11	2:H:122:PHE:HZ	1.50	0.72
1:A:430:SER:HB2	1:A:432:PRO:HD2	1.72	0.71
1:B:430:SER:HB2	1:B:432:PRO:HD2	1.72	0.70
1:B:453:VAL:CG1	2:H:122:PHE:HZ	2.05	0.70
1:D:430:SER:HB2	1:D:432:PRO:HD2	1.72	0.69
1:C:430:SER:HB2	1:C:432:PRO:HD2	1.72	0.69
1:D:332:ASP:OD1	1:D:376:LYS:NZ	2.28	0.67
1:C:178:ASP:N	1:C:178:ASP:OD1	2.29	0.65
1:C:170:ARG:NH2	1:D:178:ASP:OD2	2.31	0.63
1:B:290:SER:C	1:B:292:SER:H	2.02	0.62
1:A:462:SER:OG	1:B:439:VAL:HG11	2.00	0.61
1:B:107:VAL:HG22	1:B:116:GLU:HG2	1.84	0.60
1:A:255:THR:O	1:A:255:THR:OG1	2.21	0.58
1:B:170:ARG:NH2	1:C:178:ASP:OD2	2.37	0.58
1:B:168:ARG:HD3	1:B:170:ARG:HH21	1.68	0.57
1:A:250:ILE:O	1:A:254:GLU:HB2	2.05	0.56
2:H:44:GLY:HA3	3:L:103:SER:HA	1.87	0.56
1:B:420:GLU:HB3	1:B:425:THR:HG21	1.88	0.56
1:D:313:ARG:HG2	1:D:323:PHE:HE1	1.70	0.55
1:D:420:GLU:HB3	1:D:425:THR:HG21	1.88	0.55
3:L:23:SER:HA	3:L:71:SER:HA	1.88	0.55
1:C:420:GLU:HB3	1:C:425:THR:HG21	1.88	0.55
1:C:251:PHE:HE2	1:C:371:VAL:HG23	1.72	0.55
2:H:21:THR:HA	2:H:79:SER:HA	1.88	0.54
1:A:420:GLU:HB3	1:A:425:THR:HG21	1.88	0.54
1:C:171:ARG:NH1	1:C:175:VAL:O	2.41	0.54
1:C:160:LEU:O	1:C:164:GLN:HG2	2.08	0.53
1:C:168:ARG:HD3	1:C:170:ARG:HH21	1.74	0.52
1:B:181:SER:O	1:B:184:ILE:HG22	2.10	0.52
1:A:227:PRO:HA	1:A:233:ALA:HB1	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:MET:HG3	1:B:464:CYS:SG	2.51	0.51
1:D:247:SER:OG	1:D:373:ARG:NH1	2.44	0.51
1:C:442:MET:HG3	1:C:464:CYS:SG	2.51	0.51
1:C:290:SER:C	1:C:292:SER:H	2.14	0.51
1:B:327:ILE:HD12	1:B:327:ILE:H	1.75	0.51
3:L:22:CYS:O	3:L:72:ALA:N	2.41	0.51
1:D:256:LEU:HD12	1:D:257:PRO:HD2	1.92	0.51
1:A:442:MET:HG3	1:A:464:CYS:SG	2.51	0.50
1:D:442:MET:HG3	1:D:464:CYS:SG	2.51	0.50
1:D:294:PRO:HA	1:D:297:VAL:HG12	1.94	0.50
1:C:220:VAL:HA	1:C:223:LEU:HB2	1.93	0.50
1:C:247:SER:OG	1:C:373:ARG:NH1	2.44	0.50
1:D:129:LEU:O	1:D:136:ARG:HB3	2.11	0.50
1:A:181:SER:O	1:A:184:ILE:HG12	2.12	0.50
1:A:439:VAL:HG11	1:D:462:SER:OG	2.13	0.49
1:C:181:SER:O	1:C:184:ILE:HG12	2.12	0.49
1:A:129:LEU:O	1:A:136:ARG:HB3	2.13	0.48
1:B:290:SER:C	1:B:292:SER:N	2.66	0.48
1:A:236:ILE:HA	1:A:239:VAL:HG22	1.95	0.48
1:A:420:GLU:HB3	1:A:425:THR:CG2	2.44	0.48
1:A:359:SER:HA	1:A:362:ILE:HB	1.96	0.48
1:B:420:GLU:HB3	1:B:425:THR:CG2	2.44	0.48
1:C:462:SER:OG	1:D:439:VAL:HG11	2.14	0.48
1:A:213:ARG:HA	1:A:218:ARG:HD3	1.95	0.47
1:B:303:ILE:HG23	1:B:336:ILE:HD11	1.96	0.47
1:B:426:SER:OG	2:H:122:PHE:CZ	2.66	0.47
1:C:420:GLU:HB3	1:C:425:THR:CG2	2.44	0.47
1:D:420:GLU:HB3	1:D:425:THR:CG2	2.44	0.47
1:A:377:LEU:HD12	1:A:377:LEU:HA	1.80	0.46
1:C:153:ARG:N	1:C:154:PRO:HD2	2.30	0.46
1:D:211:LEU:HB3	1:D:213:ARG:HD2	1.98	0.46
1:D:124:GLN:HG3	1:D:125:PHE:HD1	1.81	0.46
1:B:208:GLU:O	1:B:210:PRO:HD3	2.16	0.45
1:D:140:PHE:HB2	1:D:147:TYR:CD2	2.52	0.45
1:A:126:PRO:O	1:A:132:ASP:HB2	2.17	0.45
1:A:213:ARG:HA	1:A:218:ARG:HB2	1.99	0.45
1:A:359:SER:HB2	1:A:363:LEU:HG	1.98	0.45
1:C:130:LEU:O	1:C:136:ARG:HD3	2.17	0.44
1:B:377:LEU:HD12	1:B:377:LEU:HA	1.86	0.44
3:L:89:CYS:O	3:L:102:GLY:N	2.51	0.44
1:A:174:ASN:OD1	1:A:174:ASN:N	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.81	0.44
1:B:227:PRO:HA	1:B:233:ALA:HB1	2.00	0.44
1:B:336:ILE:HD12	1:B:336:ILE:HA	1.84	0.44
1:A:223:LEU:HD11	1:A:232:PRO:HB2	1.98	0.44
1:B:232:PRO:O	1:B:236:ILE:HG12	2.18	0.43
1:B:144:ARG:HH21	1:B:148:PHE:HB2	1.82	0.43
1:B:230:SER:OG	1:B:231:GLY:N	2.52	0.43
1:B:432:PRO:HG2	1:C:256:LEU:HD13	1.99	0.43
1:C:311:LEU:HA	1:C:311:LEU:HD23	1.75	0.43
1:A:400:LEU:HD23	1:A:400:LEU:HA	1.81	0.43
2:H:268:CYS:CB	3:L:215:CYS:CB	2.97	0.43
1:C:432:PRO:HD3	1:D:255:THR:OG1	2.19	0.43
1:D:133:PRO:HA	1:D:136:ARG:HG2	2.01	0.42
1:D:367:ARG:O	1:D:370:ARG:HB2	2.19	0.42
1:A:135:ARG:HE	1:A:135:ARG:HB2	1.61	0.42
1:B:117:THR:OG1	1:B:118:GLN:N	2.51	0.42
2:H:132:LEU:H	2:H:132:LEU:HG	1.76	0.42
3:L:169:SER:O	3:L:177:ALA:N	2.51	0.42
1:A:111:SER:HB3	1:A:153:ARG:HG2	2.01	0.42
1:D:256:LEU:HD12	1:D:256:LEU:HA	1.80	0.42
2:H:22:CYS:N	2:H:78:PHE:O	2.49	0.42
1:A:244:ILE:HD13	1:A:377:LEU:HD13	2.00	0.42
1:B:212:PRO:O	1:B:218:ARG:HB2	2.19	0.42
1:A:367:ARG:O	1:A:370:ARG:HB2	2.19	0.42
1:B:364:ARG:HE	1:B:364:ARG:HB3	1.68	0.42
1:B:376:LYS:HB3	1:B:376:LYS:HE3	1.85	0.42
1:C:238:ILE:HD13	1:C:238:ILE:HA	1.77	0.42
1:B:204:LEU:HB2	1:B:489:ARG:HD2	2.02	0.41
1:C:313:ARG:HH11	1:C:313:ARG:HD2	1.67	0.41
1:B:340:PHE:HD1	1:B:340:PHE:HA	1.72	0.41
1:C:107:VAL:HB	1:C:146:GLU:HG2	2.02	0.41
1:A:160:LEU:HD12	1:A:160:LEU:HA	1.90	0.41
1:B:343:LEU:HD12	1:B:343:LEU:HA	1.80	0.41
1:C:250:ILE:HA	1:C:250:ILE:HD13	1.78	0.41
1:C:407:ILE:HG23	1:D:374:ILE:HD12	2.01	0.41
2:H:128:MET:HE2	2:H:128:MET:HB2	1.74	0.41
2:H:190:LEU:O	2:H:234:VAL:N	2.38	0.41
1:B:171:ARG:NH1	1:B:175:VAL:O	2.54	0.41
1:B:255:THR:O	1:B:255:THR:OG1	2.25	0.41
1:C:418:PHE:CZ	1:D:367:ARG:HG2	2.55	0.41
2:H:98:VAL:HA	2:H:152:VAL:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:SER:OG	1:A:231:GLY:N	2.52	0.40
1:A:314:PHE:O	1:A:320:LYS:HE3	2.21	0.40
1:B:426:SER:OG	2:H:122:PHE:CE2	2.73	0.40
1:C:400:LEU:HD23	1:C:400:LEU:HA	1.80	0.40
1:D:340:PHE:HD1	1:D:340:PHE:HA	1.72	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	344/856 (40%)	328 (95%)	16 (5%)	0	100	100
1	B	344/856 (40%)	325 (94%)	19 (6%)	0	100	100
1	C	344/856 (40%)	321 (93%)	23 (7%)	0	100	100
1	D	344/856 (40%)	319 (93%)	25 (7%)	0	100	100
2	H	255/270 (94%)	234 (92%)	21 (8%)	0	100	100
3	L	211/216 (98%)	193 (92%)	18 (8%)	0	100	100
All	All	1842/3910 (47%)	1720 (93%)	122 (7%)	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	A	311/724 (43%)	295 (95%)	16 (5%)	20	46
1	B	311/724 (43%)	302 (97%)	9 (3%)	37	61
1	C	311/724 (43%)	293 (94%)	18 (6%)	17	42
1	D	311/724 (43%)	298 (96%)	13 (4%)	25	51
2	H	33/239 (14%)	31 (94%)	2 (6%)	15	40
All	All	1277/3135 (41%)	1219 (96%)	58 (4%)	26	50

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	125	PHE
1	A	144	ARG
1	A	145	ASN
1	A	194	MET
1	A	201	GLU
1	A	204	LEU
1	A	211	LEU
1	A	308	PHE
1	A	336	ILE
1	A	377	LEU
1	A	406	PHE
1	A	413	SER
1	A	416	VAL
1	A	422	ASP
1	A	430	SER
1	B	153	ARG
1	B	219	GLN
1	B	223	LEU
1	B	363	LEU
1	B	406	PHE
1	B	413	SER
1	B	416	VAL
1	B	422	ASP
1	B	430	SER
1	C	119	LEU
1	C	122	LEU
1	C	127	GLU
1	C	150	ASP
1	C	151	ARG
1	C	153	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	163	TYR
1	C	183	GLU
1	C	209	ARG
1	C	299	GLU
1	C	341	ILE
1	C	360	LEU
1	C	382	LYS
1	C	406	PHE
1	C	413	SER
1	C	416	VAL
1	C	422	ASP
1	C	430	SER
1	D	106	VAL
1	D	119	LEU
1	D	121	THR
1	D	164	GLN
1	D	174	ASN
1	D	220	VAL
1	D	222	LEU
1	D	365	VAL
1	D	406	PHE
1	D	413	SER
1	D	416	VAL
1	D	422	ASP
1	D	430	SER
2	H	132	LEU
2	H	136	ARG

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

Mol	Chain	Res	Type
1	A	124	GLN
1	A	145	ASN
1	A	164	GLN
1	B	145	ASN
1	C	124	GLN
1	C	164	GLN
1	C	451	HIS

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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

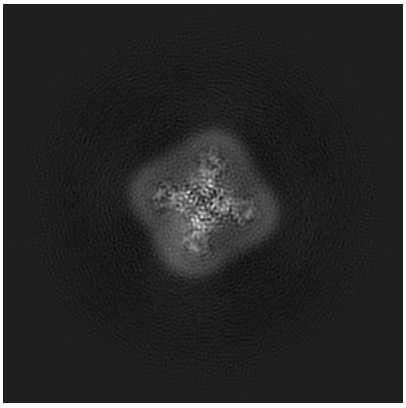
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25414. These allow visual inspection of the internal detail of the map and identification of artifacts.

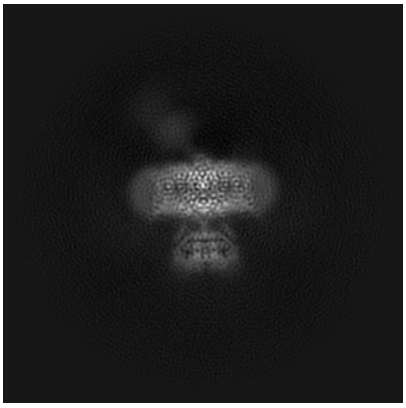
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

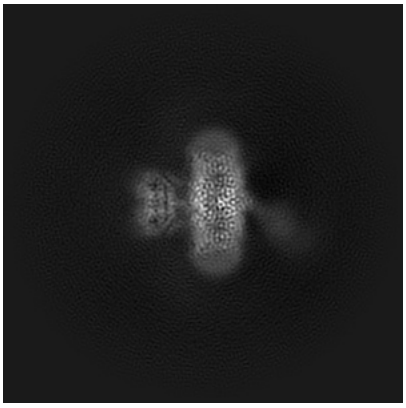
6.1.1 Primary map



X



Y

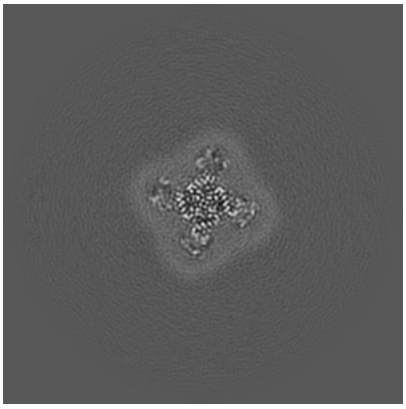


Z

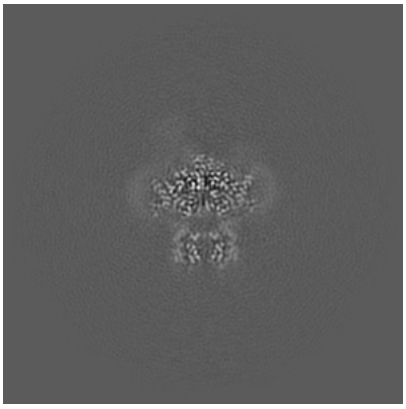
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

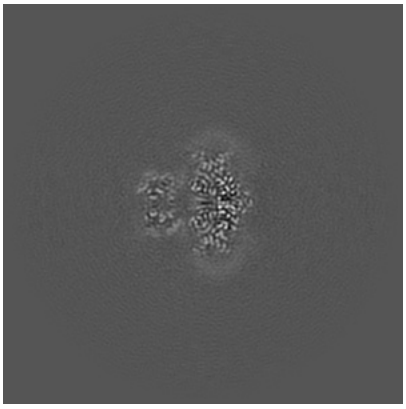
6.2.1 Primary map



X Index: 220



Y Index: 220

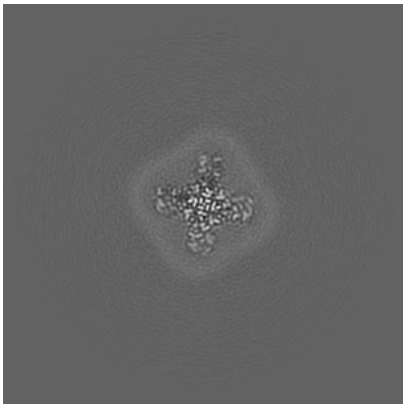


Z Index: 220

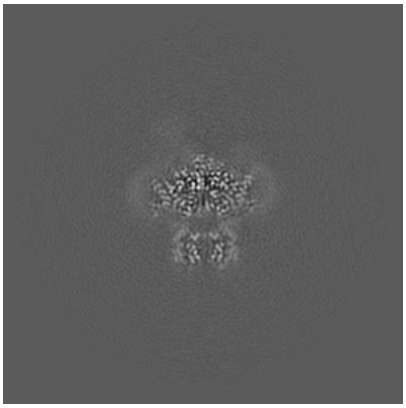
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

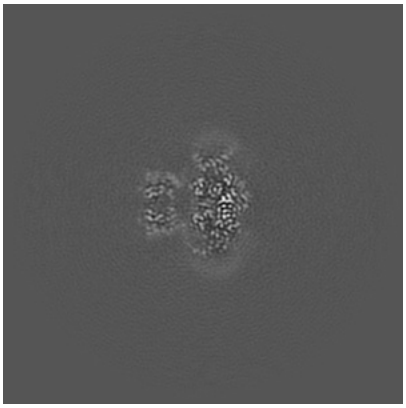
6.3.1 Primary map



X Index: 243



Y Index: 220

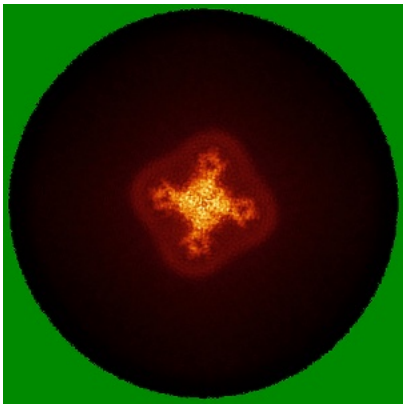


Z Index: 223

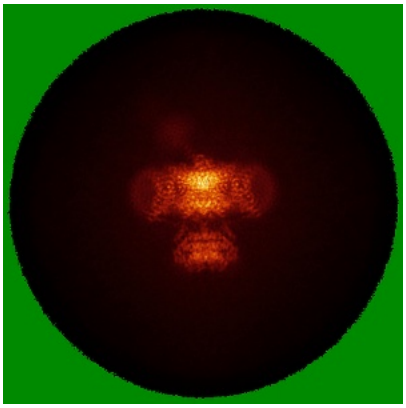
The images above show the largest variance slices of the map in three orthogonal directions.

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

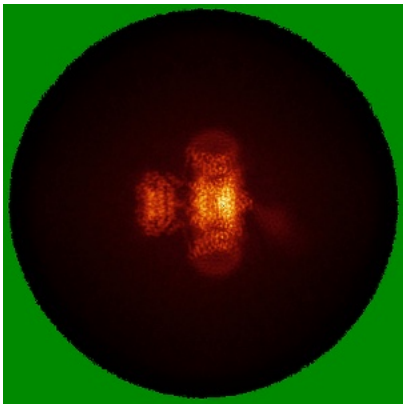
6.4.1 Primary map



X



Y



Z

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 0.227. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

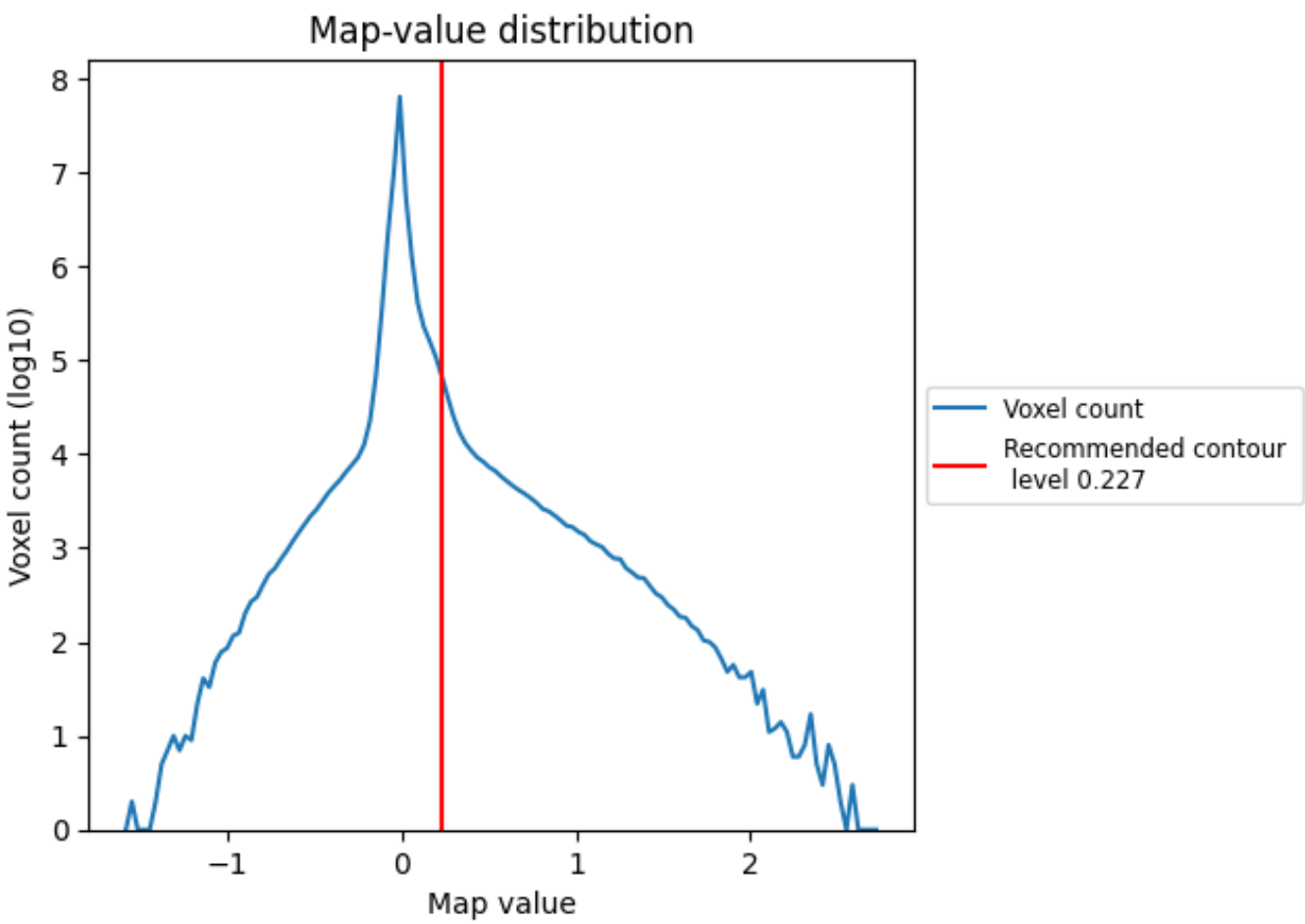
6.6 Mask visualisation (i)

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

7 Map analysis (i)

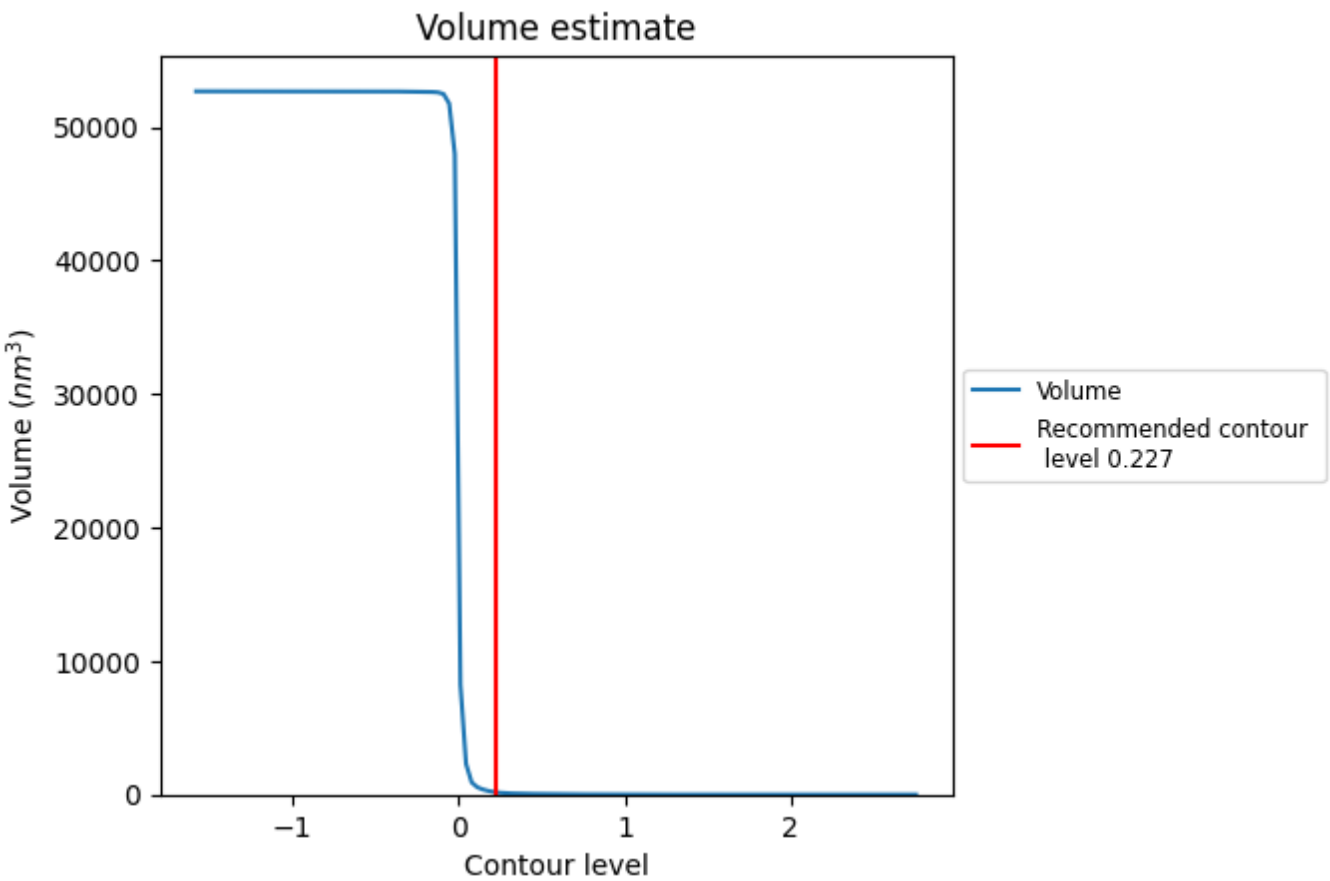
This section contains the results of statistical analysis of the map.

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.

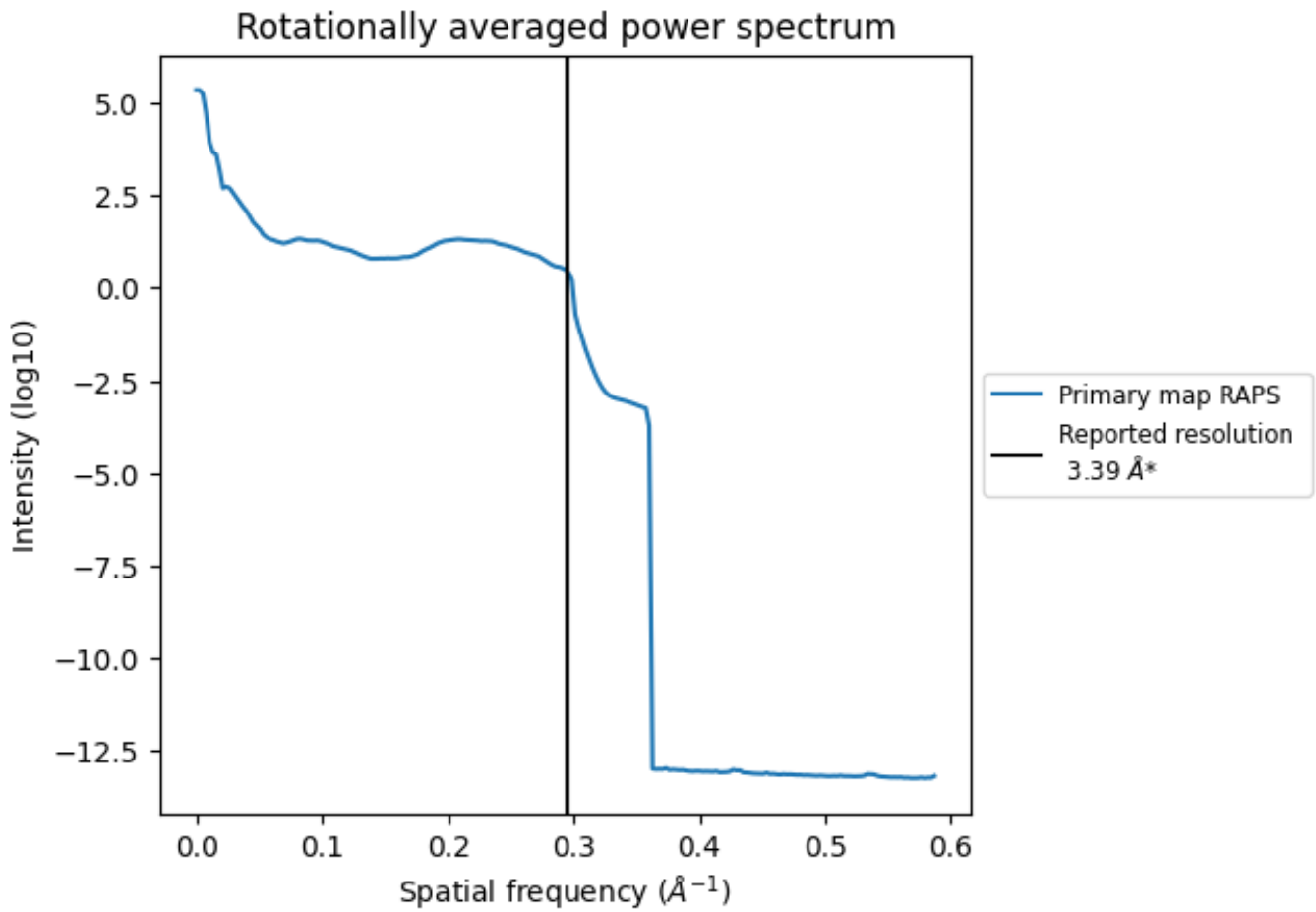
7.2 Volume estimate (i)



The volume at the recommended contour level is 168 nm^3; this corresponds to an approximate mass of 151 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)

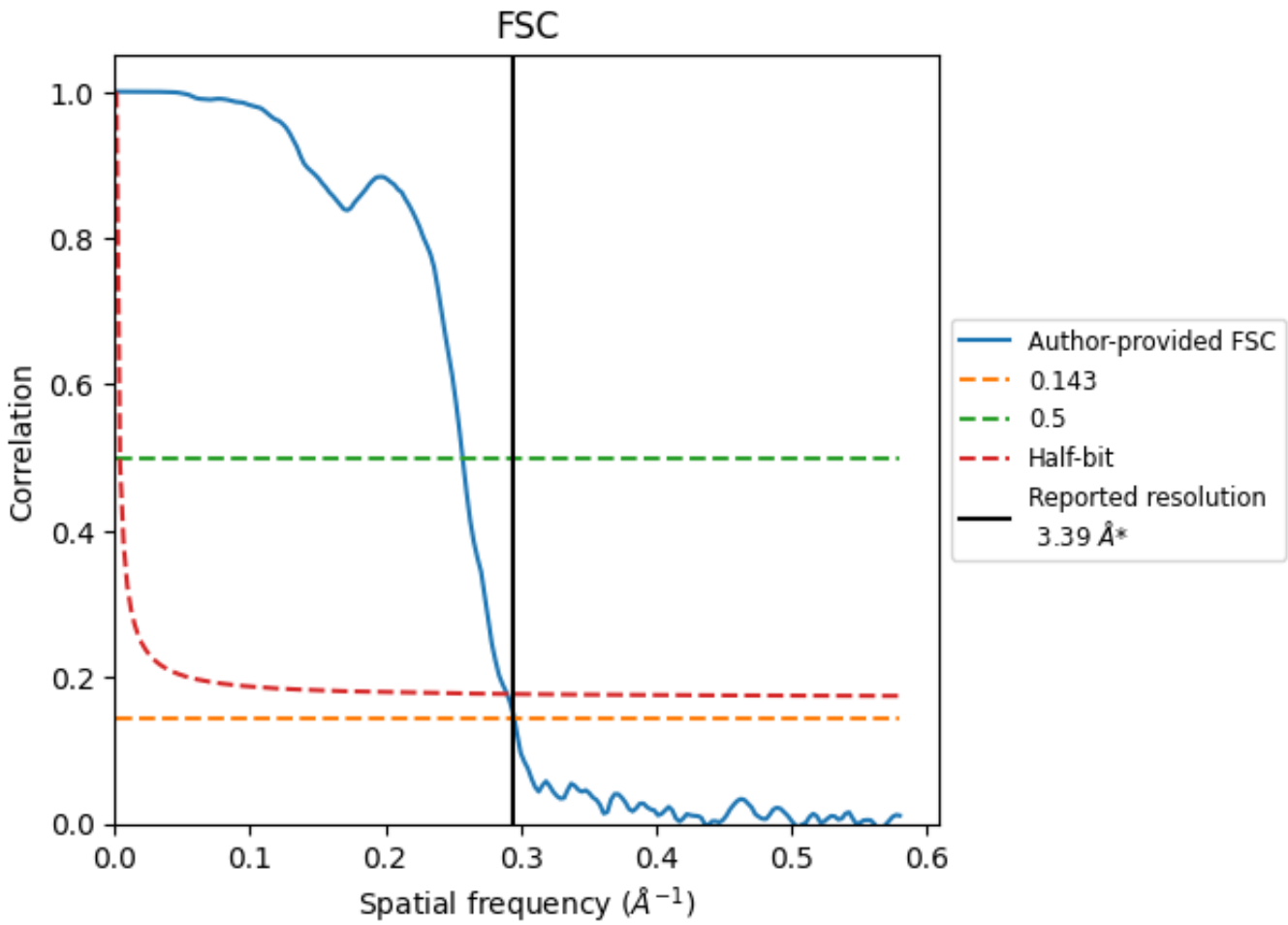


*Reported resolution corresponds to spatial frequency of 0.295 Å^{-1}

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 0.295 Å^{-1}

8.2 Resolution estimates (i)

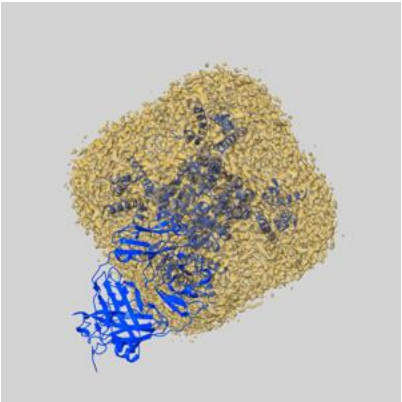
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	3.39	3.89	3.45
Unmasked-calculated*	-	-	-

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

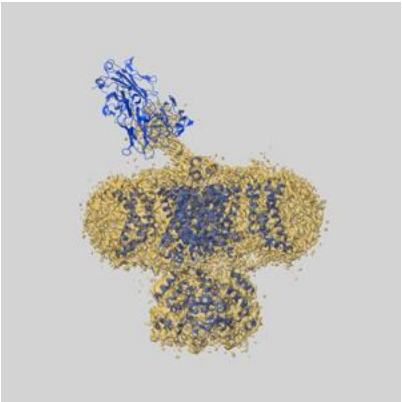
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25414 and PDB model 7SSV. Per-residue inclusion information can be found in section 3 on page 10.

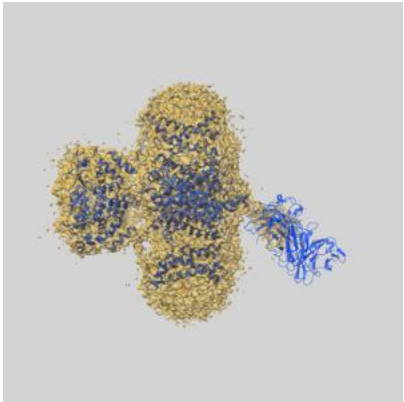
9.1 Map-model overlay (i)



X



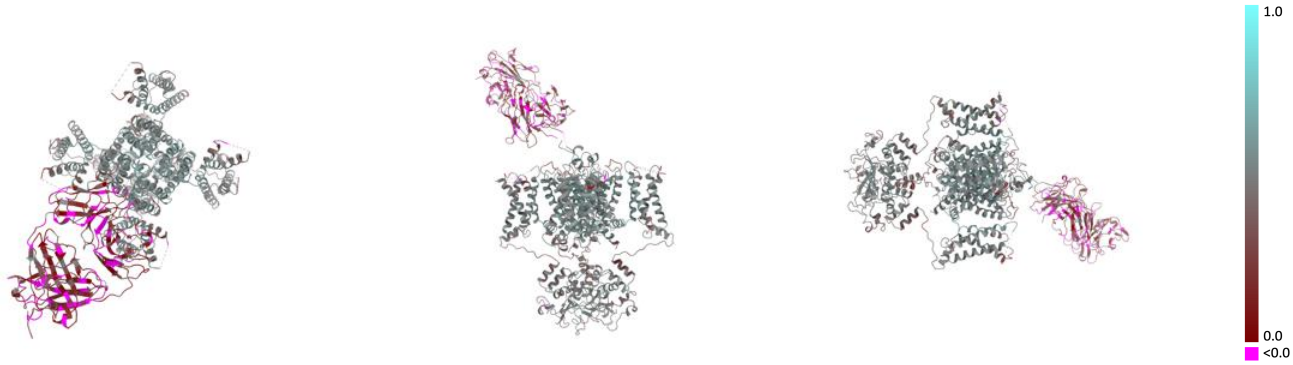
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.227 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.

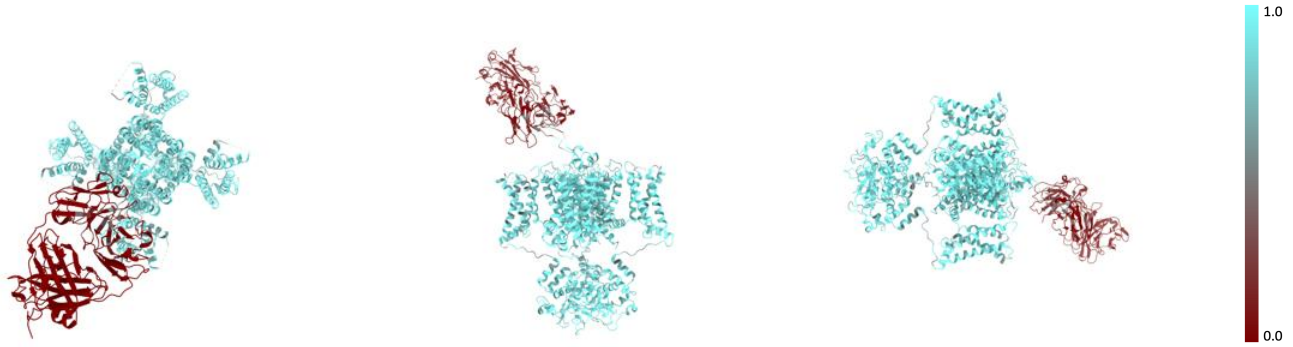
9.2 Q-score mapped to coordinate model (i)



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.

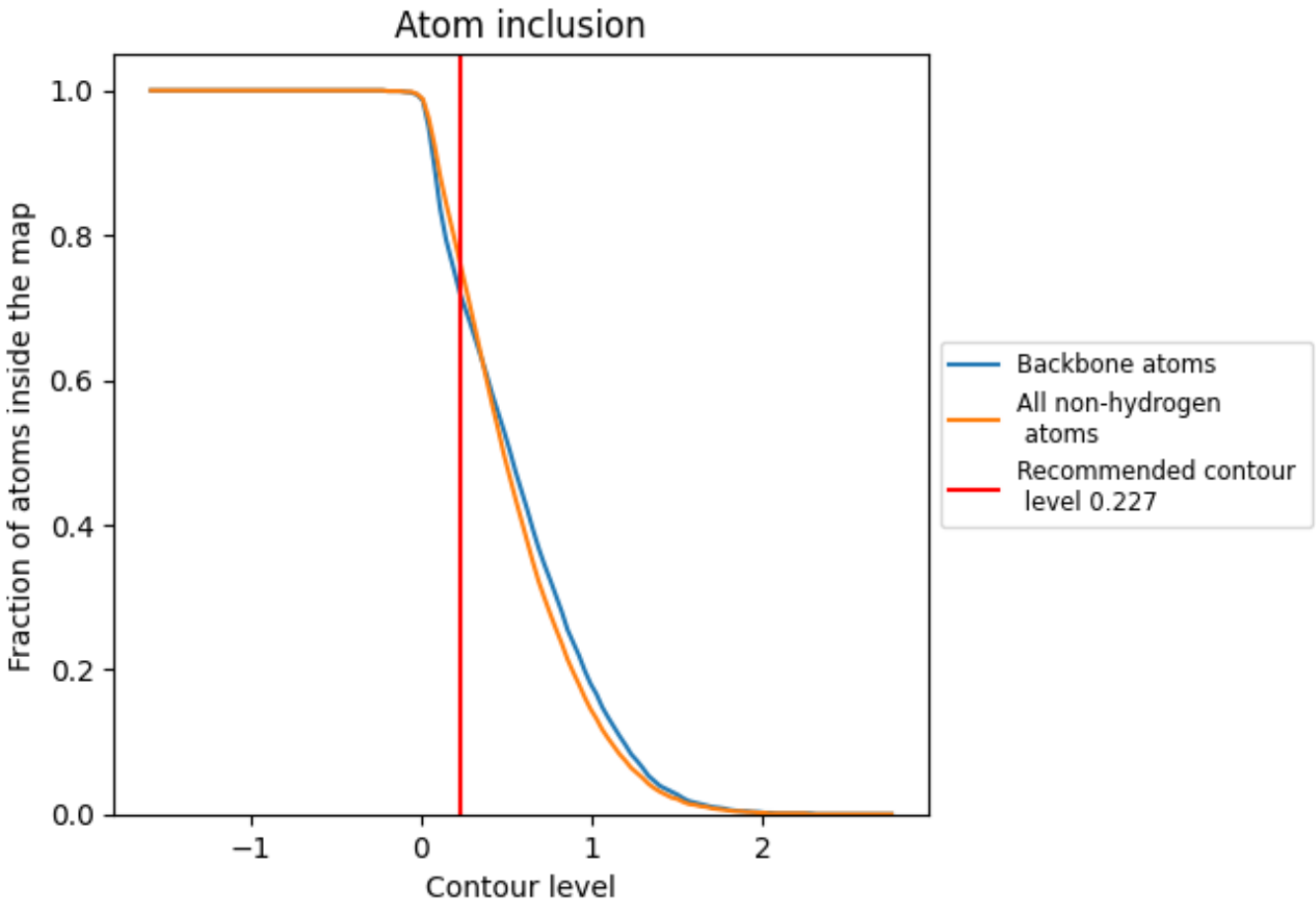
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.227).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.227) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7630	0.4410
A	0.8950	0.4970
B	0.9000	0.4870
C	0.9040	0.4900
D	0.9010	0.4940
H	0.2120	0.2200
L	0.0420	0.1740