



Full wwPDB EM Validation Report ⓘ

Aug 8, 2023 – 04:19 PM JST

PDB ID : 8HIR
EMDB ID : EMD-34827
Title : potassium channels
Authors : Jiang, D.H.; Zhang, J.T.
Deposited on : 2022-11-21
Resolution : 3.18 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

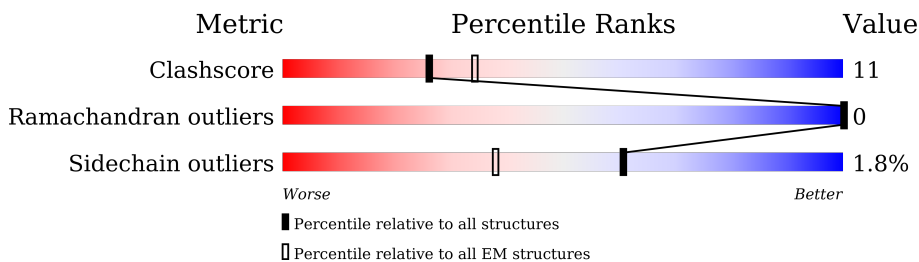
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1235	
1	B	1235	
1	C	1235	
1	D	1235	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 29168 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 channel subfamily T member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	918	7278	4716	1212	1298	52	0	0
1	B	918	7278	4716	1212	1298	52	0	0
1	C	918	7278	4716	1212	1298	52	0	0
1	D	918	7278	4716	1212	1298	52	0	0

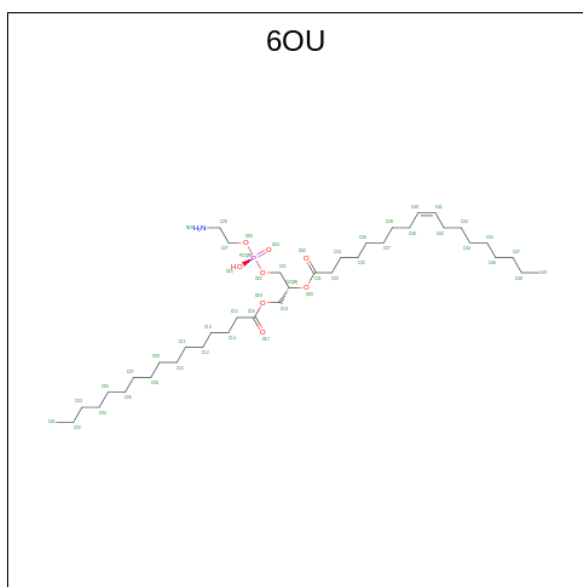
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
3	A	4	Total	K	0
			4	4	

- Molecule 4 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: C₃₉H₇₆NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C 11 11	0
4	B	1	Total C 11 11	0
4	C	1	Total C 11 11	0
4	D	1	Total C 11 11	0

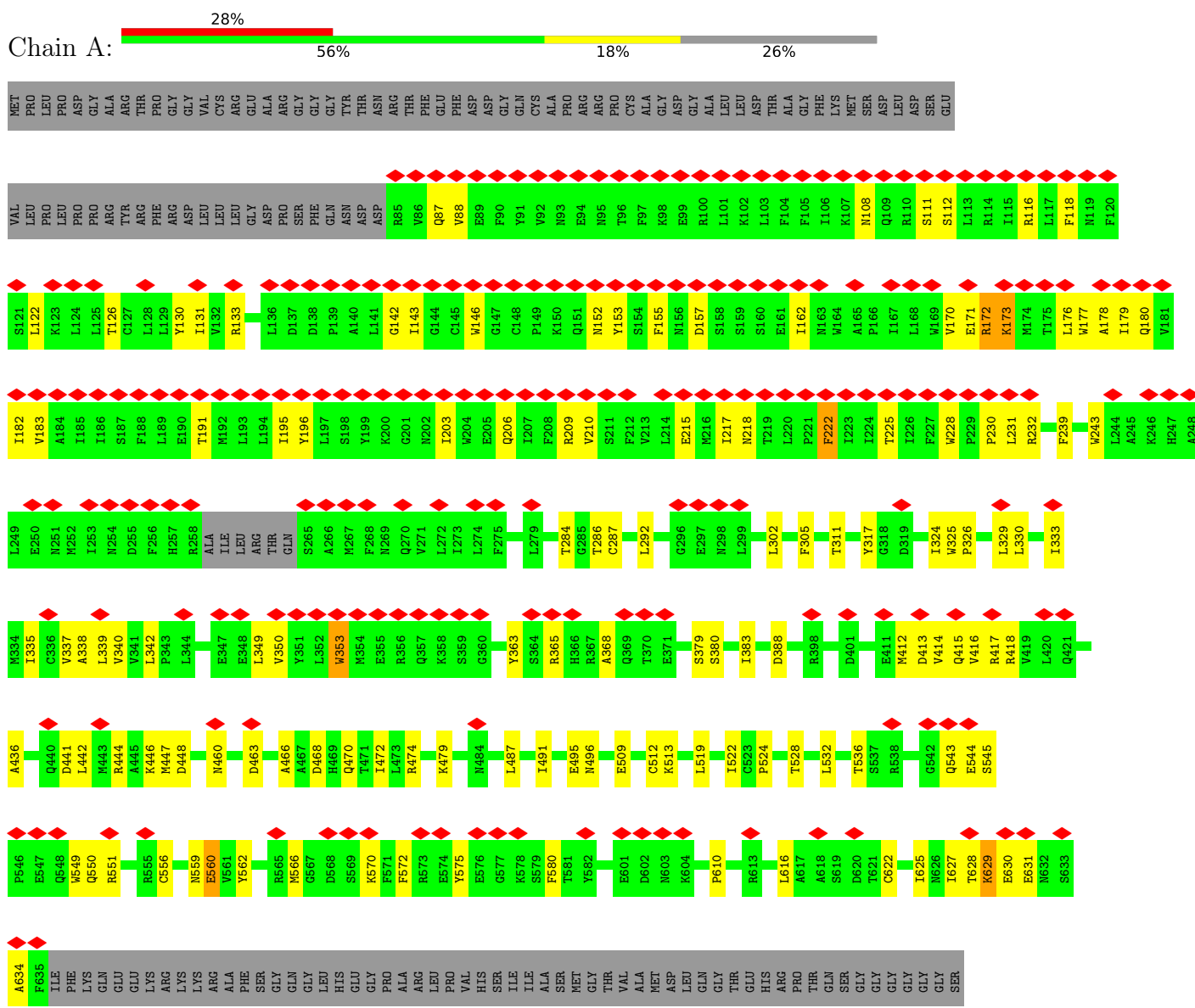
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

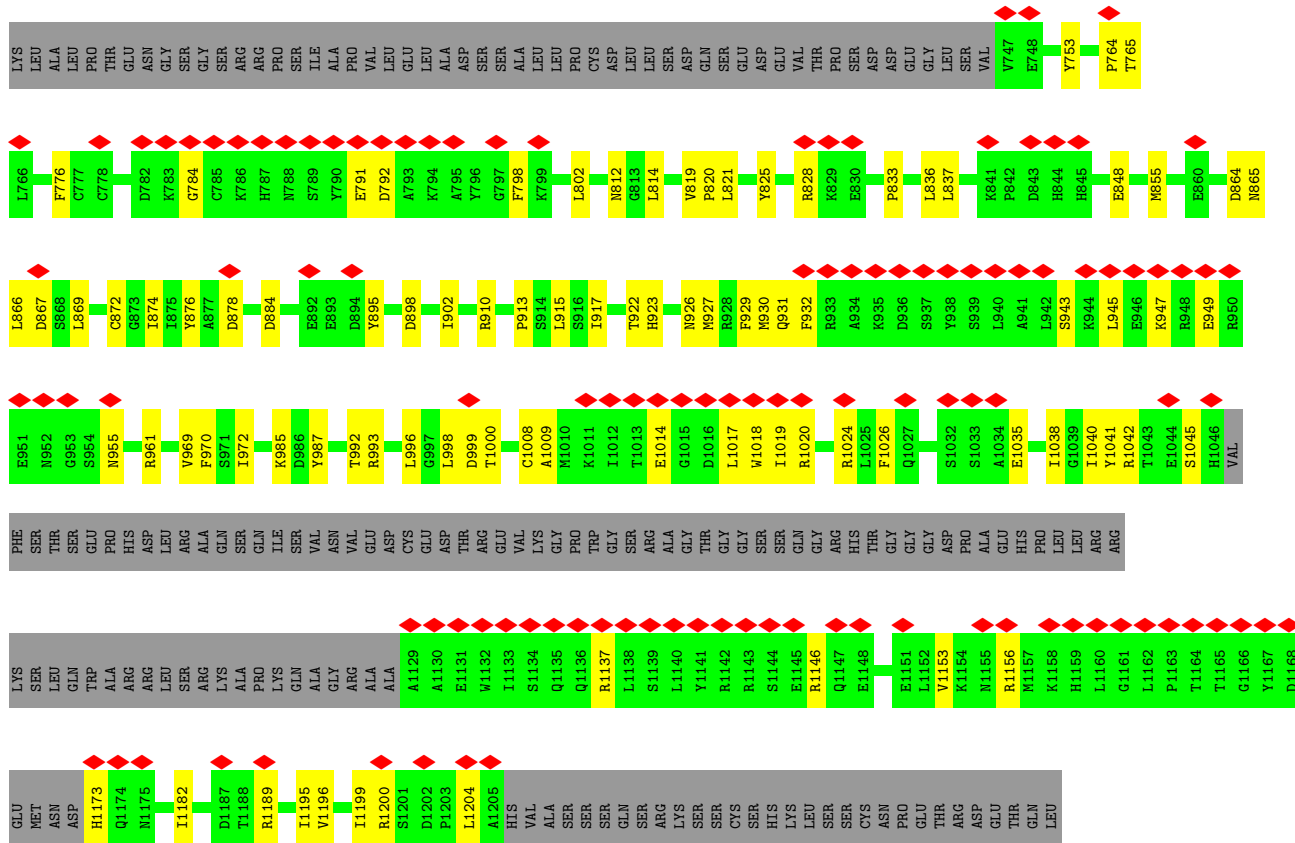
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0
5	B	1	Total Zn 1 1	0
5	C	1	Total Zn 1 1	0
5	D	1	Total Zn 1 1	0

3 Residue-property plots

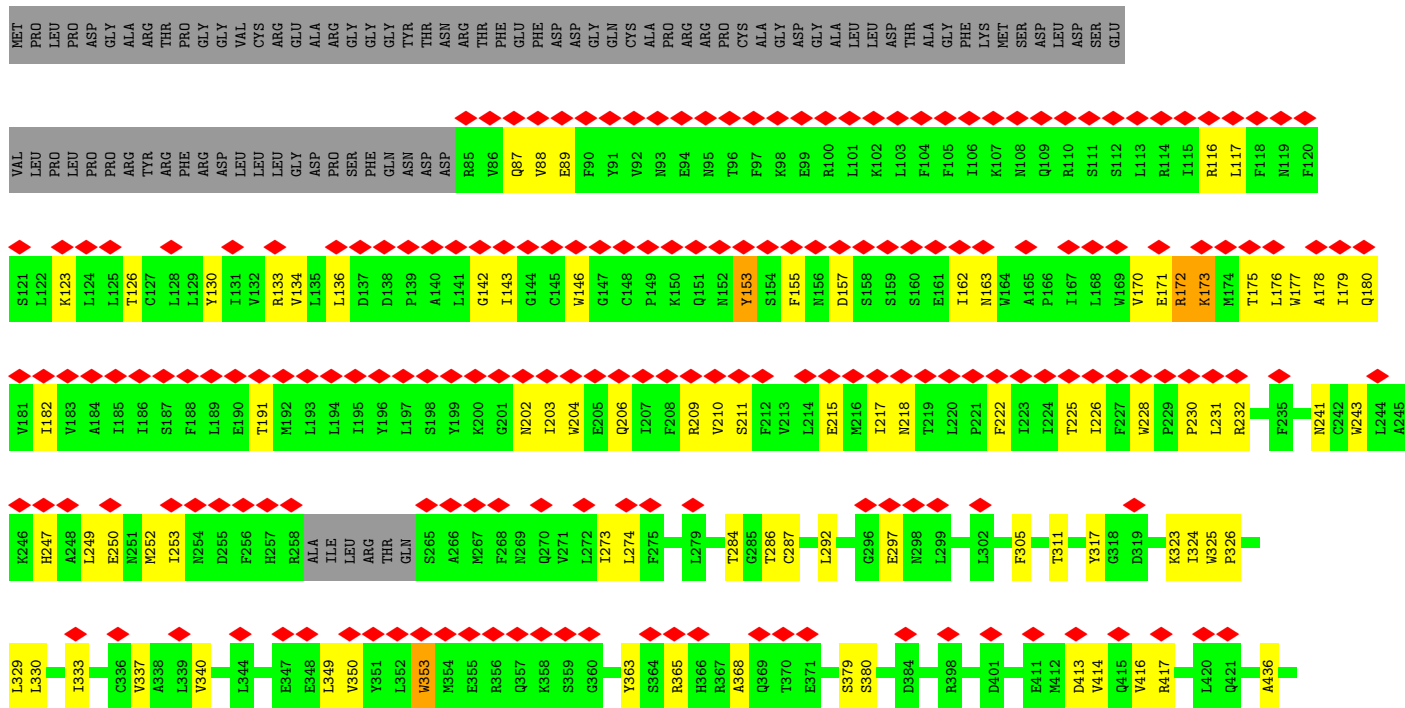
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

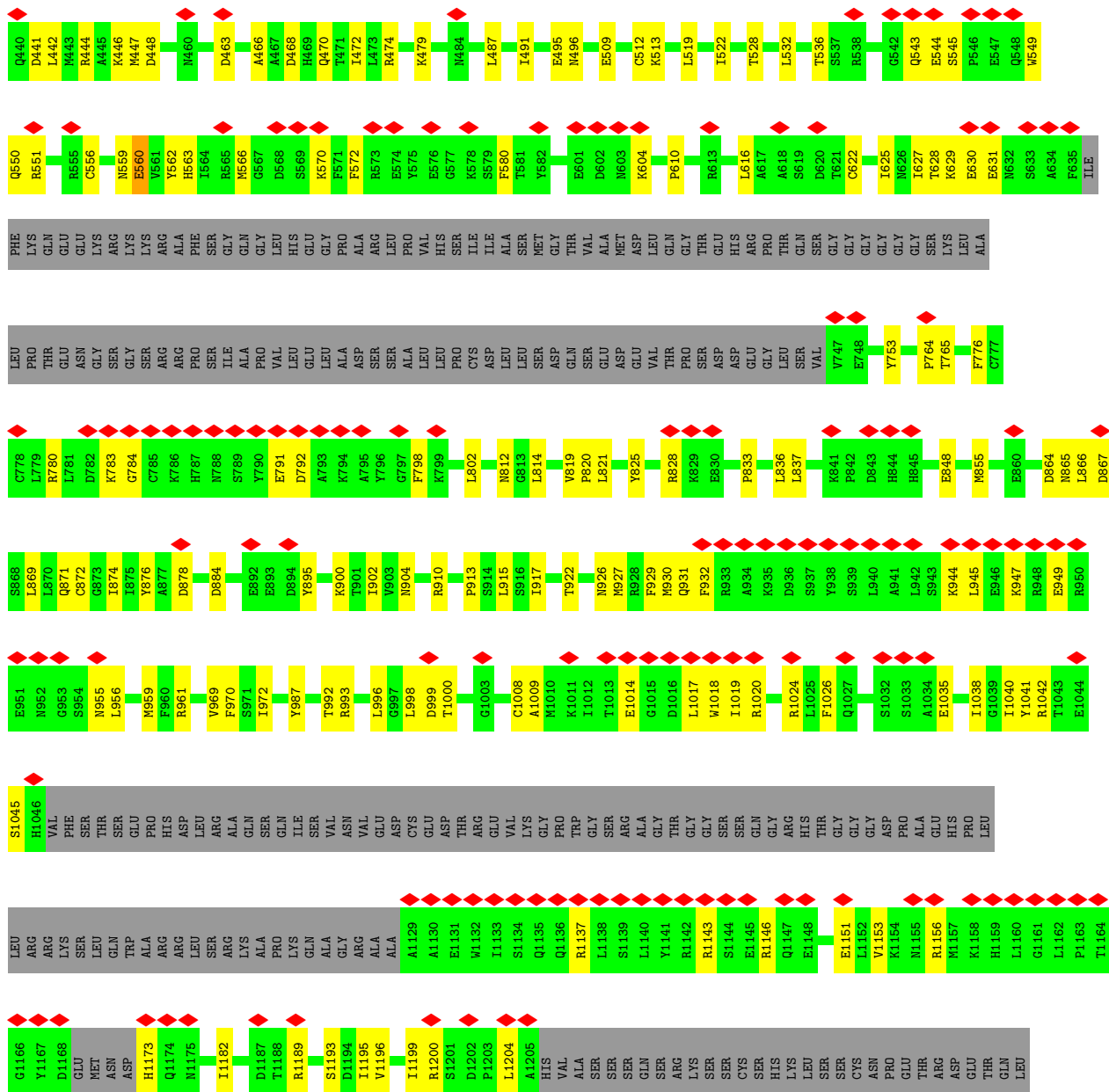
- Molecule 1: Potassium channel subfamily T member 1



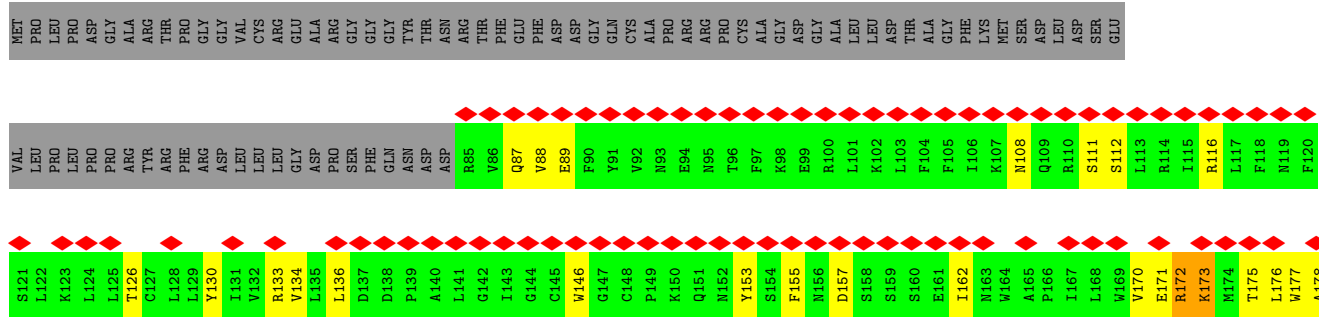


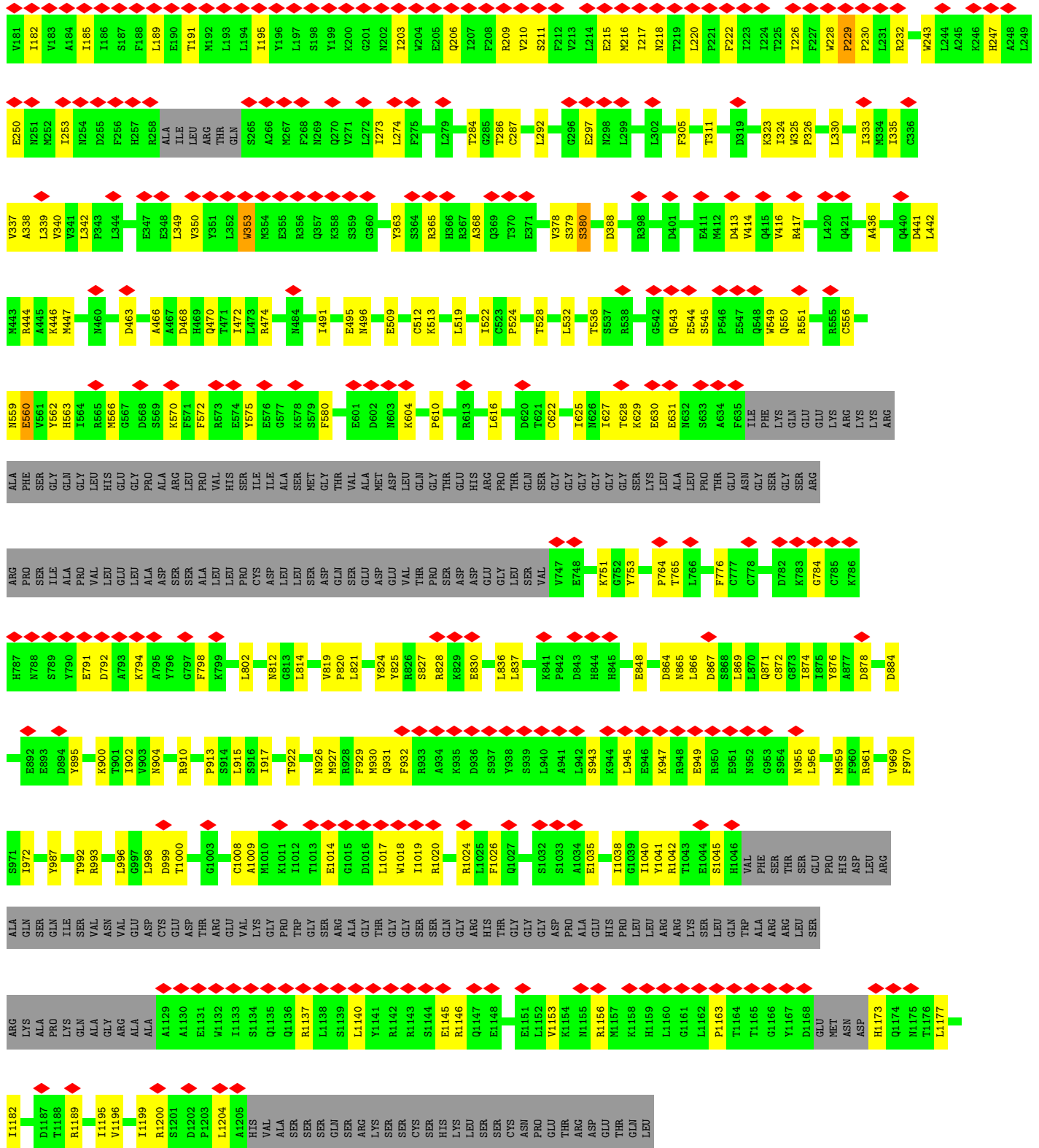
● Molecule 1: Potassium channel subfamily T member 1





• Molecule 1: Potassium channel subfamily T member 1





• Molecule 1: Potassium channel subfamily T member 1



Table showing amino acid types and their corresponding validation scores. The table is organized into several columns of colored blocks, each representing a different residue type and its associated score. The colors range from yellow to dark grey, indicating different levels of validation quality or consistency. Red diamonds are present above many of the entries, likely marking specific residues of interest.

HIS ASP LEU ARG ALA GLN SER LEU ILE VAL VAL VAL ASP CYS ASP THR ARG VAL LYS TRP SER ARG ALA LEU THR GLY TRP THR ARG HIS	S971 1972 D976 K985 D986 Y987 T992 R993 D894 R995 L996 G997 L998 D999 T1000 G1003 C1008 A1009 M1010 K1011 I1012 T1013 T1014 E1014 D1016 L1017 W1018 L1019 R1020 R1024 L1026 F1027 S1032 S1033 A1034 E1035 I1038 I1040 Y1041 R1042 T1043 S1044 S1045 H1046 VAL PHE THR SER LEU TRP ALA	G873 1874 1876 1878 1877 D876 E892 E893 D894 Y895 I902 R910 R913 P913 S914 L915 S916 I917 N926 N927 R928 F929 R930 Q931 F932 R933 A934 D936 S937 Y938 L940 A941 S942 R943 L944 L945 E946 R947 E949 E951 N952 G953 S954 N955 L956 R959 F960 R961 V969 F970	K789 784 785 786 787 788 789 790 E791 D792 A793 K794 A795 Y796 G797 F798 L802 R812 G813 L814 W819 R821 Y825 R828 R829 E830 P833 L836 L837 R841 D843 H844 H845 E848 R855 E860 D864 R866 D867 S868 L869 R871 C872	P546 E547 Q548 W549 Q550 R551 R555 C556 M559 E560 Y561 Y562 R565 M566 G567 D568 S569 K570 R573 E574 Y575 E576 G577 K578 S579 F580 T581 Y582 E601 D602 K604 P610 L616 A617 A618 S619 D620 I625 T628 K629 E630 B631 M632 S633 A634 I635 PHE LYS GLN	D441 L442 M443 R444 A445 K446 M447 D448 M460 D463 A466 A467 H468 H469 Q470 T471 I472 L473 R474 K479 M484 L487 Q490 E495 N496 K501 E509 C512 K513 L519 M520 I522 C523 P524 S527 L532 T536 S537 R538 G542 Q543 E544 S545	V337 A338 L339 V340 Y341 L342 P343 L344 E347 E348 L349 V350 Y351 L352 W353 M354 E355 R356 Q357 K358 S359 G360 Y363 R365 R366 R367 A368 Q369 T370 E371 V378 S379 S380 D384 D388 R398 D401 F411 M412 D413 V414 Q415 F416 R417 R418 W419 L420 Q421 D439 Q440	E250 M251 M252 I253 M254 D255 F256 R257 R258 ALA ILE LEU ARG THR GLN S285 A286 M287 F288 M289 Q270 V271 L272 L273 L274 F275 L279 T284 G285 T286 C287 L292 G296 E297 N298 L299 L302 F305 Y317 G318 D319 T324 D413 W325 P326 L329 L330 I333 M334 I335 G336	I182 V183 A184 I185 I186 S187 F188 L189 E190 T191 M192 L193 L194 I195 Y196 L197 S198 Y199 K200 G201 H202 I203 W204 E205 Q206 I207 F208 R209 V210 S211 F212 V213 E215 M216 L217 N218 T219 L220 P221 F222 L223 L224 T225 I226 F227 W228 P229 L231 R232 W243 L244 A245 K246 H247 L249	S121 L122 K123 L124 L125 T126 C127 L128 L129 Y130 I131 V132 R133 L134 L135 L136 D137 D138 P139 A140 G142 I143 G144 E145 W146 G147 C148 M150 Q151 M152 Y153 S154 F155 M156 R157 L158 S159 F160 F161 I162 M163 M164 A165 P166 I167 L168 W169 V170 E171 R172 K173 M174 T175 L176 W177 I179 Q180	VAL LEU PRO LEU PRO ASP GLY ALA ARG THR PRO PRO GLY VAL CYS ARG GLU ALA ARG PRO ARG GLY GLY THR THR ASN ARG THR PHE PHE ASP ASP GLY GLN CYS ALA PRO ARG ARG ARG ARG PHE THR ASP ASP ASP GLY LEU PHE LYS MET SER ASP LEU ASP ASP MET LYS M108 Q109 R110 S111 S112 L113 R114 I115 R116 R117 L118 M119 F120
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ARG	ARG	ARG	LEU	SER	ARG	ARG	LYS	ALA	PRO	LYS	GLN	ALA	GLY	ARG	ALA	ALA	A1129	A1130	E1131	W1132	I1133	S1134	Q1135	Q1136	R1137	L1138	S1139	L1140	Y1141	R1142	R1143	S1144	E1145	R1146	Q1147	E1148	E1151	L1152	Y1153	K1154	N1155	R1156	M1157	K1158	H1159	L1160	G1161	L1162	P1163	T1164	T1165	G1166	Y1167	D1168	GLU	MET	ASN	ASP	H1173	Q1174
N1175	I1182	D1187	T1188	R1189	I1195	V1196	I1199	R1200	S1201	D1202	P1203	L1204	A1205	HIS	VAL	ALA	SER	SER	SER	GLN	ARG	LYS	SER	SER	CYS	SER	HIS	LYS	LEU	SER	SER	CYS	ASN	PRO	GLU	THR	THR	ARG	ASP	GLU	THR	GLN	LEU																	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28867	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 ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.585	Depositor
Minimum map value	-2.059	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.771	Depositor
Map size (\AA)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6OU, K, ZN, NA

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	0.26	0/7451	0.52	4/10116 (0.0%)
1	B	0.26	0/7451	0.52	5/10116 (0.0%)
1	C	0.26	0/7451	0.53	6/10116 (0.1%)
1	D	0.26	0/7451	0.52	4/10116 (0.0%)
All	All	0.26	0/29804	0.52	19/40464 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	173	LYS	N-CA-CB	-10.58	91.56	110.60
1	D	172	ARG	N-CA-C	-10.39	82.95	111.00
1	B	173	LYS	N-CA-CB	-10.36	91.95	110.60
1	A	172	ARG	N-CA-C	-10.31	83.15	111.00
1	A	173	LYS	N-CA-CB	-10.29	92.08	110.60
1	B	172	ARG	N-CA-C	-10.26	83.30	111.00
1	C	172	ARG	N-CA-C	-10.26	83.31	111.00
1	D	173	LYS	N-CA-CB	-10.24	92.16	110.60
1	C	229	PRO	CA-N-CD	-8.69	99.33	111.50
1	B	173	LYS	N-CA-C	6.21	127.77	111.00
1	D	173	LYS	N-CA-C	6.14	127.57	111.00
1	A	173	LYS	N-CA-C	6.09	127.45	111.00
1	C	173	LYS	N-CA-C	5.96	127.10	111.00
1	D	157	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	157	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	157	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	136	LEU	CA-CB-CG	5.16	127.18	115.30
1	C	136	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	157	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7278	0	7219	163	0
1	B	7278	0	7219	173	0
1	C	7278	0	7219	176	0
1	D	7278	0	7219	155	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	0	0	0
4	A	11	0	0	0	0
4	B	11	0	0	0	0
4	C	11	0	0	0	0
4	D	11	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	29168	0	28876	648	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 11.

All (648) 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:D:566:MET:SD	1:D:616:LEU:HD12	1.76	1.25
1:A:566:MET:CE	1:A:622:CYS:SG	2.26	1.24
1:C:566:MET:HE1	1:C:622:CYS:SG	1.78	1.23
1:C:629:LYS:HE2	1:C:631:GLU:OE1	1.32	1.22
1:A:566:MET:HE1	1:A:622:CYS:SG	1.77	1.22
1:B:629:LYS:HE2	1:B:631:GLU:OE1	1.34	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:LYS:HG2	1:C:631:GLU:OE2	1.43	1.19
1:C:566:MET:CE	1:C:622:CYS:SG	2.30	1.18
1:B:566:MET:HE1	1:B:622:CYS:SG	1.85	1.17
1:B:566:MET:CE	1:B:622:CYS:SG	2.32	1.16
1:D:566:MET:HE2	1:D:617:ALA:O	1.46	1.15
1:B:629:LYS:HG2	1:B:631:GLU:OE2	1.49	1.09
1:C:229:PRO:HD2	1:C:230:PRO:CD	1.84	1.07
1:D:629:LYS:HG2	1:D:631:GLU:OE1	1.55	1.05
1:C:629:LYS:HE2	1:C:631:GLU:CD	1.78	1.04
1:A:566:MET:SD	1:A:572:PHE:CB	2.49	1.01
1:B:629:LYS:HE2	1:B:631:GLU:CD	1.81	1.00
1:A:566:MET:SD	1:A:572:PHE:HB2	2.03	0.98
1:A:566:MET:HE2	1:A:622:CYS:SG	2.01	0.97
1:D:566:MET:SD	1:D:616:LEU:CD1	2.53	0.97
1:B:566:MET:SD	1:B:572:PHE:CB	2.54	0.96
1:C:566:MET:SD	1:C:572:PHE:CB	2.55	0.94
1:B:566:MET:HE2	1:B:622:CYS:SG	2.05	0.94
1:C:566:MET:HE2	1:C:622:CYS:SG	2.08	0.93
1:C:629:LYS:CE	1:C:631:GLU:OE1	2.18	0.92
1:B:566:MET:SD	1:B:572:PHE:HB2	2.09	0.92
1:A:566:MET:SD	1:A:572:PHE:HB3	2.10	0.91
1:C:229:PRO:HD2	1:C:230:PRO:HD3	1.48	0.91
1:C:566:MET:SD	1:C:572:PHE:HB2	2.10	0.90
1:C:324:ILE:HG22	1:C:326:PRO:HD2	1.52	0.90
1:D:324:ILE:HG22	1:D:326:PRO:HD2	1.53	0.89
1:A:324:ILE:HG22	1:A:326:PRO:HD2	1.52	0.89
1:C:468:ASP:OD2	1:C:496:ASN:ND2	2.06	0.88
1:B:629:LYS:CE	1:B:631:GLU:OE1	2.21	0.88
1:C:566:MET:SD	1:C:572:PHE:HB3	2.14	0.88
1:B:324:ILE:HG22	1:B:326:PRO:HD2	1.53	0.88
1:B:468:ASP:OD2	1:B:496:ASN:ND2	2.06	0.88
1:B:566:MET:SD	1:B:572:PHE:HB3	2.14	0.88
1:D:509:GLU:HG3	1:D:972:ILE:HG12	1.57	0.86
1:C:509:GLU:HG3	1:C:972:ILE:HG12	1.58	0.86
1:A:509:GLU:HG3	1:A:972:ILE:HG12	1.58	0.85
1:B:566:MET:CE	1:B:616:LEU:HD11	2.06	0.85
1:B:509:GLU:HG3	1:B:972:ILE:HG12	1.58	0.85
1:A:468:ASP:OD2	1:A:496:ASN:ND2	2.10	0.84
1:B:468:ASP:OD1	1:B:491:ILE:HG13	1.78	0.83
1:C:468:ASP:OD1	1:C:491:ILE:HG13	1.79	0.82
1:A:468:ASP:OD1	1:A:491:ILE:HG13	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASP:OD2	1:A:496:ASN:CG	2.19	0.80
1:A:468:ASP:OD2	1:A:496:ASN:CB	2.29	0.80
1:B:566:MET:HE2	1:B:616:LEU:HD11	1.67	0.76
1:B:629:LYS:CG	1:B:631:GLU:OE2	2.33	0.74
1:D:566:MET:HE1	1:D:616:LEU:HB3	1.69	0.74
1:D:566:MET:CE	1:D:617:ALA:O	2.33	0.74
1:C:468:ASP:OD2	1:C:496:ASN:CB	2.37	0.73
1:C:468:ASP:OD2	1:C:496:ASN:CG	2.26	0.73
1:B:468:ASP:OD2	1:B:496:ASN:CB	2.37	0.72
1:C:566:MET:CE	1:C:616:LEU:HD11	2.19	0.72
1:D:171:GLU:C	1:D:172:ARG:O	2.22	0.72
1:B:468:ASP:OD2	1:B:496:ASN:CG	2.27	0.72
1:C:629:LYS:CG	1:C:631:GLU:OE2	2.31	0.72
1:B:566:MET:CE	1:B:616:LEU:CD1	2.69	0.70
1:A:171:GLU:C	1:A:172:ARG:O	2.23	0.68
1:D:566:MET:SD	1:D:616:LEU:CG	2.81	0.68
1:B:566:MET:HE3	1:B:616:LEU:HD11	1.74	0.68
1:B:162:ILE:HD12	1:B:324:ILE:HG21	1.76	0.68
1:B:930:MET:HG3	1:B:969:VAL:HG21	1.76	0.68
1:B:171:GLU:C	1:B:172:ARG:O	2.24	0.68
1:C:146:TRP:HB3	1:C:230:PRO:HA	1.76	0.68
1:A:566:MET:CE	1:A:616:LEU:HD11	2.24	0.67
1:C:171:GLU:C	1:C:172:ARG:O	2.24	0.67
1:D:930:MET:HG3	1:D:969:VAL:HG21	1.77	0.67
1:C:162:ILE:HD12	1:C:324:ILE:HG21	1.76	0.66
1:B:173:LYS:HD3	1:B:176:LEU:HD23	1.76	0.66
1:A:930:MET:HG3	1:A:969:VAL:HG21	1.77	0.66
1:C:930:MET:HG3	1:C:969:VAL:HG21	1.77	0.66
1:B:472:ILE:HD11	1:B:496:ASN:HB3	1.78	0.66
1:C:765:THR:HG23	1:C:1000:THR:HG21	1.78	0.66
1:D:162:ILE:HD12	1:D:324:ILE:HG21	1.77	0.65
1:B:765:THR:HG23	1:B:1000:THR:HG21	1.78	0.65
1:C:472:ILE:HD11	1:C:496:ASN:HB3	1.78	0.64
1:D:472:ILE:HD11	1:D:496:ASN:HB3	1.78	0.64
1:C:927:MET:HE3	1:C:961:ARG:HG3	1.80	0.64
1:A:162:ILE:HD12	1:A:324:ILE:HG21	1.79	0.64
1:B:566:MET:HE2	1:B:616:LEU:CD1	2.26	0.64
1:A:1038:ILE:HD11	1:A:1199:ILE:HD11	1.80	0.64
1:B:1038:ILE:HD11	1:B:1199:ILE:HD11	1.80	0.64
1:D:765:THR:HG23	1:D:1000:THR:HG21	1.80	0.64
1:C:1038:ILE:HD11	1:C:1199:ILE:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:ARG:NH2	1:A:1189:ARG:O	2.31	0.63
1:D:1042:ARG:NH2	1:D:1189:ARG:O	2.31	0.63
1:D:1038:ILE:HD11	1:D:1199:ILE:HD11	1.80	0.63
1:C:1042:ARG:NH2	1:C:1189:ARG:O	2.31	0.63
1:A:472:ILE:HD11	1:A:496:ASN:HB3	1.81	0.62
1:A:765:THR:HG23	1:A:1000:THR:HG21	1.80	0.62
1:B:864:ASP:OD1	1:B:865:ASN:N	2.31	0.62
1:A:468:ASP:OD1	1:A:491:ILE:CG1	2.47	0.62
1:A:243:TRP:HE1	1:A:284:THR:HG21	1.65	0.62
1:C:229:PRO:HD2	1:C:230:PRO:HD2	1.78	0.62
1:D:927:MET:HE3	1:D:961:ARG:HG3	1.82	0.62
1:B:468:ASP:OD1	1:B:491:ILE:CG1	2.47	0.62
1:A:1008:CYS:SG	1:A:1009:ALA:N	2.73	0.62
1:D:243:TRP:HE1	1:D:284:THR:HG21	1.65	0.62
1:D:864:ASP:OD1	1:D:865:ASN:N	2.31	0.62
1:A:631:GLU:OE1	1:A:631:GLU:N	2.22	0.61
1:A:864:ASP:OD1	1:A:865:ASN:N	2.31	0.61
1:B:413:ASP:OD2	1:B:414:VAL:N	2.33	0.61
1:C:243:TRP:HE1	1:C:284:THR:HG21	1.65	0.61
1:C:864:ASP:OD1	1:C:865:ASN:N	2.31	0.61
1:C:566:MET:HE3	1:C:616:LEU:HD11	1.82	0.61
1:D:228:TRP:HB3	1:D:230:PRO:HD2	1.82	0.61
1:C:413:ASP:OD2	1:C:414:VAL:N	2.34	0.61
1:B:1008:CYS:SG	1:B:1009:ALA:N	2.73	0.61
1:A:470:GLN:HG2	1:D:895:TYR:HE2	1.65	0.61
1:C:895:TYR:HE2	1:D:470:GLN:HG2	1.66	0.61
1:A:228:TRP:HB3	1:A:230:PRO:HD2	1.82	0.61
1:A:895:TYR:HE2	1:B:470:GLN:HG2	1.65	0.61
1:A:286:THR:HG22	1:A:305:PHE:HA	1.83	0.61
1:A:566:MET:HE3	1:A:616:LEU:HD11	1.83	0.61
1:B:243:TRP:HE1	1:B:284:THR:HG21	1.65	0.61
1:B:1042:ARG:NH2	1:B:1189:ARG:O	2.34	0.61
1:D:180:GLN:HB3	1:D:222:PHE:HE2	1.66	0.60
1:D:413:ASP:OD2	1:D:414:VAL:N	2.34	0.60
1:D:629:LYS:CG	1:D:631:GLU:OE1	2.42	0.60
1:D:1008:CYS:SG	1:D:1009:ALA:N	2.73	0.60
1:B:513:LYS:HG3	1:B:970:PHE:HE2	1.66	0.60
1:C:1008:CYS:SG	1:C:1009:ALA:N	2.74	0.60
1:A:495:GLU:OE1	1:A:812:ASN:ND2	2.34	0.60
1:A:513:LYS:HG3	1:A:970:PHE:HE2	1.66	0.60
1:C:867:ASP:HB3	1:C:1156:ARG:HH21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLN:NE2	1:D:88:VAL:O	2.34	0.60
1:D:286:THR:HG22	1:D:305:PHE:HA	1.84	0.60
1:C:286:THR:HG22	1:C:305:PHE:HA	1.83	0.60
1:D:910:ARG:O	1:D:1146:ARG:NH2	2.35	0.60
1:A:87:GLN:NE2	1:A:88:VAL:O	2.34	0.60
1:B:895:TYR:HE2	1:C:470:GLN:HG2	1.65	0.60
1:D:180:GLN:HB3	1:D:222:PHE:CE2	2.37	0.60
1:C:910:ARG:O	1:C:1146:ARG:NH2	2.35	0.60
1:B:286:THR:HG22	1:B:305:PHE:HA	1.83	0.60
1:B:495:GLU:OE1	1:B:812:ASN:ND2	2.35	0.60
1:A:413:ASP:OD2	1:A:414:VAL:N	2.34	0.60
1:B:867:ASP:HB3	1:B:1156:ARG:HH21	1.65	0.60
1:C:513:LYS:HG3	1:C:970:PHE:HE2	1.66	0.59
1:D:867:ASP:HB3	1:D:1156:ARG:HH21	1.67	0.59
1:A:910:ARG:O	1:A:1146:ARG:NH2	2.35	0.59
1:C:566:MET:HE2	1:C:616:LEU:HD11	1.83	0.59
1:D:495:GLU:OE1	1:D:812:ASN:ND2	2.35	0.59
1:D:513:LYS:HG3	1:D:970:PHE:HE2	1.66	0.59
1:C:468:ASP:OD1	1:C:491:ILE:CG1	2.48	0.59
1:C:931:GLN:OE1	1:C:931:GLN:N	2.36	0.59
1:C:495:GLU:OE1	1:C:812:ASN:ND2	2.35	0.59
1:B:228:TRP:HB3	1:B:230:PRO:HD2	1.83	0.58
1:B:566:MET:HE3	1:B:616:LEU:CD1	2.31	0.58
1:B:931:GLN:N	1:B:931:GLN:OE1	2.35	0.58
1:B:910:ARG:O	1:B:1146:ARG:NH2	2.35	0.58
1:A:867:ASP:HB3	1:A:1156:ARG:HH21	1.66	0.58
1:C:325:TRP:CG	1:C:326:PRO:HD3	2.38	0.58
1:A:913:PRO:HB2	1:A:1173:HIS:HB2	1.86	0.58
1:B:87:GLN:NE2	1:B:88:VAL:O	2.37	0.57
1:C:87:GLN:NE2	1:C:88:VAL:O	2.37	0.57
1:C:178:ALA:O	1:C:182:ILE:HG13	2.04	0.57
1:C:913:PRO:HB2	1:C:1173:HIS:HB2	1.87	0.57
1:B:913:PRO:HB2	1:B:1173:HIS:HB2	1.87	0.57
1:D:448:ASP:OD1	1:D:448:ASP:N	2.32	0.57
1:B:325:TRP:CG	1:B:326:PRO:HD3	2.39	0.57
1:D:913:PRO:HB2	1:D:1173:HIS:HB2	1.87	0.57
1:D:325:TRP:CG	1:D:326:PRO:HD3	2.40	0.57
1:C:566:MET:CE	1:C:616:LEU:CD1	2.83	0.57
1:B:203:ILE:HG13	1:B:203:ILE:O	2.04	0.56
1:B:1018:TRP:O	1:B:1024:ARG:NH2	2.38	0.56
1:C:1018:TRP:O	1:C:1024:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1018:TRP:O	1:D:1024:ARG:NH2	2.39	0.56
1:D:1035:GLU:OE2	1:D:1200:ARG:NE	2.36	0.56
1:B:559:ASN:HB3	1:B:625:ILE:HG22	1.88	0.56
1:A:1035:GLU:OE2	1:A:1200:ARG:NE	2.36	0.56
1:B:153:TYR:HD2	1:B:163:ASN:HD22	1.53	0.56
1:D:931:GLN:OE1	1:D:931:GLN:N	2.36	0.56
1:A:180:GLN:HB3	1:A:222:PHE:CE2	2.41	0.56
1:A:325:TRP:CG	1:A:326:PRO:HD3	2.41	0.56
1:A:1018:TRP:O	1:A:1024:ARG:NH2	2.39	0.56
1:B:146:TRP:HB3	1:B:230:PRO:HA	1.87	0.56
1:A:559:ASN:HB3	1:A:625:ILE:HG22	1.88	0.55
1:C:325:TRP:CD1	1:C:326:PRO:HD3	2.40	0.55
1:C:1040:ILE:HG12	1:C:1196:VAL:HG22	1.89	0.55
1:D:178:ALA:O	1:D:182:ILE:HG13	2.06	0.55
1:D:1040:ILE:HG12	1:D:1196:VAL:HG22	1.89	0.55
1:A:178:ALA:O	1:A:182:ILE:HG13	2.06	0.55
1:B:325:TRP:CD1	1:B:326:PRO:HD3	2.41	0.55
1:D:559:ASN:HB3	1:D:625:ILE:HG22	1.89	0.55
1:A:1137:ARG:HH11	1:B:1204:LEU:HD12	1.71	0.55
1:B:1137:ARG:HH11	1:C:1204:LEU:HD12	1.71	0.55
1:D:631:GLU:OE1	1:D:631:GLU:N	2.23	0.55
1:A:927:MET:HE3	1:A:961:ARG:HG3	1.89	0.55
1:A:1204:LEU:HD12	1:D:1137:ARG:HH11	1.72	0.55
1:C:559:ASN:HB3	1:C:625:ILE:HG22	1.89	0.55
1:B:1040:ILE:HG12	1:B:1196:VAL:HG22	1.88	0.54
1:C:869:LEU:HD22	1:C:874:ILE:HD12	1.90	0.54
1:B:178:ALA:O	1:B:182:ILE:HG13	2.08	0.54
1:C:195:ILE:HD13	1:C:206:GLN:HB3	1.90	0.54
1:A:130:TYR:HE2	1:A:287:CYS:HB3	1.72	0.54
1:B:463:ASP:HB3	1:B:466:ALA:HB3	1.90	0.54
1:D:203:ILE:O	1:D:203:ILE:HG13	2.08	0.54
1:A:463:ASP:HB3	1:A:466:ALA:HB3	1.90	0.54
1:A:1040:ILE:HG12	1:A:1196:VAL:HG22	1.89	0.54
1:C:1137:ARG:HH11	1:D:1204:LEU:HD12	1.72	0.54
1:A:195:ILE:HD13	1:A:206:GLN:HB3	1.90	0.54
1:D:566:MET:SD	1:D:616:LEU:HG	2.48	0.54
1:B:350:VAL:HA	1:B:353:TRP:HB2	1.91	0.53
1:C:1035:GLU:OE2	1:C:1200:ARG:NE	2.35	0.53
1:A:203:ILE:HG13	1:A:203:ILE:O	2.08	0.53
1:A:335:ILE:O	1:A:339:LEU:HD12	2.09	0.53
1:C:463:ASP:HB3	1:C:466:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:GLN:OE1	1:A:931:GLN:N	2.35	0.53
1:C:556:CYS:O	1:C:559:ASN:ND2	2.42	0.53
1:A:566:MET:HE2	1:A:616:LEU:HD11	1.91	0.53
1:C:350:VAL:HA	1:C:353:TRP:HB2	1.91	0.53
1:D:463:ASP:HB3	1:D:466:ALA:HB3	1.90	0.53
1:B:869:LEU:HD22	1:B:874:ILE:HD12	1.91	0.53
1:D:335:ILE:O	1:D:339:LEU:HD12	2.09	0.53
1:D:566:MET:CE	1:D:616:LEU:HB3	2.36	0.53
1:A:556:CYS:O	1:A:559:ASN:ND2	2.41	0.53
1:A:629:LYS:HG2	1:A:631:GLU:OE1	2.08	0.53
1:B:556:CYS:O	1:B:559:ASN:ND2	2.41	0.53
1:B:1035:GLU:OE2	1:B:1200:ARG:NE	2.35	0.52
1:D:556:CYS:O	1:D:559:ASN:ND2	2.41	0.52
1:C:203:ILE:O	1:C:203:ILE:HG13	2.10	0.52
1:C:566:MET:HE2	1:C:616:LEU:CD1	2.40	0.52
1:C:335:ILE:O	1:C:339:LEU:HD12	2.10	0.52
1:C:180:GLN:HB3	1:C:222:PHE:HE2	1.74	0.52
1:A:330:LEU:HA	1:A:333:ILE:HG22	1.92	0.52
1:D:195:ILE:HD13	1:D:206:GLN:HB3	1.92	0.52
1:D:869:LEU:HD22	1:D:874:ILE:HD12	1.91	0.52
1:A:350:VAL:HA	1:A:353:TRP:HB2	1.91	0.51
1:A:543:GLN:NE2	1:A:551:ARG:O	2.42	0.51
1:D:350:VAL:HA	1:D:353:TRP:HB2	1.92	0.51
1:A:869:LEU:HD22	1:A:874:ILE:HD12	1.92	0.51
1:B:317:TYR:OH	1:C:311:THR:OG1	2.29	0.51
1:B:448:ASP:OD1	1:B:448:ASP:N	2.40	0.51
1:B:927:MET:HE3	1:B:961:ARG:HG3	1.92	0.51
1:C:155:PHE:CE1	1:C:324:ILE:HD11	2.46	0.51
1:C:133:ARG:NH1	1:C:170:VAL:HG21	2.26	0.51
1:D:330:LEU:HA	1:D:333:ILE:HG22	1.93	0.51
1:B:902:ILE:HD13	1:B:929:PHE:HB2	1.93	0.51
1:C:333:ILE:O	1:C:337:VAL:HG12	2.11	0.51
1:C:330:LEU:HA	1:C:333:ILE:HG22	1.93	0.51
1:D:225:THR:OG1	1:D:231:LEU:O	2.28	0.51
1:B:203:ILE:HD12	1:B:206:GLN:HB2	1.93	0.51
1:B:209:ARG:HE	1:B:210:VAL:H	1.59	0.51
1:B:629:LYS:HE2	1:B:631:GLU:OE2	2.11	0.50
1:A:902:ILE:HD13	1:A:929:PHE:HB2	1.93	0.50
1:C:902:ILE:HD13	1:C:929:PHE:HB2	1.94	0.50
1:D:146:TRP:HB3	1:D:230:PRO:HA	1.93	0.50
1:A:898:ASP:OD2	1:A:926:ASN:ND2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:ILE:HD11	1:D:821:LEU:HD23	1.92	0.50
1:B:155:PHE:CE1	1:B:324:ILE:HD11	2.47	0.50
1:D:441:ASP:HA	1:D:444:ARG:HD3	1.93	0.50
1:D:902:ILE:HD13	1:D:929:PHE:HB2	1.94	0.50
1:B:330:LEU:HA	1:B:333:ILE:HG22	1.93	0.50
1:C:173:LYS:HB2	1:C:176:LEU:HD12	1.92	0.50
1:A:333:ILE:O	1:A:337:VAL:HG12	2.12	0.50
1:B:191:THR:HG21	1:B:215:GLU:OE1	2.12	0.50
1:D:155:PHE:CE1	1:D:324:ILE:HD11	2.46	0.50
1:A:545:SER:HB2	1:A:945:LEU:HD21	1.94	0.50
1:A:566:MET:CE	1:A:616:LEU:CD1	2.88	0.50
1:B:333:ILE:O	1:B:337:VAL:HG12	2.11	0.50
1:C:180:GLN:HB3	1:C:222:PHE:CE2	2.47	0.50
1:A:932:PHE:CD2	1:A:932:PHE:O	2.65	0.50
1:A:448:ASP:N	1:A:448:ASP:OD1	2.43	0.49
1:A:519:LEU:HD11	1:A:996:LEU:HA	1.94	0.49
1:C:932:PHE:CD2	1:C:932:PHE:O	2.65	0.49
1:D:776:PHE:HZ	1:D:848:GLU:HG2	1.77	0.49
1:C:172:ARG:NH1	1:C:232:ARG:O	2.45	0.49
1:C:209:ARG:HE	1:C:210:VAL:H	1.59	0.49
1:C:274:LEU:HD22	1:C:349:LEU:HD22	1.94	0.49
1:D:543:GLN:NE2	1:D:551:ARG:O	2.44	0.49
1:A:191:THR:HG21	1:A:215:GLU:OE1	2.12	0.49
1:A:441:ASP:HA	1:A:444:ARG:HD3	1.93	0.49
1:A:753:TYR:CD1	1:A:764:PRO:HB2	2.47	0.49
1:A:866:LEU:HD21	1:A:1153:VAL:HG22	1.94	0.49
1:B:776:PHE:HZ	1:B:848:GLU:HG2	1.77	0.49
1:B:866:LEU:HD21	1:B:1153:VAL:HG22	1.95	0.49
1:B:932:PHE:O	1:B:932:PHE:CD2	2.65	0.49
1:C:513:LYS:HB2	1:C:972:ILE:HD13	1.94	0.49
1:D:753:TYR:CD1	1:D:764:PRO:HB2	2.48	0.49
1:A:155:PHE:CE1	1:A:324:ILE:HD11	2.47	0.49
1:A:329:LEU:HD21	1:D:302:LEU:HD11	1.93	0.49
1:A:513:LYS:HB2	1:A:972:ILE:HD13	1.94	0.49
1:C:337:VAL:HA	1:C:340:VAL:HG22	1.94	0.49
1:D:519:LEU:HD11	1:D:996:LEU:HA	1.94	0.49
1:A:180:GLN:HB3	1:A:222:PHE:HE2	1.77	0.49
1:B:522:ILE:HD11	1:B:821:LEU:HD23	1.94	0.49
1:C:1000:THR:O	1:C:1000:THR:OG1	2.30	0.49
1:D:333:ILE:O	1:D:337:VAL:HG12	2.12	0.49
1:D:1000:THR:O	1:D:1000:THR:OG1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ILE:HD11	1:A:821:LEU:HD23	1.93	0.49
1:A:146:TRP:HB3	1:A:230:PRO:HA	1.95	0.49
1:C:126:THR:O	1:C:180:GLN:NE2	2.45	0.49
1:C:203:ILE:HD12	1:C:206:GLN:HB2	1.95	0.49
1:C:441:ASP:HA	1:C:444:ARG:HD3	1.94	0.49
1:D:932:PHE:O	1:D:932:PHE:CD2	2.65	0.49
1:C:631:GLU:OE2	1:C:631:GLU:N	2.31	0.49
1:D:126:THR:OG1	1:D:180:GLN:OE1	2.28	0.49
1:D:513:LYS:HB2	1:D:972:ILE:HD13	1.95	0.49
1:A:776:PHE:HZ	1:A:848:GLU:HG2	1.78	0.49
1:C:545:SER:HB2	1:C:945:LEU:HD21	1.94	0.49
1:D:191:THR:HG21	1:D:215:GLU:OE1	2.13	0.49
1:B:513:LYS:HB2	1:B:972:ILE:HD13	1.94	0.49
1:C:519:LEU:HD11	1:C:996:LEU:HA	1.95	0.49
1:B:225:THR:OG1	1:B:231:LEU:O	2.28	0.48
1:C:522:ILE:HD11	1:C:821:LEU:HD23	1.94	0.48
1:C:631:GLU:CD	1:C:631:GLU:H	2.16	0.48
1:C:866:LEU:HD21	1:C:1153:VAL:HG22	1.95	0.48
1:D:177:TRP:HZ2	1:D:226:ILE:HA	1.76	0.48
1:A:225:THR:OG1	1:A:231:LEU:O	2.27	0.48
1:B:441:ASP:HA	1:B:444:ARG:HD3	1.94	0.48
1:C:543:GLN:NE2	1:C:551:ARG:O	2.42	0.48
1:D:209:ARG:HE	1:D:210:VAL:H	1.61	0.48
1:A:311:THR:OG1	1:D:317:TYR:OH	2.29	0.48
1:B:317:TYR:HH	1:C:311:THR:HG1	1.53	0.48
1:B:519:LEU:HD11	1:B:996:LEU:HA	1.94	0.48
1:C:837:LEU:HD13	1:C:872:CYS:SG	2.54	0.48
1:D:217:ILE:HD12	1:D:218:ASN:N	2.29	0.48
1:A:203:ILE:HD12	1:A:206:GLN:HB2	1.95	0.48
1:B:274:LEU:HD22	1:B:349:LEU:HD22	1.95	0.48
1:D:349:LEU:O	1:D:353:TRP:N	2.47	0.48
1:D:544:GLU:N	1:D:544:GLU:OE1	2.47	0.48
1:D:956:LEU:HB2	1:D:959:MET:HE2	1.95	0.48
1:A:349:LEU:O	1:A:353:TRP:N	2.47	0.48
1:C:560:GLU:HB2	1:C:562:TYR:CE2	2.49	0.48
1:D:325:TRP:CD1	1:D:326:PRO:HD3	2.48	0.48
1:A:217:ILE:HD12	1:A:218:ASN:N	2.29	0.47
1:A:317:TYR:OH	1:B:311:THR:OG1	2.28	0.47
1:B:545:SER:HB2	1:B:945:LEU:HD21	1.96	0.47
1:A:325:TRP:CD1	1:A:326:PRO:HD3	2.49	0.47
1:A:544:GLU:N	1:A:544:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:NH1	1:B:232:ARG:O	2.46	0.47
1:B:1143:ARG:NH1	1:B:1151:GLU:OE1	2.47	0.47
1:C:228:TRP:HB3	1:C:230:PRO:HD2	1.95	0.47
1:A:337:VAL:HA	1:A:340:VAL:HG22	1.96	0.47
1:A:133:ARG:NH1	1:A:170:VAL:HG21	2.30	0.47
1:A:902:ILE:HD11	1:A:926:ASN:HB3	1.96	0.47
1:B:202:ASN:O	1:B:203:ILE:C	2.52	0.47
1:C:544:GLU:OE1	1:C:544:GLU:N	2.47	0.47
1:C:566:MET:HE3	1:C:616:LEU:CD1	2.43	0.47
1:D:866:LEU:HD21	1:D:1153:VAL:HG22	1.96	0.47
1:A:837:LEU:HD13	1:A:872:CYS:SG	2.55	0.47
1:D:837:LEU:HD13	1:D:872:CYS:SG	2.54	0.47
1:A:833:PRO:HG3	1:A:855:MET:HE2	1.96	0.47
1:B:116:ARG:HG2	1:B:116:ARG:HH11	1.80	0.47
1:B:217:ILE:HD12	1:B:218:ASN:N	2.30	0.47
1:C:292:LEU:HD12	1:C:330:LEU:HD22	1.97	0.47
1:C:753:TYR:CD1	1:C:764:PRO:HB2	2.49	0.47
1:C:776:PHE:HZ	1:C:848:GLU:HG2	1.78	0.47
1:D:126:THR:O	1:D:180:GLN:NE2	2.48	0.47
1:A:442:LEU:HD22	1:A:447:MET:HG3	1.97	0.47
1:A:468:ASP:OD1	1:A:491:ILE:CD1	2.63	0.47
1:A:993:ARG:HH12	1:A:999:ASP:HB3	1.80	0.47
1:B:566:MET:HG2	1:B:616:LEU:HD12	1.97	0.47
1:D:442:LEU:HD22	1:D:447:MET:HG3	1.97	0.47
1:D:1019:ILE:HA	1:D:1024:ARG:HH21	1.80	0.47
1:A:126:THR:O	1:A:180:GLN:NE2	2.47	0.47
1:B:1000:THR:O	1:B:1000:THR:OG1	2.29	0.47
1:D:292:LEU:HD12	1:D:330:LEU:HD22	1.97	0.47
1:B:442:LEU:HD22	1:B:447:MET:HG3	1.97	0.47
1:B:956:LEU:HB2	1:B:959:MET:HE2	1.97	0.47
1:D:203:ILE:HD12	1:D:206:GLN:HB2	1.96	0.47
1:A:173:LYS:HB2	1:A:176:LEU:HD12	1.97	0.47
1:B:837:LEU:HD13	1:B:872:CYS:SG	2.55	0.47
1:D:173:LYS:HB2	1:D:176:LEU:HD12	1.95	0.47
1:D:628:THR:OG1	1:D:629:LYS:N	2.48	0.47
1:C:349:LEU:O	1:C:353:TRP:N	2.49	0.46
1:C:414:VAL:HA	1:C:417:ARG:HG3	1.96	0.46
1:A:1019:ILE:HA	1:A:1024:ARG:HH21	1.80	0.46
1:C:993:ARG:HH12	1:C:999:ASP:HB3	1.81	0.46
1:D:902:ILE:HD11	1:D:926:ASN:HB3	1.97	0.46
1:A:566:MET:HE3	1:A:616:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:PHE:CE2	1:A:610:PRO:HD2	2.51	0.46
1:A:927:MET:HB2	1:A:927:MET:HE2	1.48	0.46
1:B:627:ILE:HB	1:C:89:GLU:HG2	1.97	0.46
1:B:833:PRO:HG3	1:B:855:MET:HE2	1.97	0.46
1:D:133:ARG:NH1	1:D:170:VAL:HG21	2.30	0.46
1:D:580:PHE:CE2	1:D:610:PRO:HD2	2.51	0.46
1:A:112:SER:O	1:A:116:ARG:HG3	2.16	0.46
1:A:209:ARG:HE	1:A:210:VAL:H	1.61	0.46
1:A:628:THR:OG1	1:A:629:LYS:N	2.49	0.46
1:C:580:PHE:CE2	1:C:610:PRO:HD2	2.51	0.46
1:D:337:VAL:HA	1:D:340:VAL:HG22	1.96	0.46
1:B:349:LEU:O	1:B:353:TRP:N	2.48	0.46
1:B:126:THR:O	1:B:180:GLN:NE2	2.47	0.46
1:C:191:THR:HG21	1:C:215:GLU:OE1	2.16	0.46
1:C:442:LEU:HD22	1:C:447:MET:HG3	1.97	0.46
1:C:956:LEU:HB2	1:C:959:MET:HE2	1.97	0.46
1:B:133:ARG:NH1	1:B:170:VAL:HG21	2.31	0.46
1:B:993:ARG:HH12	1:B:999:ASP:HB3	1.81	0.46
1:C:130:TYR:O	1:C:134:VAL:HG12	2.16	0.46
1:D:993:ARG:HH12	1:D:999:ASP:HB3	1.80	0.46
1:B:544:GLU:N	1:B:544:GLU:OE1	2.47	0.46
1:B:580:PHE:CE2	1:B:610:PRO:HD2	2.51	0.46
1:A:130:TYR:CD2	1:A:239:PHE:HB3	2.52	0.45
1:B:286:THR:HG21	1:B:305:PHE:HD1	1.82	0.45
1:C:1019:ILE:HA	1:C:1024:ARG:HH21	1.80	0.45
1:B:202:ASN:O	1:B:204:TRP:N	2.49	0.45
1:C:175:THR:O	1:C:179:ILE:HG13	2.17	0.45
1:C:286:THR:HG21	1:C:305:PHE:HD1	1.82	0.45
1:C:379:SER:HB2	1:C:474:ARG:NH2	2.32	0.45
1:C:794:LYS:HG2	1:C:1163:PRO:HD2	1.97	0.45
1:A:566:MET:HE2	1:A:616:LEU:CD1	2.46	0.45
1:C:253:ILE:HG21	1:C:273:ILE:HD11	1.97	0.45
1:C:814:LEU:HD21	1:C:836:LEU:HD22	1.99	0.45
1:D:814:LEU:HD21	1:D:836:LEU:HD22	1.99	0.45
1:A:152:ASN:OD1	1:A:152:ASN:O	2.34	0.45
1:A:286:THR:HG21	1:A:305:PHE:HD1	1.81	0.45
1:B:753:TYR:CD1	1:B:764:PRO:HB2	2.51	0.45
1:C:604:LYS:HB2	1:C:604:LYS:HE2	1.71	0.45
1:D:112:SER:O	1:D:116:ARG:HG3	2.16	0.45
1:D:379:SER:HB2	1:D:474:ARG:NH2	2.32	0.45
1:D:784:GLY:N	1:D:791:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:833:PRO:HG3	1:D:855:MET:HE1	1.99	0.45
1:B:175:THR:O	1:B:179:ILE:HG13	2.17	0.45
1:B:784:GLY:N	1:B:791:GLU:OE1	2.50	0.45
1:B:814:LEU:HD21	1:B:836:LEU:HD22	1.99	0.45
1:D:828:ARG:HB3	1:D:828:ARG:NH1	2.31	0.45
1:A:814:LEU:HD21	1:A:836:LEU:HD22	1.99	0.45
1:A:828:ARG:HB3	1:A:828:ARG:NH1	2.31	0.45
1:B:1019:ILE:HA	1:B:1024:ARG:HH21	1.80	0.45
1:C:217:ILE:HD12	1:C:218:ASN:N	2.31	0.45
1:A:413:ASP:HB3	1:A:416:VAL:HG23	1.99	0.45
1:A:784:GLY:N	1:A:791:GLU:OE1	2.50	0.45
1:D:130:TYR:O	1:D:134:VAL:HG12	2.16	0.45
1:B:628:THR:OG1	1:B:629:LYS:N	2.50	0.44
1:A:992:THR:O	1:A:996:LEU:HG	2.18	0.44
1:B:414:VAL:HA	1:B:417:ARG:HG3	1.98	0.44
1:B:631:GLU:OE2	1:B:631:GLU:N	2.42	0.44
1:B:902:ILE:HD11	1:B:926:ASN:HB3	1.98	0.44
1:C:902:ILE:HD11	1:C:926:ASN:HB3	1.99	0.44
1:D:414:VAL:HA	1:D:417:ARG:HG3	1.99	0.44
1:A:414:VAL:HA	1:A:417:ARG:HG3	1.99	0.44
1:B:116:ARG:HG2	1:B:116:ARG:NH1	2.32	0.44
1:B:130:TYR:O	1:B:134:VAL:HG12	2.18	0.44
1:A:302:LEU:HD11	1:B:329:LEU:HD21	1.97	0.44
1:B:927:MET:HB2	1:B:927:MET:HE2	1.47	0.44
1:C:378:VAL:HG12	1:C:380:SER:H	1.83	0.44
1:D:130:TYR:HE2	1:D:287:CYS:HB3	1.83	0.44
1:D:413:ASP:HB3	1:D:416:VAL:HG23	2.00	0.44
1:A:884:ASP:OD2	1:A:922:THR:OG1	2.26	0.44
1:B:468:ASP:OD1	1:B:491:ILE:CD1	2.65	0.44
1:C:112:SER:O	1:C:116:ARG:HG3	2.17	0.44
1:C:628:THR:OG1	1:C:629:LYS:N	2.50	0.44
1:D:286:THR:HG21	1:D:305:PHE:HD1	1.82	0.44
1:A:172:ARG:HG2	1:A:173:LYS:H	1.83	0.44
1:B:543:GLN:NE2	1:B:551:ARG:O	2.45	0.44
1:B:884:ASP:OD2	1:B:922:THR:OG1	2.27	0.44
1:D:1014:GLU:H	1:D:1014:GLU:CD	2.21	0.44
1:B:604:LYS:HB2	1:B:604:LYS:HE2	1.69	0.44
1:C:130:TYR:HE2	1:C:287:CYS:HB3	1.83	0.44
1:C:468:ASP:OD1	1:C:491:ILE:CD1	2.65	0.44
1:B:292:LEU:HD12	1:B:330:LEU:HD22	2.00	0.44
1:B:1008:CYS:SG	1:B:1200:ARG:NH1	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1014:GLU:H	1:B:1014:GLU:CD	2.21	0.44
1:B:992:THR:O	1:B:996:LEU:HG	2.18	0.43
1:A:512:CYS:HA	1:A:998:LEU:HD11	2.01	0.43
1:B:177:TRP:HZ2	1:B:226:ILE:HA	1.83	0.43
1:C:927:MET:HB2	1:C:927:MET:HE2	1.44	0.43
1:B:133:ARG:HG3	1:B:172:ARG:HG3	2.00	0.43
1:D:378:VAL:HG12	1:D:380:SER:H	1.83	0.43
1:A:460:ASN:HD21	1:A:923:HIS:CE1	2.36	0.43
1:A:1017:LEU:HD12	1:A:1017:LEU:HA	1.83	0.43
1:D:992:THR:O	1:D:996:LEU:HG	2.18	0.43
1:A:292:LEU:HD12	1:A:330:LEU:HD22	2.00	0.43
1:A:549:TRP:CE2	1:A:550:GLN:HG3	2.54	0.43
1:C:784:GLY:N	1:C:791:GLU:OE1	2.51	0.43
1:D:172:ARG:NH1	1:D:232:ARG:O	2.52	0.43
1:A:627:ILE:HB	1:B:89:GLU:HG2	1.99	0.43
1:A:1014:GLU:CD	1:A:1014:GLU:H	2.21	0.43
1:A:108:ASN:ND2	1:A:111:SER:OG	2.51	0.43
1:A:985:LYS:HG2	1:A:987:TYR:OH	2.18	0.43
1:B:549:TRP:CE2	1:B:550:GLN:HG3	2.54	0.43
1:D:368:ALA:HB2	1:D:446:LYS:HG3	2.01	0.43
1:A:365:ARG:HA	1:A:446:LYS:HE2	2.01	0.43
1:A:1000:THR:O	1:A:1000:THR:OG1	2.30	0.43
1:B:123:LYS:HD2	1:B:241:ASN:HB3	2.01	0.43
1:B:297:GLU:HG2	1:B:323:LYS:HD2	2.00	0.43
1:B:365:ARG:HA	1:B:446:LYS:HE2	2.00	0.43
1:C:798:PHE:HD2	1:C:802:LEU:HD11	1.84	0.43
1:B:172:ARG:HG2	1:B:173:LYS:H	1.84	0.43
1:C:177:TRP:HZ2	1:C:226:ILE:HA	1.84	0.43
1:C:338:ALA:O	1:C:342:LEU:HB2	2.19	0.43
1:C:627:ILE:HB	1:D:89:GLU:HG2	2.01	0.43
1:C:751:LYS:NZ	1:C:824:TYR:HB2	2.34	0.43
1:D:338:ALA:O	1:D:342:LEU:HB2	2.19	0.43
1:D:479:LYS:HD3	1:D:487:LEU:HD12	2.01	0.43
1:A:338:ALA:O	1:A:342:LEU:HB2	2.19	0.43
1:C:992:THR:O	1:C:996:LEU:HG	2.18	0.43
1:D:172:ARG:HG2	1:D:173:LYS:H	1.84	0.43
1:A:1008:CYS:SG	1:A:1200:ARG:NH1	2.91	0.42
1:B:130:TYR:HE2	1:B:287:CYS:HB3	1.83	0.42
1:C:827:SER:HB2	1:C:830:GLU:HB3	2.00	0.42
1:C:1014:GLU:H	1:C:1014:GLU:CD	2.21	0.42
1:C:1145:GLU:HB2	1:D:501:LYS:HZ1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:549:TRP:CE2	1:C:550:GLN:HG3	2.54	0.42
1:D:985:LYS:HG2	1:D:987:TYR:OH	2.19	0.42
1:D:176:LEU:O	1:D:180:GLN:HB2	2.19	0.42
1:D:545:SER:OG	1:D:945:LEU:HD21	2.19	0.42
1:A:172:ARG:NH1	1:A:232:ARG:O	2.53	0.42
1:A:798:PHE:HD2	1:A:802:LEU:HD11	1.84	0.42
1:C:133:ARG:HG3	1:C:172:ARG:HG3	2.00	0.42
1:C:570:LYS:HG2	1:C:630:GLU:OE2	2.20	0.42
1:D:133:ARG:HG3	1:D:172:ARG:HG3	2.00	0.42
1:D:247:HIS:HA	1:D:250:GLU:OE2	2.20	0.42
1:D:566:MET:SD	1:D:616:LEU:HB3	2.60	0.42
1:A:479:LYS:HD3	1:A:487:LEU:HD12	2.01	0.42
1:A:560:GLU:HB2	1:A:562:TYR:CE2	2.54	0.42
1:B:368:ALA:HB2	1:B:446:LYS:HG3	2.00	0.42
1:B:532:LEU:HD12	1:B:1182:ILE:HD11	2.02	0.42
1:B:798:PHE:HD2	1:B:802:LEU:HD11	1.85	0.42
1:C:536:THR:O	1:C:955:ASN:ND2	2.52	0.42
1:C:998:LEU:HD23	1:C:998:LEU:HA	1.89	0.42
1:D:175:THR:O	1:D:179:ILE:HG13	2.20	0.42
1:D:819:VAL:HB	1:D:820:PRO:HD3	2.01	0.42
1:A:368:ALA:HB2	1:A:446:LYS:HG3	2.01	0.42
1:A:931:GLN:HG2	1:A:932:PHE:H	1.85	0.42
1:B:337:VAL:HA	1:B:340:VAL:HG22	2.00	0.42
1:B:512:CYS:HA	1:B:998:LEU:HD11	2.02	0.42
1:C:1041:TYR:HB3	1:C:1195:ILE:HB	2.02	0.42
1:D:108:ASN:ND2	1:D:111:SER:OG	2.53	0.42
1:D:520:ASN:ND2	1:D:527:SER:OG	2.47	0.42
1:D:798:PHE:HD2	1:D:802:LEU:HD11	1.84	0.42
1:B:828:ARG:HB3	1:B:828:ARG:CZ	2.49	0.42
1:B:867:ASP:HB3	1:B:1156:ARG:NH2	2.34	0.42
1:C:172:ARG:HG2	1:C:173:LYS:H	1.85	0.42
1:C:532:LEU:HD12	1:C:1182:ILE:HD11	2.02	0.42
1:D:560:GLU:HB2	1:D:562:TYR:CE2	2.54	0.42
1:A:177:TRP:CZ3	1:A:232:ARG:HD3	2.54	0.42
1:A:532:LEU:HD12	1:A:1182:ILE:HD11	2.02	0.42
1:C:368:ALA:HB2	1:C:446:LYS:HG3	2.01	0.42
1:D:363:TYR:HB3	1:D:444:ARG:O	2.20	0.42
1:D:532:LEU:HD12	1:D:1182:ILE:HD11	2.02	0.42
1:D:549:TRP:CE2	1:D:550:GLN:HG3	2.54	0.42
1:D:943:SER:O	1:D:947:LYS:HG3	2.20	0.42
1:B:117:LEU:HD22	1:B:252:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:944:LYS:HA	1:B:947:LYS:HE2	2.01	0.42
1:C:819:VAL:HB	1:C:820:PRO:HD3	2.02	0.42
1:C:884:ASP:OD2	1:C:922:THR:OG1	2.27	0.42
1:C:900:LYS:HE2	1:C:904:ASN:HD21	1.85	0.42
1:C:1020:ARG:HB2	1:C:1020:ARG:NH1	2.35	0.42
1:D:536:THR:O	1:D:955:ASN:ND2	2.53	0.42
1:D:931:GLN:HG2	1:D:932:PHE:H	1.85	0.42
1:A:524:PRO:HG3	1:A:1195:ILE:HD13	2.01	0.42
1:A:536:THR:O	1:A:955:ASN:ND2	2.53	0.42
1:A:1041:TYR:HB3	1:A:1195:ILE:HB	2.02	0.42
1:B:570:LYS:HG2	1:B:630:GLU:OE2	2.20	0.42
1:A:179:ILE:H	1:A:179:ILE:HG13	1.61	0.41
1:B:247:HIS:HA	1:B:250:GLU:OE2	2.20	0.41
1:B:479:LYS:HD3	1:B:487:LEU:HD12	2.01	0.41
1:C:108:ASN:ND2	1:C:111:SER:OG	2.53	0.41
1:C:363:TYR:HB3	1:C:444:ARG:O	2.20	0.41
1:C:512:CYS:HA	1:C:998:LEU:HD11	2.02	0.41
1:D:512:CYS:HA	1:D:998:LEU:HD11	2.01	0.41
1:D:945:LEU:O	1:D:949:GLU:HG2	2.20	0.41
1:D:1041:TYR:HB3	1:D:1195:ILE:HB	2.02	0.41
1:A:1020:ARG:HB2	1:A:1020:ARG:NH1	2.35	0.41
1:B:413:ASP:HB3	1:B:416:VAL:HG23	2.02	0.41
1:B:1020:ARG:NH1	1:B:1020:ARG:HB2	2.35	0.41
1:B:1041:TYR:HB3	1:B:1195:ILE:HB	2.02	0.41
1:C:365:ARG:HA	1:C:446:LYS:HE2	2.02	0.41
1:C:436:ALA:HB3	1:C:474:ARG:HD3	2.02	0.41
1:C:1008:CYS:SG	1:C:1200:ARG:NH1	2.91	0.41
1:D:117:LEU:HD22	1:D:252:MET:SD	2.60	0.41
1:A:363:TYR:HB3	1:A:444:ARG:O	2.20	0.41
1:D:1020:ARG:NH1	1:D:1020:ARG:HB2	2.35	0.41
1:A:118:PHE:O	1:A:122:LEU:HB2	2.21	0.41
1:A:130:TYR:CE2	1:A:239:PHE:HD2	2.38	0.41
1:A:867:ASP:HB3	1:A:1156:ARG:NH2	2.35	0.41
1:A:943:SER:O	1:A:947:LYS:HG3	2.21	0.41
1:B:249:LEU:O	1:B:252:MET:HB2	2.20	0.41
1:B:253:ILE:HG21	1:B:273:ILE:HD11	2.03	0.41
1:C:413:ASP:HB3	1:C:416:VAL:HG23	2.02	0.41
1:D:177:TRP:CZ3	1:D:232:ARG:HD3	2.56	0.41
1:D:867:ASP:HB3	1:D:1156:ARG:NH2	2.35	0.41
1:A:819:VAL:HB	1:A:820:PRO:HD3	2.01	0.41
1:B:1017:LEU:HD12	1:B:1017:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:TRP:CZ2	1:C:226:ILE:HA	2.55	0.41
1:C:247:HIS:HA	1:C:250:GLU:OE2	2.21	0.41
1:C:828:ARG:CZ	1:C:828:ARG:HB3	2.50	0.41
1:D:1140:LEU:HD23	1:D:1140:LEU:HA	1.89	0.41
1:B:900:LYS:HE2	1:B:904:ASN:HD21	1.86	0.41
1:D:524:PRO:HG3	1:D:1195:ILE:HD13	2.02	0.41
1:B:536:THR:O	1:B:955:ASN:ND2	2.53	0.41
1:B:819:VAL:HB	1:B:820:PRO:HD3	2.02	0.41
1:C:297:GLU:HG2	1:C:323:LYS:HD2	2.02	0.41
1:C:563:HIS:HB3	1:C:987:TYR:CZ	2.56	0.41
1:C:931:GLN:HG2	1:C:932:PHE:H	1.86	0.41
1:C:945:LEU:O	1:C:949:GLU:HG2	2.20	0.41
1:D:490:GLN:HE22	1:D:976:ASP:HA	1.85	0.41
1:D:945:LEU:HD23	1:D:945:LEU:HA	1.92	0.41
1:A:122:LEU:HG	1:A:183:VAL:HG22	2.03	0.41
1:B:363:TYR:HB3	1:B:444:ARG:O	2.20	0.41
1:B:528:THR:O	1:B:532:LEU:HG	2.21	0.41
1:B:915:LEU:HD23	1:B:917:ILE:HG12	2.02	0.41
1:C:528:THR:O	1:C:532:LEU:HG	2.21	0.41
1:C:549:TRP:CE2	1:C:1177:LEU:HD21	2.56	0.41
1:C:1017:LEU:HD12	1:C:1017:LEU:HA	1.82	0.41
1:D:915:LEU:HD23	1:D:917:ILE:HG12	2.03	0.41
1:D:1144:SER:H	1:D:1147:GLN:HE21	1.69	0.41
1:A:142:GLY:O	1:A:143:ILE:HD13	2.21	0.41
1:A:570:LYS:HG2	1:A:630:GLU:OE2	2.20	0.41
1:B:563:HIS:HB3	1:B:987:TYR:CZ	2.55	0.41
1:B:867:ASP:O	1:B:871:GLN:HG3	2.21	0.41
1:B:945:LEU:O	1:B:949:GLU:HG2	2.21	0.41
1:C:185:ILE:HG22	1:C:189:LEU:HD23	2.01	0.41
1:C:867:ASP:O	1:C:871:GLN:HG3	2.21	0.41
1:C:943:SER:O	1:C:947:LYS:HG3	2.20	0.41
1:C:1140:LEU:HD23	1:C:1140:LEU:HA	1.89	0.41
1:D:197:LEU:HA	1:D:197:LEU:HD12	1.85	0.41
1:A:131:ILE:HD13	1:A:131:ILE:HA	1.91	0.41
1:A:350:VAL:HG12	1:A:353:TRP:HD1	1.86	0.41
1:A:945:LEU:O	1:A:949:GLU:HG2	2.21	0.41
1:B:142:GLY:O	1:B:143:ILE:HD13	2.21	0.41
1:B:436:ALA:HB3	1:B:474:ARG:HD3	2.03	0.41
1:B:560:GLU:HB2	1:B:562:TYR:CE2	2.55	0.41
1:C:209:ARG:HG3	1:C:211:SER:H	1.86	0.41
1:C:629:LYS:HE2	1:C:631:GLU:OE2	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ILE:HD13	1:D:131:ILE:HA	1.91	0.41
1:D:142:GLY:O	1:D:143:ILE:HD13	2.21	0.41
1:D:365:ARG:HA	1:D:446:LYS:HE2	2.02	0.41
1:A:436:ALA:HB3	1:A:474:ARG:HD3	2.03	0.40
1:B:468:ASP:OD2	1:B:496:ASN:HB2	2.19	0.40
1:D:1008:CYS:SG	1:D:1200:ARG:NH1	2.91	0.40
1:A:468:ASP:OD2	1:A:496:ASN:HB3	2.17	0.40
1:A:572:PHE:HA	1:A:575:TYR:CE1	2.57	0.40
1:A:634:ALA:H	1:B:87:GLN:HE22	1.69	0.40
1:B:209:ARG:HG3	1:B:211:SER:H	1.86	0.40
1:C:216:MET:O	1:C:220:LEU:HB2	2.22	0.40
1:C:536:THR:HA	1:C:560:GLU:OE2	2.20	0.40
1:C:572:PHE:HA	1:C:575:TYR:CE1	2.57	0.40
1:A:528:THR:O	1:A:532:LEU:HG	2.21	0.40
1:B:173:LYS:CD	1:B:176:LEU:HD23	2.47	0.40
1:B:631:GLU:CD	1:B:631:GLU:H	2.17	0.40
1:B:931:GLN:HG2	1:B:932:PHE:H	1.85	0.40
1:C:915:LEU:HD23	1:C:917:ILE:HG12	2.03	0.40
1:A:383:ILE:HG21	1:A:415:GLN:OE1	2.22	0.40
1:A:631:GLU:H	1:A:631:GLU:CD	2.18	0.40
1:B:780:ARG:NH1	1:B:783:LYS:HB3	2.37	0.40
1:A:915:LEU:HD23	1:A:917:ILE:HG12	2.02	0.40
1:C:524:PRO:HG3	1:C:1195:ILE:HD13	2.02	0.40
1:D:177:TRP:CZ2	1:D:226:ILE:HA	2.57	0.40
1:D:439:ASP:O	1:D:443:MET:HG3	2.21	0.40
1:D:867:ASP:O	1:D:871:GLN:HG3	2.21	0.40
1:D:1017:LEU:HD12	1:D:1017:LEU:HA	1.83	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	908/1235 (74%)	883 (97%)	25 (3%)	0	100	100
1	B	908/1235 (74%)	882 (97%)	26 (3%)	0	100	100
1	C	908/1235 (74%)	881 (97%)	27 (3%)	0	100	100
1	D	908/1235 (74%)	883 (97%)	25 (3%)	0	100	100
All	All	3632/4940 (74%)	3529 (97%)	103 (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	790/1086 (73%)	773 (98%)	17 (2%)	52	78
1	B	790/1086 (73%)	777 (98%)	13 (2%)	62	83
1	C	790/1086 (73%)	779 (99%)	11 (1%)	67	85
1	D	790/1086 (73%)	773 (98%)	17 (2%)	52	78
All	All	3160/4344 (73%)	3102 (98%)	58 (2%)	61	81

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

Mol	Chain	Res	Type
1	A	153	TYR
1	A	196	TYR
1	A	222	PHE
1	A	353	TRP
1	A	379	SER
1	A	380	SER
1	A	388	ASP
1	A	412	MET
1	A	418	ARG
1	A	560	GLU
1	A	629	LYS
1	A	792	ASP
1	A	825	TYR

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Mol	Chain	Res	Type
1	A	876	TYR
1	A	878	ASP
1	A	1026	PHE
1	A	1045	SER
1	B	153	TYR
1	B	222	PHE
1	B	353	TRP
1	B	379	SER
1	B	380	SER
1	B	560	GLU
1	B	792	ASP
1	B	825	TYR
1	B	876	TYR
1	B	878	ASP
1	B	1026	PHE
1	B	1045	SER
1	B	1193	SER
1	C	153	TYR
1	C	353	TRP
1	C	380	SER
1	C	388	ASP
1	C	560	GLU
1	C	792	ASP
1	C	825	TYR
1	C	876	TYR
1	C	878	ASP
1	C	1026	PHE
1	C	1045	SER
1	D	153	TYR
1	D	163	ASN
1	D	222	PHE
1	D	329	LEU
1	D	353	TRP
1	D	380	SER
1	D	388	ASP
1	D	412	MET
1	D	418	ARG
1	D	468	ASP
1	D	560	GLU
1	D	792	ASP
1	D	825	TYR
1	D	843	ASP

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Mol	Chain	Res	Type
1	D	876	TYR
1	D	878	ASP
1	D	1026	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	119	ASN
1	A	151	GLN
1	A	241	ASN
1	A	291	HIS
1	A	369	GLN
1	A	490	GLN
1	A	496	ASN
1	A	505	HIS
1	A	871	GLN
1	A	879	ASN
1	A	904	ASN
1	A	923	HIS
1	A	955	ASN
1	A	1147	GLN
1	B	108	ASN
1	B	119	ASN
1	B	151	GLN
1	B	241	ASN
1	B	291	HIS
1	B	369	GLN
1	B	490	GLN
1	B	496	ASN
1	B	871	GLN
1	B	879	ASN
1	B	904	ASN
1	B	923	HIS
1	B	955	ASN
1	B	1147	GLN
1	C	108	ASN
1	C	119	ASN
1	C	151	GLN
1	C	241	ASN
1	C	291	HIS
1	C	369	GLN

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Mol	Chain	Res	Type
1	C	490	GLN
1	C	496	ASN
1	C	505	HIS
1	C	871	GLN
1	C	879	ASN
1	C	904	ASN
1	C	923	HIS
1	C	955	ASN
1	C	1147	GLN
1	D	108	ASN
1	D	119	ASN
1	D	151	GLN
1	D	241	ASN
1	D	291	HIS
1	D	369	GLN
1	D	490	GLN
1	D	505	HIS
1	D	871	GLN
1	D	879	ASN
1	D	904	ASN
1	D	923	HIS
1	D	955	ASN
1	D	1147	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	6OU	D	1301	-	10,10,48	0.27	0	9,9,53	0.24	0
4	6OU	B	1301	-	10,10,48	0.27	0	9,9,53	0.25	0
4	6OU	C	1301	-	10,10,48	0.27	0	9,9,53	0.24	0
4	6OU	A	1306	-	10,10,48	0.27	0	9,9,53	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6OU	D	1301	-	-	1/8/8/52	-
4	6OU	B	1301	-	-	1/8/8/52	-
4	6OU	C	1301	-	-	1/8/8/52	-
4	6OU	A	1306	-	-	1/8/8/52	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

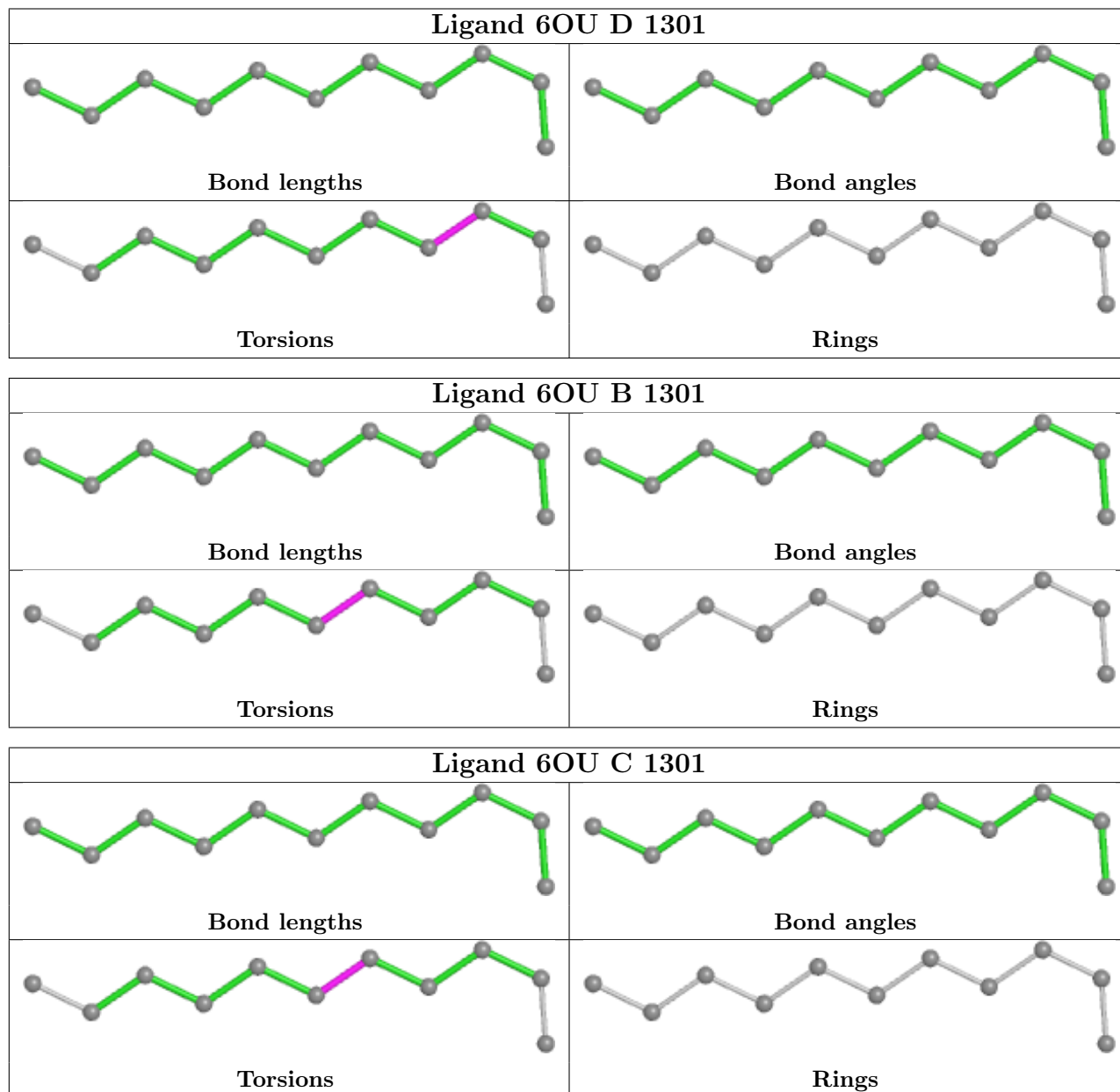
Mol	Chain	Res	Type	Atoms
4	B	1301	6OU	C42-C43-C44-C45
4	C	1301	6OU	C42-C43-C44-C45
4	A	1306	6OU	C42-C43-C44-C45
4	D	1301	6OU	C40-C41-C42-C43

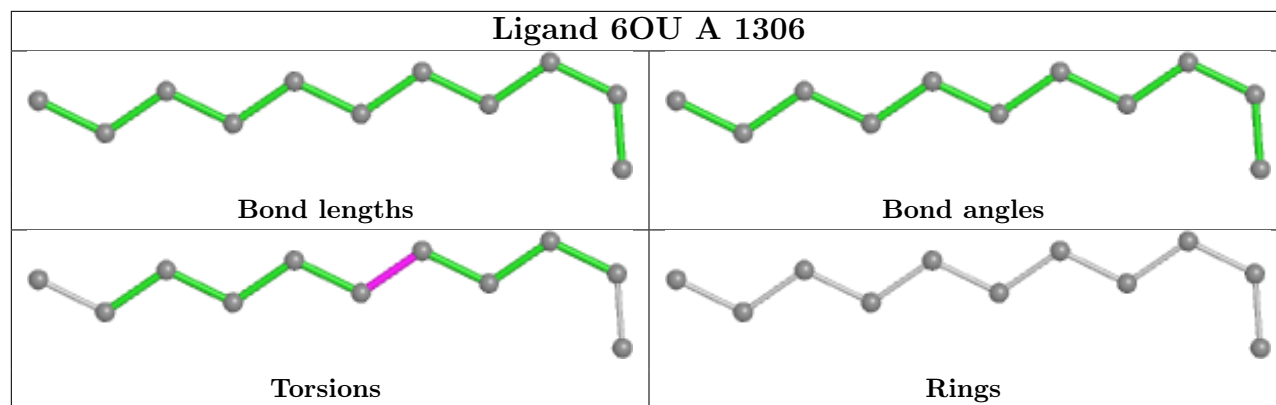
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

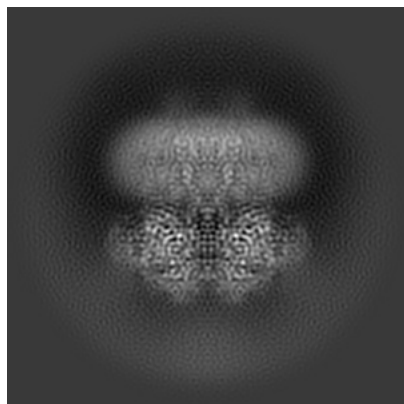
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34827. These allow visual inspection of the internal detail of the map and identification of artifacts.

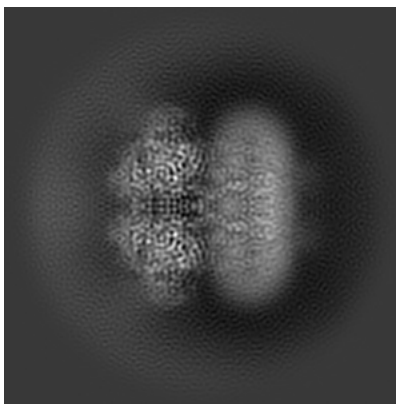
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

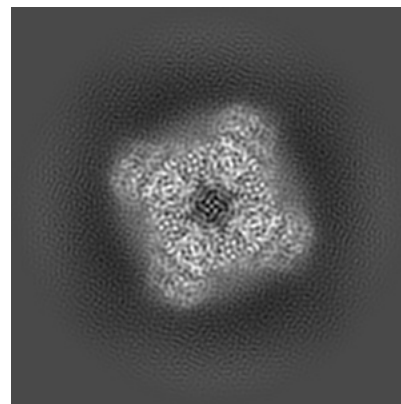
6.1.1 Primary map



X

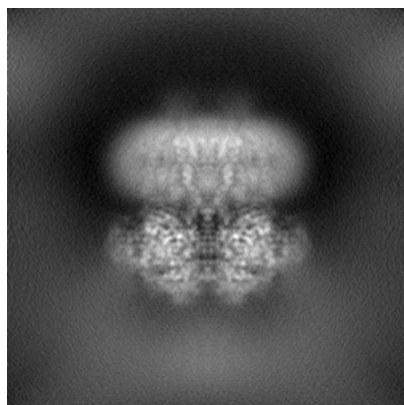


Y

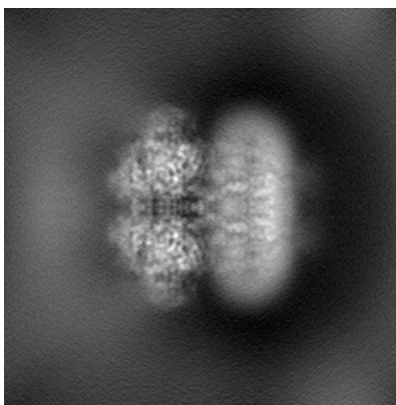


Z

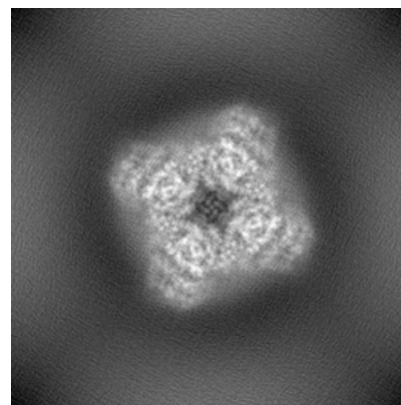
6.1.2 Raw map



X



Y

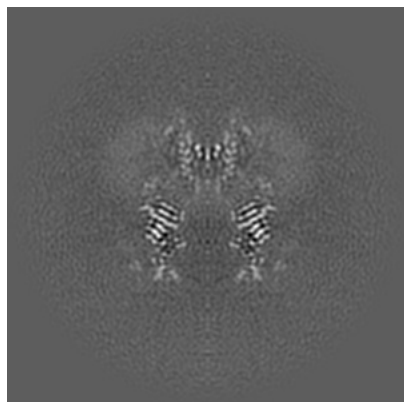


Z

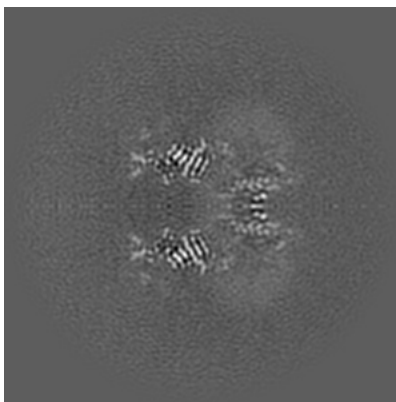
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

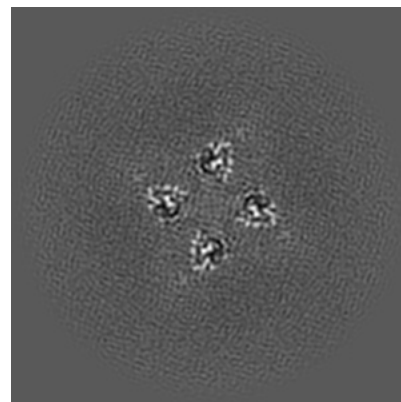
6.2.1 Primary map



X Index: 128

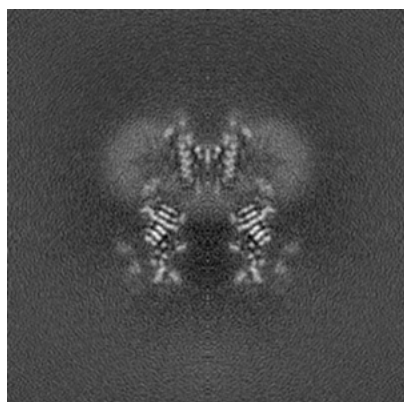


Y Index: 128

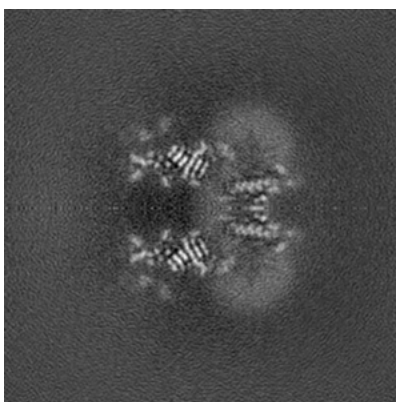


Z Index: 128

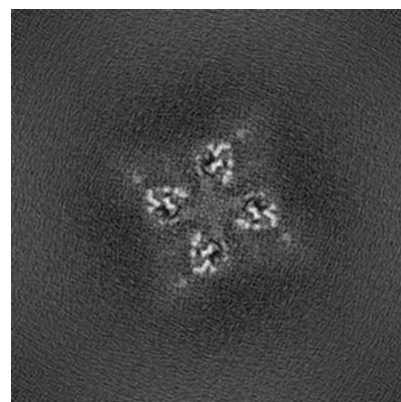
6.2.2 Raw map



X Index: 128



Y Index: 128

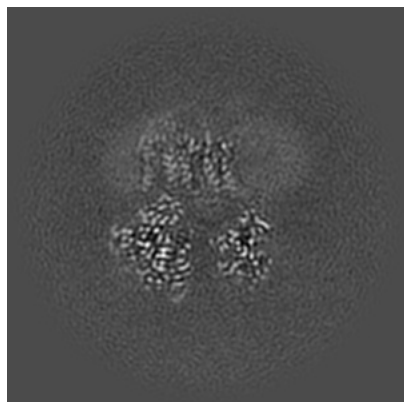


Z Index: 128

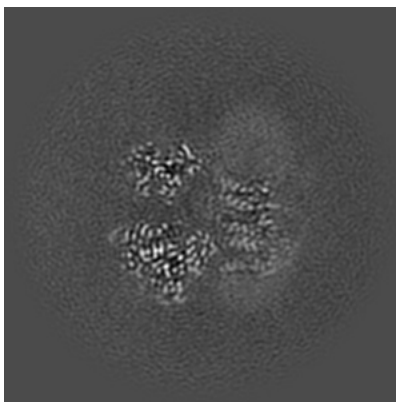
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

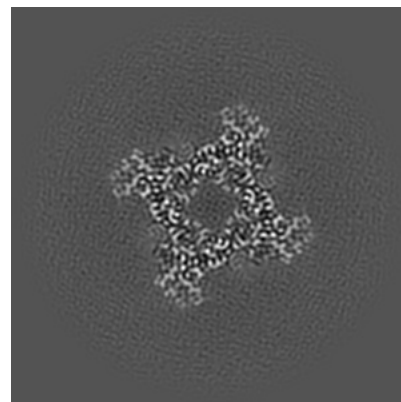
6.3.1 Primary map



X Index: 116

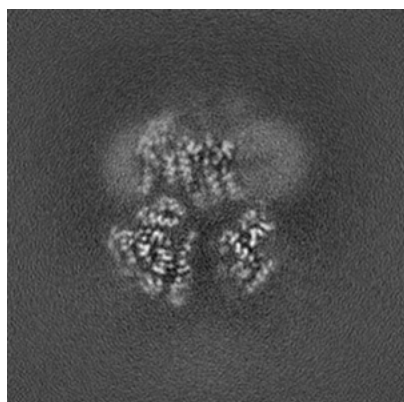


Y Index: 140

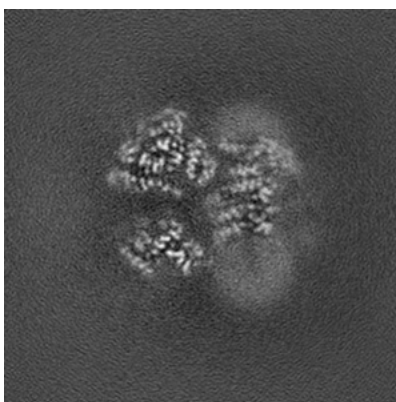


Z Index: 108

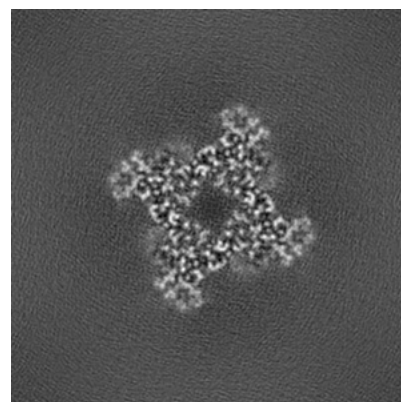
6.3.2 Raw map



X Index: 117



Y Index: 117

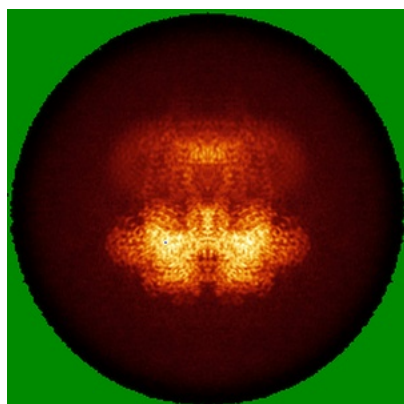


Z Index: 108

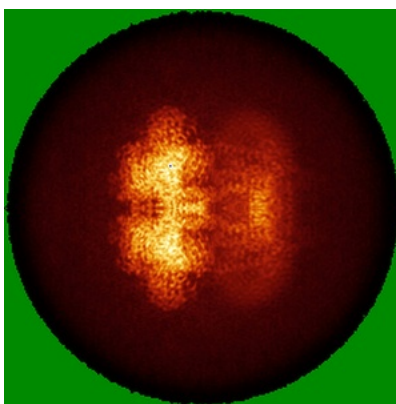
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

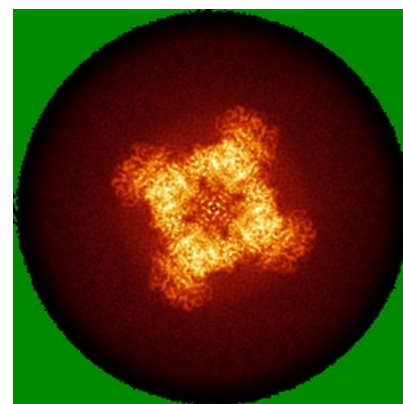
6.4.1 Primary map



X

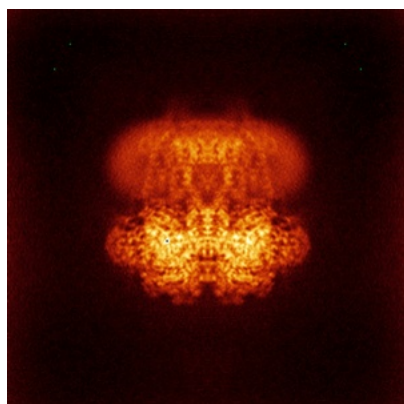


Y

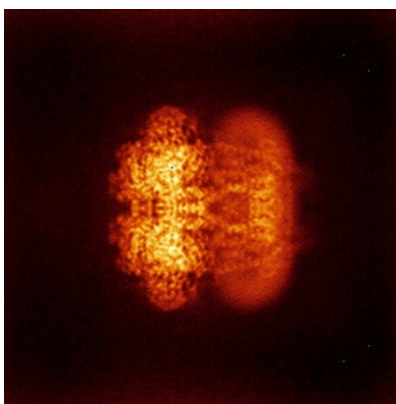


Z

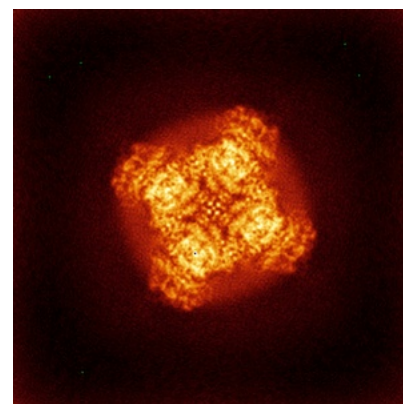
6.4.2 Raw map



X



Y

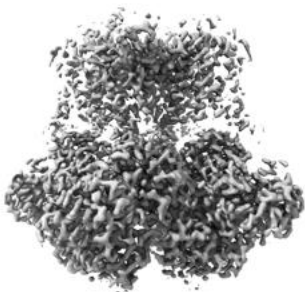


Z

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](#)

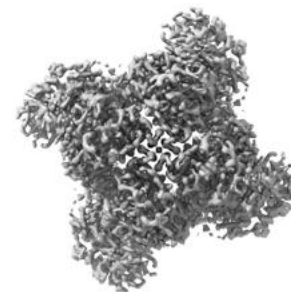
6.5.1 Primary map



X



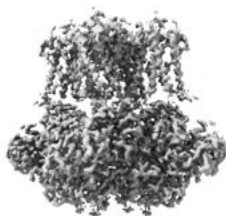
Y



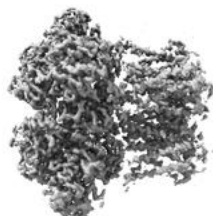
Z

The images above show the 3D surface view of the map at the recommended contour level 0.771. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

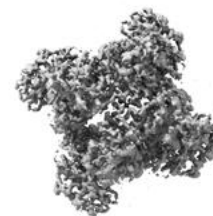
6.5.2 Raw map



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.

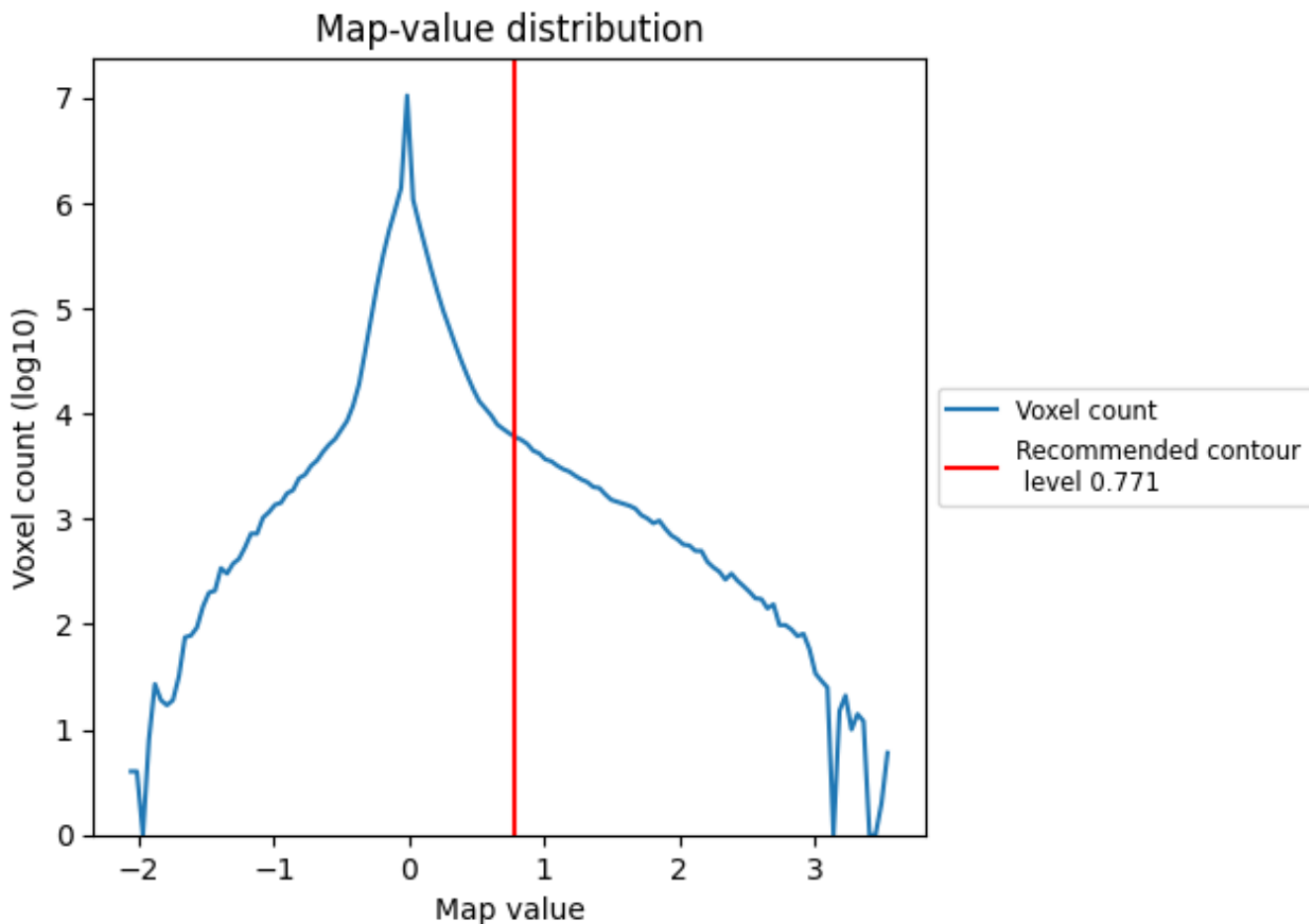
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

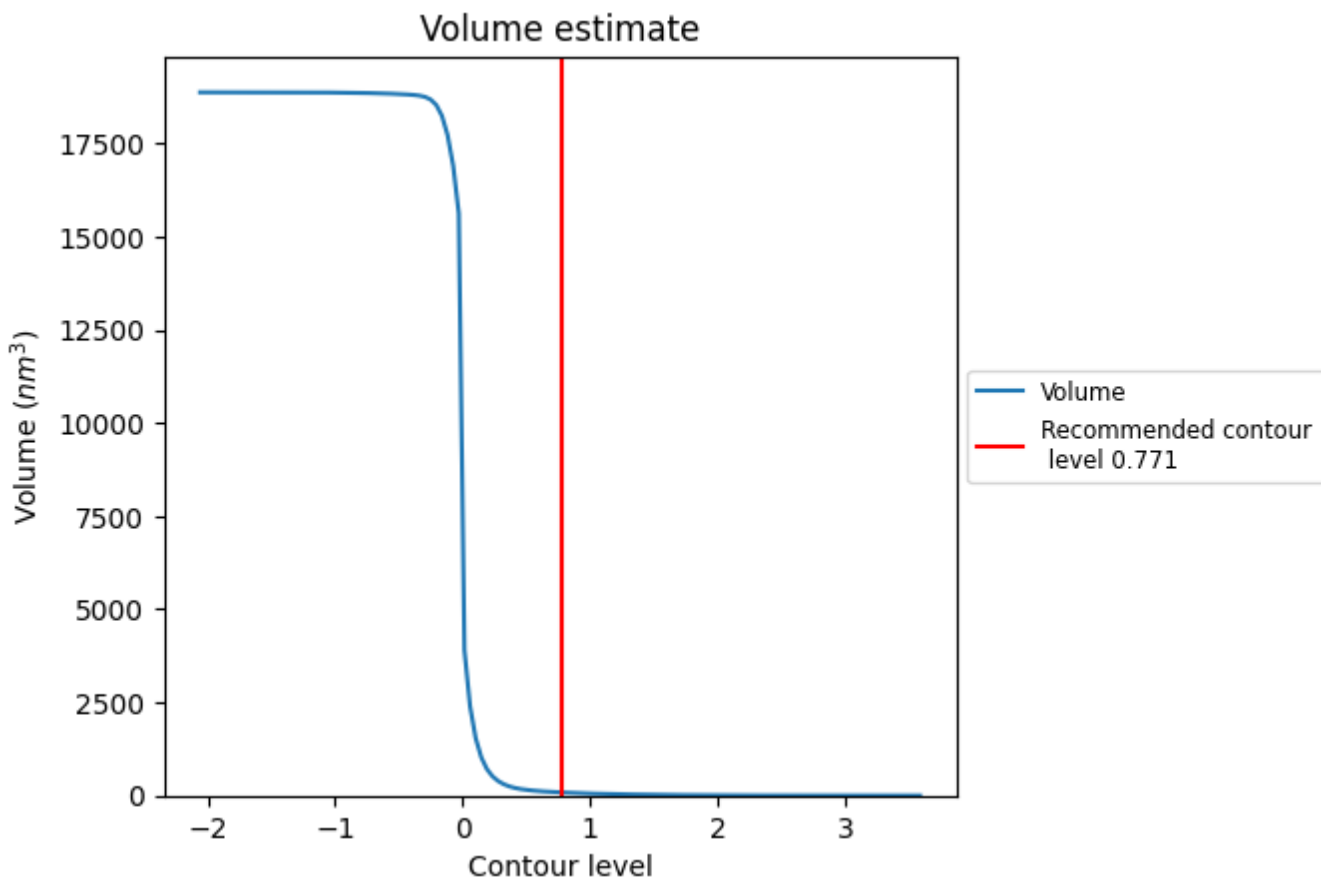
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

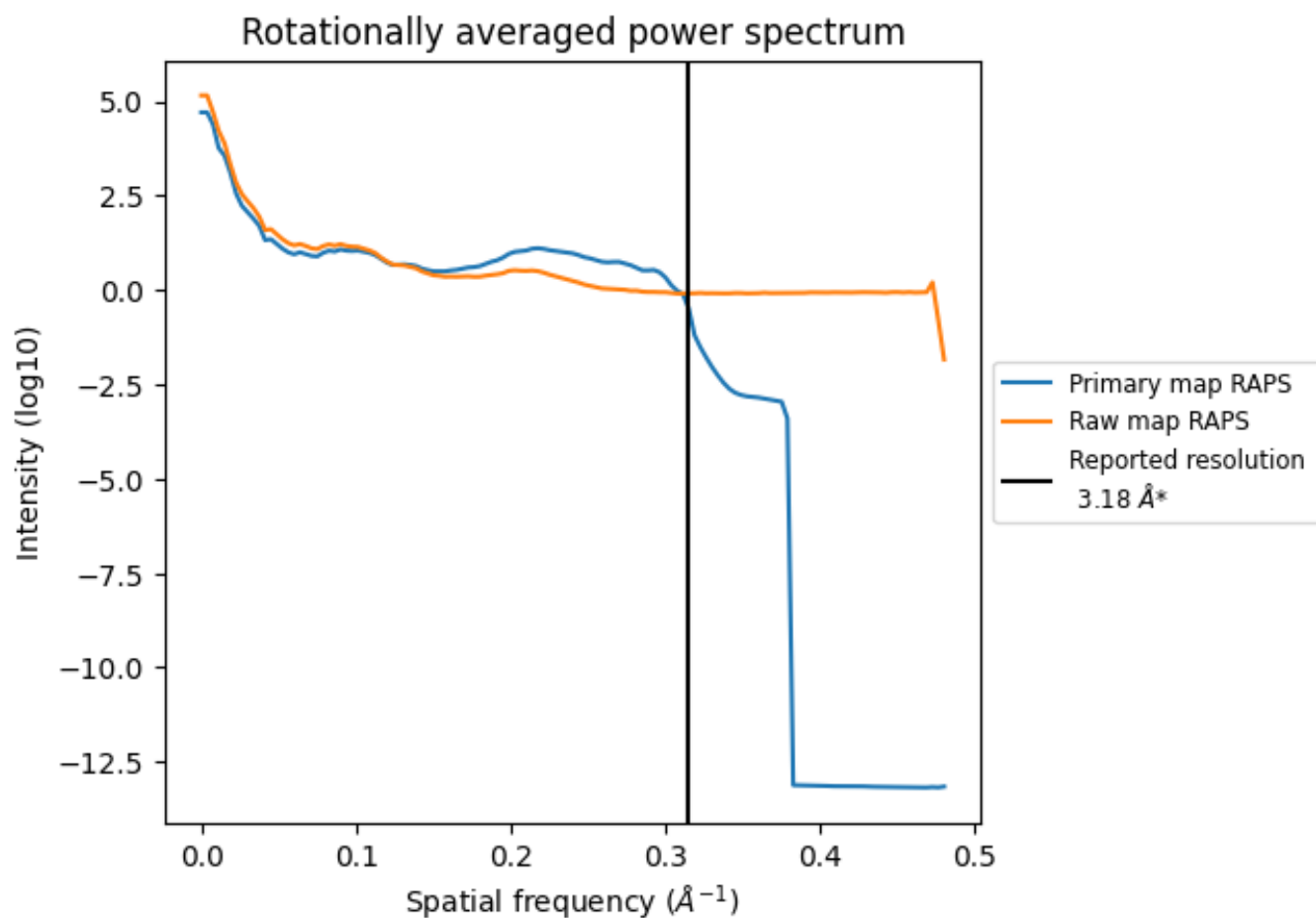
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 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](#)

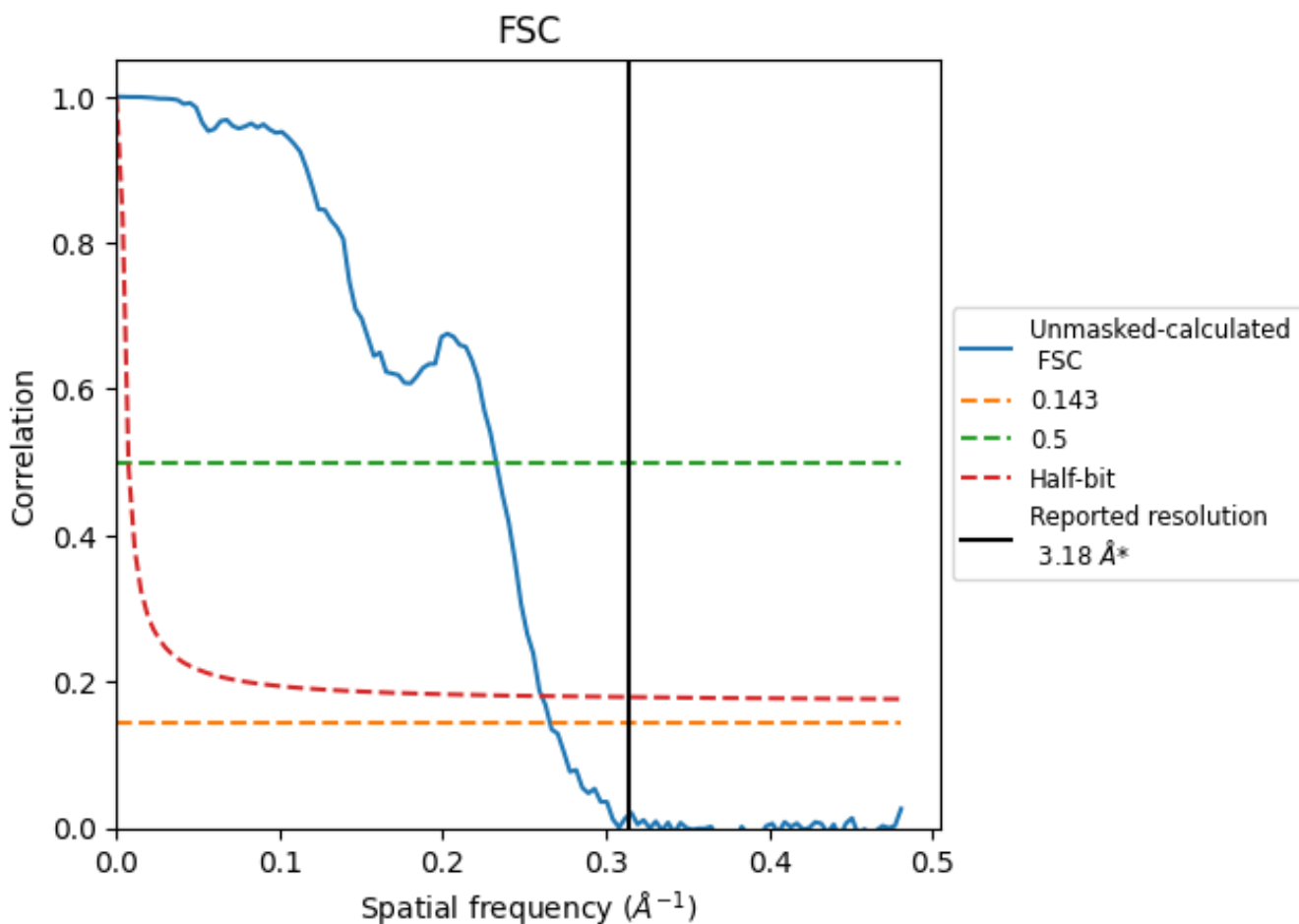


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.314 \AA^{-1}

8.2 Resolution estimates [i](#)

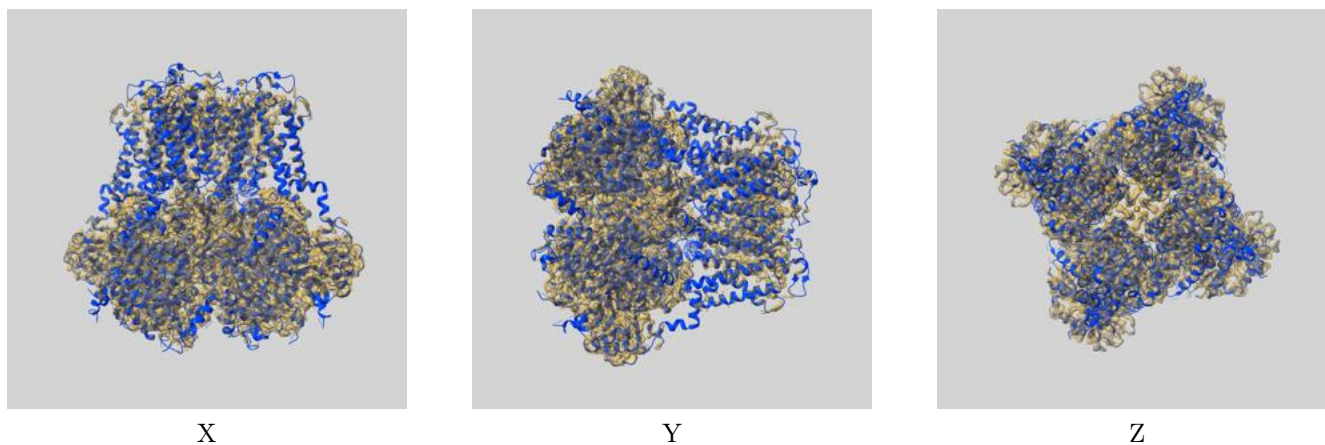
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	4.30	3.84

*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 3.76 differs from the reported value 3.18 by more than 10 %

9 Map-model fit [i](#)

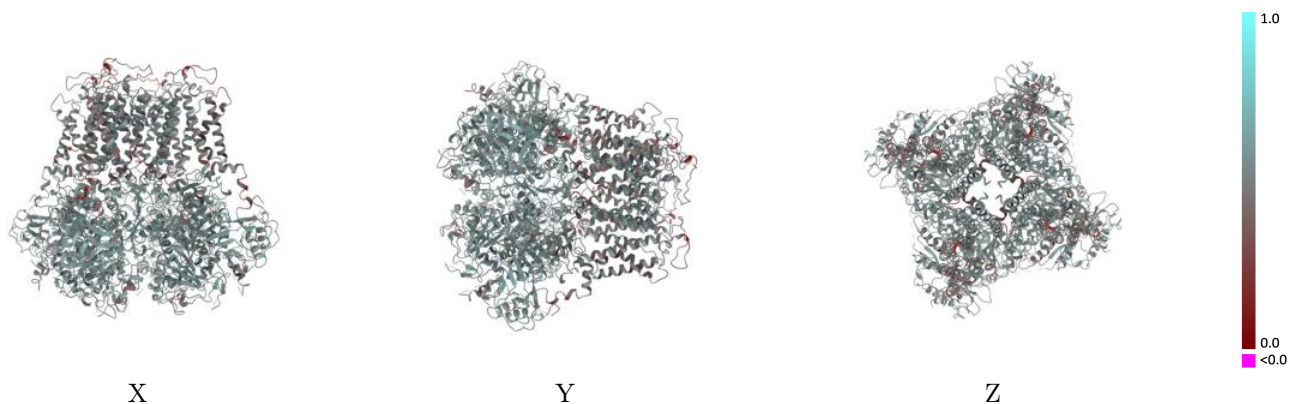
This section contains information regarding the fit between EMDB map EMD-34827 and PDB model 8HIR. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



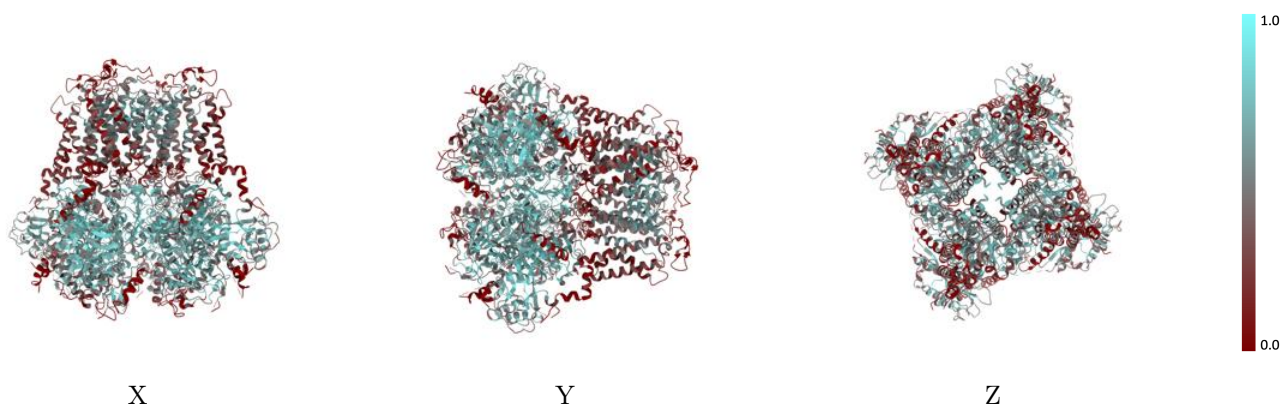
The images above show the 3D surface view of the map at the recommended contour level 0.771 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



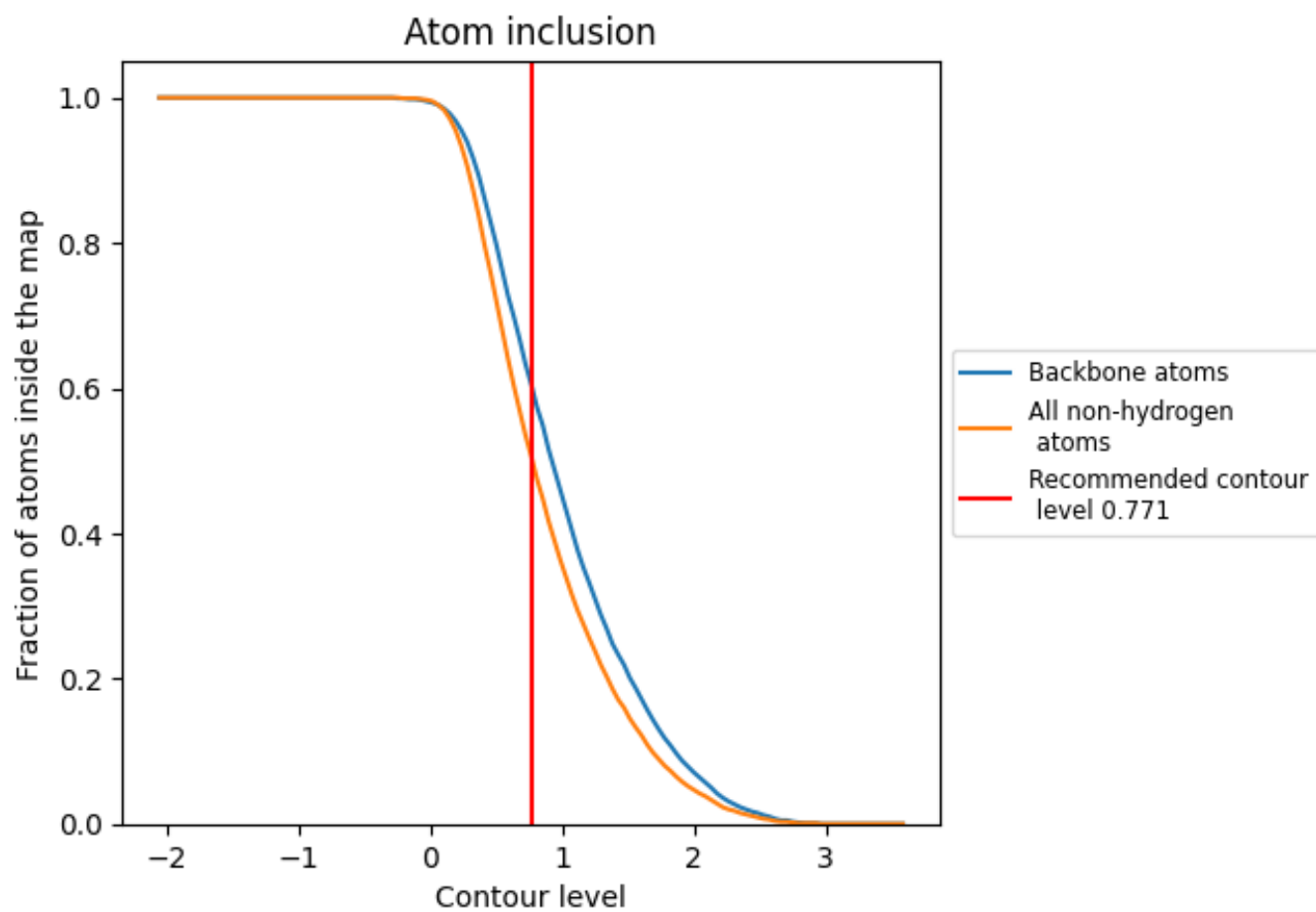
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.771).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.771) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	█ 0.5010	█ 0.5180
A	█ 0.5020	█ 0.5190
B	█ 0.5010	█ 0.5180
C	█ 0.5010	█ 0.5180
D	█ 0.5010	█ 0.5180

