Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 02:08 am BST

PDB ID	:	30LA / pdb_000030la
EMDB ID	:	EMD-57866
Title	:	Human Trpm4 with calcium at 37 degrees celsius
Authors	:	Schneiter, D.; Ekundayo, B.E.; Stahlberg, H.; Abriel, H.
Deposited on	:	2026-05-01
Resolution	:	3.00 Å(reported)
Based on initial model	:	9B8W

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:

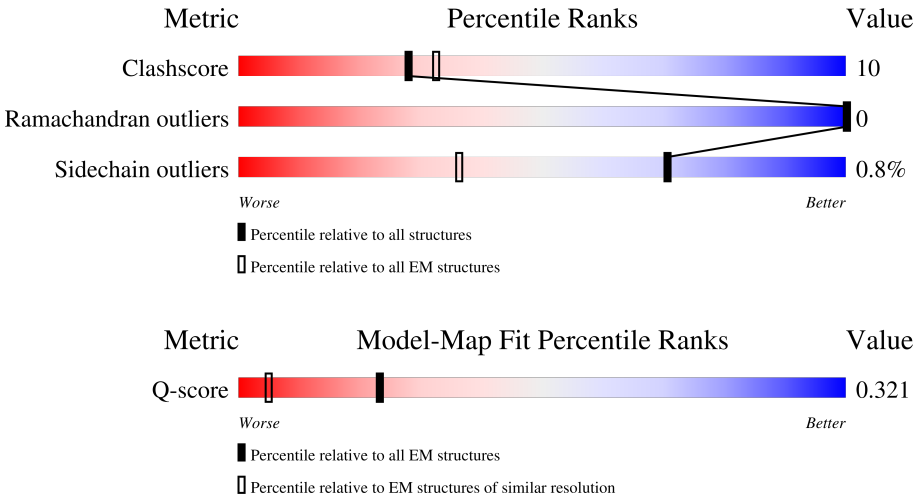
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.00 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	14081 (2.50 - 3.50)

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	1214	27% 65% 16% 18%
1	B	1214	27% 65% 16% 18%
1	C	1214	27% 65% 17% 18%
1	D	1214	27% 65% 16% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 30252 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 Transient receptor potential cation channel subfamily M member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	993	Total 7562	C 4898	N 1336	O 1290	S 38	0	0
1	B	993	Total 7562	C 4898	N 1336	O 1290	S 38	0	0
1	C	993	Total 7562	C 4898	N 1336	O 1290	S 38	0	0
1	D	993	Total 7562	C 4898	N 1336	O 1290	S 38	0	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Ca 1	0
2	B	1	Total 1	Ca 1	0
2	C	1	Total 1	Ca 1	0
2	D	1	Total 1	Ca 1	0

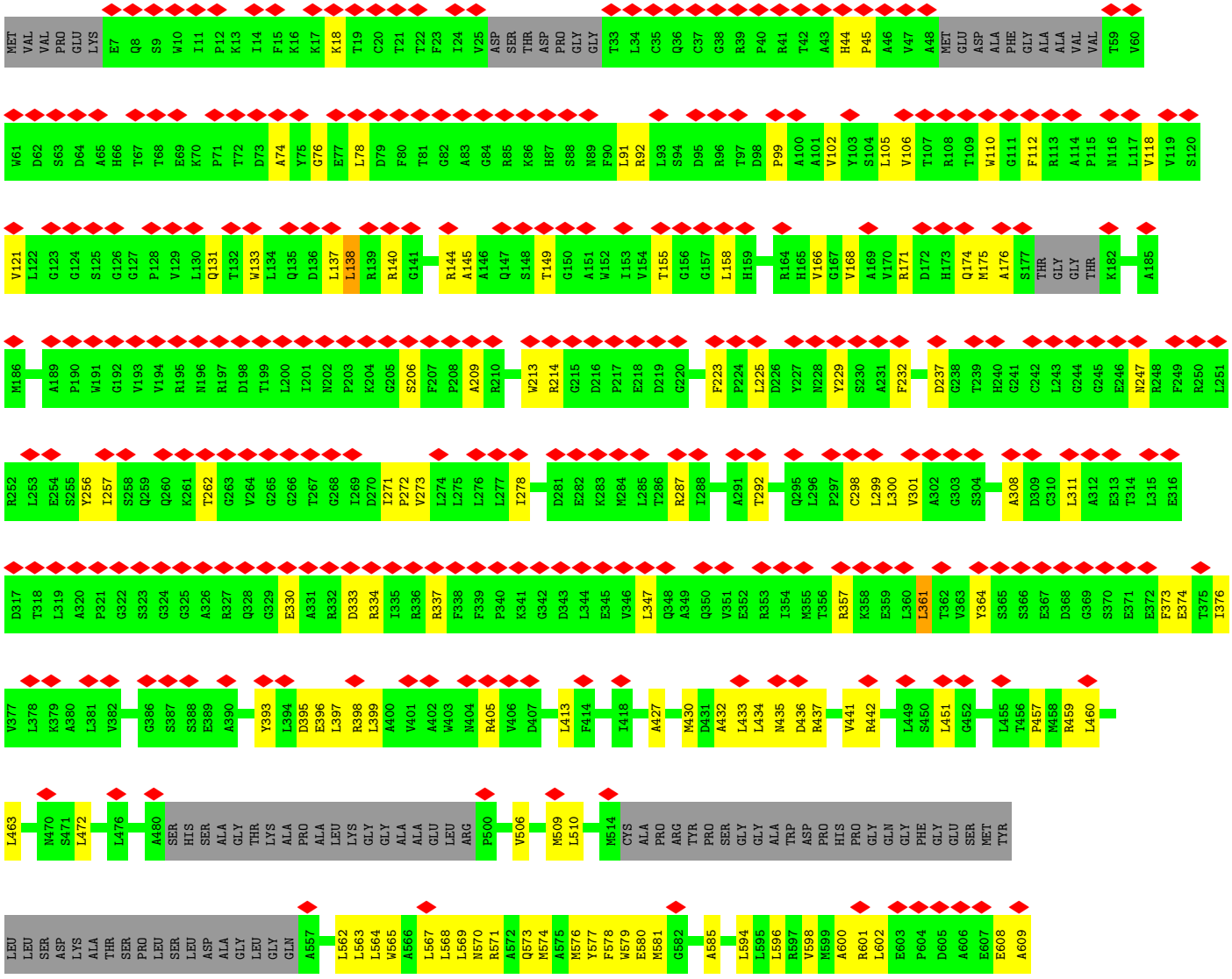
3 Residue-property plots (i)

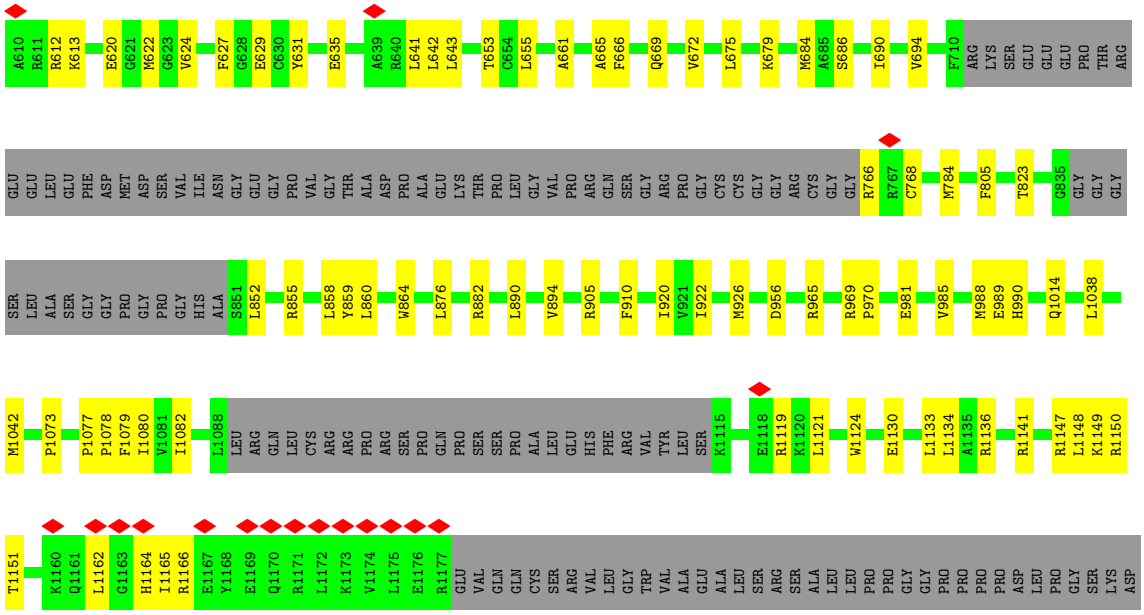
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transient receptor potential cation channel subfamily M member 4

Chain A:



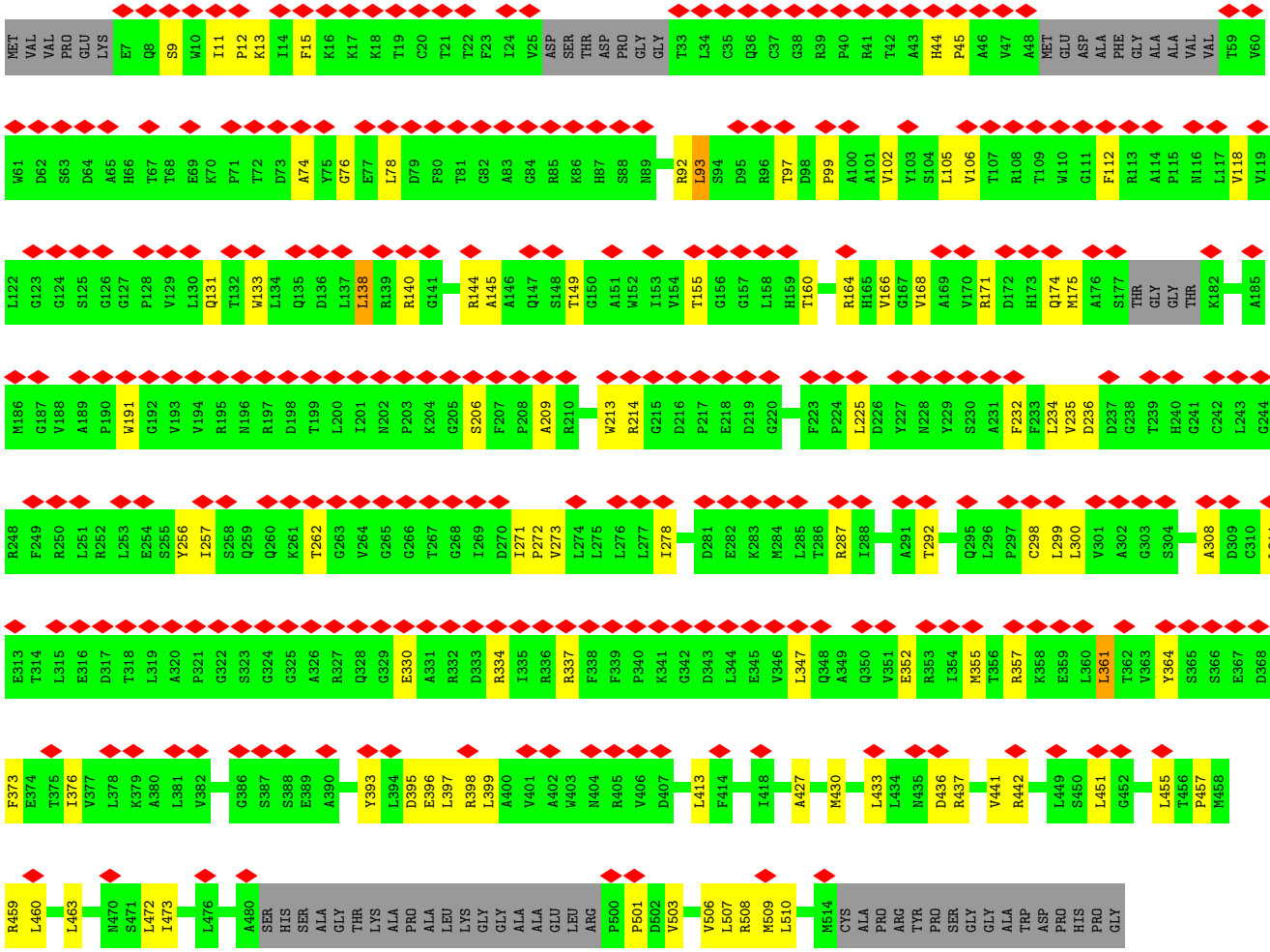


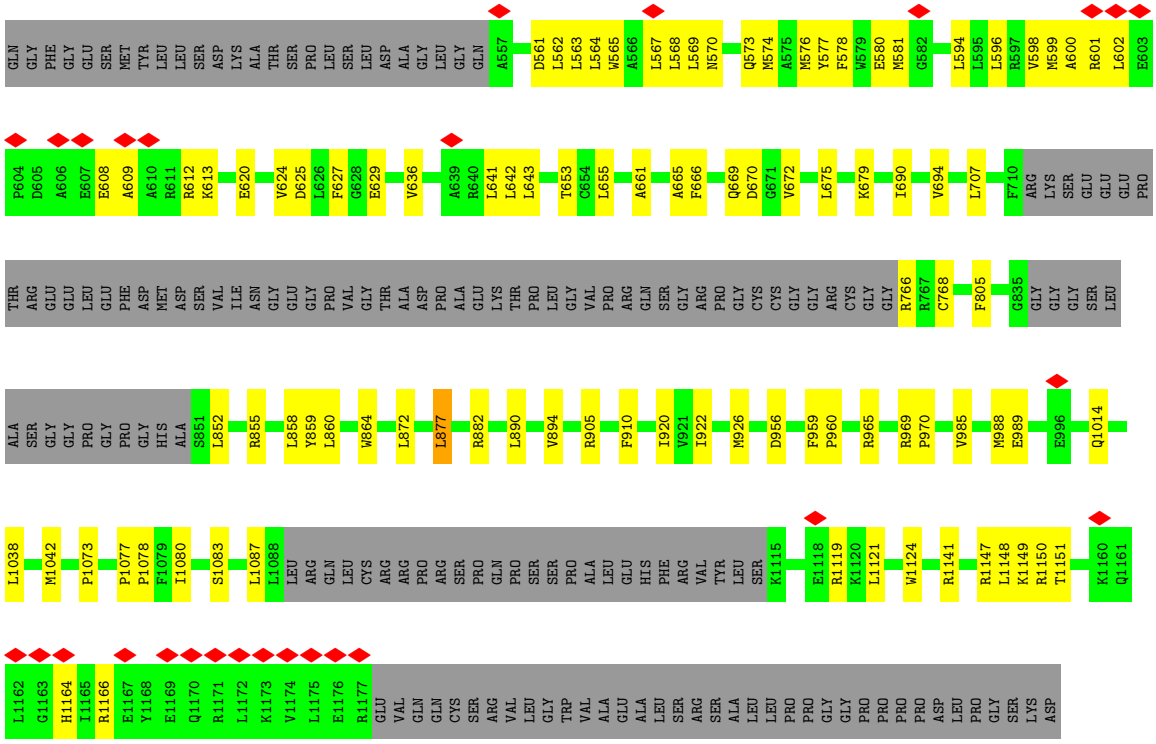


• Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain B:



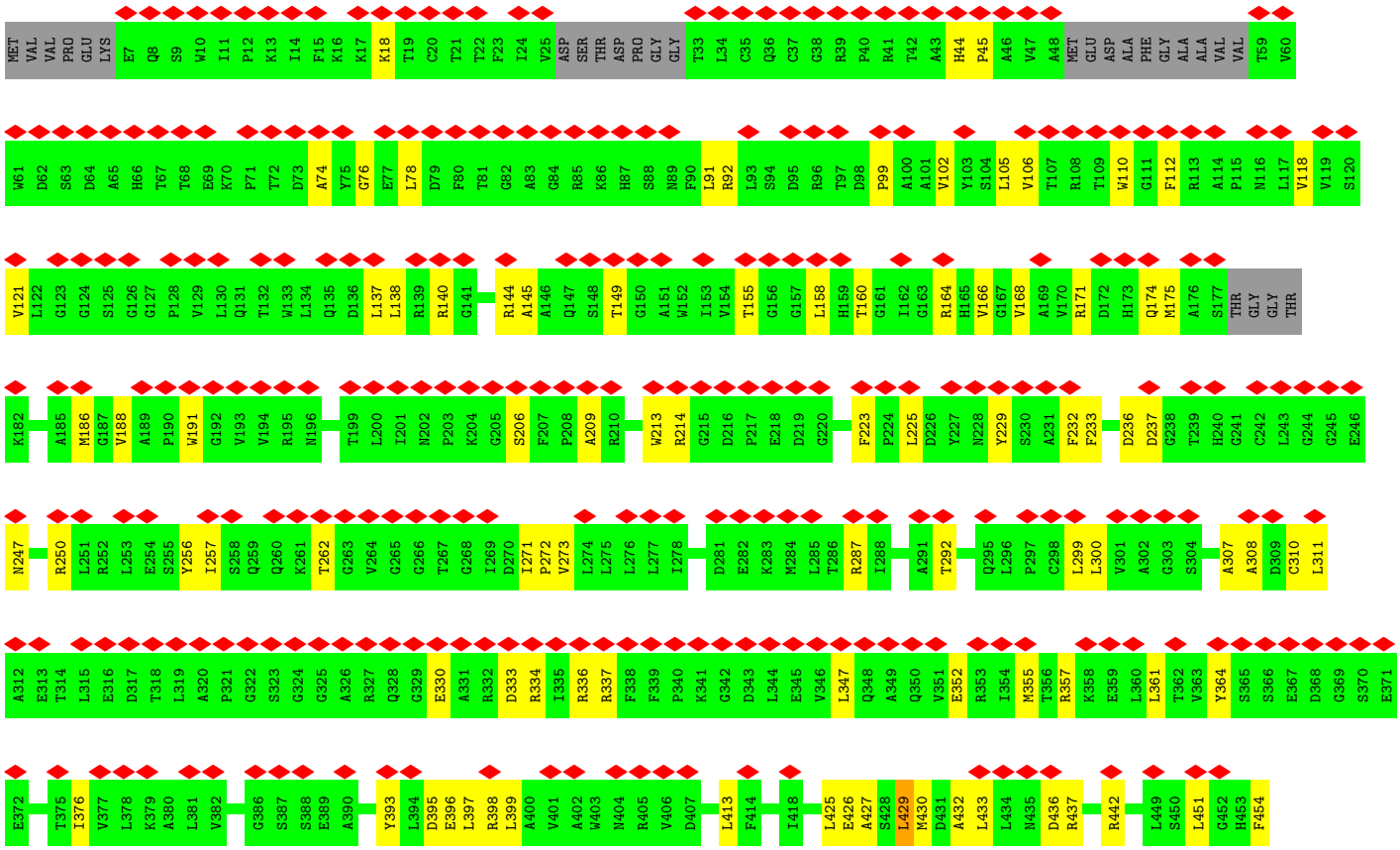


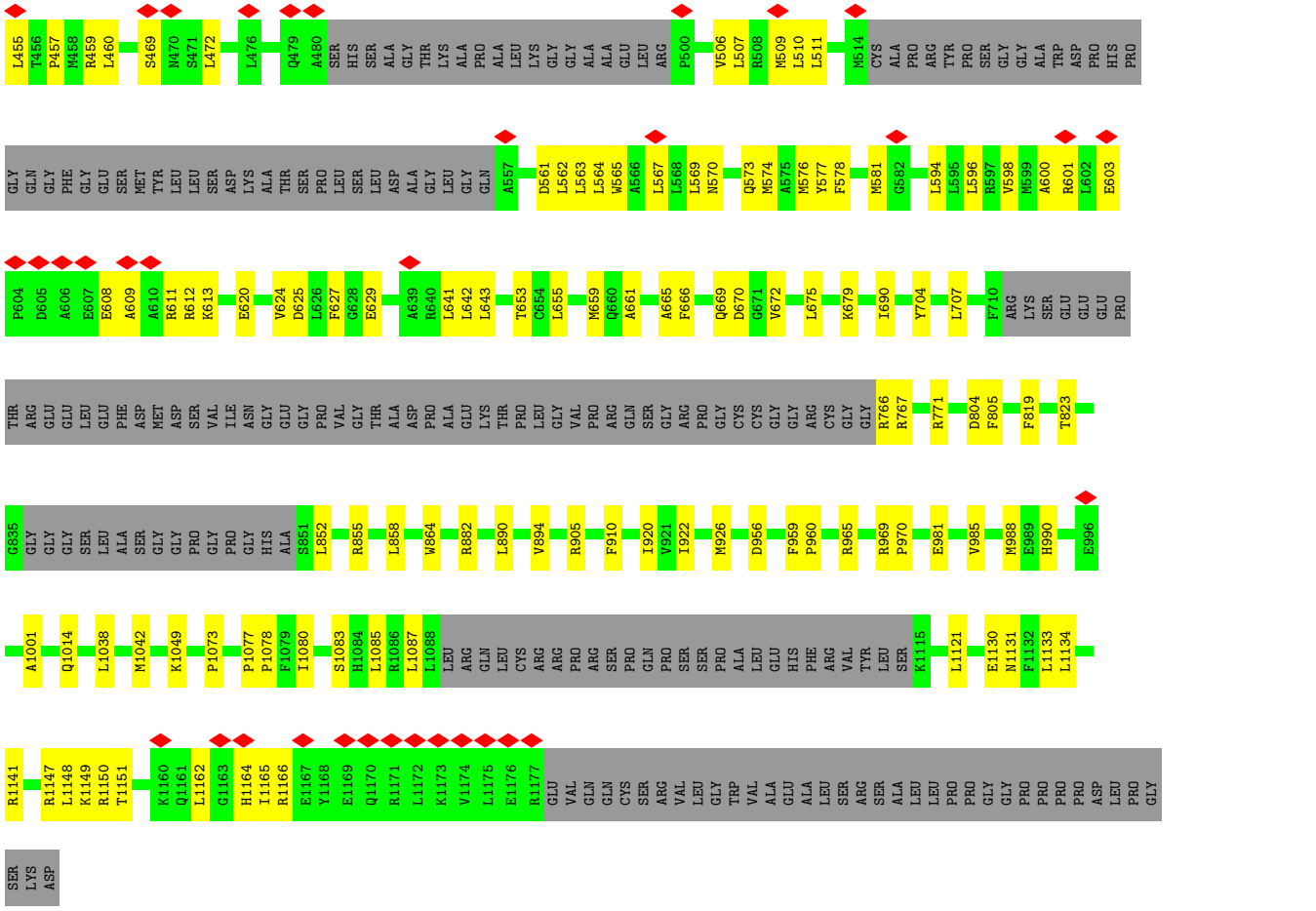


• Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain C:



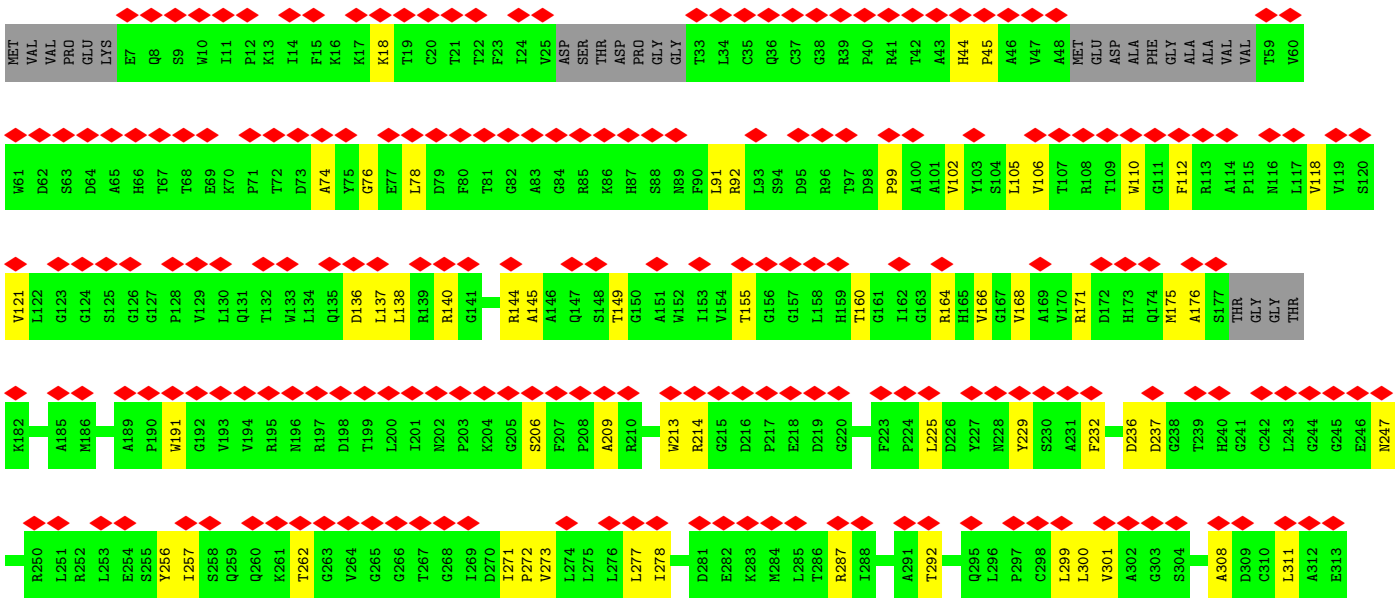


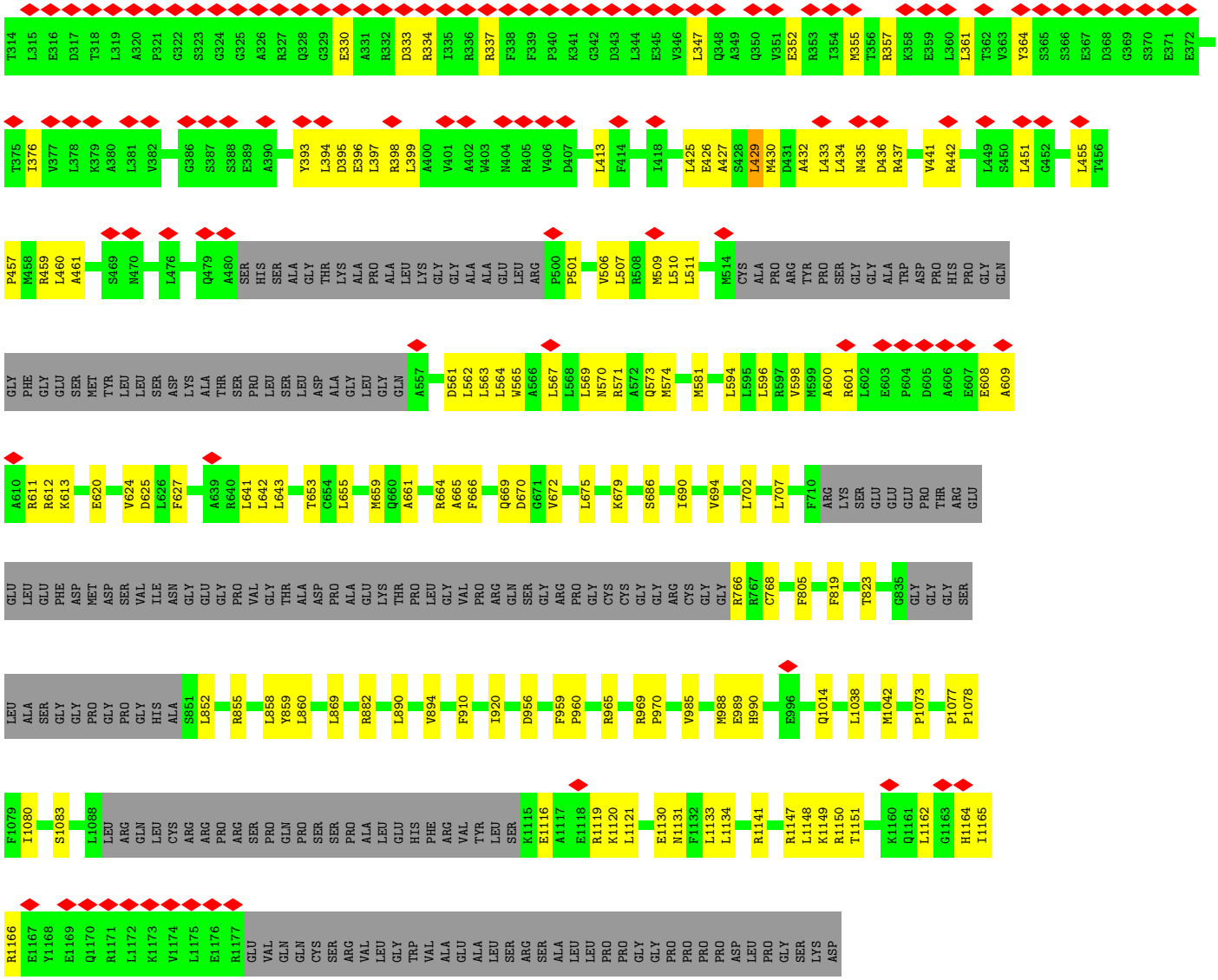


• Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain D:






T314 L315 E316 D317 T318 L319 A320 P321 G322 S323 G324 G325 A326 R327 Q328 G329 E330 A331 R332 D333 R334 I335 R336 R337 F338 F339 P340 K341 G342 D343 L344 E345 V346 L347 Q348 A349 Q350 V351 E352 R353 I354 M355 T356 R357 K358 E359 L360 L361 T362 V363 Y364 S365 S366 E367 D368 G369 S370 E371 E372
T375 I376 V377 L378 K379 A380 L381 V382 G386 S387 S388 E389 A390 Y393 L394 D395 E396 L397 R398 L399 A400 V401 A402 W403 N404 R405 V406 D407 L413 F414 I418 L425 E426 A427 S428 L429 M430 D431 A432 L433 L434 N435 D436 R437 V441 R442 L449 S450 L451 G452 L455 T456
P457 M458 R459 L460 A461 S469 N470 L476 Q479 A480 SER HIS SER ALA GLY THR LYS ALA PRO ALA LEU LYS GLY GLY ALA ALA GLU LEU ARG P500 P501 V506 L507 R508 M509 L510 L511 M514 CYS ALA PRO ARG TYR PRO SER GLY GLY ALA TRP ASP PRO HIS PRO GLY GLN
GLY PHE GLY GLU SER MET TYR LEU LEU SER ASP LYS ALA THR SER PRO LEU SER LEU ASP ALA GLY LEU GLY GLN A557 D561 L562 L563 L564 W565 A566 L567 L568 L569 N570 R571 A572 Q573 M574 M581 L594 L595 L596 R597 V598 M599 A600 R601 L602 E603 P604 D605 A606 E607 E608 A609
A610 R611 R612 K613 E620 V624 D625 L626 F627 A639 R640 L641 L642 L643 T653 C654 L655 M659 Q660 A661 R664 A665 F666 Q669 D670 G671 V672 L675 K679 S686 I690 V694 L702 L707 F710 ARG LYS SER GLU GLU GLU PRO THR ARG GLU
GLU LEU GLU PHE ASP MET ASP SER VAL ILE ASN GLY GLU GLY PRO VAL GLY THR ALA ASP PRO ALA GLU LYS THR PRO LEU GLY VAL PRO ARG GLN SER GLY ARG PRO GLY CYS CYS GLY GLY ARG CYS GLY GLY R766 R767 C768 F805 F819 T823 G835 GLY GLY GLY SER
LEU ALA SER GLY GLY PRO GLY PRO GLY HIS ALA S851 L852 R855 L858 Y859 L860 L869 R882 L890 V894 F910 I920 D956 F959 P960 R965 R969 P970 V985 M988 E989 H990 E996 Q1014 L1038 M1042 P1073 P1077 P1078
F1079 I1080 S1083 L1088 LEU ARG GLN LEU CYS ARG ARG PRO ARG SER PRO GLN PRO SER SER PRO ALA LEU GLU HIS PHE ARG VAL TYR LEU SER K1115 E1116 A1117 E1118 R1119 K1120 L1121 E1130 N1131 F1132 L1133 L1134 R1141 R1147 L1148 K1149 R1150 T1151 K1160 Q1161 L1162 G1163 H1164 I1165
R1166 E1167 Y1168 E1169 Q1170 R1171 L1172 K1173 V1174 L1175 E1176 R1177 GLU VAL GLN GLN CYS SER ARG VAL LEU GLY TRP VAL ALA GLU ALA LEU SER ARG SER ALA LEU LEU PRO PRO GLY GLY PRO PRO PRO PRO ASP LEU PRO GLY SER LYS ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.382	Depositor
Minimum map value	-0.169	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	365.19998, 365.19998, 365.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9129999, 0.9129999, 0.9129999	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/7737	0.41	0/10521
1	B	0.16	0/7737	0.41	0/10521
1	C	0.16	0/7737	0.40	1/10521 (0.0%)
1	D	0.16	0/7737	0.39	0/10521
All	All	0.16	0/30948	0.40	1/42084 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	469	SER	CB-CA-C	-5.67	110.02	116.54

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	7562	0	7425	145	0
1	B	7562	0	7425	145	0
1	C	7562	0	7425	150	0
1	D	7562	0	7425	150	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	30252	0	29700	573	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 10.

All (573) 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:C:300:LEU:HD21	1:C:308:ALA:HB1	1.49	0.91
1:B:13:LYS:HE2	1:B:13:LYS:H	1.38	0.88
1:A:300:LEU:HD21	1:A:308:ALA:HB1	1.60	0.82
1:A:1073:PRO:HB2	1:A:1080:ILE:HD11	1.61	0.82
1:B:300:LEU:HD21	1:B:308:ALA:HB1	1.60	0.82
1:D:300:LEU:HD21	1:D:308:ALA:HB1	1.59	0.82
1:B:565:TRP:HE1	1:B:569:LEU:HD22	1.51	0.75
1:A:435:ASN:HB2	1:A:437:ARG:HD3	1.68	0.75
1:D:214:ARG:H	1:D:214:ARG:HD3	1.51	0.74
1:B:168:VAL:HA	1:B:171:ARG:HG3	1.70	0.74
1:A:214:ARG:HD3	1:A:214:ARG:H	1.52	0.74
1:C:214:ARG:H	1:C:214:ARG:HD3	1.52	0.73
1:B:214:ARG:H	1:B:214:ARG:HD3	1.52	0.72
1:C:574:MET:HE3	1:C:574:MET:HA	1.71	0.72
1:A:171:ARG:O	1:A:175:MET:HG3	1.90	0.72
1:A:690:ILE:HD12	1:A:690:ILE:H	1.56	0.71
1:D:435:ASN:HB2	1:D:437:ARG:HD3	1.71	0.71
1:B:574:MET:HE3	1:B:574:MET:HA	1.73	0.70
1:C:76:GLY:HA3	1:C:206:SER:HB2	1.72	0.70
1:A:565:TRP:HE1	1:A:569:LEU:HD22	1.56	0.70
1:D:430:MET:HE1	1:D:459:ARG:HG2	1.74	0.69
1:C:175:MET:HG2	1:D:1120:LYS:HE2	1.73	0.69
1:C:1149:LYS:HD3	1:D:1147:ARG:HH12	1.58	0.69
1:D:455:LEU:HD11	1:D:460:LEU:HD23	1.76	0.68
1:B:690:ILE:HD12	1:B:690:ILE:H	1.59	0.67
1:D:337:ARG:HD3	1:D:347:LEU:HD11	1.76	0.67
1:D:609:ALA:O	1:D:613:LYS:HG2	1.95	0.67
1:C:472:LEU:HD21	1:C:603:GLU:HG3	1.76	0.67
1:C:653:THR:HG22	1:C:655:LEU:H	1.59	0.67
1:C:609:ALA:O	1:C:613:LYS:HG2	1.94	0.67
1:B:337:ARG:HD3	1:B:347:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:GLY:HA3	1:D:206:SER:HB2	1.77	0.67
1:A:506:VAL:O	1:A:510:LEU:HD12	1.94	0.67
1:A:76:GLY:HA3	1:A:206:SER:HB2	1.77	0.66
1:B:433:LEU:HB3	1:B:565:TRP:HH2	1.60	0.66
1:C:337:ARG:HD3	1:C:347:LEU:HD11	1.77	0.66
1:D:171:ARG:O	1:D:175:MET:HG3	1.95	0.66
1:B:364:TYR:HD1	1:B:376:ILE:HG13	1.60	0.66
1:A:337:ARG:HD3	1:A:347:LEU:HD11	1.76	0.66
1:A:653:THR:HG22	1:A:655:LEU:H	1.61	0.66
1:B:653:THR:HG22	1:B:655:LEU:H	1.61	0.65
1:D:574:MET:HE3	1:D:574:MET:HA	1.76	0.65
1:B:76:GLY:HA3	1:B:206:SER:HB2	1.79	0.65
1:A:574:MET:HE3	1:A:574:MET:HA	1.79	0.65
1:D:653:THR:HG22	1:D:655:LEU:H	1.61	0.65
1:B:609:ALA:O	1:B:613:LYS:HG2	1.97	0.65
1:C:145:ALA:O	1:C:149:THR:HG22	1.97	0.65
1:A:564:LEU:O	1:A:568:LEU:HD12	1.95	0.65
1:A:145:ALA:O	1:A:149:THR:HG22	1.97	0.64
1:C:690:ILE:HD12	1:C:690:ILE:H	1.62	0.64
1:A:155:THR:HG21	1:A:166:VAL:HG21	1.80	0.64
1:B:506:VAL:O	1:B:510:LEU:HD12	1.97	0.64
1:D:168:VAL:HA	1:D:171:ARG:HG2	1.80	0.64
1:A:609:ALA:O	1:A:613:LYS:HG2	1.98	0.63
1:D:581:MET:HE3	1:D:581:MET:HA	1.80	0.63
1:D:292:THR:HG22	1:D:357:ARG:HE	1.63	0.63
1:D:364:TYR:HD1	1:D:376:ILE:HG13	1.64	0.62
1:D:985:VAL:HA	1:D:988:MET:HE2	1.81	0.62
1:B:13:LYS:HE2	1:B:13:LYS:N	2.12	0.62
1:C:292:THR:HG22	1:C:357:ARG:HE	1.64	0.62
1:C:433:LEU:HB3	1:C:565:TRP:HH2	1.63	0.62
1:C:330:GLU:O	1:C:334:ARG:HG2	2.01	0.61
1:D:1119:ARG:HH12	1:D:1120:LYS:HE3	1.64	0.61
1:B:985:VAL:HG23	1:B:988:MET:HE2	1.82	0.61
1:D:397:LEU:HB3	1:D:413:LEU:HD13	1.82	0.61
1:B:74:ALA:HB3	1:B:92:ARG:HB3	1.82	0.61
1:C:581:MET:HE3	1:C:581:MET:HA	1.80	0.61
1:D:565:TRP:HE1	1:D:569:LEU:HD22	1.65	0.61
1:B:393:TYR:O	1:B:397:LEU:HD23	2.01	0.61
1:C:144:ARG:HH22	1:D:1131:ASN:HD21	1.49	0.61
1:B:330:GLU:O	1:B:334:ARG:HG2	2.01	0.60
1:A:292:THR:HG22	1:A:357:ARG:HE	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:THR:HG22	1:B:357:ARG:HE	1.66	0.60
1:C:985:VAL:HA	1:C:988:MET:HE2	1.84	0.60
1:B:155:THR:HG21	1:B:166:VAL:HG21	1.82	0.60
1:B:581:MET:HE3	1:B:581:MET:HA	1.84	0.60
1:A:330:GLU:O	1:A:334:ARG:HG2	2.01	0.60
1:A:433:LEU:HB3	1:A:565:TRP:HH2	1.66	0.60
1:B:213:TRP:H	1:B:213:TRP:CD1	2.20	0.60
1:C:393:TYR:O	1:C:397:LEU:HD23	2.01	0.60
1:D:330:GLU:O	1:D:334:ARG:HG2	2.00	0.60
1:A:1141:ARG:HH11	1:A:1150:ARG:HH12	1.50	0.59
1:C:1141:ARG:HH11	1:C:1150:ARG:HH12	1.50	0.59
1:A:393:TYR:O	1:A:397:LEU:HD23	2.02	0.59
1:C:168:VAL:HA	1:C:171:ARG:HG2	1.83	0.59
1:C:74:ALA:HB3	1:C:92:ARG:HB3	1.85	0.59
1:C:364:TYR:HD1	1:C:376:ILE:HG13	1.66	0.59
1:A:213:TRP:CD1	1:A:213:TRP:H	2.21	0.58
1:D:155:THR:HG21	1:D:166:VAL:HG21	1.83	0.58
1:B:262:THR:HG21	1:B:398:ARG:HH12	1.67	0.58
1:A:74:ALA:HB3	1:A:92:ARG:HB3	1.85	0.58
1:C:956:ASP:HB2	1:C:965:ARG:HH22	1.67	0.58
1:D:506:VAL:O	1:D:510:LEU:HG	2.03	0.58
1:D:213:TRP:H	1:D:213:TRP:CD1	2.20	0.58
1:D:361:LEU:H	1:D:361:LEU:HD23	1.69	0.58
1:B:956:ASP:HB2	1:B:965:ARG:HH22	1.69	0.58
1:C:160:THR:HA	1:C:164:ARG:HE	1.69	0.58
1:B:118:VAL:HG21	1:B:257:ILE:HG21	1.86	0.58
1:B:1141:ARG:HH11	1:B:1150:ARG:HH12	1.52	0.58
1:A:262:THR:HG21	1:A:398:ARG:HH12	1.67	0.57
1:C:1073:PRO:HB2	1:C:1080:ILE:HD11	1.87	0.57
1:B:1073:PRO:HB2	1:B:1080:ILE:HD11	1.86	0.57
1:C:213:TRP:CD1	1:C:213:TRP:H	2.20	0.57
1:C:262:THR:HG21	1:C:398:ARG:HH12	1.69	0.57
1:C:852:LEU:HA	1:C:855:ARG:HE	1.68	0.57
1:A:852:LEU:HA	1:A:855:ARG:HE	1.69	0.57
1:B:298:CYS:HB3	1:B:361:LEU:HD22	1.86	0.57
1:D:1141:ARG:HH11	1:D:1150:ARG:HH12	1.52	0.56
1:A:298:CYS:HB3	1:A:361:LEU:HD22	1.86	0.56
1:A:567:LEU:HD12	1:A:596:LEU:HD11	1.88	0.56
1:B:852:LEU:HA	1:B:855:ARG:HE	1.69	0.56
1:A:985:VAL:HA	1:A:988:MET:HE2	1.88	0.56
1:D:1073:PRO:HB2	1:D:1080:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:LEU:HD23	1:C:361:LEU:H	1.69	0.56
1:D:852:LEU:HA	1:D:855:ARG:HE	1.69	0.56
1:C:155:THR:HG21	1:C:166:VAL:HG21	1.86	0.56
1:C:430:MET:HE1	1:C:459:ARG:HG2	1.88	0.56
1:C:171:ARG:HB2	1:C:175:MET:HE3	1.87	0.56
1:B:168:VAL:HB	1:B:171:ARG:NH2	2.21	0.55
1:C:78:LEU:HA	1:C:209:ALA:HB3	1.87	0.55
1:D:433:LEU:HB3	1:D:565:TRP:HH2	1.70	0.55
1:C:118:VAL:HG21	1:C:257:ILE:HG21	1.87	0.55
1:D:74:ALA:HB3	1:D:92:ARG:HB3	1.86	0.55
1:A:168:VAL:HA	1:A:171:ARG:HG2	1.86	0.55
1:A:563:LEU:O	1:A:567:LEU:HD22	2.06	0.55
1:C:506:VAL:O	1:C:510:LEU:HG	2.07	0.55
1:A:1038:LEU:O	1:A:1042:MET:HG3	2.07	0.55
1:D:567:LEU:HD12	1:D:596:LEU:HD11	1.89	0.55
1:D:956:ASP:HB2	1:D:965:ARG:HH22	1.71	0.55
1:A:118:VAL:HG21	1:A:257:ILE:HG21	1.87	0.55
1:B:15:PHE:CD1	1:B:93:LEU:HD11	2.42	0.55
1:C:565:TRP:CD1	1:C:569:LEU:HD13	2.42	0.55
1:A:922:ILE:HG22	1:A:926:MET:HE2	1.89	0.54
1:D:118:VAL:HG21	1:D:257:ILE:HG21	1.88	0.54
1:D:985:VAL:HG21	1:D:1014:GLN:HB3	1.90	0.54
1:B:567:LEU:HD12	1:B:596:LEU:HD21	1.89	0.54
1:C:922:ILE:HG22	1:C:926:MET:HE2	1.89	0.54
1:A:956:ASP:HB2	1:A:965:ARG:HH22	1.72	0.54
1:D:506:VAL:HA	1:D:509:MET:SD	2.48	0.54
1:A:581:MET:HE3	1:A:581:MET:HA	1.90	0.54
1:B:576:MET:HE3	1:B:576:MET:C	2.32	0.54
1:D:78:LEU:HA	1:D:209:ALA:HB3	1.90	0.54
1:B:78:LEU:HA	1:B:209:ALA:HB3	1.90	0.53
1:B:299:LEU:HD11	1:B:376:ILE:HG22	1.89	0.53
1:B:922:ILE:HG22	1:B:926:MET:HE2	1.89	0.53
1:C:565:TRP:HE1	1:C:569:LEU:HD22	1.73	0.53
1:A:78:LEU:HA	1:A:209:ALA:HB3	1.91	0.53
1:A:594:LEU:HB2	1:A:661:ALA:HB2	1.90	0.53
1:B:568:LEU:HA	1:B:599:MET:HE1	1.91	0.53
1:B:594:LEU:HB2	1:B:661:ALA:HB2	1.90	0.53
1:B:1038:LEU:O	1:B:1042:MET:HG3	2.09	0.53
1:B:985:VAL:HG21	1:B:1014:GLN:HB3	1.91	0.53
1:C:472:LEU:H	1:C:472:LEU:HD12	1.73	0.53
1:B:121:VAL:HB	1:B:155:THR:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:PHE:CZ	1:A:643:LEU:HD21	2.43	0.53
1:D:594:LEU:HB2	1:D:661:ALA:HB2	1.90	0.53
1:C:1166:ARG:HH21	1:D:1164:HIS:CE1	2.27	0.52
1:D:262:THR:HG21	1:D:398:ARG:HH12	1.72	0.52
1:D:1038:LEU:O	1:D:1042:MET:HG3	2.08	0.52
1:B:642:LEU:HD23	1:B:1121:LEU:HD21	1.91	0.52
1:D:627:PHE:CZ	1:D:643:LEU:HD21	2.45	0.52
1:B:160:THR:C	1:B:164:ARG:HG2	2.35	0.52
1:C:766:ARG:HE	1:C:767:ARG:H	1.57	0.52
1:A:364:TYR:HD1	1:A:376:ILE:HG13	1.75	0.52
1:A:441:VAL:HG11	1:A:574:MET:SD	2.50	0.52
1:B:144:ARG:HH22	1:C:1131:ASN:HD21	1.57	0.52
1:C:985:VAL:HG21	1:C:1014:GLN:HB3	1.92	0.52
1:A:463:LEU:HD13	1:A:565:TRP:CZ3	2.45	0.52
1:A:1149:LYS:NZ	1:B:1147:ARG:HH22	2.08	0.52
1:B:643:LEU:HD12	1:B:675:LEU:HD23	1.92	0.52
1:B:1166:ARG:HH21	1:C:1164:HIS:CE1	2.27	0.52
1:D:138:LEU:HD21	1:D:278:ILE:HD11	1.92	0.52
1:D:620:GLU:OE1	1:D:665:ALA:HB3	2.10	0.52
1:A:158:LEU:HD13	1:A:223:PHE:HD2	1.74	0.52
1:A:1130:GLU:HA	1:A:1133:LEU:HG	1.92	0.51
1:D:121:VAL:HB	1:D:155:THR:HG22	1.92	0.51
1:A:1147:ARG:NH2	1:D:1149:LYS:HE3	2.26	0.51
1:B:600:ALA:HB2	1:B:612:ARG:HB2	1.93	0.51
1:C:969:ARG:HB3	1:C:970:PRO:HD3	1.92	0.51
1:C:1130:GLU:HA	1:C:1133:LEU:HG	1.92	0.51
1:D:262:THR:HG21	1:D:398:ARG:HH22	1.75	0.51
1:A:985:VAL:HG21	1:A:1014:GLN:HB3	1.92	0.51
1:C:121:VAL:HB	1:C:155:THR:HG22	1.92	0.51
1:C:620:GLU:OE2	1:C:665:ALA:HB3	2.10	0.51
1:B:102:VAL:O	1:B:105:LEU:HG	2.10	0.51
1:C:105:LEU:HD11	1:C:233:PHE:HZ	1.76	0.51
1:C:426:GLU:O	1:C:430:MET:HG2	2.11	0.51
1:C:455:LEU:HD11	1:C:460:LEU:HD23	1.92	0.51
1:A:262:THR:HG22	1:A:271:ILE:HG12	1.93	0.51
1:A:600:ALA:HB2	1:A:612:ARG:HB2	1.92	0.51
1:A:1166:ARG:HH21	1:B:1164:HIS:CE1	2.29	0.51
1:B:145:ALA:O	1:B:149:THR:HG22	2.11	0.51
1:B:509:MET:C	1:B:509:MET:HE2	2.34	0.51
1:C:627:PHE:CZ	1:C:643:LEU:HD21	2.45	0.51
1:D:426:GLU:O	1:D:430:MET:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1130:GLU:HA	1:D:1133:LEU:HG	1.93	0.51
1:B:451:LEU:HD11	1:B:562:LEU:HD11	1.91	0.51
1:B:608:GLU:O	1:B:612:ARG:HG3	2.11	0.51
1:A:576:MET:C	1:A:576:MET:HE3	2.36	0.50
1:B:561:ASP:O	1:B:564:LEU:HD12	2.11	0.50
1:D:395:ASP:O	1:D:399:LEU:HG	2.11	0.50
1:D:563:LEU:O	1:D:567:LEU:HD22	2.10	0.50
1:B:247:ASN:HB3	1:B:287:ARG:HD3	1.94	0.50
1:C:594:LEU:HB2	1:C:661:ALA:HB2	1.94	0.50
1:D:160:THR:C	1:D:164:ARG:HG2	2.36	0.50
1:C:576:MET:C	1:C:576:MET:HE3	2.36	0.50
1:A:247:ASN:HB3	1:A:287:ARG:HD3	1.94	0.50
1:A:570:ASN:OD1	1:A:612:ARG:HG2	2.12	0.50
1:B:627:PHE:CE1	1:B:643:LEU:HD21	2.47	0.50
1:A:102:VAL:O	1:A:105:LEU:HG	2.12	0.50
1:A:121:VAL:HB	1:A:155:THR:HG22	1.92	0.50
1:C:262:THR:HG21	1:C:398:ARG:HH22	1.77	0.50
1:A:299:LEU:HD21	1:A:364:TYR:HB2	1.92	0.50
1:C:397:LEU:HB3	1:C:413:LEU:HD13	1.94	0.50
1:A:579:TRP:CZ2	1:A:585:ALA:HB1	2.47	0.49
1:B:641:LEU:HB3	1:B:1121:LEU:HD22	1.93	0.49
1:B:1119:ARG:HG2	1:B:1119:ARG:HH11	1.76	0.49
1:C:561:ASP:O	1:C:564:LEU:HD12	2.12	0.49
1:A:395:ASP:O	1:A:399:LEU:HG	2.12	0.49
1:B:164:ARG:O	1:B:168:VAL:HG13	2.12	0.49
1:B:262:THR:HG21	1:B:398:ARG:HH22	1.77	0.49
1:B:262:THR:HG22	1:B:271:ILE:HG12	1.94	0.49
1:C:395:ASP:O	1:C:399:LEU:HG	2.12	0.49
1:D:451:LEU:HD11	1:D:562:LEU:HD11	1.94	0.49
1:C:118:VAL:HB	1:C:273:VAL:HG22	1.94	0.49
1:B:455:LEU:HD11	1:B:460:LEU:HD23	1.95	0.49
1:A:608:GLU:O	1:A:612:ARG:HG3	2.12	0.49
1:D:145:ALA:O	1:D:149:THR:HG22	2.12	0.49
1:B:567:LEU:HD12	1:B:596:LEU:HD11	1.95	0.49
1:C:102:VAL:O	1:C:105:LEU:HG	2.12	0.49
1:A:262:THR:HG21	1:A:398:ARG:HH22	1.78	0.49
1:B:174:GLN:NE2	1:B:175:MET:HE3	2.28	0.49
1:B:99:PRO:HG2	1:B:256:TYR:CD1	2.48	0.49
1:B:564:LEU:O	1:B:568:LEU:HG	2.12	0.49
1:D:608:GLU:O	1:D:612:ARG:HG3	2.13	0.49
1:A:99:PRO:HG2	1:A:256:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:LEU:HD12	1:C:596:LEU:HD11	1.95	0.49
1:C:990:HIS:HA	1:C:1001:ALA:HA	1.95	0.49
1:D:442:ARG:HH21	1:D:573:GLN:NE2	2.10	0.49
1:A:442:ARG:HH21	1:A:573:GLN:NE2	2.10	0.49
1:A:642:LEU:HD23	1:A:1121:LEU:HD21	1.95	0.49
1:C:168:VAL:HG12	1:C:171:ARG:NH1	2.28	0.49
1:C:262:THR:HG22	1:C:271:ILE:HG12	1.94	0.49
1:D:102:VAL:O	1:D:105:LEU:HG	2.13	0.48
1:A:138:LEU:HD21	1:A:278:ILE:HD11	1.95	0.48
1:B:397:LEU:HB3	1:B:413:LEU:HD13	1.95	0.48
1:B:620:GLU:OE2	1:B:665:ALA:HB3	2.12	0.48
1:C:567:LEU:HD12	1:C:596:LEU:HD21	1.94	0.48
1:D:136:ASP:O	1:D:140:ARG:HG3	2.14	0.48
1:C:608:GLU:O	1:C:612:ARG:HG3	2.13	0.48
1:B:12:PRO:HD2	1:B:13:LYS:NZ	2.27	0.48
1:C:1133:LEU:HD12	1:C:1134:LEU:N	2.28	0.48
1:D:805:PHE:CZ	1:D:882:ARG:HG3	2.49	0.48
1:A:620:GLU:OE1	1:A:665:ALA:HB3	2.13	0.48
1:A:910:PHE:HB2	1:A:920:ILE:HD11	1.96	0.48
1:C:805:PHE:CZ	1:C:882:ARG:HG3	2.49	0.48
1:D:272:PRO:HD3	1:D:395:ASP:HB2	1.95	0.48
1:D:393:TYR:HA	1:D:396:GLU:OE1	2.13	0.48
1:C:576:MET:HE3	1:C:577:TYR:N	2.29	0.48
1:D:262:THR:HG22	1:D:271:ILE:HG12	1.96	0.48
1:B:168:VAL:HB	1:B:171:ARG:CZ	2.43	0.48
1:B:395:ASP:O	1:B:399:LEU:HG	2.13	0.48
1:C:188:VAL:HG21	1:C:250:ARG:HD3	1.96	0.48
1:A:118:VAL:HB	1:A:273:VAL:HG22	1.95	0.48
1:B:118:VAL:HB	1:B:273:VAL:HG22	1.96	0.48
1:B:433:LEU:HD13	1:B:565:TRP:HZ3	1.78	0.48
1:C:99:PRO:HG2	1:C:256:TYR:CD2	2.49	0.48
1:A:397:LEU:HB3	1:A:413:LEU:HD13	1.96	0.47
1:C:247:ASN:HB3	1:C:287:ARG:HD3	1.96	0.47
1:B:1148:LEU:HA	1:B:1151:THR:HG22	1.96	0.47
1:D:247:ASN:HB3	1:D:287:ARG:HD3	1.96	0.47
1:C:299:LEU:HD11	1:C:376:ILE:HG22	1.97	0.47
1:B:427:ALA:HA	1:B:430:MET:HG3	1.97	0.47
1:C:442:ARG:HH21	1:C:573:GLN:NE2	2.12	0.47
1:D:570:ASN:OD1	1:D:612:ARG:HG2	2.14	0.47
1:A:1162:LEU:HA	1:A:1165:ILE:HD12	1.96	0.47
1:D:118:VAL:HB	1:D:273:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:MET:HE3	1:A:577:TYR:N	2.29	0.47
1:B:437:ARG:O	1:B:441:VAL:HG12	2.14	0.47
1:C:1038:LEU:O	1:C:1042:MET:HG3	2.15	0.47
1:A:624:VAL:HG22	1:A:666:PHE:HA	1.97	0.47
1:A:805:PHE:CZ	1:A:882:ARG:HG3	2.50	0.47
1:C:562:LEU:HB3	1:C:578:PHE:CE2	2.49	0.47
1:C:563:LEU:HD13	1:C:567:LEU:CD2	2.45	0.47
1:D:1148:LEU:HA	1:D:1151:THR:HG22	1.96	0.47
1:B:563:LEU:HD13	1:B:567:LEU:CD2	2.45	0.47
1:C:299:LEU:HD21	1:C:364:TYR:HB2	1.96	0.47
1:B:168:VAL:HA	1:B:171:ARG:CG	2.41	0.47
1:B:191:TRP:HB3	1:B:236:ASP:HA	1.97	0.47
1:B:570:ASN:OD1	1:B:612:ARG:HG2	2.14	0.47
1:D:437:ARG:O	1:D:441:VAL:HG12	2.15	0.47
1:D:509:MET:C	1:D:509:MET:HE2	2.40	0.47
1:B:1149:LYS:HA	1:C:1147:ARG:HH12	1.80	0.47
1:A:171:ARG:O	1:A:174:GLN:HG3	2.16	0.46
1:B:442:ARG:HH21	1:B:573:GLN:HE22	1.61	0.46
1:B:463:LEU:HD13	1:B:565:TRP:CZ3	2.49	0.46
1:C:186:MET:HE1	1:C:188:VAL:HG13	1.98	0.46
1:C:855:ARG:HA	1:C:858:LEU:HG	1.97	0.46
1:D:561:ASP:O	1:D:564:LEU:HD12	2.15	0.46
1:D:969:ARG:HB3	1:D:970:PRO:HD3	1.97	0.46
1:A:299:LEU:HD11	1:A:376:ILE:HG22	1.97	0.46
1:A:427:ALA:HA	1:A:430:MET:HG3	1.98	0.46
1:B:138:LEU:HD21	1:B:278:ILE:HD11	1.97	0.46
1:C:436:ASP:C	1:C:437:ARG:HD2	2.41	0.46
1:C:598:VAL:O	1:C:601:ARG:HG2	2.16	0.46
1:A:509:MET:C	1:A:509:MET:HE2	2.40	0.46
1:B:473:ILE:HD13	1:B:568:LEU:HB3	1.97	0.46
1:C:191:TRP:HB3	1:C:236:ASP:HA	1.98	0.46
1:B:299:LEU:HD21	1:B:364:TYR:HB2	1.95	0.46
1:C:1148:LEU:HA	1:C:1151:THR:HG22	1.97	0.46
1:B:805:PHE:CZ	1:B:882:ARG:HG3	2.51	0.46
1:B:969:ARG:HB3	1:B:970:PRO:HD3	1.97	0.46
1:D:441:VAL:HG11	1:D:574:MET:SD	2.56	0.46
1:B:442:ARG:HH21	1:B:573:GLN:NE2	2.14	0.46
1:C:352:GLU:O	1:C:355:MET:HG2	2.16	0.46
1:A:374:GLU:HB2	1:A:405:ARG:NH1	2.31	0.46
1:B:106:VAL:HG13	1:B:112:PHE:HD2	1.80	0.46
1:D:168:VAL:HG12	1:D:171:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1119:ARG:HH22	1:D:1120:LYS:HE3	1.81	0.46
1:A:437:ARG:HD2	1:A:437:ARG:N	2.30	0.46
1:C:642:LEU:HD23	1:C:642:LEU:HA	1.75	0.46
1:D:99:PRO:HG2	1:D:256:TYR:CD2	2.49	0.46
1:C:570:ASN:OD1	1:C:612:ARG:HG2	2.15	0.46
1:D:598:VAL:O	1:D:601:ARG:HG2	2.16	0.46
1:D:642:LEU:HD23	1:D:1121:LEU:HD21	1.98	0.46
1:C:160:THR:C	1:C:164:ARG:HG2	2.41	0.45
1:D:106:VAL:HG13	1:D:112:PHE:HD2	1.81	0.45
1:A:451:LEU:HD11	1:A:562:LEU:HD11	1.98	0.45
1:B:562:LEU:HB3	1:B:578:PHE:CE2	2.51	0.45
1:A:969:ARG:HB3	1:A:970:PRO:HD3	1.97	0.45
1:A:641:LEU:HB3	1:A:1121:LEU:HD22	1.98	0.45
1:D:570:ASN:HD21	1:D:611:ARG:HD2	1.81	0.45
1:D:675:LEU:O	1:D:679:LYS:HG2	2.17	0.45
1:A:106:VAL:HG13	1:A:112:PHE:HD2	1.80	0.45
1:A:642:LEU:HD23	1:A:642:LEU:HA	1.75	0.45
1:A:675:LEU:O	1:A:679:LYS:HG2	2.17	0.45
1:A:1149:LYS:HZ3	1:B:1147:ARG:HH22	1.64	0.45
1:C:256:TYR:CD1	1:C:256:TYR:N	2.85	0.45
1:D:311:LEU:H	1:D:311:LEU:HD22	1.82	0.45
1:D:1077:PRO:N	1:D:1078:PRO:HD2	2.31	0.45
1:A:374:GLU:HB2	1:A:405:ARG:HH12	1.82	0.45
1:A:1077:PRO:N	1:A:1078:PRO:HD2	2.32	0.45
1:A:1148:LEU:HA	1:A:1151:THR:HG22	1.98	0.45
1:B:459:ARG:O	1:B:463:LEU:HG	2.16	0.45
1:B:675:LEU:O	1:B:679:LYS:HG2	2.16	0.45
1:C:451:LEU:HD11	1:C:562:LEU:HD11	1.97	0.45
1:B:11:ILE:HB	1:B:12:PRO:HD3	1.99	0.45
1:C:1077:PRO:N	1:C:1078:PRO:HD2	2.31	0.45
1:D:509:MET:HE1	1:D:510:LEU:HD23	1.99	0.45
1:B:93:LEU:HD12	1:B:97:THR:HG21	1.99	0.44
1:B:598:VAL:O	1:B:601:ARG:HG2	2.17	0.44
1:C:675:LEU:O	1:C:679:LYS:HG2	2.16	0.44
1:A:1149:LYS:HE2	1:A:1149:LYS:HB2	1.79	0.44
1:D:563:LEU:HD13	1:D:567:LEU:HD21	1.97	0.44
1:D:1133:LEU:HD12	1:D:1134:LEU:N	2.33	0.44
1:C:106:VAL:HG13	1:C:112:PHE:HD2	1.81	0.44
1:D:299:LEU:HD21	1:D:364:TYR:HB2	1.98	0.44
1:D:641:LEU:HB3	1:D:1121:LEU:HD22	1.98	0.44
1:A:565:TRP:NE1	1:A:569:LEU:HD22	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:LEU:HD12	1:B:877:LEU:HA	1.84	0.44
1:C:437:ARG:HD2	1:C:437:ARG:N	2.31	0.44
1:D:299:LEU:HD11	1:D:376:ILE:HG22	1.99	0.44
1:D:702:LEU:HD12	1:D:702:LEU:HA	1.76	0.44
1:D:766:ARG:HG3	1:D:768:CYS:H	1.82	0.44
1:B:299:LEU:HD13	1:B:373:PHE:HE2	1.83	0.44
1:C:311:LEU:HD22	1:C:311:LEU:H	1.82	0.44
1:D:432:ALA:HA	1:D:437:ARG:HG2	1.99	0.44
1:D:1141:ARG:NH1	1:D:1150:ARG:HH12	2.16	0.44
1:A:459:ARG:O	1:A:463:LEU:HG	2.17	0.44
1:A:766:ARG:HG3	1:A:768:CYS:H	1.83	0.44
1:B:1119:ARG:HG2	1:B:1119:ARG:NH1	2.31	0.44
1:C:642:LEU:HD23	1:C:1121:LEU:HD21	2.00	0.44
1:C:18:LYS:HD2	1:C:237:ASP:HA	1.99	0.44
1:C:624:VAL:HG22	1:C:666:PHE:HA	2.00	0.44
1:D:140:ARG:O	1:D:144:ARG:HB2	2.17	0.44
1:B:624:VAL:HG22	1:B:666:PHE:HA	1.98	0.44
1:B:890:LEU:O	1:B:894:VAL:HG12	2.18	0.44
1:B:910:PHE:HB2	1:B:920:ILE:HD11	1.99	0.44
1:B:1077:PRO:N	1:B:1078:PRO:HD2	2.32	0.44
1:B:437:ARG:HD2	1:B:437:ARG:N	2.32	0.44
1:A:629:GLU:C	1:A:629:GLU:OE1	2.61	0.43
1:B:225:LEU:HB3	1:B:232:PHE:CE2	2.53	0.43
1:C:641:LEU:HB3	1:C:1121:LEU:HD22	2.00	0.43
1:A:890:LEU:O	1:A:894:VAL:HG12	2.18	0.43
1:C:457:PRO:O	1:C:460:LEU:HD12	2.18	0.43
1:A:565:TRP:CD1	1:A:569:LEU:HD13	2.53	0.43
1:A:598:VAL:O	1:A:601:ARG:HG2	2.17	0.43
1:C:158:LEU:HD13	1:C:223:PHE:HD2	1.83	0.43
1:C:707:LEU:HD23	1:C:707:LEU:HA	1.82	0.43
1:D:256:TYR:N	1:D:256:TYR:CD1	2.84	0.43
1:D:437:ARG:HD2	1:D:437:ARG:N	2.32	0.43
1:B:436:ASP:C	1:B:437:ARG:HD2	2.43	0.43
1:B:507:LEU:HD12	1:B:508:ARG:N	2.34	0.43
1:C:432:ALA:HA	1:C:437:ARG:HG2	1.99	0.43
1:D:18:LYS:HD2	1:D:237:ASP:HA	2.00	0.43
1:D:425:LEU:O	1:D:429:LEU:HD12	2.18	0.43
1:D:565:TRP:CD1	1:D:569:LEU:HD13	2.53	0.43
1:A:433:LEU:HD13	1:A:565:TRP:HZ3	1.83	0.43
1:C:509:MET:HE2	1:C:509:MET:C	2.43	0.43
1:C:669:GLN:HG3	1:C:672:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:TYR:HB2	1:D:232:PHE:CZ	2.54	0.43
1:D:653:THR:HG22	1:D:655:LEU:N	2.32	0.43
1:A:272:PRO:HD3	1:A:395:ASP:HB2	2.01	0.43
1:D:352:GLU:HA	1:D:355:MET:SD	2.59	0.43
1:A:311:LEU:HD22	1:A:311:LEU:H	1.82	0.43
1:B:643:LEU:O	1:B:653:THR:HG23	2.19	0.43
1:C:272:PRO:HD3	1:C:395:ASP:HB2	2.00	0.43
1:C:629:GLU:C	1:C:629:GLU:OE1	2.62	0.43
1:D:457:PRO:HA	1:D:460:LEU:HG	2.01	0.43
1:A:1164:HIS:CD2	1:D:1166:ARG:HH21	2.37	0.43
1:B:44:HIS:CD2	1:B:45:PRO:HD2	2.54	0.43
1:B:433:LEU:HD13	1:B:565:TRP:CZ3	2.53	0.43
1:B:472:LEU:HD11	1:B:602:LEU:HD23	2.01	0.43
1:D:869:LEU:HD12	1:D:869:LEU:HA	1.87	0.43
1:D:890:LEU:O	1:D:894:VAL:HG12	2.19	0.43
1:A:18:LYS:HD2	1:A:237:ASP:HA	2.00	0.42
1:A:44:HIS:CD2	1:A:45:PRO:HD2	2.54	0.42
1:B:629:GLU:OE1	1:B:629:GLU:C	2.61	0.42
1:C:425:LEU:O	1:C:429:LEU:HD12	2.19	0.42
1:D:707:LEU:HD23	1:D:707:LEU:HA	1.84	0.42
1:A:168:VAL:HG12	1:A:171:ARG:NH1	2.33	0.42
1:A:472:LEU:HD11	1:A:602:LEU:HD23	2.01	0.42
1:B:272:PRO:HD3	1:B:395:ASP:HB2	2.01	0.42
1:D:225:LEU:HB3	1:D:232:PHE:CE2	2.54	0.42
1:D:563:LEU:HD13	1:D:567:LEU:CD2	2.49	0.42
1:A:864:TRP:HB3	1:A:905:ARG:NH1	2.34	0.42
1:B:670:ASP:OD1	1:B:670:ASP:N	2.53	0.42
1:C:1149:LYS:HD3	1:D:1147:ARG:NH1	2.31	0.42
1:C:1162:LEU:HA	1:C:1165:ILE:HD12	2.01	0.42
1:D:642:LEU:HG	1:D:1121:LEU:HD11	2.01	0.42
1:D:664:ARG:HH11	1:D:664:ARG:HG2	1.84	0.42
1:D:989:GLU:HG2	1:D:990:HIS:N	2.33	0.42
1:A:176:ALA:HA	1:B:1124:TRP:HD1	1.85	0.42
1:A:256:TYR:N	1:A:256:TYR:CD2	2.87	0.42
1:A:631:TYR:CZ	1:A:635:GLU:HG2	2.54	0.42
1:C:766:ARG:NE	1:C:767:ARG:H	2.16	0.42
1:C:819:PHE:O	1:C:823:THR:HG23	2.19	0.42
1:C:910:PHE:HB2	1:C:920:ILE:HD11	2.01	0.42
1:C:1049:LYS:HB3	1:C:1049:LYS:HE3	1.80	0.42
1:A:1079:PHE:O	1:A:1082:ILE:HG22	2.20	0.42
1:A:1147:ARG:HH22	1:D:1149:LYS:HE3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:ARG:HG3	1:B:768:CYS:H	1.84	0.42
1:C:307:ALA:HA	1:C:337:ARG:HD2	2.00	0.42
1:D:642:LEU:HD23	1:D:642:LEU:HA	1.76	0.42
1:D:669:GLN:HG3	1:D:672:VAL:HG23	2.01	0.42
1:B:256:TYR:N	1:B:256:TYR:CD2	2.87	0.42
1:C:229:TYR:HB2	1:C:232:PHE:CZ	2.54	0.42
1:C:429:LEU:HD13	1:C:454:PHE:HE2	1.84	0.42
1:D:140:ARG:HH12	1:D:144:ARG:NH1	2.18	0.42
1:D:461:ALA:HA	1:D:501:PRO:HG3	2.01	0.42
1:A:225:LEU:HB3	1:A:232:PHE:CE2	2.55	0.42
1:B:625:ASP:OD2	1:B:625:ASP:C	2.62	0.42
1:B:859:TYR:CD2	1:B:860:LEU:HD12	2.55	0.42
1:C:44:HIS:CD2	1:C:45:PRO:HD2	2.54	0.42
1:C:625:ASP:OD1	1:C:625:ASP:C	2.63	0.42
1:A:1124:TRP:HD1	1:D:176:ALA:HA	1.84	0.42
1:A:1136:ARG:HH11	1:A:1136:ARG:HG3	1.84	0.42
1:B:872:LEU:HD23	1:B:872:LEU:HA	1.89	0.42
1:C:426:GLU:HA	1:C:454:PHE:CZ	2.54	0.42
1:C:704:TYR:CE2	1:C:771:ARG:HD3	2.55	0.42
1:C:852:LEU:HA	1:C:855:ARG:NE	2.35	0.42
1:D:333:ASP:O	1:D:337:ARG:HB2	2.20	0.42
1:D:427:ALA:HA	1:D:430:MET:HG2	2.01	0.42
1:D:1116:GLU:O	1:D:1119:ARG:HG3	2.20	0.42
1:B:580:GLU:OE1	1:B:580:GLU:C	2.63	0.42
1:C:570:ASN:HD21	1:C:611:ARG:HD2	1.85	0.42
1:C:959:PHE:HB3	1:C:960:PRO:HD3	2.02	0.42
1:C:1141:ARG:NH1	1:C:1150:ARG:HH12	2.14	0.42
1:D:394:LEU:HA	1:D:397:LEU:HD23	2.01	0.42
1:D:852:LEU:HA	1:D:855:ARG:NE	2.35	0.42
1:A:1141:ARG:NH1	1:A:1150:ARG:HH12	2.17	0.42
1:B:855:ARG:HA	1:B:858:LEU:HG	2.02	0.42
1:C:171:ARG:O	1:C:174:GLN:HG3	2.20	0.42
1:D:624:VAL:HG22	1:D:666:PHE:HA	2.01	0.42
1:A:433:LEU:HD13	1:A:565:TRP:CZ3	2.55	0.41
1:A:694:VAL:HB	1:A:784:MET:HE1	2.01	0.41
1:D:44:HIS:CD2	1:D:45:PRO:HD2	2.55	0.41
1:D:91:LEU:HD13	1:D:110:TRP:HZ2	1.85	0.41
1:A:563:LEU:HD13	1:A:567:LEU:CD2	2.50	0.41
1:A:622:MET:SD	1:A:622:MET:C	3.03	0.41
1:A:1133:LEU:HD12	1:A:1134:LEU:N	2.35	0.41
1:A:1147:ARG:HH12	1:D:1149:LYS:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:PRO:HB2	1:B:503:VAL:HG13	2.02	0.41
1:B:864:TRP:HB3	1:B:905:ARG:NH1	2.35	0.41
1:D:140:ARG:HB3	1:D:140:ARG:CZ	2.50	0.41
1:D:430:MET:O	1:D:434:LEU:HG	2.20	0.41
1:D:819:PHE:O	1:D:823:THR:HG23	2.20	0.41
1:D:910:PHE:HB2	1:D:920:ILE:HD11	2.02	0.41
1:A:229:TYR:HB2	1:A:232:PHE:CZ	2.55	0.41
1:A:430:MET:O	1:A:434:LEU:HG	2.20	0.41
1:A:562:LEU:HB3	1:A:578:PHE:CE2	2.56	0.41
1:A:580:GLU:C	1:A:580:GLU:OE1	2.63	0.41
1:A:669:GLN:HG3	1:A:672:VAL:HG23	2.03	0.41
1:C:225:LEU:HB3	1:C:232:PHE:CE2	2.55	0.41
1:D:436:ASP:C	1:D:437:ARG:HD2	2.46	0.41
1:D:859:TYR:CD2	1:D:860:LEU:HD12	2.56	0.41
1:B:9:SER:O	1:B:13:LYS:HE3	2.20	0.41
1:C:670:ASP:OD1	1:C:670:ASP:N	2.52	0.41
1:D:1162:LEU:HA	1:D:1165:ILE:HD12	2.03	0.41
1:A:106:VAL:O	1:A:112:PHE:HB2	2.21	0.41
1:B:140:ARG:O	1:B:144:ARG:HB2	2.20	0.41
1:B:653:THR:HG22	1:B:655:LEU:N	2.33	0.41
1:C:91:LEU:HD13	1:C:110:TRP:HZ2	1.85	0.41
1:A:299:LEU:HD13	1:A:373:PHE:HE1	1.86	0.41
1:A:436:ASP:C	1:A:437:ARG:HD2	2.46	0.41
1:C:393:TYR:HA	1:C:396:GLU:OE1	2.21	0.41
1:C:472:LEU:CD2	1:C:603:GLU:HG3	2.47	0.41
1:C:864:TRP:HB3	1:C:905:ARG:NH1	2.36	0.41
1:D:352:GLU:O	1:D:355:MET:HG2	2.20	0.41
1:D:690:ILE:O	1:D:694:VAL:HG12	2.20	0.41
1:A:140:ARG:O	1:A:144:ARG:HB2	2.20	0.41
1:A:457:PRO:HA	1:A:460:LEU:HG	2.03	0.41
1:A:855:ARG:HA	1:A:858:LEU:HG	2.03	0.41
1:D:191:TRP:HB3	1:D:236:ASP:HA	2.02	0.41
1:D:670:ASP:OD1	1:D:670:ASP:N	2.51	0.41
1:A:432:ALA:HA	1:A:437:ARG:HG2	2.02	0.41
1:A:684:MET:HE2	1:A:684:MET:HB2	1.87	0.41
1:A:1119:ARG:CZ	1:A:1119:ARG:HB3	2.49	0.41
1:B:92:ARG:HB2	1:B:234:LEU:HD12	2.02	0.41
1:B:131:GLN:HB3	1:B:133:TRP:CD1	2.56	0.41
1:C:138:LEU:HD21	1:C:166:VAL:HG12	2.02	0.41
1:C:140:ARG:O	1:C:144:ARG:HB2	2.20	0.41
1:C:160:THR:HA	1:C:164:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:THR:HG22	1:C:655:LEU:N	2.32	0.41
1:D:625:ASP:OD2	1:D:625:ASP:C	2.63	0.41
1:A:131:GLN:HB3	1:A:133:TRP:CD1	2.55	0.41
1:A:333:ASP:O	1:A:337:ARG:HB2	2.20	0.41
1:A:823:THR:HG22	1:A:1080:ILE:HG22	2.02	0.41
1:B:393:TYR:HA	1:B:396:GLU:OE1	2.21	0.41
1:B:669:GLN:HG3	1:B:672:VAL:HG23	2.02	0.41
1:B:1147:ARG:HG2	1:B:1147:ARG:HH11	1.86	0.41
1:C:310:CYS:HB2	1:C:336:ARG:HB3	2.03	0.41
1:C:507:LEU:O	1:C:511:LEU:HG	2.20	0.41
1:C:890:LEU:O	1:C:894:VAL:HG12	2.20	0.41
1:D:507:LEU:O	1:D:511:LEU:HG	2.20	0.41
1:D:569:LEU:HB3	1:D:571:ARG:HE	1.86	0.41
1:D:959:PHE:HB3	1:D:960:PRO:HD3	2.02	0.41
1:A:300:LEU:HD22	1:A:301:VAL:H	1.86	0.41
1:A:569:LEU:HD23	1:A:571:ARG:HH21	1.86	0.41
1:A:859:TYR:CD2	1:A:860:LEU:HD12	2.56	0.41
1:B:352:GLU:O	1:B:355:MET:HG2	2.21	0.41
1:C:333:ASP:O	1:C:337:ARG:HB2	2.21	0.41
1:C:427:ALA:HA	1:C:430:MET:HG2	2.02	0.41
1:B:457:PRO:HA	1:B:460:LEU:HG	2.03	0.40
1:C:106:VAL:O	1:C:112:PHE:HB2	2.21	0.40
1:C:565:TRP:NE1	1:C:569:LEU:HD22	2.35	0.40
1:C:600:ALA:HB2	1:C:612:ARG:HB2	2.03	0.40
1:C:608:GLU:HA	1:C:611:ARG:NH1	2.36	0.40
1:C:981:GLU:OE1	1:C:981:GLU:C	2.64	0.40
1:D:164:ARG:O	1:D:168:VAL:HG13	2.20	0.40
1:D:277:LEU:HB3	1:D:300:LEU:HD23	2.03	0.40
1:D:300:LEU:HD22	1:D:301:VAL:H	1.85	0.40
1:A:91:LEU:HD13	1:A:110:TRP:HZ2	1.86	0.40
1:A:393:TYR:HA	1:A:396:GLU:OE1	2.20	0.40
1:A:989:GLU:HG2	1:A:990:HIS:N	2.36	0.40
1:B:311:LEU:H	1:B:311:LEU:HD22	1.85	0.40
1:B:576:MET:HE3	1:B:577:TYR:N	2.35	0.40
1:B:707:LEU:HA	1:B:707:LEU:HD23	1.82	0.40
1:B:959:PHE:HB3	1:B:960:PRO:HD3	2.02	0.40
1:C:164:ARG:O	1:C:168:VAL:HG13	2.20	0.40
1:D:106:VAL:O	1:D:112:PHE:HB2	2.21	0.40
1:D:442:ARG:HH21	1:D:573:GLN:HE22	1.69	0.40
1:A:876:LEU:HD12	1:A:876:LEU:HA	1.82	0.40
1:A:981:GLU:C	1:A:981:GLU:OE1	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:TRP:CD1	1:B:569:LEU:HD13	2.57	0.40
1:B:690:ILE:O	1:B:694:VAL:HG12	2.22	0.40
1:B:1141:ARG:NH1	1:B:1150:ARG:HH12	2.17	0.40
1:A:405:ARG:N	1:A:405:ARG:HE	2.19	0.40
1:B:235:VAL:HG21	1:B:246:GLU:HB2	2.04	0.40
1:D:600:ALA:HB2	1:D:612:ARG:HB2	2.03	0.40
1:C:563:LEU:O	1:C:567:LEU:HD22	2.22	0.40
1:D:337:ARG:HE	1:D:337:ARG:HB3	1.70	0.40
1:D:855:ARG:HA	1:D:858:LEU:HG	2.03	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	975/1214 (80%)	942 (97%)	33 (3%)	0	100	100
1	B	975/1214 (80%)	943 (97%)	32 (3%)	0	100	100
1	C	975/1214 (80%)	948 (97%)	27 (3%)	0	100	100
1	D	975/1214 (80%)	943 (97%)	32 (3%)	0	100	100
All	All	3900/4856 (80%)	3776 (97%)	124 (3%)	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	743/1000 (74%)	739 (100%)	4 (0%)	81 89
1	B	743/1000 (74%)	735 (99%)	8 (1%)	65 83
1	C	743/1000 (74%)	736 (99%)	7 (1%)	70 85
1	D	743/1000 (74%)	738 (99%)	5 (1%)	76 86
All	All	2972/4000 (74%)	2948 (99%)	24 (1%)	70 86

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	138	LEU
1	A	361	LEU
1	A	686	SER
1	B	93	LEU
1	B	138	LEU
1	B	361	LEU
1	B	636	VAL
1	B	877	LEU
1	B	989	GLU
1	B	1083	SER
1	B	1087	LEU
1	C	137	LEU
1	C	429	LEU
1	C	659	MET
1	C	804	ASP
1	C	1083	SER
1	C	1085	LEU
1	C	1087	LEU
1	D	137	LEU
1	D	429	LEU
1	D	659	MET
1	D	686	SER
1	D	1083	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	293	GLN
1	A	350	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	447	HIS
1	A	475	ASN
1	A	806	GLN
1	A	1007	GLN
1	A	1014	GLN
1	A	1017	ASN
1	A	1032	ASN
1	B	44	HIS
1	B	293	GLN
1	B	350	GLN
1	B	475	ASN
1	B	774	HIS
1	B	806	GLN
1	B	1014	GLN
1	B	1017	ASN
1	C	44	HIS
1	C	350	GLN
1	C	447	HIS
1	C	806	GLN
1	C	980	GLN
1	C	1007	GLN
1	C	1014	GLN
1	D	44	HIS
1	D	350	GLN
1	D	447	HIS
1	D	475	ASN
1	D	806	GLN
1	D	1007	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

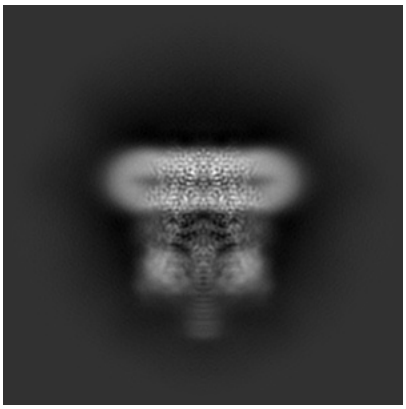
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-57866. These allow visual inspection of the internal detail of the map and identification of artifacts.

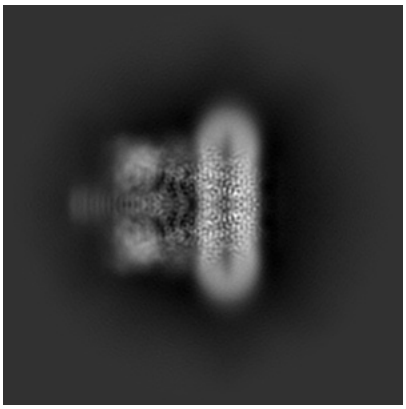
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

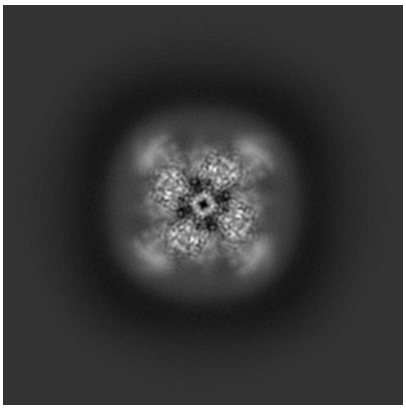
6.1.1 Primary map



X

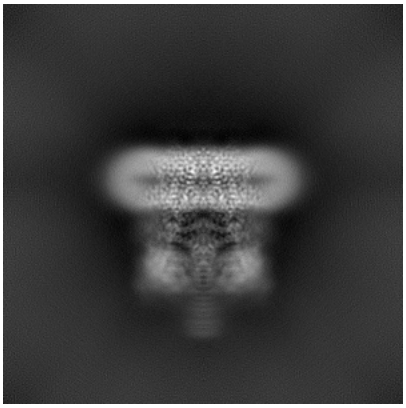


Y

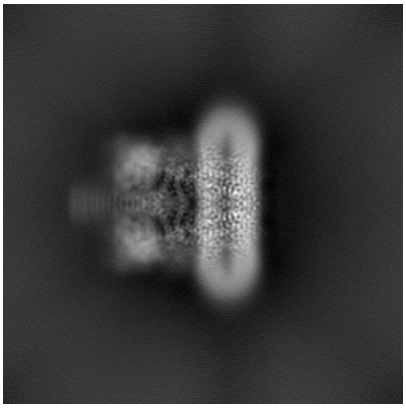


Z

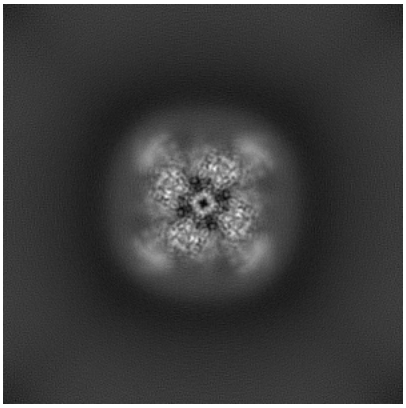
6.1.2 Raw map



X



Y

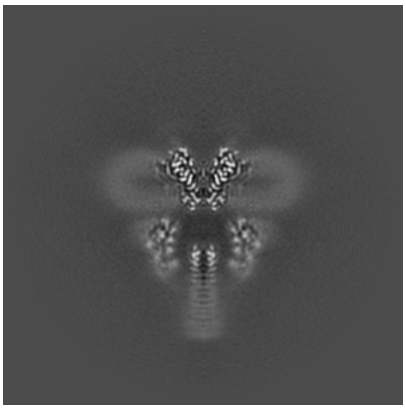


Z

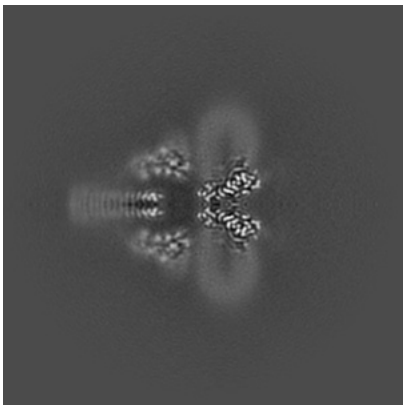
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

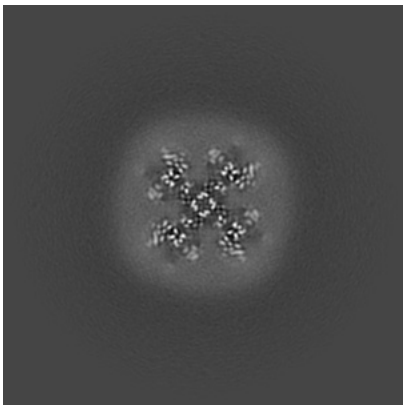
6.2.1 Primary map



X Index: 200

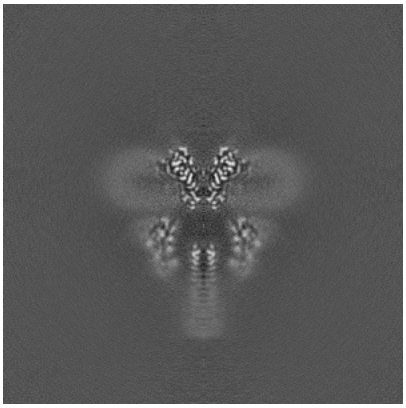


Y Index: 200

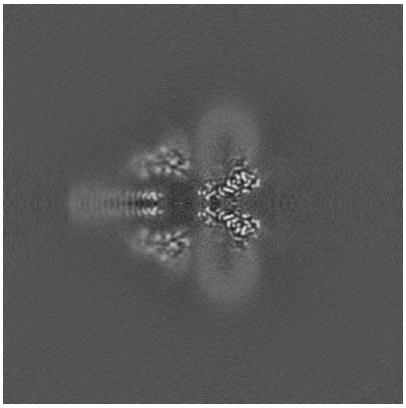


Z Index: 200

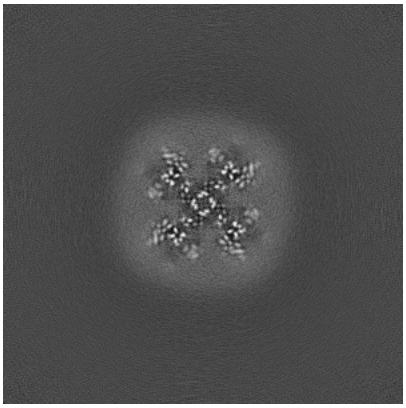
6.2.2 Raw map



X Index: 200



Y Index: 200

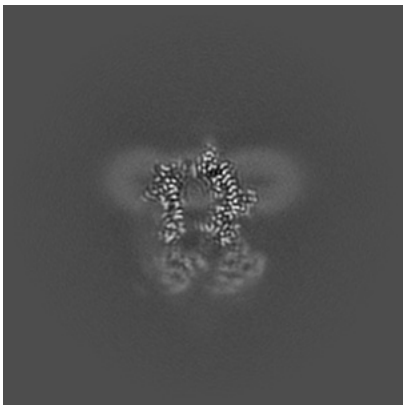


Z Index: 200

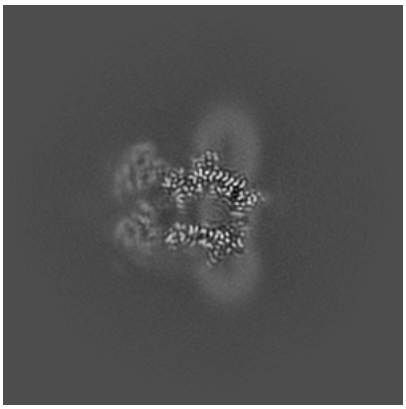
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

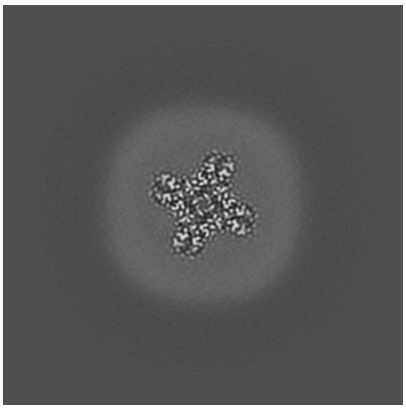
6.3.1 Primary map



X Index: 172

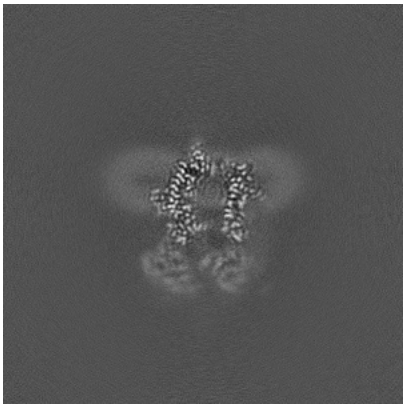


Y Index: 228

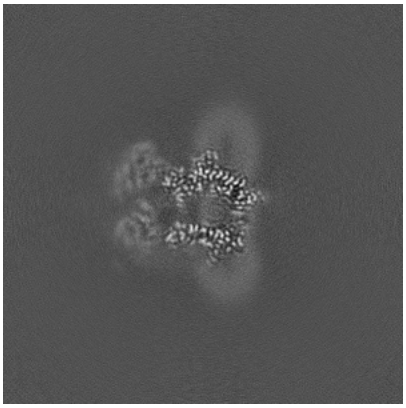


Z Index: 236

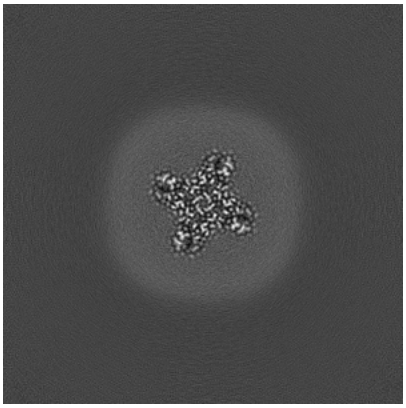
6.3.2 Raw map



X Index: 228



Y Index: 228

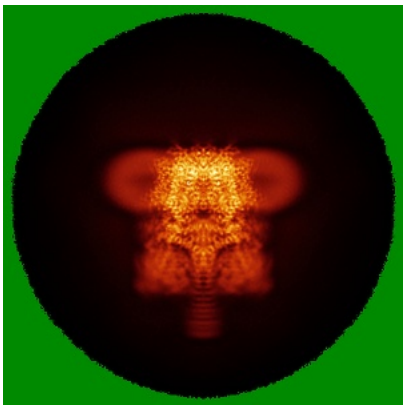


Z Index: 235

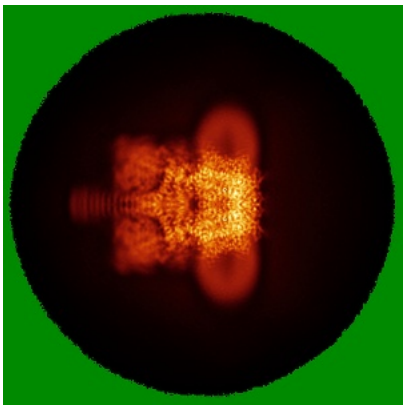
The images above show the largest variance slices of the map in three orthogonal directions.

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

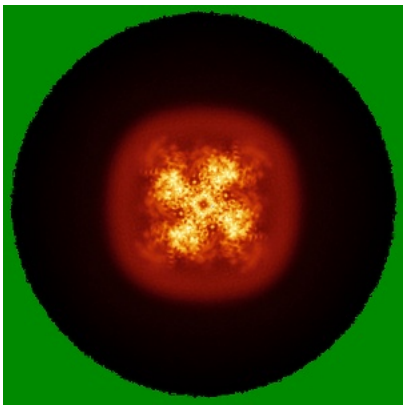
6.4.1 Primary map



X

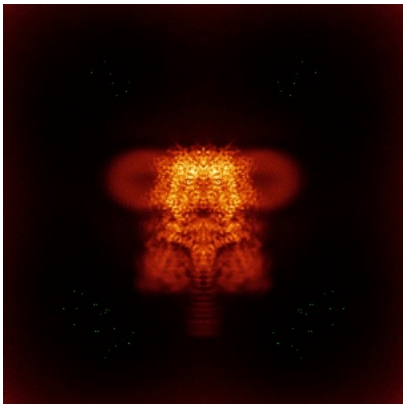


Y

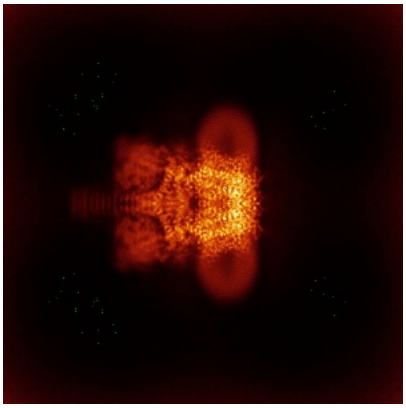


Z

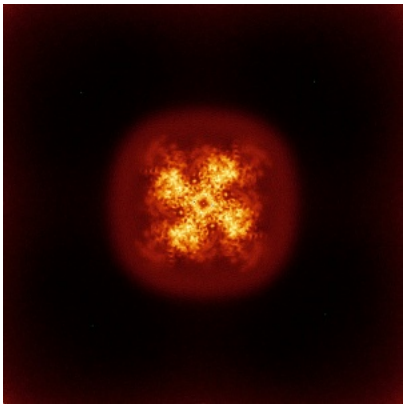
6.4.2 Raw map



X



Y

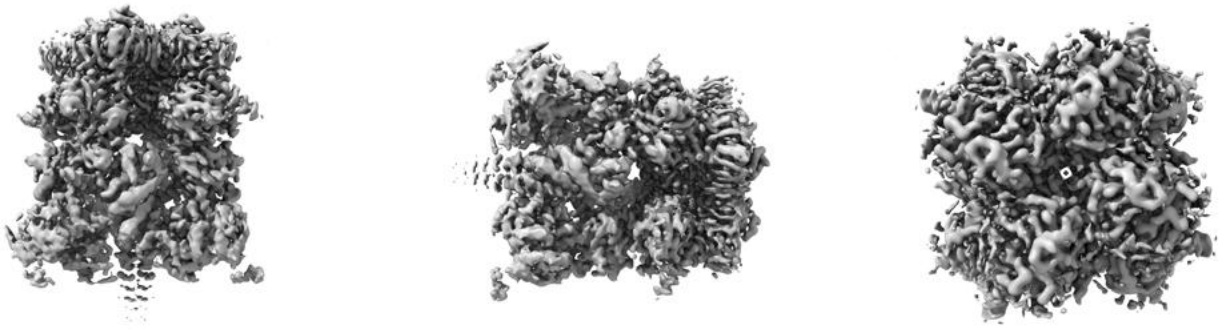


Z

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)

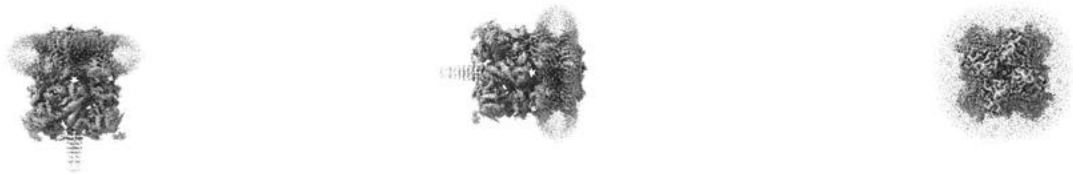
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

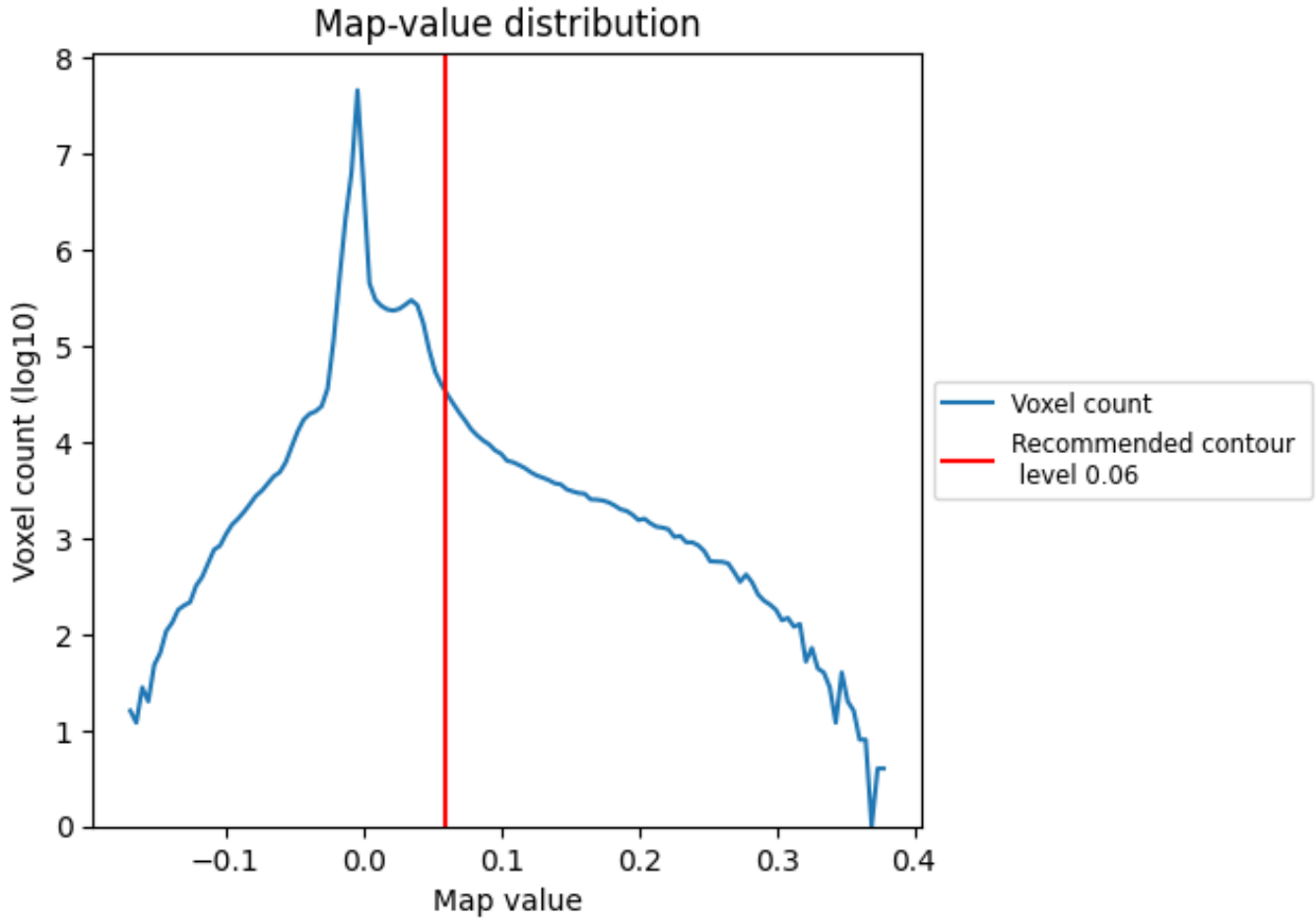
6.6 Mask visualisation (i)

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

7 Map analysis

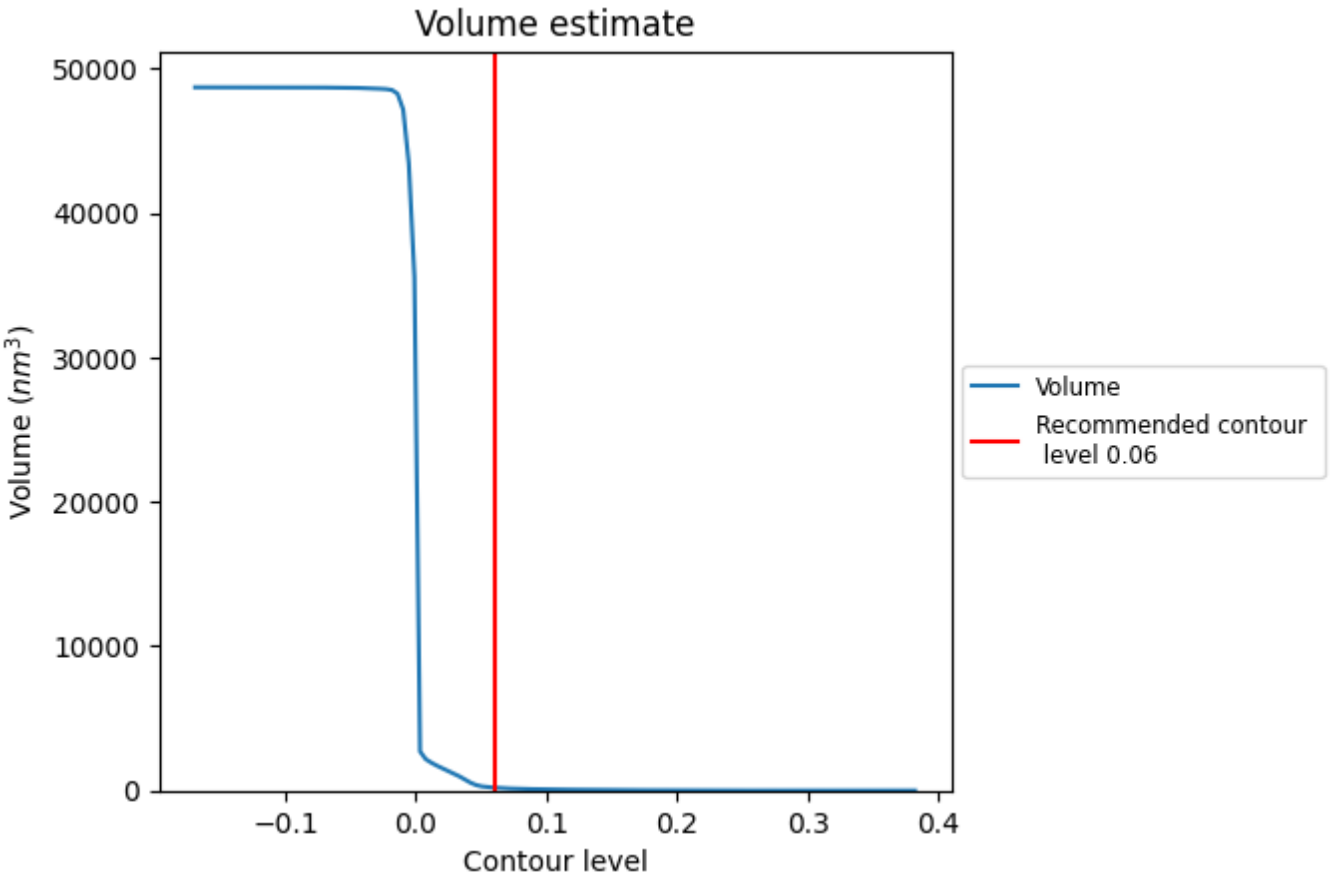
This section contains the results of statistical analysis of the map.

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.

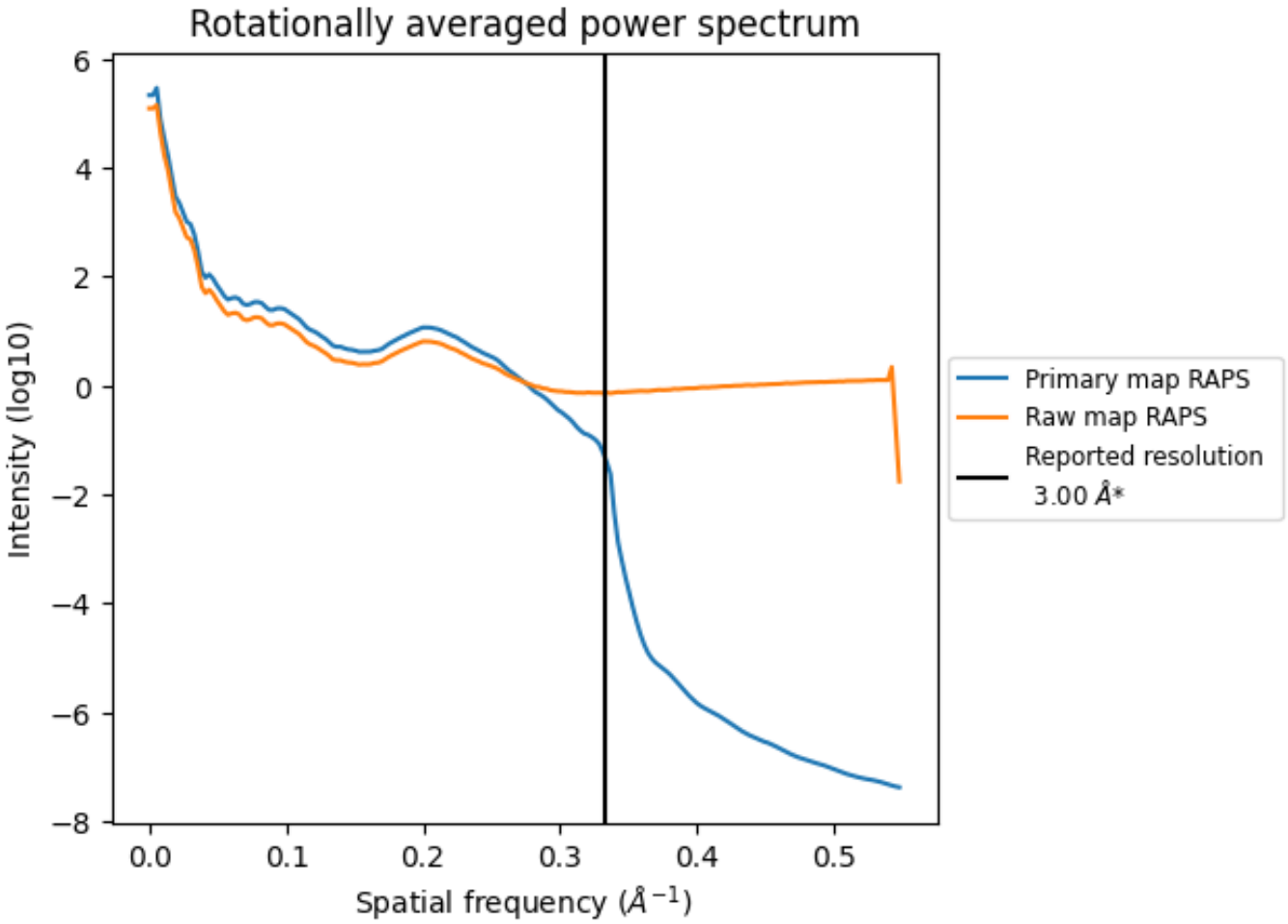
7.2 Volume estimate (i)



The volume at the recommended contour level is 200 nm^3; this corresponds to an approximate mass of 181 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)

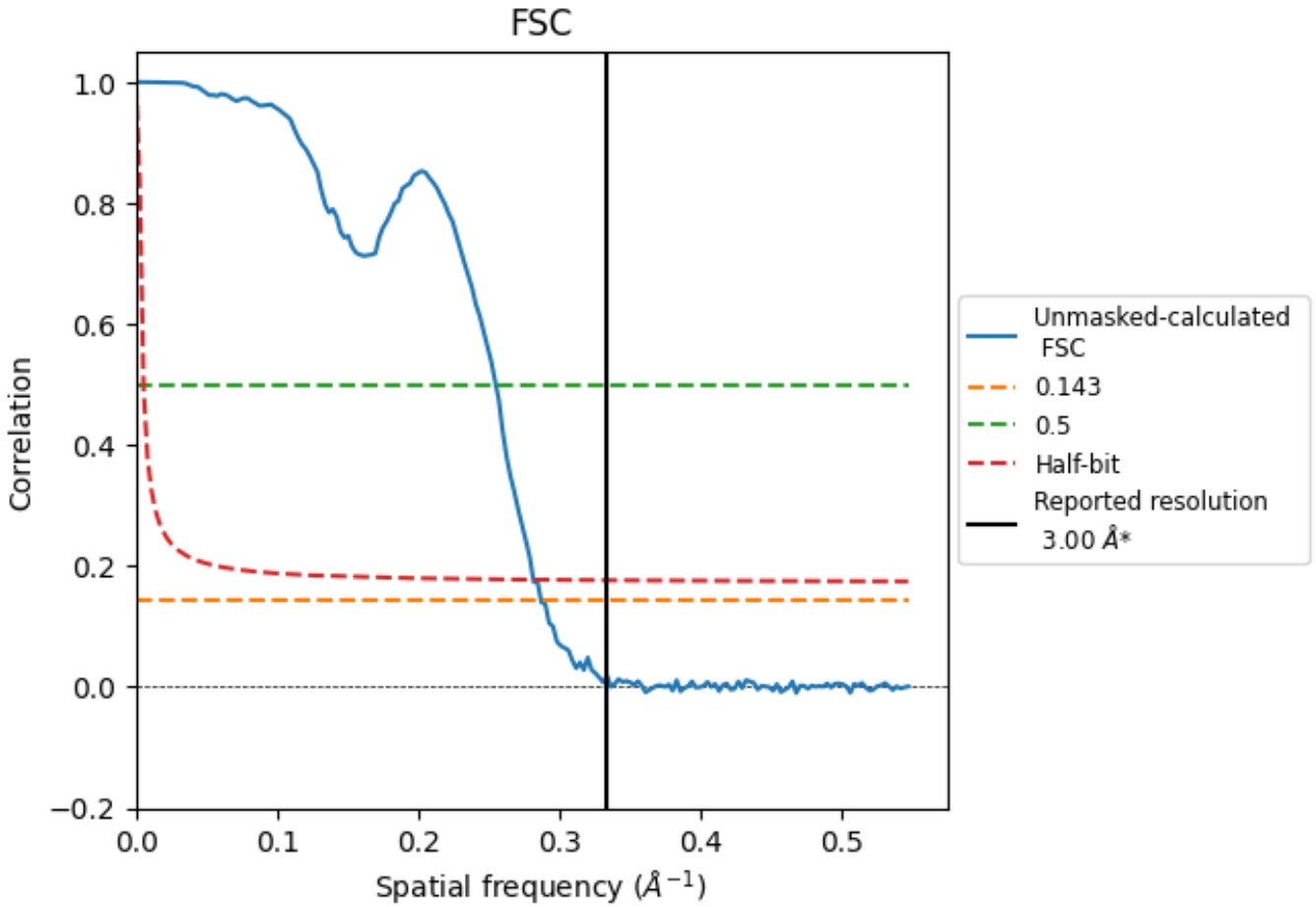


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

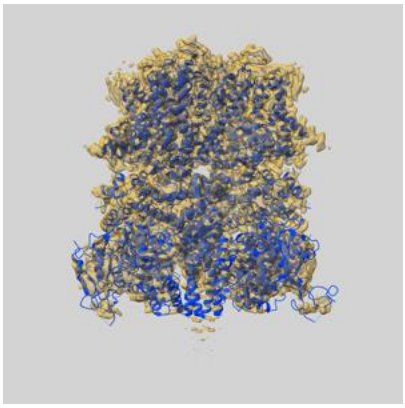
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.48	3.92	3.55

*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 3.48 differs from the reported value 3.0 by more than 10 %

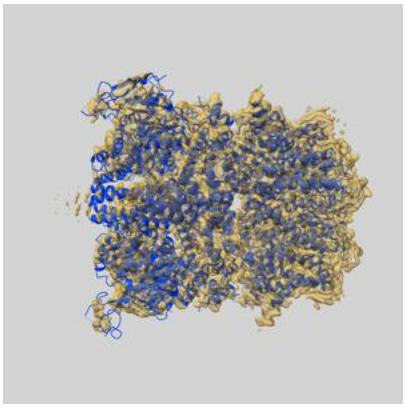
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-57866 and PDB model 30LA. Per-residue inclusion information can be found in section 3 on page 4.

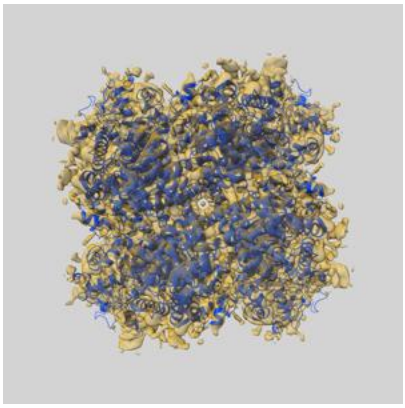
9.1 Map-model overlay



X



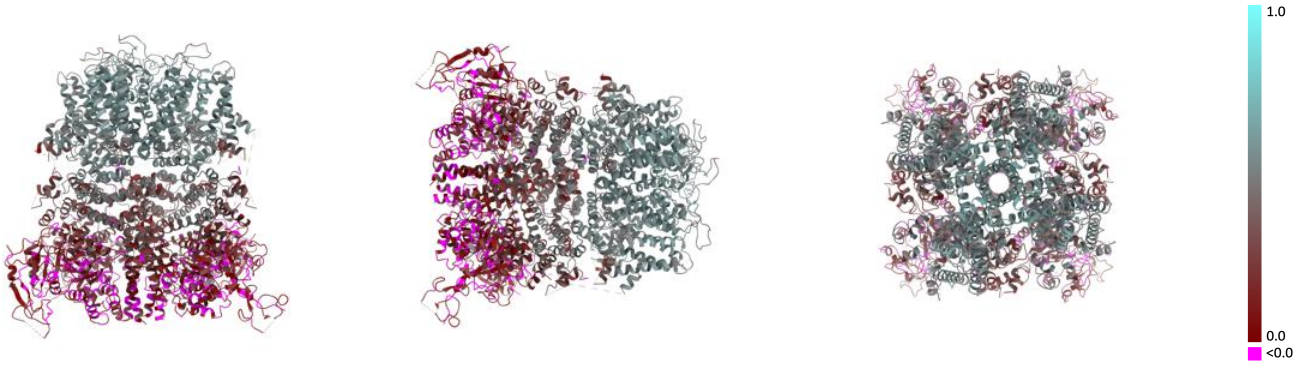
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

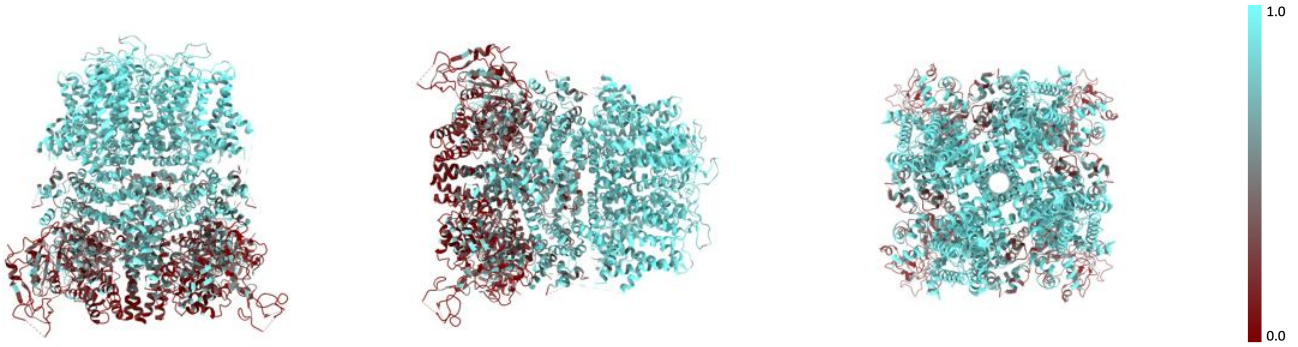
9.2 Q-score mapped to coordinate model (i)



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.

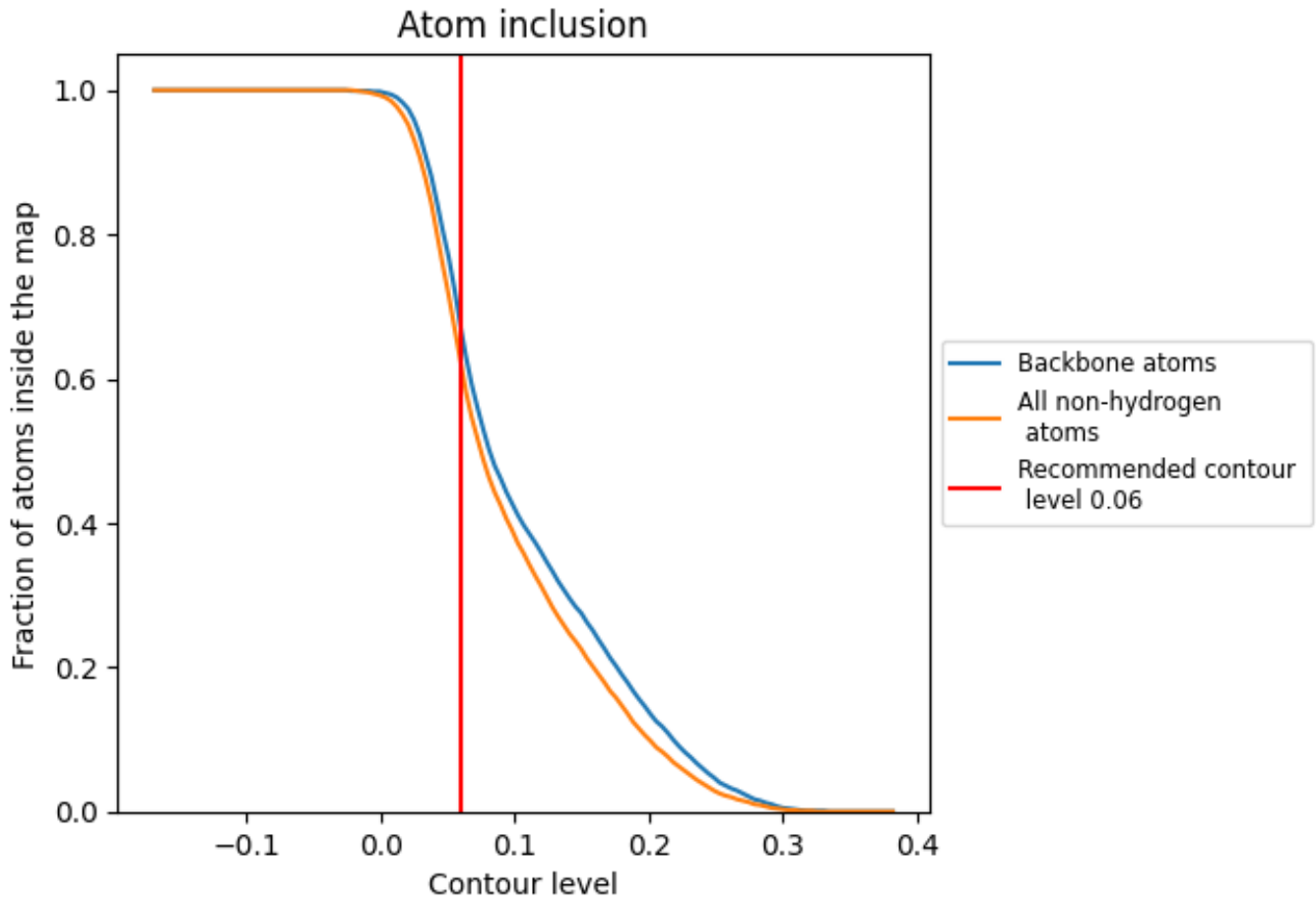
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 62% 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 (0.06) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6160	0.3210
A	0.6160	0.3210
B	0.6160	0.3190
C	0.6160	0.3210
D	0.6180	0.3220