Full wwPDB EM Validation Report ⓘ

May 2, 2023 – 10:19 AM EDT

PDB ID	:	8GHG
EMDB ID	:	EMD-40045
Title	:	Cryo-EM structure of hSlo1 in digitonin, Ca2+-free and EDTA-free
Authors	:	Tao, X.; Zhao, C.; MacKinnon, R.
Deposited on	:	2023-03-10
Resolution	:	3.30 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:

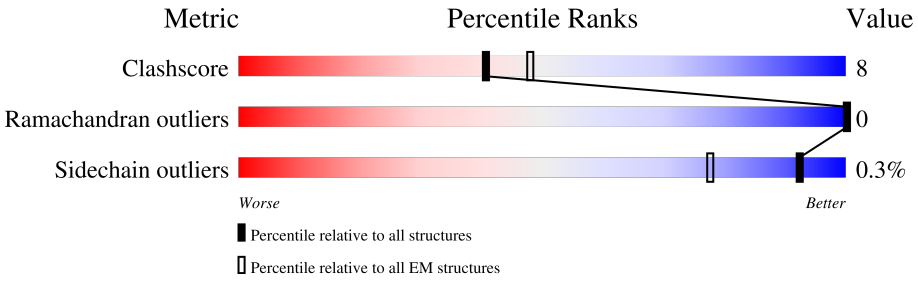
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1072	10% 59% 17% 24%
1	B	1072	10% 61% 15% 24%
1	C	1072	12% 65% 15% 20%
1	D	1072	12% 64% 15% 21%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 26659 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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	816	Total	C	N	O	S	1	0
			6533	4241	1060	1189	43		
1	C	853	Total	C	N	O	S	1	0
			6802	4414	1109	1236	43		
1	B	817	Total	C	N	O	S	1	0
			6549	4254	1062	1190	43		
1	D	849	Total	C	N	O	S	1	0
			6775	4398	1105	1229	43		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q12791
A	-14	ALA	-	expression tag	UNP Q12791
A	-13	PRO	-	expression tag	UNP Q12791
A	-12	SER	-	expression tag	UNP Q12791
A	-11	ARG	-	expression tag	UNP Q12791
A	-10	LEU	-	expression tag	UNP Q12791
A	-9	GLU	-	expression tag	UNP Q12791
A	-8	GLU	-	expression tag	UNP Q12791
A	-7	GLU	-	expression tag	UNP Q12791
A	-6	LEU	-	expression tag	UNP Q12791
A	-5	ARG	-	expression tag	UNP Q12791
A	-4	ARG	-	expression tag	UNP Q12791
A	-3	ARG	-	expression tag	UNP Q12791
A	-2	LEU	-	expression tag	UNP Q12791
A	-1	THR	-	expression tag	UNP Q12791
A	0	GLU	-	expression tag	UNP Q12791
A	1	PRO	-	expression tag	UNP Q12791
C	-15	MET	-	expression tag	UNP Q12791
C	-14	ALA	-	expression tag	UNP Q12791
C	-13	PRO	-	expression tag	UNP Q12791
C	-12	SER	-	expression tag	UNP Q12791
C	-11	ARG	-	expression tag	UNP Q12791

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	LEU	-	expression tag	UNP Q12791
C	-9	GLU	-	expression tag	UNP Q12791
C	-8	GLU	-	expression tag	UNP Q12791
C	-7	GLU	-	expression tag	UNP Q12791
C	-6	LEU	-	expression tag	UNP Q12791
C	-5	ARG	-	expression tag	UNP Q12791
C	-4	ARG	-	expression tag	UNP Q12791
C	-3	ARG	-	expression tag	UNP Q12791
C	-2	LEU	-	expression tag	UNP Q12791
C	-1	THR	-	expression tag	UNP Q12791
C	0	GLU	-	expression tag	UNP Q12791
C	1	PRO	-	expression tag	UNP Q12791
B	-15	MET	-	expression tag	UNP Q12791
B	-14	ALA	-	expression tag	UNP Q12791
B	-13	PRO	-	expression tag	UNP Q12791
B	-12	SER	-	expression tag	UNP Q12791
B	-11	ARG	-	expression tag	UNP Q12791
B	-10	LEU	-	expression tag	UNP Q12791
B	-9	GLU	-	expression tag	UNP Q12791
B	-8	GLU	-	expression tag	UNP Q12791
B	-7	GLU	-	expression tag	UNP Q12791
B	-6	LEU	-	expression tag	UNP Q12791
B	-5	ARG	-	expression tag	UNP Q12791
B	-4	ARG	-	expression tag	UNP Q12791
B	-3	ARG	-	expression tag	UNP Q12791
B	-2	LEU	-	expression tag	UNP Q12791
B	-1	THR	-	expression tag	UNP Q12791
B	0	GLU	-	expression tag	UNP Q12791
B	1	PRO	-	expression tag	UNP Q12791
D	-15	MET	-	expression tag	UNP Q12791
D	-14	ALA	-	expression tag	UNP Q12791
D	-13	PRO	-	expression tag	UNP Q12791
D	-12	SER	-	expression tag	UNP Q12791
D	-11	ARG	-	expression tag	UNP Q12791
D	-10	LEU	-	expression tag	UNP Q12791
D	-9	GLU	-	expression tag	UNP Q12791
D	-8	GLU	-	expression tag	UNP Q12791
D	-7	GLU	-	expression tag	UNP Q12791
D	-6	LEU	-	expression tag	UNP Q12791
D	-5	ARG	-	expression tag	UNP Q12791
D	-4	ARG	-	expression tag	UNP Q12791
D	-3	ARG	-	expression tag	UNP Q12791

Continued on next page...

Continued from previous page...

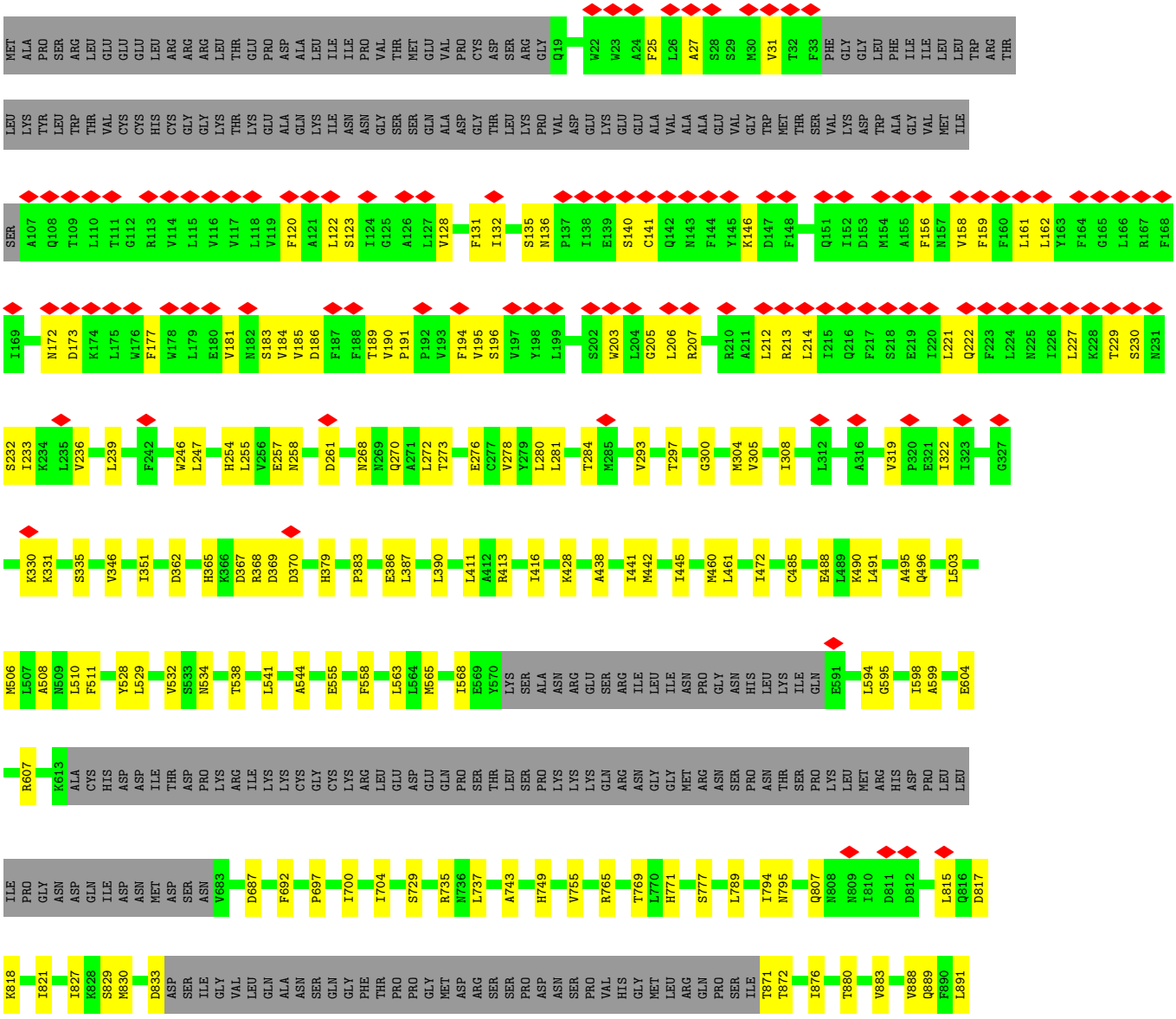
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	expression tag	UNP Q12791
D	-1	THR	-	expression tag	UNP Q12791
D	0	GLU	-	expression tag	UNP Q12791
D	1	PRO	-	expression tag	UNP Q12791

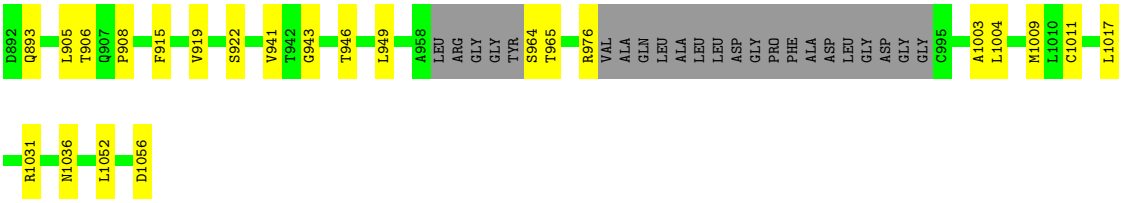
3 Residue-property plots (i)

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: Calcium-activated potassium channel subunit alpha-1

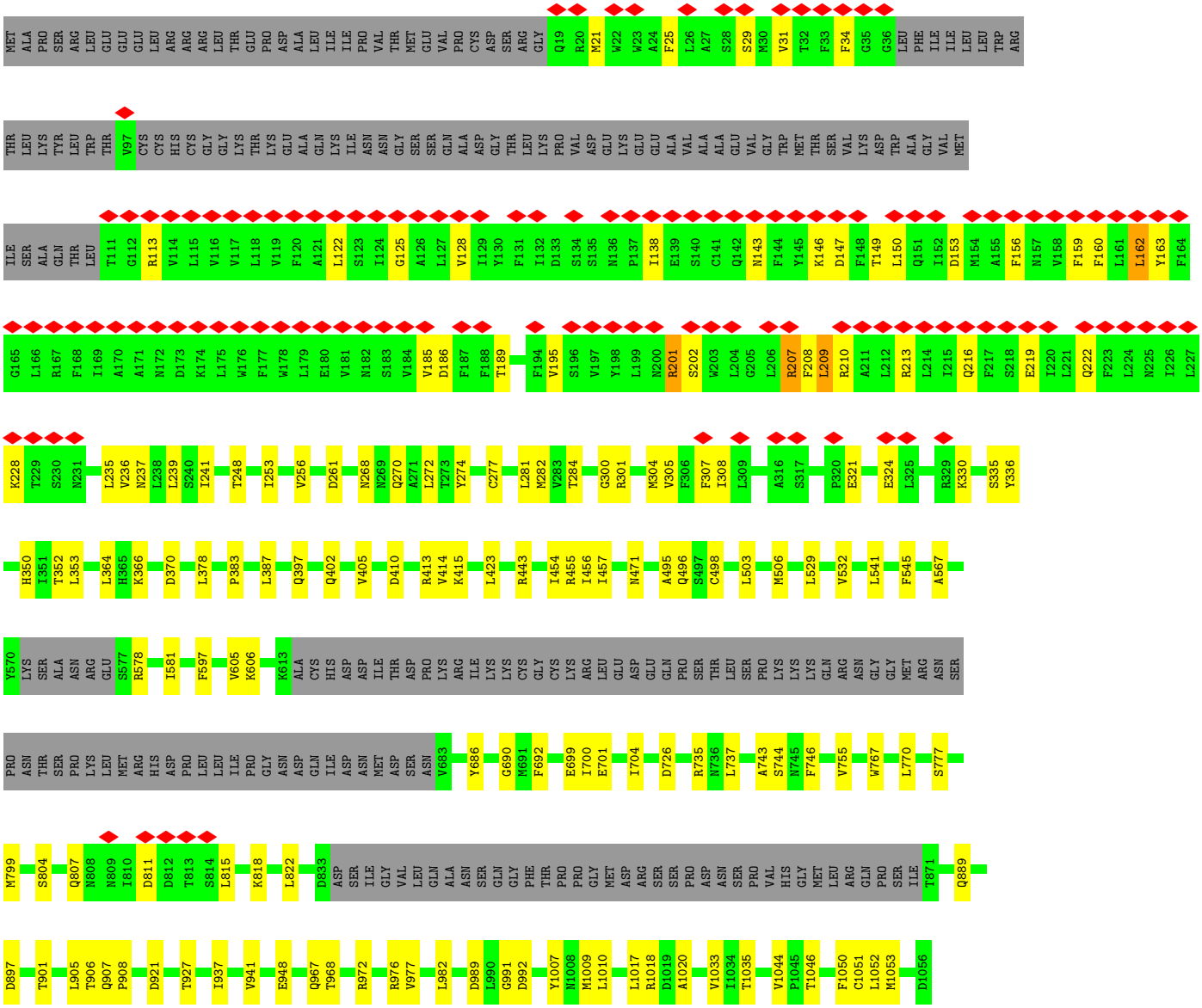
Chain A:





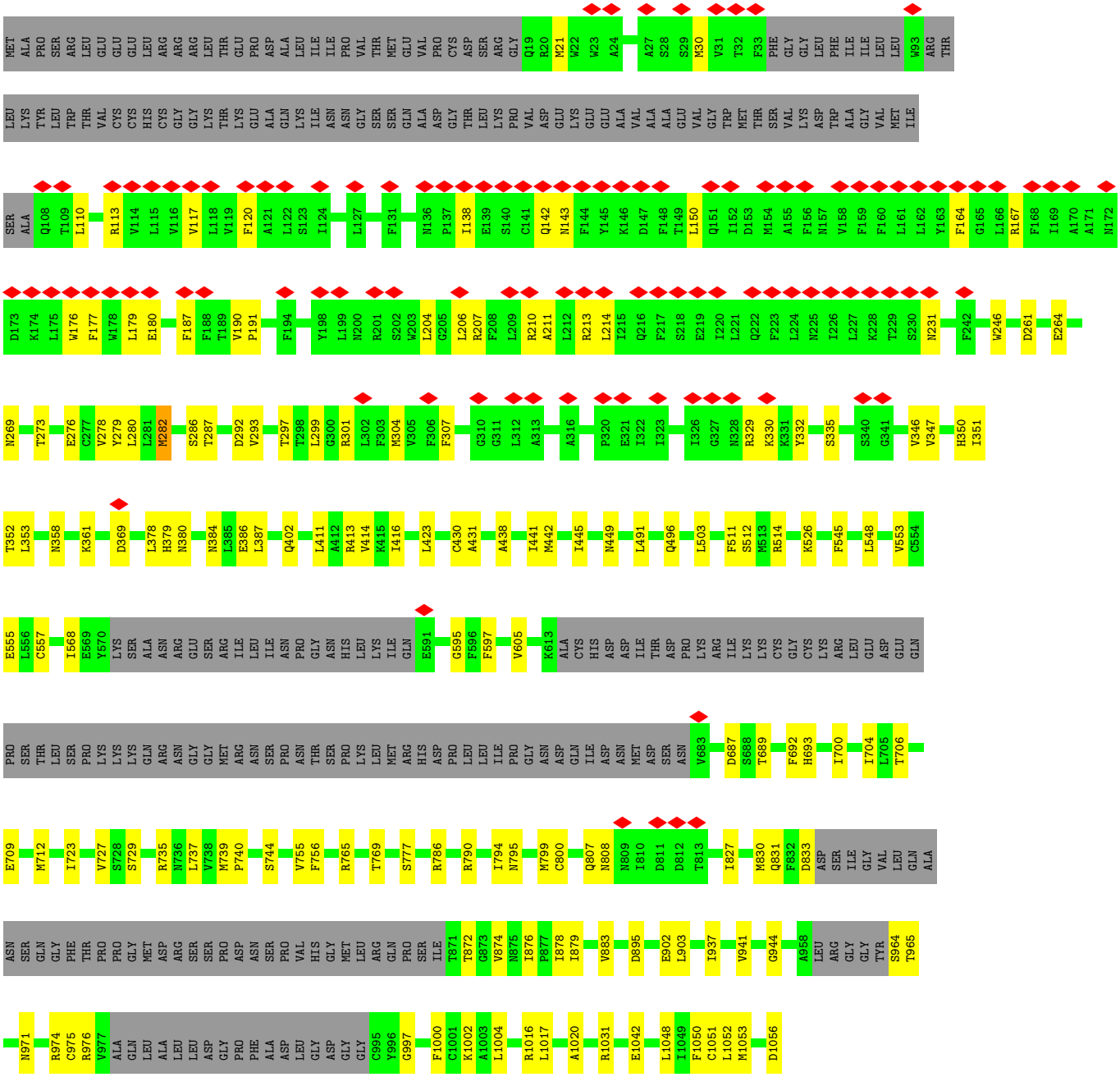
• Molecule 1: Calcium-activated potassium channel subunit alpha-1

Chain C:



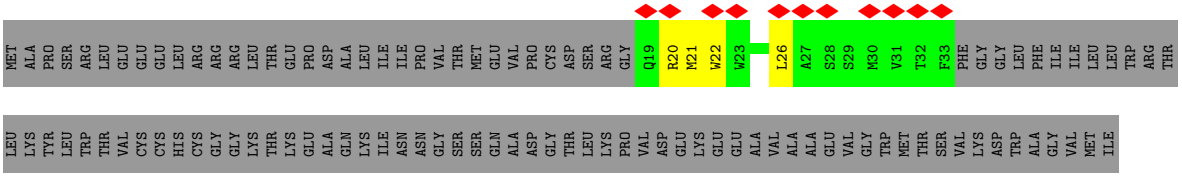
• Molecule 1: Calcium-activated potassium channel subunit alpha-1

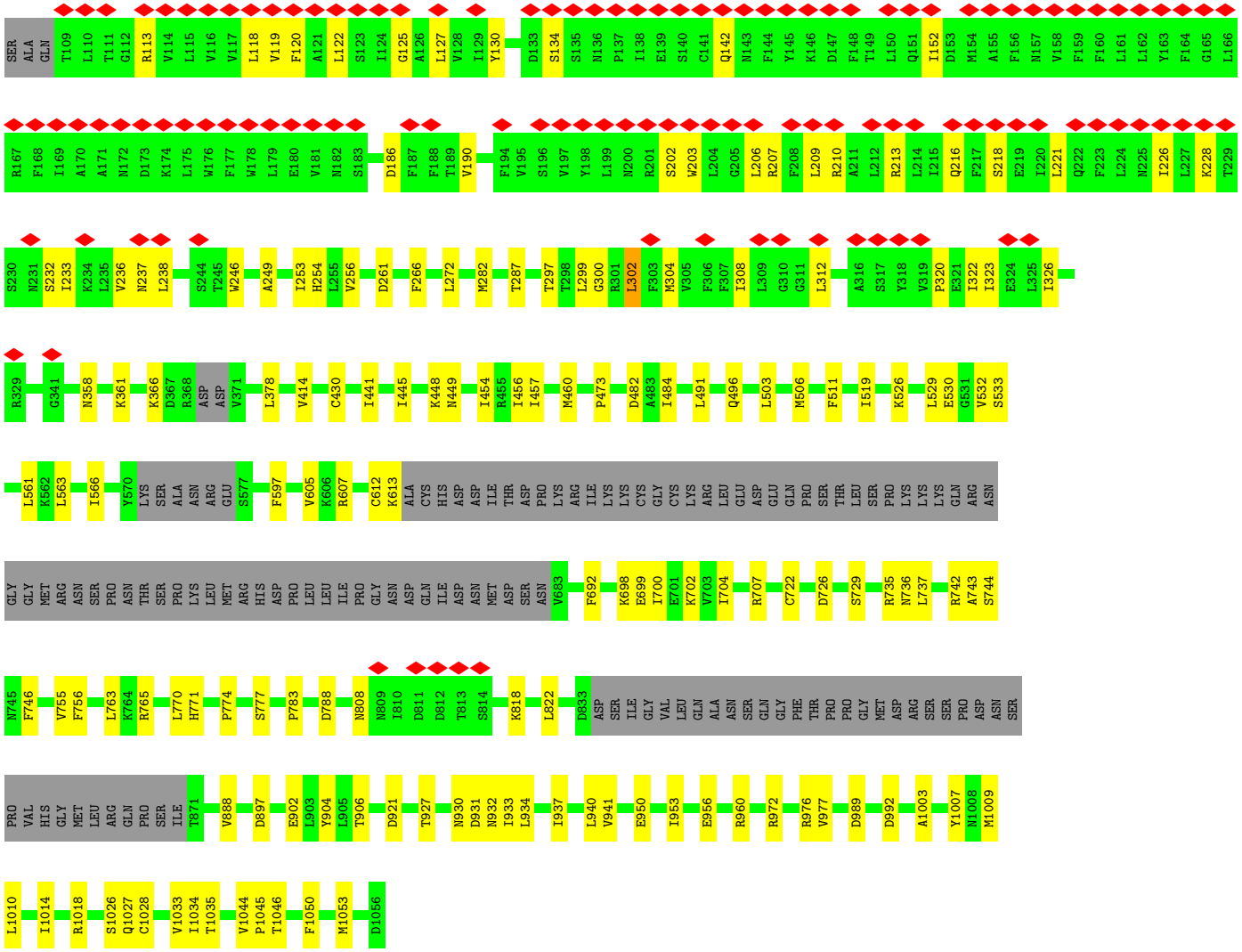
Chain B:



• Molecule 1: Calcium-activated potassium channel subunit alpha-1

Chain D:




SER ALA GLN T109 L110 T111 G112 R113 V114 L115 V116 V117 L118 V119 F120 A121 L122 S123 I124 G125 A126 L127 V128 I129 Y130 D133 S134 S135 N136 P137 I138 E139 S140 C141 Q142 N143 F144 Y145 K146 D147 F148 T149 L150 Q151 I152 D153 M154 A155 F156 N157 V158 F159 F160 L161 L162 Y163 F164 G165 L166
R167 F168 I169 A170 A171 N172 D173 K174 L175 W176 F177 W178 L179 E180 V181 N182 S183 D186 F187 F188 T189 V190 F194 V195 S196 V197 Y198 L199 N200 R201 S202 W203 L204 G205 L206 R207 F208 L209 R210 A211 L212 R213 L214 I215 Q216 F217 S218 E219 I220 L221 Q222 F223 L224 N225 I226 L227 K228 T229
S230 N231 S232 I233 K234 L235 V236 N237 L238 S244 T245 W246 A249 I253 H254 L255 V256 D261 F266 L272 M282 T287 T297 T298 L299 G300 R301 L302 F303 M304 V305 F306 F307 I308 L309 G310 G311 L312 A316 S317 Y318 V319 P320 E321 I322 I323 E324 L325 I326
R329 G341 N358 K361 K366 D367 R368 ASP ASP V371 L378 V414 C430 I441 I445 K448 N449 I454 R455 I456 I457 M460 P473 D482 A483 I484 L491 Q496 L503 M506 F511 I519 K526 L529 E530 G531 V532 S533
L561 K562 L563 I566 Y570 LYS SER ALA ASN ARG GLU S577 F597 V605 K606 R607 C612 K613 ALA CYS HIS ASP ASP ILE THR ASP PRO LYS ARG ILE LYS LYS CYS GLY CYS LYS ARG LEU GLU ASP GLU GLN PRO SER THR LEU SER PRO LYS LYS LYS GLN ARG ASN
GLY GLY MET ARG ASN SER PRO ASN THR SER PRO LYS LEU MET ARG HIS ASP PRO LEU LEU ILE PRO GLY ASN ASP GLN ILE ASP ASN MET ASP SER ASN V683 F692 K698 E699 I700 E701 K702 V703 I704 R707 C722 D726 S729 R735 N736 L737 R742 A743 S744
N745 F746 V755 F756 L763 K764 R765 L770 H771 P774 S777 P783 D788 N808 N809 I810 D811 D812 T813 S814 K818 L822 D833 ASP SER ILE GLY VAL LEU GLN ALA ASN SER GLN GLY PHE THR PRO PRO GLY MET ASP ARG SER SER PRO ASP ASN SER
PRO VAL HIS GLY MET LEU ARG GLN PRO SER ILE T871 V888 D897 E902 L903 Y904 L905 T906 D921 T927 N930 D931 N932 I933 L934 I937 L940 V941 E950 I953 E956 R960 R972 R976 V977 D989 D992 A1003 Y1007 N1008 M1009
L1010 I1014 R1018 S1026 Q1027 C1028 V1033 I1034 T1035 V1044 P1045 T1046 F1050 M1053 D1056

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	123286	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 ($e^-/Å^2$)	51.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.967	Depositor
Minimum map value	-0.314	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/6681	0.51	0/9062
1	B	0.26	0/6698	0.53	3/9085 (0.0%)
1	C	0.25	0/6957	0.52	2/9436 (0.0%)
1	D	0.26	0/6929	0.50	1/9399 (0.0%)
All	All	0.26	0/27265	0.52	6/36982 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	282	MET	CG-SD-CE	7.45	112.12	100.20
1	B	206	LEU	CA-CB-CG	5.91	128.88	115.30
1	C	209	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	30	MET	CB-CG-SD	5.25	128.15	112.40
1	D	302	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	162	LEU	CA-CB-CG	5.13	127.11	115.30

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	A	6533	0	6499	112	0
1	B	6549	0	6512	100	0
1	C	6802	0	6771	100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6775	0	6757	101	0
All	All	26659	0	26539	401	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 8.

All (401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:ILE:HG21	1:A:827:ILE:HD11	1.64	0.80
1:A:491:LEU:HD12	1:A:737:LEU:HB2	1.67	0.75
1:A:445:ILE:HD13	1:A:472:ILE:HD12	1.69	0.75
1:B:246:TRP:HZ2	1:B:278:VAL:HG13	1.51	0.74
1:B:287:THR:HB	1:D:287:THR:HB	1.71	0.72
1:D:482:ASP:HB3	1:D:934:LEU:HD13	1.70	0.71
1:C:455:ARG:NH2	1:C:927:THR:O	2.26	0.68
1:B:211:ALA:HA	1:B:214:LEU:HD23	1.76	0.67
1:B:755:VAL:HG12	1:B:777:SER:HB2	1.77	0.67
1:B:794:ILE:HG21	1:B:827:ILE:HD11	1.77	0.66
1:A:906:THR:HG22	1:A:908:PRO:HD2	1.78	0.65
1:B:800:CYS:HB3	1:B:878:ILE:HG22	1.79	0.65
1:A:346:VAL:HG21	1:A:416:ILE:HG22	1.79	0.65
1:C:29:SER:HA	1:C:195:VAL:HG21	1.77	0.65
1:B:555:GLU:HG3	1:B:1004:LEU:HB3	1.81	0.63
1:C:503:LEU:HD22	1:C:977:VAL:HG11	1.81	0.63
1:A:558:PHE:HE1	1:A:565:MET:H	1.46	0.63
1:A:1017:LEU:HA	1:A:1031:ARG:HA	1.81	0.63
1:A:132:ILE:O	1:A:136:ASN:ND2	2.31	0.62
1:A:335:SER:HA	1:A:413:ARG:HG3	1.81	0.62
1:A:815:LEU:HD12	1:A:818:LYS:HD3	1.81	0.62
1:D:454:ILE:HG23	1:D:456:ILE:HD11	1.80	0.62
1:B:727:VAL:O	1:B:765:ARG:NH1	2.33	0.62
1:D:238:LEU:HD21	1:D:322:ILE:HB	1.82	0.61
1:D:1003:ALA:HB1	1:D:1009:MET:HB2	1.82	0.61
1:B:491:LEU:HD12	1:B:737:LEU:HB2	1.83	0.61
1:A:305:VAL:HG23	1:C:282:MET:HG3	1.83	0.61
1:A:555:GLU:HA	1:A:558:PHE:HB3	1.81	0.61
1:D:744:SER:HB3	1:D:972:ARG:HD2	1.81	0.61
1:C:305:VAL:HG23	1:B:282:MET:HG3	1.82	0.60
1:C:906:THR:HG22	1:C:908:PRO:HD2	1.82	0.60
1:C:378:LEU:HD11	1:C:414:VAL:HG21	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:ASN:OD1	1:B:786:ARG:NH2	2.35	0.60
1:A:541:LEU:HD21	1:A:544:ALA:HB3	1.83	0.60
1:B:246:TRP:CZ2	1:B:278:VAL:HG13	2.35	0.60
1:B:411:LEU:HD12	1:B:416:ILE:HD13	1.82	0.60
1:C:147:ASP:HB3	1:C:150:LEU:HD23	1.84	0.60
1:A:893:GLN:HE22	1:D:473:PRO:HB2	1.67	0.59
1:A:254:HIS:O	1:A:258:ASN:ND2	2.35	0.59
1:A:383:PRO:HB3	1:A:387:LEU:HD23	1.84	0.59
1:A:976:ARG:HB3	1:A:1052:LEU:HD23	1.84	0.59
1:D:254:HIS:NE2	1:D:272:LEU:O	2.35	0.59
1:A:203:TRP:O	1:A:207:ARG:NH1	2.35	0.59
1:A:284:THR:HG21	1:A:304:MET:HE1	1.84	0.59
1:C:138:ILE:HD12	1:C:201:ARG:HH12	1.66	0.59
1:A:755:VAL:HG12	1:A:777:SER:HB2	1.83	0.59
1:D:1007:TYR:HB2	1:D:1009:MET:HG2	1.83	0.59
1:A:280:LEU:HD21	1:A:293:VAL:HG23	1.85	0.59
1:C:1017:LEU:HB2	1:C:1020:ALA:HB2	1.85	0.59
1:B:1016:ARG:NH2	1:B:1042:GLU:O	2.35	0.59
1:B:975:CYS:O	1:B:1052:LEU:N	2.34	0.58
1:D:297:THR:HG23	1:D:300:GLY:H	1.68	0.58
1:B:997:GLY:HA2	1:B:1000:PHE:CE1	2.38	0.58
1:D:930:ASN:HB3	1:D:933:ILE:HG12	1.84	0.58
1:C:597:PHE:HD2	1:C:605:VAL:HG13	1.69	0.58
1:D:118:LEU:HD23	1:D:216:GLN:HG2	1.86	0.58
1:D:1014:ILE:HB	1:D:1034:ILE:HB	1.86	0.58
1:B:117:VAL:HA	1:B:120:PHE:CE1	2.39	0.57
1:C:815:LEU:HB3	1:C:818:LYS:HD3	1.87	0.57
1:A:365:HIS:ND1	1:A:367:ASP:OD1	2.38	0.57
1:A:871:THR:OG1	1:A:872:THR:N	2.37	0.57
1:D:888:VAL:HG11	1:D:906:THR:HG21	1.86	0.57
1:B:449:ASN:ND2	1:D:897:ASP:OD2	2.32	0.57
1:A:261:ASP:OD2	1:A:268:ASN:ND2	2.39	0.56
1:D:956:GLU:OE2	1:D:960:ARG:NH1	2.38	0.56
1:D:976:ARG:NE	1:D:1053:MET:SD	2.75	0.56
1:C:304:MET:HA	1:C:307:PHE:HD2	1.70	0.56
1:A:411:LEU:HD12	1:A:416:ILE:HD13	1.88	0.56
1:D:566:ILE:HG22	1:D:1010:LEU:HD21	1.88	0.56
1:D:729:SER:O	1:D:765:ARG:NH2	2.39	0.56
1:C:222:GLN:HE22	1:C:228:LYS:HA	1.70	0.55
1:D:430:CYS:O	1:D:808:ASN:ND2	2.39	0.55
1:A:496:GLN:HB3	1:A:503:LEU:HD23	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:HD22	1:B:386:GLU:HG3	1.87	0.55
1:B:548:LEU:HB2	1:B:553:VAL:HG11	1.88	0.55
1:A:538:THR:HB	1:A:594:LEU:HD11	1.89	0.55
1:C:1007:TYR:HB2	1:C:1009:MET:HB2	1.88	0.55
1:B:142:GLN:NE2	1:B:143:ASN:O	2.40	0.55
1:C:304:MET:O	1:C:308:ILE:HG12	2.07	0.55
1:D:496:GLN:HB3	1:D:503:LEU:HD23	1.89	0.55
1:B:346:VAL:HG21	1:B:416:ILE:HG22	1.88	0.55
1:D:120:PHE:HB2	1:D:216:GLN:HE22	1.72	0.55
1:C:496:GLN:HB3	1:C:503:LEU:HD23	1.89	0.54
1:A:222:GLN:HE21	1:A:233:ILE:HG21	1.72	0.54
1:B:273:THR:OG1	1:B:276:GLU:OE1	2.23	0.54
1:B:1017:LEU:HB2	1:B:1020:ALA:HB2	1.89	0.54
1:A:273:THR:N	1:A:276:GLU:OE2	2.32	0.54
1:D:755:VAL:HG12	1:D:777:SER:HB2	1.90	0.54
1:A:510:LEU:HD22	1:A:598:ILE:HD11	1.90	0.54
1:B:430:CYS:SG	1:B:431:ALA:N	2.80	0.54
1:A:25:PHE:HA	1:A:195:VAL:HG21	1.89	0.54
1:A:729:SER:O	1:A:765:ARG:NH2	2.40	0.54
1:C:1044:VAL:HG12	1:C:1046:THR:H	1.71	0.53
1:D:261:ASP:OD1	1:D:297:THR:OG1	2.26	0.53
1:D:253:ILE:HA	1:D:256:VAL:HG12	1.90	0.53
1:D:529:LEU:HA	1:D:532:VAL:HG12	1.89	0.53
1:A:976:ARG:HA	1:A:1011:CYS:HA	1.90	0.53
1:C:495:ALA:HB2	1:C:737:LEU:HD12	1.91	0.53
1:A:735:ARG:NH1	1:A:769:THR:OG1	2.42	0.52
1:B:430:CYS:O	1:B:808:ASN:ND2	2.43	0.52
1:B:790:ARG:NH2	1:B:831:GLN:O	2.36	0.52
1:A:1017:LEU:HB3	1:A:1031:ARG:HG2	1.91	0.52
1:C:976:ARG:NE	1:C:1053:MET:SD	2.78	0.52
1:A:230:SER:HA	1:A:233:ILE:HG12	1.92	0.52
1:C:222:GLN:O	1:C:228:LYS:NZ	2.43	0.52
1:C:529:LEU:HA	1:C:532:VAL:HG12	1.91	0.52
1:C:31:VAL:HA	1:C:34:PHE:HD2	1.75	0.52
1:C:270:GLN:HB3	1:C:272:LEU:HD23	1.90	0.52
1:B:282:MET:O	1:B:286:SER:OG	2.26	0.52
1:D:746:PHE:HD1	1:D:976:ARG:HH11	1.57	0.52
1:D:506:MET:SD	1:D:1035:THR:OG1	2.61	0.52
1:C:186:ASP:HA	1:C:189:THR:HG22	1.92	0.52
1:B:709:GLU:HA	1:B:712:MET:HG3	1.92	0.52
1:D:503:LEU:HD22	1:D:977:VAL:HG11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:TYR:HA	1:C:277:CYS:SG	2.50	0.51
1:D:322:ILE:O	1:D:326:ILE:HG12	2.10	0.51
1:D:460:MET:N	1:D:484:ILE:O	2.38	0.51
1:C:402:GLN:O	1:C:413:ARG:NH2	2.42	0.51
1:A:123:SER:OG	1:A:213:ARG:NH2	2.44	0.51
1:A:272:LEU:HD12	1:A:276:GLU:HG3	1.93	0.51
1:B:795:ASN:HA	1:B:876:ILE:HD11	1.92	0.51
1:D:186:ASP:O	1:D:190:VAL:HG23	2.10	0.51
1:D:698:LYS:H	1:D:771:HIS:HB2	1.76	0.51
1:A:460:MET:HB3	1:A:485:CYS:HA	1.92	0.51
1:A:700:ILE:O	1:A:704:ILE:HG12	2.11	0.51
1:B:167:ARG:NH2	1:B:180:GLU:OE1	2.42	0.51
1:C:143:ASN:HB3	1:C:146:LYS:HB2	1.92	0.51
1:B:350:HIS:NE2	1:B:352:THR:OG1	2.44	0.50
1:B:827:ILE:HD12	1:B:830:MET:HG3	1.93	0.50
1:C:160:PHE:HA	1:C:163:TYR:CE1	2.46	0.50
1:C:405:VAL:HG11	1:C:443:ARG:HG3	1.92	0.50
1:C:982:LEU:HD13	1:C:991:GLY:HA3	1.93	0.50
1:B:21:MET:SD	1:B:21:MET:N	2.82	0.50
1:D:700:ILE:O	1:D:704:ILE:HG12	2.11	0.50
1:C:692:PHE:HD1	1:C:743:ALA:HA	1.76	0.50
1:C:506:MET:SD	1:C:1035:THR:OG1	2.65	0.50
1:B:496:GLN:HB3	1:B:503:LEU:HD23	1.93	0.50
1:B:964:SER:OG	1:B:965:THR:N	2.45	0.50
1:D:597:PHE:HD2	1:D:605:VAL:HG13	1.77	0.50
1:D:134:SER:HB2	1:D:254:HIS:HE1	1.77	0.50
1:D:218:SER:HB2	1:D:236:VAL:HG22	1.93	0.50
1:A:270:GLN:HB3	1:A:272:LEU:HD23	1.94	0.50
1:A:687:ASP:N	1:A:692:PHE:O	2.45	0.50
1:D:491:LEU:HD22	1:D:737:LEU:HB2	1.94	0.49
1:D:233:ILE:O	1:D:237:ASN:ND2	2.45	0.49
1:A:140:SER:OG	1:A:141:CYS:N	2.45	0.49
1:A:297:THR:HG23	1:A:300:GLY:H	1.78	0.49
1:C:21:MET:O	1:C:25:PHE:N	2.42	0.49
1:C:989:ASP:OD1	1:C:989:ASP:N	2.45	0.49
1:B:729:SER:O	1:B:765:ARG:NH2	2.36	0.49
1:A:120:PHE:HE1	1:A:214:LEU:HA	1.76	0.49
1:C:597:PHE:CD2	1:C:605:VAL:HG13	2.47	0.49
1:D:519:ILE:HB	1:D:526:LYS:HB3	1.94	0.49
1:D:142:GLN:HG2	1:D:202:SER:HB3	1.95	0.49
1:A:789:LEU:HD13	1:A:827:ILE:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:VAL:HG12	1:C:777:SER:HB2	1.95	0.49
1:B:358:ASN:HA	1:B:361:LYS:HG2	1.95	0.49
1:B:833:ASP:OD1	1:B:833:ASP:N	2.43	0.49
1:D:692:PHE:HD1	1:D:743:ALA:HA	1.77	0.49
1:C:457:ILE:HD13	1:C:927:THR:HG23	1.93	0.48
1:A:829:SER:HB2	1:D:473:PRO:HG3	1.94	0.48
1:A:833:ASP:N	1:A:833:ASP:OD1	2.46	0.48
1:C:1010:LEU:HD23	1:C:1052:LEU:HD12	1.95	0.48
1:B:351:ILE:HD11	1:B:379:HIS:HB2	1.95	0.48
1:A:304:MET:O	1:A:308:ILE:HG12	2.14	0.48
1:C:138:ILE:O	1:C:202:SER:OG	2.31	0.48
1:C:578:ARG:NH2	1:C:948:GLU:OE2	2.37	0.48
1:D:308:ILE:HA	1:D:312:LEU:HD23	1.95	0.48
1:A:205:GLY:HA3	1:A:255:LEU:HD12	1.95	0.48
1:C:746:PHE:HD1	1:C:976:ARG:HH11	1.62	0.48
1:B:512:SER:OG	1:B:514:ARG:NH1	2.46	0.48
1:A:508:ALA:HB1	1:A:919:VAL:HG11	1.96	0.48
1:C:364:LEU:HD11	1:C:397:GLN:HE21	1.77	0.48
1:C:921:ASP:N	1:C:921:ASP:OD1	2.47	0.48
1:C:208:PHE:CE2	1:C:248:THR:HA	2.49	0.48
1:B:380:ASN:O	1:B:402:GLN:NE2	2.46	0.48
1:B:402:GLN:O	1:B:413:ARG:NH2	2.47	0.48
1:B:692:PHE:HZ	1:B:944:GLY:HA3	1.78	0.48
1:D:457:ILE:HD13	1:D:927:THR:HG23	1.96	0.48
1:A:807:GLN:HG3	1:A:883:VAL:HG11	1.95	0.47
1:A:888:VAL:HA	1:A:891:LEU:HD23	1.95	0.47
1:C:321:GLU:HA	1:C:324:GLU:HG2	1.96	0.47
1:B:210:ARG:HB2	1:B:213:ARG:HH21	1.79	0.47
1:A:131:PHE:O	1:A:135:SER:OG	2.29	0.47
1:A:186:ASP:HA	1:A:189:THR:HG22	1.95	0.47
1:A:563:LEU:HD11	1:A:599:ALA:HB2	1.95	0.47
1:C:207:ARG:O	1:C:207:ARG:NH1	2.45	0.47
1:C:901:THR:HB	1:C:905:LEU:HD11	1.96	0.47
1:A:534:ASN:HD21	1:A:1036:ASN:HD22	1.62	0.47
1:C:606:LYS:O	1:C:606:LYS:NZ	2.47	0.47
1:A:158:VAL:HA	1:A:161:LEU:HD12	1.95	0.47
1:A:511:PHE:O	1:A:922:SER:OG	2.30	0.47
1:C:690:GLY:HA3	1:C:968:THR:HB	1.95	0.47
1:B:190:VAL:HB	1:B:191:PRO:HD3	1.97	0.47
1:B:335:SER:HA	1:B:413:ARG:HG3	1.96	0.47
1:C:1051:CYS:SG	1:C:1052:LEU:N	2.88	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HD11	1:B:293:VAL:HG23	1.97	0.47
1:D:20:ARG:HD3	1:D:266:PHE:CE2	2.50	0.47
1:D:221:LEU:HB3	1:D:226:ILE:HD12	1.97	0.47
1:D:561:LEU:HD23	1:D:607:ARG:HB3	1.96	0.47
1:A:191:PRO:HA	1:A:194:PHE:HB2	1.96	0.47
1:D:226:ILE:HG22	1:D:228:LYS:HE3	1.97	0.47
1:A:278:VAL:O	1:A:281:LEU:HG	2.15	0.46
1:C:159:PHE:HA	1:C:162:LEU:HG	1.96	0.46
1:B:330:LYS:HZ1	1:B:332:TYR:HB2	1.79	0.46
1:B:369:ASP:OD1	1:B:369:ASP:N	2.45	0.46
1:B:700:ILE:O	1:B:704:ILE:HG12	2.16	0.46
1:D:206:LEU:HD21	1:D:209:LEU:HD13	1.97	0.46
1:A:964:SER:OG	1:A:965:THR:N	2.48	0.46
1:C:992:ASP:N	1:C:992:ASP:OD1	2.48	0.46
1:A:362:ASP:O	1:A:368:ARG:NH1	2.39	0.46
1:C:410:ASP:O	1:C:414:VAL:HG23	2.16	0.46
1:D:491:LEU:HD12	1:D:736:ASN:HB3	1.98	0.46
1:D:931:ASP:N	1:D:931:ASP:OD1	2.49	0.46
1:A:485:CYS:SG	1:A:488:GLU:HB3	2.56	0.46
1:B:976:ARG:HA	1:B:1051:CYS:HA	1.97	0.46
1:A:697:PRO:HB3	1:A:771:HIS:HD2	1.81	0.46
1:C:185:VAL:HG21	1:C:209:LEU:HD13	1.97	0.46
1:B:110:LEU:HD13	1:B:113:ARG:HH21	1.80	0.46
1:D:130:TYR:HD1	1:D:207:ARG:HB3	1.79	0.46
1:A:749:HIS:CD2	1:A:749:HIS:H	2.34	0.46
1:C:498:CYS:HA	1:C:799:MET:HG2	1.98	0.46
1:B:937:ILE:O	1:B:941:VAL:HG22	2.16	0.46
1:A:27:ALA:HA	1:A:31:VAL:HB	1.97	0.46
1:A:503:LEU:HA	1:A:506:MET:HB3	1.97	0.46
1:C:889:GLN:HB2	1:C:897:ASP:HB3	1.98	0.46
1:A:186:ASP:O	1:A:190:VAL:HG22	2.16	0.46
1:C:370:ASP:N	1:C:370:ASP:OD1	2.49	0.46
1:B:735:ARG:HE	1:B:769:THR:HG1	1.59	0.45
1:D:122:LEU:HD22	1:D:152:ILE:HG21	1.98	0.45
1:A:206:LEU:HD12	1:A:255:LEU:HD11	1.98	0.45
1:A:246:TRP:HD1	1:A:247:LEU:HD22	1.82	0.45
1:B:176:TRP:HA	1:B:179:LEU:HB2	1.98	0.45
1:B:971:ASN:H	1:B:1056:ASP:HB2	1.80	0.45
1:B:974:ARG:NH1	1:B:1053:MET:SD	2.90	0.45
1:A:181:VAL:HA	1:A:184:VAL:HG22	1.99	0.45
1:A:555:GLU:HB3	1:A:1004:LEU:HD12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:ALA:HB1	1:A:1009:MET:HB3	1.97	0.45
1:A:495:ALA:HB2	1:A:737:LEU:HD12	1.98	0.45
1:A:568:ILE:HG22	1:A:595:GLY:HA2	1.98	0.45
1:D:21:MET:SD	1:D:203:TRP:NE1	2.89	0.45
1:A:369:ASP:OD1	1:A:370:ASP:N	2.49	0.45
1:A:528:TYR:HE2	1:A:905:LEU:HA	1.82	0.45
1:D:378:LEU:HD11	1:D:414:VAL:HG21	1.98	0.45
1:A:438:ALA:O	1:A:442:MET:HG2	2.17	0.45
1:A:889:GLN:O	1:D:449:ASN:ND2	2.46	0.45
1:C:146:LYS:HD3	1:C:146:LYS:HA	1.77	0.45
1:C:383:PRO:HB3	1:C:387:LEU:HD23	1.99	0.45
1:C:208:PHE:HE2	1:C:248:THR:HA	1.82	0.45
1:D:530:GLU:O	1:D:533:SER:OG	2.33	0.44
1:C:423:LEU:HD13	1:C:457:ILE:HB	1.98	0.44
1:B:301:ARG:HA	1:B:304:MET:HG3	1.98	0.44
1:D:207:ARG:HG3	1:D:210:ARG:HH11	1.82	0.44
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.78	0.44
1:C:744:SER:HB3	1:C:972:ARG:HG2	1.98	0.44
1:B:142:GLN:HG3	1:B:150:LEU:HD13	1.98	0.44
1:D:358:ASN:HA	1:D:361:LYS:HG2	1.98	0.44
1:D:20:ARG:NH2	1:D:22:TRP:HB2	2.33	0.44
1:D:448:LYS:HE2	1:D:456:ILE:HG13	2.00	0.44
1:C:967:GLN:O	1:C:968:THR:OG1	2.34	0.44
1:D:921:ASP:OD1	1:D:921:ASP:N	2.49	0.44
1:A:257:GLU:OE2	1:A:272:LEU:N	2.46	0.44
1:A:185:VAL:HG21	1:A:212:LEU:HD22	1.98	0.44
1:B:438:ALA:HB1	1:D:818:LYS:HB3	1.99	0.44
1:D:441:ILE:O	1:D:445:ILE:HG12	2.18	0.44
1:D:756:PHE:HB3	1:D:763:LEU:HD21	1.99	0.44
1:A:880:THR:HG21	1:A:891:LEU:HD11	1.99	0.44
1:C:686:TYR:HD2	1:C:744:SER:HG	1.66	0.44
1:B:261:ASP:HB2	1:B:264:GLU:HB2	2.00	0.44
1:C:541:LEU:HD12	1:C:545:PHE:HD2	1.83	0.44
1:C:907:GLN:HE21	1:C:1018:ARG:HD3	1.83	0.44
1:B:138:ILE:HG23	1:B:204:LEU:HB2	2.00	0.44
1:C:236:VAL:HA	1:C:239:LEU:HG	2.00	0.43
1:C:300:GLY:O	1:C:304:MET:HG2	2.18	0.43
1:C:454:ILE:HG23	1:C:456:ILE:HD11	2.00	0.43
1:B:545:PHE:CZ	1:B:557:CYS:HB3	2.53	0.43
1:C:281:LEU:O	1:C:284:THR:OG1	2.28	0.43
1:C:330:LYS:HE3	1:C:402:GLN:HG2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:GLN:HB2	1:B:883:VAL:HG11	2.00	0.43
1:D:992:ASP:HA	1:D:1045:PRO:HG3	2.00	0.43
1:D:1018:ARG:NH2	1:D:1028:CYS:SG	2.92	0.43
1:C:415:LYS:HB3	1:C:415:LYS:HE2	1.82	0.43
1:C:496:GLN:HG3	1:C:941:VAL:HG23	1.99	0.43
1:B:378:LEU:HD21	1:B:414:VAL:HG21	2.00	0.43
1:A:236:VAL:HA	1:A:239:LEU:HG	2.00	0.43
1:A:428:LYS:HA	1:A:461:LEU:HD21	2.00	0.43
1:C:735:ARG:HA	1:C:770:LEU:HD21	2.01	0.43
1:A:177:PHE:O	1:A:183:SER:OG	2.17	0.43
1:C:125:GLY:HA3	1:C:156:PHE:HZ	1.83	0.43
1:C:149:THR:O	1:C:153:ASP:N	2.49	0.43
1:B:1048:LEU:HD11	1:B:1050:PHE:HD2	1.82	0.43
1:C:700:ILE:O	1:C:704:ILE:HG12	2.18	0.43
1:A:441:ILE:HG21	1:C:822:LEU:HD21	2.00	0.43
1:A:827:ILE:HD12	1:A:830:MET:HG3	1.99	0.43
1:C:253:ILE:HA	1:C:256:VAL:HG22	2.00	0.43
1:D:119:VAL:HB	1:D:213:ARG:HD2	1.99	0.43
1:B:297:THR:HB	1:B:299:LEU:HD23	2.00	0.43
1:D:249:ALA:O	1:D:253:ILE:HG23	2.18	0.43
1:C:235:LEU:HD23	1:C:239:LEU:HD23	2.00	0.43
1:A:351:ILE:HG12	1:A:379:HIS:HD2	1.84	0.42
1:B:378:LEU:HD11	1:B:414:VAL:HG21	2.01	0.42
1:D:20:ARG:HH21	1:D:22:TRP:HB2	1.84	0.42
1:B:799:MET:SD	1:B:879:ILE:HG22	2.59	0.42
1:A:496:GLN:HG3	1:A:941:VAL:HA	2.01	0.42
1:C:726:ASP:OD1	1:C:726:ASP:N	2.52	0.42
1:C:937:ILE:O	1:C:941:VAL:HG12	2.19	0.42
1:B:568:ILE:HG22	1:B:595:GLY:HA2	2.01	0.42
1:B:739:MET:HB3	1:B:740:PRO:HD3	2.02	0.42
1:A:221:LEU:HD21	1:A:227:LEU:HB2	2.02	0.42
1:A:692:PHE:HE1	1:A:943:GLY:HA3	1.84	0.42
1:C:353:LEU:HD12	1:C:387:LEU:HB2	2.02	0.42
1:B:902:GLU:OE1	1:B:903:LEU:N	2.52	0.42
1:D:742:ARG:HD2	1:D:774:PRO:HD2	2.01	0.42
1:D:902:GLU:HG3	1:D:904:TYR:CE2	2.55	0.42
1:C:301:ARG:HB2	1:B:279:TYR:CD1	2.54	0.42
1:A:122:LEU:HD11	1:A:156:PHE:CD1	2.54	0.42
1:D:127:LEU:HD23	1:D:127:LEU:HA	1.88	0.42
1:D:232:SER:O	1:D:236:VAL:HG23	2.19	0.42
1:D:699:GLU:OE1	1:D:702:LYS:NZ	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:989:ASP:OD1	1:D:989:ASP:N	2.52	0.42
1:D:1026:SER:OG	1:D:1027:GLN:N	2.52	0.42
1:A:196:SER:HB2	1:A:207:ARG:HH21	1.84	0.42
1:A:330:LYS:NZ	1:A:331:LYS:O	2.39	0.42
1:B:304:MET:HA	1:B:307:PHE:HB3	2.00	0.42
1:B:597:PHE:HD2	1:B:605:VAL:HG13	1.85	0.42
1:D:299:LEU:HA	1:D:302:LEU:HD12	2.01	0.42
1:D:511:PHE:HZ	1:D:937:ILE:HD11	1.84	0.42
1:D:937:ILE:HD13	1:D:937:ILE:HA	1.83	0.42
1:A:946:THR:OG1	1:A:949:LEU:HD23	2.19	0.42
1:B:511:PHE:CZ	1:B:937:ILE:HD11	2.54	0.42
1:D:931:ASP:OD1	1:D:932:ASN:ND2	2.53	0.42
1:A:229:THR:HG23	1:A:232:SER:H	1.84	0.42
1:C:261:ASP:OD2	1:C:268:ASN:ND2	2.38	0.42
1:A:319:VAL:HA	1:A:322:ILE:HG12	2.02	0.41
1:B:687:ASP:OD2	1:B:689:THR:OG1	2.35	0.41
1:D:707:ARG:NE	1:D:788:ASP:OD1	2.52	0.41
1:D:722:CYS:HB3	1:D:783:PRO:HB3	2.02	0.41
1:D:1044:VAL:HG12	1:D:1046:THR:H	1.83	0.41
1:A:442:MET:HA	1:A:445:ILE:HG22	2.02	0.41
1:C:163:TYR:OH	1:C:213:ARG:NH2	2.53	0.41
1:B:207:ARG:O	1:B:210:ARG:NH2	2.53	0.41
1:B:1002:LYS:HD3	1:B:1002:LYS:HA	1.77	0.41
1:D:134:SER:HB2	1:D:254:HIS:CE1	2.55	0.41
1:D:612:CYS:SG	1:D:613:LYS:N	2.93	0.41
1:A:795:ASN:HA	1:A:876:ILE:HD11	2.02	0.41
1:A:817:ASP:O	1:A:821:ILE:HG12	2.20	0.41
1:C:567:ALA:HB2	1:C:581:ILE:HD13	2.01	0.41
1:B:693:HIS:CE1	1:B:744:SER:HA	2.56	0.41
1:D:496:GLN:NE2	1:D:940:LEU:O	2.52	0.41
1:D:950:GLU:HA	1:D:953:ILE:HG22	2.02	0.41
1:C:700:ILE:HB	1:C:767:TRP:CD1	2.55	0.41
1:B:167:ARG:HA	1:B:167:ARG:HD2	1.80	0.41
1:B:723:ILE:HD11	1:B:756:PHE:HD2	1.85	0.41
1:B:895:ASP:OD1	1:B:895:ASP:N	2.51	0.41
1:D:1033:VAL:HG23	1:D:1050:PHE:HE2	1.85	0.41
1:A:146:LYS:HZ2	1:A:146:LYS:HG3	1.68	0.41
1:B:706:THR:HG22	1:B:709:GLU:HG2	2.02	0.41
1:B:876:ILE:HD13	1:B:876:ILE:HA	1.92	0.41
1:D:320:PRO:O	1:D:323:ILE:HG22	2.20	0.41
1:A:172:ASN:HB3	1:A:173:ASP:H	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:GLU:HG3	1:C:701:GLU:H	1.85	0.41
1:C:811:ASP:OD1	1:C:811:ASP:N	2.54	0.41
1:A:386:GLU:O	1:A:390:LEU:HG	2.20	0.41
1:D:300:GLY:O	1:D:304:MET:HG2	2.20	0.41
1:D:496:GLN:HE21	1:D:941:VAL:HA	1.85	0.41
1:A:490:LYS:HG3	1:A:915:PHE:HE2	1.85	0.41
1:A:692:PHE:HD1	1:A:743:ALA:HA	1.86	0.41
1:C:122:LEU:HB3	1:C:210:ARG:HH11	1.86	0.41
1:C:237:ASN:O	1:C:241:ILE:HG23	2.21	0.41
1:C:350:HIS:CE1	1:C:352:THR:HG1	2.39	0.41
1:B:442:MET:HA	1:B:445:ILE:HG22	2.03	0.41
1:D:992:ASP:N	1:D:992:ASP:OD1	2.49	0.41
1:A:604:GLU:OE2	1:A:607:ARG:NH1	2.42	0.41
1:C:335:SER:OG	1:C:336:TYR:N	2.53	0.41
1:B:231:ASN:N	1:B:231:ASN:OD1	2.55	0.41
1:B:441:ILE:HG21	1:D:822:LEU:HD11	2.03	0.41
1:D:122:LEU:HG	1:D:125:GLY:HA3	2.03	0.41
1:A:159:PHE:O	1:A:162:LEU:HG	2.21	0.40
1:D:726:ASP:N	1:D:726:ASP:OD1	2.52	0.40
1:C:210:ARG:HA	1:C:213:ARG:HB2	2.03	0.40
1:C:804:SER:OG	1:C:807:GLN:HB3	2.21	0.40
1:C:1033:VAL:HG23	1:C:1050:PHE:HE2	1.85	0.40
1:B:384:ASN:O	1:B:387:LEU:N	2.53	0.40
1:D:26:LEU:HD22	1:D:26:LEU:HA	1.91	0.40
1:D:735:ARG:HA	1:D:770:LEU:HD21	2.02	0.40
1:A:351:ILE:HD11	1:A:379:HIS:HB2	2.03	0.40
1:B:164:PHE:HE1	1:B:187:PHE:CE1	2.40	0.40
1:B:167:ARG:HB3	1:B:177:PHE:HE1	1.87	0.40
1:B:330:LYS:HA	1:B:330:LYS:HD2	1.87	0.40
1:B:511:PHE:CE2	1:B:937:ILE:HD11	2.55	0.40
1:D:246:TRP:HZ2	1:D:282:MET:HB2	1.86	0.40
1:A:529:LEU:HA	1:A:532:VAL:HG12	2.02	0.40
1:A:1056:ASP:OD1	1:A:1056:ASP:N	2.46	0.40
1:B:292:ASP:N	1:B:292:ASP:OD1	2.53	0.40
1:B:347:VAL:HG22	1:B:423:LEU:HB2	2.03	0.40
1:B:526:LYS:HB3	1:B:526:LYS:HE2	1.91	0.40
1:D:563:LEU:HD21	1:D:597:PHE:CG	2.57	0.40
1:C:216:GLN:O	1:C:219:GLU:HG2	2.22	0.40
1:B:269:ASN:N	1:B:269:ASN:OD1	2.54	0.40
1:B:872:THR:HG23	1:B:874:VAL:HG12	2.02	0.40
1:B:1017:LEU:HG	1:B:1031:ARG:HE	1.86	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	803/1072 (75%)	750 (93%)	53 (7%)	0	100	100
1	B	803/1072 (75%)	761 (95%)	42 (5%)	0	100	100
1	C	843/1072 (79%)	805 (96%)	38 (4%)	0	100	100
1	D	838/1072 (78%)	796 (95%)	42 (5%)	0	100	100
All	All	3287/4288 (77%)	3112 (95%)	175 (5%)	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	724/943 (77%)	723 (100%)	1 (0%)	93	97
1	B	726/943 (77%)	725 (100%)	1 (0%)	93	97
1	C	750/943 (80%)	745 (99%)	5 (1%)	84	90
1	D	747/943 (79%)	745 (100%)	2 (0%)	92	96
All	All	2947/3772 (78%)	2938 (100%)	9 (0%)	92	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	C	113	ARG
1	C	128	VAL
1	C	201	ARG
1	C	207	ARG
1	C	366	LYS
1	B	329	ARG
1	D	113	ARG
1	D	366	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	200	ASN
1	A	222	GLN
1	A	258	ASN
1	A	462	GLN
1	A	468	HIS
1	A	534	ASN
1	A	749	HIS
1	A	816	GLN
1	A	893	GLN
1	A	930	ASN
1	A	967	GLN
1	C	402	GLN
1	C	464	HIS
1	C	534	ASN
1	C	907	GLN
1	B	108	GLN
1	B	344	HIS
1	B	465	ASN
1	B	468	HIS
1	B	496	GLN
1	B	509	ASN
1	B	808	ASN
1	B	1008	ASN
1	D	216	GLN
1	D	222	GLN
1	D	225	ASN
1	D	534	ASN
1	D	693	HIS
1	D	745	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	808	ASN
1	D	932	ASN
1	D	971	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

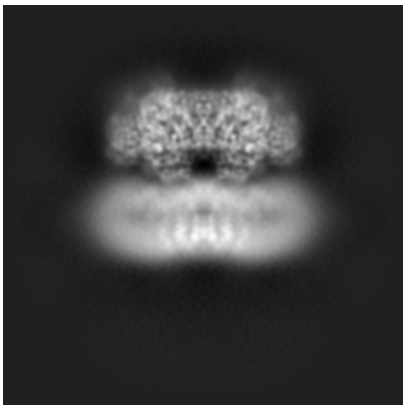
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40045. These allow visual inspection of the internal detail of the map and identification of artifacts.

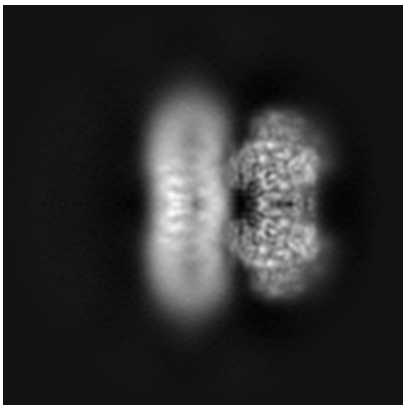
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

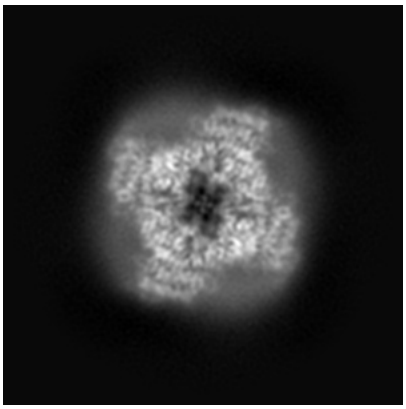
6.1.1 Primary map



X

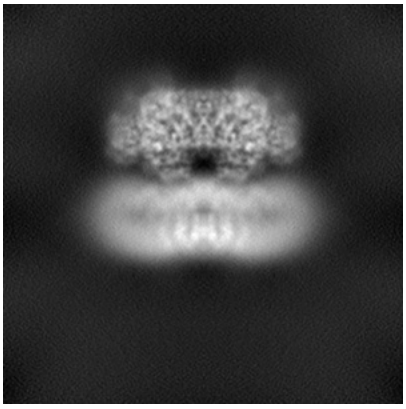


Y

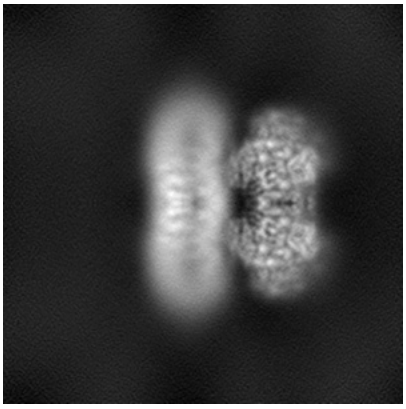


Z

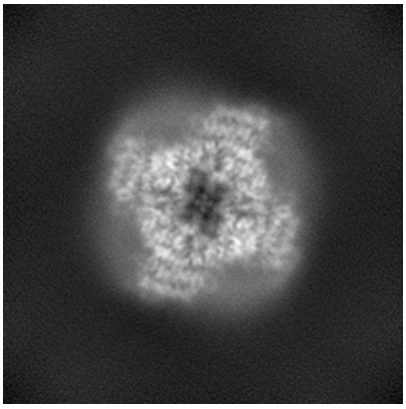
6.1.2 Raw map



X



Y

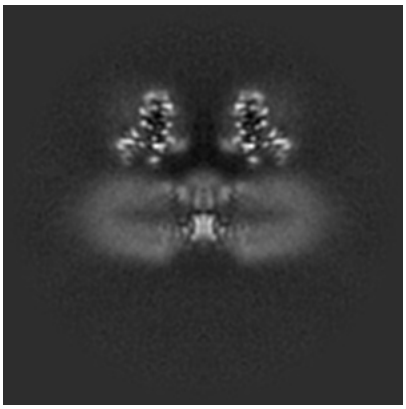


Z

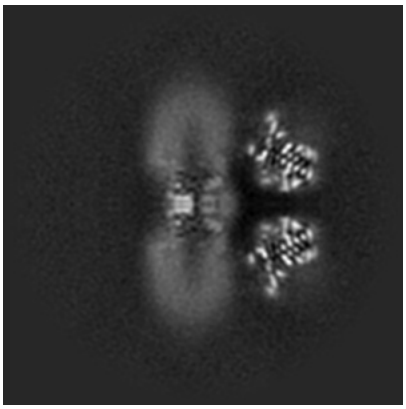
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

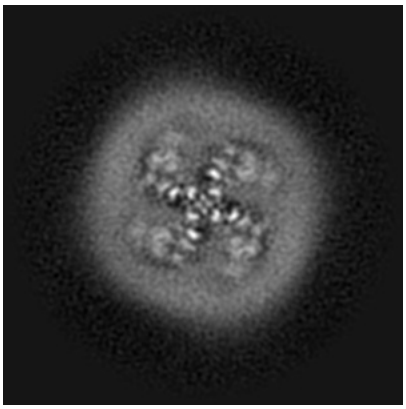
6.2.1 Primary map



X Index: 128

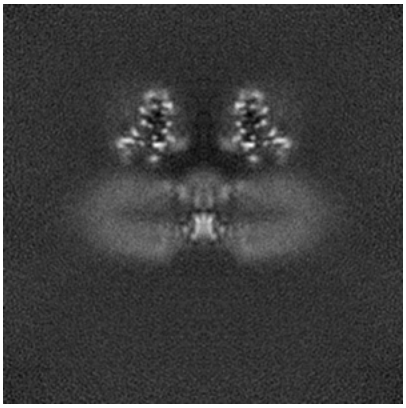


Y Index: 128

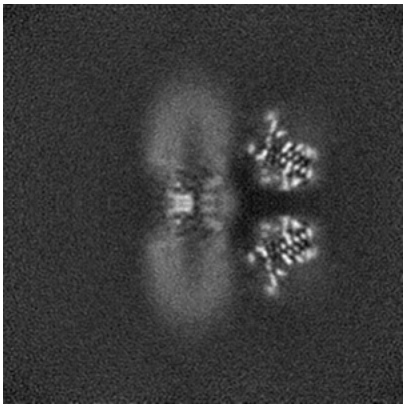


Z Index: 128

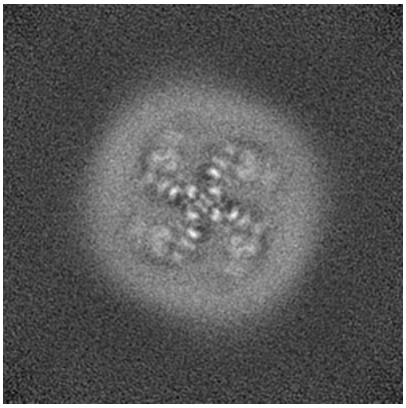
6.2.2 Raw map



X Index: 128



Y Index: 128

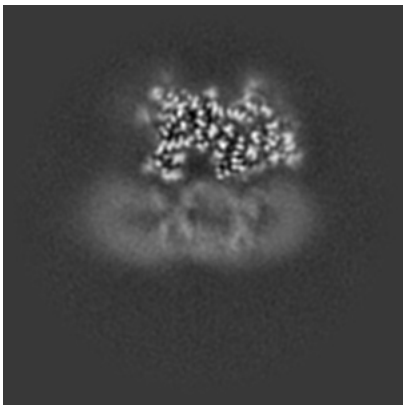


Z Index: 128

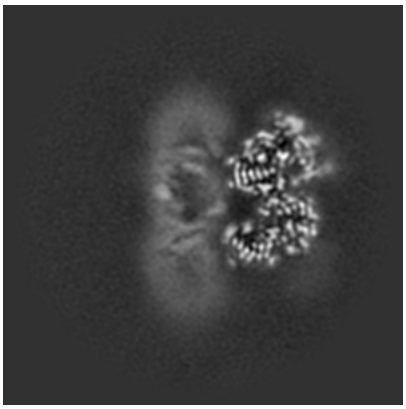
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

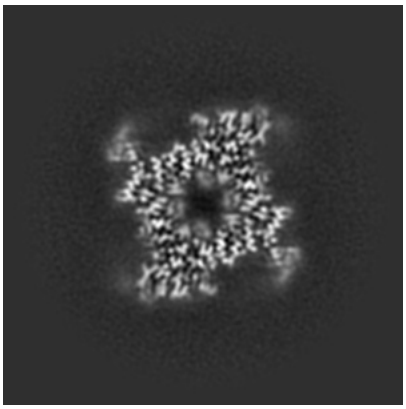
6.3.1 Primary map



X Index: 156

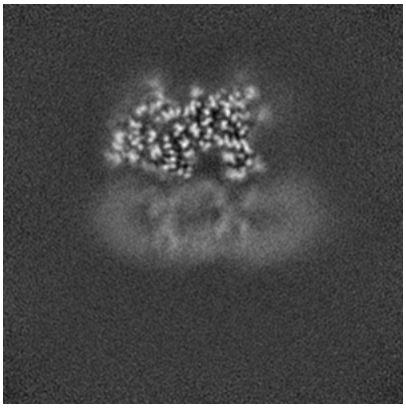


Y Index: 105

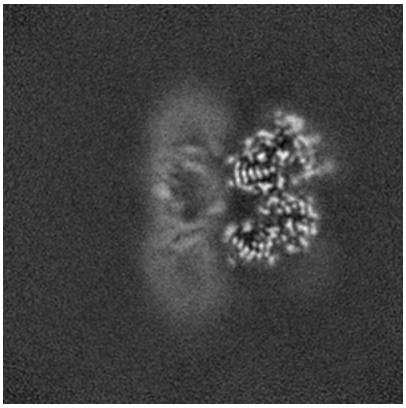


Z Index: 166

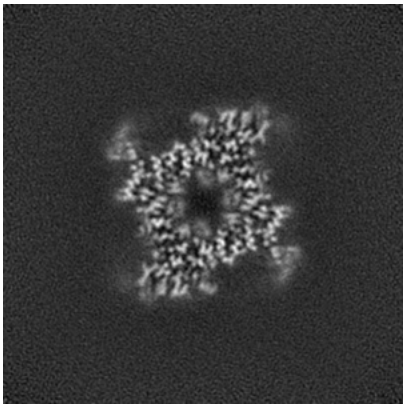
6.3.2 Raw map



X Index: 100



Y Index: 105

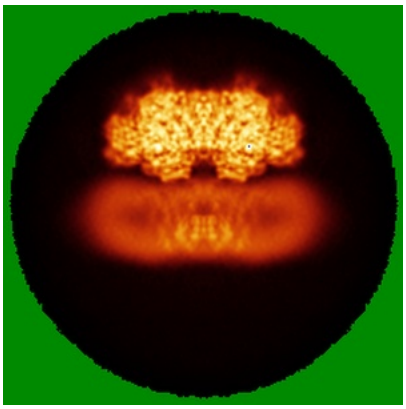


Z Index: 166

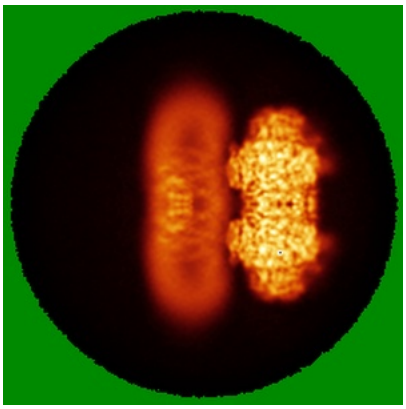
The images above show the largest variance slices of the map in three orthogonal directions.

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

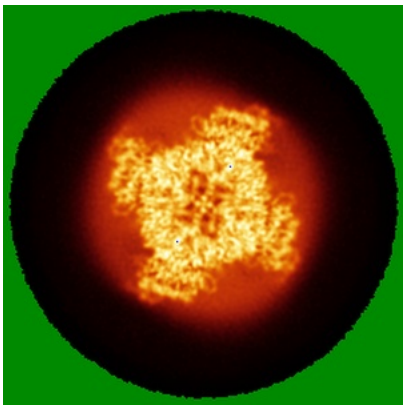
6.4.1 Primary map



X

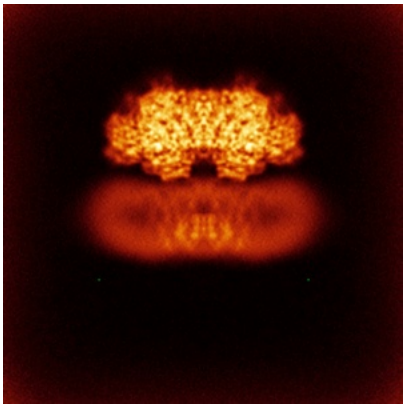


Y

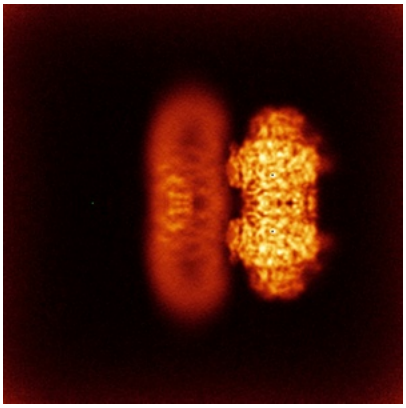


Z

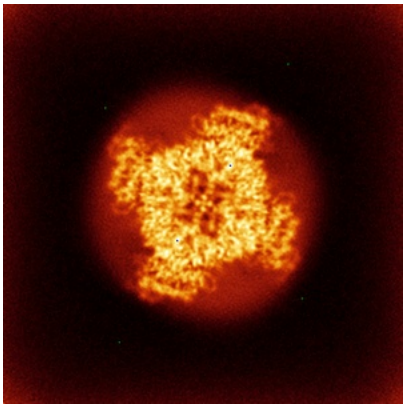
6.4.2 Raw map



X



Y

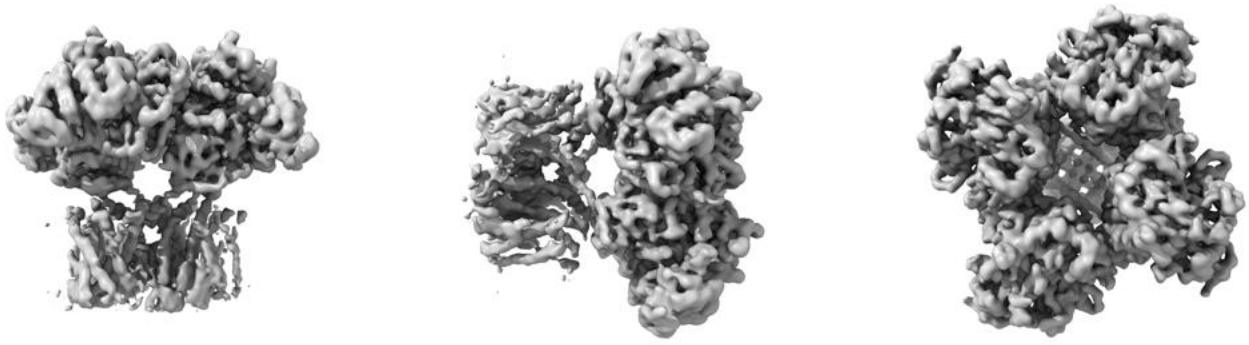


Z

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 0.28. 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.

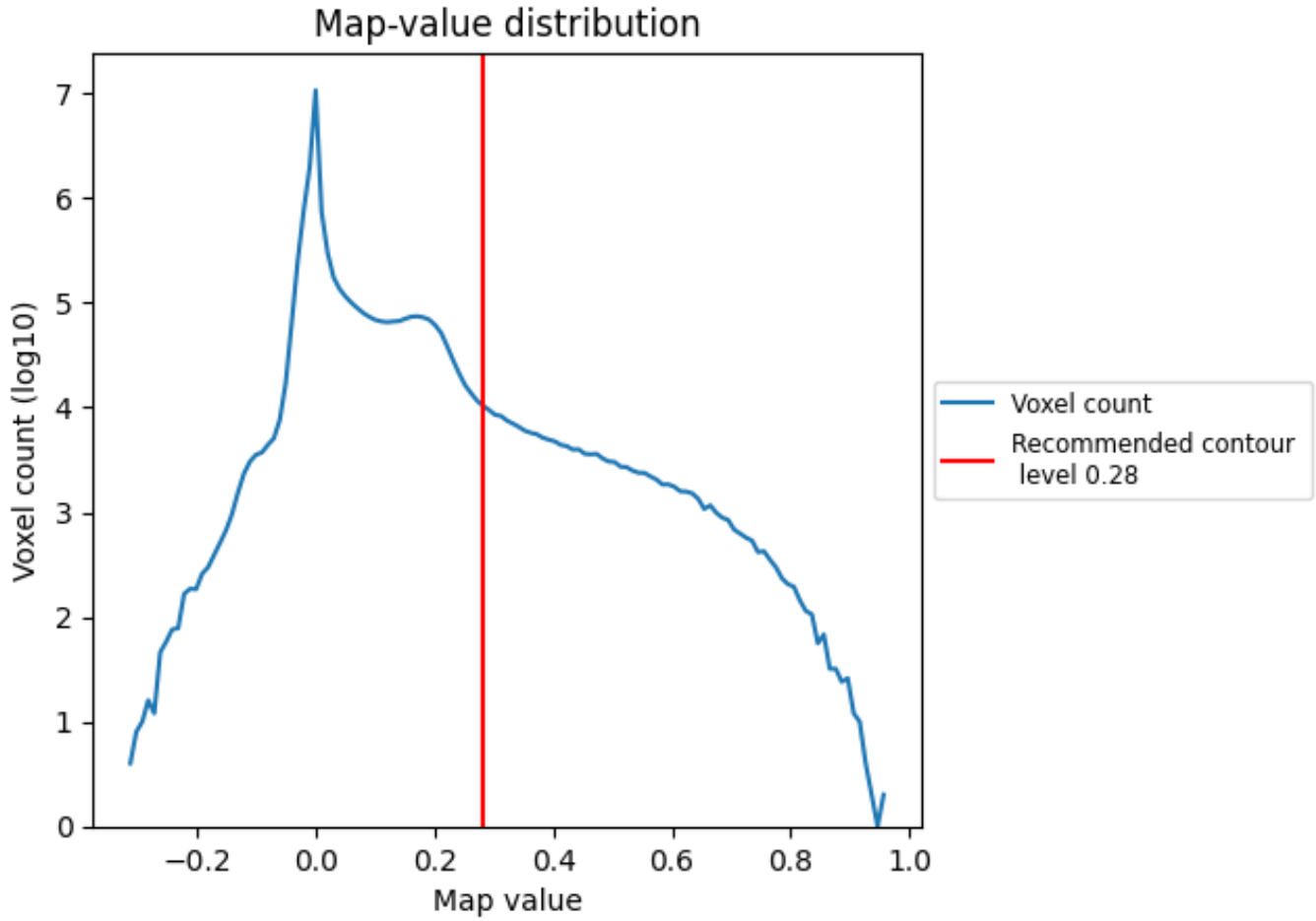
6.6 Mask visualisation (i)

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

7 Map analysis

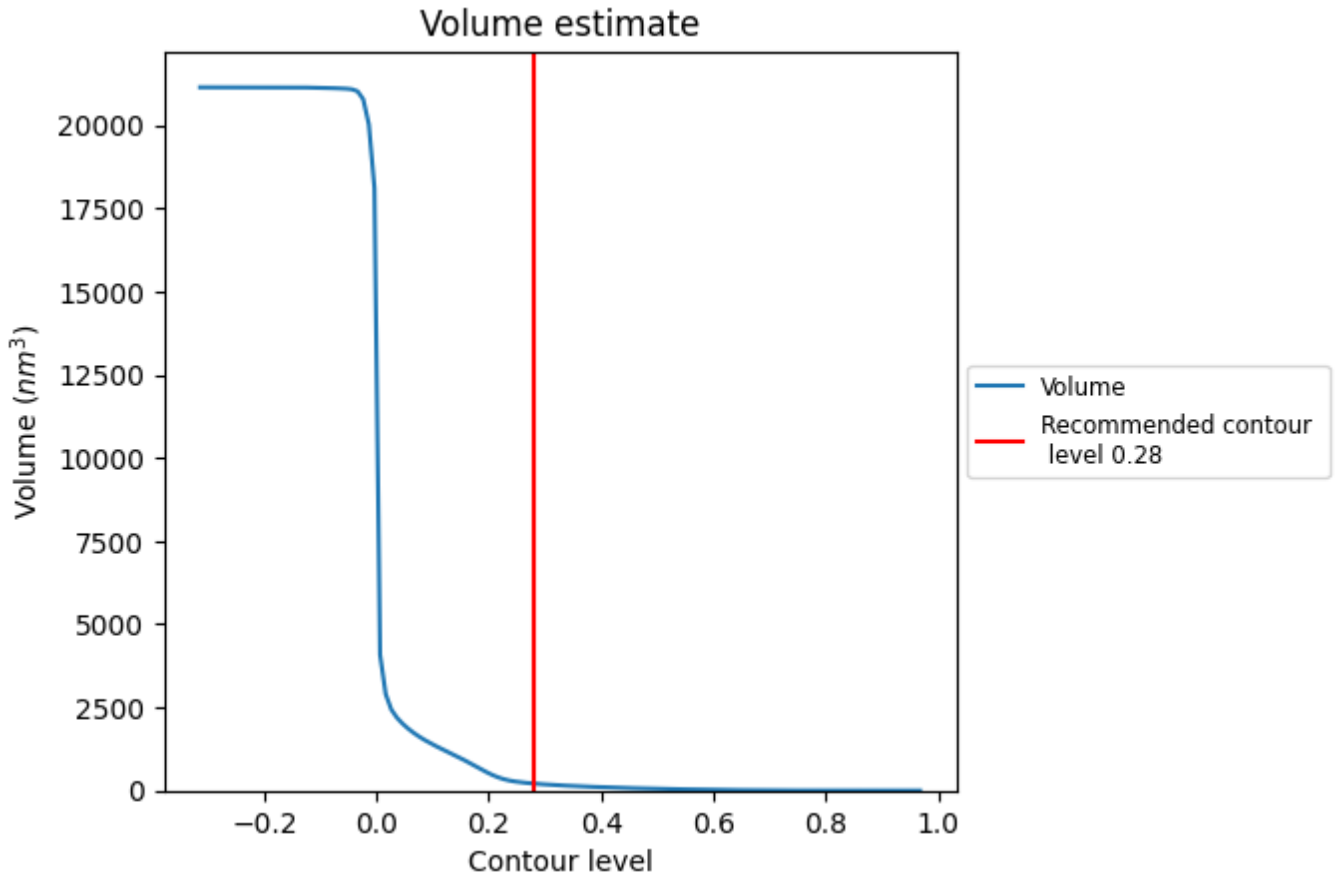
This section contains the results of statistical analysis of the map.

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.

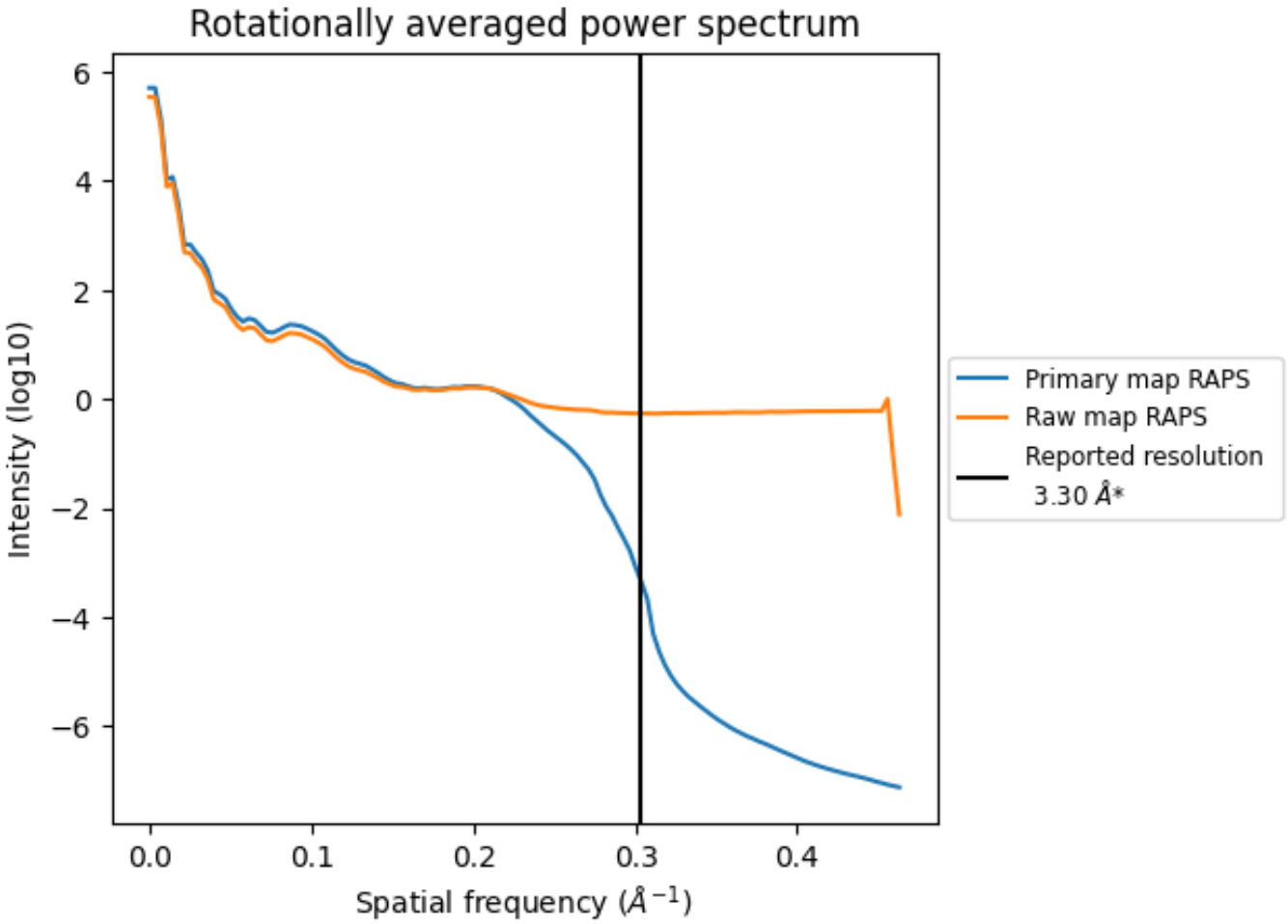
7.2 Volume estimate



The volume at the recommended contour level is 210 nm^3; this corresponds to an approximate mass of 190 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)

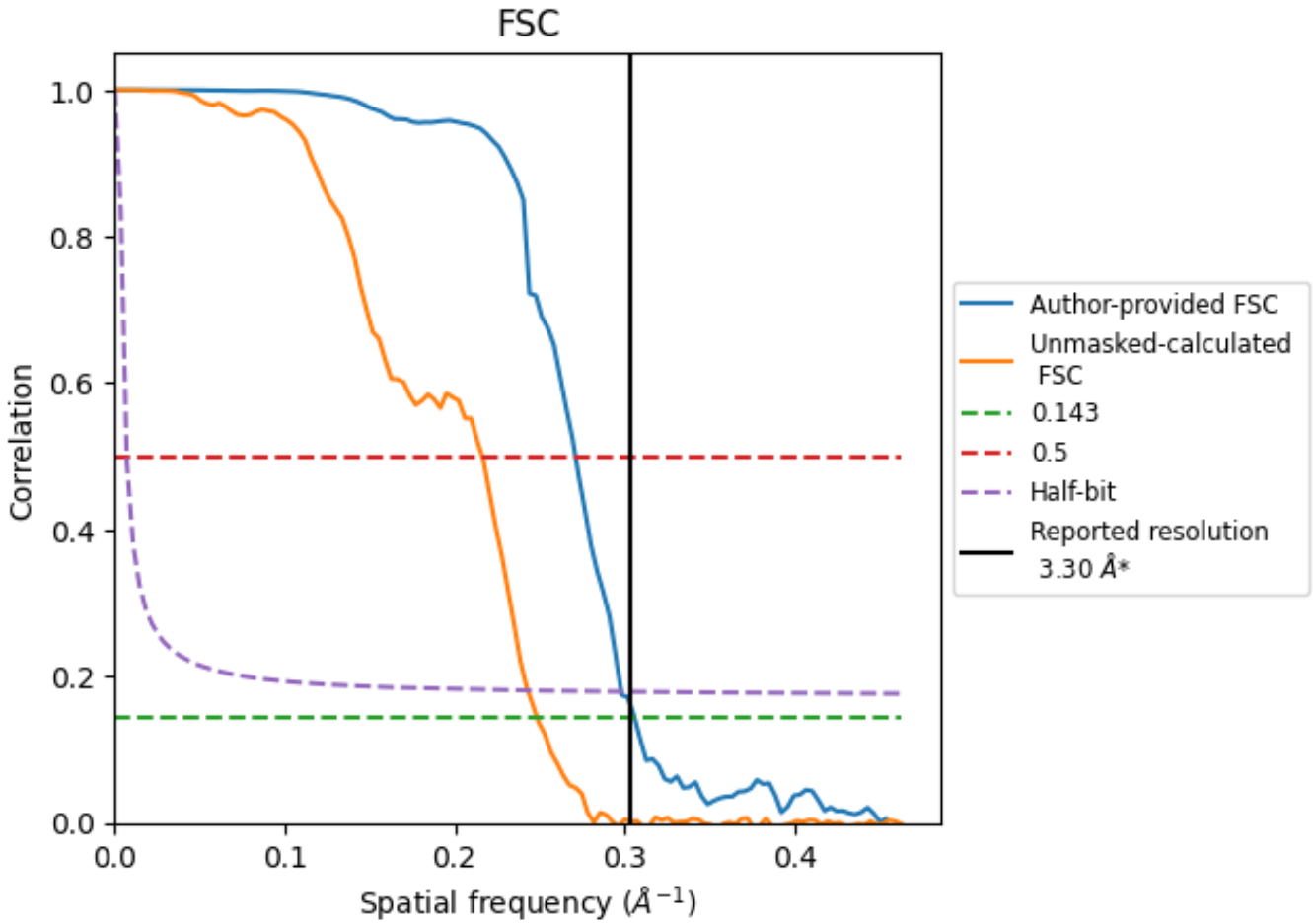


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

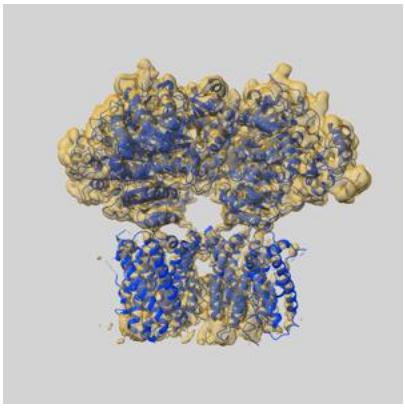
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.69	3.35
Unmasked-calculated*	4.02	4.62	4.11

*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 4.02 differs from the reported value 3.3 by more than 10 %

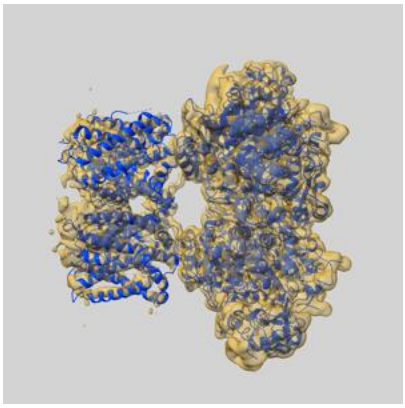
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40045 and PDB model 8GHG. Per-residue inclusion information can be found in section 3 on page 6.

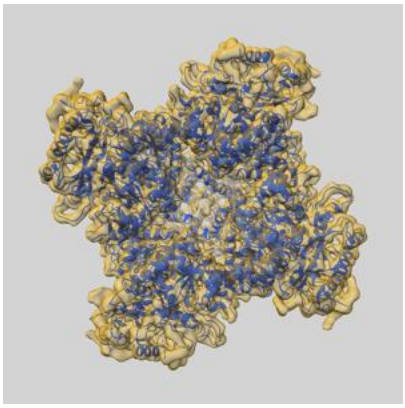
9.1 Map-model overlay



X



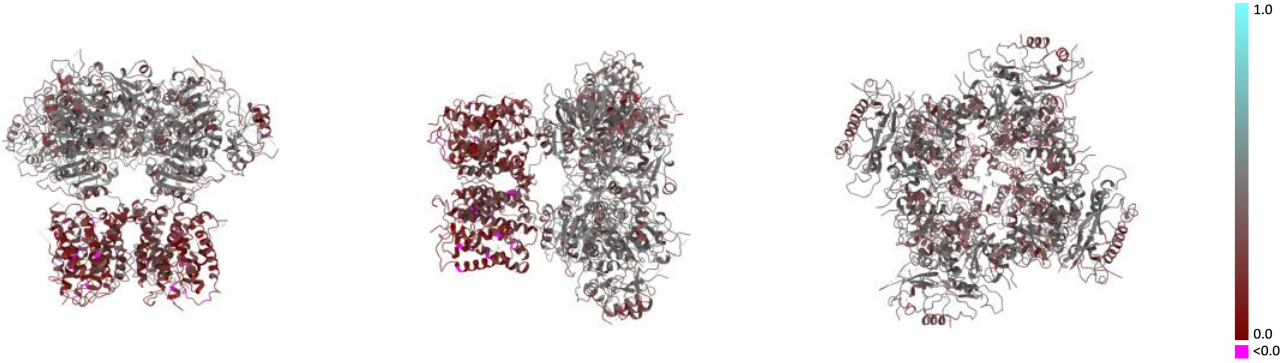
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 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.

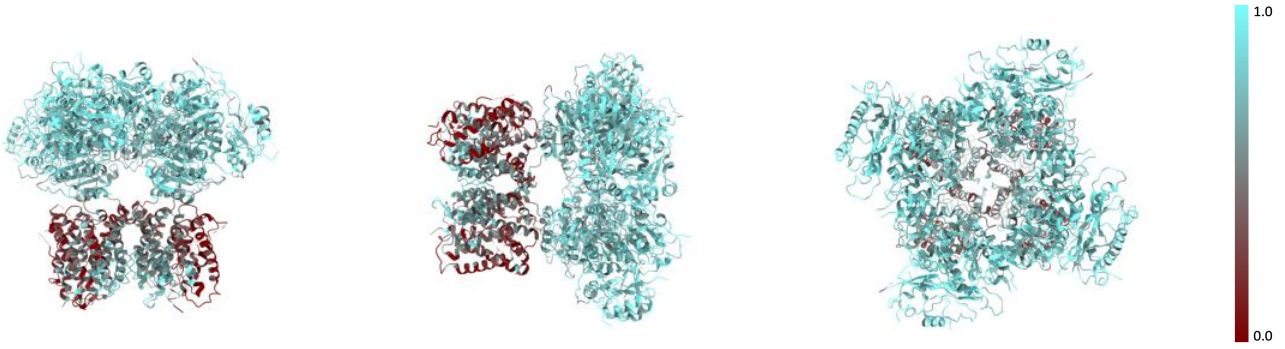
9.2 Q-score mapped to coordinate model (i)



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.

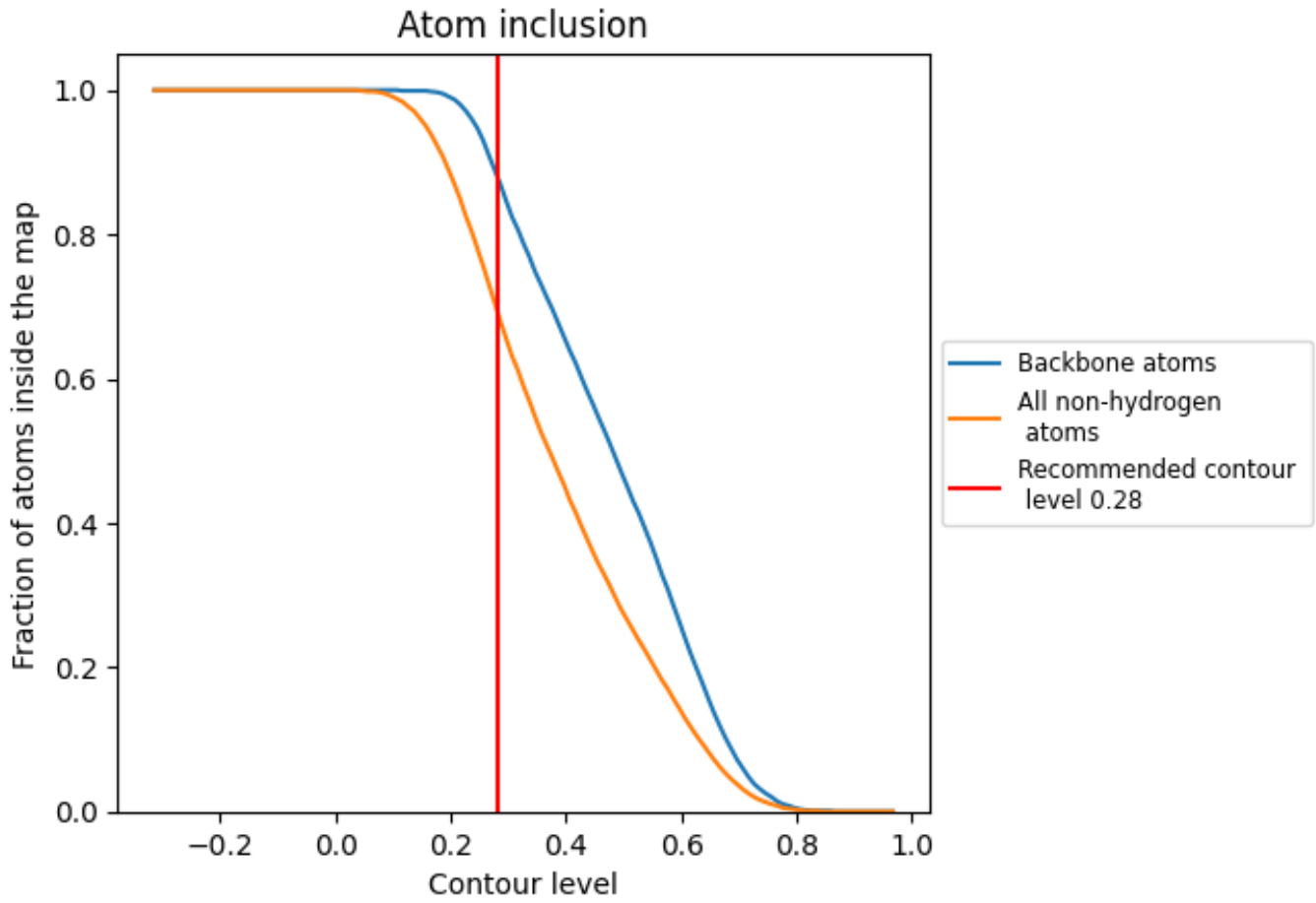
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.3570
A	0.7050	0.3560
B	0.6980	0.3540
C	0.6900	0.3580
D	0.6890	0.3580