



## Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 05:08 PM JST

PDB ID : 7XNI  
EMDB ID : EMD-33316  
Title : human KCNQ1-CaM in apo state  
Authors : Ma, D.; Guo, J.  
Deposited on : 2022-04-28  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

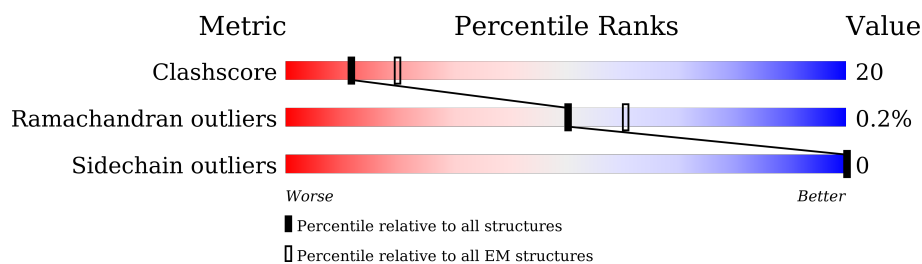
# 1 Overall quality at a glance

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)
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  $\geq 3$ , 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	692	
1	B	692	
1	D	692	
1	G	692	
2	C	177	
2	E	177	
2	F	177	
2	H	177	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31368 atoms, of which 15652 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 KQT member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	348	Total	C	H	N	O	S	0	0
			5712	1851	2891	492	467	11		
1	B	348	Total	C	H	N	O	S	0	0
			5712	1851	2891	492	467	11		
1	D	348	Total	C	H	N	O	S	0	0
			5712	1851	2891	492	467	11		
1	G	348	Total	C	H	N	O	S	0	0
			5712	1851	2891	492	467	11		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	677	LEU	-	expression tag	UNP P51787
A	678	GLU	-	expression tag	UNP P51787
A	679	GLY	-	expression tag	UNP P51787
A	680	GLY	-	expression tag	UNP P51787
A	681	SER	-	expression tag	UNP P51787
A	682	SER	-	expression tag	UNP P51787
A	683	GLY	-	expression tag	UNP P51787
A	684	GLY	-	expression tag	UNP P51787
A	685	TRP	-	expression tag	UNP P51787
A	686	SER	-	expression tag	UNP P51787
A	687	HIS	-	expression tag	UNP P51787
A	688	PRO	-	expression tag	UNP P51787
A	689	GLN	-	expression tag	UNP P51787
A	690	PHE	-	expression tag	UNP P51787
A	691	GLU	-	expression tag	UNP P51787
A	692	LYS	-	expression tag	UNP P51787
B	677	LEU	-	expression tag	UNP P51787
B	678	GLU	-	expression tag	UNP P51787
B	679	GLY	-	expression tag	UNP P51787
B	680	GLY	-	expression tag	UNP P51787
B	681	SER	-	expression tag	UNP P51787
B	682	SER	-	expression tag	UNP P51787

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Chain	Residue	Modelled	Actual	Comment	Reference
B	683	GLY	-	expression tag	UNP P51787
B	684	GLY	-	expression tag	UNP P51787
B	685	TRP	-	expression tag	UNP P51787
B	686	SER	-	expression tag	UNP P51787
B	687	HIS	-	expression tag	UNP P51787
B	688	PRO	-	expression tag	UNP P51787
B	689	GLN	-	expression tag	UNP P51787
B	690	PHE	-	expression tag	UNP P51787
B	691	GLU	-	expression tag	UNP P51787
B	692	LYS	-	expression tag	UNP P51787
D	677	LEU	-	expression tag	UNP P51787
D	678	GLU	-	expression tag	UNP P51787
D	679	GLY	-	expression tag	UNP P51787
D	680	GLY	-	expression tag	UNP P51787
D	681	SER	-	expression tag	UNP P51787
D	682	SER	-	expression tag	UNP P51787
D	683	GLY	-	expression tag	UNP P51787
D	684	GLY	-	expression tag	UNP P51787
D	685	TRP	-	expression tag	UNP P51787
D	686	SER	-	expression tag	UNP P51787
D	687	HIS	-	expression tag	UNP P51787
D	688	PRO	-	expression tag	UNP P51787
D	689	GLN	-	expression tag	UNP P51787
D	690	PHE	-	expression tag	UNP P51787
D	691	GLU	-	expression tag	UNP P51787
D	692	LYS	-	expression tag	UNP P51787
G	677	LEU	-	expression tag	UNP P51787
G	678	GLU	-	expression tag	UNP P51787
G	679	GLY	-	expression tag	UNP P51787
G	680	GLY	-	expression tag	UNP P51787
G	681	SER	-	expression tag	UNP P51787
G	682	SER	-	expression tag	UNP P51787
G	683	GLY	-	expression tag	UNP P51787
G	684	GLY	-	expression tag	UNP P51787
G	685	TRP	-	expression tag	UNP P51787
G	686	SER	-	expression tag	UNP P51787
G	687	HIS	-	expression tag	UNP P51787
G	688	PRO	-	expression tag	UNP P51787
G	689	GLN	-	expression tag	UNP P51787
G	690	PHE	-	expression tag	UNP P51787
G	691	GLU	-	expression tag	UNP P51787
G	692	LYS	-	expression tag	UNP P51787

- Molecule 2 is a protein called Calmodulin-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	144	Total	C	H	N	O	S	0	0
			2130	682	1022	180	237	9		
2	E	144	Total	C	H	N	O	S	0	0
			2130	682	1022	180	237	9		
2	F	144	Total	C	H	N	O	S	0	0
			2130	682	1022	180	237	9		
2	H	144	Total	C	H	N	O	S	0	0
			2130	682	1022	180	237	9		

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	150	LEU	-	expression tag	UNP P0DP25
C	151	GLU	-	expression tag	UNP P0DP25
C	152	GLY	-	expression tag	UNP P0DP25
C	153	GLY	-	expression tag	UNP P0DP25
C	154	SER	-	expression tag	UNP P0DP25
C	155	SER	-	expression tag	UNP P0DP25
C	156	GLY	-	expression tag	UNP P0DP25
C	157	GLY	-	expression tag	UNP P0DP25
C	158	LEU	-	expression tag	UNP P0DP25
C	159	VAL	-	expression tag	UNP P0DP25
C	160	PRO	-	expression tag	UNP P0DP25
C	161	ARG	-	expression tag	UNP P0DP25
C	162	GLY	-	expression tag	UNP P0DP25
C	163	SER	-	expression tag	UNP P0DP25
C	164	GLY	-	expression tag	UNP P0DP25
C	165	GLY	-	expression tag	UNP P0DP25
C	166	SER	-	expression tag	UNP P0DP25
C	167	SER	-	expression tag	UNP P0DP25
C	168	GLY	-	expression tag	UNP P0DP25
C	169	GLY	-	expression tag	UNP P0DP25
C	170	HIS	-	expression tag	UNP P0DP25
C	171	HIS	-	expression tag	UNP P0DP25
C	172	HIS	-	expression tag	UNP P0DP25
C	173	HIS	-	expression tag	UNP P0DP25
C	174	HIS	-	expression tag	UNP P0DP25
C	175	HIS	-	expression tag	UNP P0DP25
C	176	HIS	-	expression tag	UNP P0DP25
C	177	HIS	-	expression tag	UNP P0DP25
E	150	LEU	-	expression tag	UNP P0DP25
E	151	GLU	-	expression tag	UNP P0DP25

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Chain	Residue	Modelled	Actual	Comment	Reference
E	152	GLY	-	expression tag	UNP P0DP25
E	153	GLY	-	expression tag	UNP P0DP25
E	154	SER	-	expression tag	UNP P0DP25
E	155	SER	-	expression tag	UNP P0DP25
E	156	GLY	-	expression tag	UNP P0DP25
E	157	GLY	-	expression tag	UNP P0DP25
E	158	LEU	-	expression tag	UNP P0DP25
E	159	VAL	-	expression tag	UNP P0DP25
E	160	PRO	-	expression tag	UNP P0DP25
E	161	ARG	-	expression tag	UNP P0DP25
E	162	GLY	-	expression tag	UNP P0DP25
E	163	SER	-	expression tag	UNP P0DP25
E	164	GLY	-	expression tag	UNP P0DP25
E	165	GLY	-	expression tag	UNP P0DP25
E	166	SER	-	expression tag	UNP P0DP25
E	167	SER	-	expression tag	UNP P0DP25
E	168	GLY	-	expression tag	UNP P0DP25
E	169	GLY	-	expression tag	UNP P0DP25
E	170	HIS	-	expression tag	UNP P0DP25
E	171	HIS	-	expression tag	UNP P0DP25
E	172	HIS	-	expression tag	UNP P0DP25
E	173	HIS	-	expression tag	UNP P0DP25
E	174	HIS	-	expression tag	UNP P0DP25
E	175	HIS	-	expression tag	UNP P0DP25
E	176	HIS	-	expression tag	UNP P0DP25
E	177	HIS	-	expression tag	UNP P0DP25
F	150	LEU	-	expression tag	UNP P0DP25
F	151	GLU	-	expression tag	UNP P0DP25
F	152	GLY	-	expression tag	UNP P0DP25
F	153	GLY	-	expression tag	UNP P0DP25
F	154	SER	-	expression tag	UNP P0DP25
F	155	SER	-	expression tag	UNP P0DP25
F	156	GLY	-	expression tag	UNP P0DP25
F	157	GLY	-	expression tag	UNP P0DP25
F	158	LEU	-	expression tag	UNP P0DP25
F	159	VAL	-	expression tag	UNP P0DP25
F	160	PRO	-	expression tag	UNP P0DP25
F	161	ARG	-	expression tag	UNP P0DP25
F	162	GLY	-	expression tag	UNP P0DP25
F	163	SER	-	expression tag	UNP P0DP25
F	164	GLY	-	expression tag	UNP P0DP25
F	165	GLY	-	expression tag	UNP P0DP25

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Chain	Residue	Modelled	Actual	Comment	Reference
F	166	SER	-	expression tag	UNP P0DP25
F	167	SER	-	expression tag	UNP P0DP25
F	168	GLY	-	expression tag	UNP P0DP25
F	169	GLY	-	expression tag	UNP P0DP25
F	170	HIS	-	expression tag	UNP P0DP25
F	171	HIS	-	expression tag	UNP P0DP25
F	172	HIS	-	expression tag	UNP P0DP25
F	173	HIS	-	expression tag	UNP P0DP25
F	174	HIS	-	expression tag	UNP P0DP25
F	175	HIS	-	expression tag	UNP P0DP25
F	176	HIS	-	expression tag	UNP P0DP25
F	177	HIS	-	expression tag	UNP P0DP25
H	150	LEU	-	expression tag	UNP P0DP25
H	151	GLU	-	expression tag	UNP P0DP25
H	152	GLY	-	expression tag	UNP P0DP25
H	153	GLY	-	expression tag	UNP P0DP25
H	154	SER	-	expression tag	UNP P0DP25
H	155	SER	-	expression tag	UNP P0DP25
H	156	GLY	-	expression tag	UNP P0DP25
H	157	GLY	-	expression tag	UNP P0DP25
H	158	LEU	-	expression tag	UNP P0DP25
H	159	VAL	-	expression tag	UNP P0DP25
H	160	PRO	-	expression tag	UNP P0DP25
H	161	ARG	-	expression tag	UNP P0DP25
H	162	GLY	-	expression tag	UNP P0DP25
H	163	SER	-	expression tag	UNP P0DP25
H	164	GLY	-	expression tag	UNP P0DP25
H	165	GLY	-	expression tag	UNP P0DP25
H	166	SER	-	expression tag	UNP P0DP25
H	167	SER	-	expression tag	UNP P0DP25
H	168	GLY	-	expression tag	UNP P0DP25
H	169	GLY	-	expression tag	UNP P0DP25
H	170	HIS	-	expression tag	UNP P0DP25
H	171	HIS	-	expression tag	UNP P0DP25
H	172	HIS	-	expression tag	UNP P0DP25
H	173	HIS	-	expression tag	UNP P0DP25
H	174	HIS	-	expression tag	UNP P0DP25
H	175	HIS	-	expression tag	UNP P0DP25
H	176	HIS	-	expression tag	UNP P0DP25
H	177	HIS	-	expression tag	UNP P0DP25



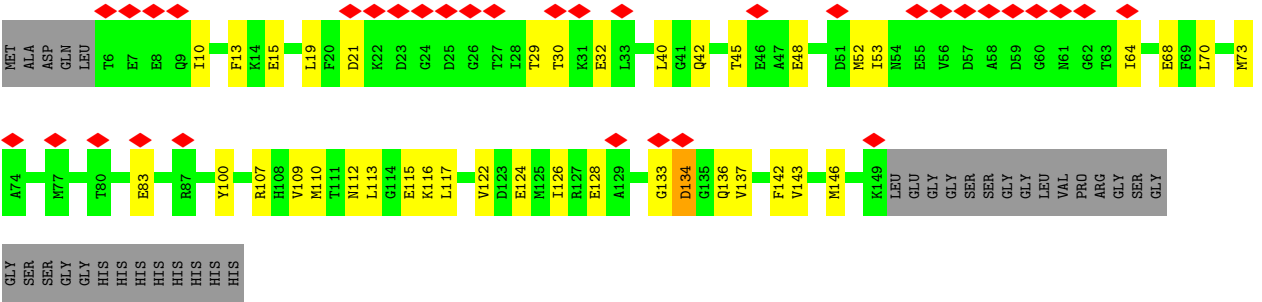




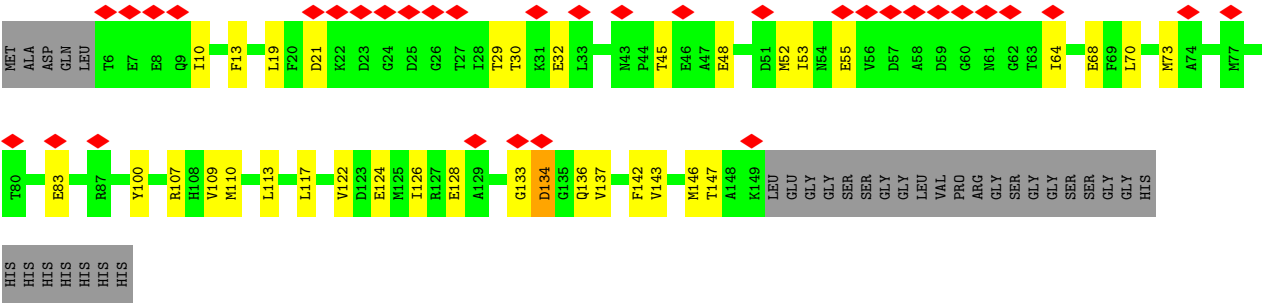








● Molecule 2: Calmodulin-3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169344	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 ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	-1100	Depositor
Maximum defocus (nm)	-1300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.023	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0088	Depositor
Map size (Å)	243.36002, 243.36002, 243.36002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.60	0/2891	0.78	2/3913 (0.1%)
1	B	0.60	0/2891	0.78	2/3913 (0.1%)
1	D	0.60	0/2891	0.78	2/3913 (0.1%)
1	G	0.60	0/2891	0.78	2/3913 (0.1%)
2	C	0.43	0/1120	0.58	0/1507
2	E	0.43	0/1120	0.58	0/1507
2	F	0.43	0/1120	0.58	0/1507
2	H	0.43	0/1120	0.58	0/1507
All	All	0.56	0/16044	0.73	8/21680 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	522	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	D	522	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	B	522	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	A	522	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	G	522	TYR	CB-CG-CD2	5.38	124.23	121.00
1	A	522	TYR	CB-CG-CD2	5.37	124.22	121.00
1	D	522	TYR	CB-CG-CD2	5.37	124.22	121.00
1	B	522	TYR	CB-CG-CD2	5.32	124.19	121.00

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	2821	2891	2891	142	0
1	B	2821	2891	2891	145	0
1	D	2821	2891	2891	143	0
1	G	2821	2891	2891	144	0
2	C	1108	1022	1022	31	0
2	E	1108	1022	1022	30	0
2	F	1108	1022	1022	32	0
2	H	1108	1022	1022	29	0
All	All	15716	15652	15652	617	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 20.

All (617) 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:G:366:ARG:NH2	1:G:534:LYS:O	2.06	0.89
1:A:509:HIS:HB3	2:C:19:LEU:HD21	1.55	0.89
1:B:366:ARG:NH2	1:B:534:LYS:O	2.06	0.88
1:A:366:ARG:NH2	1:A:534:LYS:O	2.06	0.88
1:D:366:ARG:NH2	1:D:534:LYS:O	2.06	0.87
1:B:509:HIS:HB3	2:F:19:LEU:HD21	1.64	0.78
1:G:166:PHE:O	1:G:169:THR:OG1	2.03	0.77
1:B:166:PHE:O	1:B:169:THR:OG1	2.03	0.76
1:A:166:PHE:O	1:A:169:THR:OG1	2.03	0.76
1:D:166:PHE:O	1:D:169:THR:OG1	2.03	0.76
1:B:170:GLU:OE1	1:B:174:ARG:NH2	2.19	0.76
1:D:170:GLU:OE1	1:D:174:ARG:NH2	2.19	0.76
1:A:170:GLU:OE1	1:A:174:ARG:NH2	2.19	0.76
1:G:170:GLU:OE1	1:G:174:ARG:NH2	2.19	0.74
1:B:520:MET:SD	2:F:52:MET:HB3	2.28	0.74
1:A:516:VAL:HG22	2:C:73:MET:HE3	1.69	0.74
1:G:330:SER:O	1:G:334:VAL:HG12	1.87	0.73
1:D:142:LEU:HD23	1:D:145:ILE:HD12	1.71	0.73
1:D:330:SER:O	1:D:334:VAL:HG12	1.87	0.73
1:A:142:LEU:HD23	1:A:145:ILE:HD12	1.71	0.73
1:A:330:SER:O	1:A:334:VAL:HG12	1.87	0.73
1:B:330:SER:O	1:B:334:VAL:HG12	1.87	0.73
1:G:142:LEU:HD23	1:G:145:ILE:HD12	1.71	0.72
1:A:295:GLU:OE1	1:A:318:LYS:HA	1.90	0.72
1:B:295:GLU:OE1	1:B:318:LYS:HA	1.90	0.72
1:B:142:LEU:HD23	1:B:145:ILE:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:GLU:OE1	1:G:318:LYS:HA	1.90	0.71
1:D:295:GLU:OE1	1:D:318:LYS:HA	1.90	0.71
1:G:284:GLU:OE2	1:G:322:THR:OG1	2.06	0.69
1:B:278:TYR:CE2	1:B:282:LEU:HD11	2.28	0.69
1:G:278:TYR:CE2	1:G:282:LEU:HD11	2.28	0.69
1:D:278:TYR:CE2	1:D:282:LEU:HD11	2.28	0.68
1:A:278:TYR:CE2	1:A:282:LEU:HD11	2.28	0.68
1:D:284:GLU:OE2	1:D:322:THR:OG1	2.06	0.67
1:A:161:ILE:O	1:A:165:VAL:HG23	1.95	0.67
1:B:161:ILE:O	1:B:165:VAL:HG23	1.95	0.67
1:A:289:ASN:OD1	1:A:290:GLU:N	2.28	0.67
1:B:333:SER:OG	1:B:334:VAL:N	2.27	0.67
1:D:333:SER:OG	1:D:334:VAL:N	2.27	0.67
1:G:289:ASN:OD1	1:G:290:GLU:N	2.28	0.66
1:A:233:LEU:HD23	1:A:237:ARG:HH21	1.61	0.66
1:G:333:SER:OG	1:G:334:VAL:N	2.27	0.66
1:D:289:ASN:N	1:D:293:ARG:O	2.29	0.66
1:G:289:ASN:N	1:G:293:ARG:O	2.29	0.66
1:B:289:ASN:OD1	1:B:290:GLU:N	2.28	0.66
1:D:289:ASN:OD1	1:D:290:GLU:N	2.28	0.66
1:G:161:ILE:O	1:G:165:VAL:HG23	1.95	0.66
1:D:233:LEU:HD23	1:D:237:ARG:HH21	1.61	0.65
1:B:233:LEU:HD23	1:B:237:ARG:HH21	1.61	0.65
1:D:161:ILE:O	1:D:165:VAL:HG23	1.95	0.65
1:D:113:PHE:O	1:D:117:PRO:HB3	1.97	0.65
1:A:333:SER:OG	1:A:334:VAL:N	2.27	0.65
1:G:113:PHE:O	1:G:117:PRO:HB3	1.97	0.65
1:A:113:PHE:O	1:A:117:PRO:HB3	1.97	0.65
1:G:233:LEU:HD23	1:G:237:ARG:HH21	1.61	0.65
1:B:113:PHE:O	1:B:117:PRO:HB3	1.97	0.64
1:A:516:VAL:HG22	2:C:73:MET:CE	2.28	0.64
1:A:284:GLU:OE2	1:A:322:THR:OG1	2.06	0.63
1:B:250:LEU:O	1:B:253:SER:OG	2.13	0.63
1:A:376:GLN:OE1	2:C:115:GLU:HB2	1.99	0.62
1:B:284:GLU:OE2	1:B:322:THR:OG1	2.06	0.62
1:G:509:HIS:HB3	2:H:19:LEU:HD21	1.82	0.62
1:B:556:ILE:HG21	1:G:555:ARG:CG	2.30	0.62
1:A:289:ASN:N	1:A:293:ARG:O	2.29	0.61
1:G:184:TYR:HE1	1:G:192:ARG:HG2	1.65	0.60
1:B:289:ASN:N	1:B:293:ARG:O	2.29	0.60
1:A:184:TYR:HE1	1:A:192:ARG:HG2	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LYS:O	1:B:561:ARG:HG3	2.02	0.60
1:A:557:LYS:O	1:A:561:ARG:HG3	2.02	0.59
1:D:184:TYR:HE1	1:D:192:ARG:HG2	1.66	0.59
1:B:200:ILE:O	1:B:204:ILE:HG13	2.03	0.59
1:G:557:LYS:O	1:G:561:ARG:HG3	2.02	0.59
1:D:389:SER:OG	1:D:391:THR:HG22	2.03	0.59
1:A:389:SER:OG	1:A:391:THR:HG22	2.03	0.59
1:G:519:ARG:HG2	1:G:523:PHE:CE2	2.38	0.59
1:D:200:ILE:O	1:D:204:ILE:HG13	2.03	0.59
1:D:519:ARG:HG2	1:D:523:PHE:CE2	2.38	0.59
1:D:557:LYS:O	1:D:561:ARG:HG3	2.02	0.59
1:A:519:ARG:HG2	1:A:523:PHE:CE2	2.38	0.59
1:A:200:ILE:O	1:A:204:ILE:HG13	2.03	0.58
1:B:389:SER:OG	1:B:391:THR:HG22	2.03	0.58
1:G:200:ILE:O	1:G:204:ILE:HG13	2.03	0.58
1:B:520:MET:O	1:B:524:VAL:HG23	2.03	0.58
1:B:519:ARG:HG2	1:B:523:PHE:CE2	2.38	0.58
1:A:520:MET:O	1:A:524:VAL:HG23	2.03	0.58
1:B:184:TYR:HB3	1:B:193:PHE:HB2	1.86	0.57
1:D:250:LEU:O	1:D:253:SER:OG	2.13	0.57
1:G:520:MET:O	1:G:524:VAL:HG23	2.03	0.57
1:D:516:VAL:HG22	2:E:73:MET:HE3	1.86	0.57
1:G:370:ALA:O	1:G:373:SER:OG	2.23	0.57
1:G:389:SER:OG	1:G:391:THR:HG22	2.03	0.57
1:B:374:LEU:O	1:B:377:THR:OG1	2.22	0.57
1:B:376:GLN:HG3	2:F:117:LEU:HD11	1.85	0.57
1:G:250:LEU:O	1:G:253:SER:OG	2.13	0.57
1:G:184:TYR:HB3	1:G:193:PHE:HB2	1.86	0.57
2:C:48:GLU:O	2:C:52:MET:HG3	2.05	0.57
1:B:104:THR:O	1:B:107:GLN:HG2	2.05	0.57
1:B:376:GLN:OE1	2:F:115:GLU:HB2	2.04	0.57
1:G:104:THR:O	1:G:107:GLN:HG2	2.05	0.57
1:A:184:TYR:HB3	1:A:193:PHE:HB2	1.86	0.57
1:B:370:ALA:O	1:B:373:SER:OG	2.23	0.57
1:D:192:ARG:O	1:D:195:ARG:HB2	2.05	0.57
1:D:520:MET:O	1:D:524:VAL:HG23	2.04	0.57
1:G:192:ARG:O	1:G:195:ARG:HB2	2.05	0.57
1:B:556:ILE:HG21	1:G:555:ARG:HG3	1.87	0.57
1:B:201:ILE:O	1:B:205:VAL:HG23	2.05	0.57
1:D:201:ILE:O	1:D:205:VAL:HG23	2.05	0.57
2:F:48:GLU:O	2:F:52:MET:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:253:SER:OG	1:G:254:VAL:N	2.38	0.57
1:A:192:ARG:O	1:A:195:ARG:HB2	2.05	0.56
1:B:253:SER:OG	1:B:254:VAL:N	2.38	0.56
1:A:370:ALA:O	1:A:373:SER:OG	2.23	0.56
1:B:192:ARG:O	1:B:195:ARG:HB2	2.05	0.56
1:D:537:ASP:OD1	1:D:538:VAL:N	2.38	0.56
1:A:201:ILE:O	1:A:205:VAL:HG23	2.05	0.56
1:B:516:VAL:HG22	2:F:73:MET:HE3	1.86	0.56
1:D:555:ARG:HH12	1:G:557:LYS:CE	2.19	0.56
1:A:104:THR:O	1:A:107:GLN:HG2	2.05	0.56
1:B:537:ASP:OD1	1:B:538:VAL:N	2.38	0.56
1:D:184:TYR:HB3	1:D:193:PHE:HB2	1.86	0.56
1:A:537:ASP:OD1	1:A:538:VAL:N	2.38	0.56
1:B:203:LEU:O	1:B:207:VAL:HG22	2.06	0.56
1:D:104:THR:O	1:D:107:GLN:HG2	2.05	0.56
1:G:537:ASP:OD1	1:G:538:VAL:N	2.38	0.56
1:A:253:SER:OG	1:A:254:VAL:N	2.38	0.56
1:A:270:PHE:O	1:A:273:LEU:HB3	2.06	0.56
1:D:106:VAL:O	1:D:110:VAL:HG23	2.05	0.56
2:E:48:GLU:O	2:E:52:MET:HG3	2.05	0.56
2:H:48:GLU:O	2:H:52:MET:HG3	2.05	0.56
1:D:203:LEU:O	1:D:207:VAL:HG22	2.06	0.56
1:A:556:ILE:HG21	1:B:555:ARG:CG	2.36	0.56
1:B:232:PHE:HA	1:B:235:ILE:HD12	1.88	0.56
1:B:270:PHE:O	1:B:273:LEU:HB3	2.06	0.56
1:D:270:PHE:O	1:D:273:LEU:HB3	2.06	0.56
1:G:270:PHE:O	1:G:273:LEU:HB3	2.06	0.56
1:G:374:LEU:O	1:G:377:THR:OG1	2.22	0.56
1:A:203:LEU:O	1:A:207:VAL:HG22	2.06	0.56
1:A:232:PHE:HA	1:A:235:ILE:HD12	1.88	0.56
1:A:112:ASN:OD1	1:A:116:ARG:HG3	2.07	0.55
1:G:201:ILE:O	1:G:205:VAL:HG23	2.05	0.55
1:A:106:VAL:O	1:A:110:VAL:HG23	2.05	0.55
1:G:106:VAL:O	1:G:110:VAL:HG23	2.05	0.55
1:D:112:ASN:OD1	1:D:116:ARG:HG3	2.07	0.55
1:G:112:ASN:OD1	1:G:116:ARG:HG3	2.07	0.55
1:G:203:LEU:O	1:G:207:VAL:HG22	2.06	0.55
1:G:361:GLN:HE22	1:G:535:PRO:HD3	1.72	0.55
2:E:143:VAL:O	2:E:147:THR:OG1	2.15	0.55
1:G:126:HIS:O	1:G:129:VAL:HG12	2.07	0.55
2:H:21:ASP:HA	2:H:32:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:21:ASP:HA	2:E:32:GLU:OE2	2.07	0.55
1:A:374:LEU:O	1:A:377:THR:OG1	2.22	0.55
1:B:361:GLN:HE22	1:B:535:PRO:HD3	1.72	0.55
1:D:232:PHE:HA	1:D:235:ILE:HD12	1.88	0.55
1:D:544:GLN:HE22	1:G:542:ILE:HG23	1.72	0.55
1:B:106:VAL:O	1:B:110:VAL:HG23	2.07	0.55
1:D:361:GLN:HE22	1:D:535:PRO:HD3	1.72	0.55
2:F:21:ASP:HA	2:F:32:GLU:OE2	2.07	0.54
1:B:112:ASN:OD1	1:B:116:ARG:HG3	2.07	0.54
1:D:126:HIS:O	1:D:129:VAL:HG12	2.07	0.54
1:D:370:ALA:O	1:D:373:SER:OG	2.23	0.54
1:D:374:LEU:O	1:D:377:THR:OG1	2.22	0.54
1:G:232:PHE:HA	1:G:235:ILE:HD12	1.88	0.54
1:A:361:GLN:HE22	1:A:535:PRO:HD3	1.72	0.54
2:C:10:ILE:HG22	2:C:70:LEU:HD11	1.90	0.54
2:F:10:ILE:HG22	2:F:70:LEU:HD11	1.90	0.54
1:A:250:LEU:O	1:A:253:SER:OG	2.13	0.54
2:C:21:ASP:HA	2:C:32:GLU:OE2	2.07	0.54
1:D:212:VAL:HG23	1:D:213:LEU:HD22	1.90	0.54
1:A:552:LEU:O	1:A:556:ILE:HG12	2.08	0.54
1:D:253:SER:OG	1:D:254:VAL:N	2.38	0.54
1:A:212:VAL:HG23	1:A:213:LEU:HD22	1.90	0.53
1:B:126:HIS:O	1:B:129:VAL:HG12	2.07	0.53
1:D:264:THR:HG22	1:D:268:ILE:HD11	1.90	0.53
2:H:10:ILE:HG22	2:H:70:LEU:HD11	1.90	0.53
1:D:391:THR:HG21	1:D:518:ARG:HH12	1.73	0.53
1:B:264:THR:HG22	1:B:268:ILE:HD11	1.90	0.53
2:E:10:ILE:HG22	2:E:70:LEU:HD11	1.90	0.53
1:A:264:THR:HG22	1:A:268:ILE:HD11	1.90	0.53
1:G:552:LEU:O	1:G:556:ILE:HG12	2.09	0.53
1:D:212:VAL:HG23	1:D:213:LEU:CD2	2.39	0.53
1:D:552:LEU:O	1:D:556:ILE:HG12	2.08	0.53
1:A:126:HIS:O	1:A:129:VAL:HG12	2.07	0.53
1:G:356:GLN:O	1:G:360:ARG:HG2	2.09	0.53
1:A:212:VAL:HG23	1:A:213:LEU:CD2	2.39	0.53
1:A:356:GLN:O	1:A:360:ARG:HG2	2.09	0.53
1:G:212:VAL:HG23	1:G:213:LEU:CD2	2.39	0.53
1:A:391:THR:HG21	1:A:518:ARG:HH12	1.74	0.52
1:B:212:VAL:HG23	1:B:213:LEU:CD2	2.39	0.52
1:B:552:LEU:O	1:B:556:ILE:HG12	2.09	0.52
1:D:516:VAL:HG13	2:E:73:MET:CE	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:ALA:O	1:G:294:VAL:HG22	2.09	0.52
1:D:209:SER:HA	1:D:233:LEU:HD21	1.91	0.52
1:G:212:VAL:HG23	1:G:213:LEU:HD22	1.90	0.52
1:G:264:THR:HG22	1:G:268:ILE:HD11	1.90	0.52
1:A:209:SER:HA	1:A:233:LEU:HD21	1.91	0.52
1:G:209:SER:HA	1:G:233:LEU:HD21	1.91	0.52
1:B:287:ALA:O	1:B:294:VAL:HG22	2.09	0.52
1:G:376:GLN:HG3	2:H:117:LEU:HD11	1.91	0.52
1:D:509:HIS:HB3	2:E:19:LEU:HD21	1.91	0.52
1:B:391:THR:HG21	1:B:518:ARG:HH12	1.74	0.52
1:D:192:ARG:O	1:D:195:ARG:CB	2.58	0.52
1:B:212:VAL:HG23	1:B:213:LEU:HD22	1.90	0.52
1:B:512:ALA:O	1:B:516:VAL:HG23	2.10	0.52
1:A:287:ALA:O	1:A:294:VAL:HG22	2.10	0.52
1:B:192:ARG:O	1:B:195:ARG:CB	2.58	0.52
1:D:287:ALA:O	1:D:294:VAL:HG22	2.10	0.52
1:B:376:GLN:OE1	2:F:115:GLU:O	2.28	0.52
1:A:344:ALA:HA	1:D:342:LEU:CD2	2.40	0.52
2:C:124:GLU:O	2:C:128:GLU:HG2	2.10	0.51
1:G:192:ARG:O	1:G:195:ARG:CB	2.58	0.51
1:A:192:ARG:O	1:A:195:ARG:CB	2.58	0.51
1:B:131:LEU:HD23	1:B:132:ILE:HD13	1.93	0.51
1:G:227:ILE:O	1:G:230:ILE:HG22	2.11	0.51
1:G:391:THR:HG21	1:G:518:ARG:HH12	1.73	0.51
1:B:356:GLN:O	1:B:360:ARG:HG2	2.09	0.51
1:D:356:GLN:O	1:D:360:ARG:HG2	2.09	0.51
1:A:512:ALA:O	1:A:516:VAL:HG23	2.10	0.51
1:D:131:LEU:HD23	1:D:132:ILE:HD13	1.92	0.51
1:D:310:VAL:HG21	1:D:340:PHE:CE2	2.46	0.51
1:G:131:LEU:HD23	1:G:132:ILE:HD13	1.92	0.51
2:H:110:MET:O	2:H:117:LEU:HD13	2.10	0.51
1:A:131:LEU:HD23	1:A:132:ILE:HD13	1.92	0.51
1:B:227:ILE:O	1:B:230:ILE:HG22	2.11	0.51
2:E:110:MET:O	2:E:117:LEU:HD13	2.10	0.51
1:G:224:THR:HG23	1:G:225:SER:H	1.76	0.51
1:G:516:VAL:HG22	2:H:73:MET:HE3	1.91	0.51
2:H:100:TYR:HB3	2:H:136:GLN:HB3	1.92	0.51
2:E:124:GLU:O	2:E:128:GLU:HG2	2.10	0.51
1:A:310:VAL:HG21	1:A:340:PHE:CE2	2.46	0.51
1:B:209:SER:HA	1:B:233:LEU:HD21	1.91	0.51
1:B:556:ILE:HG21	1:G:555:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:THR:HG23	1:D:225:SER:H	1.76	0.51
1:G:310:VAL:HG21	1:G:340:PHE:CE2	2.46	0.51
1:G:512:ALA:O	1:G:516:VAL:HG23	2.10	0.51
2:H:133:GLY:O	2:H:134:ASP:CB	2.59	0.51
2:C:100:TYR:HB3	2:C:136:GLN:HB3	1.92	0.51
2:E:100:TYR:HB3	2:E:136:GLN:HB3	1.92	0.51
2:F:124:GLU:O	2:F:128:GLU:HG2	2.10	0.51
2:H:45:THR:HB	2:H:48:GLU:HG2	1.93	0.51
2:C:45:THR:HB	2:C:48:GLU:HG2	1.92	0.50
2:F:100:TYR:HB3	2:F:136:GLN:HB3	1.92	0.50
1:B:224:THR:HG23	1:B:225:SER:H	1.76	0.50
1:B:542:ILE:HG23	1:G:544:GLN:HE22	1.75	0.50
2:F:110:MET:O	2:F:117:LEU:HD13	2.10	0.50
1:D:227:ILE:O	1:D:230:ILE:HG22	2.11	0.50
1:D:512:ALA:O	1:D:516:VAL:HG23	2.10	0.50
1:D:354:LYS:O	1:D:357:GLN:HG2	2.12	0.50
2:H:124:GLU:O	2:H:128:GLU:HG2	2.10	0.50
1:A:224:THR:HG23	1:A:225:SER:H	1.76	0.50
1:B:184:TYR:HA	1:B:189:GLY:CA	2.42	0.50
1:B:270:PHE:O	1:B:274:ILE:HG12	2.12	0.50
1:B:310:VAL:HG21	1:B:340:PHE:CE2	2.46	0.50
1:A:227:ILE:O	1:A:230:ILE:HG22	2.11	0.50
1:A:270:PHE:O	1:A:274:ILE:HG12	2.12	0.50
1:B:354:LYS:O	1:B:357:GLN:HG2	2.12	0.50
2:C:110:MET:O	2:C:117:LEU:HD13	2.10	0.50
1:G:520:MET:SD	2:H:52:MET:HB3	2.52	0.50
1:A:537:ASP:OD1	1:A:538:VAL:HG22	2.12	0.50
1:D:537:ASP:OD1	1:D:538:VAL:HG22	2.12	0.50
1:A:184:TYR:HA	1:A:189:GLY:CA	2.42	0.50
1:D:184:TYR:HA	1:D:189:GLY:CA	2.42	0.50
2:E:45:THR:HB	2:E:48:GLU:HG2	1.93	0.50
2:E:133:GLY:O	2:E:134:ASP:CB	2.59	0.50
1:G:184:TYR:HA	1:G:189:GLY:CA	2.42	0.50
1:G:305:TRP:CD1	1:G:318:LYS:O	2.65	0.50
1:B:161:ILE:HA	1:B:164:VAL:HG12	1.94	0.50
2:F:133:GLY:O	2:F:134:ASP:CB	2.59	0.50
2:C:133:GLY:O	2:C:134:ASP:CB	2.59	0.49
1:D:527:LYS:HD3	2:E:55:GLU:OE2	2.11	0.49
1:D:555:ARG:CG	1:G:556:ILE:HG21	2.42	0.49
1:G:327:THR:O	1:G:330:SER:OG	2.28	0.49
1:G:354:LYS:O	1:G:357:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:ILE:HA	1:G:164:VAL:HG12	1.95	0.49
1:G:270:PHE:O	1:G:274:ILE:HG12	2.12	0.49
1:G:529:PHE:O	1:G:532:ALA:N	2.45	0.49
1:G:537:ASP:OD1	1:G:538:VAL:HG22	2.12	0.49
1:A:305:TRP:CD1	1:A:318:LYS:O	2.65	0.49
1:A:342:LEU:CD2	1:B:344:ALA:HA	2.43	0.49
1:B:305:TRP:CD1	1:B:318:LYS:O	2.65	0.49
1:G:115:GLU:C	1:G:117:PRO:HD3	2.33	0.49
1:A:354:LYS:O	1:A:357:GLN:HG2	2.12	0.49
1:B:225:SER:HA	1:B:228:ARG:HB2	1.95	0.49
1:D:115:GLU:C	1:D:117:PRO:HD3	2.33	0.49
1:D:225:SER:HA	1:D:228:ARG:HB2	1.95	0.49
1:G:527:LYS:HD3	2:H:55:GLU:OE2	2.12	0.49
1:A:327:THR:O	1:A:330:SER:OG	2.28	0.49
1:A:376:GLN:HG3	2:C:117:LEU:HD11	1.95	0.49
1:A:529:PHE:O	1:A:532:ALA:N	2.45	0.49
1:B:115:GLU:C	1:B:117:PRO:HD3	2.33	0.49
1:B:537:ASP:OD1	1:B:538:VAL:HG22	2.12	0.49
1:D:270:PHE:O	1:D:274:ILE:HG12	2.12	0.49
1:D:305:TRP:CD1	1:D:318:LYS:O	2.65	0.49
2:F:45:THR:HB	2:F:48:GLU:HG2	1.93	0.49
1:A:225:SER:HA	1:A:228:ARG:HB2	1.95	0.49
1:D:184:TYR:CD2	1:D:193:PHE:HD2	2.31	0.49
1:D:344:ALA:HA	1:G:342:LEU:CD2	2.42	0.49
1:D:529:PHE:O	1:D:532:ALA:N	2.45	0.49
1:A:161:ILE:HA	1:A:164:VAL:HG12	1.94	0.48
1:B:187:LEU:HD23	1:B:188:TRP:CD1	2.48	0.48
1:B:529:PHE:O	1:B:532:ALA:N	2.45	0.48
1:D:305:TRP:HD1	1:D:318:LYS:HB2	1.78	0.48
1:G:225:SER:HA	1:G:228:ARG:HB2	1.95	0.48
1:A:187:LEU:HD23	1:A:188:TRP:CD1	2.48	0.48
1:A:239:LEU:HD12	1:A:239:LEU:O	2.13	0.48
1:A:520:MET:SD	2:C:52:MET:HB3	2.53	0.48
1:G:187:LEU:HD23	1:G:188:TRP:CD1	2.48	0.48
1:A:556:ILE:HG21	1:B:555:ARG:HG3	1.94	0.48
1:B:305:TRP:HD1	1:B:318:LYS:HB2	1.78	0.48
1:D:187:LEU:HD23	1:D:188:TRP:CD1	2.48	0.48
1:D:276:SER:O	1:D:280:VAL:HG23	2.13	0.48
1:A:115:GLU:C	1:A:117:PRO:HD3	2.33	0.48
1:G:239:LEU:HD12	1:G:239:LEU:O	2.13	0.48
1:A:276:SER:O	1:A:280:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:TYR:CD2	1:B:193:PHE:HD2	2.31	0.48
1:G:184:TYR:CD2	1:G:193:PHE:HD2	2.31	0.48
1:A:184:TYR:CD2	1:A:193:PHE:HD2	2.31	0.48
1:D:161:ILE:HA	1:D:164:VAL:HG12	1.94	0.48
1:A:278:TYR:O	1:A:282:LEU:HG	2.14	0.48
1:G:276:SER:O	1:G:280:VAL:HG23	2.13	0.48
1:A:395:TYR:CE1	2:C:40:LEU:HB3	2.49	0.48
1:B:516:VAL:HG22	2:F:73:MET:CE	2.43	0.48
1:D:239:LEU:O	1:D:239:LEU:HD12	2.13	0.48
1:G:305:TRP:HD1	1:G:318:LYS:HB2	1.78	0.48
1:A:305:TRP:HD1	1:A:318:LYS:HB2	1.78	0.48
1:B:239:LEU:O	1:B:239:LEU:HD12	2.13	0.48
1:B:276:SER:O	1:B:280:VAL:HG23	2.13	0.48
1:A:120:TRP:CZ3	1:A:121:LYS:HG2	2.49	0.48
1:D:310:VAL:CG2	1:D:340:PHE:CE2	2.97	0.48
1:B:267:TYR:OH	1:G:239:LEU:O	2.31	0.47
1:D:516:VAL:HG22	2:E:73:MET:CE	2.44	0.47
1:B:120:TRP:CZ3	1:B:121:LYS:HG2	2.50	0.47
1:D:555:ARG:HH12	1:G:557:LYS:HE3	1.79	0.47
1:G:120:TRP:CZ3	1:G:121:LYS:HG2	2.50	0.47
1:G:250:LEU:O	1:G:254:VAL:HG23	2.15	0.47
1:A:555:ARG:CG	1:D:556:ILE:HG21	2.45	0.47
1:D:120:TRP:CZ3	1:D:121:LYS:HG2	2.49	0.47
1:D:239:LEU:O	1:G:267:TYR:OH	2.31	0.47
1:D:526:LYS:NZ	2:E:82:SER:HB2	2.30	0.47
1:A:310:VAL:CG2	1:A:340:PHE:CE2	2.97	0.47
1:A:250:LEU:O	1:A:254:VAL:HG23	2.15	0.47
1:A:556:ILE:HG21	1:B:555:ARG:HG2	1.95	0.47
1:B:278:TYR:O	1:B:282:LEU:HG	2.14	0.47
1:A:317:ASP:OD1	1:A:317:ASP:N	2.48	0.47
1:G:278:TYR:O	1:G:282:LEU:HG	2.14	0.47
1:B:250:LEU:O	1:B:254:VAL:HG23	2.15	0.47
1:B:317:ASP:N	1:B:317:ASP:OD1	2.48	0.47
1:B:514:ILE:O	1:B:518:ARG:HG3	2.15	0.47
1:G:514:ILE:O	1:G:518:ARG:HG3	2.15	0.47
1:G:234:GLN:HA	1:G:234:GLN:NE2	2.30	0.47
1:G:310:VAL:CG2	1:G:340:PHE:CE2	2.97	0.47
1:B:234:GLN:HA	1:B:234:GLN:NE2	2.30	0.47
1:D:245:GLY:HA2	1:D:248:TRP:HD1	1.80	0.47
1:G:245:GLY:HA2	1:G:248:TRP:HD1	1.80	0.47
1:A:542:ILE:HG23	1:B:544:GLN:HE22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:CG2	1:B:340:PHE:CE2	2.97	0.47
2:C:142:PHE:O	2:C:146:MET:HG2	2.15	0.47
1:D:187:LEU:CD2	1:D:188:TRP:CD1	2.98	0.47
2:E:83:GLU:HG3	2:E:143:VAL:CG1	2.45	0.47
1:B:245:GLY:HA2	1:B:248:TRP:HD1	1.80	0.46
2:C:83:GLU:HG3	2:C:143:VAL:CG1	2.45	0.46
1:D:278:TYR:O	1:D:282:LEU:HG	2.14	0.46
2:F:142:PHE:O	2:F:146:MET:HG2	2.15	0.46
1:A:245:GLY:HA2	1:A:248:TRP:HD1	1.80	0.46
1:D:250:LEU:O	1:D:254:VAL:HG23	2.15	0.46
2:H:142:PHE:O	2:H:146:MET:HG2	2.15	0.46
1:A:544:GLN:HE22	1:D:542:ILE:HG23	1.80	0.46
1:B:187:LEU:CD2	1:B:188:TRP:CD1	2.98	0.46
1:B:278:TYR:HA	1:B:299:TYR:HE1	1.80	0.46
1:B:538:VAL:CG2	1:G:536:TYR:HB2	2.45	0.46
1:D:120:TRP:O	1:D:124:VAL:HG23	2.16	0.46
1:D:514:ILE:O	1:D:518:ARG:HG3	2.15	0.46
1:G:187:LEU:CD2	1:G:188:TRP:CD1	2.98	0.46
1:B:120:TRP:O	1:B:124:VAL:HG23	2.16	0.46
1:B:342:LEU:CD2	1:G:344:ALA:HA	2.46	0.46
1:D:234:GLN:HA	1:D:234:GLN:NE2	2.30	0.46
2:E:142:PHE:O	2:E:146:MET:HG2	2.15	0.46
1:A:187:LEU:CD2	1:A:188:TRP:CD1	2.98	0.46
1:B:190:ARG:O	1:B:193:PHE:HB3	2.16	0.46
1:D:190:ARG:O	1:D:193:PHE:HB3	2.16	0.46
1:D:317:ASP:OD1	1:D:317:ASP:N	2.48	0.46
1:G:171:TYR:O	1:G:174:ARG:HB3	2.16	0.46
1:G:176:TRP:O	1:G:190:ARG:NH2	2.40	0.46
1:B:171:TYR:O	1:B:174:ARG:HB3	2.16	0.46
1:D:278:TYR:HA	1:D:299:TYR:HE1	1.80	0.46
1:D:171:TYR:O	1:D:174:ARG:HB3	2.16	0.46
1:G:190:ARG:O	1:G:193:PHE:HB3	2.16	0.46
1:A:234:GLN:NE2	1:A:234:GLN:HA	2.30	0.46
1:A:278:TYR:HA	1:A:299:TYR:HE1	1.80	0.46
1:G:120:TRP:O	1:G:124:VAL:HG23	2.16	0.46
1:G:131:LEU:O	1:G:135:VAL:HG23	2.16	0.46
1:G:376:GLN:CG	2:H:117:LEU:HD11	2.45	0.46
1:A:176:TRP:O	1:A:190:ARG:NH2	2.40	0.46
1:G:317:ASP:N	1:G:317:ASP:OD1	2.48	0.46
2:H:83:GLU:HG3	2:H:143:VAL:CG1	2.45	0.46
1:A:514:ILE:O	1:A:518:ARG:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:O	1:A:174:ARG:HB3	2.16	0.45
1:A:523:PHE:CE1	2:C:75:ARG:NH1	2.83	0.45
1:B:131:LEU:O	1:B:135:VAL:HG23	2.16	0.45
1:A:120:TRP:O	1:A:124:VAL:HG23	2.16	0.45
1:A:514:ILE:HA	1:A:517:ILE:HG12	1.99	0.45
1:A:131:LEU:O	1:A:135:VAL:HG23	2.16	0.45
1:B:514:ILE:HA	1:B:517:ILE:HG12	1.99	0.45
2:E:29:THR:HG22	2:E:30:THR:N	2.32	0.45
1:G:278:TYR:HA	1:G:299:TYR:HE1	1.80	0.45
1:A:190:ARG:O	1:A:193:PHE:HB3	2.16	0.45
1:D:131:LEU:O	1:D:135:VAL:HG23	2.16	0.45
1:G:366:ARG:HD2	1:G:532:ALA:HA	1.99	0.45
1:B:158:TRP:O	1:B:162:VAL:HG23	2.17	0.45
1:B:366:ARG:HD2	1:B:532:ALA:HA	1.98	0.45
1:B:557:LYS:CE	1:G:555:ARG:HH12	2.30	0.45
2:F:83:GLU:HG3	2:F:143:VAL:CG1	2.45	0.45
1:D:158:TRP:O	1:D:162:VAL:HG23	2.17	0.45
1:A:538:VAL:CG2	1:B:536:TYR:HB2	2.46	0.45
1:A:344:ALA:HA	1:D:342:LEU:HD21	1.99	0.45
1:B:129:VAL:O	1:B:133:VAL:HG22	2.17	0.45
1:B:140:SER:HA	1:B:156:LEU:HD22	1.98	0.45
1:G:129:VAL:O	1:G:133:VAL:HG22	2.17	0.45
1:G:140:SER:HA	1:G:156:LEU:HD22	1.98	0.45
1:G:167:PHE:O	1:G:170:GLU:HG3	2.17	0.45
1:B:167:PHE:O	1:B:170:GLU:HG3	2.17	0.45
1:A:158:TRP:O	1:A:162:VAL:HG23	2.17	0.44
1:B:179:GLY:HA3	1:B:190:ARG:NH2	2.32	0.44
1:B:199:SER:O	1:B:202:ASP:OD1	2.36	0.44
1:B:327:THR:O	1:B:330:SER:OG	2.28	0.44
2:C:29:THR:HG22	2:C:30:THR:N	2.32	0.44
1:G:514:ILE:HA	1:G:517:ILE:HG12	1.99	0.44
1:D:368:ILE:HB	1:D:369:PRO:HD3	1.99	0.44
1:A:366:ARG:HD2	1:A:532:ALA:HA	1.98	0.44
1:A:368:ILE:HB	1:A:369:PRO:HD3	1.99	0.44
1:D:129:VAL:O	1:D:133:VAL:HG22	2.17	0.44
1:D:199:SER:O	1:D:202:ASP:OD1	2.36	0.44
1:D:366:ARG:HD2	1:D:532:ALA:HA	1.99	0.44
1:G:295:GLU:OE1	1:G:318:LYS:HG2	2.18	0.44
2:C:109:VAL:HG13	2:C:113:LEU:HD12	1.99	0.44
1:D:167:PHE:O	1:D:170:GLU:HG3	2.17	0.44
1:D:179:GLY:HA3	1:D:190:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:ARG:HG3	1:G:556:ILE:HG21	1.98	0.44
1:A:129:VAL:O	1:A:133:VAL:HG22	2.17	0.44
1:A:140:SER:HA	1:A:156:LEU:HD22	1.98	0.44
1:A:167:PHE:O	1:A:170:GLU:HG3	2.17	0.44
1:A:295:GLU:OE1	1:A:318:LYS:HG2	2.18	0.44
2:E:137:VAL:HG21	2:E:142:PHE:CE2	2.53	0.44
2:F:29:THR:HG22	2:F:30:THR:N	2.32	0.44
1:G:205:VAL:HG22	1:G:236:LEU:HD23	2.00	0.44
1:G:368:ILE:HB	1:G:369:PRO:HD3	1.99	0.44
1:B:510:HIS:CD2	2:F:40:LEU:HD21	2.53	0.44
1:B:563:LEU:HD23	1:G:562:ARG:CG	2.47	0.44
2:C:137:VAL:HG21	2:C:142:PHE:CE2	2.53	0.44
1:D:327:THR:O	1:D:330:SER:OG	2.28	0.44
1:G:158:TRP:O	1:G:162:VAL:HG23	2.17	0.44
1:G:199:SER:O	1:G:202:ASP:OD1	2.36	0.44
1:B:382:TYR:CD1	2:F:146:MET:HA	2.53	0.44
1:D:140:SER:HA	1:D:156:LEU:HD22	1.98	0.44
1:D:284:GLU:OE1	1:D:322:THR:HG23	2.18	0.44
1:G:284:GLU:OE1	1:G:322:THR:HG23	2.18	0.44
1:B:205:VAL:HG22	1:B:236:LEU:HD23	2.00	0.44
1:G:364:PHE:CE2	1:G:533:ARG:O	2.71	0.44
2:H:109:VAL:HG13	2:H:113:LEU:HD12	1.99	0.44
1:D:140:SER:HB3	1:D:156:LEU:HD11	2.01	0.43
1:D:289:ASN:OD1	1:D:290:GLU:HG3	2.18	0.43
1:D:376:GLN:HG3	2:E:117:LEU:HD11	1.99	0.43
1:D:514:ILE:HA	1:D:517:ILE:HG12	1.99	0.43
2:F:109:VAL:HG13	2:F:113:LEU:HD12	1.99	0.43
1:G:371:ALA:O	1:G:375:ILE:HG12	2.18	0.43
1:D:371:ALA:O	1:D:375:ILE:HG12	2.18	0.43
2:F:137:VAL:HG21	2:F:142:PHE:CE2	2.53	0.43
2:H:29:THR:HG22	2:H:30:THR:N	2.32	0.43
1:A:284:GLU:OE1	1:A:322:THR:HG23	2.18	0.43
1:B:371:ALA:O	1:B:375:ILE:HG12	2.18	0.43
1:G:140:SER:HB3	1:G:156:LEU:HD11	2.01	0.43
1:A:199:SER:O	1:A:202:ASP:OD1	2.36	0.43
1:A:342:LEU:HD21	1:B:344:ALA:HA	2.00	0.43
1:B:284:GLU:OE1	1:B:322:THR:HG23	2.18	0.43
1:B:295:GLU:OE1	1:B:318:LYS:HG2	2.18	0.43
1:B:368:ILE:HB	1:B:369:PRO:HD3	1.99	0.43
1:D:295:GLU:OE1	1:D:318:LYS:HG2	2.18	0.43
1:A:179:GLY:HA3	1:A:190:ARG:NH2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:GLU:O	1:B:547:GLN:HG3	2.19	0.43
1:D:118:THR:HG22	1:D:119:GLY:H	1.84	0.43
1:D:364:PHE:CE2	1:D:533:ARG:O	2.71	0.43
2:E:109:VAL:HG13	2:E:113:LEU:HD12	1.99	0.43
1:G:289:ASN:OD1	1:G:290:GLU:HG3	2.18	0.43
1:A:371:ALA:O	1:A:375:ILE:HG12	2.18	0.43
1:B:118:THR:HG22	1:B:119:GLY:H	1.84	0.43
1:D:523:PHE:CE1	2:E:75:ARG:NH1	2.86	0.43
1:A:140:SER:HB3	1:A:156:LEU:HD11	2.00	0.43
1:A:313:ILE:O	1:D:314:GLY:HA3	2.18	0.43
1:A:543:GLU:O	1:A:547:GLN:HG3	2.19	0.43
1:B:176:TRP:O	1:B:190:ARG:NH2	2.40	0.43
1:B:224:THR:HG23	1:B:225:SER:N	2.34	0.43
1:B:364:PHE:CE2	1:B:533:ARG:O	2.71	0.43
2:C:13:PHE:CZ	2:C:73:MET:HB3	2.54	0.43
2:F:13:PHE:CZ	2:F:73:MET:HB3	2.54	0.43
1:G:179:GLY:HA3	1:G:190:ARG:NH2	2.32	0.43
1:G:516:VAL:HG22	2:H:73:MET:CE	2.48	0.43
1:A:289:ASN:OD1	1:A:290:GLU:HG3	2.18	0.43
1:B:289:ASN:OD1	1:B:290:GLU:HG3	2.18	0.43
1:D:205:VAL:HG22	1:D:236:LEU:HD23	2.00	0.43
1:B:561:ARG:O	1:B:564:ASP:HB3	2.19	0.43
1:D:243:ARG:HG3	1:D:243:ARG:O	2.19	0.43
1:D:391:THR:OG1	1:D:518:ARG:NH2	2.52	0.43
1:D:561:ARG:O	1:D:564:ASP:HB3	2.19	0.43
2:E:13:PHE:CZ	2:E:73:MET:HB3	2.54	0.43
1:A:224:THR:HG23	1:A:225:SER:N	2.34	0.42
1:A:376:GLN:HE21	1:A:380:ARG:NH2	2.17	0.42
1:D:174:ARG:HD3	1:D:243:ARG:NH2	2.34	0.42
1:D:224:THR:HG23	1:D:225:SER:N	2.34	0.42
1:D:376:GLN:HE21	1:D:380:ARG:NH2	2.17	0.42
1:G:376:GLN:HE21	1:G:380:ARG:NH2	2.17	0.42
1:G:376:GLN:NE2	2:H:117:LEU:HD12	2.33	0.42
1:G:561:ARG:O	1:G:564:ASP:HB3	2.19	0.42
1:A:364:PHE:CE2	1:A:533:ARG:O	2.71	0.42
1:B:140:SER:HB3	1:B:156:LEU:HD11	2.00	0.42
1:G:224:THR:HG23	1:G:225:SER:N	2.34	0.42
1:A:243:ARG:O	1:A:243:ARG:HG3	2.19	0.42
1:B:376:GLN:HE21	1:B:380:ARG:NH2	2.17	0.42
1:G:243:ARG:O	1:G:243:ARG:HG3	2.19	0.42
1:G:543:GLU:O	1:G:547:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:VAL:HG21	2:H:142:PHE:CE2	2.53	0.42
1:A:118:THR:HG22	1:A:119:GLY:H	1.84	0.42
1:A:391:THR:OG1	1:A:518:ARG:NH2	2.52	0.42
1:A:536:TYR:HB2	1:D:538:VAL:CG2	2.49	0.42
1:D:543:GLU:O	1:D:547:GLN:HG3	2.19	0.42
1:G:118:THR:HG22	1:G:119:GLY:H	1.84	0.42
1:G:137:LEU:HA	1:G:140:SER:HG	1.84	0.42
2:H:13:PHE:CZ	2:H:73:MET:HB3	2.54	0.42
1:A:561:ARG:O	1:A:564:ASP:HB3	2.19	0.42
1:B:174:ARG:HD3	1:B:243:ARG:NH2	2.34	0.42
1:A:314:GLY:HA3	1:B:313:ILE:O	2.20	0.42
1:A:120:TRP:O	1:A:124:VAL:CG2	2.68	0.42
1:A:205:VAL:HG22	1:A:236:LEU:HD23	2.00	0.42
1:A:376:GLN:OE1	2:C:115:GLU:O	2.37	0.42
1:B:395:TYR:CE1	2:F:42:GLN:OE1	2.73	0.42
1:G:391:THR:OG1	1:G:518:ARG:NH2	2.52	0.42
2:H:143:VAL:O	2:H:147:THR:OG1	2.15	0.42
1:B:267:TYR:HE1	1:G:241:VAL:HG12	1.84	0.42
2:C:30:THR:HG22	2:C:53:ILE:HD12	2.02	0.42
1:G:174:ARG:HD3	1:G:243:ARG:NH2	2.34	0.42
1:B:120:TRP:O	1:B:124:VAL:CG2	2.68	0.42
1:D:555:ARG:NH1	1:G:557:LYS:CE	2.82	0.42
2:F:64:ILE:HA	2:F:68:GLU:OE1	2.20	0.42
2:H:30:THR:HG22	2:H:53:ILE:HD12	2.02	0.42
2:C:122:VAL:O	2:C:126:ILE:HG12	2.20	0.42
1:D:176:TRP:O	1:D:190:ARG:NH2	2.40	0.42
1:D:344:ALA:HA	1:G:342:LEU:HD21	2.02	0.42
1:D:376:GLN:OE1	2:E:115:GLU:HB2	2.19	0.42
2:F:30:THR:HG22	2:F:53:ILE:HD12	2.02	0.42
2:F:107:ARG:HG3	2:F:122:VAL:HG11	2.02	0.42
2:F:122:VAL:O	2:F:126:ILE:HG12	2.20	0.42
2:H:122:VAL:O	2:H:126:ILE:HG12	2.20	0.42
1:A:174:ARG:HD3	1:A:243:ARG:NH2	2.34	0.41
2:C:64:ILE:HA	2:C:68:GLU:OE1	2.20	0.41
2:C:137:VAL:HG21	2:C:142:PHE:HE2	1.85	0.41
2:E:64:ILE:HA	2:E:68:GLU:OE1	2.20	0.41
2:H:64:ILE:HA	2:H:68:GLU:OE1	2.20	0.41
1:A:137:LEU:HA	1:A:140:SER:HG	1.85	0.41
1:B:391:THR:OG1	1:B:518:ARG:NH2	2.52	0.41
2:E:30:THR:HG22	2:E:53:ILE:HD12	2.02	0.41
1:A:312:THR:OG1	1:D:312:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ARG:O	1:B:243:ARG:HG3	2.19	0.41
1:B:538:VAL:HG23	1:G:536:TYR:HB2	2.03	0.41
2:F:137:VAL:HG21	2:F:142:PHE:HE2	1.85	0.41
2:H:107:ARG:HG3	2:H:122:VAL:HG11	2.02	0.41
1:A:555:ARG:HG2	1:D:556:ILE:HG21	2.02	0.41
2:E:122:VAL:O	2:E:126:ILE:HG12	2.20	0.41
1:G:131:LEU:O	1:G:134:LEU:HB3	2.21	0.41
1:G:323:TRP:CZ3	1:G:324:VAL:HG22	2.56	0.41
1:A:323:TRP:CZ3	1:A:324:VAL:HG22	2.56	0.41
1:A:555:ARG:HH12	1:D:557:LYS:CE	2.33	0.41
1:B:131:LEU:O	1:B:134:LEU:HB3	2.21	0.41
2:E:137:VAL:HG21	2:E:142:PHE:HE2	1.85	0.41
1:A:204:ILE:HA	1:A:207:VAL:HG22	2.02	0.41
2:C:107:ARG:HG3	2:C:122:VAL:HG11	2.02	0.41
2:E:107:ARG:HG3	2:E:122:VAL:HG11	2.02	0.41
1:G:120:TRP:O	1:G:124:VAL:CG2	2.68	0.41
1:A:344:ALA:HA	1:D:342:LEU:HD23	2.02	0.41
1:B:376:GLN:CG	2:F:117:LEU:HD11	2.50	0.41
1:D:323:TRP:CZ3	1:D:324:VAL:HG22	2.56	0.41
1:A:131:LEU:O	1:A:134:LEU:HB3	2.21	0.41
1:A:230:ILE:HD12	1:A:230:ILE:HA	1.91	0.41
1:A:288:VAL:HG22	1:A:289:ASN:O	2.21	0.41
1:B:542:ILE:HG12	1:G:544:GLN:NE2	2.36	0.41
1:G:288:VAL:HG22	1:G:289:ASN:O	2.21	0.41
1:A:239:LEU:O	1:D:267:TYR:OH	2.36	0.41
1:A:278:TYR:HA	1:A:299:TYR:CE1	2.56	0.41
1:B:323:TRP:CZ3	1:B:324:VAL:HG22	2.56	0.41
2:C:110:MET:HB3	2:C:117:LEU:HD22	2.02	0.41
2:C:112:ASN:O	2:C:116:LYS:HE2	2.21	0.41
1:D:120:TRP:O	1:D:124:VAL:CG2	2.68	0.41
1:D:204:ILE:HA	1:D:207:VAL:HG22	2.02	0.41
2:F:112:ASN:O	2:F:116:LYS:HE2	2.21	0.41
1:G:204:ILE:HA	1:G:207:VAL:HG22	2.02	0.41
1:B:278:TYR:HA	1:B:299:TYR:CE1	2.56	0.41
1:B:288:VAL:HG22	1:B:289:ASN:O	2.21	0.41
1:D:357:GLN:O	1:D:361:GLN:HG2	2.21	0.41
1:G:227:ILE:HG22	1:G:231:ARG:NH1	2.36	0.41
1:B:531:GLN:C	1:B:533:ARG:H	2.25	0.40
1:B:563:LEU:HD23	1:G:562:ARG:HG3	2.03	0.40
1:A:557:LYS:CE	1:B:555:ARG:HH12	2.34	0.40
2:H:137:VAL:HG21	2:H:142:PHE:HE2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HG22	1:A:231:ARG:NH1	2.36	0.40
1:D:130:PHE:HA	1:D:133:VAL:HG22	2.04	0.40
2:H:110:MET:HB3	2:H:117:LEU:HD22	2.02	0.40
1:B:204:ILE:HA	1:B:207:VAL:HG22	2.02	0.40
1:B:208:ALA:O	1:B:212:VAL:HG22	2.22	0.40
2:C:103:ALA:HB2	2:C:131:ILE:HD11	2.04	0.40
1:D:131:LEU:O	1:D:134:LEU:HB3	2.21	0.40
1:D:208:ALA:O	1:D:212:VAL:HG22	2.22	0.40
1:D:227:ILE:HG22	1:D:231:ARG:NH1	2.36	0.40
1:G:396:ILE:HD12	1:G:396:ILE:HA	1.95	0.40
1:G:540:ASP:O	1:G:544:GLN:HG2	2.22	0.40
1:B:137:LEU:HA	1:B:140:SER:HG	1.85	0.40
1:D:245:GLY:HA2	1:D:248:TRP:CD1	2.57	0.40
1:D:288:VAL:HG22	1:D:289:ASN:O	2.21	0.40
2:E:15:GLU:O	2:E:19:LEU:HD13	2.22	0.40
2:F:15:GLU:O	2:F:19:LEU:HD13	2.22	0.40
1:G:357:GLN:O	1:G:361:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	342/692 (49%)	323 (94%)	19 (6%)	0	100	100
1	B	342/692 (49%)	324 (95%)	18 (5%)	0	100	100
1	D	342/692 (49%)	323 (94%)	19 (6%)	0	100	100
1	G	342/692 (49%)	323 (94%)	19 (6%)	0	100	100
2	C	142/177 (80%)	138 (97%)	3 (2%)	1 (1%)	22	61
2	E	142/177 (80%)	138 (97%)	3 (2%)	1 (1%)	22	61
2	F	142/177 (80%)	138 (97%)	3 (2%)	1 (1%)	22	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	142/177 (80%)	138 (97%)	3 (2%)	1 (1%)	22	61
All	All	1936/3476 (56%)	1845 (95%)	87 (4%)	4 (0%)	50	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	134	ASP
2	E	134	ASP
2	F	134	ASP
2	H	134	ASP

### 5.3.2 Protein sidechains ⓘ

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	297/579 (51%)	297 (100%)	0	100	100
1	B	297/579 (51%)	297 (100%)	0	100	100
1	D	297/579 (51%)	297 (100%)	0	100	100
1	G	297/579 (51%)	297 (100%)	0	100	100
2	C	115/146 (79%)	115 (100%)	0	100	100
2	E	115/146 (79%)	115 (100%)	0	100	100
2	F	115/146 (79%)	115 (100%)	0	100	100
2	H	115/146 (79%)	115 (100%)	0	100	100
All	All	1648/2900 (57%)	1648 (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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	GLN
1	A	544	GLN

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Mol	Chain	Res	Type
1	B	234	GLN
1	B	361	GLN
1	B	510	HIS
1	B	544	GLN
2	C	108	HIS
1	D	361	GLN
1	D	544	GLN
2	E	112	ASN
1	G	234	GLN
1	G	361	GLN
1	G	376	GLN
1	G	544	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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

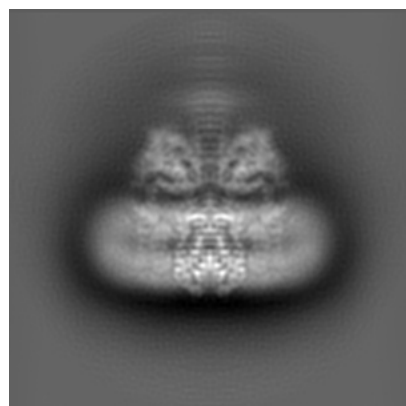
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33316. These allow visual inspection of the internal detail of the map and identification of artifacts.

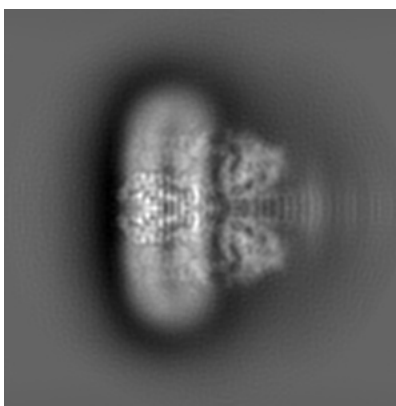
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

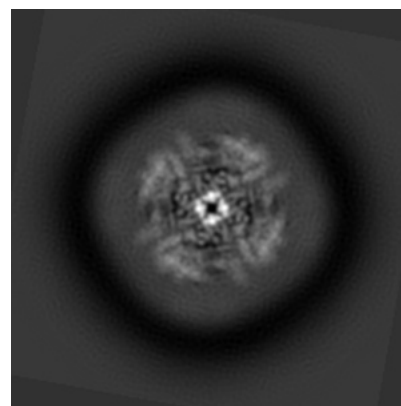
#### 6.1.1 Primary map



X

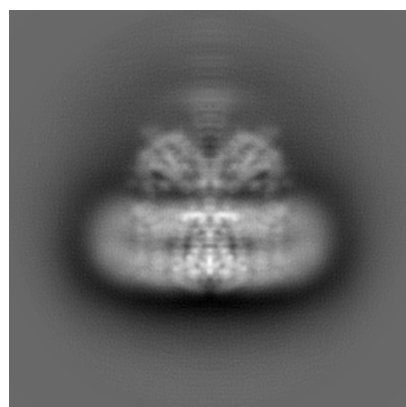


Y

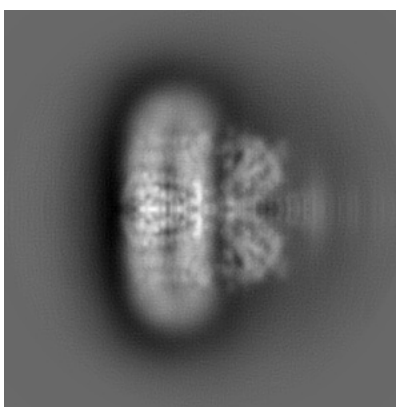


Z

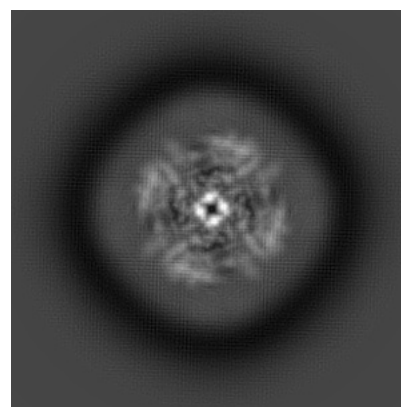
#### 6.1.2 Raw map



X



Y

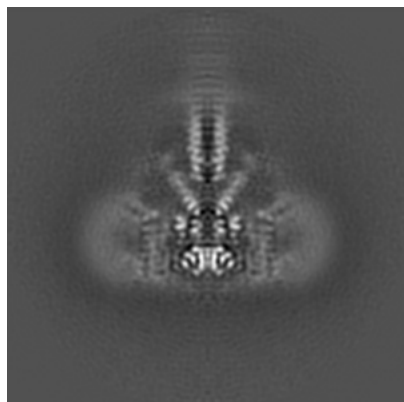


Z

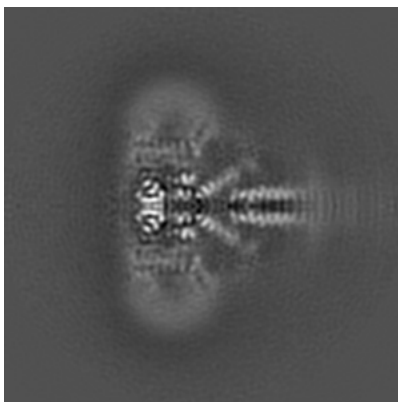
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

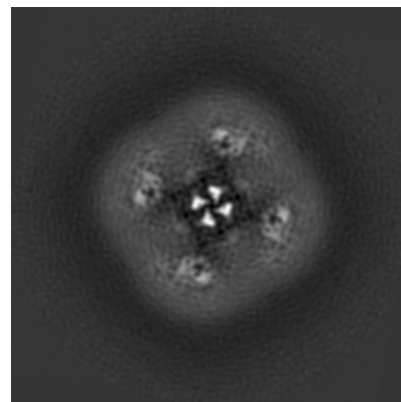
### 6.2.1 Primary map



X Index: 120

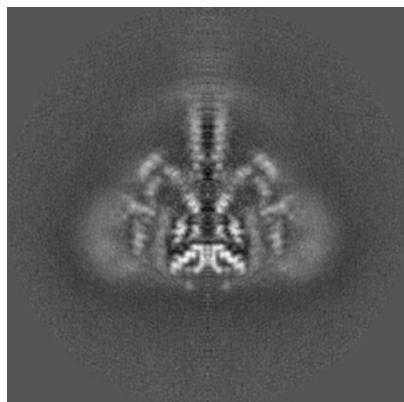


Y Index: 120

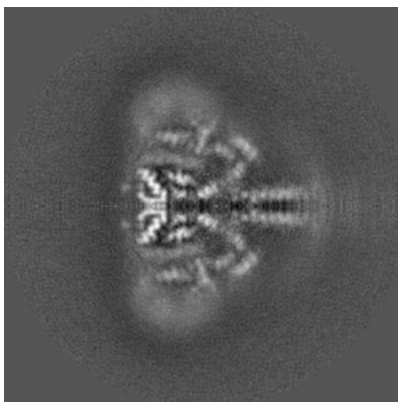


Z Index: 120

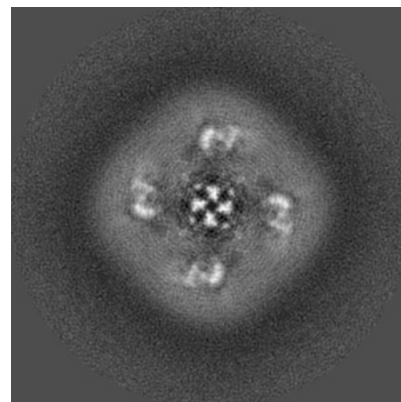
### 6.2.2 Raw map



X Index: 120



Y Index: 120

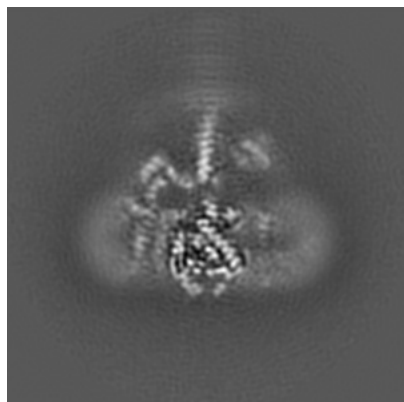


Z Index: 120

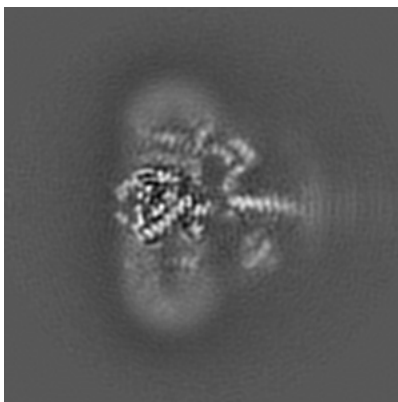
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

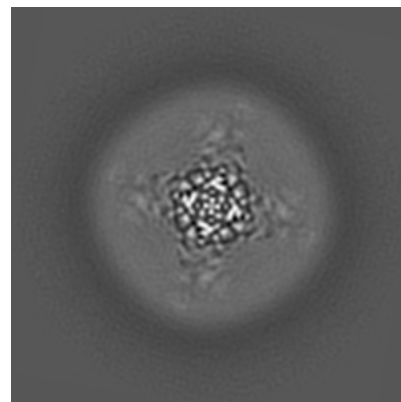
### 6.3.1 Primary map



X Index: 113

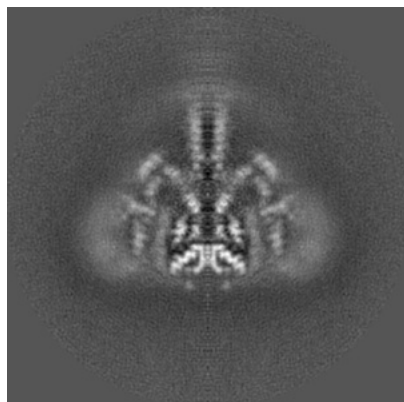


Y Index: 113

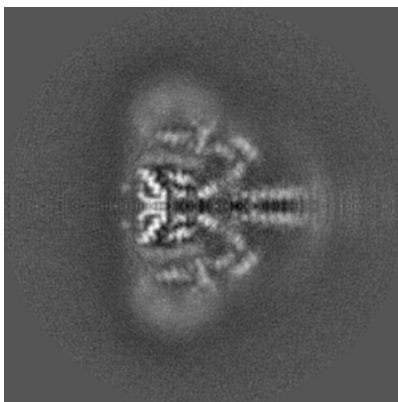


Z Index: 86

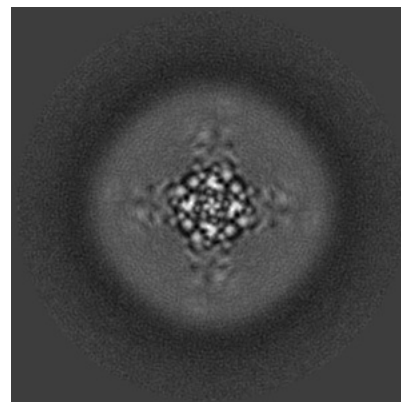
### 6.3.2 Raw map



X Index: 120



Y Index: 120

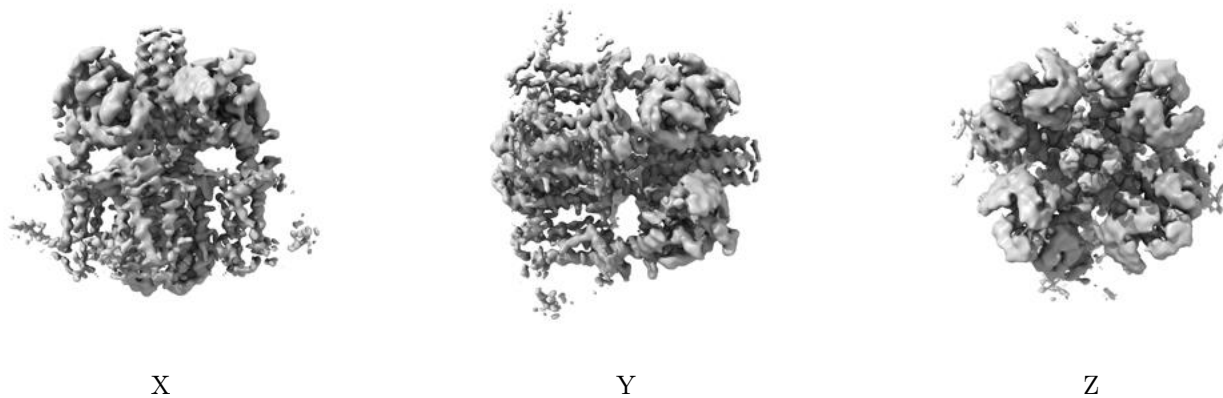


Z Index: 88

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

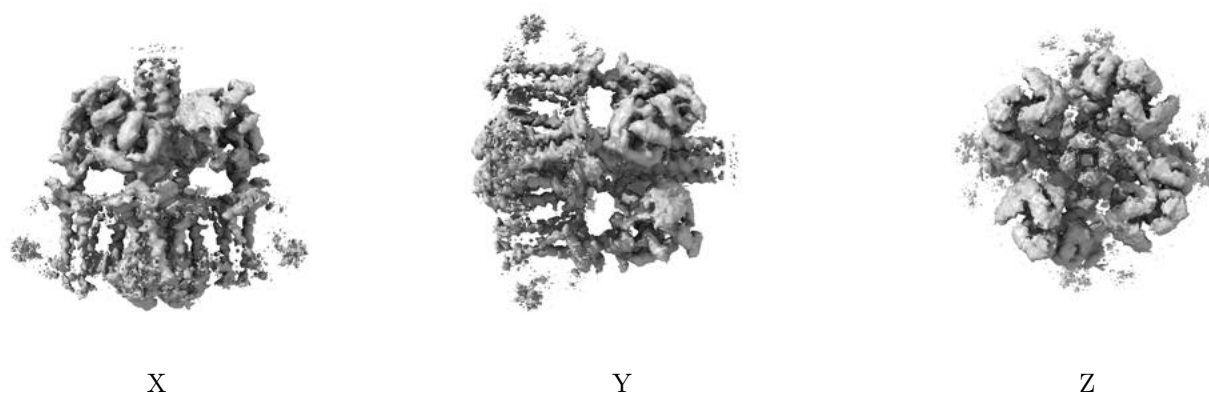
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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.

## 6.5 Mask visualisation [i](#)

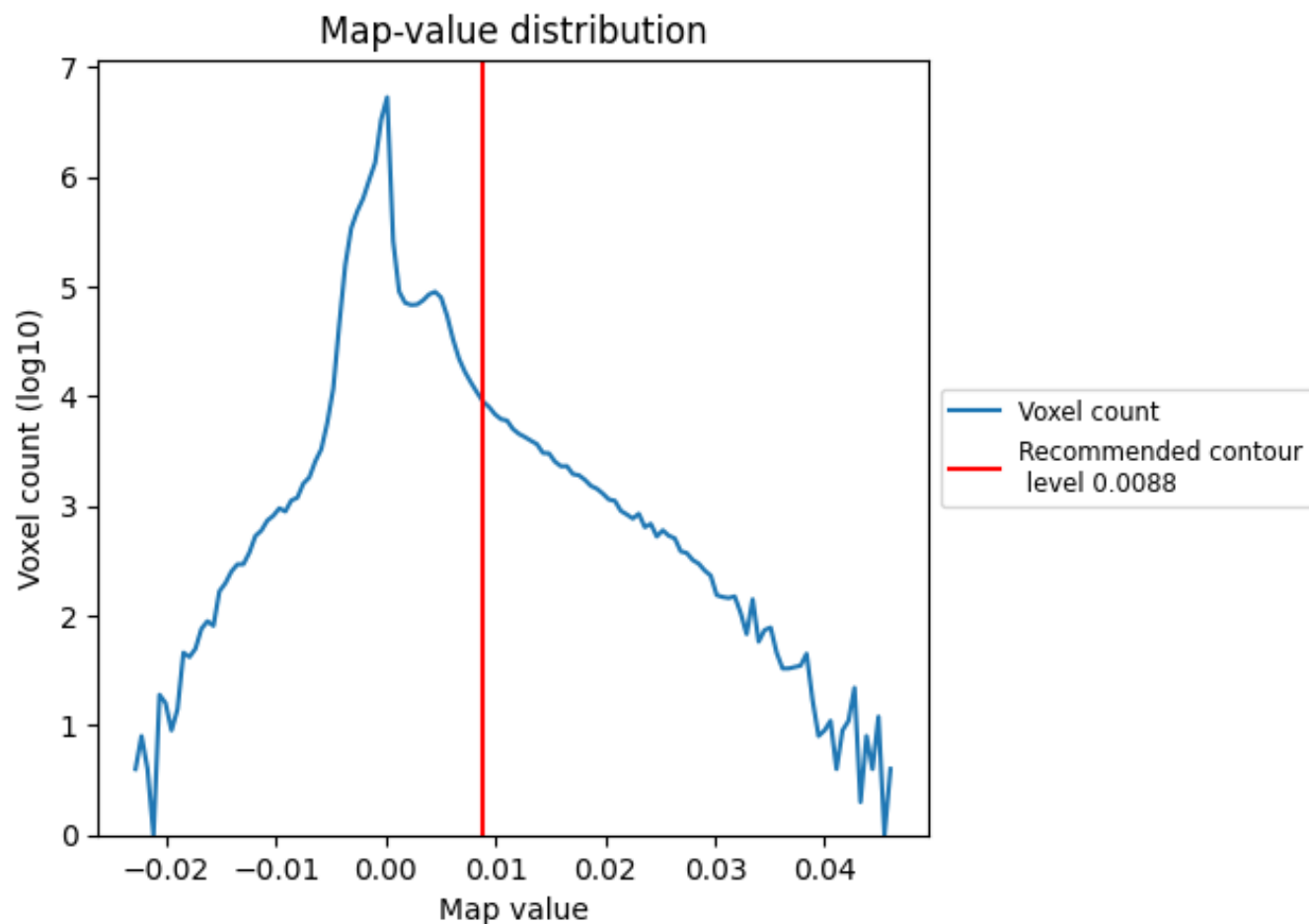
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

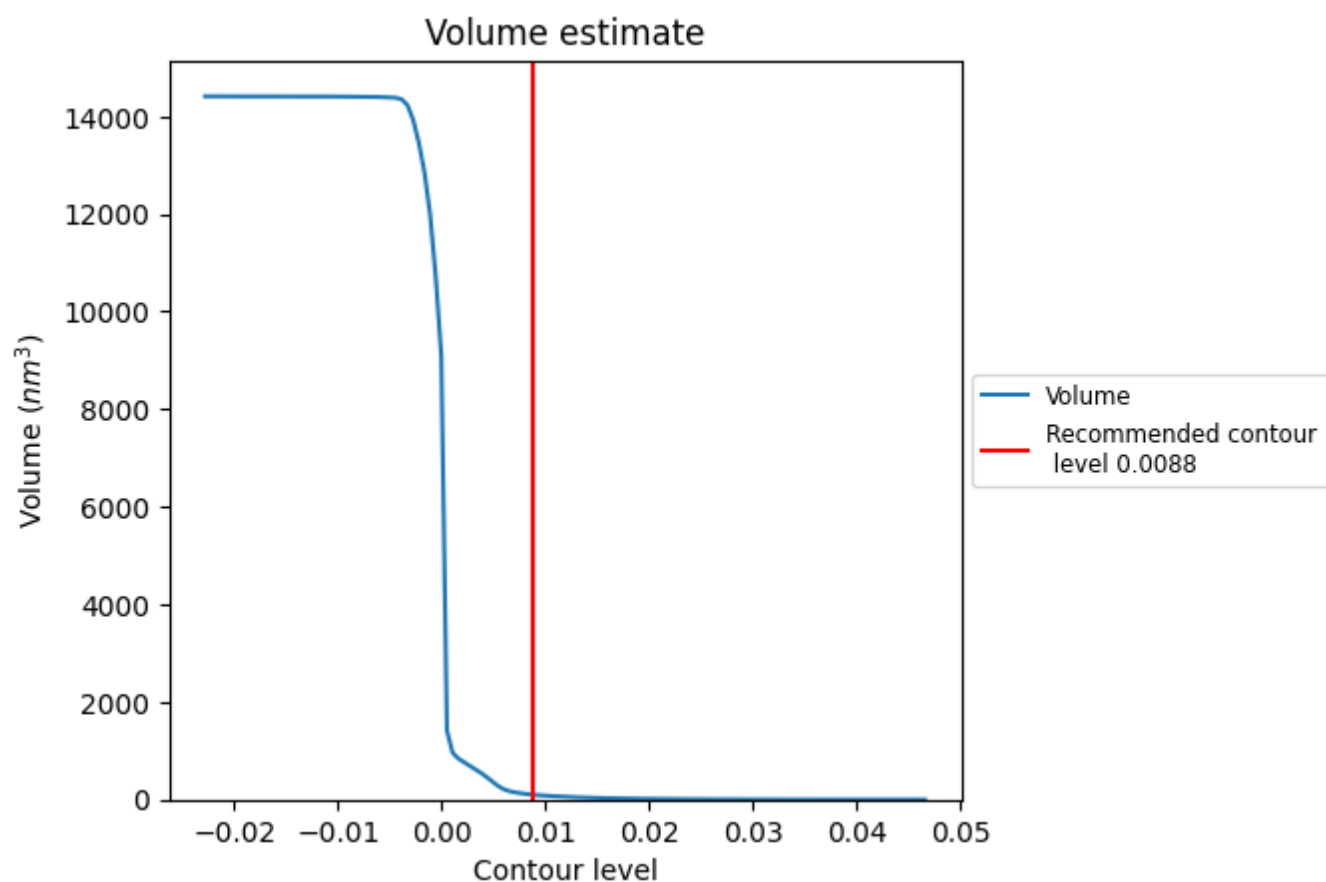
This section contains the results of statistical analysis of the map.

### 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.

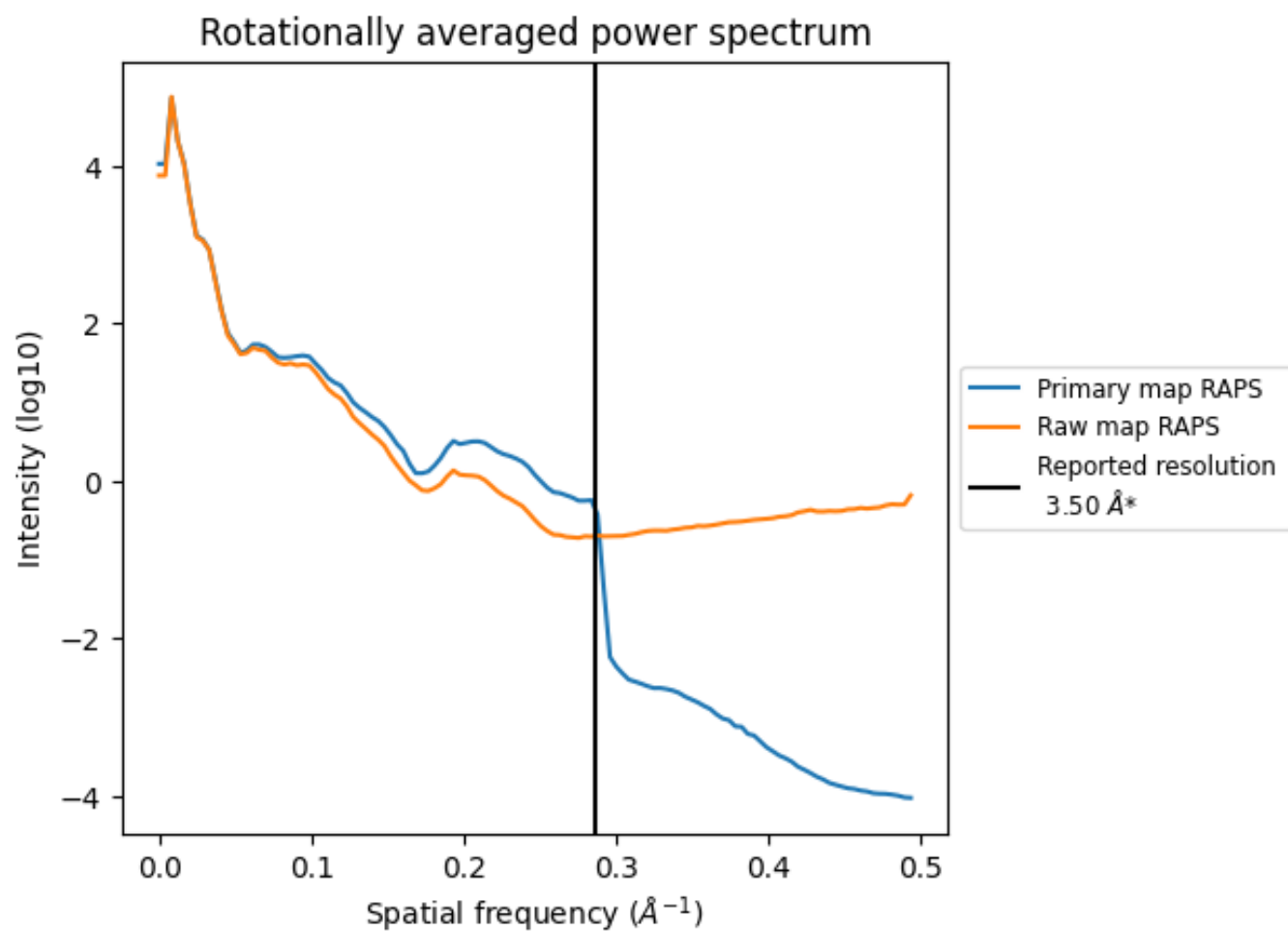
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm<sup>3</sup>; this corresponds to an approximate mass of 89 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 ⓘ

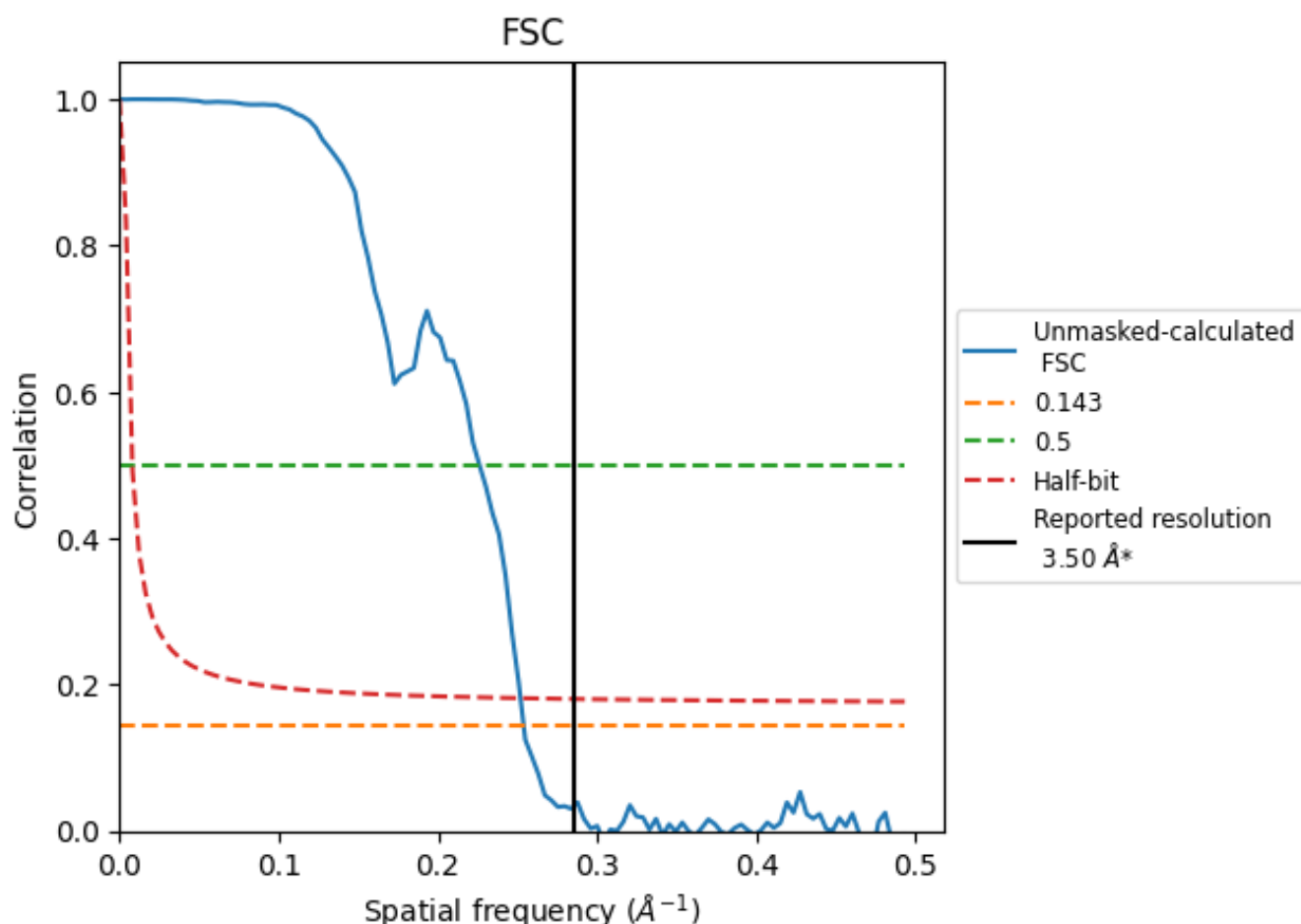


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 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 0.286  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

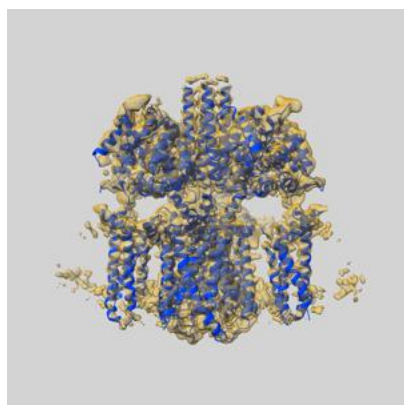
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	4.42	3.97

\*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 3.94 differs from the reported value 3.5 by more than 10 %

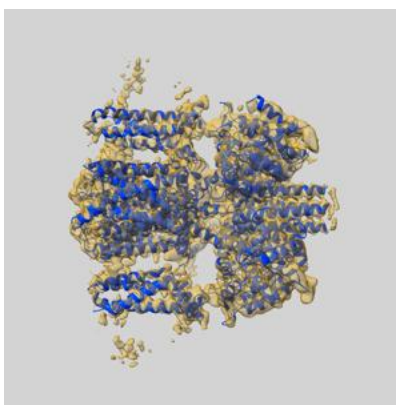
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33316 and PDB model 7XNI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

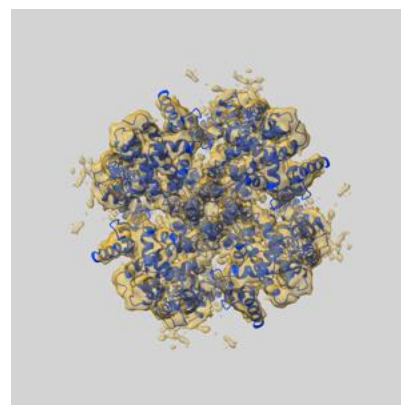
### 9.1 Map-model overlay [i](#)



X



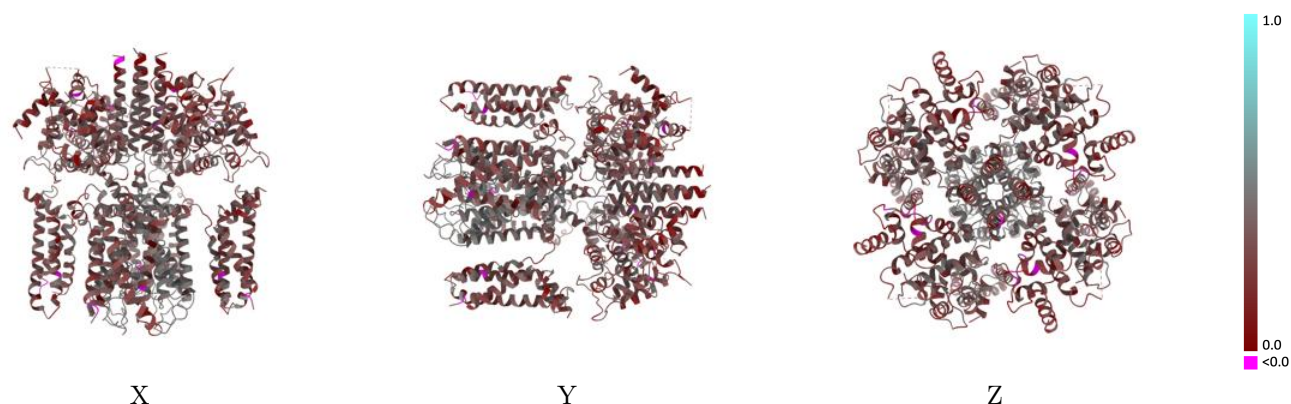
Y



Z

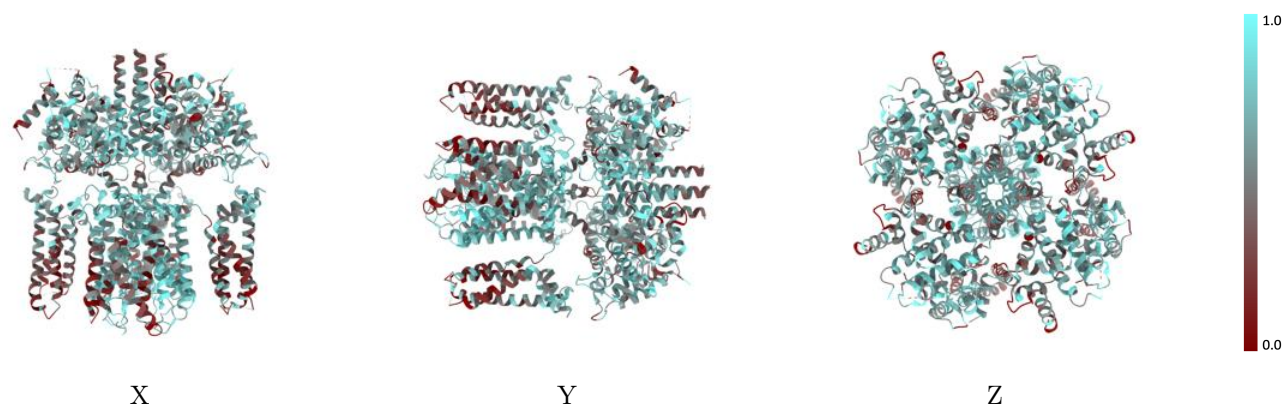
The images above show the 3D surface view of the map at the recommended contour level 0.0088 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



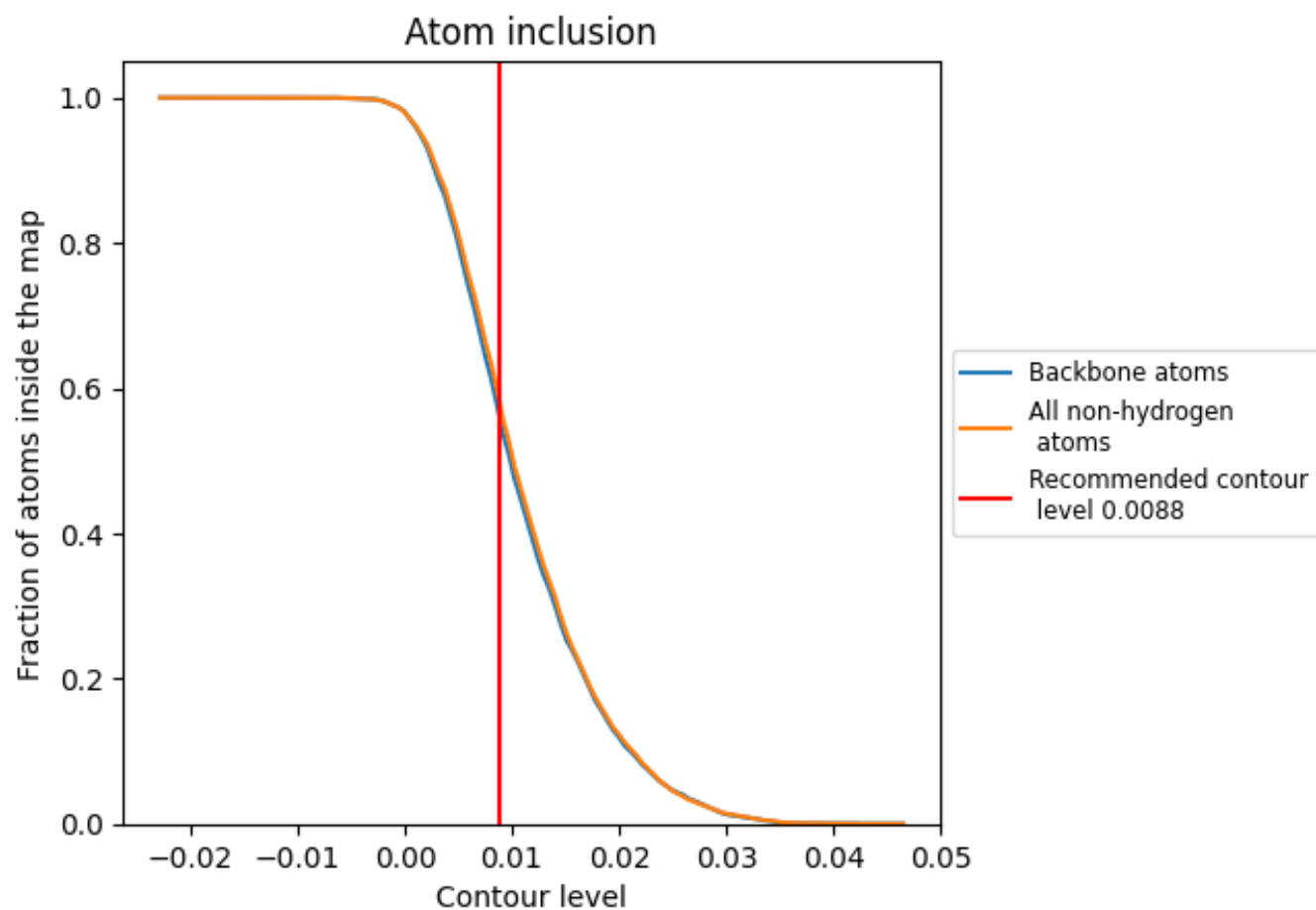
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0088).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 59% 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 (0.0088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5858	<div></div> 0.3150
A	<div></div> 0.6163	<div></div> 0.3400
B	<div></div> 0.6188	<div></div> 0.3410
C	<div></div> 0.5384	<div></div> 0.2510
D	<div></div> 0.6163	<div></div> 0.3370
E	<div></div> 0.5466	<div></div> 0.2580
F	<div></div> 0.5475	<div></div> 0.2490
G	<div></div> 0.6192	<div></div> 0.3400
H	<div></div> 0.5439	<div></div> 0.2570

