Full wwPDB EM Validation Report

Mar 6, 2026 – 03:43 PM UTC

PDB ID	:	7YIH / pdb_00007yih
EMDB ID	:	EMD-33859
Title	:	Human KCNH5 open state
Authors	:	Zhang, M.F.
Deposited on	:	2022-07-16
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

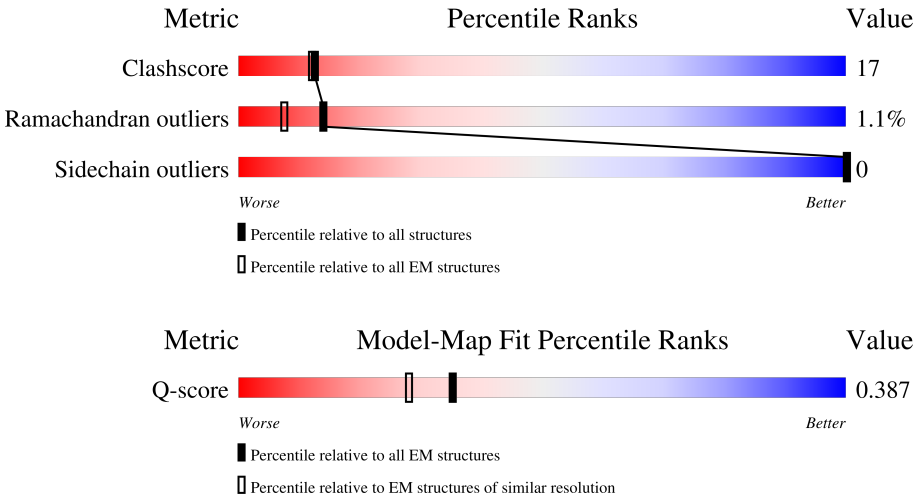
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	988	19% 46% 20% • 33%
1	B	988	19% 46% 20% • 33%
1	C	988	19% 46% 20% 33%
1	D	988	19% 46% 20% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21321 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Potassium voltage-gated channel subfamily H member 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	660	Total	C	N	O	S	0	0
			5328	3449	886	961	32		
1	B	660	Total	C	N	O	S	0	0
			5328	3449	886	961	32		
1	C	660	Total	C	N	O	S	0	0
			5328	3449	886	961	32		
1	D	660	Total	C	N	O	S	0	0
			5328	3449	886	961	32		

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

Mol	Chain	Residues	Atoms		AltConf
2	A	5	Total	K	0
			5	5	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	O	0
			1	1	
3	B	1	Total	O	0
			1	1	
3	C	1	Total	O	0
			1	1	
3	D	1	Total	O	0
			1	1	

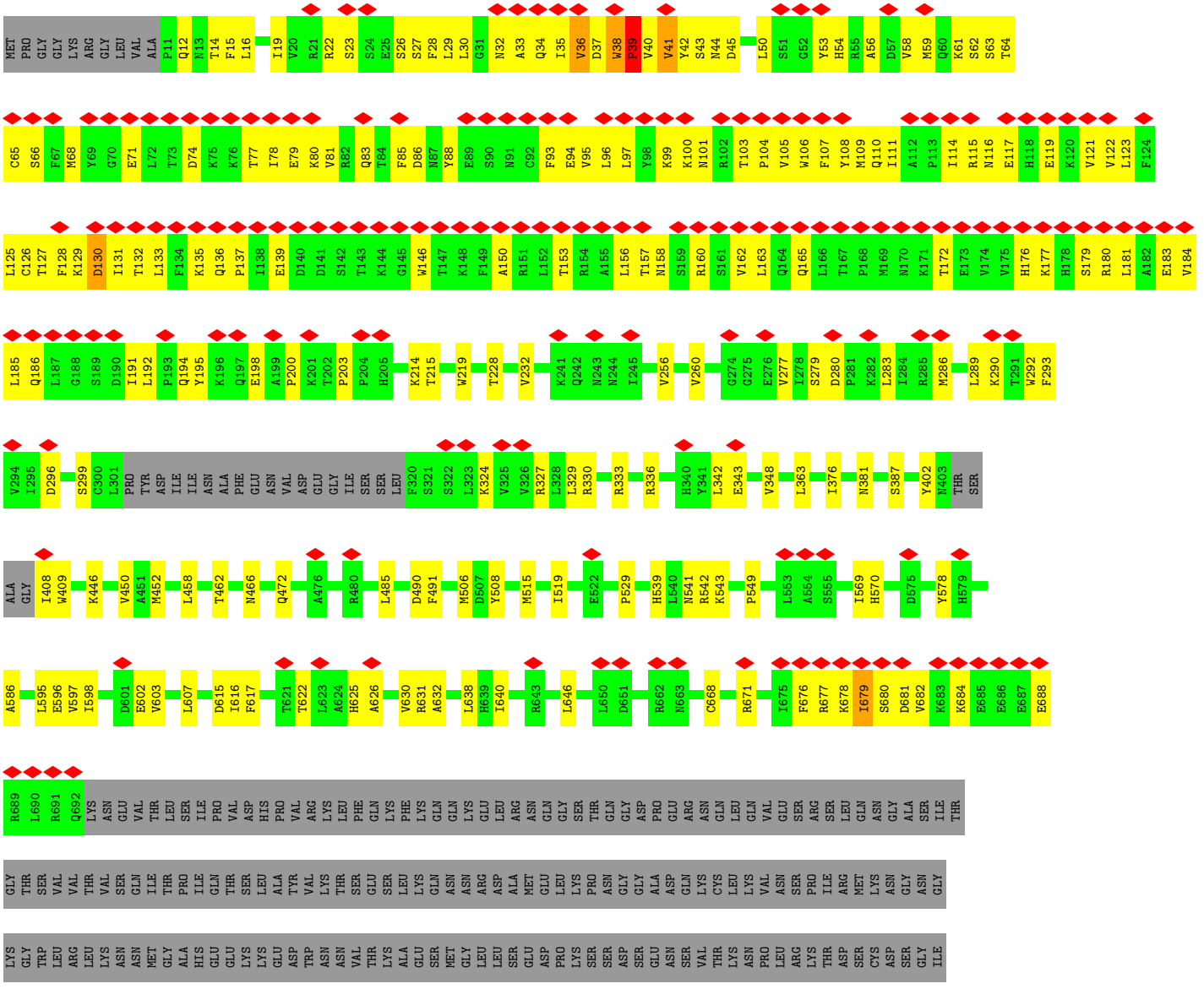
3 Residue-property plots (i)

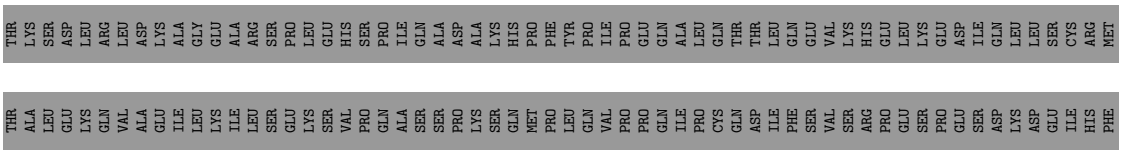
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Potassium voltage-gated channel subfamily H member 5

Chain A:



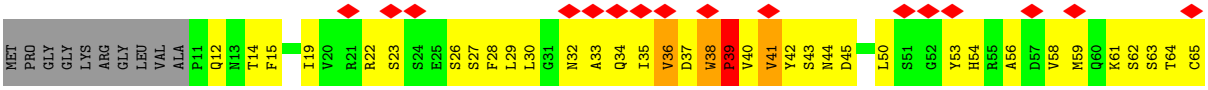


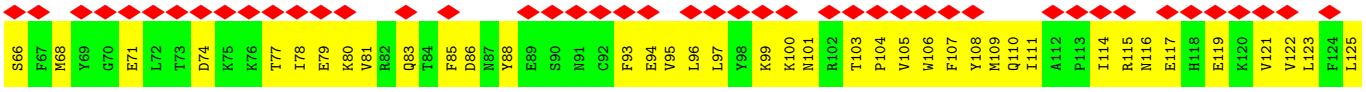


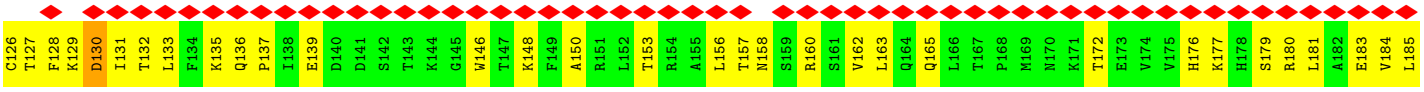
• Molecule 1: Potassium voltage-gated channel subfamily H member 5

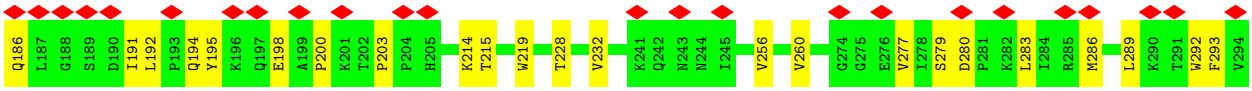
Chain B:



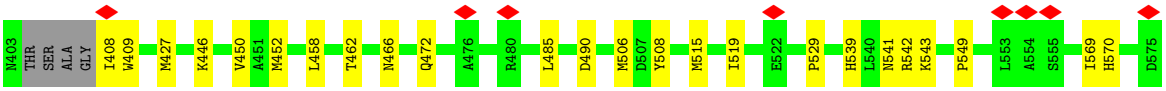


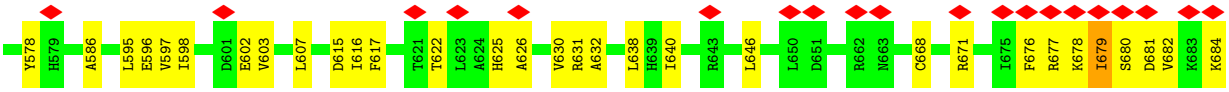


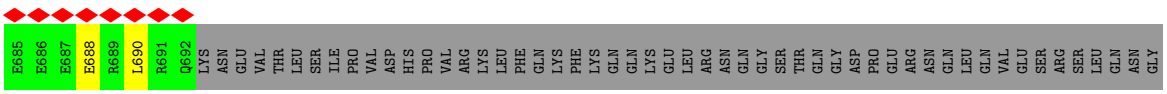


















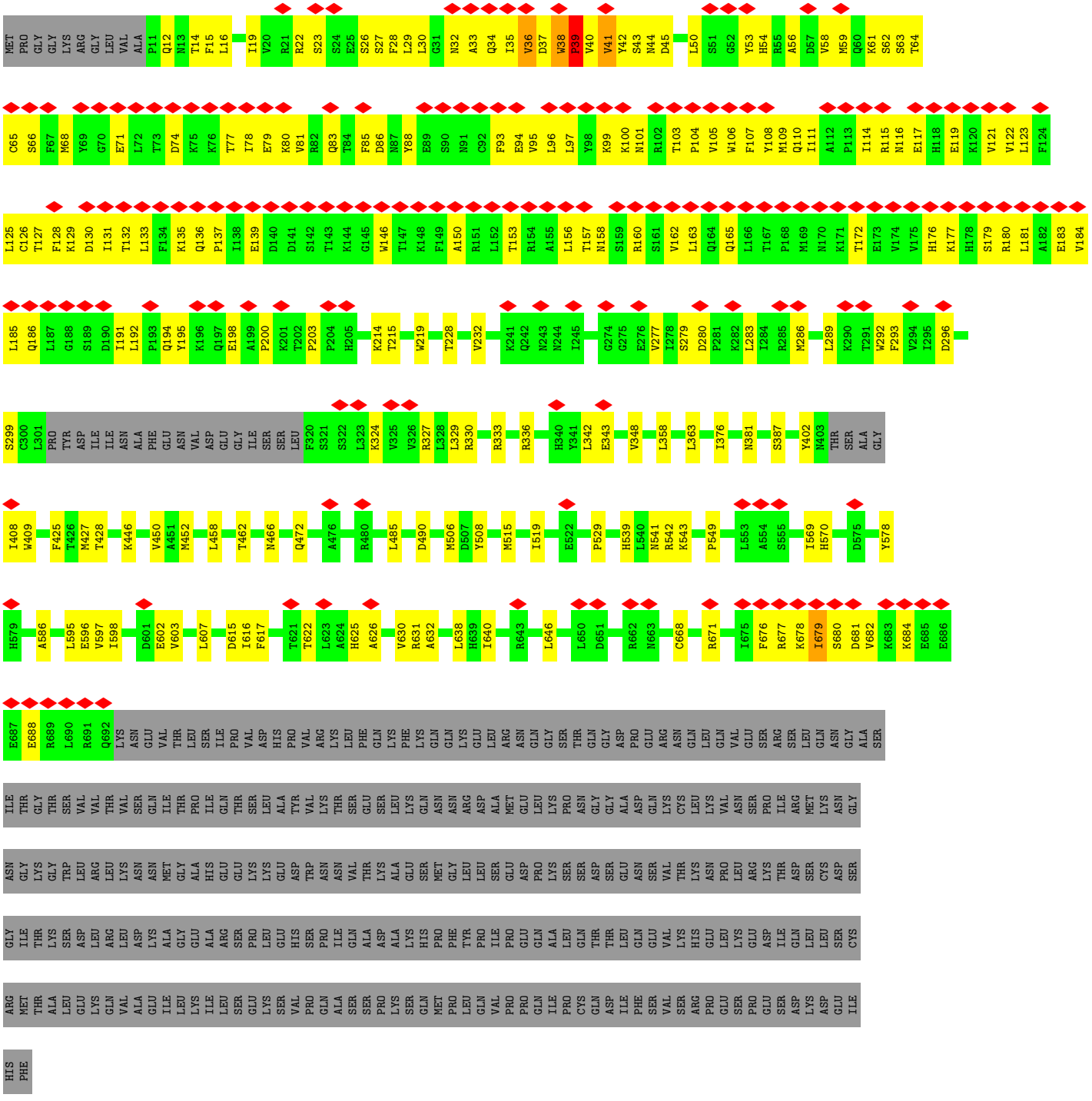




• Molecule 1: Potassium voltage-gated channel subfamily H member 5

Chain C:

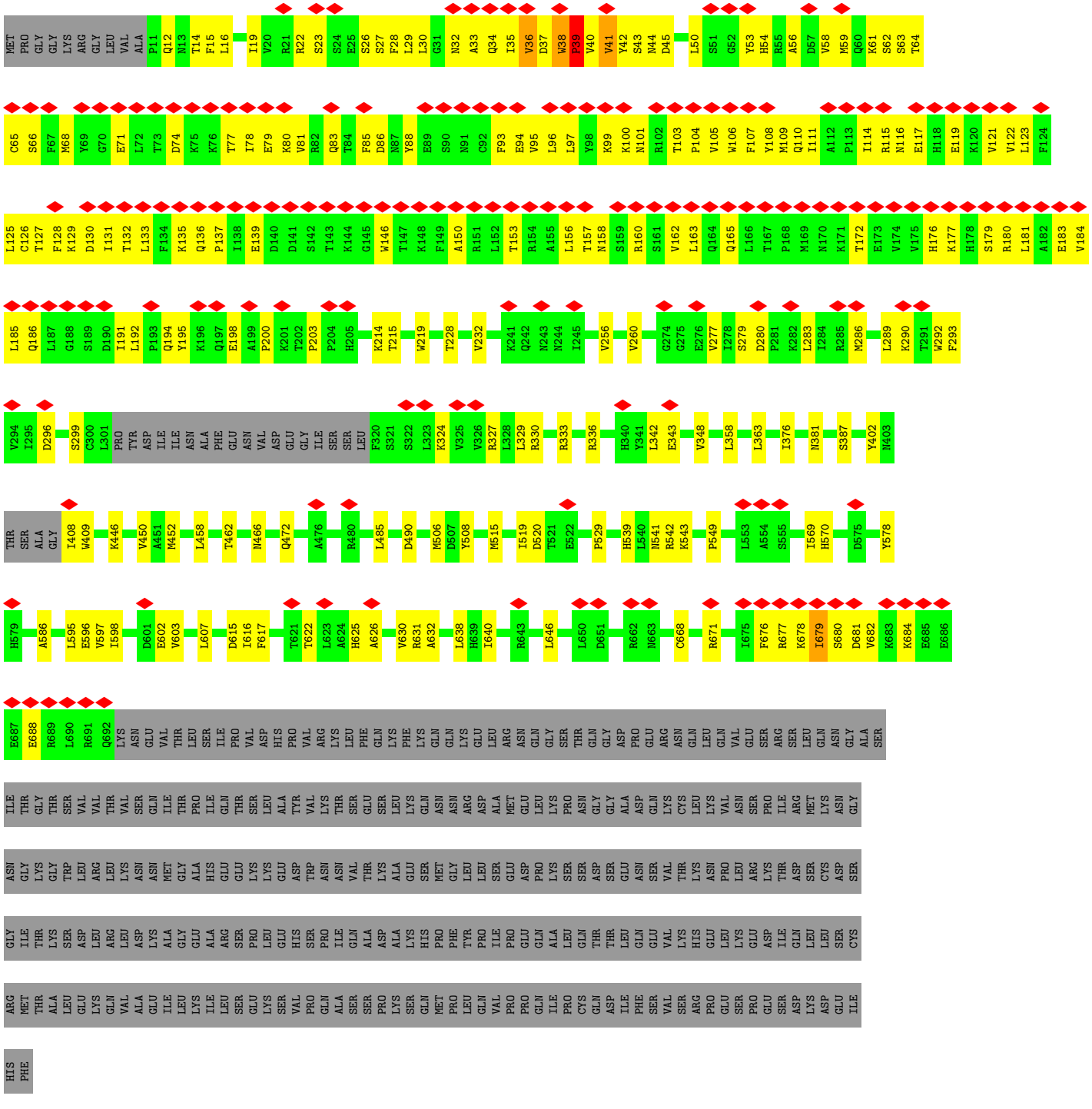




• Molecule 1: Potassium voltage-gated channel subfamily H member 5

Chain D:




MET PRO GLY GLY LYS ARG GLY LEU VAL ALA P11 Q12 N13 T14 F15 L16 I19 V20 R21 R22 S23 S24 E25 S26 S27 F28 L29 L30 G31 N32 A33 Q34 I35 V36 D37 W38 P39 V40 V41 Y42 S43 N44 D45 L50 S51 G52 Y53 H54 R55 A56 D57 V58 M59 Q60 K61 S62 S63 T64
C65 S66 F67 M68 Y69 G70 E71 L72 T73 D74 K75 K76 T77 I78 E79 K80 V81 R82 Q83 T84 F85 D86 M87 Y88 E89 S90 N91 C92 F93 E94 V95 L96 L97 Y98 K99 K100 N101 R102 T103 P104 V105 W106 F107 Y108 M109 Q110 I111 A112 P113 I114 R115 N116 E117 H118 E119 K120 V121 V122 L123 F124
L125 C126 T127 F128 K129 D130 I131 T132 L133 F134 K135 Q136 P137 I138 E139 D140 D141 S142 T143 K144 G145 W146 T147 K148 F149 A150 R151 L152 T153 R154 A155 L156 T157 N158 S159 R160 S161 V162 L163 Q164 Q165 L166 T167 P168 M169 N170 K171 T172 E173 V174 V175 H176 K177 H178 S179 R180 L181 A182 E183 V184
L185 Q186 L187 G188 S189 D190 I191 L192 P193 Q194 Y195 K196 Q197 E198 A199 P200 K201 T202 P203 P204 H205 K214 T215 W219 T228 V232 K241 Q242 N243 N244 I245 V256 V260 G274 G275 E276 V277 I278 S279 D280 P281 K282 L283 I284 R285 M286 L289 K290 T291 W292 F293
V294 I295 D296 S299 C300 L301 PRO TYR ASP ILE ILE ASN ALA PHE GLU ASN VAL ASP GLU GLY ILE SER SER LEU F320 S321 S322 L323 K324 V325 V326 R327 L328 L329 R330 R333 R336 H340 Y341 L342 E343 V348 L358 L363 I376 N381 S387 Y402 W403
THR SER ALA GLY I408 W409 K446 V450 A451 W452 L458 T462 N466 Q472 A476 R480 L485 D490 M506 D507 Y508 M515 I519 D520 T521 E522 P529 H539 L540 N541 R542 K543 P549 L553 A554 S555 I569 H570 D575 Y578
H579 A586 L595 E596 V597 I598 D601 E602 V603 L607 D615 I616 F617 T621 T622 L623 A624 H625 A626 V630 R631 A632 L638 H639 I640 R643 L646 L650 D651 R662 N663 C668 R671 I675 F676 R677 K678 I679 S680 D681 V682 K683 K684 E685 E686
E687 E688 R689 L690 R691 Q692 LYS ASN GLU VAL THR LEU SER ILE PRO VAL ASP HIS PRO VAL ARG LYS LEU PHE GLN LYS PHE LYS GLN GLN LYS GLU LEU ARG ASN GLN GLY SER THR GLN GLY ASP PRO GLU ARG ASN GLN LEU GLN VAL GLU SER ARG SER LEU GLN ASN GLY ALA SER
ILE THR GLY THR SER VAL VAL THR VAL SER GLN ILE THR PRO ILE GLN THR SER LEU ALA TYR VAL LYS THR SER GLU SER LEU LYS GLN ASN ASN ARG ASP ALA MET GLU LEU LYS PRO ASN GLY GLY ALA ASP GLN LYS CYS LEU LYS VAL ASN SER PRO ILE ARG MET LYS ASN GLY
ASN GLY LYS GLY TRP LEU ARG LEU LYS ASN ASN MET GLY ALA HIS GLU GLU LYS LYS GLU ASP TRP ASN ASN VAL THR LYS ALA GLU SER MET GLY LEU LEU SER GLU ASP PRO LYS SER SER ASP SER GLU ASN SER VAL THR LYS ASN PRO LEU LEU ARG LYS THR ASP SER CYS ASP SER
GLY ILE THR LYS SER ASP LEU ARG LEU ASP LYS ALA GLY GLU ALA ARG SER PRO LEU GLU HIS SER PRO ILE GLN ALA LEU ASP ALA LYS SER HIS PRO PHE TYR PRO ILE PRO GLU GLN ALA LEU GLN GLU VAL LYS HIS GLU LEU LYS GLU ASP ILE GLN LEU LEU SER CYS
ARG MET THR ALA LEU GLU LYS GLN VAL ALA GLU ILE LEU LYS ILE LEU SER GLU LYS SER VAL PRO GLN ALA SER SER PRO ALA LYS SER GLN MET PRO LEU GLN VAL PRO PRO GLN ILE PRO CYS GLN ASP ILE PHE SER VAL SER ARG PRO GLU SER PRO GLU SER ASP LYS ASP GLU ILE
HIS PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63387	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.386	Depositor
Minimum map value	-1.609	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	339.59998, 339.59998, 339.59998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8489999, 0.8489999, 0.8489999	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.18	0/5451	0.46	2/7396 (0.0%)
1	B	0.18	0/5451	0.46	2/7396 (0.0%)
1	C	0.18	0/5451	0.46	2/7396 (0.0%)
1	D	0.18	0/5451	0.46	2/7396 (0.0%)
All	All	0.18	0/21804	0.46	8/29584 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	PRO	N-CA-C	5.62	124.04	112.47
1	B	39	PRO	N-CA-C	5.62	124.04	112.47
1	C	39	PRO	N-CA-C	5.62	124.04	112.47
1	D	39	PRO	N-CA-C	5.62	124.04	112.47
1	A	549	PRO	CA-N-CD	-5.20	104.72	112.00
1	B	549	PRO	CA-N-CD	-5.20	104.72	112.00
1	C	549	PRO	CA-N-CD	-5.20	104.72	112.00
1	D	549	PRO	CA-N-CD	-5.20	104.72	112.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	PRO	Peptide
1	A	679	ILE	Peptide
1	B	39	PRO	Peptide
1	B	679	ILE	Peptide
1	C	39	PRO	Peptide
1	C	679	ILE	Peptide
1	D	39	PRO	Peptide
1	D	679	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5328	0	5364	204	0
1	B	5328	0	5364	209	0
1	C	5328	0	5364	207	0
1	D	5328	0	5364	210	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	21321	0	21456	718	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 17.

All (718) 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:36:VAL:HB	1:D:677:ARG:HB3	1.43	1.00
1:A:677:ARG:HB3	1:D:36:VAL:HB	1.43	1.00
1:B:36:VAL:HB	1:C:677:ARG:HB3	1.43	1.00
1:A:36:VAL:HB	1:B:677:ARG:HB3	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ALA:HA	1:C:680:SER:H	1.32	0.94
1:C:33:ALA:HA	1:D:680:SER:H	1.32	0.94
1:A:33:ALA:HA	1:B:680:SER:H	1.32	0.92
1:A:680:SER:H	1:D:33:ALA:HA	1.32	0.92
1:B:38:TRP:N	1:C:677:ARG:O	2.07	0.88
1:A:38:TRP:N	1:B:677:ARG:O	2.07	0.87
1:C:38:TRP:N	1:D:677:ARG:O	2.07	0.87
1:B:34:GLN:H	1:C:678:LYS:HB3	1.40	0.87
1:A:677:ARG:O	1:D:38:TRP:N	2.07	0.87
1:C:34:GLN:H	1:D:678:LYS:HB3	1.40	0.87
1:A:34:GLN:H	1:B:678:LYS:HB3	1.40	0.86
1:B:597:VAL:HG12	1:B:630:VAL:HG12	1.58	0.86
1:C:94:GLU:HB3	1:C:106:TRP:HB3	1.58	0.85
1:A:597:VAL:HG12	1:A:630:VAL:HG12	1.58	0.85
1:D:94:GLU:HB3	1:D:106:TRP:HB3	1.58	0.85
1:A:678:LYS:HB3	1:D:34:GLN:H	1.40	0.84
1:A:94:GLU:HB3	1:A:106:TRP:HB3	1.58	0.84
1:D:597:VAL:HG12	1:D:630:VAL:HG12	1.58	0.84
1:B:94:GLU:HB3	1:B:106:TRP:HB3	1.58	0.83
1:C:597:VAL:HG12	1:C:630:VAL:HG12	1.58	0.83
1:D:104:PRO:HD3	1:D:139:GLU:HG2	1.64	0.80
1:C:104:PRO:HD3	1:C:139:GLU:HG2	1.64	0.79
1:A:28:PHE:HB2	1:A:42:TYR:HB2	1.65	0.79
1:B:35:ILE:HA	1:C:682:VAL:HG13	1.65	0.78
1:A:682:VAL:HG13	1:D:35:ILE:HA	1.65	0.78
1:B:104:PRO:HD3	1:B:139:GLU:HG2	1.64	0.78
1:B:28:PHE:HB2	1:B:42:TYR:HB2	1.65	0.78
1:A:677:ARG:C	1:D:38:TRP:HD1	1.92	0.77
1:B:38:TRP:HD1	1:C:677:ARG:C	1.92	0.77
1:C:38:TRP:HD1	1:D:677:ARG:C	1.92	0.77
1:D:28:PHE:HB2	1:D:42:TYR:HB2	1.65	0.77
1:A:104:PRO:HD3	1:A:139:GLU:HG2	1.64	0.77
1:A:38:TRP:HD1	1:B:677:ARG:C	1.92	0.77
1:C:28:PHE:HB2	1:C:42:TYR:HB2	1.65	0.76
1:C:35:ILE:HA	1:D:682:VAL:HG13	1.65	0.76
1:A:35:ILE:HA	1:B:682:VAL:HG13	1.65	0.75
1:D:58:VAL:HG11	1:D:66:SER:H	1.53	0.73
1:A:58:VAL:HG11	1:A:66:SER:H	1.53	0.73
1:C:58:VAL:HG11	1:C:66:SER:H	1.53	0.72
1:B:58:VAL:HG11	1:B:66:SER:H	1.53	0.72
1:D:68:MET:HE3	1:D:97:LEU:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:N	1:C:678:LYS:O	2.23	0.71
1:A:68:MET:HE3	1:A:97:LEU:HB3	1.72	0.71
1:A:678:LYS:HB2	1:D:35:ILE:H	1.55	0.71
1:B:37:ASP:HB3	1:B:62:SER:HA	1.72	0.71
1:C:35:ILE:H	1:D:678:LYS:HB2	1.55	0.71
1:B:68:MET:HE3	1:B:97:LEU:HB3	1.72	0.71
1:C:68:MET:HE3	1:C:97:LEU:HB3	1.72	0.71
1:A:678:LYS:O	1:D:36:VAL:N	2.23	0.71
1:B:38:TRP:HB2	1:C:678:LYS:HA	1.73	0.71
1:C:36:VAL:N	1:D:678:LYS:O	2.23	0.71
1:A:35:ILE:H	1:B:678:LYS:HB2	1.55	0.71
1:C:37:ASP:HB3	1:C:62:SER:HA	1.72	0.70
1:A:36:VAL:N	1:B:678:LYS:O	2.23	0.70
1:A:38:TRP:HB2	1:B:678:LYS:HA	1.73	0.70
1:B:35:ILE:H	1:C:678:LYS:HB2	1.55	0.70
1:A:37:ASP:HB3	1:A:62:SER:HA	1.72	0.70
1:D:37:ASP:HB3	1:D:62:SER:HA	1.72	0.70
1:A:38:TRP:CD1	1:B:678:LYS:HG3	2.27	0.70
1:B:38:TRP:CD1	1:C:678:LYS:HG3	2.27	0.70
1:A:678:LYS:HG3	1:D:38:TRP:CD1	2.27	0.69
1:C:38:TRP:CD1	1:D:678:LYS:HG3	2.27	0.69
1:A:678:LYS:HA	1:D:38:TRP:HB2	1.73	0.69
1:C:38:TRP:HB2	1:D:678:LYS:HA	1.73	0.69
1:B:79:GLU:HG3	1:B:83:GLN:HB2	1.76	0.67
1:B:99:LYS:HZ1	1:B:157:THR:H	1.40	0.67
1:C:79:GLU:HG3	1:C:83:GLN:HB2	1.76	0.67
1:A:79:GLU:HG3	1:A:83:GLN:HB2	1.76	0.67
1:A:99:LYS:HZ2	1:A:156:LEU:HA	1.59	0.67
1:A:132:THR:HB	1:A:156:LEU:HD13	1.78	0.66
1:A:58:VAL:HG12	1:A:62:SER:HB3	1.78	0.66
1:B:132:THR:HB	1:B:156:LEU:HD13	1.78	0.66
1:D:79:GLU:HG3	1:D:83:GLN:HB2	1.76	0.66
1:C:58:VAL:HG12	1:C:62:SER:HB3	1.78	0.66
1:B:58:VAL:HG12	1:B:62:SER:HB3	1.78	0.65
1:C:132:THR:HB	1:C:156:LEU:HD13	1.78	0.65
1:D:596:GLU:OE2	1:D:631:ARG:NH2	2.30	0.65
1:D:58:VAL:HG12	1:D:62:SER:HB3	1.78	0.65
1:B:133:LEU:HD11	1:B:153:THR:HA	1.77	0.65
1:D:132:THR:HB	1:D:156:LEU:HD13	1.78	0.65
1:B:596:GLU:OE2	1:B:631:ARG:NH2	2.30	0.65
1:A:133:LEU:HD11	1:A:153:THR:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:GLU:OE2	1:C:631:ARG:NH2	2.30	0.65
1:A:34:GLN:H	1:B:678:LYS:CB	2.09	0.65
1:A:596:GLU:OE2	1:A:631:ARG:NH2	2.30	0.65
1:D:133:LEU:HD11	1:D:153:THR:HA	1.77	0.65
1:B:34:GLN:H	1:C:678:LYS:CB	2.09	0.64
1:C:99:LYS:HZ2	1:C:156:LEU:HA	1.62	0.64
1:C:163:LEU:HD13	1:C:179:SER:HB3	1.79	0.64
1:C:133:LEU:HD11	1:C:153:THR:HA	1.77	0.64
1:D:99:LYS:HZ2	1:D:156:LEU:HA	1.61	0.64
1:B:115:ARG:HH12	1:B:119:GLU:HG3	1.62	0.64
1:C:39:PRO:HA	1:C:61:LYS:HA	1.80	0.64
1:D:39:PRO:HA	1:D:61:LYS:HA	1.80	0.64
1:A:39:PRO:HA	1:A:61:LYS:HA	1.80	0.63
1:C:35:ILE:O	1:D:678:LYS:N	2.31	0.63
1:D:163:LEU:HD13	1:D:179:SER:HB3	1.79	0.63
1:A:163:LEU:HD13	1:A:179:SER:HB3	1.79	0.63
1:A:678:LYS:N	1:D:35:ILE:O	2.31	0.63
1:B:35:ILE:O	1:C:678:LYS:N	2.31	0.63
1:A:81:VAL:HB	1:A:95:VAL:HG12	1.81	0.63
1:A:678:LYS:CB	1:D:34:GLN:H	2.09	0.63
1:C:115:ARG:HH12	1:C:119:GLU:HG3	1.62	0.63
1:A:35:ILE:O	1:B:678:LYS:N	2.31	0.63
1:A:115:ARG:HH12	1:A:119:GLU:HG3	1.62	0.63
1:B:163:LEU:HD13	1:B:179:SER:HB3	1.79	0.63
1:C:34:GLN:H	1:D:678:LYS:CB	2.09	0.63
1:B:39:PRO:HA	1:B:61:LYS:HA	1.80	0.62
1:C:81:VAL:HB	1:C:95:VAL:HG12	1.81	0.62
1:D:81:VAL:HB	1:D:95:VAL:HG12	1.81	0.62
1:A:29:LEU:HB3	1:A:126:CYS:HB2	1.81	0.62
1:B:81:VAL:HB	1:B:95:VAL:HG12	1.81	0.62
1:C:108:TYR:H	1:C:131:ILE:HG12	1.65	0.62
1:C:466:ASN:OD1	1:D:472:GLN:NE2	2.32	0.62
1:D:108:TYR:H	1:D:131:ILE:HG12	1.65	0.62
1:D:116:ASN:ND2	1:D:122:VAL:O	2.33	0.62
1:A:108:TYR:H	1:A:131:ILE:HG12	1.65	0.62
1:B:569:ILE:HD13	1:B:640:ILE:HD11	1.82	0.62
1:C:569:ILE:HD13	1:C:640:ILE:HD11	1.82	0.62
1:C:116:ASN:ND2	1:C:122:VAL:O	2.33	0.62
1:A:569:ILE:HD13	1:A:640:ILE:HD11	1.82	0.62
1:A:466:ASN:OD1	1:B:472:GLN:NE2	2.32	0.62
1:B:108:TYR:H	1:B:131:ILE:HG12	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASN:ND2	1:B:122:VAL:O	2.33	0.62
1:B:466:ASN:OD1	1:C:472:GLN:NE2	2.32	0.62
1:C:29:LEU:HB3	1:C:126:CYS:HB2	1.81	0.62
1:D:115:ARG:HH12	1:D:119:GLU:HG3	1.62	0.61
1:B:29:LEU:HB3	1:B:126:CYS:HB2	1.81	0.61
1:D:29:LEU:HB3	1:D:126:CYS:HB2	1.81	0.61
1:D:569:ILE:HD13	1:D:640:ILE:HD11	1.82	0.61
1:B:402:TYR:HE1	1:B:408:ILE:HB	1.66	0.61
1:A:402:TYR:HE1	1:A:408:ILE:HB	1.66	0.61
1:A:215:THR:HG23	1:A:219:TRP:CZ3	2.36	0.61
1:B:215:THR:HG23	1:B:219:TRP:CZ3	2.36	0.61
1:D:402:TYR:HE1	1:D:408:ILE:HB	1.66	0.61
1:A:39:PRO:HD3	1:A:61:LYS:HG2	1.83	0.61
1:B:39:PRO:HD3	1:B:61:LYS:HG2	1.83	0.61
1:D:215:THR:HG23	1:D:219:TRP:CZ3	2.36	0.61
1:B:56:ALA:HA	1:B:61:LYS:NZ	2.16	0.61
1:A:116:ASN:ND2	1:A:122:VAL:O	2.33	0.60
1:C:39:PRO:HD3	1:C:61:LYS:HG2	1.83	0.60
1:D:39:PRO:HD3	1:D:61:LYS:HG2	1.83	0.60
1:C:215:THR:HG23	1:C:219:TRP:CZ3	2.36	0.60
1:B:36:VAL:O	1:C:679:ILE:HA	2.02	0.60
1:A:472:GLN:NE2	1:D:466:ASN:OD1	2.32	0.60
1:C:402:TYR:HE1	1:C:408:ILE:HB	1.66	0.59
1:A:56:ALA:HA	1:A:61:LYS:NZ	2.16	0.59
1:D:56:ALA:HA	1:D:61:LYS:NZ	2.16	0.59
1:C:34:GLN:O	1:D:681:ASP:HB3	2.03	0.59
1:C:56:ALA:HA	1:C:61:LYS:NZ	2.16	0.59
1:A:679:ILE:HA	1:D:36:VAL:O	2.02	0.59
1:B:135:LYS:HG3	1:B:136:GLN:H	1.68	0.59
1:A:135:LYS:HG3	1:A:136:GLN:H	1.68	0.59
1:C:36:VAL:O	1:D:679:ILE:HA	2.02	0.59
1:D:135:LYS:HG3	1:D:136:GLN:H	1.68	0.59
1:C:135:LYS:HG3	1:C:136:GLN:H	1.68	0.58
1:A:681:ASP:HB3	1:D:34:GLN:O	2.03	0.58
1:A:36:VAL:O	1:B:679:ILE:HA	2.02	0.58
1:B:50:LEU:HD13	1:B:157:THR:HB	1.86	0.58
1:A:34:GLN:O	1:B:681:ASP:HB3	2.03	0.58
1:C:50:LEU:HD13	1:C:157:THR:HB	1.86	0.58
1:A:30:LEU:HB3	1:A:123:LEU:HG	1.86	0.58
1:B:176:HIS:O	1:B:180:ARG:NH2	2.37	0.58
1:C:106:TRP:H	1:C:135:LYS:NZ	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HB3	1:B:123:LEU:HG	1.86	0.57
1:B:34:GLN:O	1:C:681:ASP:HB3	2.03	0.57
1:C:30:LEU:HB3	1:C:123:LEU:HG	1.86	0.57
1:D:176:HIS:O	1:D:180:ARG:NH2	2.37	0.57
1:A:176:HIS:O	1:A:180:ARG:NH2	2.37	0.57
1:B:106:TRP:H	1:B:135:LYS:NZ	2.02	0.57
1:A:681:ASP:HB3	1:D:34:GLN:HA	1.87	0.57
1:C:34:GLN:HA	1:D:681:ASP:HB3	1.87	0.57
1:D:30:LEU:HB3	1:D:123:LEU:HG	1.86	0.57
1:D:74:ASP:N	1:D:77:THR:OG1	2.38	0.57
1:B:34:GLN:HA	1:C:681:ASP:HB3	1.87	0.57
1:C:299:SER:HB3	1:C:329:LEU:HB2	1.87	0.57
1:A:74:ASP:N	1:A:77:THR:OG1	2.38	0.57
1:A:97:LEU:HB2	1:A:107:PHE:HZ	1.70	0.57
1:B:74:ASP:N	1:B:77:THR:OG1	2.38	0.57
1:B:299:SER:HB3	1:B:329:LEU:HB2	1.87	0.57
1:D:106:TRP:H	1:D:135:LYS:NZ	2.02	0.57
1:D:299:SER:HB3	1:D:329:LEU:HB2	1.87	0.57
1:A:34:GLN:HA	1:B:681:ASP:HB3	1.87	0.57
1:A:177:LYS:HB3	1:A:181:LEU:HB3	1.87	0.57
1:C:176:HIS:O	1:C:180:ARG:NH2	2.37	0.57
1:D:50:LEU:HD13	1:D:157:THR:HB	1.86	0.57
1:C:81:VAL:H	1:C:95:VAL:HB	1.70	0.57
1:A:106:TRP:H	1:A:135:LYS:NZ	2.02	0.56
1:B:97:LEU:HB2	1:B:107:PHE:HZ	1.70	0.56
1:A:50:LEU:HD13	1:A:157:THR:HB	1.86	0.56
1:D:177:LYS:HB3	1:D:181:LEU:HB3	1.87	0.56
1:A:299:SER:HB3	1:A:329:LEU:HB2	1.87	0.56
1:C:74:ASP:N	1:C:77:THR:OG1	2.38	0.56
1:C:97:LEU:HB2	1:C:107:PHE:HZ	1.70	0.56
1:C:177:LYS:HB3	1:C:181:LEU:HB3	1.87	0.56
1:A:81:VAL:H	1:A:95:VAL:HB	1.70	0.56
1:C:56:ALA:HA	1:C:61:LYS:HZ3	1.70	0.56
1:A:39:PRO:HB3	1:A:41:VAL:HG23	1.88	0.56
1:B:177:LYS:HB3	1:B:181:LEU:HB3	1.87	0.56
1:C:39:PRO:HB3	1:C:41:VAL:HG23	1.88	0.56
1:D:110:GLN:OE1	1:D:184:VAL:N	2.39	0.56
1:B:81:VAL:H	1:B:95:VAL:HB	1.70	0.56
1:D:39:PRO:HB3	1:D:41:VAL:HG23	1.88	0.55
1:D:97:LEU:HB2	1:D:107:PHE:HZ	1.70	0.55
1:D:81:VAL:H	1:D:95:VAL:HB	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HA	1:A:293:PHE:HB2	1.89	0.55
1:D:289:LEU:HA	1:D:293:PHE:HB2	1.89	0.55
1:A:22:ARG:HH22	1:A:191:ILE:HA	1.72	0.55
1:B:39:PRO:HB3	1:B:41:VAL:HG23	1.88	0.55
1:C:86:ASP:HB3	1:D:679:ILE:HD11	1.89	0.55
1:B:22:ARG:HH22	1:B:191:ILE:HA	1.72	0.54
1:B:110:GLN:OE1	1:B:184:VAL:N	2.39	0.54
1:A:176:HIS:CE1	1:A:177:LYS:HE3	2.43	0.54
1:A:679:ILE:HD11	1:D:86:ASP:HB3	1.89	0.54
1:B:86:ASP:HB3	1:C:679:ILE:HD11	1.89	0.54
1:D:176:HIS:CE1	1:D:177:LYS:HE3	2.43	0.54
1:A:56:ALA:HA	1:A:61:LYS:HZ3	1.73	0.54
1:B:114:ILE:HG22	1:B:125:LEU:HB2	1.90	0.54
1:C:289:LEU:HA	1:C:293:PHE:HB2	1.89	0.54
1:A:86:ASP:HB3	1:B:679:ILE:HD11	1.89	0.54
1:B:289:LEU:HA	1:B:293:PHE:HB2	1.89	0.54
1:C:110:GLN:OE1	1:C:184:VAL:N	2.39	0.54
1:A:586:ALA:HB1	1:A:640:ILE:HG23	1.89	0.54
1:C:176:HIS:CE1	1:C:177:LYS:HE3	2.43	0.54
1:D:586:ALA:HB1	1:D:640:ILE:HG23	1.89	0.54
1:B:176:HIS:CE1	1:B:177:LYS:HE3	2.43	0.53
1:A:114:ILE:HG22	1:A:125:LEU:HB2	1.90	0.53
1:B:179:SER:HA	1:B:183:GLU:HB2	1.91	0.53
1:A:179:SER:HA	1:A:183:GLU:HB2	1.91	0.53
1:B:117:GLU:HB3	1:B:195:TYR:HD2	1.74	0.53
1:A:676:PHE:HB2	1:D:38:TRP:NE1	2.24	0.53
1:C:114:ILE:HG22	1:C:125:LEU:HB2	1.90	0.53
1:B:38:TRP:NE1	1:C:676:PHE:HB2	2.24	0.53
1:B:586:ALA:HB1	1:B:640:ILE:HG23	1.89	0.53
1:D:615:ASP:OD2	1:D:671:ARG:NH1	2.42	0.53
1:A:110:GLN:OE1	1:A:184:VAL:N	2.39	0.53
1:C:179:SER:HA	1:C:183:GLU:HB2	1.91	0.53
1:A:65:CYS:HB2	1:A:85:PHE:HE2	1.74	0.53
1:A:117:GLU:HB3	1:A:195:TYR:HD2	1.74	0.53
1:B:615:ASP:OD2	1:B:671:ARG:NH1	2.42	0.53
1:D:22:ARG:HH22	1:D:191:ILE:HA	1.72	0.53
1:D:114:ILE:HG22	1:D:125:LEU:HB2	1.90	0.53
1:A:146:TRP:HB3	1:A:150:ALA:HB3	1.91	0.53
1:B:519:ILE:HD11	1:C:490:ASP:HB3	1.92	0.53
1:C:117:GLU:HB3	1:C:195:TYR:HD2	1.74	0.53
1:C:586:ALA:HB1	1:C:640:ILE:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:GLU:HB3	1:D:195:TYR:HD2	1.74	0.53
1:B:15:PHE:HB3	1:B:42:TYR:HE2	1.74	0.52
1:C:146:TRP:HB3	1:C:150:ALA:HB3	1.91	0.52
1:A:127:THR:HG22	1:A:129:LYS:HZ2	1.74	0.52
1:A:615:ASP:OD2	1:A:671:ARG:NH1	2.42	0.52
1:B:44:ASN:OD1	1:B:45:ASP:N	2.43	0.52
1:B:146:TRP:HB3	1:B:150:ALA:HB3	1.91	0.52
1:C:65:CYS:HB2	1:C:85:PHE:HE2	1.74	0.52
1:B:27:SER:O	1:B:29:LEU:N	2.42	0.52
1:B:283:LEU:HA	1:B:286:MET:HE2	1.92	0.52
1:C:27:SER:O	1:C:29:LEU:N	2.42	0.52
1:A:15:PHE:HB3	1:A:42:TYR:HE2	1.74	0.52
1:B:99:LYS:HD3	1:B:101:ASN:H	1.74	0.52
1:C:38:TRP:NE1	1:D:676:PHE:HB2	2.24	0.52
1:C:615:ASP:OD2	1:C:671:ARG:NH1	2.42	0.52
1:D:80:LYS:HB3	1:D:93:PHE:HB3	1.91	0.52
1:D:146:TRP:HB3	1:D:150:ALA:HB3	1.91	0.52
1:D:99:LYS:HD3	1:D:101:ASN:H	1.74	0.52
1:D:179:SER:HA	1:D:183:GLU:HB2	1.91	0.52
1:A:38:TRP:NE1	1:B:676:PHE:HB2	2.24	0.52
1:C:22:ARG:HH22	1:C:191:ILE:HA	1.72	0.52
1:C:44:ASN:OD1	1:C:45:ASP:N	2.43	0.52
1:C:519:ILE:HD11	1:D:490:ASP:HB3	1.92	0.52
1:D:65:CYS:HB2	1:D:85:PHE:HE2	1.74	0.52
1:A:123:LEU:O	1:A:194:GLN:HB2	2.10	0.52
1:C:80:LYS:HB3	1:C:93:PHE:HB3	1.91	0.52
1:D:44:ASN:OD1	1:D:45:ASP:N	2.43	0.52
1:A:27:SER:HB2	1:A:128:PHE:HB2	1.91	0.52
1:A:283:LEU:HA	1:A:286:MET:HE2	1.92	0.52
1:C:41:VAL:HG12	1:C:42:TYR:N	2.25	0.52
1:C:123:LEU:O	1:C:194:GLN:HB2	2.10	0.52
1:D:12:GLN:HB3	1:D:198:GLU:HB2	1.92	0.52
1:A:12:GLN:HB3	1:A:198:GLU:HB2	1.92	0.52
1:A:99:LYS:HD3	1:A:101:ASN:H	1.74	0.52
1:B:27:SER:HB2	1:B:128:PHE:HB2	1.91	0.52
1:B:41:VAL:HG12	1:B:42:TYR:N	2.25	0.52
1:B:12:GLN:HB3	1:B:198:GLU:HB2	1.92	0.52
1:C:631:ARG:HG2	1:C:632:ALA:H	1.75	0.52
1:C:283:LEU:HA	1:C:286:MET:HE2	1.92	0.51
1:D:631:ARG:HG2	1:D:632:ALA:H	1.75	0.51
1:A:80:LYS:HB3	1:A:93:PHE:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ASP:HB3	1:D:519:ILE:HD11	1.92	0.51
1:B:123:LEU:O	1:B:194:GLN:HB2	2.10	0.51
1:C:12:GLN:HB3	1:C:198:GLU:HB2	1.92	0.51
1:C:99:LYS:HD3	1:C:101:ASN:H	1.74	0.51
1:D:41:VAL:HG12	1:D:42:TYR:N	2.25	0.51
1:A:44:ASN:OD1	1:A:45:ASP:N	2.43	0.51
1:B:80:LYS:HB3	1:B:93:PHE:HB3	1.91	0.51
1:D:27:SER:O	1:D:29:LEU:N	2.42	0.51
1:A:41:VAL:HG12	1:A:42:TYR:N	2.25	0.51
1:C:125:LEU:HD11	1:C:191:ILE:HB	1.93	0.51
1:D:123:LEU:O	1:D:194:GLN:HB2	2.10	0.51
1:D:27:SER:HB2	1:D:128:PHE:HB2	1.91	0.51
1:A:27:SER:O	1:A:29:LEU:N	2.42	0.51
1:A:114:ILE:HG23	1:A:194:GLN:HB3	1.93	0.51
1:B:631:ARG:HG2	1:B:632:ALA:H	1.75	0.51
1:C:15:PHE:HB3	1:C:42:TYR:HE2	1.74	0.51
1:D:283:LEU:HA	1:D:286:MET:HE2	1.92	0.51
1:A:78:ILE:HG13	1:A:79:GLU:N	2.26	0.51
1:A:519:ILE:HD11	1:B:490:ASP:HB3	1.92	0.51
1:B:65:CYS:HB2	1:B:85:PHE:HE2	1.74	0.51
1:B:127:THR:HG22	1:B:129:LYS:NZ	2.26	0.51
1:D:78:ILE:HG13	1:D:79:GLU:N	2.26	0.51
1:D:125:LEU:HD11	1:D:191:ILE:HB	1.93	0.51
1:A:125:LEU:HD11	1:A:191:ILE:HB	1.93	0.50
1:C:27:SER:HB2	1:C:128:PHE:HB2	1.91	0.50
1:A:127:THR:HG22	1:A:129:LYS:NZ	2.26	0.50
1:D:15:PHE:HB3	1:D:42:TYR:HE2	1.74	0.50
1:D:99:LYS:HD3	1:D:100:LYS:N	2.27	0.50
1:A:64:THR:HA	1:A:85:PHE:HD2	1.77	0.50
1:A:631:ARG:HG2	1:A:632:ALA:H	1.75	0.50
1:B:64:THR:HA	1:B:85:PHE:HD2	1.77	0.50
1:C:64:THR:HA	1:C:85:PHE:HD2	1.77	0.50
1:D:114:ILE:HG23	1:D:194:GLN:HB3	1.93	0.50
1:C:99:LYS:HD3	1:C:100:LYS:N	2.27	0.50
1:C:114:ILE:HG23	1:C:194:GLN:HB3	1.93	0.50
1:D:127:THR:HG22	1:D:129:LYS:NZ	2.26	0.50
1:B:78:ILE:HG13	1:B:79:GLU:N	2.26	0.50
1:B:114:ILE:HG23	1:B:194:GLN:HB3	1.93	0.50
1:B:615:ASP:OD1	1:B:616:ILE:N	2.45	0.50
1:C:127:THR:HG22	1:C:129:LYS:NZ	2.26	0.50
1:B:99:LYS:HD3	1:B:100:LYS:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:THR:HA	1:D:85:PHE:HD2	1.77	0.50
1:D:615:ASP:OD1	1:D:616:ILE:N	2.45	0.50
1:A:203:PRO:HD3	1:A:279:SER:HB3	1.94	0.49
1:C:38:TRP:CE2	1:D:676:PHE:HB2	2.47	0.49
1:D:625:HIS:CG	1:D:626:ALA:H	2.30	0.49
1:A:99:LYS:HD3	1:A:100:LYS:N	2.27	0.49
1:A:615:ASP:OD1	1:A:616:ILE:N	2.45	0.49
1:A:625:HIS:CG	1:A:626:ALA:H	2.30	0.49
1:B:38:TRP:HE3	1:B:39:PRO:HG2	1.78	0.49
1:B:125:LEU:HD11	1:B:191:ILE:HB	1.93	0.49
1:B:203:PRO:HD3	1:B:279:SER:HB3	1.94	0.49
1:C:38:TRP:HE3	1:C:39:PRO:HG2	1.78	0.49
1:C:106:TRP:H	1:C:135:LYS:HZ1	1.60	0.49
1:C:43:SER:OG	1:C:59:MET:SD	2.70	0.49
1:A:116:ASN:N	1:A:194:GLN:HE21	2.10	0.49
1:D:203:PRO:HD3	1:D:279:SER:HB3	1.94	0.49
1:C:625:HIS:CG	1:C:626:ALA:H	2.30	0.49
1:D:116:ASN:N	1:D:194:GLN:HE21	2.10	0.49
1:B:43:SER:OG	1:B:59:MET:SD	2.70	0.49
1:B:625:HIS:CG	1:B:626:ALA:H	2.30	0.49
1:C:78:ILE:HG13	1:C:79:GLU:N	2.26	0.49
1:C:615:ASP:OD1	1:C:616:ILE:N	2.45	0.49
1:D:43:SER:OG	1:D:59:MET:SD	2.70	0.49
1:A:676:PHE:HB2	1:D:38:TRP:CE2	2.47	0.49
1:B:200:PRO:HB3	1:B:277:VAL:HG21	1.94	0.49
1:C:116:ASN:N	1:C:194:GLN:HE21	2.10	0.49
1:A:43:SER:OG	1:A:59:MET:SD	2.70	0.49
1:B:38:TRP:CE2	1:C:676:PHE:HB2	2.47	0.49
1:B:56:ALA:HA	1:B:61:LYS:HZ3	1.77	0.49
1:A:38:TRP:CE2	1:B:676:PHE:HB2	2.47	0.48
1:D:38:TRP:HE3	1:D:39:PRO:HG2	1.78	0.48
1:D:200:PRO:HB3	1:D:277:VAL:HG21	1.94	0.48
1:C:203:PRO:HD3	1:C:279:SER:HB3	1.94	0.48
1:A:38:TRP:HE3	1:A:39:PRO:HG2	1.78	0.48
1:A:200:PRO:HB3	1:A:277:VAL:HG21	1.94	0.48
1:C:200:PRO:HB3	1:C:277:VAL:HG21	1.94	0.48
1:C:26:SER:HB2	1:C:127:THR:HG23	1.95	0.48
1:D:26:SER:HB2	1:D:127:THR:HG23	1.95	0.48
1:D:78:ILE:HG13	1:D:79:GLU:H	1.79	0.48
1:D:342:LEU:HD22	1:D:348:VAL:HG22	1.96	0.48
1:A:529:PRO:HG3	1:B:508:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:PRO:HG3	1:C:508:TYR:CZ	2.49	0.48
1:C:162:VAL:HG12	1:C:163:LEU:HD12	1.96	0.48
1:A:78:ILE:HG13	1:A:79:GLU:H	1.79	0.48
1:A:342:LEU:HD22	1:A:348:VAL:HG22	1.96	0.48
1:B:95:VAL:HG22	1:B:96:LEU:H	1.79	0.48
1:B:116:ASN:N	1:B:194:GLN:HE21	2.10	0.48
1:C:78:ILE:HG13	1:C:79:GLU:H	1.79	0.48
1:C:156:LEU:HD11	1:C:158:ASN:HB2	1.96	0.48
1:D:133:LEU:HB2	1:D:156:LEU:HD22	1.96	0.47
1:A:508:TYR:CZ	1:D:529:PRO:HG3	2.49	0.47
1:A:677:ARG:C	1:D:38:TRP:CD1	2.83	0.47
1:B:109:MET:HE3	1:B:111:ILE:HD11	1.97	0.47
1:B:156:LEU:HD11	1:B:158:ASN:HB2	1.96	0.47
1:B:342:LEU:HD22	1:B:348:VAL:HG22	1.96	0.47
1:C:133:LEU:HB2	1:C:156:LEU:HD22	1.96	0.47
1:A:26:SER:HB2	1:A:127:THR:HG23	1.95	0.47
1:A:37:ASP:H	1:B:677:ARG:C	2.23	0.47
1:A:110:GLN:OE1	1:A:183:GLU:N	2.48	0.47
1:A:133:LEU:HB2	1:A:156:LEU:HD22	1.96	0.47
1:B:127:THR:HG22	1:B:129:LYS:HZ2	1.80	0.47
1:C:342:LEU:HD22	1:C:348:VAL:HG22	1.96	0.47
1:A:677:ARG:C	1:D:37:ASP:H	2.23	0.47
1:B:162:VAL:HG12	1:B:163:LEU:HD12	1.96	0.47
1:D:156:LEU:HD11	1:D:158:ASN:HB2	1.96	0.47
1:A:156:LEU:HD11	1:A:158:ASN:HB2	1.96	0.47
1:B:78:ILE:HG13	1:B:79:GLU:H	1.79	0.47
1:B:99:LYS:HZ1	1:B:156:LEU:HA	1.79	0.47
1:B:133:LEU:HB2	1:B:156:LEU:HD22	1.96	0.47
1:C:529:PRO:HG3	1:D:508:TYR:CZ	2.49	0.47
1:A:622:THR:OG1	1:A:671:ARG:NH2	2.48	0.47
1:B:26:SER:HB2	1:B:127:THR:HG23	1.95	0.47
1:B:41:VAL:HG12	1:B:42:TYR:CD1	2.50	0.47
1:D:41:VAL:HG12	1:D:42:TYR:CD1	2.50	0.47
1:A:35:ILE:C	1:B:678:LYS:H	2.22	0.47
1:A:105:VAL:HG22	1:A:132:THR:HG23	1.97	0.47
1:A:678:LYS:H	1:D:35:ILE:C	2.22	0.47
1:C:194:GLN:OE1	1:C:194:GLN:N	2.41	0.47
1:D:105:VAL:HG22	1:D:132:THR:HG23	1.97	0.47
1:D:110:GLN:OE1	1:D:183:GLU:N	2.48	0.47
1:D:122:VAL:HG12	1:D:123:LEU:HD12	1.97	0.47
1:D:162:VAL:HG12	1:D:163:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:THR:OG1	1:D:671:ARG:NH2	2.48	0.47
1:A:41:VAL:HG12	1:A:42:TYR:CD1	2.50	0.47
1:C:41:VAL:HG12	1:C:42:TYR:CD1	2.50	0.47
1:C:109:MET:HE3	1:C:111:ILE:HD11	1.97	0.47
1:C:110:GLN:OE1	1:C:183:GLU:N	2.48	0.47
1:C:122:VAL:HG12	1:C:123:LEU:HD12	1.97	0.47
1:A:40:VAL:HB	1:A:63:SER:HA	1.97	0.47
1:B:97:LEU:HB2	1:B:107:PHE:CZ	2.50	0.47
1:D:109:MET:HE3	1:D:111:ILE:HD11	1.97	0.47
1:A:38:TRP:CD1	1:B:677:ARG:C	2.83	0.47
1:A:569:ILE:HD11	1:A:638:LEU:HD12	1.97	0.47
1:C:105:VAL:HG22	1:C:132:THR:HG23	1.97	0.47
1:D:95:VAL:HG22	1:D:96:LEU:H	1.79	0.47
1:D:569:ILE:HD11	1:D:638:LEU:HD12	1.97	0.47
1:A:12:GLN:HG3	1:A:14:THR:HG23	1.97	0.46
1:B:37:ASP:H	1:C:677:ARG:C	2.23	0.46
1:B:40:VAL:HB	1:B:63:SER:HA	1.97	0.46
1:C:35:ILE:C	1:D:678:LYS:H	2.22	0.46
1:C:95:VAL:HG22	1:C:96:LEU:H	1.79	0.46
1:C:215:THR:O	1:C:219:TRP:HE3	1.98	0.46
1:A:95:VAL:HG22	1:A:96:LEU:H	1.79	0.46
1:B:622:THR:OG1	1:B:671:ARG:NH2	2.48	0.46
1:C:292:TRP:CE2	1:C:336:ARG:HD2	2.51	0.46
1:D:56:ALA:HA	1:D:61:LYS:HZ3	1.79	0.46
1:A:381:ASN:OD1	1:A:409:TRP:NE1	2.47	0.46
1:D:65:CYS:H	1:D:85:PHE:HD2	1.64	0.46
1:D:106:TRP:H	1:D:135:LYS:HZ1	1.64	0.46
1:D:292:TRP:CE2	1:D:336:ARG:HD2	2.51	0.46
1:A:162:VAL:HG12	1:A:163:LEU:HD12	1.96	0.46
1:B:35:ILE:C	1:C:678:LYS:H	2.22	0.46
1:C:622:THR:OG1	1:C:671:ARG:NH2	2.48	0.46
1:B:65:CYS:H	1:B:85:PHE:HD2	1.64	0.46
1:C:214:LYS:HD2	1:C:214:LYS:HA	1.75	0.46
1:B:32:ASN:HB2	1:C:678:LYS:HG2	1.98	0.46
1:B:122:VAL:HG12	1:B:123:LEU:HD12	1.97	0.46
1:C:65:CYS:H	1:C:85:PHE:HD2	1.64	0.46
1:C:569:ILE:HD11	1:C:638:LEU:HD12	1.98	0.46
1:A:215:THR:O	1:A:219:TRP:HE3	1.98	0.46
1:A:292:TRP:CE2	1:A:336:ARG:HD2	2.51	0.46
1:B:105:VAL:HG22	1:B:132:THR:HG23	1.97	0.46
1:B:110:GLN:OE1	1:B:183:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ASN:HB2	1:D:678:LYS:HG2	1.98	0.46
1:C:40:VAL:HB	1:C:63:SER:HA	1.97	0.46
1:D:12:GLN:HG3	1:D:14:THR:HG23	1.97	0.46
1:D:97:LEU:HB2	1:D:107:PHE:CZ	2.50	0.46
1:A:539:HIS:O	1:A:542:ARG:HB2	2.16	0.46
1:C:541:ASN:O	1:C:543:LYS:N	2.49	0.46
1:D:539:HIS:O	1:D:542:ARG:HB2	2.16	0.46
1:A:65:CYS:H	1:A:85:PHE:HD2	1.64	0.46
1:A:122:VAL:HG12	1:A:123:LEU:HD12	1.97	0.46
1:B:215:THR:O	1:B:219:TRP:HE3	1.98	0.46
1:C:34:GLN:OE1	1:C:35:ILE:HG12	2.16	0.46
1:C:37:ASP:H	1:D:677:ARG:C	2.23	0.46
1:D:290:LYS:HB3	1:D:290:LYS:HE3	1.79	0.46
1:D:541:ASN:O	1:D:543:LYS:N	2.49	0.46
1:A:280:ASP:N	1:A:280:ASP:OD1	2.48	0.46
1:B:541:ASN:O	1:B:543:LYS:N	2.49	0.46
1:A:485:LEU:HD22	1:A:506:MET:HE1	1.98	0.45
1:B:569:ILE:HD11	1:B:638:LEU:HD12	1.98	0.45
1:C:539:HIS:O	1:C:542:ARG:HB2	2.16	0.45
1:D:86:ASP:HA	1:D:88:TYR:CE1	2.51	0.45
1:D:194:GLN:OE1	1:D:194:GLN:N	2.41	0.45
1:D:485:LEU:HD22	1:D:506:MET:HE1	1.98	0.45
1:B:86:ASP:HA	1:B:88:TYR:CE1	2.51	0.45
1:B:381:ASN:OD1	1:B:409:TRP:NE1	2.47	0.45
1:D:62:SER:OG	1:D:64:THR:O	2.34	0.45
1:A:86:ASP:HA	1:A:88:TYR:CE1	2.51	0.45
1:A:116:ASN:OD1	1:A:121:VAL:N	2.50	0.45
1:A:160:ARG:HH21	1:A:165:GLN:C	2.25	0.45
1:B:129:LYS:HA	1:B:129:LYS:HD3	1.77	0.45
1:B:292:TRP:CE2	1:B:336:ARG:HD2	2.51	0.45
1:D:34:GLN:OE1	1:D:35:ILE:HG12	2.16	0.45
1:D:40:VAL:HB	1:D:63:SER:HA	1.97	0.45
1:D:116:ASN:OD1	1:D:121:VAL:N	2.50	0.45
1:A:22:ARG:HD2	1:A:23:SER:N	2.32	0.45
1:C:86:ASP:HA	1:C:88:TYR:CE1	2.51	0.45
1:C:116:ASN:OD1	1:C:121:VAL:N	2.50	0.45
1:D:19:ILE:HG22	1:D:192:LEU:HD23	1.98	0.45
1:D:520:ASP:OD1	1:D:520:ASP:N	2.49	0.45
1:A:32:ASN:HB2	1:B:678:LYS:HG2	1.98	0.45
1:A:109:MET:HE3	1:A:111:ILE:HD11	1.97	0.45
1:B:34:GLN:OE1	1:B:35:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ARG:HH21	1:C:165:GLN:C	2.25	0.45
1:D:381:ASN:OD1	1:D:409:TRP:NE1	2.47	0.45
1:A:34:GLN:OE1	1:A:35:ILE:HG12	2.16	0.45
1:A:595:LEU:O	1:A:607:LEU:N	2.50	0.45
1:C:19:ILE:HG22	1:C:192:LEU:HD23	1.98	0.45
1:B:19:ILE:HG22	1:B:192:LEU:HD23	1.98	0.45
1:D:280:ASP:OD1	1:D:280:ASP:N	2.48	0.45
1:D:324:LYS:HA	1:D:327:ARG:HB3	1.99	0.45
1:A:678:LYS:HG2	1:D:32:ASN:HB2	1.98	0.45
1:B:12:GLN:HG3	1:B:14:THR:HG23	1.97	0.45
1:B:15:PHE:HB3	1:B:42:TYR:CE2	2.52	0.45
1:C:280:ASP:N	1:C:280:ASP:OD1	2.48	0.45
1:C:485:LEU:HD22	1:C:506:MET:HE1	1.98	0.45
1:B:22:ARG:HD2	1:B:23:SER:N	2.32	0.45
1:B:38:TRP:CD1	1:C:677:ARG:C	2.83	0.45
1:C:324:LYS:HA	1:C:327:ARG:HB3	1.99	0.45
1:C:595:LEU:O	1:C:607:LEU:N	2.50	0.45
1:B:539:HIS:O	1:B:542:ARG:HB2	2.16	0.45
1:C:12:GLN:HG3	1:C:14:THR:HG23	1.97	0.45
1:A:19:ILE:HG22	1:A:192:LEU:HD23	1.98	0.44
1:A:30:LEU:HD12	1:A:41:VAL:HG21	1.99	0.44
1:A:194:GLN:OE1	1:A:194:GLN:N	2.41	0.44
1:A:541:ASN:O	1:A:543:LYS:N	2.49	0.44
1:C:30:LEU:HD12	1:C:41:VAL:HG21	1.99	0.44
1:D:160:ARG:HH21	1:D:165:GLN:C	2.25	0.44
1:D:215:THR:O	1:D:219:TRP:HE3	1.98	0.44
1:C:22:ARG:HD2	1:C:23:SER:N	2.32	0.44
1:C:597:VAL:HG11	1:C:668:CYS:SG	2.57	0.44
1:D:22:ARG:HD2	1:D:23:SER:N	2.32	0.44
1:D:598:ILE:HG12	1:D:603:VAL:HG12	2.00	0.44
1:B:35:ILE:C	1:C:678:LYS:O	2.60	0.44
1:B:116:ASN:OD1	1:B:121:VAL:N	2.50	0.44
1:A:290:LYS:HB3	1:A:290:LYS:HE3	1.79	0.44
1:B:485:LEU:HD22	1:B:506:MET:HE1	1.98	0.44
1:C:15:PHE:HB3	1:C:42:TYR:CE2	2.52	0.44
1:C:62:SER:OG	1:C:64:THR:O	2.34	0.44
1:C:215:THR:HG23	1:C:219:TRP:HZ3	1.81	0.44
1:D:232:VAL:HG13	1:D:324:LYS:HB3	2.00	0.44
1:D:595:LEU:O	1:D:607:LEU:N	2.50	0.44
1:A:597:VAL:HG11	1:A:668:CYS:SG	2.57	0.44
1:A:678:LYS:O	1:D:35:ILE:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:HH21	1:B:165:GLN:C	2.25	0.44
1:B:342:LEU:O	1:B:343:GLU:HG2	2.18	0.44
1:C:598:ILE:HG12	1:C:603:VAL:HG12	2.00	0.44
1:A:35:ILE:C	1:B:678:LYS:O	2.60	0.44
1:B:598:ILE:HG12	1:B:603:VAL:HG12	2.00	0.44
1:C:35:ILE:C	1:D:678:LYS:O	2.60	0.44
1:D:71:GLU:HB2	1:D:96:LEU:HD21	2.00	0.44
1:A:39:PRO:HB3	1:A:41:VAL:CG2	2.47	0.44
1:C:39:PRO:HB3	1:C:41:VAL:CG2	2.47	0.44
1:C:342:LEU:O	1:C:343:GLU:HG2	2.18	0.44
1:D:15:PHE:HB3	1:D:42:TYR:CE2	2.52	0.44
1:A:15:PHE:HB3	1:A:42:TYR:CE2	2.52	0.44
1:B:597:VAL:HG11	1:B:668:CYS:SG	2.57	0.44
1:C:97:LEU:HB2	1:C:107:PHE:CZ	2.50	0.44
1:A:232:VAL:HG13	1:A:324:LYS:HB3	2.00	0.44
1:B:62:SER:OG	1:B:64:THR:O	2.34	0.44
1:B:595:LEU:O	1:B:607:LEU:N	2.50	0.44
1:D:39:PRO:HB3	1:D:41:VAL:CG2	2.47	0.44
1:D:597:VAL:HG11	1:D:668:CYS:SG	2.57	0.44
1:A:22:ARG:HD2	1:A:22:ARG:C	2.43	0.43
1:A:71:GLU:HB2	1:A:96:LEU:HD21	2.00	0.43
1:A:296:ASP:OD1	1:A:333:ARG:NH2	2.51	0.43
1:B:214:LYS:HD2	1:B:214:LYS:HA	1.75	0.43
1:C:99:LYS:HZ1	1:C:157:THR:H	1.65	0.43
1:B:38:TRP:CE3	1:B:39:PRO:HD2	2.53	0.43
1:B:296:ASP:OD1	1:B:333:ARG:NH2	2.51	0.43
1:C:71:GLU:HB2	1:C:96:LEU:HD21	2.00	0.43
1:D:22:ARG:HD2	1:D:22:ARG:C	2.43	0.43
1:A:598:ILE:HG12	1:A:603:VAL:HG12	2.00	0.43
1:B:324:LYS:HA	1:B:327:ARG:HB3	1.99	0.43
1:C:172:THR:HG22	1:C:176:HIS:HD2	1.83	0.43
1:D:342:LEU:O	1:D:343:GLU:HG2	2.18	0.43
1:A:28:PHE:N	1:A:42:TYR:O	2.52	0.43
1:A:38:TRP:CE3	1:A:39:PRO:HD2	2.53	0.43
1:A:97:LEU:HB2	1:A:107:PHE:CZ	2.50	0.43
1:A:172:THR:HG22	1:A:176:HIS:HD2	1.83	0.43
1:B:28:PHE:N	1:B:42:TYR:O	2.52	0.43
1:C:22:ARG:HD2	1:C:22:ARG:C	2.43	0.43
1:C:232:VAL:HG13	1:C:324:LYS:HB3	2.00	0.43
1:D:172:THR:HG22	1:D:176:HIS:HD2	1.83	0.43
1:D:30:LEU:HD12	1:D:41:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD12	1:B:41:VAL:HG21	1.99	0.43
1:B:99:LYS:HZ1	1:B:157:THR:N	2.10	0.43
1:B:232:VAL:HG13	1:B:324:LYS:HB3	2.00	0.43
1:C:515:MET:HE1	1:C:570:HIS:CE1	2.54	0.43
1:D:363:LEU:HD13	1:D:452:MET:HG3	2.01	0.43
1:A:363:LEU:HD13	1:A:452:MET:HG3	2.01	0.43
1:A:684:LYS:O	1:A:688:GLU:HG2	2.19	0.43
1:B:363:LEU:HD13	1:B:452:MET:HG3	2.01	0.43
1:D:214:LYS:HD2	1:D:214:LYS:HA	1.75	0.43
1:C:578:TYR:H	1:C:630:VAL:CG2	2.32	0.43
1:D:615:ASP:CG	1:D:671:ARG:HD3	2.44	0.43
1:A:96:LEU:HA	1:A:105:VAL:O	2.19	0.43
1:A:324:LYS:HA	1:A:327:ARG:HB3	1.99	0.43
1:A:615:ASP:CG	1:A:671:ARG:HD3	2.44	0.43
1:B:71:GLU:HB2	1:B:96:LEU:HD21	2.00	0.43
1:B:578:TYR:H	1:B:630:VAL:CG2	2.32	0.43
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.83	0.43
1:C:363:LEU:HD13	1:C:452:MET:HG3	2.01	0.43
1:D:38:TRP:CE3	1:D:39:PRO:HD2	2.53	0.43
1:D:96:LEU:HA	1:D:105:VAL:O	2.19	0.43
1:D:515:MET:HE1	1:D:570:HIS:CE1	2.54	0.43
1:A:74:ASP:HB2	1:A:77:THR:HG23	2.01	0.42
1:B:515:MET:HE1	1:B:570:HIS:CE1	2.54	0.42
1:C:38:TRP:CE3	1:C:39:PRO:HD2	2.53	0.42
1:D:74:ASP:HB2	1:D:77:THR:HG23	2.01	0.42
1:D:127:THR:HG22	1:D:129:LYS:HZ2	1.84	0.42
1:A:185:LEU:HD12	1:A:186:GLN:HG3	2.01	0.42
1:B:446:LYS:O	1:B:450:VAL:HG13	2.19	0.42
1:D:28:PHE:N	1:D:42:TYR:O	2.52	0.42
1:D:129:LYS:HA	1:D:129:LYS:HD3	1.77	0.42
1:D:327:ARG:NH1	1:D:330:ARG:HH12	2.18	0.42
1:A:214:LYS:HD2	1:A:214:LYS:HA	1.75	0.42
1:B:39:PRO:HB3	1:B:41:VAL:CG2	2.47	0.42
1:C:28:PHE:N	1:C:42:TYR:O	2.52	0.42
1:C:96:LEU:HA	1:C:105:VAL:O	2.19	0.42
1:D:684:LYS:O	1:D:688:GLU:HG2	2.19	0.42
1:B:22:ARG:HD2	1:B:22:ARG:C	2.43	0.42
1:B:172:THR:HG22	1:B:176:HIS:HD2	1.83	0.42
1:B:194:GLN:OE1	1:B:194:GLN:N	2.41	0.42
1:C:617:PHE:HD2	1:C:646:LEU:HD23	1.85	0.42
1:D:446:LYS:O	1:D:450:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:NH1	1:A:330:ARG:HH12	2.18	0.42
1:A:342:LEU:O	1:A:343:GLU:HG2	2.18	0.42
1:A:515:MET:HE1	1:A:570:HIS:CE1	2.54	0.42
1:B:615:ASP:CG	1:B:671:ARG:HD3	2.44	0.42
1:B:617:PHE:HD2	1:B:646:LEU:HD23	1.85	0.42
1:D:228:THR:HG21	1:D:330:ARG:NH2	2.35	0.42
1:B:96:LEU:HA	1:B:105:VAL:O	2.19	0.42
1:C:485:LEU:HD23	1:C:485:LEU:HA	1.90	0.42
1:C:615:ASP:CG	1:C:671:ARG:HD3	2.44	0.42
1:A:446:LYS:O	1:A:450:VAL:HG13	2.19	0.42
1:A:578:TYR:H	1:A:630:VAL:CG2	2.32	0.42
1:C:53:TYR:CE2	1:C:68:MET:HB3	2.55	0.42
1:C:631:ARG:HG2	1:C:632:ALA:N	2.35	0.42
1:B:74:ASP:HB2	1:B:77:THR:HG23	2.01	0.42
1:B:280:ASP:OD1	1:B:280:ASP:N	2.48	0.42
1:B:631:ARG:HG2	1:B:632:ALA:N	2.35	0.42
1:C:327:ARG:NH1	1:C:330:ARG:HH12	2.18	0.42
1:D:458:LEU:O	1:D:462:THR:HG23	2.20	0.42
1:D:578:TYR:H	1:D:630:VAL:CG2	2.32	0.42
1:D:631:ARG:HG2	1:D:632:ALA:N	2.35	0.42
1:A:129:LYS:HA	1:A:129:LYS:HD3	1.78	0.42
1:B:185:LEU:HD12	1:B:186:GLN:HG3	2.01	0.42
1:C:228:THR:HG21	1:C:330:ARG:NH2	2.35	0.42
1:D:215:THR:HG23	1:D:219:TRP:HZ3	1.81	0.42
1:A:228:THR:HG21	1:A:330:ARG:NH2	2.35	0.42
1:C:38:TRP:CZ3	1:D:602:GLU:HB2	2.55	0.42
1:A:53:TYR:CE2	1:A:68:MET:HB3	2.55	0.41
1:B:684:LYS:O	1:B:688:GLU:HG2	2.19	0.41
1:A:458:LEU:O	1:A:462:THR:HG23	2.20	0.41
1:B:327:ARG:NH1	1:B:330:ARG:HH12	2.18	0.41
1:C:74:ASP:HB2	1:C:77:THR:HG23	2.01	0.41
1:C:381:ASN:OD1	1:C:409:TRP:NE1	2.47	0.41
1:D:99:LYS:HZ1	1:D:157:THR:H	1.67	0.41
1:C:127:THR:HG22	1:C:129:LYS:HZ2	1.85	0.41
1:C:446:LYS:O	1:C:450:VAL:HG13	2.19	0.41
1:A:103:THR:HG21	1:A:137:PRO:HB3	2.03	0.41
1:A:631:ARG:HG2	1:A:632:ALA:N	2.35	0.41
1:A:679:ILE:HB	1:D:37:ASP:O	2.20	0.41
1:B:37:ASP:O	1:C:679:ILE:HB	2.20	0.41
1:B:53:TYR:CE2	1:B:68:MET:HB3	2.55	0.41
1:B:94:GLU:HB3	1:B:106:TRP:CB	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:THR:HG21	1:B:330:ARG:NH2	2.35	0.41
1:C:22:ARG:NH2	1:C:191:ILE:HA	2.35	0.41
1:C:684:LYS:O	1:C:688:GLU:HG2	2.19	0.41
1:D:22:ARG:NH2	1:D:191:ILE:HA	2.35	0.41
1:D:54:HIS:O	1:D:59:MET:HB3	2.21	0.41
1:D:617:PHE:HD2	1:D:646:LEU:HD23	1.85	0.41
1:B:427:MET:HE2	1:B:427:MET:HB2	1.98	0.41
1:C:37:ASP:O	1:D:679:ILE:HB	2.20	0.41
1:C:185:LEU:HD12	1:C:186:GLN:HG3	2.01	0.41
1:C:425:PHE:O	1:C:428:THR:OG1	2.32	0.41
1:D:103:THR:HG21	1:D:137:PRO:HB3	2.03	0.41
1:D:677:ARG:HA	1:D:677:ARG:HD2	1.89	0.41
1:A:37:ASP:O	1:B:679:ILE:HB	2.20	0.41
1:A:38:TRP:CZ3	1:B:602:GLU:HB2	2.55	0.41
1:A:54:HIS:O	1:A:59:MET:HB3	2.21	0.41
1:A:62:SER:OG	1:A:64:THR:O	2.34	0.41
1:A:602:GLU:HB2	1:D:38:TRP:CZ3	2.55	0.41
1:B:68:MET:HG3	1:B:97:LEU:HD22	2.03	0.41
1:C:68:MET:HG3	1:C:97:LEU:HD22	2.03	0.41
1:C:129:LYS:HA	1:C:129:LYS:HD3	1.77	0.41
1:C:296:ASP:OD1	1:C:333:ARG:NH2	2.51	0.41
1:B:38:TRP:CZ3	1:C:602:GLU:HB2	2.55	0.41
1:C:458:LEU:O	1:C:462:THR:HG23	2.20	0.41
1:D:53:TYR:CE2	1:D:68:MET:HB3	2.55	0.41
1:D:58:VAL:HA	1:D:61:LYS:O	2.20	0.41
1:D:68:MET:HG3	1:D:97:LEU:HD22	2.03	0.41
1:D:97:LEU:HD23	1:D:97:LEU:HA	1.94	0.41
1:D:108:TYR:N	1:D:131:ILE:HG12	2.34	0.41
1:A:68:MET:HG3	1:A:97:LEU:HD22	2.03	0.41
1:B:54:HIS:O	1:B:59:MET:HB3	2.21	0.41
1:B:103:THR:HG21	1:B:137:PRO:HB3	2.03	0.41
1:C:54:HIS:O	1:C:59:MET:HB3	2.21	0.41
1:C:103:THR:HG21	1:C:137:PRO:HB3	2.03	0.41
1:D:16:LEU:HB2	1:D:42:TYR:OH	2.21	0.41
1:D:185:LEU:HD12	1:D:186:GLN:HG3	2.01	0.41
1:A:617:PHE:HD2	1:A:646:LEU:HD23	1.85	0.41
1:C:597:VAL:O	1:C:597:VAL:HG23	2.21	0.41
1:B:458:LEU:O	1:B:462:THR:HG23	2.20	0.40
1:C:58:VAL:HA	1:C:61:LYS:O	2.20	0.40
1:C:427:MET:HE2	1:C:427:MET:HB2	1.98	0.40
1:D:256:VAL:O	1:D:260:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:LEU:HD23	1:D:358:LEU:HA	1.83	0.40
1:A:58:VAL:HA	1:A:61:LYS:O	2.20	0.40
1:A:106:TRP:H	1:A:135:LYS:HZ1	1.65	0.40
1:A:256:VAL:O	1:A:260:VAL:HG23	2.22	0.40
1:B:58:VAL:HA	1:B:61:LYS:O	2.20	0.40
1:B:338:LEU:HD11	1:B:351:LEU:HD11	2.04	0.40
1:A:129:LYS:O	1:A:130:ASP:HB3	2.21	0.40
1:C:16:LEU:HB2	1:C:42:TYR:OH	2.21	0.40
1:D:296:ASP:OD1	1:D:333:ARG:NH2	2.51	0.40
1:B:129:LYS:O	1:B:130:ASP:HB3	2.21	0.40
1:A:16:LEU:HB2	1:A:42:TYR:OH	2.21	0.40
1:A:491:PHE:HA	1:D:519:ILE:HD13	2.04	0.40
1:B:22:ARG:NH2	1:B:191:ILE:HA	2.35	0.40
1:B:137:PRO:HB2	1:B:148:LYS:HB3	2.04	0.40
1:B:256:VAL:O	1:B:260:VAL:HG23	2.22	0.40
1:B:677:ARG:HD2	1:B:677:ARG:HA	1.89	0.40
1:B:690:LEU:HD23	1:B:690:LEU:HA	1.96	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	654/988 (66%)	556 (85%)	91 (14%)	7 (1%)	11	43
1	B	654/988 (66%)	556 (85%)	91 (14%)	7 (1%)	11	43
1	C	654/988 (66%)	556 (85%)	91 (14%)	7 (1%)	11	43
1	D	654/988 (66%)	556 (85%)	91 (14%)	7 (1%)	11	43
All	All	2616/3952 (66%)	2224 (85%)	364 (14%)	28 (1%)	14	43

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	38	TRP
1	A	39	PRO
1	A	387	SER
1	B	36	VAL
1	B	38	TRP
1	B	39	PRO
1	B	387	SER
1	C	36	VAL
1	C	38	TRP
1	C	39	PRO
1	C	387	SER
1	D	36	VAL
1	D	38	TRP
1	D	39	PRO
1	D	387	SER
1	A	41	VAL
1	B	41	VAL
1	C	41	VAL
1	D	41	VAL
1	A	130	ASP
1	A	376	ILE
1	B	130	ASP
1	B	376	ILE
1	C	130	ASP
1	C	376	ILE
1	D	130	ASP
1	D	376	ILE

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	595/888 (67%)	595 (100%)	0	100	100
1	B	595/888 (67%)	595 (100%)	0	100	100
1	C	595/888 (67%)	595 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	595/888 (67%)	595 (100%)	0	100	100
All	All	2380/3552 (67%)	2380 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	287	ASN
1	A	663	ASN
1	B	91	ASN
1	B	287	ASN
1	B	663	ASN
1	C	287	ASN
1	C	391	GLN
1	C	663	ASN
1	D	287	ASN
1	D	663	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

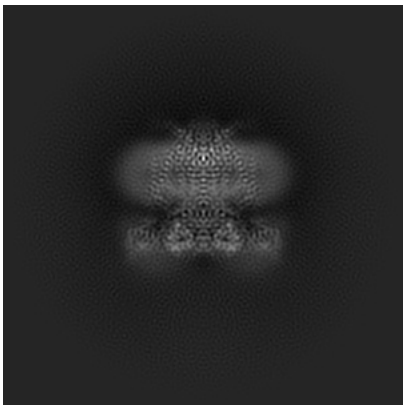
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33859. These allow visual inspection of the internal detail of the map and identification of artifacts.

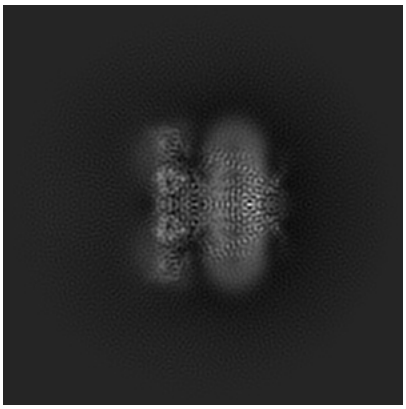
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

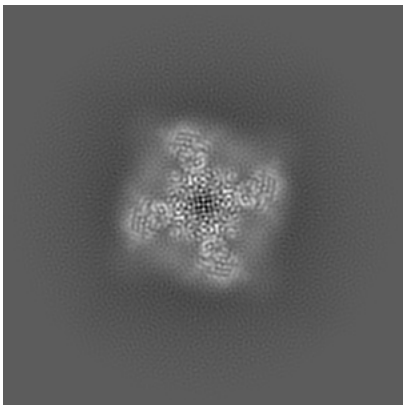
6.1.1 Primary map



X

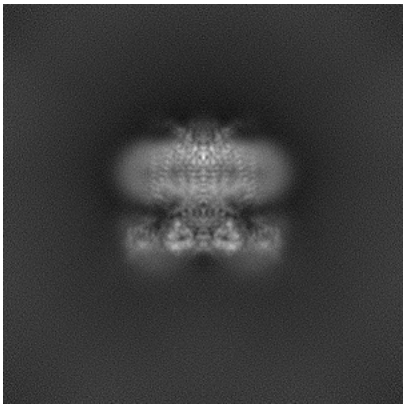


Y

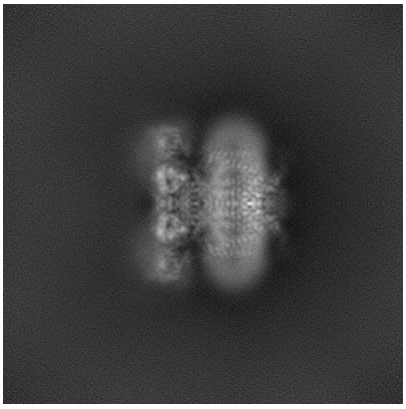


Z

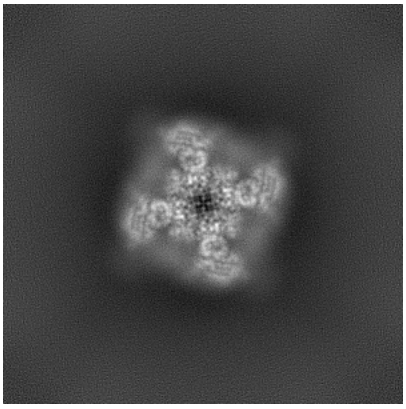
6.1.2 Raw map



X



Y

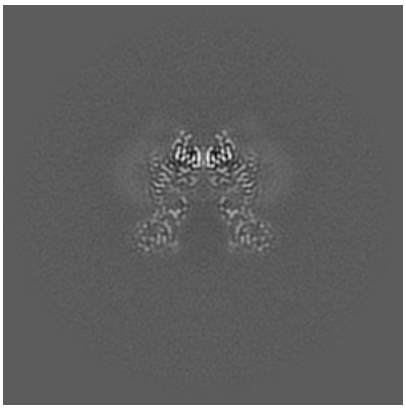


Z

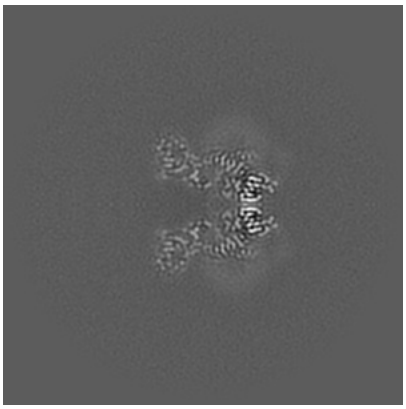
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

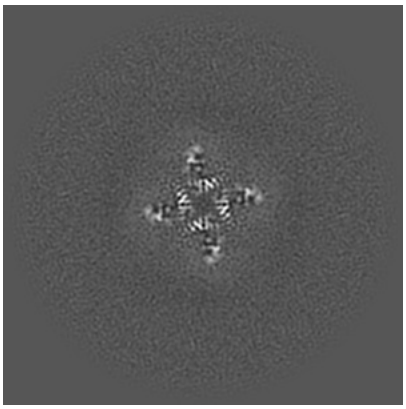
6.2.1 Primary map



X Index: 200

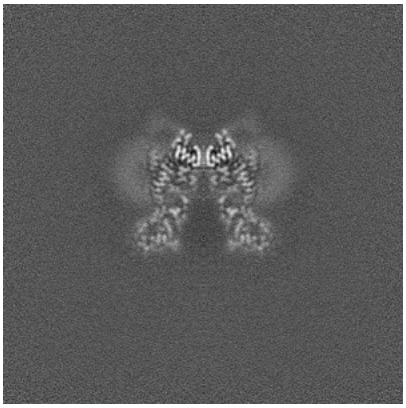


Y Index: 200

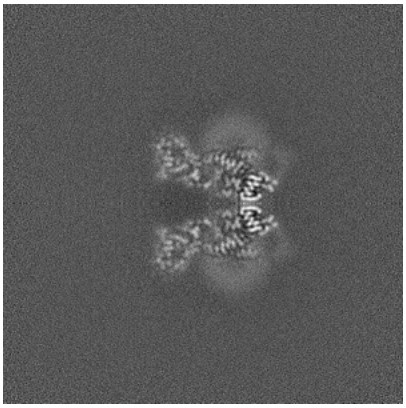


Z Index: 200

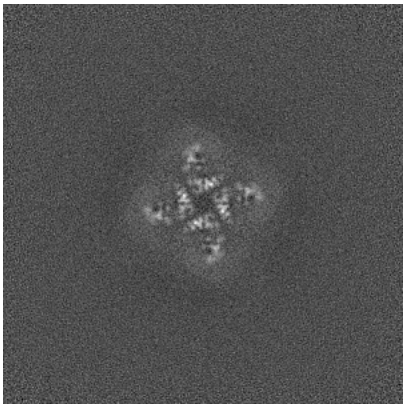
6.2.2 Raw map



X Index: 200



Y Index: 200

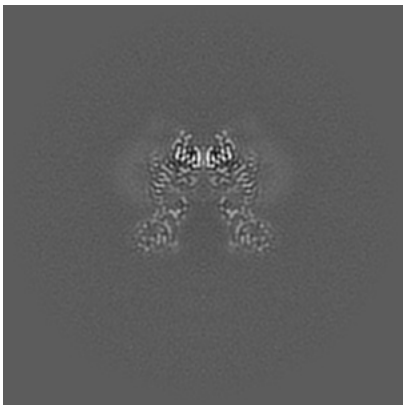


Z Index: 200

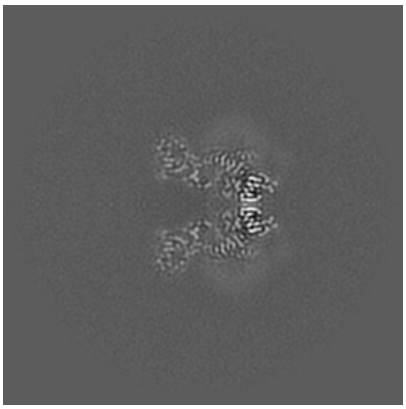
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

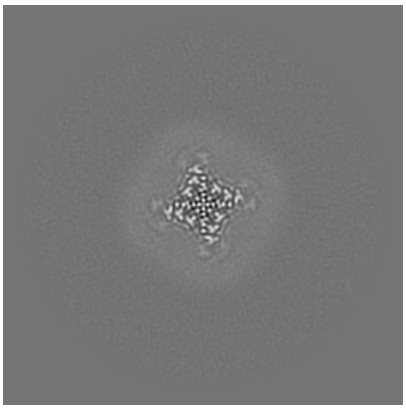
6.3.1 Primary map



X Index: 200

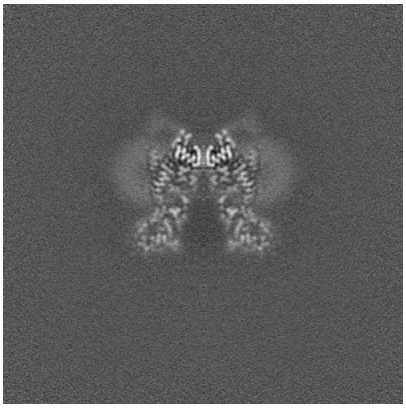


Y Index: 200

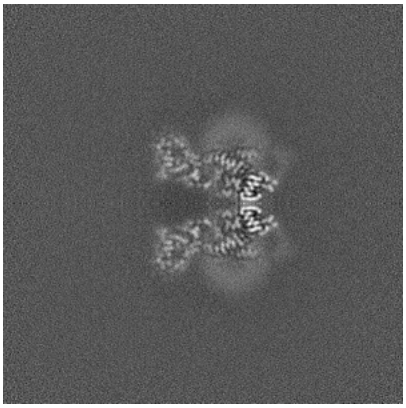


Z Index: 247

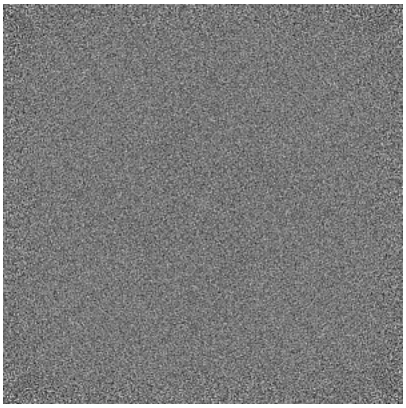
6.3.2 Raw map



X Index: 200



Y Index: 200

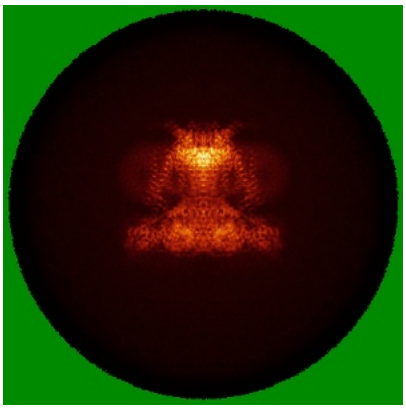


Z Index: 0

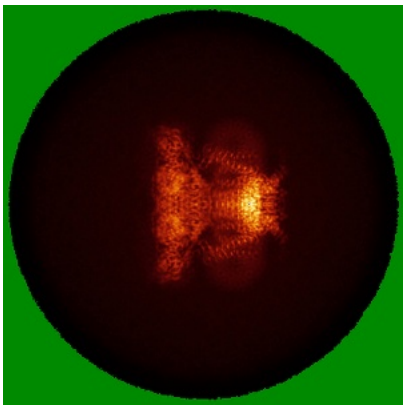
The images above show the largest variance slices of the map in three orthogonal directions.

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

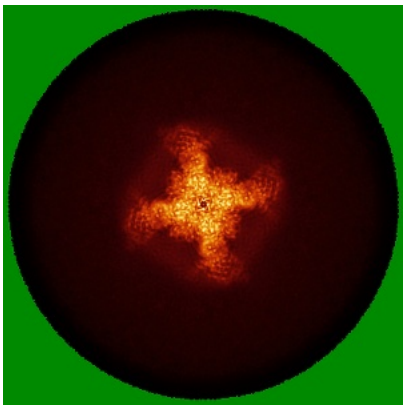
6.4.1 Primary map



X

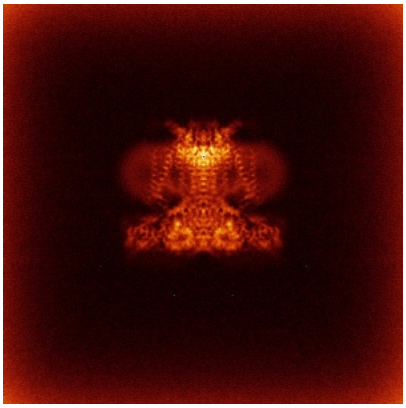


Y

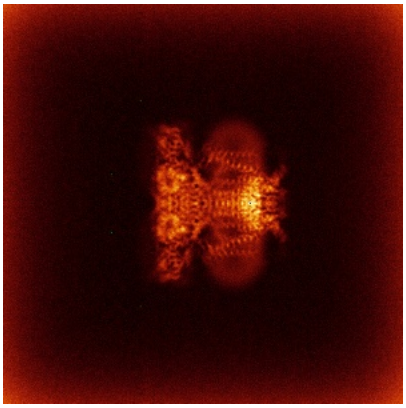


Z

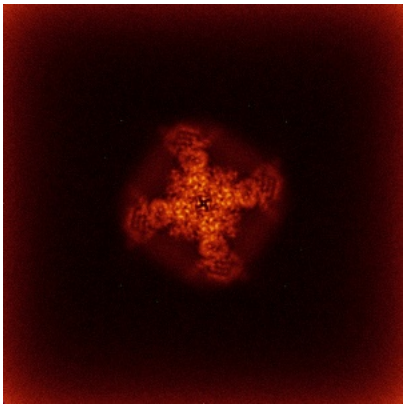
6.4.2 Raw map



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 0.25. 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.

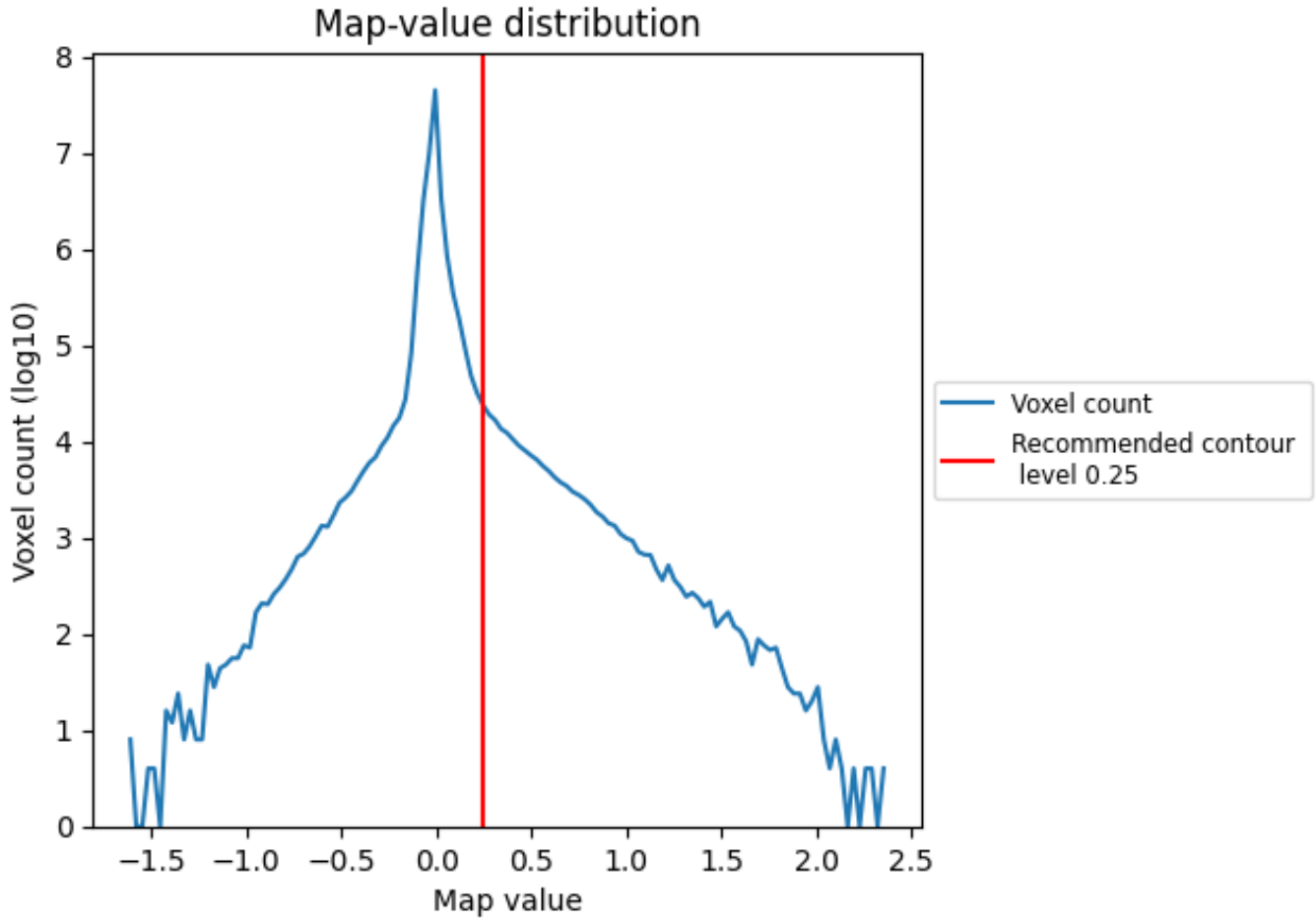
6.6 Mask visualisation (i)

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

7 Map analysis

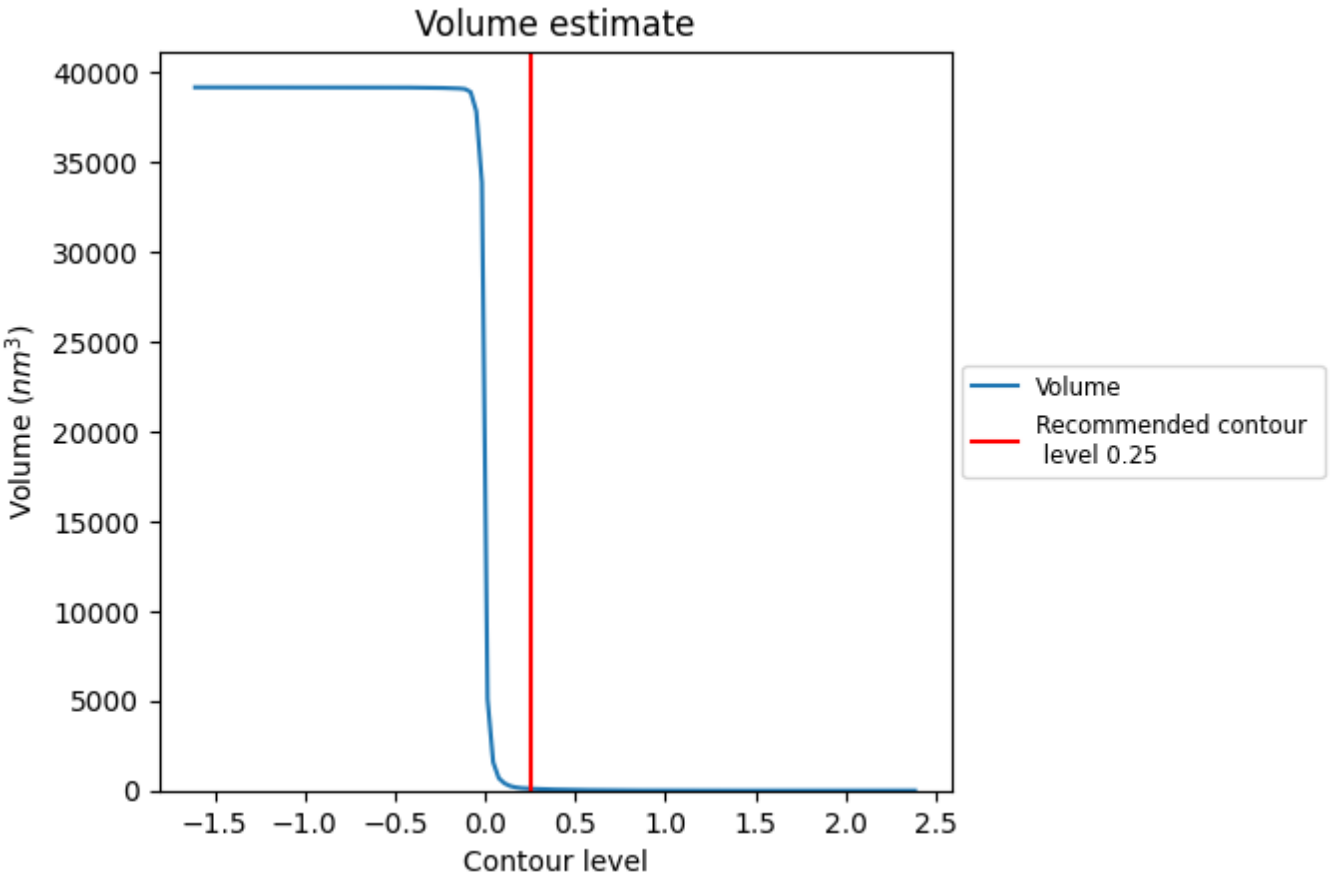
This section contains the results of statistical analysis of the map.

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.

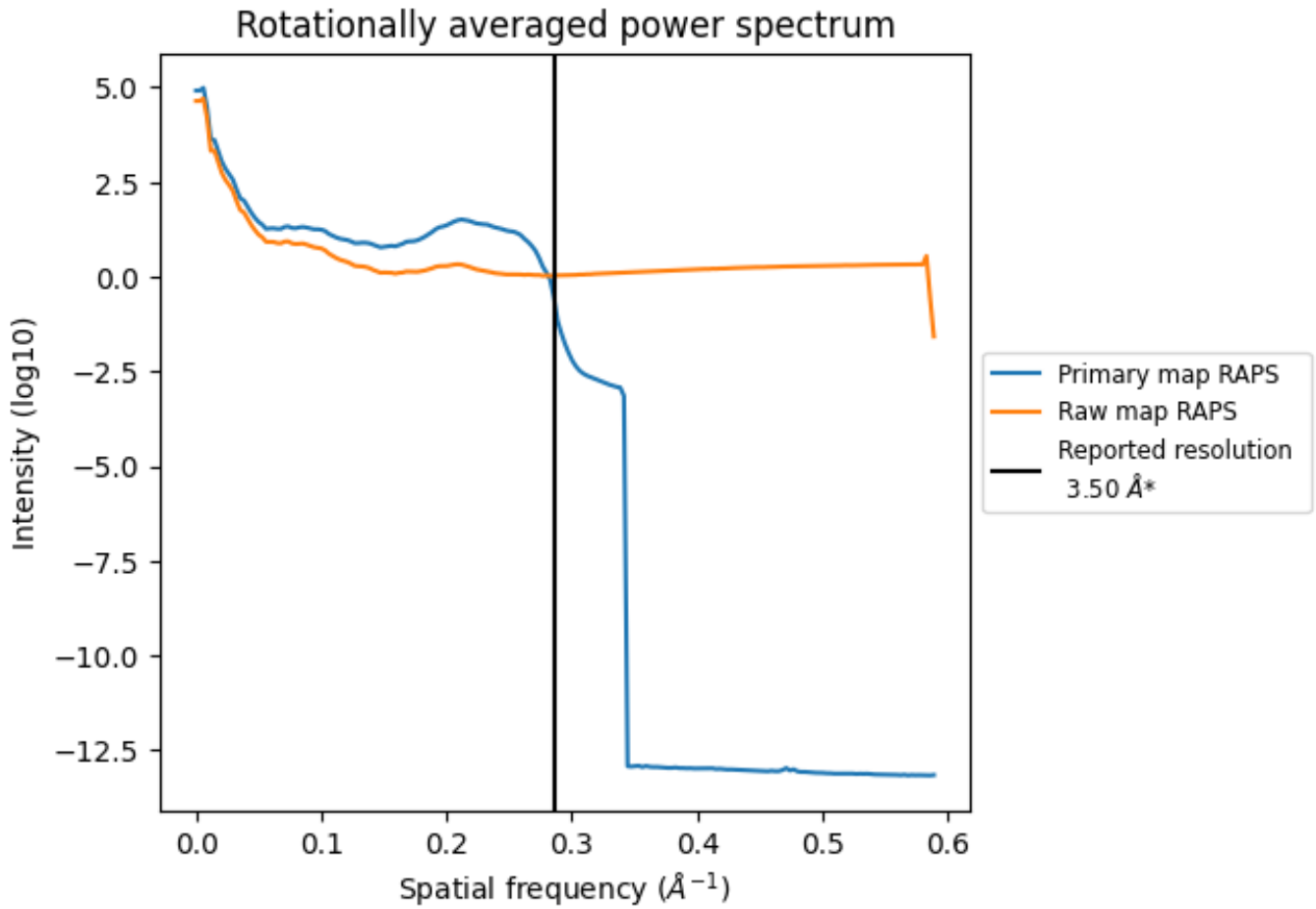
7.2 Volume estimate



The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 kDa.

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

7.3 Rotationally averaged power spectrum (i)

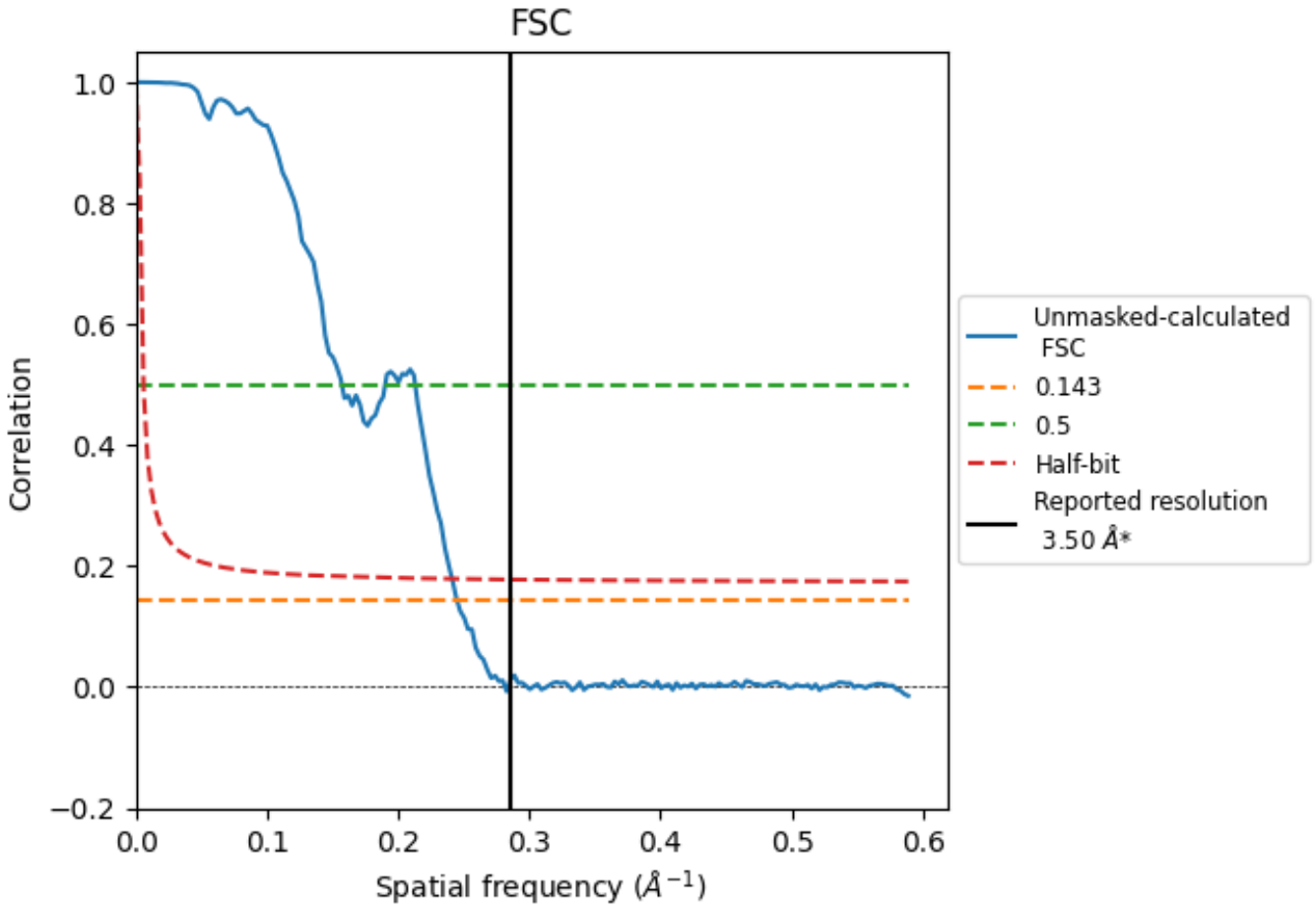


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

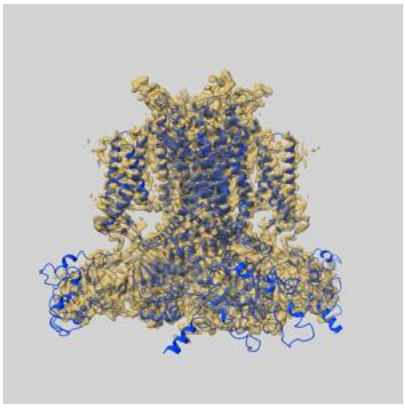
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	6.37	4.15

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

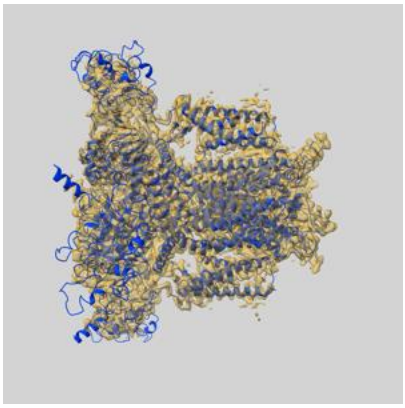
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33859 and PDB model 7YIH. Per-residue inclusion information can be found in section 3 on page 4.

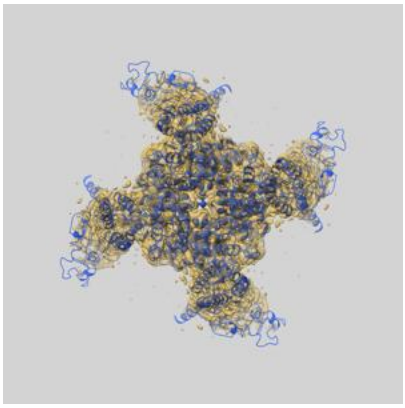
9.1 Map-model overlay



X



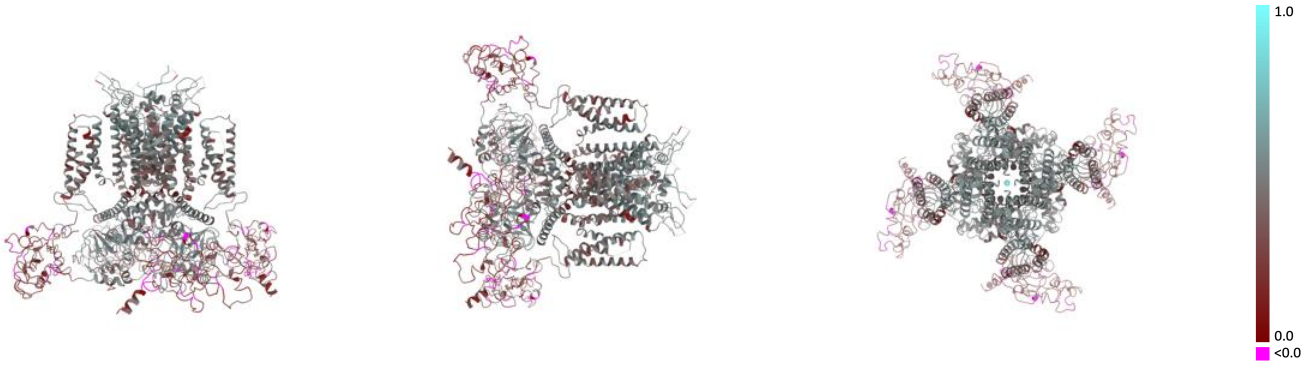
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

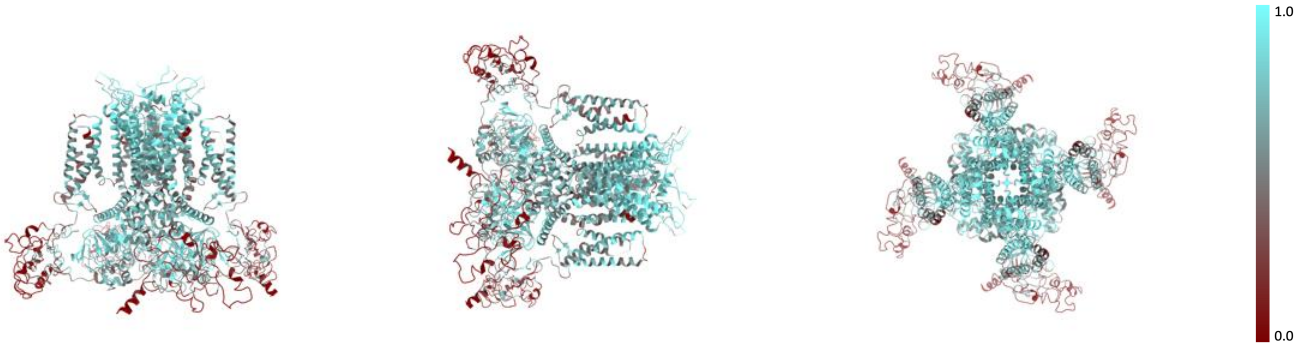
9.2 Q-score mapped to coordinate model (i)



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.

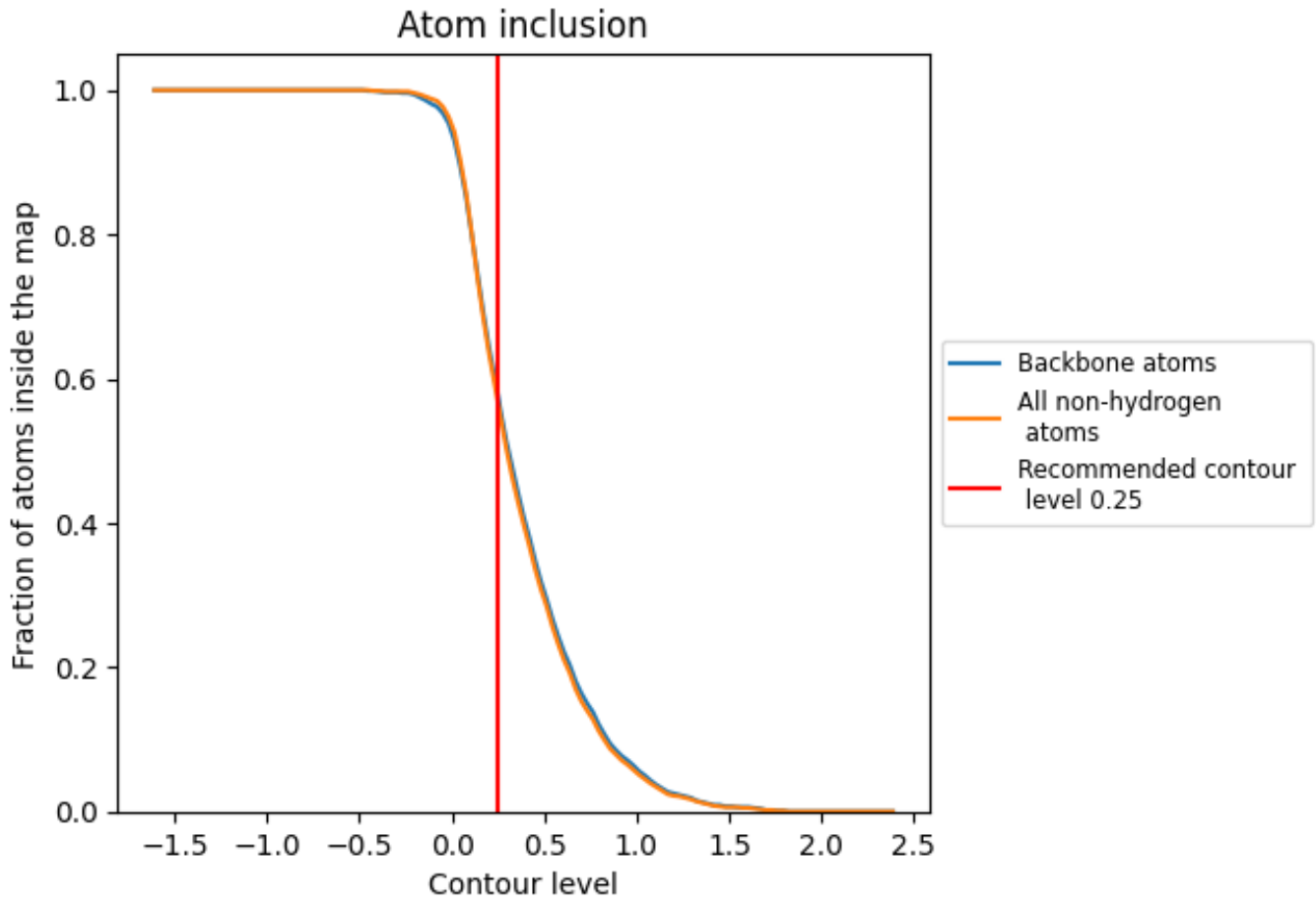
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 57% 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 (0.25) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.5670	0.3870
A	0.5740	0.3880
B	0.5730	0.3870
C	0.5730	0.3860
D	0.5730	0.3860