



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:43 PM UTC

PDB ID : 8JHK / pdb_00008jhk
EMDB ID : EMD-36271
Title : Cryo-EM structure of the DOCK5/ELMO1 complex, focused on one protomer
Authors : Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Mishima-Tsumagari, C.; Yonemochi, M.; Inoue, M.; Nakagawa, R.; Kaushik, R.; Zhang, K.Y.J.; Shirouzu, M.
Deposited on : 2023-05-23
Resolution : 4.76 Å (reported)
Based on initial models : 7DPA, 6IE1

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

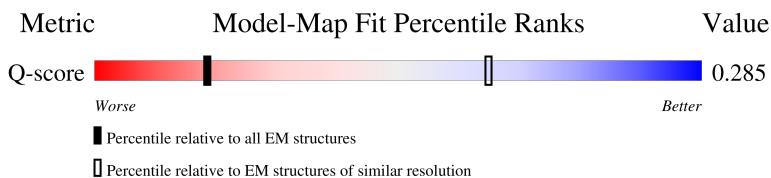
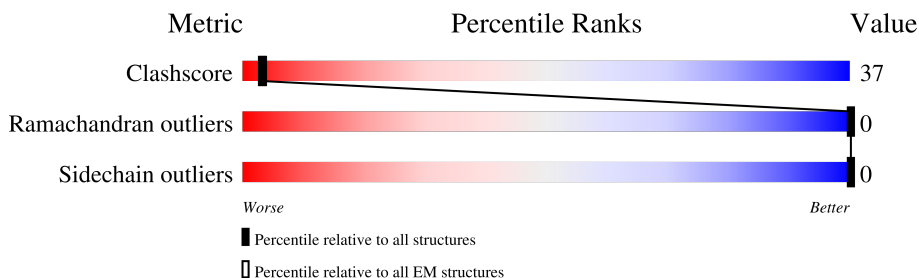
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

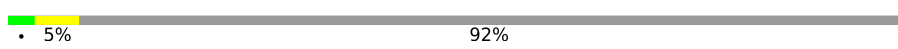
The reported resolution of this entry is 4.76 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1591 (4.26 - 5.26)

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	733	
2	B	1648	
2	E	1648	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 20512 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 Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	727	Total	C	N	O	S	0	0
			5879	3721	1009	1108	41		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q92556
A	-4	GLY	-	expression tag	UNP Q92556
A	-3	SER	-	expression tag	UNP Q92556
A	-2	GLY	-	expression tag	UNP Q92556
A	-1	GLY	-	expression tag	UNP Q92556
A	0	SER	-	expression tag	UNP Q92556

- Molecule 2 is a protein called Deducator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		
2	E	140	Total	C	N	O	S	0	0
			1197	773	197	222	5		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q9H7D0
B	-4	GLY	-	expression tag	UNP Q9H7D0
B	-3	SER	-	expression tag	UNP Q9H7D0
B	-2	GLY	-	expression tag	UNP Q9H7D0
B	-1	GLY	-	expression tag	UNP Q9H7D0
B	0	SER	-	expression tag	UNP Q9H7D0
B	1285	ARG	LYS	variant	UNP Q9H7D0
E	-5	GLY	-	expression tag	UNP Q9H7D0
E	-4	GLY	-	expression tag	UNP Q9H7D0

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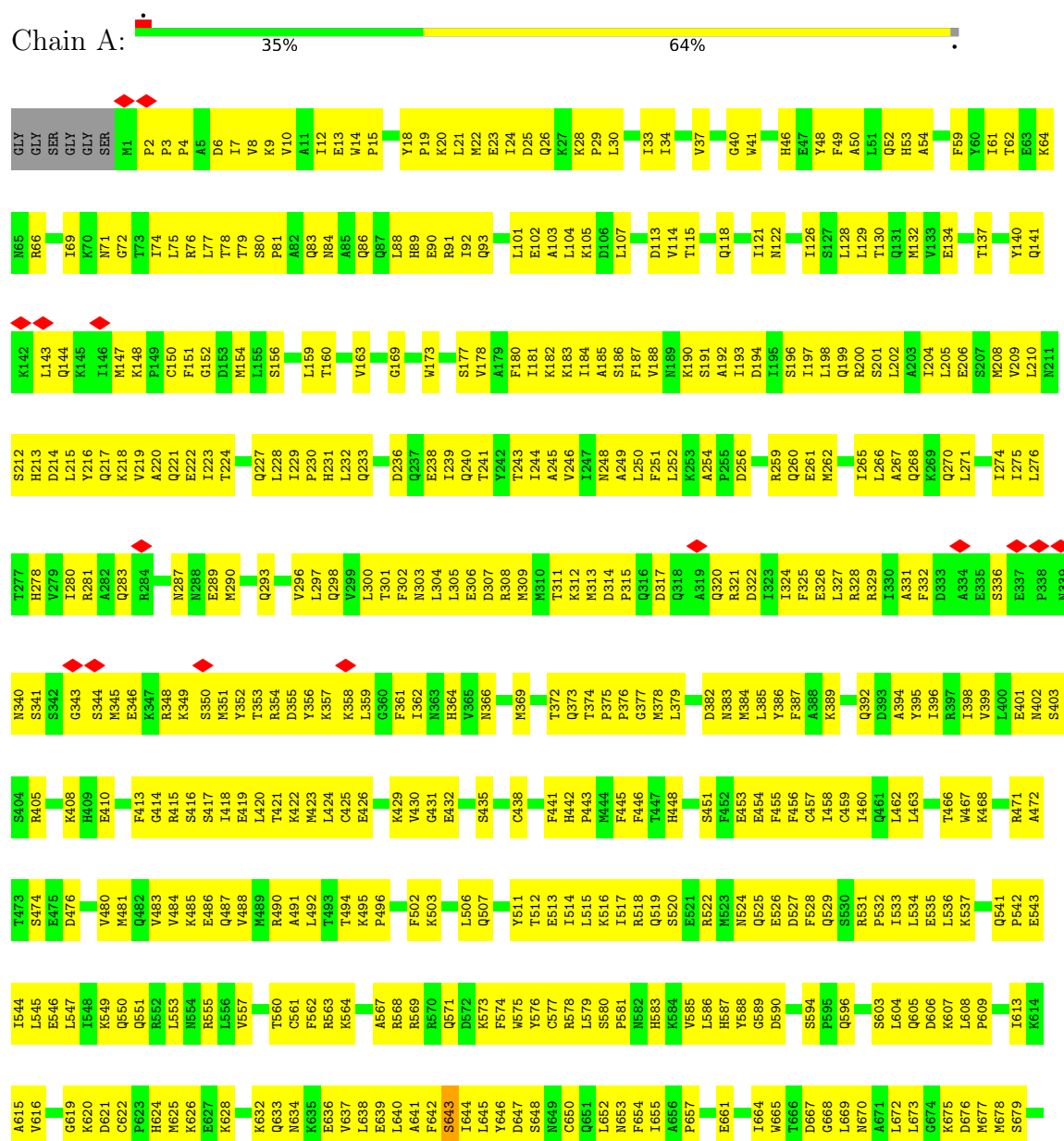
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	SER	-	expression tag	UNP Q9H7D0
E	-2	GLY	-	expression tag	UNP Q9H7D0
E	-1	GLY	-	expression tag	UNP Q9H7D0
E	0	SER	-	expression tag	UNP Q9H7D0
E	1285	ARG	LYS	variant	UNP Q9H7D0

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.

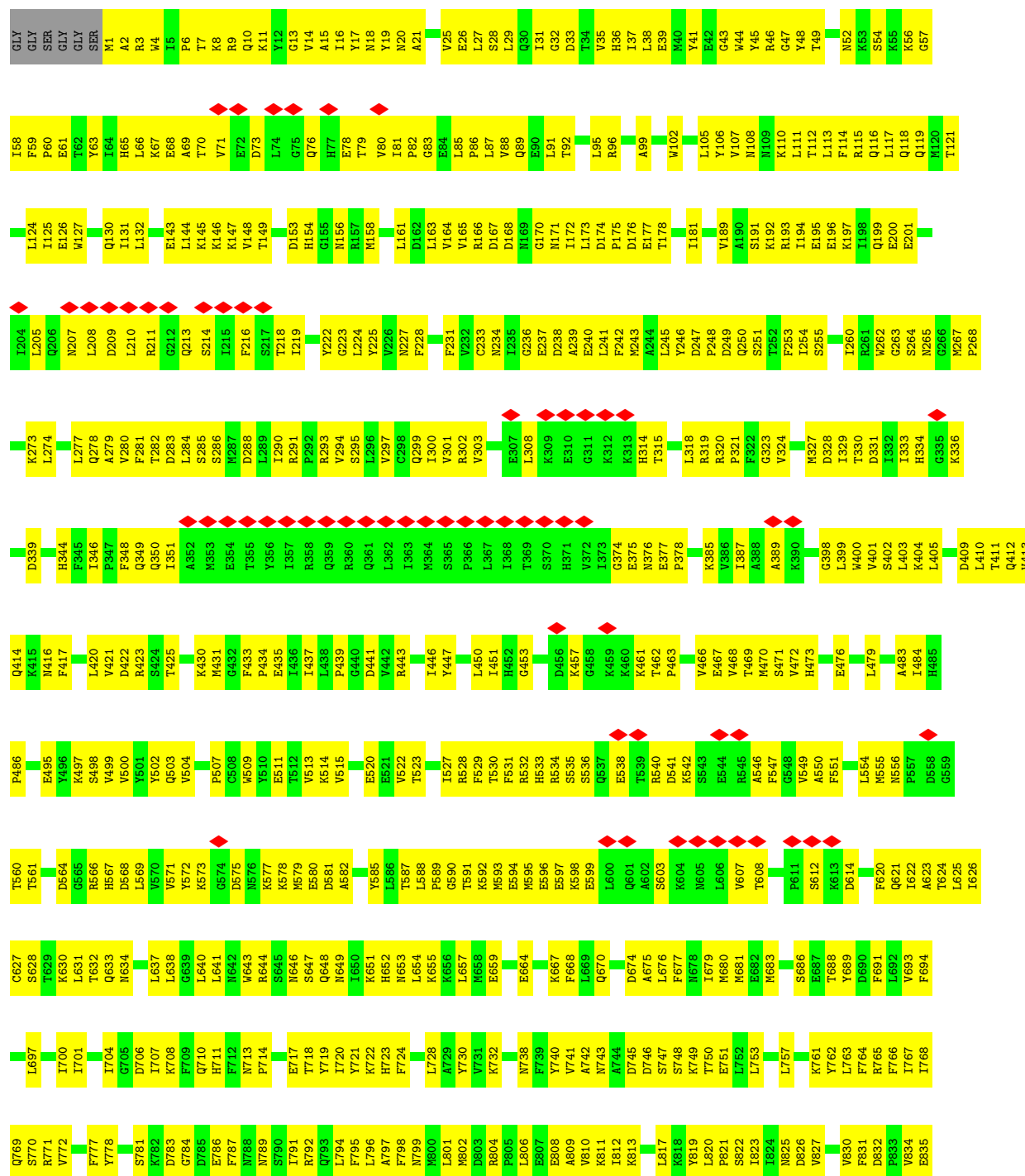
- Molecule 1: Engulfment and cell motility protein 1

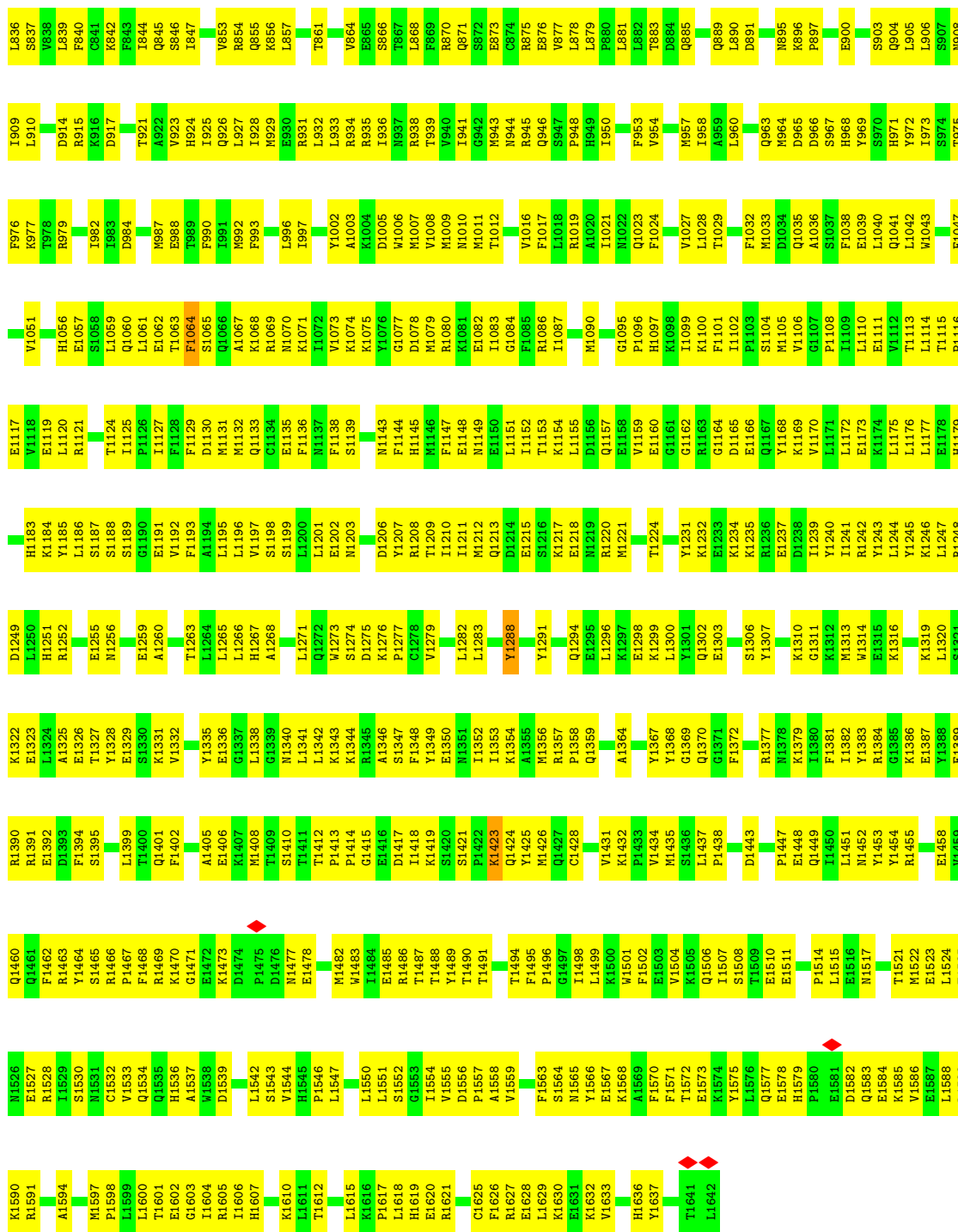




• Molecule 2: Dedicator of cytokinesis protein 5

Chain B: 39% 61%







GLU	LYS	TYR	LYS	PRO	TYR	PHE	V1332
LYS	HIS	LEU	GLU	GLU	ARG	SER	
TYR	TYR	GLN	ASN	ASN	ASN	ARG	Y1336
GLY	GLY	GLU	ALA	ALA	GLU	LEU	E1336
VAL	VAL	HIS	ILE	ILE	VAL	LEU	G1337
PRO	PRO	GLU	THR	THR	GLN	THR	L1338
THR	GLU	GLU	GLU	GLN	PHE	GLN	G1339
LEU	LEU	ASP	ASP	ASP	ASP	PHE	M1340
		GLN	GLN	GLU	ARG	PRO	L1341
		GLU	LYS	LEU	TYR	ASN	K1344
	LYS	GLY	THR	ASN	SER	ALA	R1345
	VAL	VAL	ASN	ARG	ARG	GLU	R1346
	GLU	GLU	PRO	PRO	PRO	LYS	S1347
	LEU	LEU	ARG	PHE	PHE	MET	F1348
	LEU	LEU	ILE	ARG	ARG	THR	Y1349
	LYS	LYS	SER	LYS	LYS	SER	E1350
	ARG	ARG	ASN	GLY	GLY	THR	M1351
	LEU	LEU	CYS	GLU	GLU	THR	I1352
	ILE	ILE	VAL	VAL	LYS	PRO	I1353
	ALA	ALA	GLN	ASP	ALA	PRO	K1354
	LEU	LEU	GLN	PRO	PRO	GLY	A1355
	GLN	GLN	HIS	HIS	ASP	GLU	MET
	MET	MET	ALA	ASN	ASN	ASP	ARG
	PRO	PRO	TRP	TRP	GLU	ILE	PRO
	LEU	LEU	ASP	PHE	PHE	LYS	GLN
	LEU	LEU	ARG	ALA	ALA	SER	PRO
	THR	THR	SER	THR	THR	SER	GLU
	GLU	GLU	LEU	LEU	MET	PRO	TYR
	GLY	GLY	SER	SER	TRP	LYS	PHE
	ILE	ILE	VAL	VAL	ILE	GLN	ALA
	ILE	ILE	ARG	HIS	GLU	TYR	VAL
	HIS	HIS	LEU	LEU	THR	GLN	GLY
	GLY	GLY	SER	THR	THR	CYS	TYR
	GLU	GLU	MET	THR	PHE	PHE	GLY
	LYS	LYS	LEU	LEU	THR	VAL	GLN
	LEU	LEU	LEU	THR	THR	ALA	LYS
	THR	THR	SER	SER	TYR	PRO	PRO
	GLU	GLU	GLY	GLY	TYR	VAL	LYS
	LEU	LEU	ILE	ILE	THR	VAL	ILE
	LYS	LYS	VAL	VAL	PHE	MET	PHE
	PRO	PRO	ASP	ASP	PRO	LYS	THR
	LEU	LEU	ALA	ILE	GLY	LEU	ILE
	HIS	HIS	VAL	VAL	LEU	PRO	LYS
	GLU	GLU	MET	MET	LYS	SER	ILE
	ARG	ARG	GLY	GLY	TRP	TYR	PHE
	LEU	LEU	GLY	GLY	PHE	LYS	THR
	SER	SER	PHE	PHE	GLU	ASP	TYR
	SER	SER	SER	VAL	VAL	LYS	ARG
	CYS	CYS	ASN	LYS	PRO	PRO	GLY
	PHE	PHE	TYR	GLN	GLN	VAL	LYS
	ARG	ARG	GLU	ILE	ILE	PRO	GLU
	GLU	GLU	LYS	LYS	SER	GLU	TYR
	LEU	LEU	ALA	THR	THR	GLN	GLY
	LYS	LYS	PHE	PHE	ILE	ARG	ARG
	LYS	LYS	THR	GLU	GLU	LEU	GLY
	VAL	VAL	THR	ILE	TYR	ASN	GLU
							ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	279838	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	319.2, 319.2, 319.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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	0.23	0/5992	0.53	0/8086
2	B	0.29	0/13722	0.55	2/18514 (0.0%)
2	E	0.28	0/1223	0.55	0/1643
All	All	0.27	0/20937	0.54	2/28243 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1423	LYS	CA-C-N	5.17	129.47	121.26
2	B	1423	LYS	C-N-CA	5.17	129.47	121.26

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	643	SER	Peptide
2	B	1064	PHE	Peptide
2	B	1288	TYR	Peptide

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	5879	0	5902	469	0
2	B	13436	0	13516	978	0
2	E	1197	0	1194	96	0
All	All	20512	0	20612	1515	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 37.

All (1515) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:MET:HE3	1:A:485:LYS:HG3	1.44	0.99
2:B:761:LYS:HE3	2:B:765:ARG:HE	1.32	0.95
2:B:201:GLU:O	2:B:205:LEU:HB2	1.67	0.93
2:B:36:HIS:HB2	2:B:48:TYR:HB2	1.52	0.88
2:B:1573:GLU:OE1	2:B:1577:GLN:NE2	2.05	0.88
2:E:1265:LEU:O	2:E:1269:GLU:N	2.07	0.88
2:B:1357:ARG:O	2:B:1359:GLN:NE2	2.08	0.87
2:E:1231:TYR:O	2:E:1235:LYS:N	2.09	0.86
2:B:1490:THR:HB	2:B:1506:GLN:HB3	1.56	0.86
2:B:1584:GLU:O	2:B:1588:LEU:HB2	1.74	0.86
2:B:223:GLY:HA3	2:B:280:VAL:HG13	1.58	0.85
2:B:1028:LEU:HD11	2:B:1042:LEU:HD23	1.59	0.85
2:B:664:GLU:HA	2:B:667:LYS:HD3	1.58	0.85
2:B:1597:MET:HE1	2:B:1630:LYS:HB2	1.57	0.85
2:B:1059:LEU:HD12	2:B:1116:PRO:HB2	1.58	0.84
2:B:154:HIS:HA	2:B:197:LYS:HZ3	1.42	0.83
2:B:1145:HIS:HA	2:B:1148:GLU:HG3	1.59	0.82
1:A:568:ARG:HE	1:A:569:ARG:HH22	1.27	0.82
1:A:490:ARG:NH1	1:A:513:GLU:O	2.13	0.81
1:A:144:GLN:HA	1:A:147:MET:HG3	1.62	0.80
2:B:1062:GLU:HB3	2:B:1069:ARG:HA	1.63	0.80
2:B:1372:PHE:HB2	2:B:1377:ARG:HG2	1.62	0.80
2:B:91:LEU:HD11	2:B:124:LEU:HD11	1.62	0.79
2:B:1:MET:O	2:B:4:TRP:NE1	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1418:ILE:HA	2:B:1421:SER:HB3	1.63	0.78
2:B:283:ASP:HB2	2:B:430:LYS:HB3	1.66	0.77
2:B:904:GLN:O	2:B:908:ASN:ND2	2.17	0.77
2:B:224:LEU:H	2:B:281:PHE:H	1.30	0.77
2:B:1117:GLU:OE1	2:B:1119:GLU:N	2.18	0.77
2:B:1029:THR:HA	2:B:1033:MET:HE3	1.67	0.77
2:B:1582:ASP:O	2:B:1585:LYS:NZ	2.17	0.77
2:B:323:GLY:HA3	2:B:350:GLN:HA	1.67	0.77
2:B:14:VAL:HG23	2:B:65:HIS:HB3	1.66	0.77
1:A:202:LEU:HD12	1:A:246:VAL:HG21	1.66	0.76
2:B:1111:GLU:OE1	2:B:1111:GLU:N	2.18	0.76
1:A:306:GLU:HG3	1:A:431:GLY:HA3	1.66	0.76
2:B:1530:SER:O	2:B:1534:GLN:NE2	2.19	0.76
2:B:1544:VAL:HG22	2:B:1610:LYS:HD2	1.67	0.76
2:B:1346:ALA:HB1	2:E:1339:GLY:HA2	1.66	0.75
1:A:351:MET:HG2	1:A:354:ARG:HH21	1.48	0.75
2:B:1335:TYR:HA	2:B:1338:LEU:HD23	1.69	0.75
2:B:701:ILE:HD11	2:B:762:TYR:HD2	1.51	0.75
1:A:567:ALA:HB3	1:A:573:LYS:HG2	1.68	0.75
1:A:327:LEU:HB3	1:A:384:MET:HE1	1.69	0.75
2:B:417:PHE:HB3	2:B:420:LEU:HB2	1.68	0.75
2:B:216:PHE:O	2:B:222:TYR:OH	2.06	0.74
2:B:710:GLN:O	2:B:713:ASN:ND2	2.20	0.74
1:A:238:GLU:O	1:A:241:THR:OG1	2.04	0.74
2:B:1465:SER:HA	2:B:1486:ARG:HA	1.69	0.74
1:A:209:VAL:HG11	1:A:249:ALA:HB1	1.67	0.74
2:B:966:ASP:HA	2:B:969:TYR:HD1	1.50	0.74
2:B:1466:ARG:HG3	2:B:1485:GLU:HB2	1.67	0.74
2:B:95:LEU:HD13	2:B:124:LEU:HD23	1.68	0.74
1:A:34:ILE:HG22	1:A:46:HIS:HB2	1.70	0.74
2:B:740:TYR:HB3	2:B:753:LEU:HD21	1.69	0.74
2:E:1291:TYR:HB3	2:E:1296:LEU:HD11	1.70	0.74
2:B:472:VAL:HG21	2:B:483:ALA:HB3	1.70	0.74
1:A:536:LEU:HD13	2:B:18:ASN:HD21	1.52	0.73
2:B:1215:GLU:O	2:B:1220:ARG:NH1	2.21	0.73
2:E:1248:ARG:HH11	2:E:1252:ARG:HH12	1.37	0.73
1:A:306:GLU:HA	1:A:309:MET:HG3	1.69	0.73
2:B:509:TRP:HB3	2:B:511:GLU:HB2	1.70	0.73
2:B:1298:GLU:OE1	2:B:1302:GLN:NE2	2.22	0.72
1:A:408:LYS:HE3	1:A:474:SER:HB2	1.70	0.72
2:B:1464:TYR:O	2:B:1487:THR:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1294:GLN:N	2:E:1294:GLN:OE1	2.23	0.72
2:B:1209:THR:O	2:B:1213:GLN:NE2	2.23	0.72
2:B:208:LEU:HB3	2:B:211:ARG:HE	1.53	0.72
2:B:114:PHE:O	2:B:118:GLN:NE2	2.22	0.72
2:B:1559:VAL:HG22	2:B:1629:LEU:HD11	1.72	0.72
1:A:348:ARG:HH11	1:A:351:MET:HE3	1.55	0.71
1:A:79:THR:O	1:A:84:ASN:ND2	2.23	0.71
1:A:266:LEU:HD22	1:A:271:LEU:HD22	1.72	0.71
2:B:1160:GLU:OE1	2:B:1242:ARG:NH2	2.21	0.71
1:A:670:ASN:ND2	1:A:676:ASP:O	2.21	0.71
2:B:385:LYS:O	2:B:389:ALA:N	2.23	0.71
2:B:801:LEU:O	2:B:813:LYS:NZ	2.21	0.71
2:B:809:ALA:HB1	2:B:812:ILE:HB	1.71	0.71
1:A:140:TYR:HD1	1:A:143:LEU:HD11	1.55	0.71
2:B:126:GLU:OE1	2:B:130:GLN:NE2	2.24	0.71
2:B:761:LYS:NZ	2:B:826:ASP:OD2	2.24	0.71
2:B:1460:GLN:NE2	2:B:1491:THR:O	2.24	0.71
2:B:314:HIS:ND1	2:B:536:SER:O	2.24	0.71
2:B:590:GLY:N	2:B:594:GLU:OE2	2.24	0.70
1:A:514:ILE:O	1:A:518:ARG:NH2	2.23	0.70
2:B:1377:ARG:H	2:B:1379:LYS:HE2	1.55	0.70
2:B:1169:LYS:O	2:B:1173:GLU:HG2	1.91	0.70
2:B:1391:ARG:HH12	2:B:1395:SER:HB2	1.56	0.70
2:B:166:ARG:HG2	2:B:173:LEU:HB2	1.72	0.70
1:A:212:SER:HB3	1:A:215:LEU:HD13	1.73	0.70
2:B:652:HIS:HA	2:B:655:LYS:HD2	1.73	0.70
2:B:10:GLN:NE2	2:B:68:GLU:OE2	2.25	0.70
2:B:149:THR:HG22	2:B:171:ASN:HD21	1.56	0.70
1:A:511:TYR:HD1	1:A:514:ILE:HD12	1.56	0.70
2:E:1280:PRO:HA	2:E:1283:LEU:HB2	1.74	0.70
2:B:628:SER:O	2:B:667:LYS:NZ	2.24	0.69
2:B:944:ASN:O	2:B:946:GLN:NE2	2.25	0.69
2:B:1153:THR:HG22	2:B:1157:GLN:HE22	1.57	0.69
2:B:446:ILE:HA	2:B:626:ILE:HG23	1.72	0.69
1:A:228:LEU:HA	1:A:231:HIS:HD2	1.56	0.69
2:B:654:LEU:HD13	2:B:657:LEU:HD12	1.74	0.69
2:B:1241:ILE:HA	2:B:1244:LEU:HD12	1.72	0.69
2:B:1386:LYS:HB2	2:B:1389:GLU:HB2	1.72	0.69
1:A:512:THR:O	1:A:516:LYS:N	2.26	0.69
1:A:670:ASN:OD1	1:A:675:LYS:HG3	1.92	0.69
2:B:224:LEU:HD11	2:B:245:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1238:ASP:OD1	2:E:1239:ILE:N	2.25	0.69
1:A:260:GLN:NE2	1:A:307:ASP:OD2	2.25	0.69
1:A:386:TYR:HA	1:A:389:LYS:HD2	1.75	0.69
2:B:315:THR:HA	2:B:538:GLU:HG3	1.74	0.69
2:B:819:TYR:O	2:B:822:SER:OG	2.10	0.69
1:A:356:TYR:HB3	1:A:361:PHE:HB2	1.73	0.69
1:A:287:ASN:HB2	1:A:290:MET:H	1.58	0.69
1:A:541:GLN:HA	1:A:544:ILE:HG12	1.75	0.69
2:B:273:LYS:HB3	2:B:277:LEU:HD21	1.75	0.69
2:B:717:GLU:OE2	2:B:765:ARG:NH1	2.25	0.68
2:B:927:LEU:HD12	2:B:931:ARG:HH22	1.57	0.68
1:A:25:ASP:O	1:A:66:ARG:NH2	2.26	0.68
2:B:154:HIS:NE2	2:B:201:GLU:OE2	2.25	0.68
2:B:871:GLN:HG3	2:B:875:ARG:HB2	1.76	0.68
1:A:720:TYR:C	2:B:1:MET:H1	2.00	0.68
2:B:8:LYS:HA	2:B:11:LYS:HD3	1.75	0.68
2:B:864:VAL:HG21	2:B:909:ILE:HG22	1.74	0.68
1:A:518:ARG:O	1:A:522:ARG:NH2	2.26	0.68
2:B:1488:THR:HB	2:B:1508:SER:HB2	1.73	0.68
1:A:62:THR:HG23	1:A:64:LYS:H	1.58	0.68
1:A:408:LYS:HB3	1:A:474:SER:H	1.58	0.68
2:B:36:HIS:HB3	2:B:38:LEU:HD21	1.76	0.68
2:B:1237:GLU:OE1	2:B:1237:GLU:N	2.27	0.68
1:A:441:PHE:HD2	1:A:443:PRO:HD3	1.59	0.67
2:B:1056:HIS:ND1	2:B:1057:GLU:OE2	2.26	0.67
2:B:1384:ARG:HH21	2:B:1495:PHE:HB3	1.60	0.67
2:B:1573:GLU:O	2:B:1577:GLN:NE2	2.28	0.67
2:B:228:PHE:HE2	2:B:399:LEU:HB2	1.59	0.67
2:B:1067:ALA:O	2:B:1071:LYS:N	2.24	0.67
2:B:1458:GLU:HA	2:B:1495:PHE:O	1.94	0.67
1:A:20:LYS:HB2	1:A:22:MET:HE1	1.77	0.67
2:B:1135:GLU:O	2:B:1139:SER:N	2.28	0.67
2:B:1347:SER:O	2:B:1350:GLU:HG3	1.94	0.67
2:B:675:ALA:O	2:B:679:ILE:HD12	1.94	0.67
2:B:1024:PHE:HA	2:B:1027:VAL:HG12	1.77	0.67
1:A:61:ILE:HG21	1:A:69:ILE:HD11	1.77	0.67
1:A:541:GLN:HB3	1:A:545:LEU:HD23	1.75	0.67
2:B:789:ASN:HA	2:B:792:ARG:HD2	1.76	0.67
1:A:202:LEU:HD13	1:A:205:LEU:HD12	1.76	0.66
2:B:1452:ASN:HA	2:B:1455:ARG:HG2	1.77	0.66
2:B:1389:GLU:OE2	2:B:1394:PHE:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ARG:NH2	2:B:48:TYR:OH	2.28	0.66
2:B:1117:GLU:OE2	2:B:1121:ARG:N	2.22	0.66
2:E:1249:ASP:OD1	2:E:1252:ARG:NH1	2.28	0.66
1:A:245:ALA:N	1:A:293:GLN:HE22	1.94	0.66
2:B:1406:GLU:OE2	2:B:1423:LYS:HG3	1.95	0.66
1:A:147:MET:HB2	1:A:150:CYS:HB2	1.78	0.66
2:B:720:ILE:HA	2:B:724:PHE:HB2	1.78	0.66
2:B:1102:ILE:O	2:B:1106:VAL:HG13	1.96	0.66
1:A:214:ASP:HA	1:A:217:GLN:HG2	1.77	0.66
1:A:230:PRO:HA	1:A:233:GLN:HG2	1.77	0.66
1:A:276:LEU:HA	1:A:280:ILE:HB	1.76	0.65
2:B:972:TYR:HA	2:B:975:THR:HB	1.77	0.65
2:B:941:ILE:O	2:B:944:ASN:ND2	2.29	0.65
2:B:1604:ILE:HG23	2:B:1619:HIS:HE2	1.60	0.65
2:E:1301:TYR:HE1	2:E:1320:LEU:HD22	1.60	0.65
1:A:359:LEU:HD22	1:A:413:PHE:H	1.60	0.65
2:B:409:ASP:OD1	2:B:411:THR:OG1	2.12	0.65
2:B:144:LEU:HD23	2:B:147:LYS:HE2	1.79	0.65
2:B:1364:ALA:HA	2:B:1382:ILE:HG13	1.79	0.65
2:B:1583:GLN:O	2:B:1583:GLN:NE2	2.29	0.65
2:E:1248:ARG:NH1	2:E:1249:ASP:OD1	2.28	0.65
2:B:1466:ARG:NH1	2:B:1467:PRO:O	2.28	0.65
2:E:1328:TYR:HA	2:E:1332:VAL:HG12	1.78	0.65
1:A:10:VAL:HG11	1:A:75:LEU:HD13	1.78	0.65
2:B:875:ARG:HD2	2:B:924:HIS:CG	2.32	0.65
2:B:1065:SER:OG	2:B:1068:LYS:N	2.28	0.65
2:B:965:ASP:OD1	2:B:966:ASP:N	2.28	0.65
2:E:1283:LEU:O	2:E:1285:ARG:NH1	2.28	0.65
2:B:231:PHE:CE2	2:B:233:CYS:HB3	2.32	0.64
1:A:233:GLN:OE1	1:A:278:HIS:NE2	2.29	0.64
1:A:677:MET:O	1:A:678:MET:HE2	1.96	0.64
1:A:18:TYR:O	1:A:41:TRP:NE1	2.26	0.64
2:B:1406:GLU:OE1	2:B:1425:TYR:HD1	1.80	0.64
2:B:1575:TYR:OH	2:B:1585:LYS:HB2	1.97	0.64
1:A:177:SER:H	1:A:180:PHE:HB2	1.61	0.64
1:A:241:THR:O	1:A:293:GLN:NE2	2.31	0.64
2:B:730:TYR:HB2	2:B:767:ILE:HG23	1.79	0.64
2:B:1612:THR:H	2:B:1615:LEU:HB2	1.61	0.64
1:A:169:GLY:HA2	1:A:173:TRP:HZ2	1.62	0.64
1:A:198:LEU:HD11	1:A:231:HIS:CE1	2.32	0.64
2:B:1567:GLU:HG2	2:B:1568:LYS:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HZ3	1:A:40:GLY:HA3	1.62	0.64
2:B:450:LEU:HB2	2:B:511:GLU:HB3	1.79	0.64
2:B:1356:MET:O	2:B:1357:ARG:NH1	2.31	0.64
2:E:1301:TYR:O	2:E:1305:ILE:HG12	1.98	0.64
2:B:1432:LYS:HB3	2:B:1463:ARG:HG2	1.80	0.64
2:B:462:THR:HB	2:B:503:GLN:HG2	1.80	0.64
2:B:640:LEU:HD11	2:B:657:LEU:HD21	1.79	0.64
2:B:934:ARG:NH1	2:B:938:ARG:HB2	2.13	0.64
1:A:442:HIS:HA	1:A:495:LYS:HZ3	1.63	0.64
2:B:17:TYR:HA	2:B:31:ILE:HG23	1.80	0.64
2:B:1175:LEU:O	2:B:1179:HIS:ND1	2.31	0.64
1:A:251:PHE:O	1:A:259:ARG:NH2	2.31	0.63
2:B:417:PHE:O	2:B:421:VAL:N	2.26	0.63
2:B:1575:TYR:CZ	2:B:1585:LYS:HD2	2.34	0.63
2:B:1059:LEU:O	2:B:1063:THR:OG1	2.09	0.63
2:B:795:PHE:HD2	2:B:839:LEU:HB3	1.62	0.63
2:B:1151:LEU:O	2:B:1155:LEU:HG	1.99	0.63
1:A:54:ALA:HB2	1:A:76:ARG:H	1.63	0.63
1:A:327:LEU:HD21	1:A:385:LEU:HD23	1.81	0.63
1:A:563:ARG:HB2	1:A:655:ILE:HG21	1.81	0.63
1:A:722:PHE:HD1	2:B:1:MET:H2	1.45	0.63
2:B:102:TRP:HA	2:B:105:LEU:HB2	1.80	0.63
1:A:281:ARG:O	1:A:283:GLN:NE2	2.31	0.63
1:A:503:LYS:HD3	1:A:506:LEU:HD12	1.81	0.63
2:B:628:SER:HB2	2:B:631:LEU:HD22	1.80	0.63
2:B:670:GLN:NE2	2:B:674:ASP:OD2	2.31	0.63
2:B:1340:ASN:HA	2:B:1343:LYS:NZ	2.14	0.63
1:A:256:ASP:HA	1:A:259:ARG:HD3	1.80	0.62
2:B:172:ILE:O	2:B:174:ASP:N	2.32	0.62
2:B:451:ILE:HD12	2:B:621:GLN:HE22	1.63	0.62
1:A:86:GLN:HA	1:A:89:HIS:CD2	2.34	0.62
2:B:900:GLU:O	2:B:904:GLN:HG2	2.00	0.62
1:A:202:LEU:HA	1:A:205:LEU:HD12	1.80	0.62
1:A:346:GLU:N	1:A:346:GLU:OE1	2.33	0.62
1:A:560:THR:H	1:A:665:TRP:HZ2	1.46	0.62
1:A:646:TYR:N	1:A:650:CYS:O	2.30	0.62
2:B:653:ASN:O	2:B:657:LEU:HG	2.00	0.62
2:B:789:ASN:OD1	2:B:792:ARG:NH1	2.32	0.62
2:B:1073:VAL:O	2:B:1077:GLY:N	2.32	0.62
2:B:225:TYR:HB3	2:B:404:LYS:H	1.64	0.62
2:E:1307:TYR:O	2:E:1311:GLY:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:PHE:N	1:A:575:TRP:O	2.33	0.62
2:B:170:GLY:HA3	2:B:173:LEU:HD13	1.80	0.62
2:B:599:GLU:O	2:B:603:SER:N	2.33	0.62
2:B:1536:HIS:CE1	2:B:1610:LYS:HD3	2.34	0.62
1:A:118:GLN:NE2	1:A:122:ASN:OD1	2.32	0.62
1:A:265:ILE:O	1:A:268:GLN:HG2	1.99	0.62
1:A:551:GLN:O	1:A:555:ARG:HG2	2.00	0.62
1:A:328:ARG:HD3	1:A:348:ARG:HH22	1.64	0.62
1:A:541:GLN:O	1:A:545:LEU:N	2.23	0.62
2:B:79:THR:HB	2:B:85:LEU:HG	1.81	0.62
2:B:446:ILE:HG23	2:B:626:ILE:HG12	1.81	0.62
1:A:366:ASN:HB2	1:A:369:MET:HE3	1.82	0.61
2:B:327:MET:SD	2:B:346:ILE:HG13	2.40	0.61
1:A:382:ASP:HA	1:A:385:LEU:HD12	1.83	0.61
1:A:383:ASN:ND2	1:A:453:GLU:HA	2.16	0.61
1:A:622:CYS:HB2	1:A:625:MET:HG3	1.81	0.61
2:B:768:ILE:HD12	2:B:830:VAL:HG21	1.81	0.61
1:A:677:MET:O	1:A:683:ARG:NH1	2.33	0.61
2:B:433:PHE:HA	2:B:443:ARG:HH12	1.65	0.61
2:B:810:VAL:HG23	2:B:811:LYS:H	1.65	0.61
1:A:271:LEU:HA	1:A:274:ILE:HG22	1.82	0.61
1:A:356:TYR:HD1	1:A:359:LEU:HB2	1.65	0.61
2:B:112:THR:O	2:B:116:GLN:NE2	2.34	0.61
2:B:319:ARG:NH2	2:B:498:SER:O	2.33	0.61
2:B:1607:HIS:HD2	2:B:1619:HIS:CD2	2.18	0.61
1:A:344:SER:OG	1:A:346:GLU:OE1	2.15	0.61
1:A:491:ALA:O	1:A:494:THR:OG1	2.18	0.61
2:B:1328:TYR:HB3	2:B:1338:LEU:HD22	1.82	0.61
2:E:1242:ARG:HH12	2:E:1284:GLN:HA	1.64	0.61
1:A:2:PRO:HG2	1:A:3:PRO:HD3	1.83	0.61
2:B:14:VAL:HG13	2:B:67:LYS:HD3	1.83	0.61
2:B:450:LEU:O	2:B:511:GLU:N	2.34	0.61
2:B:1486:ARG:NH1	2:B:1510:GLU:OE2	2.34	0.61
1:A:91:ARG:HB2	1:A:103:ALA:HB2	1.82	0.61
1:A:522:ARG:O	1:A:525:GLN:HG3	2.01	0.61
1:A:578:ARG:HB3	1:A:587:HIS:HB2	1.81	0.61
2:B:172:ILE:O	2:B:175:PRO:HD3	2.01	0.61
2:B:677:PHE:HA	2:B:680:MET:HG3	1.83	0.61
2:B:973:ILE:HA	2:B:976:PHE:CE1	2.34	0.61
2:B:208:LEU:O	2:B:211:ARG:NE	2.33	0.61
2:B:556:ASN:N	2:B:560:THR:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:993:PHE:O	2:B:996:LEU:N	2.33	0.61
2:B:1465:SER:HB2	2:B:1486:ARG:HG2	1.82	0.61
1:A:309:MET:HB3	1:A:379:LEU:HD23	1.81	0.61
2:B:607:VAL:HG12	2:B:608:THR:HG23	1.83	0.61
1:A:692:MET:HE2	1:A:692:MET:HA	1.82	0.60
2:B:86:PRO:O	2:B:89:GLN:HG2	2.00	0.60
2:B:596:GLU:HA	2:B:599:GLU:HG2	1.82	0.60
1:A:21:LEU:HD11	2:B:1356:MET:HB2	1.82	0.60
1:A:398:ILE:HD13	1:A:401:GLU:OE2	2.00	0.60
2:B:376:ASN:ND2	2:B:502:TYR:O	2.35	0.60
2:B:239:ALA:HA	2:B:302:ARG:HA	1.83	0.60
1:A:715:LYS:C	2:B:44:TRP:HE1	2.09	0.60
2:B:248:PRO:HB3	2:B:387:ILE:HG21	1.82	0.60
2:B:1243:TYR:O	2:B:1247:LEU:HD23	2.01	0.60
2:E:1277:PRO:HG2	2:E:1290:VAL:HG22	1.82	0.60
2:B:634:ASN:OD1	2:B:637:LEU:N	2.31	0.60
2:E:1298:GLU:OE1	2:E:1302:GLN:NE2	2.33	0.60
2:B:1007:MET:HB2	2:B:1011:MET:HE1	1.84	0.60
2:B:1082:GLU:OE2	2:B:1082:GLU:N	2.22	0.60
1:A:340:ASN:ND2	1:A:351:MET:SD	2.75	0.60
2:B:1539:ASP:HB3	2:B:1542:LEU:HD12	1.84	0.60
1:A:313:MET:HB2	1:A:378:MET:SD	2.42	0.60
2:E:1225:VAL:HA	2:E:1228:LEU:HD12	1.82	0.60
2:B:233:CYS:SG	2:B:234:ASN:N	2.75	0.60
2:B:1434:VAL:HA	2:B:1463:ARG:HH22	1.66	0.60
2:E:1221:MET:O	2:E:1224:THR:OG1	2.19	0.60
1:A:90:GLU:HA	1:A:93:GLN:OE1	2.02	0.59
2:B:569:LEU:HD11	2:B:622:ILE:HG12	1.84	0.59
1:A:441:PHE:CD2	1:A:443:PRO:HD3	2.37	0.59
1:A:557:VAL:HA	1:A:579:LEU:HB3	1.84	0.59
2:B:1368:TYR:CZ	2:B:1414:PRO:HB3	2.37	0.59
2:B:1536:HIS:HA	2:B:1542:LEU:HD13	1.84	0.59
2:B:795:PHE:HA	2:B:798:PHE:HD2	1.68	0.59
1:A:587:HIS:ND1	1:A:606:ASP:OD1	2.36	0.59
2:B:534:ARG:NE	2:B:541:ASP:OD1	2.31	0.59
2:B:1136:PHE:CD1	2:B:1186:LEU:HD22	2.38	0.59
2:B:1159:VAL:O	2:B:1208:ARG:NH2	2.17	0.59
2:B:1165:ASP:O	2:B:1168:TYR:HB3	2.02	0.59
2:B:1307:TYR:O	2:B:1311:GLY:N	2.35	0.59
1:A:262:MET:O	1:A:266:LEU:HG	2.03	0.59
2:B:16:ILE:HG12	2:B:65:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1258:THR:OG1	2:E:1259:GLU:OE1	2.21	0.59
1:A:88:LEU:O	1:A:92:ILE:HG12	2.02	0.59
2:E:1224:THR:O	2:E:1228:LEU:HG	2.02	0.59
2:B:1369:GLY:HA2	2:B:1418:ILE:HG13	1.85	0.59
2:E:1228:LEU:HB3	2:E:1240:TYR:HE1	1.67	0.59
2:B:189:VAL:O	2:B:193:ARG:HG2	2.03	0.58
2:B:1401:GLN:O	2:B:1401:GLN:NE2	2.35	0.58
2:B:954:VAL:HA	2:B:957:MET:HE3	1.85	0.58
2:B:1117:GLU:CD	2:B:1120:LEU:HG	2.28	0.58
1:A:289:GLU:O	1:A:293:GLN:HG2	2.03	0.58
2:B:1328:TYR:HA	2:B:1332:VAL:HG22	1.84	0.58
2:B:966:ASP:HA	2:B:969:TYR:CD1	2.35	0.58
2:B:1383:TYR:CD2	2:B:1501:TRP:HB3	2.38	0.58
2:B:1469:ARG:HG3	2:B:1478:GLU:HG2	1.86	0.58
2:B:1532:CYS:O	2:B:1536:HIS:HB2	2.03	0.58
2:B:1607:HIS:HE1	2:B:1615:LEU:HD13	1.68	0.58
1:A:141:GLN:HA	1:A:144:GLN:HB3	1.85	0.58
2:B:909:ILE:HG13	2:B:910:LEU:N	2.18	0.58
2:B:592:LYS:HA	2:B:595:MET:HG2	1.85	0.58
2:B:801:LEU:HD23	2:B:804:ARG:HH21	1.68	0.58
1:A:374:THR:HG22	1:A:377:GLY:HA3	1.84	0.58
2:B:587:THR:O	2:B:598:LYS:NZ	2.36	0.58
2:B:1449:GLN:HA	2:B:1452:ASN:HD21	1.69	0.58
2:B:473:HIS:HE2	2:B:528:ARG:HB3	1.69	0.58
2:B:569:LEU:HD12	2:B:620:PHE:HD2	1.69	0.58
2:B:931:ARG:C	2:B:935:ARG:HE	2.12	0.58
2:B:1327:THR:O	2:B:1331:LYS:HB2	2.03	0.58
2:B:3:ARG:HB3	2:B:41:TYR:CE1	2.39	0.57
2:B:594:GLU:HA	2:B:597:GLU:HG3	1.86	0.57
2:B:1370:GLN:HA	2:B:1377:ARG:HH21	1.69	0.57
1:A:137:THR:O	1:A:141:GLN:NE2	2.37	0.57
1:A:328:ARG:NH2	1:A:355:ASP:HB2	2.19	0.57
2:B:929:MET:HE1	2:B:968:HIS:HB3	1.86	0.57
2:B:958:ILE:HB	2:B:1016:VAL:HG21	1.86	0.57
1:A:147:MET:SD	1:A:151:PHE:HB2	2.44	0.57
1:A:181:ILE:HD11	1:A:222:GLU:HB2	1.86	0.57
2:B:484:ILE:HA	2:B:515:VAL:HG12	1.85	0.57
2:B:1008:VAL:O	2:B:1012:THR:HG23	2.05	0.57
2:B:1172:LEU:HG	2:B:1176:LEU:HD23	1.85	0.57
2:B:1231:TYR:O	2:B:1235:LYS:N	2.38	0.57
2:B:1525:THR:OG1	2:B:1528:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1555:VAL:HA	2:B:1559:VAL:HG23	1.85	0.57
2:B:1590:LYS:NZ	2:B:1637:TYR:O	2.37	0.57
2:E:1316:LYS:HG3	2:E:1319:LYS:HE3	1.86	0.57
1:A:54:ALA:HB3	1:A:74:ILE:HG23	1.85	0.57
1:A:567:ALA:HB1	1:A:571:GLN:HB2	1.85	0.57
2:B:1183:HIS:CE1	2:B:1186:LEU:HB3	2.39	0.57
1:A:53:HIS:N	1:A:59:PHE:O	2.29	0.57
2:B:706:ASP:OD1	2:B:708:LYS:N	2.35	0.57
2:B:463:PRO:HD2	2:B:503:GLN:HB3	1.86	0.57
2:B:575:ASP:OD2	2:B:578:LYS:N	2.32	0.57
2:B:470:MET:SD	2:B:484:ILE:HG12	2.45	0.57
2:B:1336:GLU:O	2:B:1340:ASN:ND2	2.37	0.57
1:A:6:ASP:O	1:A:26:GLN:N	2.35	0.57
1:A:28:LYS:O	1:A:66:ARG:NH1	2.37	0.57
1:A:276:LEU:HA	1:A:280:ILE:HD12	1.85	0.57
2:B:412:GLN:O	2:B:416:ASN:N	2.36	0.57
2:B:1195:LEU:O	2:B:1198:SER:OG	2.20	0.57
2:B:1245:TYR:HH	2:B:1267:HIS:CD2	2.22	0.57
1:A:194:ASP:HB3	1:A:197:ILE:HD12	1.87	0.57
1:A:486:GLU:O	1:A:490:ARG:HG3	2.04	0.57
2:B:44:TRP:HA	2:B:60:PRO:HA	1.87	0.57
2:B:1136:PHE:HA	2:B:1139:SER:HB2	1.87	0.57
2:B:1431:VAL:HG12	2:B:1464:TYR:HB2	1.87	0.57
2:E:1268:ALA:HA	2:E:1271:LEU:HD13	1.85	0.57
2:B:166:ARG:NH1	2:B:168:ASP:H	2.03	0.56
2:B:1232:LYS:HB2	2:B:1240:TYR:HE1	1.70	0.56
1:A:9:LYS:N	1:A:71:ASN:OD1	2.37	0.56
1:A:20:LYS:NZ	1:A:40:GLY:HA3	2.20	0.56
1:A:503:LYS:O	1:A:507:GLN:NE2	2.38	0.56
2:B:15:ALA:C	2:B:65:HIS:HB2	2.30	0.56
2:B:1207:TYR:O	2:B:1211:ILE:HG12	2.04	0.56
1:A:13:GLU:HG3	1:A:19:PRO:HB3	1.86	0.56
1:A:232:LEU:HD22	1:A:275:ILE:HD13	1.86	0.56
1:A:266:LEU:O	1:A:270:GLN:N	2.38	0.56
2:B:68:GLU:N	2:B:78:GLU:OE2	2.38	0.56
2:B:294:VAL:HB	2:B:330:THR:HA	1.87	0.56
2:B:466:VAL:HG22	2:B:547:PHE:HZ	1.70	0.56
2:B:763:LEU:HA	2:B:766:PHE:HD1	1.70	0.56
1:A:49:PHE:HA	1:A:79:THR:HA	1.86	0.56
1:A:485:LYS:HD2	1:A:488:VAL:HB	1.86	0.56
2:B:472:VAL:HA	2:B:527:ILE:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:TYR:HB3	2:B:28:SER:HA	1.88	0.56
2:B:969:TYR:HA	2:B:973:ILE:HB	1.87	0.56
2:B:1328:TYR:HB3	2:B:1338:LEU:CD2	2.35	0.56
2:B:60:PRO:HG2	2:B:63:TYR:HB2	1.88	0.56
2:B:840:PHE:O	2:B:844:ILE:HG22	2.05	0.56
2:B:939:THR:O	2:B:943:MET:HG3	2.06	0.56
2:B:1273:TRP:HE3	2:B:1294:GLN:HG3	1.70	0.56
2:B:569:LEU:HD21	2:B:622:ILE:HG12	1.87	0.56
2:B:1117:GLU:OE2	2:B:1120:LEU:HG	2.06	0.56
2:B:1249:ASP:OD1	2:B:1252:ARG:NH2	2.25	0.56
2:B:1617:PRO:O	2:B:1620:GLU:HG3	2.06	0.56
2:B:984:ASP:O	2:B:987:MET:HB2	2.05	0.56
2:B:1600:LEU:HB2	2:B:1626:PHE:HE2	1.70	0.56
2:B:817:LEU:HD11	2:B:855:GLN:HB3	1.88	0.55
2:B:1356:MET:SD	2:B:1358:PRO:HD3	2.46	0.55
1:A:306:GLU:HA	1:A:309:MET:CG	2.37	0.55
1:A:443:PRO:HD2	1:A:495:LYS:NZ	2.20	0.55
1:A:615:ALA:HB3	1:A:645:LEU:HD23	1.87	0.55
1:A:9:LYS:O	1:A:72:GLY:N	2.37	0.55
2:B:441:ASP:O	2:B:443:ARG:HG3	2.06	0.55
2:B:750:THR:O	2:B:753:LEU:N	2.39	0.55
2:B:854:ARG:HA	2:B:857:LEU:HD12	1.88	0.55
2:B:1115:THR:O	2:B:1121:ARG:NH2	2.39	0.55
2:B:1329:GLU:HB3	2:B:1338:LEU:HD11	1.88	0.55
2:B:1566:TYR:O	2:B:1570:PHE:HB2	2.07	0.55
1:A:49:PHE:HB3	1:A:77:LEU:HD11	1.88	0.55
1:A:52:GLN:OE1	1:A:76:ARG:NH1	2.36	0.55
1:A:546:GLU:HG2	1:A:549:LYS:HE3	1.88	0.55
2:B:3:ARG:HD3	2:B:3:ARG:O	2.07	0.55
2:B:143:GLU:HG3	2:B:147:LYS:HZ3	1.72	0.55
2:B:1017:PHE:O	2:B:1021:ILE:HG12	2.07	0.55
2:E:1251:HIS:NE2	2:E:1256:ASN:HB2	2.21	0.55
1:A:220:ALA:HA	1:A:223:ILE:HD12	1.88	0.55
1:A:387:PHE:CZ	1:A:457:CYS:HB3	2.42	0.55
2:B:929:MET:HE3	2:B:973:ILE:HD11	1.88	0.55
2:B:1232:LYS:HB2	2:B:1240:TYR:CE1	2.41	0.55
2:B:1477:ASN:HD22	2:B:1565:ASN:HA	1.72	0.55
2:B:1491:THR:HG22	2:B:1504:VAL:HA	1.88	0.55
2:E:1216:SER:O	2:E:1220:ARG:N	2.28	0.55
1:A:293:GLN:HA	1:A:296:VAL:HG12	1.89	0.55
2:B:228:PHE:CE2	2:B:399:LEU:HB2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ALA:HB2	1:A:81:PRO:HD3	1.88	0.55
1:A:496:PRO:HG2	1:A:502:PHE:HD1	1.72	0.55
2:B:283:ASP:O	2:B:430:LYS:HD2	2.07	0.55
1:A:303:ASN:HA	1:A:306:GLU:HB2	1.89	0.55
2:B:167:ASP:OD1	2:B:168:ASP:N	2.39	0.55
2:B:339:ASP:O	2:B:404:LYS:NZ	2.32	0.55
2:B:495:GLU:OE2	2:B:497:LYS:HE3	2.07	0.55
2:B:795:PHE:CD2	2:B:839:LEU:HB3	2.41	0.55
1:A:302:PHE:HB3	1:A:431:GLY:N	2.22	0.54
1:A:325:PHE:HZ	1:A:341:SER:HA	1.72	0.54
1:A:448:HIS:HB3	1:A:451:SER:HB3	1.89	0.54
2:B:1234:LYS:C	2:B:1235:LYS:HG2	2.32	0.54
1:A:531:ARG:HD2	1:A:535:GLU:HG2	1.89	0.54
1:A:580:SER:O	1:A:583:HIS:ND1	2.39	0.54
2:B:1196:LEU:O	2:B:1199:SER:OG	2.25	0.54
2:B:1279:VAL:HG21	2:B:1282:LEU:HD23	1.89	0.54
2:B:1536:HIS:HE1	2:B:1610:LYS:HD3	1.72	0.54
2:B:1060:GLN:HG2	2:B:1061:LEU:N	2.22	0.54
1:A:325:PHE:O	1:A:329:ARG:HG2	2.07	0.54
2:B:227:ASN:HB3	2:B:402:SER:H	1.72	0.54
2:B:976:PHE:HB2	2:B:982:ILE:HD13	1.89	0.54
2:B:1210:ILE:HA	2:B:1213:GLN:HE21	1.71	0.54
2:B:1217:LYS:HA	2:B:1220:ARG:HG3	1.90	0.54
2:E:1318:ILE:HG22	2:E:1322:LYS:HZ2	1.72	0.54
1:A:519:GLN:HA	1:A:522:ARG:HD3	1.89	0.54
1:A:224:THR:H	1:A:227:GLN:NE2	2.06	0.54
1:A:527:ASP:HB3	1:A:533:ILE:HG21	1.89	0.54
2:B:530:THR:HG22	2:B:549:VAL:HG22	1.88	0.54
2:B:533:HIS:HB2	2:B:547:PHE:CD2	2.43	0.54
2:B:932:LEU:HA	2:B:935:ARG:HB2	1.89	0.54
2:B:149:THR:HG22	2:B:171:ASN:ND2	2.23	0.54
2:B:285:SER:N	2:B:288:ASP:OD2	2.35	0.54
2:B:896:LYS:HG3	2:B:897:PRO:HD3	1.90	0.54
2:B:992:MET:O	2:B:996:LEU:HD23	2.08	0.54
2:B:1372:PHE:CZ	2:B:1424:GLN:HB3	2.43	0.54
2:B:1448:GLU:HA	2:B:1451:LEU:HD12	1.88	0.54
1:A:553:LEU:O	1:A:557:VAL:HG23	2.07	0.54
2:B:127:TRP:O	2:B:131:ILE:HG12	2.08	0.54
2:B:1002:TYR:HB2	2:B:1010:ASN:HD21	1.72	0.54
1:A:7:ILE:C	1:A:23:GLU:HB3	2.33	0.54
1:A:208:MET:HG2	1:A:215:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ARG:HA	1:A:418:ILE:HG22	1.90	0.54
2:B:450:LEU:HB3	2:B:620:PHE:HZ	1.73	0.54
2:B:564:ASP:HB3	2:B:625:LEU:HD23	1.89	0.54
2:B:589:PRO:HG3	2:B:598:LYS:HD2	1.90	0.54
2:B:686:SER:HB3	2:B:689:TYR:HB2	1.90	0.54
2:B:1063:THR:HG23	2:B:1069:ARG:HH12	1.72	0.54
2:B:1114:LEU:HD12	2:B:1164:GLY:HA2	1.89	0.54
2:B:1464:TYR:N	2:B:1487:THR:O	2.41	0.54
2:E:1221:MET:O	2:E:1225:VAL:HG23	2.08	0.54
1:A:639:GLU:N	1:A:639:GLU:OE1	2.40	0.54
2:B:143:GLU:HA	2:B:146:LYS:HE3	1.90	0.54
2:B:193:ARG:NH2	2:B:196:GLU:OE2	2.41	0.54
2:B:532:ARG:HA	2:B:546:ALA:HA	1.90	0.54
1:A:419:GLU:O	1:A:423:MET:HG2	2.07	0.53
2:B:764:PHE:CZ	2:B:827:VAL:HG22	2.43	0.53
1:A:329:ARG:HH21	1:A:336:SER:HB3	1.73	0.53
2:B:145:LYS:O	2:B:149:THR:HG23	2.09	0.53
2:B:881:LEU:O	2:B:885:GLN:NE2	2.41	0.53
2:B:1313:MET:SD	2:B:1453:TYR:OH	2.65	0.53
1:A:290:MET:HE2	1:A:293:GLN:HG3	1.90	0.53
1:A:309:MET:HE2	1:A:376:PRO:HA	1.90	0.53
2:B:853:VAL:O	2:B:856:LYS:HG2	2.09	0.53
2:B:1040:LEU:HD22	2:B:1043:TRP:CH2	2.43	0.53
2:B:1283:LEU:HG	2:B:1288:TYR:HD1	1.73	0.53
2:B:1080:ARG:HA	2:B:1083:ILE:HD12	1.89	0.53
2:B:1579:HIS:NE2	2:B:1585:LYS:HD3	2.24	0.53
1:A:325:PHE:HA	1:A:348:ARG:NH2	2.23	0.53
1:A:422:LYS:O	1:A:426:GLU:HG2	2.08	0.53
2:B:422:ASP:OD1	2:B:425:THR:OG1	2.22	0.53
2:B:1193:PHE:O	2:B:1197:VAL:HG23	2.09	0.53
2:B:1314:TRP:HZ3	2:B:1357:ARG:HD3	1.72	0.53
1:A:398:ILE:HA	1:A:401:GLU:HG2	1.90	0.53
2:B:701:ILE:HD12	2:B:704:ILE:HD12	1.90	0.53
2:B:1009:MET:O	2:B:1012:THR:OG1	2.23	0.53
1:A:329:ARG:HH12	1:A:348:ARG:CZ	2.21	0.53
2:B:900:GLU:O	2:B:903:SER:OG	2.20	0.53
2:B:1032:PHE:HA	2:B:1036:ALA:HB3	1.91	0.53
1:A:50:ALA:HB2	1:A:80:SER:HA	1.91	0.53
1:A:327:LEU:HD13	1:A:384:MET:SD	2.49	0.53
1:A:387:PHE:CE1	1:A:457:CYS:HB3	2.44	0.53
2:B:1062:GLU:O	2:B:1069:ARG:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LYS:N	1:A:573:LYS:O	2.42	0.53
2:B:83:GLY:C	2:B:86:PRO:HD2	2.34	0.53
2:B:246:TYR:HB2	2:B:253:PHE:CD1	2.44	0.53
2:B:875:ARG:HA	2:B:879:LEU:HD13	1.91	0.53
2:B:1189:SER:O	2:B:1192:VAL:HG22	2.09	0.53
2:E:1232:LYS:HE3	2:E:1240:TYR:CE1	2.44	0.53
1:A:214:ASP:OD1	1:A:214:ASP:N	2.39	0.53
1:A:383:ASN:HD22	1:A:453:GLU:HA	1.73	0.53
1:A:562:PHE:HB2	1:A:575:TRP:CE2	2.44	0.53
2:B:45:TYR:N	2:B:59:PHE:O	2.40	0.53
2:B:473:HIS:NE2	2:B:528:ARG:HB3	2.24	0.53
2:B:651:LYS:HG3	2:B:652:HIS:H	1.73	0.53
2:B:1157:GLN:O	2:B:1160:GLU:HG2	2.09	0.53
2:E:1322:LYS:HG2	2:E:1345:ARG:NH1	2.23	0.53
1:A:543:GLU:O	1:A:547:LEU:HG	2.09	0.52
1:A:702:GLU:N	1:A:702:GLU:OE1	2.41	0.52
1:A:722:PHE:HB2	1:A:725:ASP:HA	1.91	0.52
2:E:1220:ARG:O	2:E:1224:THR:HG23	2.08	0.52
2:B:1061:LEU:HA	2:B:1064:PHE:CE2	2.44	0.52
2:B:1368:TYR:O	2:B:1425:TYR:N	2.42	0.52
2:B:1584:GLU:O	2:B:1588:LEU:CB	2.55	0.52
1:A:178:VAL:O	1:A:181:ILE:HG22	2.09	0.52
1:A:420:LEU:HD11	1:A:481:MET:HE2	1.90	0.52
1:A:588:TYR:N	1:A:603:SER:OG	2.42	0.52
2:B:528:ARG:HA	2:B:551:PHE:CB	2.39	0.52
2:B:1115:THR:C	2:B:1121:ARG:HH21	2.18	0.52
2:B:1628:GLU:O	2:B:1632:LYS:HG2	2.09	0.52
2:B:567:HIS:CD2	2:B:624:THR:HG1	2.28	0.52
2:B:931:ARG:C	2:B:932:LEU:HD12	2.35	0.52
2:B:1417:ASP:OD1	2:B:1418:ILE:N	2.43	0.52
2:E:1272:GLN:OE1	2:E:1293:GLN:NE2	2.40	0.52
2:E:1318:ILE:HG22	2:E:1322:LYS:NZ	2.24	0.52
1:A:386:TYR:HE1	1:A:454:GLU:HB3	1.73	0.52
1:A:682:THR:O	1:A:686:LEU:HD23	2.09	0.52
2:B:13:GLY:HA2	2:B:67:LYS:HG2	1.92	0.52
2:B:889:GLN:OE1	2:B:895:ASN:ND2	2.22	0.52
2:B:1523:GLU:O	2:B:1527:GLU:HG2	2.10	0.52
1:A:20:LYS:HG2	1:A:41:TRP:CZ2	2.45	0.52
1:A:328:ARG:HA	1:A:331:ALA:HB3	1.91	0.52
2:B:154:HIS:HA	2:B:197:LYS:NZ	2.19	0.52
2:B:253:PHE:HE1	2:B:297:VAL:HG11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:943:MET:HA	2:B:945:ARG:NH1	2.24	0.52
2:B:1490:THR:O	2:B:1506:GLN:N	2.42	0.52
2:B:1600:LEU:HB2	2:B:1626:PHE:CE2	2.45	0.52
2:E:1249:ASP:HA	2:E:1252:ARG:NH1	2.25	0.52
1:A:354:ARG:O	1:A:357:LYS:HG2	2.10	0.52
2:B:1:MET:HE2	2:B:41:TYR:CE2	2.45	0.52
2:B:108:ASN:O	2:B:110:LYS:N	2.39	0.52
1:A:143:LEU:HD12	1:A:147:MET:HG2	1.92	0.52
2:B:143:GLU:O	2:B:147:LYS:HG2	2.09	0.52
1:A:199:GLN:OE1	1:A:200:ARG:NH1	2.43	0.52
1:A:687:ASP:OD1	1:A:688:THR:N	2.42	0.52
2:B:175:PRO:C	2:B:177:GLU:H	2.16	0.52
2:B:711:HIS:O	2:B:714:PRO:HD2	2.10	0.52
2:B:809:ALA:O	2:B:813:LYS:HG3	2.10	0.52
1:A:7:ILE:HA	1:A:24:ILE:C	2.35	0.52
1:A:118:GLN:HA	1:A:121:ILE:HD12	1.92	0.52
2:B:903:SER:HB3	2:B:953:PHE:CE2	2.45	0.52
2:B:915:ARG:NE	2:B:917:ASP:OD1	2.38	0.52
2:B:1468:PHE:HB3	2:B:1483:TRP:HB2	1.91	0.52
2:B:1517:ASN:O	2:B:1521:THR:HG23	2.10	0.52
2:E:1231:TYR:O	2:E:1234:LYS:N	2.42	0.52
2:B:6:PRO:HG3	2:B:39:GLU:HG2	1.91	0.51
2:B:923:VAL:O	2:B:926:GLN:HB3	2.11	0.51
1:A:637:VAL:O	1:A:641:ALA:N	2.41	0.51
1:A:706:ILE:HD11	2:B:65:HIS:CE1	2.45	0.51
2:B:225:TYR:HA	2:B:279:ALA:O	2.09	0.51
2:B:288:ASP:OD1	2:B:291:ARG:NH2	2.43	0.51
2:B:1183:HIS:CG	2:B:1184:LYS:N	2.78	0.51
1:A:48:TYR:HB3	1:A:83:GLN:HG3	1.91	0.51
1:A:91:ARG:HD3	1:A:102:GLU:OE2	2.09	0.51
1:A:353:THR:HA	1:A:364:HIS:CG	2.45	0.51
2:E:1335:TYR:HA	2:E:1338:LEU:HD23	1.93	0.51
2:B:1099:ILE:HA	2:B:1102:ILE:CD1	2.41	0.51
2:B:1348:PHE:O	2:B:1352:ILE:HG13	2.10	0.51
1:A:198:LEU:HD22	1:A:239:ILE:HD11	1.91	0.51
1:A:669:LEU:HA	1:A:672:LEU:HD12	1.91	0.51
1:A:14:TRP:CD1	1:A:15:PRO:HD2	2.46	0.51
1:A:325:PHE:HA	1:A:348:ARG:HH21	1.76	0.51
1:A:336:SER:HB3	1:A:340:ASN:HD21	1.75	0.51
1:A:634:ASN:ND2	1:A:636:GLU:OE2	2.44	0.51
2:B:697:LEU:HA	2:B:700:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1291:TYR:CD2	2:B:1296:LEU:HD21	2.46	0.51
2:B:1342:LEU:HD11	2:E:1346:ALA:HB2	1.92	0.51
1:A:308:ARG:HH21	1:A:379:LEU:HD11	1.76	0.51
2:B:1135:GLU:OE1	2:B:1144:PHE:HB2	2.11	0.51
2:E:1272:GLN:H	2:E:1293:GLN:NE2	2.09	0.51
2:E:1277:PRO:HG3	2:E:1292:THR:HA	1.92	0.51
2:B:52:ASN:OD1	2:B:54:SER:OG	2.22	0.51
2:B:315:THR:HB	2:B:318:LEU:HD12	1.92	0.51
2:B:575:ASP:OD2	2:B:577:LYS:N	2.44	0.51
1:A:206:GLU:O	1:A:210:LEU:HG	2.10	0.51
1:A:443:PRO:HA	1:A:446:PHE:CD2	2.46	0.51
1:A:578:ARG:HH12	1:A:581:PRO:HD3	1.76	0.51
2:B:319:ARG:HB3	2:B:499:VAL:HG13	1.93	0.51
2:B:688:THR:HA	2:B:691:PHE:CD2	2.46	0.51
2:B:827:VAL:HG11	2:B:836:LEU:HD13	1.93	0.51
2:B:1148:GLU:OE2	2:B:1149:ASN:ND2	2.44	0.51
2:B:1447:PRO:HB2	2:B:1449:GLN:NE2	2.25	0.51
2:B:806:LEU:HG	2:B:810:VAL:HA	1.93	0.50
2:B:1043:TRP:HB3	2:B:1047:PHE:CE2	2.46	0.50
2:E:1266:LEU:HA	2:E:1269:GLU:HB3	1.93	0.50
1:A:511:TYR:CD1	1:A:514:ILE:HD12	2.43	0.50
2:B:111:LEU:O	2:B:115:ARG:NE	2.43	0.50
2:B:197:LYS:HA	2:B:200:GLU:HG2	1.92	0.50
2:B:471:SER:OG	2:B:473:HIS:NE2	2.44	0.50
2:B:592:LYS:O	2:B:595:MET:N	2.45	0.50
2:B:1299:LYS:HA	2:B:1302:GLN:OE1	2.11	0.50
2:E:1336:GLU:H	2:E:1336:GLU:CD	2.18	0.50
1:A:8:VAL:H	1:A:24:ILE:H	1.60	0.50
1:A:101:LEU:O	1:A:105:LYS:HG3	2.11	0.50
1:A:588:TYR:CZ	1:A:605:GLN:HG2	2.46	0.50
2:B:88:VAL:O	2:B:92:THR:HG23	2.11	0.50
2:E:1335:TYR:HA	2:E:1338:LEU:HB2	1.94	0.50
1:A:373:GLN:HE21	1:A:418:ILE:HG12	1.75	0.50
1:A:376:PRO:HD3	1:A:422:LYS:HB3	1.93	0.50
1:A:423:MET:HE1	1:A:481:MET:HG3	1.92	0.50
1:A:563:ARG:HH21	1:A:573:LYS:HE2	1.76	0.50
1:A:589:GLY:HA3	1:A:604:LEU:HD13	1.93	0.50
1:A:673:LEU:HB2	1:A:675:LYS:NZ	2.26	0.50
1:A:700:ASP:HB3	2:B:14:VAL:HG11	1.92	0.50
2:B:224:LEU:HD21	2:B:284:LEU:HD12	1.93	0.50
2:B:572:TYR:HB2	2:B:579:MET:HE1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:987:MET:HE1	2:B:1041:GLN:HE22	1.75	0.50
2:B:1462:PHE:O	2:B:1488:THR:HA	2.12	0.50
1:A:332:PHE:CZ	1:A:355:ASP:HB3	2.46	0.50
1:A:605:GLN:OE1	1:A:605:GLN:N	2.44	0.50
2:B:268:PRO:HG2	2:B:274:LEU:HB2	1.93	0.50
2:B:781:SER:OG	2:B:784:GLY:N	2.44	0.50
2:B:823:ILE:O	2:B:827:VAL:HG23	2.11	0.50
2:B:1102:ILE:H	2:B:1102:ILE:HD12	1.75	0.50
2:B:1136:PHE:HA	2:B:1139:SER:CB	2.42	0.50
1:A:305:LEU:O	1:A:308:ARG:HG3	2.12	0.50
1:A:542:PRO:O	1:A:546:GLU:HB3	2.10	0.50
2:B:222:TYR:HB3	2:B:405:LEU:HD12	1.93	0.50
2:B:802:MET:HE1	2:B:846:SER:C	2.37	0.50
2:B:1612:THR:HG22	2:B:1615:LEU:HB2	1.93	0.50
1:A:312:LYS:NZ	1:A:372:THR:O	2.45	0.50
1:A:445:PHE:HD1	1:A:451:SER:HB2	1.76	0.50
2:B:68:GLU:HB3	2:B:76:GLN:HG2	1.93	0.50
2:B:451:ILE:O	2:B:509:TRP:N	2.23	0.50
2:B:659:GLU:N	2:B:659:GLU:OE1	2.45	0.50
2:B:871:GLN:HG2	2:B:875:ARG:NH1	2.26	0.50
1:A:178:VAL:O	1:A:182:LYS:HG2	2.12	0.50
2:B:176:ASP:HB3	2:B:178:THR:HG23	1.94	0.50
2:B:594:GLU:O	2:B:597:GLU:HG3	2.12	0.50
2:B:706:ASP:OD1	2:B:707:ILE:N	2.45	0.50
2:B:798:PHE:HA	2:B:801:LEU:HD12	1.94	0.50
2:B:881:LEU:HD23	2:B:885:GLN:OE1	2.12	0.50
2:B:1166:GLU:O	2:B:1169:LYS:HG2	2.12	0.50
2:B:1242:ARG:O	2:B:1246:LYS:HG2	2.11	0.50
1:A:208:MET:SD	1:A:215:LEU:HB3	2.52	0.50
2:B:224:LEU:HG	2:B:281:PHE:HB2	1.93	0.50
2:B:467:GLU:OE1	2:B:534:ARG:NH1	2.45	0.50
2:B:538:GLU:OE1	2:B:542:LYS:NZ	2.27	0.50
2:B:787:PHE:CE2	2:B:791:ILE:HD11	2.47	0.50
2:B:1275:ASP:HA	2:B:1294:GLN:NE2	2.27	0.50
2:B:1432:LYS:O	2:B:1463:ARG:N	2.40	0.50
2:E:1238:ASP:O	2:E:1242:ARG:HG2	2.12	0.50
2:B:375:GLU:HB2	2:B:502:TYR:H	1.76	0.49
2:B:1040:LEU:HD22	2:B:1043:TRP:HH2	1.77	0.49
2:B:1340:ASN:HB3	2:B:1344:LYS:HZ1	1.76	0.49
2:B:1482:MET:N	2:B:1514:PRO:HG3	2.26	0.49
2:B:1618:LEU:HD23	2:B:1621:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:PHE:CZ	2:B:56:LYS:HE3	2.46	0.49
2:B:70:THR:HG22	2:B:71:VAL:H	1.76	0.49
2:B:612:SER:OG	2:B:614:ASP:OD1	2.27	0.49
2:B:632:THR:HG21	2:B:638:LEU:HD21	1.93	0.49
2:B:701:ILE:HD11	2:B:762:TYR:CD2	2.38	0.49
2:B:1063:THR:HA	2:B:1069:ARG:NH1	2.27	0.49
2:B:1276:LYS:HD3	2:B:1277:PRO:HD2	1.94	0.49
1:A:12:ILE:O	1:A:20:LYS:N	2.44	0.49
1:A:526:GLU:O	1:A:529:GLN:HG2	2.11	0.49
1:A:586:LEU:HD23	1:A:608:LEU:HB3	1.95	0.49
2:B:116:GLN:HA	2:B:119:GLN:CD	2.36	0.49
2:B:333:ILE:HG22	2:B:405:LEU:HD21	1.94	0.49
2:B:648:GLN:O	2:B:651:LYS:NZ	2.40	0.49
2:B:891:ASP:OD1	2:B:938:ARG:NH2	2.45	0.49
2:B:1102:ILE:HG21	2:B:1147:PHE:HB2	1.94	0.49
2:B:1323:GLU:HA	2:B:1326:GLU:HG3	1.93	0.49
2:E:1232:LYS:HE2	2:E:1232:LYS:HA	1.94	0.49
2:E:1295:GLU:O	2:E:1298:GLU:HG3	2.12	0.49
1:A:312:LYS:NZ	1:A:374:THR:H	2.10	0.49
1:A:551:GLN:NE2	1:A:555:ARG:HH11	2.11	0.49
2:B:7:THR:HG22	2:B:9:ARG:H	1.77	0.49
2:B:238:ASP:HB2	2:B:303:VAL:HB	1.94	0.49
2:B:348:PHE:HB2	2:B:398:GLY:HA2	1.94	0.49
2:B:582:ALA:HA	2:B:585:TYR:CE1	2.47	0.49
2:B:1283:LEU:HG	2:B:1288:TYR:CD1	2.48	0.49
2:B:1607:HIS:CE1	2:B:1615:LEU:HD13	2.48	0.49
1:A:152:GLY:O	1:A:197:ILE:HD11	2.13	0.49
1:A:480:VAL:O	1:A:484:VAL:HG23	2.12	0.49
1:A:528:PHE:HZ	1:A:690:LEU:HD22	1.77	0.49
2:B:831:PHE:CE2	2:B:835:GLU:HB3	2.48	0.49
2:B:934:ARG:HH11	2:B:938:ARG:HB2	1.77	0.49
2:B:1241:ILE:HD11	2:B:1282:LEU:HD13	1.94	0.49
2:B:1251:HIS:O	2:B:1255:GLU:N	2.46	0.49
2:B:1412:THR:OG1	2:B:1413:PRO:HD3	2.12	0.49
1:A:113:ASP:OD1	1:A:114:VAL:N	2.45	0.49
1:A:271:LEU:O	1:A:275:ILE:HG12	2.13	0.49
1:A:394:ALA:O	1:A:398:ILE:HG12	2.13	0.49
1:A:399:VAL:HA	1:A:402:ASN:HD21	1.78	0.49
1:A:616:VAL:HG22	1:A:644:ILE:HD13	1.94	0.49
2:B:196:GLU:HA	2:B:199:GLN:HG2	1.94	0.49
2:B:211:ARG:NH2	2:B:336:LYS:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:PRO:HG2	2:B:437:ILE:HG12	1.94	0.49
2:B:528:ARG:HA	2:B:551:PHE:HB3	1.93	0.49
2:B:746:ASP:O	2:B:750:THR:HG23	2.13	0.49
2:B:154:HIS:O	2:B:158:MET:HE3	2.12	0.49
2:B:641:LEU:O	2:B:644:ARG:NH1	2.40	0.49
2:B:1551:LEU:HA	2:B:1554:ILE:HD12	1.95	0.49
1:A:186:SER:OG	1:A:190:LYS:NZ	2.44	0.49
1:A:575:TRP:CD1	1:A:575:TRP:H	2.31	0.49
2:B:47:GLY:H	2:B:56:LYS:NZ	2.11	0.49
2:B:69:ALA:N	2:B:78:GLU:OE2	2.45	0.49
2:B:794:LEU:HG	2:B:798:PHE:HE2	1.76	0.49
2:B:1079:MET:O	2:B:1083:ILE:HG13	2.12	0.49
2:B:1468:PHE:CZ	2:B:1470:LYS:HB3	2.47	0.49
2:E:1248:ARG:HH11	2:E:1252:ARG:NH1	2.09	0.49
1:A:86:GLN:HA	1:A:89:HIS:HD2	1.77	0.49
1:A:398:ILE:O	1:A:402:ASN:ND2	2.45	0.49
1:A:467:TRP:NE1	1:A:472:ALA:O	2.45	0.49
2:B:35:VAL:HG23	2:B:37:ILE:HG13	1.94	0.49
2:B:73:ASP:HB3	2:B:82:PRO:HB3	1.95	0.49
2:B:1627:ARG:O	2:B:1630:LYS:HB3	2.13	0.49
2:E:1245:TYR:OH	2:E:1267:HIS:NE2	2.43	0.49
1:A:163:VAL:HG12	1:A:204:ILE:HD11	1.95	0.49
2:B:57:GLY:HA3	2:B:59:PHE:CZ	2.47	0.49
2:B:431:MET:HE1	2:B:625:LEU:O	2.12	0.49
2:B:740:TYR:HA	2:B:749:LYS:HE2	1.95	0.49
2:B:993:PHE:O	2:B:997:ILE:HD12	2.13	0.49
2:B:1105:MET:C	2:B:1108:PRO:HD2	2.38	0.49
2:B:1121:ARG:O	2:B:1125:ILE:HG12	2.12	0.49
2:B:1384:ARG:NH2	2:B:1495:PHE:HB3	2.28	0.49
2:E:1304:ILE:HA	2:E:1307:TYR:CD2	2.48	0.49
1:A:676:ASP:OD2	1:A:677:MET:N	2.45	0.48
2:B:125:ILE:HG13	2:B:126:GLU:N	2.27	0.48
2:B:241:LEU:HD23	2:B:260:ILE:HD12	1.94	0.48
2:B:1056:HIS:HD1	2:B:1057:GLU:CD	2.18	0.48
2:B:1155:LEU:O	2:B:1159:VAL:HG23	2.12	0.48
2:B:1166:GLU:O	2:B:1170:VAL:HG23	2.13	0.48
2:B:1169:LYS:O	2:B:1172:LEU:HB3	2.12	0.48
2:B:1415:GLY:O	2:B:1419:LYS:HG3	2.13	0.48
2:B:1585:LYS:HG3	2:B:1586:VAL:H	1.77	0.48
1:A:198:LEU:O	1:A:202:LEU:HD23	2.13	0.48
1:A:229:ILE:HG21	1:A:274:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:PHE:CZ	2:B:58:ILE:HD11	2.48	0.48
2:B:121:THR:O	2:B:125:ILE:HG23	2.12	0.48
2:B:209:ASP:CG	2:B:213:GLN:HE21	2.20	0.48
2:B:718:THR:O	2:B:722:LYS:HB2	2.13	0.48
2:B:1071:LYS:HA	2:B:1074:LYS:HZ2	1.77	0.48
2:B:1546:PRO:O	2:B:1550:LEU:HG	2.12	0.48
2:B:1602:GLU:OE1	2:B:1605:ARG:NH2	2.45	0.48
2:B:1604:ILE:HG23	2:B:1619:HIS:NE2	2.27	0.48
2:E:1321:SER:OG	2:E:1345:ARG:NE	2.44	0.48
1:A:159:LEU:HB3	1:A:200:ARG:HB3	1.95	0.48
2:B:549:VAL:HB	2:B:579:MET:HB3	1.95	0.48
2:B:1071:LYS:HA	2:B:1075:LYS:HZ3	1.78	0.48
2:B:1449:GLN:HA	2:B:1452:ASN:ND2	2.29	0.48
1:A:216:TYR:OH	1:A:250:LEU:O	2.23	0.48
1:A:245:ALA:H	1:A:293:GLN:HE22	1.57	0.48
1:A:531:ARG:O	1:A:535:GLU:N	2.39	0.48
2:B:143:GLU:HG3	2:B:147:LYS:NZ	2.29	0.48
2:B:533:HIS:C	2:B:534:ARG:HD2	2.38	0.48
2:B:964:MET:HE2	2:B:969:TYR:CE1	2.48	0.48
2:B:1176:LEU:HD12	2:B:1177:LEU:N	2.29	0.48
2:B:1392:GLU:OE1	2:B:1392:GLU:N	2.30	0.48
2:B:1410:SER:O	2:B:1413:PRO:HD2	2.13	0.48
1:A:201:SER:O	1:A:205:LEU:HG	2.13	0.48
1:A:325:PHE:CZ	1:A:341:SER:HA	2.48	0.48
1:A:468:LYS:NZ	1:A:471:ARG:HH21	2.11	0.48
1:A:503:LYS:HA	1:A:506:LEU:HD12	1.95	0.48
1:A:534:LEU:HD12	1:A:537:LYS:HE3	1.94	0.48
1:A:619:GLY:H	1:A:642:PHE:HB2	1.77	0.48
2:B:1191:GLU:O	2:B:1195:LEU:HG	2.12	0.48
2:B:1583:GLN:HE22	2:B:1586:VAL:HG12	1.78	0.48
1:A:376:PRO:HG2	1:A:421:THR:HB	1.95	0.48
2:B:561:THR:HG21	2:B:631:LEU:HB2	1.95	0.48
2:B:837:SER:HB2	2:B:878:LEU:HD11	1.95	0.48
1:A:156:SER:O	1:A:160:THR:HG23	2.14	0.48
1:A:414:GLY:O	1:A:417:SER:OG	2.29	0.48
1:A:580:SER:HB2	1:A:587:HIS:NE2	2.29	0.48
1:A:657:PRO:HD2	1:A:661:GLU:OE2	2.14	0.48
1:A:719:ASN:O	2:B:1:MET:HA	2.14	0.48
2:B:116:GLN:HA	2:B:119:GLN:OE1	2.14	0.48
2:B:339:ASP:OD1	2:B:404:LYS:NZ	2.46	0.48
2:B:640:LEU:HD11	2:B:657:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:896:LYS:CG	2:B:897:PRO:HD3	2.44	0.48
2:B:1136:PHE:C	2:B:1139:SER:H	2.22	0.48
1:A:185:ALA:HB2	1:A:222:GLU:OE1	2.14	0.48
1:A:481:MET:HE3	1:A:485:LYS:HG2	1.95	0.48
1:A:562:PHE:HB2	1:A:575:TRP:NE1	2.29	0.48
2:B:4:TRP:CH2	2:B:46:ARG:HG3	2.49	0.48
2:B:20:ASN:OD1	2:B:21:ALA:N	2.47	0.48
2:B:231:PHE:HD1	2:B:399:LEU:HB3	1.77	0.48
2:B:1028:LEU:HA	2:B:1032:PHE:HD2	1.77	0.48
2:B:1288:TYR:HA	2:B:1291:TYR:CE2	2.49	0.48
2:B:1344:LYS:O	2:B:1347:SER:OG	2.26	0.48
2:B:1522:MET:SD	2:B:1566:TYR:OH	2.71	0.48
2:B:1566:TYR:HA	2:B:1570:PHE:CD2	2.49	0.48
2:B:154:HIS:CD2	2:B:197:LYS:HD2	2.49	0.48
2:B:228:PHE:HA	2:B:400:TRP:O	2.13	0.48
2:B:730:TYR:HB3	2:B:770:SER:HB3	1.96	0.48
2:B:777:PHE:HB3	2:B:778:TYR:HD2	1.77	0.48
2:B:1340:ASN:HA	2:B:1343:LYS:HZ3	1.79	0.48
1:A:113:ASP:OD2	1:A:115:THR:OG1	2.25	0.48
1:A:297:LEU:HA	1:A:300:LEU:HG	1.96	0.48
1:A:311:THR:O	1:A:378:MET:HE1	2.13	0.48
1:A:350:SER:O	1:A:354:ARG:HG2	2.14	0.48
1:A:484:VAL:O	1:A:488:VAL:HG23	2.14	0.48
2:B:112:THR:OG1	2:B:113:LEU:N	2.47	0.48
2:B:591:THR:N	2:B:594:GLU:OE2	2.28	0.48
2:B:630:LYS:HA	2:B:668:PHE:HZ	1.79	0.48
2:B:751:GLU:N	2:B:751:GLU:OE1	2.44	0.48
2:B:1101:PHE:O	2:B:1105:MET:HG3	2.13	0.48
2:B:1307:TYR:HA	2:B:1310:LYS:HG2	1.95	0.48
2:B:1425:TYR:O	2:B:1426:MET:HE2	2.14	0.48
1:A:302:PHE:O	1:A:306:GLU:HG2	2.13	0.47
1:A:531:ARG:O	1:A:535:GLU:HG3	2.14	0.47
2:B:746:ASP:OD2	2:B:748:SER:OG	2.25	0.47
2:B:1101:PHE:HB3	2:B:1105:MET:HG2	1.95	0.47
2:E:1304:ILE:HA	2:E:1307:TYR:HD2	1.78	0.47
1:A:256:ASP:O	1:A:259:ARG:HB2	2.15	0.47
1:A:375:PRO:HA	1:A:376:PRO:HA	1.46	0.47
1:A:443:PRO:HD2	1:A:495:LYS:HZ1	1.78	0.47
1:A:483:VAL:HG12	1:A:487:GLN:HE22	1.79	0.47
2:B:45:TYR:O	2:B:59:PHE:N	2.47	0.47
2:B:80:VAL:HG23	2:B:81:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:831:PHE:HE2	2:B:835:GLU:HB3	1.79	0.47
2:B:1130:ASP:O	2:B:1133:GLN:NE2	2.47	0.47
1:A:248:ASN:HD22	1:A:300:LEU:HD11	1.79	0.47
1:A:349:LYS:HA	1:A:352:TYR:CD2	2.50	0.47
1:A:562:PHE:O	1:A:574:PHE:HA	2.15	0.47
1:A:568:ARG:HE	1:A:569:ARG:NH2	2.06	0.47
1:A:667:ASP:HA	1:A:670:ASN:HB3	1.97	0.47
2:B:18:ASN:HA	2:B:29:LEU:O	2.14	0.47
2:B:246:TYR:OH	2:B:251:SER:HA	2.14	0.47
2:B:295:SER:HA	2:B:328:ASP:HA	1.96	0.47
2:B:592:LYS:O	2:B:595:MET:HG2	2.13	0.47
2:B:1078:ASP:OD1	2:B:1080:ARG:HG3	2.14	0.47
2:B:1260:ALA:O	2:B:1263:THR:OG1	2.32	0.47
2:B:1353:ILE:HG13	2:E:1335:TYR:HB2	1.96	0.47
2:B:1387:GLU:H	2:B:1387:GLU:CD	2.21	0.47
2:B:1575:TYR:HA	2:B:1578:GLU:CD	2.39	0.47
1:A:22:MET:HE3	1:A:22:MET:HB3	1.72	0.47
1:A:392:GLN:O	1:A:396:ILE:HG12	2.13	0.47
2:B:225:TYR:O	2:B:403:LEU:HA	2.14	0.47
2:B:327:MET:HE1	2:B:344:HIS:HB3	1.95	0.47
2:B:535:SER:HB2	2:B:540:ARG:HH11	1.79	0.47
2:B:1326:GLU:HA	2:B:1329:GLU:HG3	1.96	0.47
2:E:1296:LEU:O	2:E:1300:LEU:HG	2.14	0.47
2:E:1347:SER:HA	2:E:1350:GLU:OE2	2.14	0.47
2:E:1228:LEU:HA	2:E:1231:TYR:HD2	1.77	0.47
1:A:193:ILE:HD11	1:A:198:LEU:HB2	1.96	0.47
1:A:261:GLU:O	1:A:265:ILE:HG12	2.14	0.47
2:B:99:ALA:HA	2:B:102:TRP:NE1	2.30	0.47
2:B:302:ARG:HH12	2:B:308:LEU:H	1.63	0.47
2:B:1184:LYS:O	2:B:1187:SER:N	2.33	0.47
2:B:1325:ALA:HB2	2:B:1341:LEU:HD11	1.95	0.47
2:B:1583:GLN:NE2	2:B:1586:VAL:HG12	2.30	0.47
1:A:6:ASP:O	1:A:26:GLN:HG2	2.15	0.47
1:A:187:PHE:HB3	1:A:193:ILE:HD13	1.97	0.47
1:A:218:LYS:HA	1:A:221:GLN:OE1	2.14	0.47
1:A:417:SER:HA	1:A:456:PHE:HZ	1.78	0.47
1:A:542:PRO:O	1:A:546:GLU:CB	2.62	0.47
2:B:410:LEU:O	2:B:414:GLN:HB2	2.14	0.47
2:B:528:ARG:HD3	2:B:585:TYR:OH	2.15	0.47
2:B:761:LYS:HD3	2:B:822:SER:O	2.15	0.47
2:B:842:LYS:HA	2:B:845:GLN:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:853:VAL:HG23	2:B:854:ARG:N	2.30	0.47
2:B:921:THR:HA	2:B:924:HIS:ND1	2.30	0.47
2:B:979:ARG:O	2:B:982:ILE:HG22	2.15	0.47
2:B:1024:PHE:O	2:B:1028:LEU:HD23	2.15	0.47
2:B:1136:PHE:CG	2:B:1186:LEU:HD22	2.50	0.47
2:B:1273:TRP:CE3	2:B:1294:GLN:HG3	2.50	0.47
2:E:1312:LYS:HG3	2:E:1312:LYS:O	2.14	0.47
1:A:160:THR:HG22	1:A:200:ARG:HE	1.79	0.47
2:B:10:GLN:O	2:B:37:ILE:HB	2.14	0.47
2:B:92:THR:O	2:B:96:ARG:HG3	2.15	0.47
2:B:719:TYR:O	2:B:723:HIS:N	2.44	0.47
2:B:802:MET:HE1	2:B:846:SER:O	2.15	0.47
2:B:1003:ALA:C	2:B:1005:ASP:H	2.21	0.47
2:B:1057:GLU:O	2:B:1080:ARG:NH1	2.47	0.47
2:E:1350:GLU:HA	2:E:1353:ILE:HG12	1.97	0.47
1:A:643:SER:OG	1:A:653:ASN:HA	2.15	0.47
2:B:11:LYS:HG3	2:B:38:LEU:HD23	1.96	0.47
2:B:293:ARG:NH2	2:B:328:ASP:OD2	2.48	0.47
2:B:572:TYR:HB3	2:B:614:ASP:O	2.15	0.47
2:B:1212:MET:SD	2:B:1212:MET:N	2.82	0.47
2:B:1399:LEU:HD12	2:B:1405:ALA:HB1	1.97	0.47
2:B:1494:THR:HG22	2:B:1495:PHE:O	2.15	0.47
2:E:1268:ALA:O	2:E:1271:LEU:HB2	2.15	0.47
1:A:20:LYS:HD3	1:A:22:MET:SD	2.55	0.47
2:B:376:ASN:HA	2:B:504:VAL:HG22	1.95	0.47
2:B:746:ASP:CG	2:B:748:SER:HG	2.23	0.47
2:B:1145:HIS:HA	2:B:1148:GLU:CG	2.36	0.47
2:B:1237:GLU:O	2:B:1240:TYR:HB3	2.14	0.47
2:B:1316:LYS:NZ	2:B:1319:LYS:HD2	2.30	0.47
2:B:1340:ASN:HA	2:B:1343:LYS:HZ2	1.78	0.47
1:A:126:ILE:HD12	1:A:126:ILE:H	1.81	0.46
1:A:495:LYS:HA	1:A:495:LYS:HD2	1.64	0.46
2:B:3:ARG:HB3	2:B:41:TYR:CD1	2.50	0.46
2:B:832:ASP:OD2	2:B:835:GLU:N	2.46	0.46
2:B:1234:LYS:HD2	2:B:1234:LYS:HA	1.68	0.46
2:B:1265:LEU:O	2:B:1268:ALA:N	2.48	0.46
2:B:1565:ASN:OD1	2:B:1565:ASN:N	2.46	0.46
2:B:1606:ILE:O	2:B:1610:LYS:HG3	2.15	0.46
1:A:332:PHE:HA	1:A:399:VAL:HG11	1.96	0.46
2:B:14:VAL:HA	2:B:33:ASP:O	2.16	0.46
2:B:27:LEU:O	2:B:29:LEU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:861:THR:HA	2:B:864:VAL:HG12	1.97	0.46
2:B:1101:PHE:O	2:B:1104:SER:OG	2.25	0.46
2:B:1166:GLU:OE1	2:B:1166:GLU:N	2.33	0.46
2:B:1597:MET:HE2	2:B:1626:PHE:CE1	2.49	0.46
2:E:1275:ASP:OD1	2:E:1275:ASP:N	2.48	0.46
2:B:286:SER:O	2:B:290:ILE:HG23	2.16	0.46
2:B:825:ASN:OD1	2:B:826:ASP:N	2.48	0.46
2:B:834:VAL:O	2:B:837:SER:OG	2.25	0.46
2:E:1295:GLU:HA	2:E:1298:GLU:HG3	1.97	0.46
1:A:151:PHE:HD1	1:A:154:MET:HE3	1.80	0.46
1:A:160:THR:HG22	1:A:200:ARG:NE	2.30	0.46
2:B:192:LYS:HA	2:B:195:GLU:CD	2.40	0.46
2:B:504:VAL:O	2:B:507:PRO:HD3	2.15	0.46
2:B:1547:LEU:O	2:B:1551:LEU:HG	2.16	0.46
1:A:54:ALA:HB3	1:A:74:ILE:O	2.15	0.46
1:A:144:GLN:O	1:A:148:LYS:HG2	2.15	0.46
2:B:156:ASN:HA	2:B:161:LEU:HB2	1.98	0.46
2:B:324:VAL:N	2:B:349:GLN:O	2.48	0.46
2:B:522:VAL:HG23	2:B:554:LEU:HD13	1.98	0.46
2:B:742:ALA:O	2:B:804:ARG:NH2	2.49	0.46
2:B:801:LEU:HA	2:B:804:ARG:HE	1.80	0.46
1:A:455:PHE:HZ	1:A:492:LEU:HD21	1.80	0.46
2:B:789:ASN:O	2:B:792:ARG:N	2.48	0.46
2:B:868:LEU:HD12	2:B:868:LEU:HA	1.61	0.46
2:B:1095:GLY:HA3	2:B:1096:PRO:HD3	1.81	0.46
2:B:1452:ASN:OD1	2:B:1453:TYR:N	2.48	0.46
2:B:1468:PHE:N	2:B:1483:TRP:O	2.41	0.46
2:B:1471:GLY:O	2:B:1473:LYS:HG2	2.16	0.46
2:B:1607:HIS:CE1	2:B:1615:LEU:HB3	2.49	0.46
2:E:1354:LYS:HA	2:E:1354:LYS:HD2	1.75	0.46
1:A:7:ILE:HA	1:A:24:ILE:O	2.15	0.46
1:A:457:CYS:O	1:A:460:ILE:HG22	2.15	0.46
2:B:567:HIS:NE2	2:B:624:THR:OG1	2.43	0.46
2:B:875:ARG:HG3	2:B:879:LEU:HD13	1.98	0.46
1:A:524:ASN:OD1	1:A:525:GLN:N	2.48	0.46
2:B:242:PHE:HB2	2:B:299:GLN:O	2.15	0.46
2:B:247:ASP:OD2	2:B:291:ARG:HB3	2.16	0.46
2:B:528:ARG:NH1	2:B:580:GLU:OE2	2.49	0.46
2:B:798:PHE:O	2:B:801:LEU:HB2	2.15	0.46
2:B:1220:ARG:O	2:B:1224:THR:HG22	2.15	0.46
2:B:1466:ARG:O	2:B:1485:GLU:N	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HH22	1:A:355:ASP:HB2	1.81	0.46
1:A:632:LYS:HG3	1:A:633:GLN:OE1	2.16	0.46
1:A:719:ASN:O	2:B:2:ALA:N	2.48	0.46
2:B:181:ILE:HD12	2:B:181:ILE:H	1.81	0.46
2:B:191:SER:O	2:B:194:ILE:HB	2.15	0.46
2:B:214:SER:O	2:B:218:THR:HG23	2.15	0.46
2:B:414:GLN:HA	2:B:423:ARG:HH21	1.81	0.46
2:B:1006:TRP:N	2:B:1006:TRP:CD1	2.82	0.46
2:B:1070:ASN:O	2:B:1074:LYS:HG2	2.15	0.46
1:A:668:GLY:O	1:A:672:LEU:HG	2.16	0.46
2:B:241:LEU:HB3	2:B:260:ILE:HB	1.98	0.46
2:B:471:SER:HB2	2:B:479:LEU:HD11	1.98	0.46
2:B:834:VAL:HG22	2:B:873:GLU:HB2	1.98	0.46
2:B:1215:GLU:C	2:B:1220:ARG:HH11	2.24	0.46
1:A:435:SER:OG	1:A:438:CYS:SG	2.58	0.45
1:A:563:ARG:HB2	1:A:655:ILE:CG2	2.45	0.45
2:B:870:ARG:HA	2:B:870:ARG:HH11	1.81	0.45
2:B:1392:GLU:H	2:B:1392:GLU:CD	2.20	0.45
2:B:1563:PHE:O	2:B:1566:TYR:HB2	2.15	0.45
1:A:324:ILE:O	1:A:328:ARG:HG2	2.14	0.45
1:A:340:ASN:HA	1:A:343:GLY:HA3	1.98	0.45
1:A:719:ASN:HB2	2:B:2:ALA:HB3	1.98	0.45
2:B:738:ASN:HA	2:B:741:VAL:HG12	1.99	0.45
2:B:972:TYR:C	2:B:975:THR:H	2.23	0.45
2:B:1391:ARG:NH2	2:B:1392:GLU:HA	2.31	0.45
2:B:1564:SER:HA	2:B:1567:GLU:OE2	2.16	0.45
2:B:1618:LEU:HA	2:B:1621:ARG:HH11	1.82	0.45
2:E:1328:TYR:HD2	2:E:1338:LEU:HD13	1.81	0.45
1:A:578:ARG:HH12	1:A:580:SER:HA	1.81	0.45
2:B:99:ALA:HA	2:B:102:TRP:CD1	2.51	0.45
2:B:115:ARG:HA	2:B:118:GLN:HE21	1.82	0.45
2:B:166:ARG:NH1	2:B:167:ASP:OD1	2.49	0.45
2:B:713:ASN:O	2:B:717:GLU:HG2	2.15	0.45
2:B:1274:SER:O	2:B:1294:GLN:NE2	2.48	0.45
2:B:1598:PRO:O	2:B:1601:THR:OG1	2.23	0.45
1:A:259:ARG:HA	1:A:262:MET:HE2	1.98	0.45
1:A:561:CYS:SG	1:A:576:TYR:HB3	2.56	0.45
1:A:575:TRP:HB3	1:A:590:ASP:HB2	1.99	0.45
1:A:615:ALA:O	1:A:644:ILE:HD12	2.16	0.45
1:A:723:VAL:H	2:B:4:TRP:HD1	1.64	0.45
2:B:19:TYR:HB3	2:B:27:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:TYR:HA	2:B:253:PHE:HA	1.99	0.45
2:B:439:PRO:HD3	2:B:711:HIS:HB3	1.97	0.45
2:B:945:ARG:NH1	2:B:948:PRO:HG3	2.31	0.45
2:B:950:ILE:O	2:B:954:VAL:HG23	2.16	0.45
1:A:483:VAL:O	1:A:487:GLN:NE2	2.49	0.45
2:B:106:TYR:CD2	2:B:107:VAL:N	2.84	0.45
2:B:144:LEU:O	2:B:148:VAL:HG23	2.16	0.45
2:B:694:PHE:O	2:B:697:LEU:HG	2.15	0.45
2:B:948:PRO:O	2:B:950:ILE:HD12	2.16	0.45
2:B:1499:LEU:HD11	2:B:1501:TRP:CH2	2.52	0.45
1:A:2:PRO:O	1:A:4:PRO:HD3	2.17	0.45
2:B:166:ARG:HH12	2:B:168:ASP:HB2	1.81	0.45
2:B:346:ILE:HD11	2:B:401:VAL:HG22	1.98	0.45
2:B:588:LEU:HA	2:B:598:LYS:HZ1	1.81	0.45
2:B:753:LEU:O	2:B:757:LEU:HG	2.16	0.45
2:B:873:GLU:N	2:B:873:GLU:OE1	2.49	0.45
2:B:1401:GLN:HG3	2:B:1402:PHE:CD2	2.52	0.45
2:B:1482:MET:C	2:B:1514:PRO:HB3	2.41	0.45
1:A:30:LEU:HG	1:A:34:ILE:HD11	1.99	0.45
1:A:315:PRO:C	1:A:321:ARG:HH12	2.24	0.45
2:B:102:TRP:HB3	2:B:117:LEU:HD23	1.99	0.45
2:B:228:PHE:HZ	2:B:231:PHE:HB2	1.82	0.45
2:B:594:GLU:HA	2:B:597:GLU:CG	2.47	0.45
2:B:646:ASN:HA	2:B:648:GLN:HE22	1.82	0.45
2:B:689:TYR:O	2:B:693:VAL:HG23	2.16	0.45
2:B:1567:GLU:HG2	2:B:1568:LYS:N	2.31	0.45
2:B:1588:LEU:HD12	2:B:1591:ARG:HD3	1.98	0.45
2:B:1607:HIS:HA	2:B:1610:LYS:HB2	1.99	0.45
2:B:1597:MET:HE2	2:B:1626:PHE:CZ	2.52	0.45
1:A:130:THR:HG22	1:A:134:GLU:OE1	2.17	0.45
1:A:180:PHE:O	1:A:183:LYS:HG3	2.17	0.45
1:A:298:GLN:O	1:A:301:THR:OG1	2.34	0.45
1:A:720:TYR:O	2:B:1:MET:N	2.40	0.45
2:B:320:ARG:HD3	2:B:500:VAL:HB	1.99	0.45
2:B:566:ARG:HA	2:B:623:ALA:HA	1.98	0.45
2:B:1086:ARG:HG2	2:B:1086:ARG:HH11	1.82	0.45
1:A:628:LYS:HB2	1:A:633:GLN:HB2	1.99	0.45
2:B:95:LEU:HD11	2:B:121:THR:HG23	1.99	0.45
2:B:132:LEU:HA	2:B:132:LEU:HD23	1.68	0.45
2:B:743:ASN:HB2	2:B:749:LYS:HZ3	1.82	0.45
2:B:934:ARG:HB3	2:B:935:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1033:MET:H	2:B:1035:GLN:HE21	1.64	0.45
2:E:1280:PRO:O	2:E:1285:ARG:NH1	2.33	0.45
1:A:248:ASN:ND2	1:A:300:LEU:HD11	2.32	0.44
1:A:405:ARG:O	1:A:410:GLU:HB3	2.16	0.44
1:A:463:LEU:HD23	1:A:463:LEU:C	2.42	0.44
1:A:621:ASP:O	1:A:626:LYS:NZ	2.49	0.44
2:B:25:VAL:HG23	2:B:26:GLU:OE2	2.17	0.44
2:B:447:TYR:HE2	2:B:627:CYS:HB2	1.81	0.44
2:B:457:LYS:HB3	2:B:461:LYS:HA	1.99	0.44
2:B:926:GLN:O	2:B:929:MET:HB3	2.16	0.44
2:E:1299:LYS:O	2:E:1303:GLU:OE1	2.35	0.44
1:A:20:LYS:NZ	1:A:37:VAL:O	2.48	0.44
2:B:1563:PHE:O	2:B:1566:TYR:N	2.50	0.44
2:E:1249:ASP:HA	2:E:1252:ARG:HH11	1.82	0.44
1:A:358:LYS:HE2	1:A:403:SER:HA	1.99	0.44
1:A:609:PRO:HG2	1:A:613:ILE:HG12	1.98	0.44
2:B:210:LEU:HD23	2:B:213:GLN:NE2	2.33	0.44
2:B:294:VAL:HG12	2:B:329:ILE:HG13	1.99	0.44
2:B:447:TYR:CD1	2:B:514:LYS:HG3	2.52	0.44
2:B:993:PHE:CD2	2:B:1021:ILE:HD11	2.53	0.44
1:A:647:ASP:O	1:A:648:SER:OG	2.33	0.44
1:A:691:SER:HA	1:A:694:ILE:HD11	2.00	0.44
2:B:56:LYS:HA	2:B:56:LYS:HD2	1.77	0.44
2:B:253:PHE:CE1	2:B:297:VAL:HG11	2.52	0.44
2:B:640:LEU:O	2:B:643:TRP:HD1	2.00	0.44
2:B:1320:LEU:HA	2:B:1323:GLU:OE2	2.16	0.44
1:A:466:THR:HG21	1:A:484:VAL:HG13	1.98	0.44
2:B:905:LEU:O	2:B:909:ILE:HG23	2.18	0.44
2:B:1552:SER:HA	2:B:1555:VAL:HG12	1.98	0.44
2:B:1625:CYS:HA	2:B:1628:GLU:HG3	2.00	0.44
1:A:216:TYR:HA	1:A:219:VAL:HG12	2.00	0.44
1:A:219:VAL:O	1:A:223:ILE:HG13	2.18	0.44
1:A:229:ILE:O	1:A:232:LEU:N	2.47	0.44
1:A:232:LEU:HD21	1:A:278:HIS:HB2	1.99	0.44
1:A:536:LEU:HD13	2:B:18:ASN:ND2	2.26	0.44
2:B:85:LEU:HA	2:B:88:VAL:HG22	1.99	0.44
2:B:581:ASP:OD1	2:B:581:ASP:N	2.50	0.44
2:B:747:SER:HA	2:B:750:THR:HG23	2.00	0.44
2:B:837:SER:HB2	2:B:878:LEU:CD1	2.47	0.44
2:B:868:LEU:HG	2:B:871:GLN:OE1	2.18	0.44
2:B:933:LEU:HD23	2:B:960:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1483:TRP:H	2:B:1483:TRP:CD1	2.36	0.44
2:B:1533:VAL:O	2:B:1537:ALA:N	2.51	0.44
2:E:1242:ARG:HH22	2:E:1284:GLN:HA	1.82	0.44
2:E:1283:LEU:HD13	2:E:1291:TYR:HB2	1.99	0.44
1:A:29:PRO:O	1:A:33:ILE:HG12	2.18	0.44
2:B:7:THR:HB	2:B:10:GLN:OE1	2.18	0.44
2:B:319:ARG:C	2:B:320:ARG:HH11	2.25	0.44
2:B:945:ARG:O	2:B:948:PRO:HD2	2.18	0.44
2:B:1367:TYR:HH	2:B:1383:TYR:HH	1.55	0.44
2:E:1242:ARG:O	2:E:1246:LYS:HG3	2.17	0.44
1:A:20:LYS:HE3	1:A:41:TRP:CE3	2.53	0.44
1:A:104:LEU:HD21	1:A:154:MET:O	2.18	0.44
1:A:267:ALA:C	1:A:270:GLN:H	2.26	0.44
1:A:302:PHE:HB3	1:A:431:GLY:H	1.81	0.44
1:A:362:ILE:HD11	1:A:415:ARG:HH12	1.81	0.44
1:A:455:PHE:O	1:A:458:ILE:HG22	2.17	0.44
1:A:717:PRO:HD2	2:B:1:MET:HE3	2.00	0.44
2:B:301:VAL:HG22	2:B:321:PRO:HA	2.00	0.44
2:B:375:GLU:HB2	2:B:502:TYR:N	2.32	0.44
2:B:591:THR:HG22	2:B:592:LYS:N	2.32	0.44
2:B:984:ASP:O	2:B:988:GLU:HG3	2.17	0.44
2:B:1043:TRP:HE1	2:B:1090:MET:HE3	1.83	0.44
1:A:49:PHE:HD2	1:A:79:THR:HA	1.82	0.44
1:A:213:HIS:O	1:A:217:GLN:NE2	2.41	0.44
1:A:542:PRO:HA	1:A:545:LEU:HG	1.98	0.44
2:B:61:GLU:CD	2:B:61:GLU:H	2.26	0.44
2:B:926:GLN:HA	2:B:929:MET:HE2	2.00	0.44
2:B:932:LEU:N	2:B:935:ARG:HH21	2.14	0.44
2:B:1036:ALA:O	2:B:1040:LEU:HD21	2.18	0.44
2:B:1263:THR:HG22	2:B:1498:ILE:HB	2.00	0.44
2:B:1306:SER:O	2:B:1310:LYS:NZ	2.47	0.44
2:B:1438:PRO:HG3	2:B:1454:TYR:CD2	2.53	0.44
2:B:1448:GLU:CD	2:B:1452:ASN:HD22	2.26	0.44
2:E:1344:LYS:O	2:E:1347:SER:OG	2.25	0.44
1:A:50:ALA:O	1:A:77:LEU:HD12	2.18	0.43
1:A:266:LEU:HA	1:A:271:LEU:HD13	2.00	0.43
1:A:287:ASN:HB2	1:A:290:MET:HG2	2.00	0.43
2:B:153:ASP:OD1	2:B:164:VAL:HG22	2.18	0.43
2:B:225:TYR:CE1	2:B:278:GLN:HA	2.54	0.43
2:B:237:GLU:HG3	2:B:308:LEU:HD21	1.99	0.43
2:B:471:SER:HB2	2:B:479:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:532:ARG:HD2	2:B:534:ARG:CZ	2.48	0.43
2:B:568:ASP:HB2	2:B:592:LYS:CG	2.48	0.43
2:B:914:ASP:HB2	2:B:963:GLN:NE2	2.33	0.43
2:B:1542:LEU:HD23	2:B:1543:SER:N	2.32	0.43
1:A:185:ALA:HA	1:A:188:VAL:HG22	1.99	0.43
1:A:459:CYS:O	1:A:462:LEU:HB3	2.18	0.43
1:A:476:ASP:O	1:A:480:VAL:N	2.28	0.43
2:B:21:ALA:HA	2:B:27:LEU:HA	2.00	0.43
2:B:1197:VAL:O	2:B:1201:LEU:HD23	2.18	0.43
2:B:1554:ILE:O	2:B:1558:ALA:HB3	2.18	0.43
2:E:1270:LEU:O	2:E:1272:GLN:NE2	2.50	0.43
2:E:1300:LEU:O	2:E:1304:ILE:HD12	2.18	0.43
1:A:191:SER:OG	1:A:192:ALA:N	2.51	0.43
1:A:425:CYS:SG	1:A:430:VAL:HB	2.59	0.43
2:B:106:TYR:CG	2:B:107:VAL:N	2.86	0.43
2:B:191:SER:O	2:B:195:GLU:OE1	2.35	0.43
2:B:592:LYS:O	2:B:593:MET:C	2.59	0.43
2:B:883:THR:HG21	2:B:931:ARG:HE	1.83	0.43
2:B:1299:LYS:O	2:B:1303:GLU:OE1	2.36	0.43
2:B:1320:LEU:HD23	2:B:1323:GLU:OE2	2.19	0.43
2:B:1567:GLU:HA	2:B:1571:PHE:CD2	2.53	0.43
1:A:585:VAL:HG23	1:A:607:LYS:HD2	2.01	0.43
1:A:594:SER:OG	1:A:596:GLN:HG3	2.18	0.43
2:B:236:GLY:C	2:B:264:SER:HB2	2.44	0.43
2:B:240:GLU:O	2:B:300:ILE:HG23	2.18	0.43
2:B:434:PRO:HG2	2:B:437:ILE:HG23	1.99	0.43
2:B:529:PHE:N	2:B:550:ALA:O	2.28	0.43
2:B:681:MET:HE1	2:B:728:LEU:H	1.83	0.43
2:B:967:SER:O	2:B:971:HIS:HB2	2.18	0.43
2:B:1299:LYS:HE2	2:B:1299:LYS:HB2	1.77	0.43
2:B:1482:MET:O	2:B:1514:PRO:HB3	2.17	0.43
2:E:1279:VAL:O	2:E:1283:LEU:HD23	2.18	0.43
1:A:50:ALA:N	1:A:78:THR:O	2.49	0.43
1:A:351:MET:HA	1:A:354:ARG:HE	1.84	0.43
1:A:453:GLU:OE1	1:A:453:GLU:N	2.50	0.43
1:A:534:LEU:O	1:A:537:LYS:HG2	2.17	0.43
2:B:277:LEU:HA	2:B:277:LEU:HD23	1.76	0.43
2:B:783:ASP:HA	2:B:786:GLU:CD	2.43	0.43
2:B:853:VAL:HG23	2:B:854:ARG:H	1.83	0.43
2:B:924:HIS:O	2:B:928:ILE:HG13	2.18	0.43
2:B:1221:MET:HE3	2:B:1501:TRP:HH2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1266:LEU:CD2	2:B:1498:ILE:HG21	2.48	0.43
2:B:1632:LYS:HA	2:B:1636:HIS:HB3	1.99	0.43
1:A:317:ASP:HB2	1:A:320:GLN:HB3	2.00	0.43
1:A:492:LEU:HD22	1:A:502:PHE:CZ	2.53	0.43
1:A:578:ARG:NH1	1:A:580:SER:HA	2.33	0.43
1:A:661:GLU:HA	1:A:664:ILE:HD12	2.01	0.43
1:A:716:GLU:HG3	2:B:44:TRP:CE2	2.54	0.43
2:B:70:THR:HG22	2:B:71:VAL:N	2.32	0.43
2:B:331:ASP:HA	2:B:334:HIS:ND1	2.34	0.43
2:B:1082:GLU:O	2:B:1086:ARG:HG2	2.19	0.43
2:B:1097:HIS:HB3	2:B:1100:LYS:HZ3	1.83	0.43
2:B:1340:ASN:HB3	2:B:1344:LYS:NZ	2.33	0.43
2:B:1478:GLU:O	2:B:1478:GLU:HG3	2.18	0.43
2:E:1265:LEU:CD2	2:E:1304:ILE:HD13	2.48	0.43
1:A:229:ILE:HD11	1:A:271:LEU:HD11	1.99	0.43
1:A:383:ASN:HB3	1:A:387:PHE:CZ	2.54	0.43
2:B:375:GLU:HB2	2:B:502:TYR:HB2	2.00	0.43
2:B:439:PRO:HD3	2:B:711:HIS:CB	2.49	0.43
2:B:1133:GLN:O	2:B:1136:PHE:HB3	2.18	0.43
2:B:1206:ASP:HA	2:B:1209:THR:HG22	1.99	0.43
2:B:1240:TYR:CD2	2:B:1244:LEU:HD11	2.53	0.43
2:B:1471:GLY:N	2:B:1473:LYS:HE3	2.34	0.43
2:B:1477:ASN:ND2	2:B:1565:ASN:HA	2.33	0.43
1:A:9:LYS:H	2:B:1390:ARG:HH21	1.65	0.43
1:A:140:TYR:CD1	1:A:143:LEU:HD11	2.45	0.43
1:A:196:SER:HA	1:A:199:GLN:CD	2.44	0.43
1:A:248:ASN:O	1:A:252:LEU:HG	2.18	0.43
1:A:317:ASP:O	1:A:321:ARG:HG2	2.18	0.43
1:A:331:ALA:HB2	1:A:395:TYR:OH	2.18	0.43
2:B:19:TYR:CZ	2:B:59:PHE:HD1	2.36	0.43
2:B:351:ILE:HD13	2:B:374:GLY:O	2.18	0.43
2:B:801:LEU:O	2:B:804:ARG:HG3	2.19	0.43
2:B:810:VAL:HG23	2:B:811:LYS:N	2.32	0.43
2:B:990:PHE:HD2	2:B:1042:LEU:HD11	1.84	0.43
2:B:1099:ILE:HD13	2:B:1138:PHE:HB2	1.99	0.43
1:A:236:ASP:O	1:A:239:ILE:HG22	2.18	0.43
1:A:329:ARG:NE	1:A:340:ASN:OD1	2.51	0.43
1:A:378:MET:SD	1:A:378:MET:N	2.92	0.43
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.90	0.43
2:B:37:ILE:HG23	2:B:45:TYR:HB3	2.00	0.43
2:B:43:GLY:C	2:B:44:TRP:CD1	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:LEU:HD13	2:B:1005:ASP:HB3	2.00	0.43
2:B:507:PRO:HG2	2:B:509:TRP:CH2	2.54	0.43
2:B:592:LYS:HD3	2:B:595:MET:SD	2.58	0.43
2:B:1169:LYS:NZ	2:B:1198:SER:O	2.44	0.43
2:E:1228:LEU:HB3	2:E:1240:TYR:CE1	2.51	0.43
1:A:695:LYS:HA	1:A:698:LEU:HG	2.01	0.43
2:B:468:VAL:HB	2:B:498:SER:HB3	2.01	0.43
2:B:479:LEU:HA	2:B:479:LEU:HD12	1.72	0.43
2:B:529:PHE:O	2:B:550:ALA:N	2.35	0.43
2:B:1019:ARG:O	2:B:1023:GLN:HG2	2.19	0.43
2:B:1189:SER:HB3	2:B:1193:PHE:CE2	2.54	0.43
2:B:1489:TYR:CE1	2:B:1507:ILE:HG23	2.54	0.43
2:B:1632:LYS:O	2:B:1636:HIS:HB3	2.19	0.43
2:E:1228:LEU:O	2:E:1232:LYS:HG2	2.19	0.43
1:A:159:LEU:HD12	1:A:197:ILE:HG23	2.01	0.42
1:A:670:ASN:HA	1:A:675:LYS:NZ	2.34	0.42
2:B:1:MET:SD	2:B:58:ILE:HG21	2.59	0.42
2:B:288:ASP:HA	2:B:291:ARG:HE	1.83	0.42
2:B:649:ASN:O	2:B:652:HIS:N	2.52	0.42
2:B:855:GLN:OE1	2:B:855:GLN:N	2.39	0.42
2:B:972:TYR:HH	2:B:977:LYS:HZ2	1.59	0.42
2:B:1154:LYS:HE2	2:B:1157:GLN:OE1	2.19	0.42
2:B:1162:GLY:HA2	2:B:1208:ARG:NE	2.34	0.42
2:B:1183:HIS:CG	2:B:1184:LYS:H	2.37	0.42
2:B:1415:GLY:O	2:B:1418:ILE:HG22	2.19	0.42
2:E:1242:ARG:HD3	2:E:1242:ARG:N	2.33	0.42
2:E:1245:TYR:HA	2:E:1248:ARG:HE	1.84	0.42
1:A:74:ILE:O	1:A:75:LEU:HD12	2.19	0.42
1:A:240:GLN:O	1:A:244:ILE:HG12	2.19	0.42
1:A:313:MET:SD	1:A:378:MET:HG3	2.59	0.42
2:B:234:ASN:OD1	2:B:265:ASN:HA	2.19	0.42
2:B:637:LEU:O	2:B:640:LEU:HB2	2.20	0.42
2:B:809:ALA:HB3	2:B:813:LYS:HE3	2.01	0.42
2:B:1320:LEU:HA	2:B:1323:GLU:CD	2.45	0.42
2:B:1485:GLU:HG3	2:B:1511:GLU:HB3	2.01	0.42
2:B:1514:PRO:HA	2:B:1517:ASN:HD22	1.83	0.42
2:E:1306:SER:O	2:E:1309:ASP:HB2	2.19	0.42
1:A:385:LEU:HD22	1:A:389:LYS:HZ1	1.83	0.42
1:A:531:ARG:HG2	1:A:708:ASP:CG	2.44	0.42
2:B:468:VAL:HG22	2:B:531:PHE:CE1	2.54	0.42
2:B:820:LEU:HG	2:B:840:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1007:MET:SD	2:B:1008:VAL:N	2.92	0.42
2:B:1193:PHE:HA	2:B:1196:LEU:HD12	2.01	0.42
2:B:1384:ARG:CZ	2:B:1496:PRO:HB3	2.49	0.42
2:B:1384:ARG:NH1	2:B:1496:PRO:HB3	2.34	0.42
2:B:1563:PHE:HB3	2:B:1637:TYR:OH	2.19	0.42
2:E:1218:GLU:O	2:E:1221:MET:HG2	2.19	0.42
1:A:216:TYR:CE1	1:A:250:LEU:HA	2.55	0.42
1:A:375:PRO:HG3	1:A:426:GLU:OE2	2.19	0.42
1:A:673:LEU:HB2	1:A:675:LYS:HZ2	1.84	0.42
2:B:676:LEU:HG	2:B:693:VAL:HG13	2.02	0.42
2:B:771:ARG:HH22	2:B:784:GLY:HA2	1.83	0.42
2:B:835:GLU:O	2:B:839:LEU:HG	2.19	0.42
2:B:1127:ILE:O	2:B:1131:MET:HG2	2.19	0.42
2:B:1192:VAL:O	2:B:1196:LEU:HG	2.19	0.42
2:B:1251:HIS:ND1	2:B:1256:ASN:HB2	2.34	0.42
2:B:1408:MET:HB3	2:B:1426:MET:O	2.20	0.42
1:A:88:LEU:HD21	1:A:107:LEU:HB2	2.01	0.42
1:A:418:ILE:O	1:A:422:LYS:HG2	2.19	0.42
1:A:531:ARG:HG3	1:A:532:PRO:HD3	2.01	0.42
1:A:562:PHE:HB3	1:A:655:ILE:O	2.20	0.42
2:B:250:GLN:NE2	2:B:291:ARG:HG2	2.35	0.42
2:B:330:THR:O	2:B:334:HIS:ND1	2.46	0.42
2:B:791:ILE:O	2:B:794:LEU:HB3	2.19	0.42
2:B:972:TYR:OH	2:B:977:LYS:NZ	2.39	0.42
2:B:1143:ASN:OD1	2:B:1145:HIS:N	2.47	0.42
2:B:1555:VAL:HG13	2:B:1556:ASP:N	2.34	0.42
1:A:180:PHE:O	1:A:184:ILE:HG12	2.19	0.42
1:A:301:THR:O	1:A:305:LEU:HG	2.19	0.42
1:A:345:MET:O	1:A:348:ARG:HB2	2.19	0.42
1:A:585:VAL:HG23	1:A:607:LYS:HA	2.02	0.42
1:A:701:LEU:HD11	2:B:32:GLY:HA3	2.02	0.42
2:B:207:ASN:C	2:B:208:LEU:HD12	2.44	0.42
2:B:861:THR:O	2:B:864:VAL:HG12	2.18	0.42
2:B:906:LEU:HA	2:B:909:ILE:HG12	2.02	0.42
2:B:987:MET:HE2	2:B:987:MET:HA	2.00	0.42
2:B:1240:TYR:O	2:B:1244:LEU:HG	2.19	0.42
2:B:1391:ARG:NH1	2:B:1395:SER:HB2	2.30	0.42
2:B:1477:ASN:HD21	2:B:1568:LYS:HB2	1.85	0.42
2:B:1618:LEU:HD23	2:B:1621:ARG:HH11	1.84	0.42
1:A:20:LYS:HE3	1:A:41:TRP:CZ3	2.54	0.42
1:A:314:ASP:HB3	1:A:317:ASP:CG	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:LYS:HG2	2:B:431:MET:N	2.35	0.42
2:B:932:LEU:O	2:B:936:ILE:HG12	2.19	0.42
2:B:1152:ILE:HD13	2:B:1155:LEU:HD12	2.02	0.42
2:B:1570:PHE:O	2:B:1575:TYR:HD2	2.03	0.42
2:B:876:GLU:HG2	2:B:877:VAL:HG13	2.02	0.42
2:B:890:LEU:HD22	2:B:935:ARG:HG3	2.02	0.42
1:A:366:ASN:O	1:A:369:MET:HG2	2.19	0.42
2:B:165:VAL:HB	2:B:174:ASP:OD2	2.20	0.42
2:B:630:LYS:HA	2:B:668:PHE:CZ	2.55	0.42
2:B:1294:GLN:N	2:B:1294:GLN:CD	2.78	0.42
2:B:1364:ALA:O	2:B:1428:CYS:HA	2.20	0.42
2:E:1242:ARG:HH12	2:E:1284:GLN:CA	2.32	0.42
1:A:259:ARG:HB3	1:A:304:LEU:HD11	2.01	0.42
1:A:376:PRO:HG2	1:A:421:THR:CB	2.49	0.42
2:B:172:ILE:C	2:B:174:ASP:H	2.27	0.42
2:B:222:TYR:O	2:B:282:THR:HA	2.20	0.42
2:B:467:GLU:HG2	2:B:500:VAL:HG22	2.01	0.42
2:B:1110:LEU:O	2:B:1114:LEU:N	2.51	0.42
2:B:1113:THR:HG22	2:B:1168:TYR:HE1	1.85	0.42
2:B:1218:GLU:OE1	2:B:1218:GLU:N	2.42	0.42
1:A:181:ILE:HG12	1:A:222:GLU:OE1	2.20	0.41
1:A:244:ILE:HB	1:A:293:GLN:NE2	2.35	0.41
1:A:541:GLN:HA	1:A:544:ILE:CG1	2.47	0.41
2:B:82:PRO:HA	2:B:85:LEU:HD23	2.01	0.41
2:B:351:ILE:HG21	2:B:374:GLY:O	2.19	0.41
2:B:413:VAL:HG12	2:B:417:PHE:HD2	1.84	0.41
2:B:471:SER:OG	2:B:528:ARG:O	2.27	0.41
2:B:870:ARG:HA	2:B:870:ARG:HD2	1.86	0.41
2:B:1525:THR:HA	2:B:1528:ARG:NE	2.34	0.41
2:B:1598:PRO:O	2:B:1602:GLU:HG2	2.19	0.41
2:B:1615:LEU:HD23	2:B:1618:LEU:HD12	2.01	0.41
2:B:102:TRP:CZ3	2:B:114:PHE:HE1	2.38	0.41
2:B:435:GLU:HB3	2:B:708:LYS:HE2	2.02	0.41
2:B:777:PHE:HB3	2:B:778:TYR:CD2	2.55	0.41
2:B:844:ILE:HD12	2:B:847:ILE:HG13	2.02	0.41
2:B:1084:GLY:HA2	2:B:1087:ILE:HD12	2.03	0.41
2:B:1268:ALA:HB2	2:B:1300:LEU:HD13	2.02	0.41
2:B:1349:TYR:HA	2:B:1352:ILE:HD12	2.02	0.41
2:B:1452:ASN:O	2:B:1455:ARG:HG2	2.20	0.41
2:E:1237:GLU:O	2:E:1241:ILE:HG12	2.20	0.41
2:E:1279:VAL:HG21	2:E:1282:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:C	1:A:304:LEU:HD11	2.45	0.41
1:A:287:ASN:O	1:A:290:MET:HB2	2.21	0.41
1:A:328:ARG:CD	1:A:348:ARG:HH22	2.30	0.41
1:A:577:CYS:HA	1:A:588:TYR:HB3	2.02	0.41
2:B:65:HIS:CG	2:B:66:LEU:H	2.38	0.41
2:B:95:LEU:HD12	2:B:95:LEU:HA	1.76	0.41
2:B:218:THR:OG1	2:B:219:ILE:N	2.53	0.41
2:B:472:VAL:HG22	2:B:484:ILE:HD11	2.02	0.41
2:B:1319:LYS:O	2:B:1322:LYS:HB2	2.20	0.41
2:B:1556:ASP:HB3	2:B:1557:PRO:HD3	2.03	0.41
2:E:1242:ARG:O	2:E:1245:TYR:HB2	2.20	0.41
1:A:144:GLN:HG2	1:A:148:LYS:HE2	2.02	0.41
1:A:515:LEU:HA	1:A:518:ARG:NH2	2.35	0.41
1:A:607:LYS:HG3	1:A:608:LEU:N	2.35	0.41
2:B:49:THR:OG1	2:B:52:ASN:N	2.52	0.41
2:B:377:GLU:HA	2:B:378:PRO:HD3	1.95	0.41
2:B:550:ALA:HB2	2:B:571:VAL:HG23	2.02	0.41
2:B:1038:PHE:C	2:B:1039:GLU:HG2	2.45	0.41
2:B:1185:TYR:O	2:B:1188:SER:OG	2.31	0.41
2:E:1320:LEU:HA	2:E:1323:GLU:OE1	2.21	0.41
2:E:1325:ALA:O	2:E:1328:TYR:HB2	2.20	0.41
1:A:118:GLN:HE21	1:A:122:ASN:CG	2.28	0.41
1:A:329:ARG:HH21	1:A:336:SER:CB	2.33	0.41
1:A:376:PRO:HD2	1:A:418:ILE:HD12	2.01	0.41
1:A:562:PHE:HE2	1:A:577:CYS:HB3	1.85	0.41
1:A:578:ARG:HH12	1:A:581:PRO:CD	2.33	0.41
2:B:14:VAL:HG12	2:B:33:ASP:C	2.45	0.41
2:B:243:MET:SD	2:B:243:MET:N	2.90	0.41
2:B:321:PRO:HD3	2:B:499:VAL:HG12	2.02	0.41
2:B:651:LYS:HE2	2:B:652:HIS:CE1	2.56	0.41
2:B:821:PRO:C	2:B:823:ILE:H	2.28	0.41
2:B:897:PRO:O	2:B:900:GLU:HG3	2.20	0.41
2:B:1129:PHE:O	2:B:1133:GLN:HG3	2.21	0.41
2:B:1144:PHE:HD2	2:B:1147:PHE:HD2	1.67	0.41
2:B:1524:LEU:O	2:B:1528:ARG:HG3	2.20	0.41
2:B:1607:HIS:CD2	2:B:1619:HIS:CD2	3.05	0.41
2:B:1633:VAL:HA	2:B:1637:TYR:HB2	2.03	0.41
2:E:1306:SER:HA	2:E:1309:ASP:OD2	2.20	0.41
1:A:18:TYR:CE1	2:B:1354:LYS:HA	2.55	0.41
1:A:262:MET:HA	1:A:265:ILE:HG12	2.01	0.41
2:B:4:TRP:CZ2	2:B:58:ILE:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LEU:O	2:B:121:THR:OG1	2.32	0.41
2:B:520:GLU:O	2:B:523:THR:OG1	2.17	0.41
2:B:567:HIS:ND1	2:B:593:MET:HE1	2.35	0.41
2:B:683:MET:HE1	2:B:686:SER:HB3	2.01	0.41
2:B:1202:GLU:HG2	2:B:1203:ASN:N	2.35	0.41
2:B:1542:LEU:O	2:B:1544:VAL:HG23	2.21	0.41
2:B:1607:HIS:O	2:B:1610:LYS:N	2.53	0.41
1:A:322:ASP:HA	1:A:325:PHE:HB3	2.02	0.41
1:A:424:LEU:HA	1:A:485:LYS:HZ1	1.86	0.41
1:A:549:LYS:HD2	1:A:550:GLN:N	2.35	0.41
1:A:711:PRO:HG2	2:B:16:ILE:HD12	2.01	0.41
2:B:224:LEU:HD12	2:B:281:PHE:HD2	1.85	0.41
2:B:245:LEU:HB2	2:B:254:ILE:HB	2.01	0.41
2:B:249:ASP:OD2	2:B:293:ARG:N	2.53	0.41
2:B:255:SER:HA	2:B:430:LYS:HA	2.02	0.41
2:B:651:LYS:HE2	2:B:652:HIS:ND1	2.35	0.41
2:B:721:TYR:O	2:B:722:LYS:HE2	2.20	0.41
2:B:1586:VAL:HA	2:B:1589:LEU:HG	2.03	0.41
1:A:93:GLN:HE21	1:A:128:LEU:CD1	2.34	0.41
1:A:487:GLN:CD	1:A:514:ILE:HG12	2.46	0.41
1:A:640:LEU:HA	1:A:640:LEU:HD23	1.88	0.41
1:A:669:LEU:HD23	1:A:672:LEU:HD12	2.01	0.41
2:B:102:TRP:CE3	2:B:114:PHE:HE1	2.39	0.41
2:B:115:ARG:O	2:B:119:GLN:HG3	2.20	0.41
2:B:263:GLY:N	2:B:267:MET:O	2.51	0.41
2:B:486:PRO:HB3	2:B:513:VAL:HG12	2.03	0.41
2:B:547:PHE:CD1	2:B:573:LYS:HE2	2.55	0.41
2:B:934:ARG:NH2	2:B:988:GLU:OE2	2.54	0.41
2:B:1124:THR:O	2:B:1127:ILE:HG22	2.19	0.41
2:B:1367:TYR:HA	2:B:1426:MET:HE1	2.02	0.41
2:B:1469:ARG:HG2	2:B:1473:LYS:NZ	2.35	0.41
2:B:1568:LYS:O	2:B:1572:THR:OG1	2.33	0.41
2:E:1308:PHE:HB3	2:E:1313:MET:O	2.20	0.41
1:A:13:GLU:N	1:A:13:GLU:OE1	2.54	0.41
1:A:129:LEU:HA	1:A:132:MET:HG3	2.03	0.41
1:A:254:ALA:HB3	1:A:259:ARG:HE	1.85	0.41
1:A:483:VAL:O	1:A:486:GLU:HB2	2.20	0.41
1:A:561:CYS:HA	1:A:576:TYR:HA	2.03	0.41
1:A:622:CYS:HB3	1:A:624:HIS:ND1	2.36	0.41
2:B:44:TRP:CB	2:B:58:ILE:HG22	2.51	0.41
2:B:108:ASN:O	2:B:110:LYS:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:THR:HB	2:B:530:THR:OG1	2.21	0.41
2:B:564:ASP:N	2:B:633:GLN:OE1	2.54	0.41
2:B:568:ASP:O	2:B:592:LYS:HG2	2.21	0.41
2:B:796:LEU:HA	2:B:799:ASN:ND2	2.36	0.41
2:B:797:ALA:O	2:B:801:LEU:HG	2.21	0.41
2:B:866:SER:C	2:B:868:LEU:H	2.28	0.41
2:B:879:LEU:HD23	2:B:928:ILE:HD11	2.03	0.41
2:B:964:MET:HE3	2:B:968:HIS:HB2	2.02	0.41
2:B:1051:VAL:HG21	2:B:1108:PRO:HB3	2.02	0.41
2:B:1239:ILE:HD11	2:B:1243:TYR:CZ	2.56	0.41
2:B:1291:TYR:HB3	2:B:1296:LEU:HD11	2.03	0.41
2:E:1291:TYR:HA	2:E:1296:LEU:HD21	2.03	0.41
1:A:12:ILE:HB	1:A:20:LYS:HG3	2.03	0.41
1:A:302:PHE:CG	1:A:430:VAL:HG13	2.56	0.41
1:A:306:GLU:CA	1:A:309:MET:HG3	2.44	0.41
1:A:351:MET:HA	1:A:354:ARG:HG2	2.03	0.41
1:A:416:SER:O	1:A:420:LEU:HD13	2.20	0.41
1:A:503:LYS:HG3	1:A:507:GLN:HE22	1.86	0.41
1:A:524:ASN:HD22	1:A:687:ASP:HB3	1.85	0.41
1:A:620:LYS:HB2	1:A:638:LEU:HD13	2.02	0.41
1:A:665:TRP:O	1:A:669:LEU:HG	2.21	0.41
2:B:457:LYS:HB3	2:B:461:LYS:HG3	2.03	0.41
2:B:476:GLU:C	2:B:582:ALA:HB1	2.46	0.41
2:B:745:ASP:N	2:B:745:ASP:OD1	2.52	0.41
2:B:1147:PHE:CZ	2:B:1151:LEU:HD22	2.56	0.41
2:B:1148:GLU:HA	2:B:1151:LEU:HB3	2.03	0.41
2:B:1268:ALA:HA	2:B:1271:LEU:HD13	2.02	0.41
2:B:1372:PHE:HB2	2:B:1377:ARG:CG	2.42	0.41
2:B:1381:PHE:HA	2:B:1502:PHE:O	2.21	0.41
2:B:1594:ALA:O	2:B:1598:PRO:HD2	2.21	0.41
1:A:232:LEU:HD12	1:A:240:GLN:HG2	2.03	0.40
1:A:251:PHE:CG	1:A:300:LEU:HD13	2.56	0.40
1:A:468:LYS:O	1:A:471:ARG:HD2	2.21	0.40
1:A:722:PHE:CD1	2:B:1:MET:N	2.89	0.40
2:B:108:ASN:C	2:B:110:LYS:HG2	2.46	0.40
2:B:231:PHE:HB3	2:B:262:TRP:NE1	2.36	0.40
2:B:643:TRP:O	2:B:647:SER:N	2.54	0.40
2:B:724:PHE:CD2	2:B:769:GLN:HB3	2.55	0.40
2:B:738:ASN:OD1	2:B:794:LEU:HA	2.20	0.40
2:B:1245:TYR:HA	2:B:1248:ARG:HG2	2.01	0.40
2:B:1300:LEU:HA	2:B:1303:GLU:OE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1418:ILE:HD12	2:B:1421:SER:HB3	2.03	0.40
2:B:1603:GLY:HA2	2:B:1606:ILE:HG22	2.03	0.40
2:E:1305:ILE:HG23	2:E:1348:PHE:HZ	1.86	0.40
1:A:30:LEU:HA	1:A:33:ILE:CG1	2.51	0.40
1:A:140:TYR:O	1:A:144:GLN:N	2.51	0.40
1:A:641:ALA:HA	1:A:654:PHE:O	2.21	0.40
2:B:701:ILE:HD12	2:B:701:ILE:HA	1.89	0.40
2:B:1259:GLU:HB3	2:B:1498:ILE:O	2.20	0.40
2:B:1443:ASP:OD1	2:B:1443:ASP:N	2.47	0.40
2:B:1575:TYR:CE1	2:B:1585:LYS:HD2	2.55	0.40
2:E:1250:LEU:O	2:E:1253:ASP:HB2	2.21	0.40
1:A:52:GLN:HG2	1:A:54:ALA:HA	2.04	0.40
1:A:239:ILE:O	1:A:243:THR:HG23	2.21	0.40
1:A:326:GLU:O	1:A:329:ARG:HB2	2.22	0.40
1:A:420:LEU:HD21	1:A:463:LEU:HD12	2.03	0.40
1:A:502:PHE:O	1:A:506:LEU:HG	2.21	0.40
1:A:517:ILE:HA	1:A:520:SER:OG	2.22	0.40
1:A:693:GLU:O	1:A:696:LEU:HG	2.20	0.40
2:B:1:MET:HE1	2:B:44:TRP:CD1	2.57	0.40
2:B:86:PRO:O	2:B:87:LEU:C	2.64	0.40
2:B:453:GLY:CA	2:B:620:PHE:HA	2.51	0.40
2:B:555:MET:O	2:B:556:ASN:ND2	2.55	0.40
2:B:1349:TYR:HD1	2:E:1335:TYR:CD2	2.39	0.40
2:B:1354:LYS:HA	2:B:1354:LYS:HE2	2.03	0.40
2:B:1514:PRO:HA	2:B:1517:ASN:HB2	2.03	0.40
2:B:1515:LEU:HD22	2:B:1575:TYR:CE1	2.56	0.40
2:B:1585:LYS:HG3	2:B:1586:VAL:N	2.36	0.40
2:E:1232:LYS:HE3	2:E:1240:TYR:CZ	2.56	0.40
1:A:61:ILE:HD13	1:A:61:ILE:HA	1.90	0.40
1:A:159:LEU:O	1:A:163:VAL:HG13	2.21	0.40
1:A:387:PHE:CE2	1:A:457:CYS:HB3	2.56	0.40
1:A:692:MET:HG3	2:B:102:TRP:HZ2	1.86	0.40
1:A:710:PRO:HB3	2:B:17:TYR:CZ	2.56	0.40
2:B:263:GLY:HA3	2:B:267:MET:SD	2.62	0.40
2:B:318:LEU:HD23	2:B:318:LEU:HA	1.94	0.40
2:B:925:ILE:O	2:B:928:ILE:N	2.55	0.40
2:B:1129:PHE:CD1	2:B:1179:HIS:HB3	2.56	0.40
2:B:1129:PHE:HA	2:B:1132:MET:HG3	2.03	0.40
2:B:1435:MET:HB3	2:B:1437:LEU:HD22	2.04	0.40
2:B:1632:LYS:O	2:B:1637:TYR:N	2.35	0.40
2:E:1299:LYS:HE2	2:E:1299:LYS:HB2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:N	1:A:23:GLU:HB3	2.37	0.40
1:A:28:LYS:C	1:A:66:ARG:HH12	2.29	0.40
1:A:331:ALA:O	1:A:399:VAL:HG21	2.21	0.40
1:A:429:LYS:HB3	1:A:432:GLU:HG3	2.02	0.40
1:A:679:SER:O	1:A:682:THR:HB	2.21	0.40
2:B:29:LEU:HD12	2:B:59:PHE:CZ	2.56	0.40
2:B:209:ASP:O	2:B:213:GLN:HG3	2.21	0.40
2:B:732:LYS:HA	2:B:732:LYS:HD3	1.94	0.40
2:B:769:GLN:HA	2:B:772:VAL:HG22	2.03	0.40
2:B:804:ARG:HD2	2:B:808:GLU:OE2	2.21	0.40
2:B:929:MET:HG3	2:B:933:LEU:HD21	2.02	0.40
2:B:1468:PHE:CZ	2:B:1470:LYS:HE3	2.56	0.40
2:E:1299:LYS:HA	2:E:1302:GLN:OE1	2.21	0.40
2:E:1321:SER:OG	2:E:1341:LEU:HD11	2.22	0.40
2:E:1348:PHE:O	2:E:1352:ILE:HG13	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	725/733 (99%)	651 (90%)	74 (10%)	0	100	100
2	B	1640/1648 (100%)	1428 (87%)	212 (13%)	0	100	100
2	E	138/1648 (8%)	129 (94%)	9 (6%)	0	100	100
All	All	2503/4029 (62%)	2208 (88%)	295 (12%)	0	100	100

There are no Ramachandran outliers to report.

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	662/664 (100%)	662 (100%)	0	100	100
2	B	1495/1497 (100%)	1495 (100%)	0	100	100
2	E	130/1497 (9%)	130 (100%)	0	100	100
All	All	2287/3658 (62%)	2287 (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 (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	231	HIS
1	A	288	ASN
1	A	293	GLN
1	A	298	GLN
1	A	402	ASN
1	A	439	ASN
1	A	464	ASN
1	A	482	GLN
1	A	487	GLN
1	A	507	GLN
1	A	705	GLN
2	B	30	GLN
2	B	65	HIS
2	B	116	GLN
2	B	118	GLN
2	B	171	ASN
2	B	199	GLN
2	B	213	GLN
2	B	265	ASN
2	B	465	ASN
2	B	648	GLN
2	B	1000	ASN
2	B	1010	ASN

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Mol	Chain	Res	Type
2	B	1041	GLN
2	B	1097	HIS
2	B	1149	ASN
2	B	1157	GLN
2	B	1213	GLN
2	B	1449	GLN
2	B	1477	ASN
2	B	1534	GLN
2	B	1536	HIS
2	B	1577	GLN
2	B	1607	HIS
2	E	1256	ASN
2	E	1281	HIS

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 oligosaccharides 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.

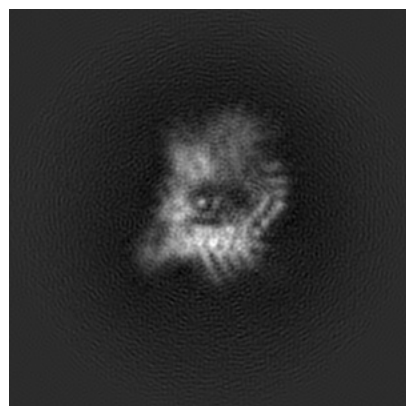
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36271. These allow visual inspection of the internal detail of the map and identification of artifacts.

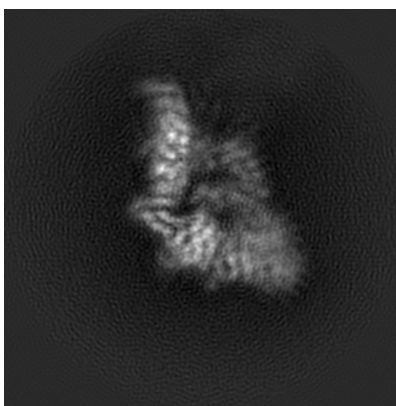
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

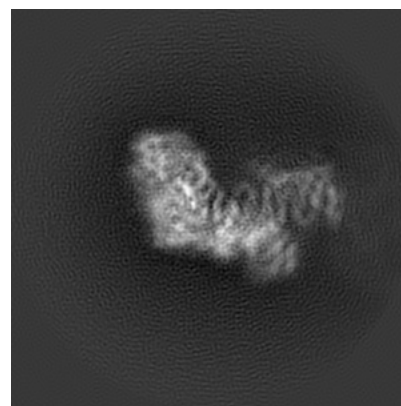
6.1.1 Primary map



X

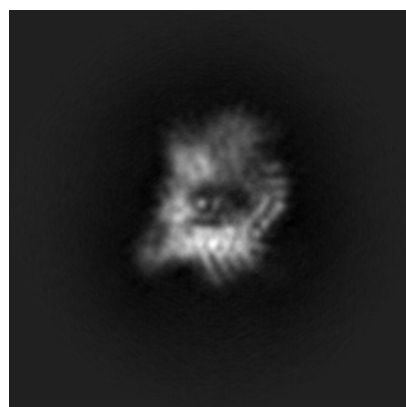


Y

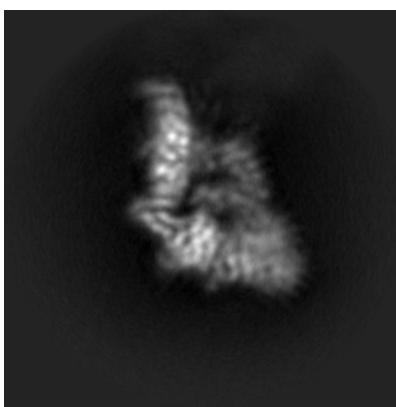


Z

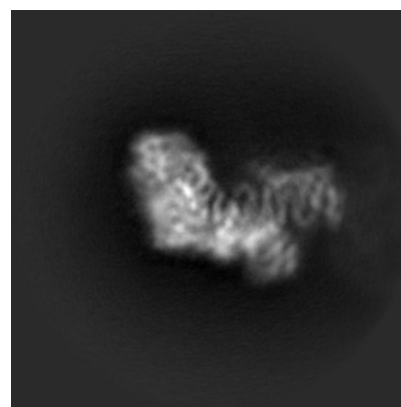
6.1.2 Raw map



X



Y

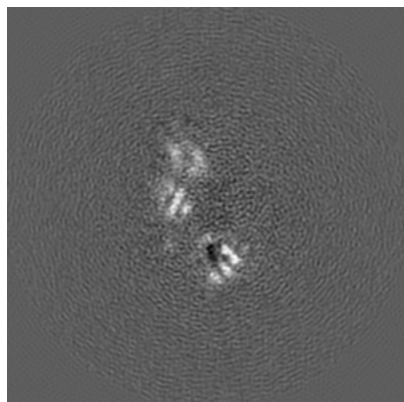


Z

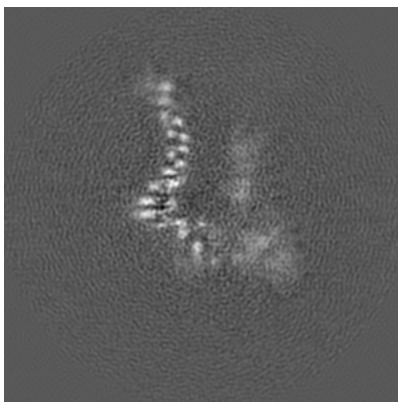
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

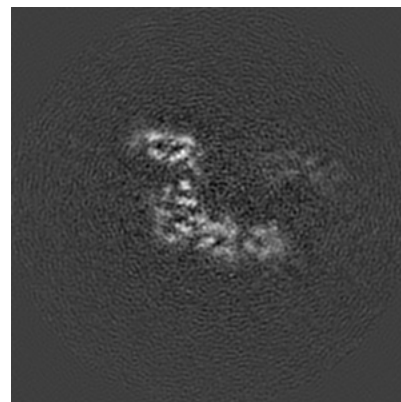
6.2.1 Primary map



X Index: 120

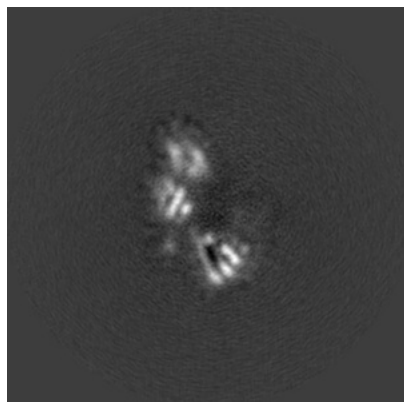


Y Index: 120

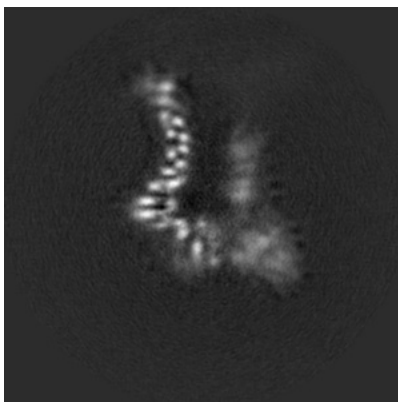


Z Index: 120

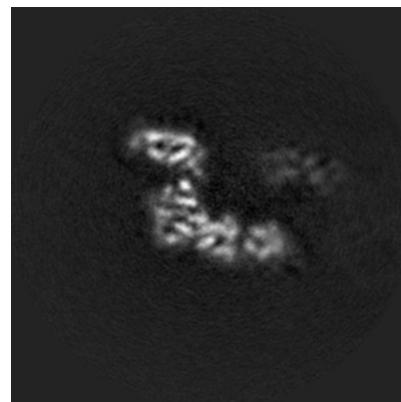
6.2.2 Raw map



X Index: 120



Y Index: 120

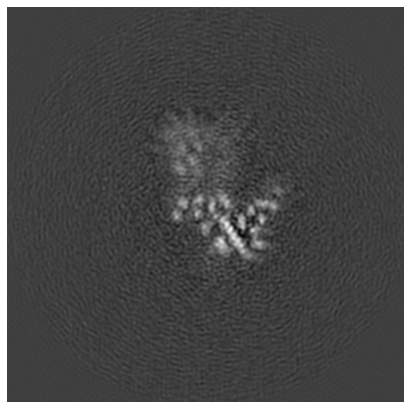


Z Index: 120

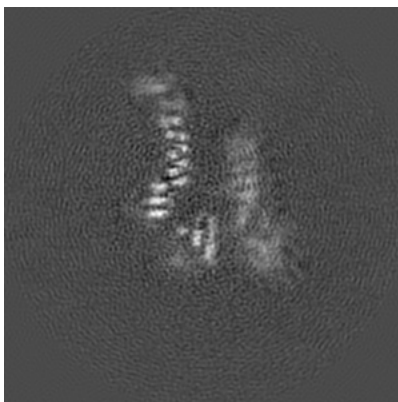
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

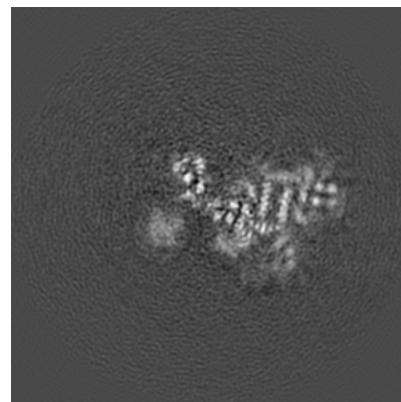
6.3.1 Primary map



X Index: 106

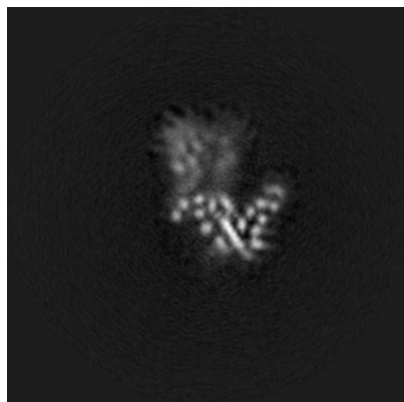


Y Index: 117

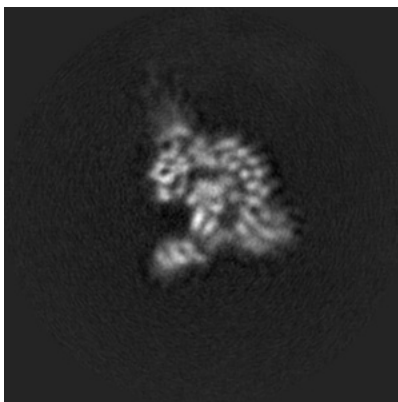


Z Index: 100

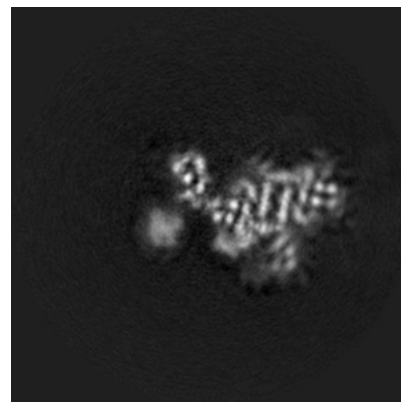
6.3.2 Raw map



X Index: 105



Y Index: 104

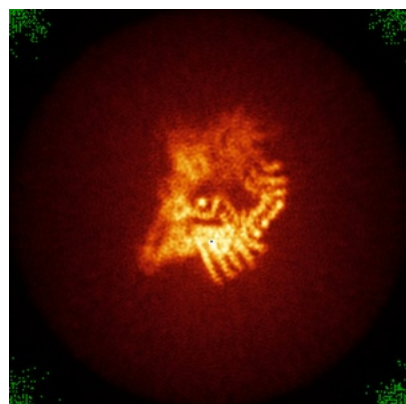


Z Index: 100

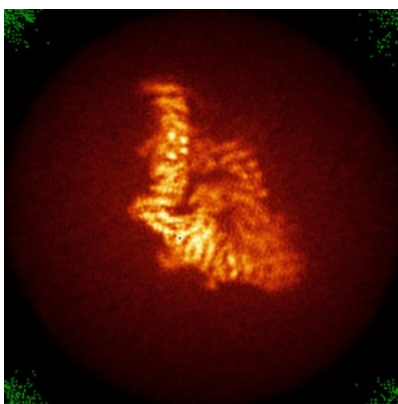
The images above show the largest variance slices of the map in three orthogonal directions.

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

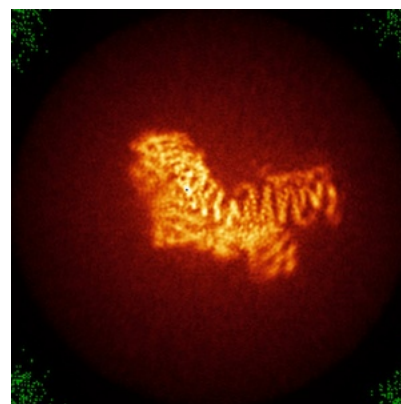
6.4.1 Primary map



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



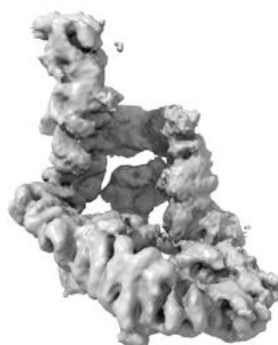
Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

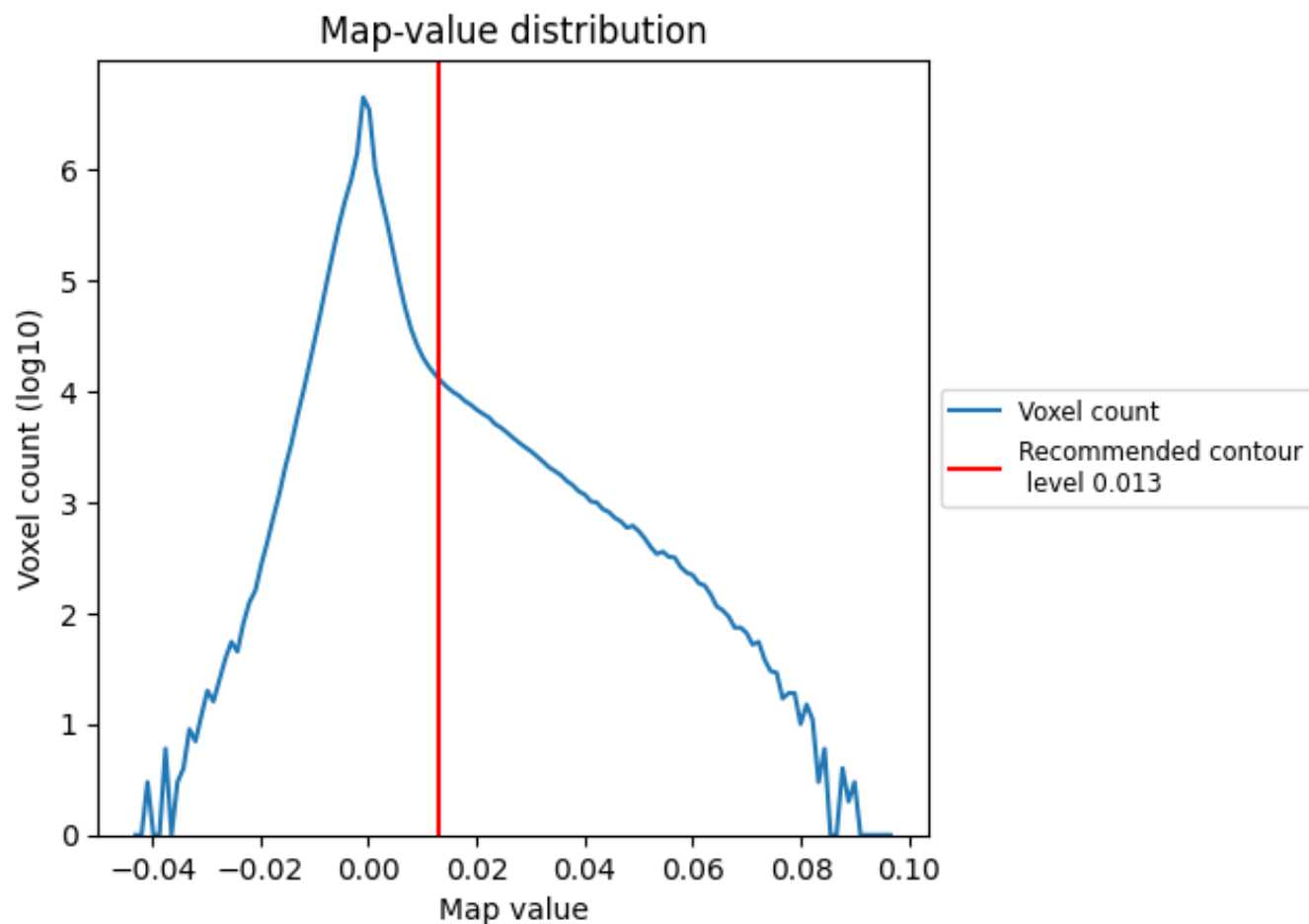
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

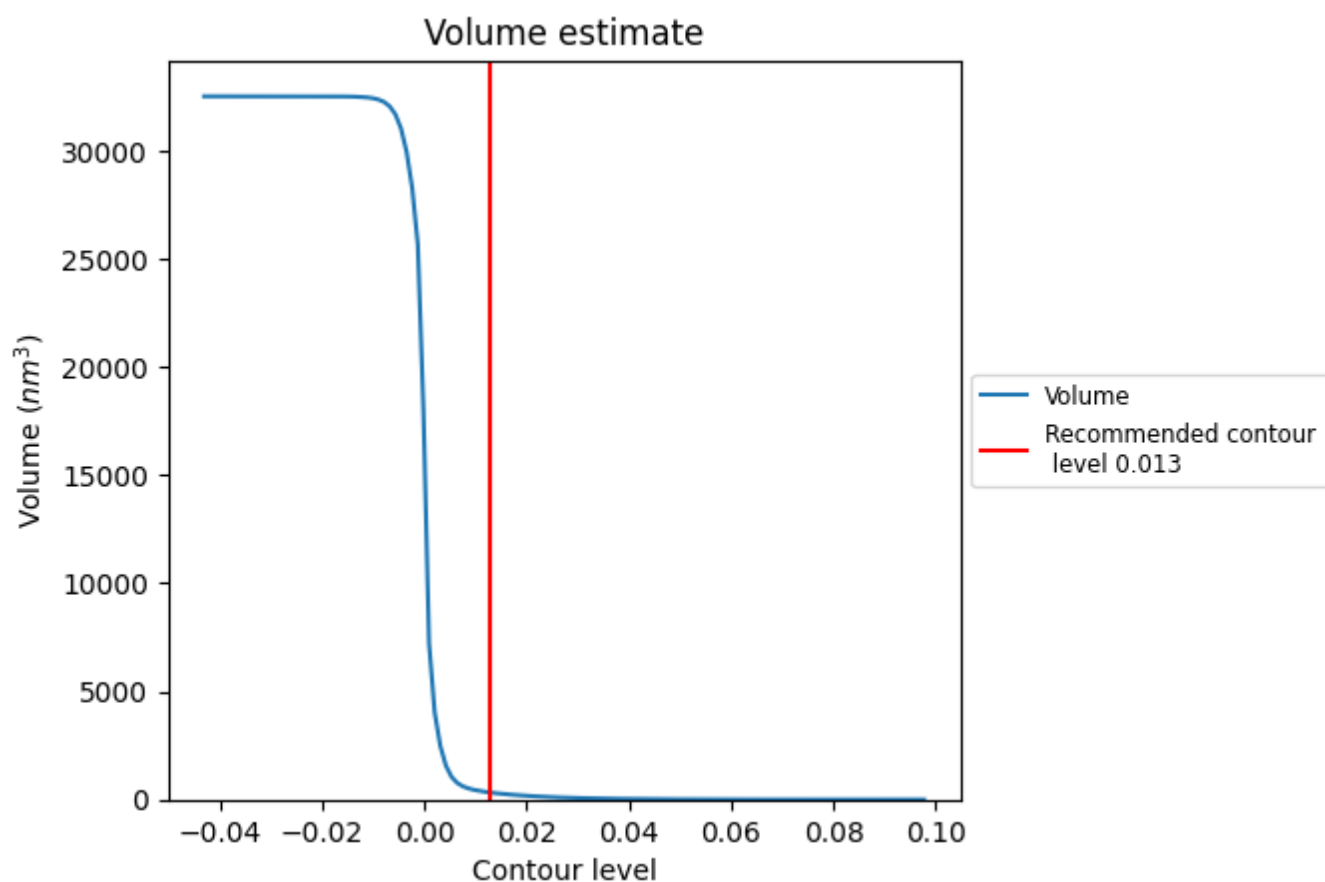
This section contains the results of statistical analysis of the map.

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.

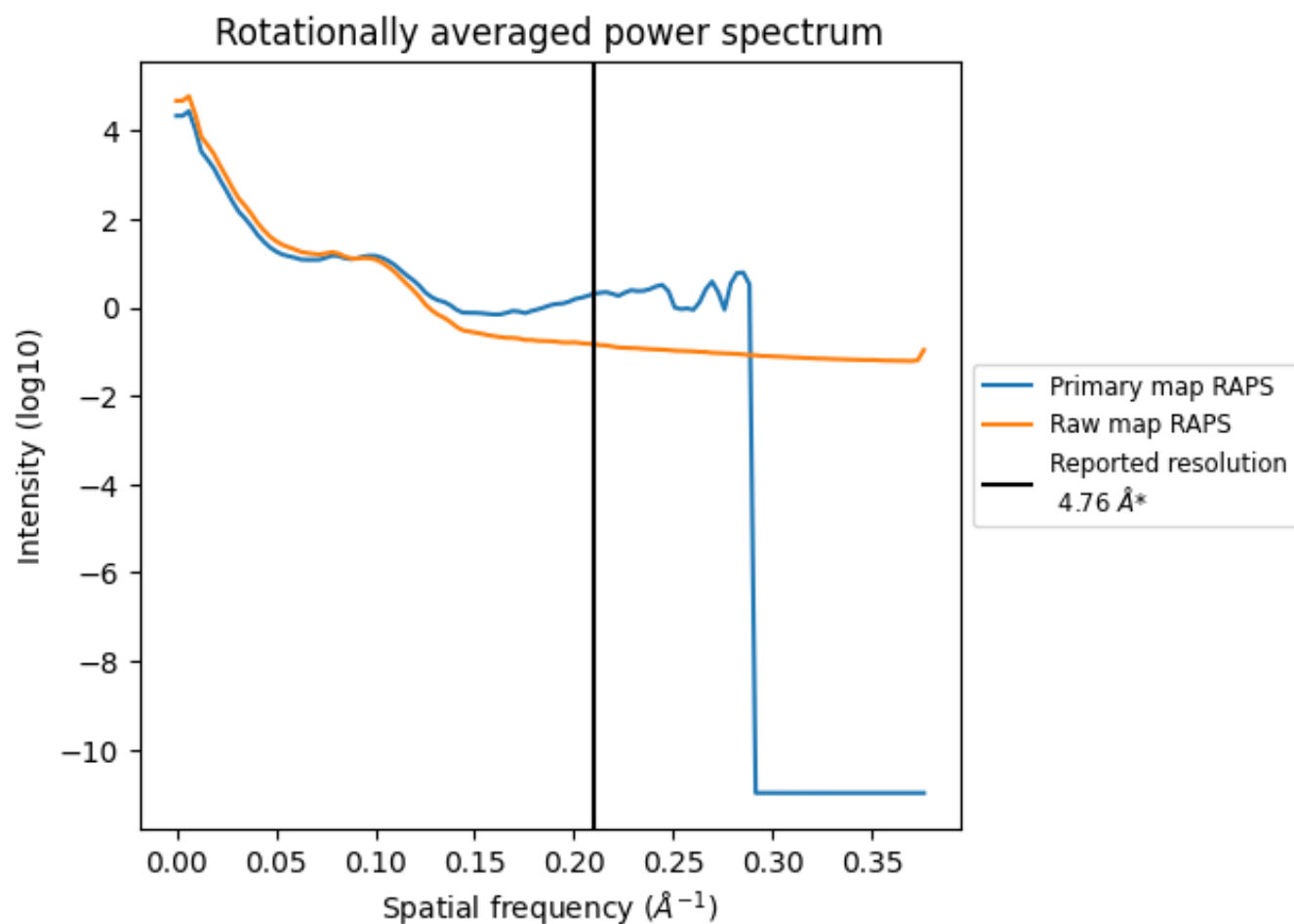
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 321 nm³; this corresponds to an approximate mass of 290 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 ⓘ

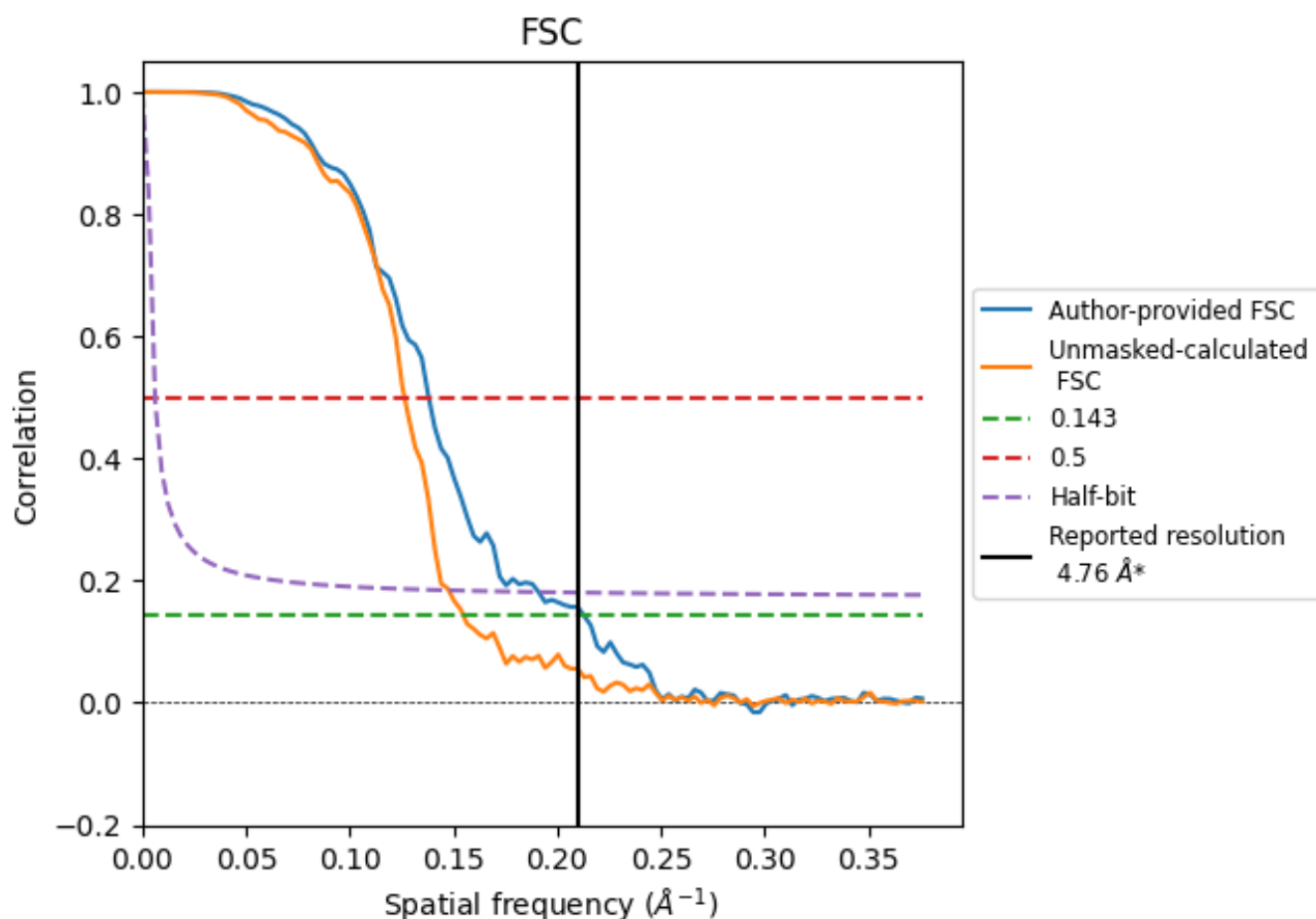


*Reported resolution corresponds to spatial frequency of 0.210 Å⁻¹

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 0.210 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

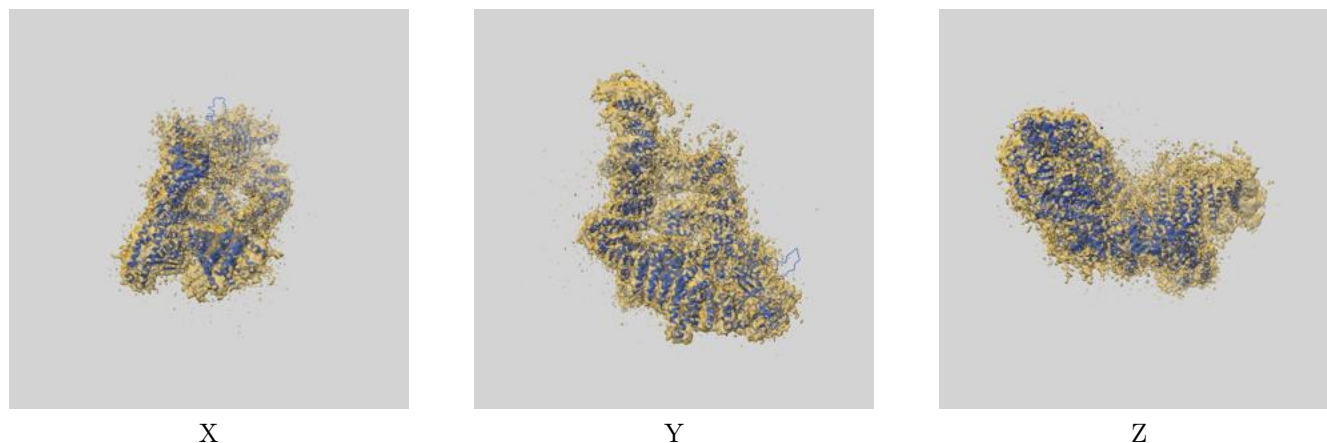
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.76	-	-
Author-provided FSC curve	4.70	7.24	5.23
Unmasked-calculated*	6.46	7.91	6.77

*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 6.46 differs from the reported value 4.76 by more than 10 %

9 Map-model fit [i](#)

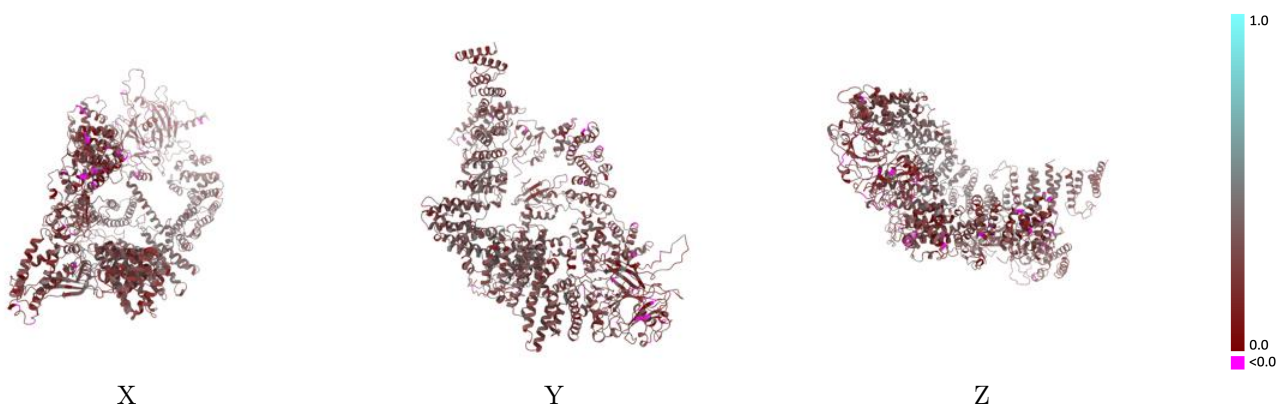
This section contains information regarding the fit between EMDB map EMD-36271 and PDB model 8JHK. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.013 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](#)

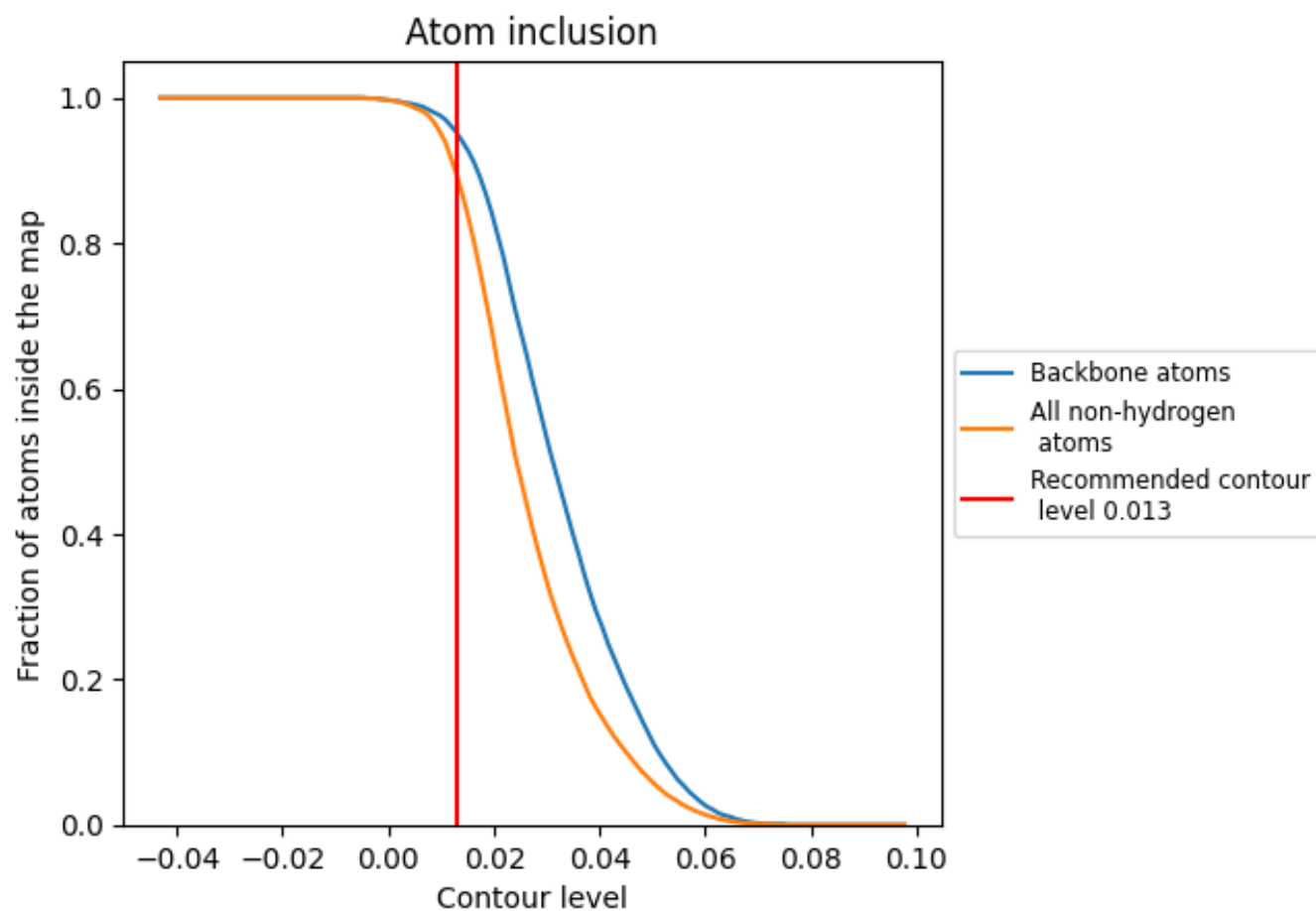


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.2850
A	0.8970	0.2590
B	0.8890	0.2980
E	0.9170	0.2750

