



Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 08:23 PM JST

PDB ID : 9L9U / pdb_00009l9u
EMDB ID : EMD-62913
Title : Arabidopsis GORK WT1
Authors : Yamanashi, T.; Kume, T.; Sekido, N.; Muraoka, Y.; Yokoyama, T.; Tanaka, Y.; Uozumi, N.
Deposited on : 2024-12-31
Resolution : 3.12 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

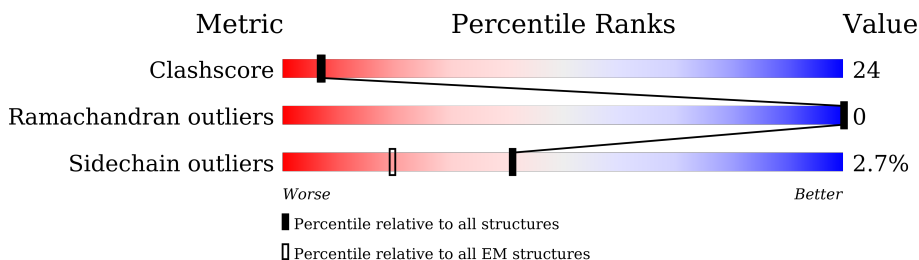
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.12 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	834	<div> <div>17%</div> <div>40%</div> <div>39%</div> <div>•</div> <div>19%</div> </div>
1	B	834	<div> <div>18%</div> <div>44%</div> <div>36%</div> <div>•</div> <div>19%</div> </div>
1	C	834	<div> <div>14%</div> <div>42%</div> <div>37%</div> <div>•</div> <div>19%</div> </div>
1	D	834	<div> <div>14%</div> <div>43%</div> <div>35%</div> <div>•</div> <div>20%</div> </div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 21836 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Potassium channel GORK.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	673	Total	C	N	O	S	0	0
			5459	3539	911	984	25		
1	B	676	Total	C	N	O	S	0	0
			5477	3551	914	987	25		
1	C	672	Total	C	N	O	S	0	0
			5453	3536	910	982	25		
1	D	671	Total	C	N	O	S	0	0
			5447	3533	909	980	25		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q94A76
A	-6	ASP	-	expression tag	UNP Q94A76
A	-5	TYR	-	expression tag	UNP Q94A76
A	-4	LYS	-	expression tag	UNP Q94A76
A	-3	ASP	-	expression tag	UNP Q94A76
A	-2	ASP	-	expression tag	UNP Q94A76
A	-1	ASP	-	expression tag	UNP Q94A76
A	0	ASP	-	expression tag	UNP Q94A76
A	1	LYS	-	expression tag	UNP Q94A76
A	821	HIS	-	expression tag	UNP Q94A76
A	822	HIS	-	expression tag	UNP Q94A76
A	823	HIS	-	expression tag	UNP Q94A76
A	824	HIS	-	expression tag	UNP Q94A76
A	825	HIS	-	expression tag	UNP Q94A76
A	826	HIS	-	expression tag	UNP Q94A76
B	-7	MET	-	initiating methionine	UNP Q94A76
B	-6	ASP	-	expression tag	UNP Q94A76
B	-5	TYR	-	expression tag	UNP Q94A76
B	-4	LYS	-	expression tag	UNP Q94A76
B	-3	ASP	-	expression tag	UNP Q94A76
B	-2	ASP	-	expression tag	UNP Q94A76
B	-1	ASP	-	expression tag	UNP Q94A76

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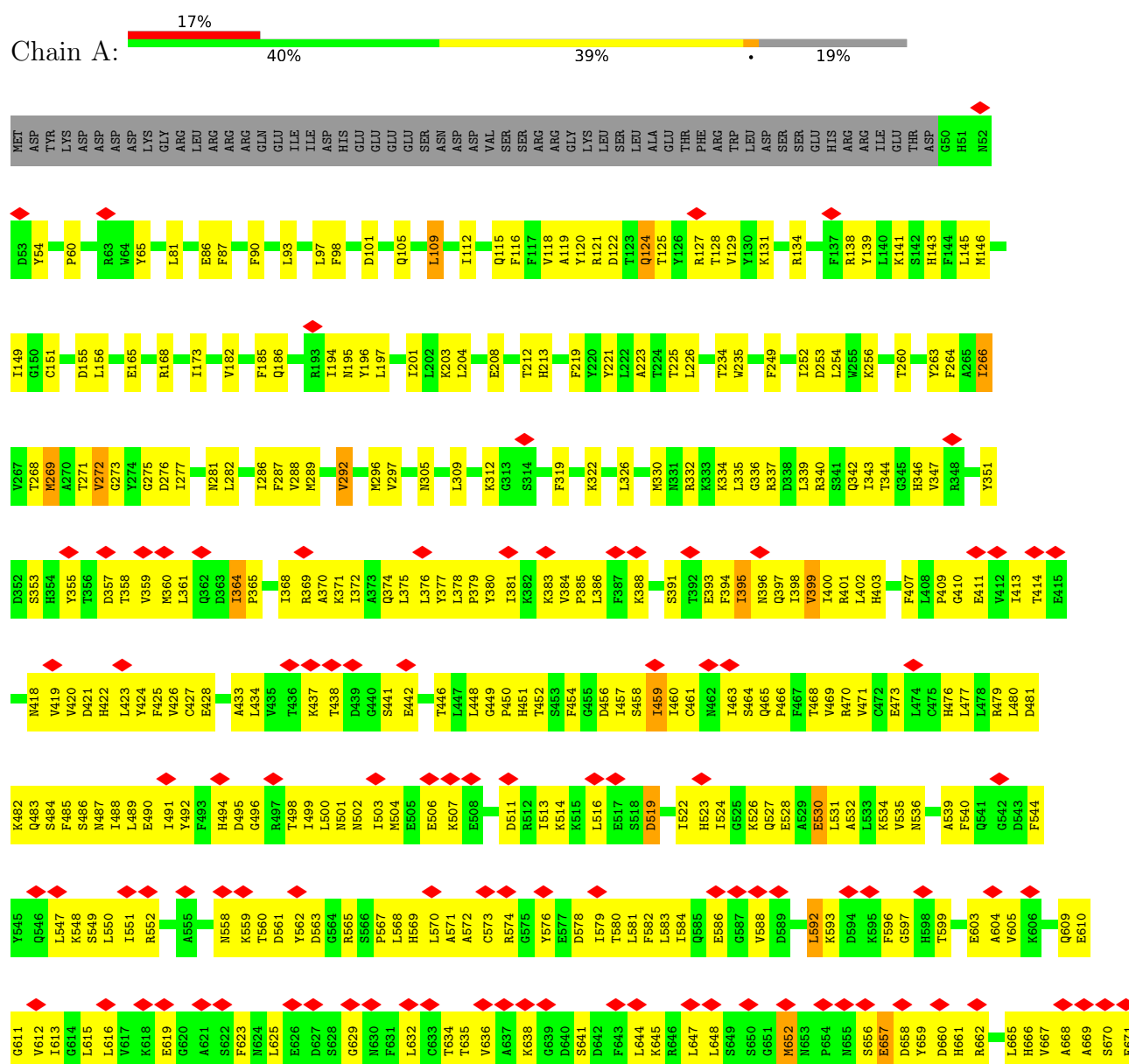
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ASP	-	expression tag	UNP Q94A76
B	1	LYS	-	expression tag	UNP Q94A76
B	821	HIS	-	expression tag	UNP Q94A76
B	822	HIS	-	expression tag	UNP Q94A76
B	823	HIS	-	expression tag	UNP Q94A76
B	824	HIS	-	expression tag	UNP Q94A76
B	825	HIS	-	expression tag	UNP Q94A76
B	826	HIS	-	expression tag	UNP Q94A76
C	-7	MET	-	initiating methionine	UNP Q94A76
C	-6	ASP	-	expression tag	UNP Q94A76
C	-5	TYR	-	expression tag	UNP Q94A76
C	-4	LYS	-	expression tag	UNP Q94A76
C	-3	ASP	-	expression tag	UNP Q94A76
C	-2	ASP	-	expression tag	UNP Q94A76
C	-1	ASP	-	expression tag	UNP Q94A76
C	0	ASP	-	expression tag	UNP Q94A76
C	1	LYS	-	expression tag	UNP Q94A76
C	821	HIS	-	expression tag	UNP Q94A76
C	822	HIS	-	expression tag	UNP Q94A76
C	823	HIS	-	expression tag	UNP Q94A76
C	824	HIS	-	expression tag	UNP Q94A76
C	825	HIS	-	expression tag	UNP Q94A76
C	826	HIS	-	expression tag	UNP Q94A76
D	-7	MET	-	initiating methionine	UNP Q94A76
D	-6	ASP	-	expression tag	UNP Q94A76
D	-5	TYR	-	expression tag	UNP Q94A76
D	-4	LYS	-	expression tag	UNP Q94A76
D	-3	ASP	-	expression tag	UNP Q94A76
D	-2	ASP	-	expression tag	UNP Q94A76
D	-1	ASP	-	expression tag	UNP Q94A76
D	0	ASP	-	expression tag	UNP Q94A76
D	1	LYS	-	expression tag	UNP Q94A76
D	821	HIS	-	expression tag	UNP Q94A76
D	822	HIS	-	expression tag	UNP Q94A76
D	823	HIS	-	expression tag	UNP Q94A76
D	824	HIS	-	expression tag	UNP Q94A76
D	825	HIS	-	expression tag	UNP Q94A76
D	826	HIS	-	expression tag	UNP Q94A76

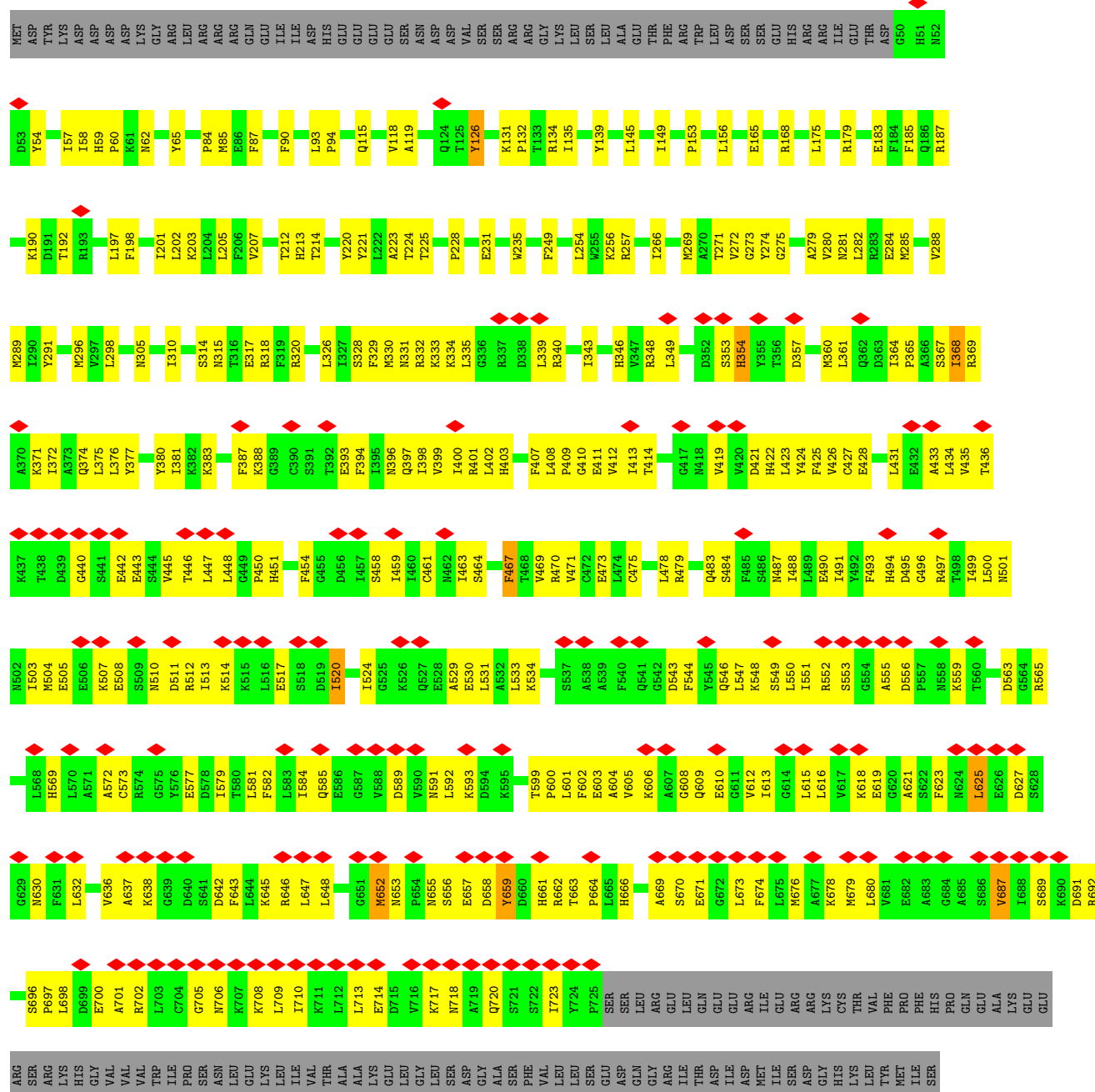
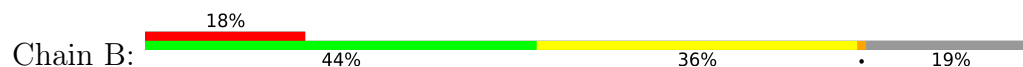
3 Residue-property plots

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

• Molecule 1: Potassium channel GORK



- Molecule 1: Potassium channel GORK



Chain D:  14% 43% 35% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26135	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.610	Depositor
Minimum map value	-0.328	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	315.19998, 315.19998, 315.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.7879999, 0.7879999, 0.7879999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/5586	0.55	0/7555
1	B	0.30	0/5605	0.50	0/7582
1	C	0.28	0/5580	0.48	0/7547
1	D	0.33	0/5574	0.55	0/7539
All	All	0.31	0/22345	0.52	0/30223

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5459	0	5475	301	0
1	B	5477	0	5488	263	0
1	C	5453	0	5470	287	0
1	D	5447	0	5465	293	0
All	All	21836	0	21898	1057	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 24.

All (1057) 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:B:514:LYS:HA	1:B:517:GLU:HG3	1.37	1.02
1:D:420:VAL:HA	1:D:465:GLN:HE21	1.27	0.98
1:C:349:LEU:HD21	1:C:406:TYR:HB2	1.48	0.96
1:A:273:GLY:HA3	1:D:272:VAL:O	1.66	0.94
1:B:601:LEU:HD22	1:B:621:ALA:HB1	1.59	0.84
1:B:361:LEU:HA	1:B:364:ILE:HD12	1.57	0.84
1:C:572:ALA:HA	1:C:612:VAL:HG11	1.60	0.83
1:C:499:ILE:HG22	1:C:503:ILE:HD11	1.60	0.81
1:A:641:SER:HB3	1:A:676:MET:HG3	1.61	0.80
1:B:664:PRO:HB2	1:B:680:LEU:HD21	1.62	0.79
1:A:428:GLU:HG3	1:A:476:HIS:HB3	1.65	0.79
1:A:275:GLY:HA3	1:D:274:TYR:O	1.83	0.79
1:A:226:LEU:HD11	1:A:281:ASN:HD22	1.47	0.78
1:C:520:ILE:HA	1:C:523:HIS:HB3	1.63	0.78
1:D:430:LEU:HD11	1:D:447:LEU:HB3	1.65	0.78
1:C:431:LEU:HB3	1:C:448:LEU:HB2	1.65	0.77
1:D:59:HIS:HD2	1:D:60:PRO:HD2	1.48	0.77
1:B:556:ASP:HB3	1:B:559:LYS:HG2	1.65	0.77
1:A:414:THR:HB	1:A:465:GLN:HE22	1.47	0.77
1:D:547:LEU:HD22	1:D:579:ILE:HG23	1.66	0.77
1:A:581:LEU:HA	1:A:584:ILE:HD12	1.67	0.76
1:C:577:GLU:HB3	1:C:615:LEU:HD11	1.65	0.76
1:B:434:LEU:HB3	1:B:442:GLU:HB3	1.65	0.76
1:A:433:ALA:HA	1:A:469:VAL:HA	1.68	0.76
1:D:420:VAL:HA	1:D:465:GLN:NE2	2.01	0.76
1:B:402:LEU:HB3	1:B:478:LEU:HD11	1.69	0.75
1:C:534:LYS:HE3	1:C:546:GLN:NE2	2.01	0.75
1:D:402:LEU:HD22	1:D:478:LEU:HG	1.67	0.75
1:A:358:THR:HA	1:A:361:LEU:HB2	1.68	0.75
1:A:434:LEU:HB3	1:A:442:GLU:HB3	1.67	0.75
1:C:431:LEU:HD12	1:C:471:VAL:HA	1.69	0.75
1:D:420:VAL:HG11	1:D:459:ILE:HG23	1.69	0.74
1:D:87:PHE:O	1:D:168:ARG:NH2	2.20	0.74
1:D:149:ILE:HG22	1:D:173:ILE:HG21	1.69	0.74
1:A:672:GLY:HA2	1:A:709:LEU:HD22	1.69	0.74
1:B:433:ALA:HB1	1:B:467:PHE:HB2	1.69	0.74
1:B:627:ASP:HB3	1:B:630:ASN:HB3	1.69	0.74
1:B:201:ILE:HG22	1:B:305:ASN:HB3	1.71	0.73
1:D:378:LEU:HD11	1:D:382:LYS:HE3	1.71	0.73
1:B:497:ARG:NH2	1:B:553:SER:HB3	2.04	0.72
1:C:381:ILE:HD11	1:C:398:ILE:HG22	1.71	0.72
1:C:330:MET:HE3	1:C:335:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:ASP:HB3	1:D:559:LYS:HG2	1.70	0.72
1:A:87:PHE:O	1:A:168:ARG:NH2	2.23	0.71
1:B:419:VAL:HA	1:B:464:SER:HA	1.70	0.71
1:B:433:ALA:HB2	1:B:469:VAL:HG22	1.73	0.71
1:B:581:LEU:HD21	1:B:615:LEU:HD22	1.72	0.71
1:A:286:ILE:HA	1:A:289:MET:HE2	1.72	0.71
1:A:330:MET:HE2	1:A:335:LEU:HB2	1.73	0.70
1:C:380:TYR:HA	1:C:383:LYS:HD2	1.74	0.70
1:B:57:ILE:HD11	1:B:132:PRO:HG3	1.74	0.70
1:B:500:LEU:HD11	1:B:524:ILE:HG12	1.73	0.70
1:C:348:ARG:HH12	1:C:352:ASP:HB2	1.55	0.69
1:D:510:ASN:HB3	1:D:513:ILE:HB	1.73	0.69
1:C:666:HIS:NE2	1:C:695:ASN:O	2.24	0.69
1:B:320:ARG:NH2	1:D:191:ASP:O	2.25	0.69
1:D:264:PHE:HB2	1:D:277:ILE:HG13	1.73	0.69
1:D:399:VAL:HA	1:D:402:LEU:HD12	1.75	0.69
1:A:623:PHE:HB3	1:A:625:LEU:HG	1.75	0.69
1:C:402:LEU:HD22	1:C:478:LEU:HB3	1.74	0.69
1:C:381:ILE:HD12	1:C:402:LEU:HD11	1.75	0.69
1:B:383:LYS:HB3	1:B:451:HIS:HB3	1.73	0.68
1:C:603:GLU:N	1:C:603:GLU:OE1	2.24	0.68
1:B:93:LEU:HD12	1:B:94:PRO:HD2	1.75	0.68
1:C:534:LYS:NZ	1:C:546:GLN:HE22	1.91	0.68
1:B:503:ILE:O	1:B:507:LYS:HG2	1.93	0.68
1:D:572:ALA:HA	1:D:612:VAL:HG11	1.75	0.68
1:B:346:HIS:CE1	1:D:365:PRO:HD3	2.29	0.68
1:D:381:ILE:HD11	1:D:478:LEU:HD23	1.75	0.68
1:B:577:GLU:HG2	1:B:612:VAL:HG23	1.74	0.68
1:A:433:ALA:HB3	1:A:446:THR:H	1.59	0.67
1:A:603:GLU:N	1:A:603:GLU:OE1	2.27	0.67
1:A:576:TYR:HB3	1:A:579:ILE:HB	1.76	0.67
1:B:549:SER:HA	1:B:552:ARG:HD2	1.75	0.67
1:D:348:ARG:NH1	1:D:352:ASP:OD2	2.22	0.67
1:A:121:ARG:HG2	1:A:128:THR:HG22	1.77	0.67
1:B:423:LEU:HB2	1:B:459:ILE:HD12	1.77	0.67
1:A:381:ILE:HG23	1:A:395:ILE:HG22	1.77	0.66
1:A:381:ILE:HD11	1:A:425:PHE:CD2	2.31	0.66
1:C:87:PHE:O	1:C:168:ARG:NH2	2.28	0.66
1:A:593:LYS:HD3	1:A:599:THR:HG23	1.78	0.66
1:B:372:ILE:HG23	1:C:335:LEU:HD11	1.77	0.66
1:A:115:GLN:HB3	1:A:139:TYR:HE2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ALA:HA	1:D:135:ILE:HD11	1.76	0.65
1:A:355:TYR:HA	1:A:358:THR:HG23	1.78	0.65
1:A:567:PRO:HB2	1:A:583:LEU:HD21	1.77	0.65
1:B:275:GLY:HA3	1:C:274:TYR:O	1.97	0.65
1:B:408:LEU:HD13	1:D:365:PRO:HG2	1.77	0.65
1:D:517:GLU:HA	1:D:520:ILE:HB	1.79	0.65
1:B:653:ASN:ND2	1:B:656:SER:OG	2.30	0.65
1:A:610:GLU:HA	1:A:613:ILE:HD12	1.79	0.64
1:A:536:ASN:ND2	1:A:570:LEU:HD11	2.12	0.64
1:C:669:ALA:HB1	1:C:701:ALA:HB2	1.79	0.64
1:C:629:GLY:HA3	1:C:657:GLU:H	1.62	0.64
1:C:90:PHE:O	1:C:168:ARG:NH2	2.31	0.64
1:C:120:TYR:HE2	1:C:135:ILE:HA	1.63	0.64
1:A:401:ARG:HE	1:A:484:SER:HB3	1.63	0.64
1:A:483:GLN:OE1	1:A:483:GLN:N	2.30	0.64
1:A:519:ASP:N	1:A:519:ASP:OD1	2.30	0.64
1:D:499:ILE:O	1:D:503:ILE:HG12	1.97	0.64
1:D:530:GLU:O	1:D:534:LYS:HG3	1.98	0.64
1:A:101:ASP:OD1	1:A:105:GLN:NE2	2.30	0.64
1:D:513:ILE:HA	1:D:516:LEU:HB2	1.80	0.64
1:A:669:ALA:HA	1:A:709:LEU:HD21	1.81	0.63
1:B:179:ARG:O	1:B:183:GLU:HG2	1.99	0.63
1:A:648:LEU:HD13	1:A:683:ALA:HB2	1.81	0.63
1:A:673:LEU:HB3	1:A:676:MET:HE2	1.79	0.63
1:B:551:ILE:HA	1:B:555:ALA:HB3	1.79	0.63
1:C:629:GLY:HA2	1:C:656:SER:HB3	1.80	0.63
1:A:420:VAL:HB	1:A:459:ILE:HG22	1.80	0.63
1:A:507:LYS:HE2	1:A:513:ILE:HG21	1.81	0.63
1:D:457:ILE:HD13	1:D:513:ILE:HG21	1.79	0.63
1:A:632:LEU:HD11	1:A:647:LEU:HD22	1.81	0.63
1:B:702:ARG:HH21	1:B:714:GLU:HG2	1.63	0.63
1:B:402:LEU:HD13	1:B:478:LEU:HD21	1.80	0.63
1:B:374:GLN:HA	1:B:399:VAL:HG11	1.81	0.63
1:A:578:ASP:OD1	1:A:579:ILE:N	2.32	0.62
1:B:126:TYR:HB2	1:C:474:LEU:HD11	1.80	0.62
1:C:60:PRO:HD3	1:C:119:ALA:HB3	1.81	0.62
1:A:282:LEU:HD13	1:D:256:LYS:HD2	1.81	0.62
1:A:271:THR:HA	1:D:272:VAL:HG13	1.80	0.62
1:A:593:LYS:HB3	1:A:597:GLY:HA2	1.80	0.62
1:B:115:GLN:HB3	1:B:139:TYR:CE2	2.35	0.62
1:B:669:ALA:HA	1:B:709:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:PHE:O	1:D:168:ARG:NH2	2.29	0.62
1:D:551:ILE:HA	1:D:555:ALA:HB3	1.81	0.62
1:B:648:LEU:HD11	1:B:680:LEU:HD12	1.80	0.62
1:A:658:ASP:OD1	1:A:659:TYR:N	2.33	0.62
1:A:272:VAL:HG13	1:C:271:THR:HA	1.81	0.62
1:B:274:TYR:O	1:D:275:GLY:HA3	2.00	0.62
1:B:499:ILE:O	1:B:503:ILE:HG13	2.00	0.62
1:C:413:ILE:HG22	1:C:414:THR:HG23	1.82	0.62
1:D:507:LYS:HG2	1:D:517:GLU:HB2	1.81	0.62
1:A:60:PRO:HD3	1:A:119:ALA:HB3	1.82	0.62
1:A:458:SER:HB2	1:A:464:SER:HA	1.81	0.62
1:D:540:PHE:HD1	1:D:574:ARG:HD3	1.65	0.62
1:D:396:ASN:O	1:D:400:ILE:HG13	2.00	0.61
1:B:368:ILE:O	1:B:372:ILE:HG13	2.00	0.61
1:C:435:VAL:O	1:C:442:GLU:HA	2.01	0.61
1:D:591:ASN:HB3	1:D:624:ASN:ND2	2.15	0.61
1:A:421:ASP:CG	1:A:422:HIS:H	2.09	0.61
1:C:233:TYR:O	1:C:281:ASN:ND2	2.33	0.61
1:C:665:LEU:HD21	1:C:685:ALA:HB1	1.81	0.61
1:D:577:GLU:OE2	1:D:577:GLU:N	2.31	0.61
1:D:601:LEU:O	1:D:605:VAL:HG13	2.01	0.61
1:D:644:LEU:O	1:D:648:LEU:HG	2.00	0.61
1:D:204:LEU:HD11	1:D:301:TYR:HB3	1.83	0.61
1:C:673:LEU:HD22	1:D:675:LEU:HD23	1.82	0.61
1:B:495:ASP:O	1:B:499:ILE:HD12	2.01	0.60
1:B:572:ALA:HB1	1:B:604:ALA:HB2	1.83	0.60
1:D:600:PRO:HB2	1:D:616:LEU:HD11	1.83	0.60
1:A:568:LEU:HD21	1:A:588:VAL:HG21	1.83	0.60
1:B:333:LYS:HD3	1:D:376:LEU:HD11	1.83	0.60
1:C:698:LEU:HD11	1:C:714:GLU:HG3	1.82	0.60
1:C:378:LEU:HD12	1:C:399:VAL:HG21	1.83	0.60
1:C:534:LYS:CE	1:C:546:GLN:NE2	2.63	0.60
1:D:335:LEU:HD22	1:D:340:ARG:HG3	1.82	0.60
1:A:420:VAL:HG12	1:A:464:SER:HB3	1.82	0.60
1:B:608:GLY:HA3	1:B:646:ARG:NH1	2.17	0.60
1:D:91:ARG:NH1	1:D:165:GLU:OE2	2.34	0.60
1:D:51:HIS:ND1	1:D:54:TYR:O	2.35	0.60
1:B:326:LEU:HG	1:B:330:MET:HE3	1.82	0.60
1:B:507:LYS:NZ	1:B:513:ILE:HG22	2.17	0.60
1:C:538:ALA:HB3	1:C:547:LEU:HD13	1.84	0.60
1:D:423:LEU:HD12	1:D:480:LEU:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ILE:HD12	1:D:364:ILE:H	1.67	0.60
1:C:434:LEU:HD22	1:C:442:GLU:HB2	1.83	0.59
1:A:692:ARG:NH1	1:D:671:GLU:OE2	2.36	0.59
1:A:422:HIS:HD2	1:A:482:LYS:H	1.49	0.59
1:B:314:SER:HB3	1:B:317:GLU:HB3	1.83	0.59
1:B:388:LYS:NZ	1:B:505:GLU:OE1	2.34	0.59
1:B:501:ASN:O	1:B:504:MET:HG2	2.02	0.59
1:B:657:GLU:HB3	1:B:661:HIS:HA	1.83	0.59
1:A:319:PHE:HA	1:A:351:TYR:CE2	2.37	0.59
1:B:461:CYS:HB2	1:B:463:ILE:HG22	1.82	0.59
1:B:637:ALA:HA	1:C:659:TYR:CD2	2.38	0.59
1:B:692:ARG:HH12	1:C:671:GLU:HG2	1.67	0.59
1:C:377:TYR:HB2	1:C:399:VAL:HG13	1.83	0.59
1:D:675:LEU:HA	1:D:678:LYS:HD3	1.85	0.59
1:A:466:PRO:HG3	1:A:516:LEU:HD11	1.85	0.59
1:A:565:ARG:NH1	1:D:563:ASP:OD1	2.35	0.59
1:B:458:SER:OG	1:B:463:ILE:O	2.20	0.59
1:B:496:GLY:HA2	1:B:499:ILE:HD12	1.84	0.59
1:C:495:ASP:O	1:C:499:ILE:HG12	2.03	0.59
1:A:535:VAL:HG22	1:A:550:LEU:HB3	1.84	0.59
1:D:520:ILE:HA	1:D:523:HIS:HB2	1.85	0.59
1:A:676:MET:SD	1:A:676:MET:N	2.76	0.59
1:C:101:ASP:O	1:C:105:GLN:NE2	2.36	0.59
1:D:669:ALA:HA	1:D:709:LEU:HD21	1.85	0.59
1:A:532:ALA:HB2	1:A:559:LYS:HG2	1.85	0.58
1:B:231:GLU:HB2	1:B:249:PHE:HE1	1.66	0.58
1:A:698:LEU:HD11	1:A:714:GLU:HG3	1.85	0.58
1:A:197:LEU:HB2	1:A:309:LEU:HD13	1.85	0.58
1:A:565:ARG:HD3	1:A:596:PHE:HD2	1.68	0.58
1:B:642:ASP:O	1:B:645:LYS:HG2	2.03	0.58
1:C:153:PRO:HB2	1:C:156:LEU:HB2	1.84	0.58
1:B:387:PHE:CZ	1:B:398:ILE:HG21	2.39	0.58
1:B:692:ARG:NH2	1:C:670:SER:O	2.37	0.58
1:A:272:VAL:O	1:C:273:GLY:HA3	2.03	0.58
1:B:673:LEU:HD13	1:B:676:MET:HE2	1.86	0.58
1:C:387:PHE:HB3	1:C:390:CYS:SG	2.44	0.58
1:C:557:PRO:HB2	1:C:588:VAL:HG21	1.85	0.58
1:C:644:LEU:HA	1:C:647:LEU:HD12	1.85	0.58
1:B:273:GLY:HA3	1:C:272:VAL:O	2.03	0.58
1:B:487:ASN:O	1:B:491:ILE:HG12	2.04	0.58
1:C:461:CYS:SG	1:C:520:ILE:HG21	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:LYS:HE2	1:D:512:ARG:HH12	1.67	0.58
1:B:520:ILE:O	1:B:524:ILE:HG13	2.04	0.58
1:B:720:GLN:HA	1:B:723:ILE:HB	1.85	0.58
1:C:364:ILE:HD12	1:C:364:ILE:H	1.68	0.58
1:D:534:LYS:HD3	1:D:550:LEU:HD11	1.86	0.58
1:D:568:LEU:HD22	1:D:588:VAL:HB	1.86	0.58
1:A:667:VAL:O	1:A:671:GLU:HG2	2.04	0.57
1:B:433:ALA:HB3	1:B:445:VAL:HG21	1.86	0.57
1:A:676:MET:HA	1:A:679:MET:HG2	1.86	0.57
1:B:507:LYS:HD3	1:B:520:ILE:HG13	1.84	0.57
1:B:659:TYR:OH	1:C:630:ASN:OD1	2.21	0.57
1:C:564:GLY:HA3	1:C:595:LYS:HG3	1.86	0.57
1:D:368:ILE:O	1:D:372:ILE:HG12	2.05	0.57
1:D:539:ALA:HA	1:D:579:ILE:HD13	1.87	0.57
1:A:526:LYS:HD3	1:A:526:LYS:N	2.19	0.57
1:B:281:ASN:ND2	1:B:284:GLU:OE2	2.36	0.57
1:B:511:ASP:HA	1:B:514:LYS:HD3	1.86	0.57
1:C:560:THR:HB	1:C:564:GLY:HA2	1.86	0.57
1:D:459:ILE:HG13	1:D:460:ILE:HG13	1.87	0.57
1:D:524:ILE:O	1:D:528:GLU:HG3	2.05	0.57
1:A:346:HIS:CD2	1:C:364:ILE:HA	2.40	0.57
1:B:493:PHE:O	1:B:497:ARG:HG3	2.05	0.57
1:D:387:PHE:CE2	1:D:398:ILE:HD13	2.40	0.57
1:D:594:ASP:OD1	1:D:598:HIS:N	2.37	0.57
1:D:644:LEU:HD12	1:D:676:MET:HE1	1.86	0.57
1:D:666:HIS:NE2	1:D:695:ASN:O	2.37	0.57
1:A:365:PRO:HD2	1:D:346:HIS:HD2	1.70	0.57
1:A:463:ILE:HG13	1:A:519:ASP:HB3	1.85	0.57
1:A:260:THR:HG23	1:A:277:ILE:HD13	1.87	0.57
1:B:377:TYR:HB3	1:B:478:LEU:HD21	1.85	0.57
1:B:483:GLN:O	1:B:487:ASN:ND2	2.38	0.57
1:B:643:PHE:HA	1:B:646:ARG:HH21	1.70	0.57
1:D:551:ILE:HD12	1:D:555:ALA:HB3	1.87	0.57
1:D:632:LEU:HD22	1:D:644:LEU:HD21	1.86	0.57
1:B:706:ASN:HB3	1:B:709:LEU:HB3	1.87	0.57
1:C:387:PHE:CE1	1:C:425:PHE:HE2	2.22	0.57
1:C:394:PHE:O	1:C:398:ILE:HG12	2.05	0.57
1:C:408:LEU:HA	1:C:474:LEU:HD23	1.85	0.57
1:A:339:LEU:HD21	1:C:372:ILE:HD13	1.86	0.57
1:B:573:CYS:HB3	1:B:603:GLU:HB3	1.85	0.57
1:C:623:PHE:HB3	1:C:625:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:PHE:O	1:A:574:ARG:NH1	2.38	0.56
1:A:648:LEU:HA	1:A:652:MET:HG3	1.86	0.56
1:D:60:PRO:HD3	1:D:119:ALA:HB3	1.86	0.56
1:C:401:ARG:HB2	1:C:480:LEU:HD11	1.87	0.56
1:D:568:LEU:HD13	1:D:583:LEU:HB2	1.87	0.56
1:A:343:ILE:O	1:A:347:VAL:HG23	2.05	0.56
1:A:401:ARG:HH22	1:D:419:VAL:HG11	1.70	0.56
1:A:665:LEU:HD21	1:A:687:VAL:HG22	1.86	0.56
1:A:673:LEU:HB3	1:A:676:MET:CE	2.35	0.56
1:C:368:ILE:O	1:C:372:ILE:HG12	2.04	0.56
1:D:285:MET:O	1:D:289:MET:HG3	2.04	0.56
1:D:500:LEU:O	1:D:504:MET:HG2	2.05	0.56
1:C:681:VAL:HG11	1:C:716:VAL:HG21	1.85	0.56
1:A:361:LEU:HD23	1:A:364:ILE:HD11	1.88	0.56
1:D:423:LEU:HD22	1:D:424:TYR:H	1.69	0.56
1:D:461:CYS:SG	1:D:520:ILE:HG23	2.46	0.56
1:D:496:GLY:HA2	1:D:499:ILE:HG12	1.88	0.56
1:A:422:HIS:CD2	1:A:481:ASP:HA	2.40	0.56
1:C:701:ALA:O	1:C:705:GLY:N	2.38	0.56
1:A:426:VAL:HA	1:A:477:LEU:HD23	1.88	0.56
1:B:593:LYS:NZ	1:B:623:PHE:O	2.37	0.56
1:D:357:ASP:O	1:D:361:LEU:HG	2.06	0.56
1:A:551:ILE:HG21	1:A:586:GLU:HG3	1.88	0.56
1:C:328:SER:O	1:C:332:ARG:HG2	2.06	0.56
1:D:154:TRP:HB2	1:D:174:ARG:HH21	1.70	0.56
1:D:226:LEU:O	1:D:250:ARG:NH2	2.38	0.56
1:D:454:PHE:CE2	1:D:469:VAL:HG11	2.41	0.56
1:B:65:TYR:OH	1:B:115:GLN:OE1	2.23	0.55
1:C:127:ARG:HE	1:C:128:THR:H	1.54	0.55
1:A:503:ILE:O	1:A:507:LYS:HD3	2.06	0.55
1:B:145:LEU:O	1:B:149:ILE:HG12	2.06	0.55
1:D:81:LEU:O	1:D:213:HIS:NE2	2.36	0.55
1:A:322:LYS:HD2	1:A:347:VAL:HG13	1.88	0.55
1:C:355:TYR:O	1:C:358:THR:HG22	2.06	0.55
1:A:86:GLU:HA	1:A:90:PHE:HD2	1.71	0.55
1:B:256:LYS:HA	1:D:282:LEU:HD21	1.88	0.55
1:D:343:ILE:O	1:D:347:VAL:HG23	2.06	0.55
1:C:421:ASP:O	1:C:422:HIS:ND1	2.40	0.55
1:C:666:HIS:HD2	1:C:700:GLU:HG3	1.71	0.55
1:D:171:LEU:HD23	1:D:174:ARG:HE	1.72	0.55
1:A:223:ALA:HB2	1:A:235:TRP:NE1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:LEU:HD21	1:C:650:SER:HB3	1.89	0.55
1:A:332:ARG:O	1:A:332:ARG:HD3	2.07	0.55
1:A:561:ASP:CG	1:A:562:TYR:H	2.14	0.55
1:A:576:TYR:O	1:A:580:THR:HG23	2.07	0.55
1:C:76:ALA:HA	1:C:108:PHE:HZ	1.72	0.55
1:C:127:ARG:HH21	1:C:128:THR:HG23	1.72	0.55
1:D:208:GLU:O	1:D:212:THR:HG23	2.07	0.55
1:D:523:HIS:O	1:D:527:GLN:HB2	2.07	0.55
1:A:149:ILE:HG22	1:A:173:ILE:HG21	1.89	0.55
1:B:346:HIS:ND1	1:D:365:PRO:HD3	2.22	0.55
1:B:435:VAL:HG22	1:B:467:PHE:HB3	1.89	0.55
1:A:584:ILE:HA	1:A:588:VAL:HG12	1.88	0.55
1:B:343:ILE:HG12	1:D:368:ILE:HG21	1.88	0.55
1:A:666:HIS:CE1	1:A:697:PRO:HD3	2.41	0.54
1:B:397:GLN:HE22	1:C:418:ASN:ND2	2.06	0.54
1:B:655:ASN:HB2	1:B:663:THR:HB	1.89	0.54
1:A:536:ASN:ND2	1:D:562:TYR:CZ	2.75	0.54
1:C:407:PHE:O	1:C:474:LEU:HA	2.08	0.54
1:D:415:GLU:HA	1:D:468:THR:HG23	1.89	0.54
1:D:452:THR:HG22	1:D:453:SER:H	1.72	0.54
1:B:394:PHE:O	1:B:398:ILE:HG12	2.06	0.54
1:D:59:HIS:CD2	1:D:60:PRO:HD2	2.37	0.54
1:D:115:GLN:HA	1:D:118:VAL:HG12	1.89	0.54
1:A:609:GLN:O	1:A:613:ILE:HG13	2.07	0.54
1:B:282:LEU:HD21	1:C:256:LYS:HA	1.89	0.54
1:C:220:TYR:OH	1:C:257:ARG:NH1	2.35	0.54
1:B:426:VAL:HG12	1:B:450:PRO:HA	1.90	0.54
1:B:632:LEU:HD21	1:B:652:MET:HE1	1.88	0.54
1:C:664:PRO:HG2	1:C:680:LEU:HD21	1.90	0.54
1:D:551:ILE:HG21	1:D:582:PHE:CE2	2.42	0.54
1:A:494:HIS:O	1:A:498:THR:OG1	2.24	0.54
1:C:648:LEU:HD23	1:C:652:MET:HB3	1.88	0.54
1:C:112:ILE:H	1:C:112:ILE:HD12	1.71	0.54
1:A:701:ALA:HB2	1:A:713:LEU:HD12	1.89	0.54
1:B:330:MET:HG2	1:B:335:LEU:HD22	1.90	0.54
1:B:484:SER:O	1:B:488:ILE:HG13	2.08	0.54
1:A:568:LEU:HD12	1:A:568:LEU:H	1.73	0.53
1:B:582:PHE:HA	1:B:585:GLN:NE2	2.23	0.53
1:C:660:ASP:HA	1:C:692:ARG:HH21	1.73	0.53
1:D:459:ILE:HD12	1:D:485:PHE:CD2	2.43	0.53
1:A:65:TYR:CZ	1:A:118:VAL:HG21	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ALA:HB2	1:B:235:TRP:NE1	2.23	0.53
1:A:146:MET:HE2	1:A:146:MET:HA	1.89	0.53
1:A:346:HIS:CD2	1:C:365:PRO:HD3	2.44	0.53
1:D:335:LEU:HD23	1:D:336:GLY:H	1.73	0.53
1:A:558:ASN:HD21	1:A:588:VAL:HA	1.71	0.53
1:B:320:ARG:HH22	1:D:191:ASP:C	2.17	0.53
1:B:331:ASN:HA	1:B:340:ARG:HH22	1.74	0.53
1:B:581:LEU:HG	1:B:615:LEU:HD13	1.90	0.53
1:C:178:VAL:O	1:C:182:VAL:HG23	2.08	0.53
1:D:456:ASP:N	1:D:456:ASP:OD1	2.41	0.53
1:D:475:CYS:SG	1:D:477:LEU:HD11	2.49	0.53
1:A:579:ILE:O	1:A:583:LEU:HD13	2.08	0.53
1:A:565:ARG:HH21	1:A:603:GLU:HG2	1.74	0.53
1:A:572:ALA:HB1	1:A:604:ALA:HB2	1.90	0.53
1:A:632:LEU:HG	1:A:644:LEU:HD11	1.89	0.53
1:B:431:LEU:HB3	1:B:448:LEU:HB2	1.90	0.53
1:D:434:LEU:HA	1:D:442:GLU:OE2	2.09	0.53
1:D:622:SER:O	1:D:624:ASN:ND2	2.40	0.53
1:D:348:ARG:HD2	1:D:351:TYR:HE1	1.74	0.53
1:D:561:ASP:OD1	1:D:563:ASP:N	2.35	0.53
1:A:407:PHE:CD1	1:A:477:LEU:HD12	2.44	0.53
1:A:423:LEU:HD23	1:A:423:LEU:H	1.74	0.53
1:A:437:LYS:HB2	1:A:441:SER:H	1.74	0.53
1:A:522:ILE:HG22	1:A:526:LYS:HE2	1.91	0.53
1:A:565:ARG:NE	1:A:569:HIS:HB3	2.23	0.53
1:C:454:PHE:CD2	1:C:469:VAL:HG21	2.44	0.53
1:B:605:VAL:HG13	1:B:646:ARG:HB2	1.91	0.52
1:A:353:SER:HB2	1:A:355:TYR:CE2	2.45	0.52
1:A:413:ILE:HD11	1:A:471:VAL:HG22	1.90	0.52
1:A:539:ALA:HA	1:A:579:ILE:HD13	1.91	0.52
1:B:54:TYR:CE1	1:B:131:LYS:HG2	2.43	0.52
1:C:413:ILE:HG21	1:C:454:PHE:CZ	2.44	0.52
1:C:503:ILE:HG22	1:C:507:LYS:HD3	1.92	0.52
1:D:675:LEU:HD12	1:D:676:MET:N	2.24	0.52
1:A:571:ALA:HB1	1:A:580:THR:HG22	1.90	0.52
1:B:266:ILE:HG21	1:D:289:MET:HA	1.91	0.52
1:B:320:ARG:HH12	1:D:192:THR:HG22	1.75	0.52
1:B:662:ARG:HH22	1:B:670:SER:HB3	1.74	0.52
1:C:335:LEU:O	1:C:340:ARG:NH1	2.41	0.52
1:D:165:GLU:OE1	1:D:168:ARG:NH1	2.39	0.52
1:D:480:LEU:HG	1:D:485:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HG21	1:B:65:TYR:HB2	1.92	0.52
1:C:500:LEU:HA	1:C:503:ILE:HG12	1.90	0.52
1:D:308:ALA:HA	1:D:311:VAL:HG12	1.91	0.52
1:D:536:ASN:ND2	1:D:561:ASP:HB3	2.25	0.52
1:B:581:LEU:HD23	1:B:584:ILE:HD12	1.91	0.52
1:D:673:LEU:HB3	1:D:676:MET:HB3	1.92	0.52
1:A:196:TYR:HD2	1:D:320:ARG:HG3	1.75	0.52
1:B:198:PHE:O	1:B:201:ILE:HG13	2.09	0.52
1:B:544:PHE:O	1:B:548:LYS:HG3	2.10	0.52
1:D:381:ILE:HG21	1:D:398:ILE:HD11	1.92	0.52
1:D:657:GLU:HG3	1:D:663:THR:HG22	1.91	0.52
1:B:357:ASP:HB3	1:C:329:PHE:HB2	1.92	0.52
1:B:412:VAL:HA	1:B:470:ARG:HA	1.92	0.52
1:B:563:ASP:OD1	1:C:565:ARG:NH1	2.43	0.52
1:C:565:ARG:HG2	1:C:594:ASP:HB2	1.92	0.52
1:C:666:HIS:CE1	1:C:697:PRO:HD3	2.45	0.52
1:A:393:GLU:O	1:A:397:GLN:HG2	2.10	0.51
1:A:413:ILE:HD12	1:A:413:ILE:H	1.74	0.51
1:A:610:GLU:CD	1:A:610:GLU:H	2.18	0.51
1:C:288:VAL:O	1:C:292:VAL:HG22	2.10	0.51
1:A:377:TYR:HB2	1:A:399:VAL:HG22	1.91	0.51
1:C:65:TYR:CE1	1:C:118:VAL:HG21	2.45	0.51
1:D:84:PRO:HG2	1:D:214:THR:HG22	1.91	0.51
1:A:368:ILE:O	1:A:372:ILE:HG12	2.11	0.51
1:A:401:ARG:HH22	1:D:419:VAL:HG21	1.76	0.51
1:A:487:ASN:O	1:A:491:ILE:HG12	2.11	0.51
1:D:102:ILE:HD11	1:D:156:LEU:HD21	1.92	0.51
1:D:315:ASN:HA	1:D:318:ARG:HD2	1.93	0.51
1:B:454:PHE:CE2	1:B:469:VAL:HG21	2.46	0.51
1:C:421:ASP:OD1	1:C:421:ASP:N	2.37	0.51
1:C:423:LEU:HB2	1:C:459:ILE:HD12	1.92	0.51
1:C:454:PHE:CE2	1:C:469:VAL:HG11	2.46	0.51
1:D:432:GLU:HG3	1:D:444:SER:HB2	1.91	0.51
1:A:424:TYR:HB2	1:A:454:PHE:CD2	2.45	0.51
1:B:547:LEU:HD21	1:B:579:ILE:HD13	1.93	0.51
1:B:589:ASP:HB3	1:B:592:LEU:HG	1.92	0.51
1:B:591:ASN:HA	1:B:600:PRO:HD2	1.93	0.51
1:C:223:ALA:HB2	1:C:235:TRP:NE1	2.25	0.51
1:C:632:LEU:HD13	1:C:652:MET:HE2	1.92	0.51
1:D:195:ASN:OD1	1:D:196:TYR:N	2.44	0.51
1:B:330:MET:HA	1:B:335:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:ASP:HB3	1:B:546:GLN:HB3	1.91	0.51
1:C:108:PHE:CE1	1:C:177:ARG:HD2	2.45	0.51
1:C:129:VAL:HG11	1:C:134:ARG:HE	1.75	0.51
1:D:526:LYS:O	1:D:530:GLU:HB3	2.10	0.51
1:A:326:LEU:HD13	1:A:343:ILE:HD11	1.93	0.51
1:B:533:LEU:HB3	1:C:533:LEU:HD23	1.93	0.51
1:C:548:LYS:HB2	1:C:548:LYS:NZ	2.26	0.51
1:D:648:LEU:HD22	1:D:683:ALA:HB2	1.92	0.51
1:D:678:LYS:HG2	1:D:679:MET:N	2.25	0.51
1:C:415:GLU:HA	1:C:468:THR:HG23	1.93	0.51
1:D:99:VAL:HG13	1:D:100:LEU:HD22	1.91	0.51
1:B:431:LEU:HD12	1:B:471:VAL:HA	1.92	0.51
1:A:165:GLU:OE2	1:A:168:ARG:NH1	2.44	0.51
1:B:280:VAL:HG13	1:C:241:LEU:HB3	1.93	0.51
1:C:533:LEU:HD21	1:C:562:TYR:HE2	1.76	0.51
1:C:634:THR:O	1:C:638:LYS:HG3	2.11	0.51
1:A:282:LEU:HD11	1:D:259:THR:HB	1.92	0.50
1:C:335:LEU:HD13	1:C:339:LEU:HD21	1.93	0.50
1:C:623:PHE:CE2	1:C:652:MET:HA	2.46	0.50
1:C:643:PHE:HB2	1:C:646:ARG:HH21	1.76	0.50
1:D:241:LEU:HD21	1:D:276:ASP:HB2	1.92	0.50
1:D:665:LEU:HA	1:D:680:LEU:HD13	1.92	0.50
1:A:511:ASP:O	1:A:514:LYS:HG2	2.11	0.50
1:C:330:MET:HE1	1:C:340:ARG:HA	1.93	0.50
1:D:387:PHE:CE1	1:D:394:PHE:HE2	2.29	0.50
1:B:249:PHE:O	1:B:257:ARG:HD2	2.11	0.50
1:B:381:ILE:HD11	1:B:402:LEU:HD11	1.92	0.50
1:B:678:LYS:HG3	1:B:679:MET:N	2.24	0.50
1:C:378:LEU:HG	1:C:382:LYS:HE3	1.94	0.50
1:D:457:ILE:HG12	1:D:507:LYS:HE2	1.94	0.50
1:A:256:LYS:NZ	1:C:233:TYR:OH	2.39	0.50
1:B:428:GLU:O	1:B:475:CYS:HA	2.11	0.50
1:C:131:LYS:HD2	1:C:132:PRO:HD2	1.91	0.50
1:D:62:ASN:ND2	1:D:64:TRP:HB2	2.26	0.50
1:A:434:LEU:HB2	1:A:468:THR:HB	1.92	0.50
1:B:220:TYR:O	1:B:224:THR:HG23	2.11	0.50
1:B:409:PRO:HG3	1:B:473:GLU:HA	1.93	0.50
1:D:514:LYS:HA	1:D:517:GLU:HB3	1.93	0.50
1:B:410:GLY:N	1:B:471:VAL:O	2.38	0.50
1:C:420:VAL:O	1:C:482:LYS:HD2	2.11	0.50
1:A:394:PHE:CE1	1:A:488:ILE:HG23	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ASP:OD1	1:A:457:ILE:N	2.43	0.50
1:C:579:ILE:O	1:C:583:LEU:HG	2.11	0.50
1:C:698:LEU:HD13	1:C:713:LEU:HB2	1.92	0.50
1:D:223:ALA:HB2	1:D:235:TRP:NE1	2.27	0.50
1:D:601:LEU:HD11	1:D:650:SER:HB3	1.92	0.50
1:A:330:MET:O	1:A:334:LYS:N	2.45	0.50
1:A:498:THR:O	1:A:502:ASN:ND2	2.45	0.50
1:A:568:LEU:HG	1:A:583:LEU:HD23	1.94	0.50
1:C:220:TYR:O	1:C:224:THR:HG23	2.12	0.50
1:D:240:LYS:NZ	1:D:247:GLU:OE2	2.45	0.50
1:A:402:LEU:HD21	1:A:425:PHE:CE2	2.47	0.50
1:A:547:LEU:HD22	1:A:579:ILE:HG23	1.94	0.50
1:B:60:PRO:HD3	1:B:119:ALA:HB3	1.94	0.49
1:C:426:VAL:HG12	1:C:450:PRO:HA	1.94	0.49
1:C:648:LEU:HA	1:C:652:MET:H	1.76	0.49
1:D:401:ARG:NH2	1:D:488:ILE:HD11	2.27	0.49
1:D:412:VAL:HG23	1:D:469:VAL:O	2.11	0.49
1:A:125:THR:HG22	1:A:127:ARG:HG3	1.94	0.49
1:A:365:PRO:HD2	1:D:346:HIS:CD2	2.47	0.49
1:B:510:ASN:HB3	1:B:513:ILE:HD12	1.94	0.49
1:C:605:VAL:HA	1:C:613:ILE:HD11	1.95	0.49
1:D:602:PHE:HA	1:D:605:VAL:HG22	1.93	0.49
1:B:90:PHE:O	1:B:168:ARG:NH1	2.45	0.49
1:B:285:MET:O	1:B:289:MET:HG3	2.12	0.49
1:B:447:LEU:HD12	1:B:447:LEU:H	1.77	0.49
1:C:401:ARG:HB2	1:C:480:LEU:CD1	2.43	0.49
1:C:644:LEU:O	1:C:648:LEU:HG	2.11	0.49
1:B:487:ASN:HA	1:B:490:GLU:CD	2.37	0.49
1:D:458:SER:HA	1:D:463:ILE:HG13	1.93	0.49
1:D:522:ILE:O	1:D:526:LYS:HG3	2.13	0.49
1:D:714:GLU:O	1:D:717:LYS:HG2	2.12	0.49
1:A:422:HIS:HB3	1:A:480:LEU:O	2.13	0.49
1:A:699:ASP:O	1:A:703:LEU:HG	2.12	0.49
1:B:396:ASN:O	1:B:400:ILE:HG13	2.13	0.49
1:B:531:LEU:HG	1:B:550:LEU:HD11	1.94	0.49
1:C:435:VAL:HG22	1:C:467:PHE:HD1	1.76	0.49
1:D:458:SER:HA	1:D:463:ILE:CG1	2.42	0.49
1:D:536:ASN:HD22	1:D:561:ASP:HB3	1.77	0.49
1:B:85:MET:HE3	1:B:213:HIS:HE1	1.78	0.49
1:B:507:LYS:HE3	1:B:517:GLU:HG2	1.93	0.49
1:D:277:ILE:HG12	1:D:277:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:LEU:O	1:D:574:ARG:HG2	2.12	0.49
1:B:365:PRO:HG3	1:C:346:HIS:CD2	2.47	0.49
1:C:254:LEU:HA	1:C:257:ARG:HH21	1.77	0.49
1:D:172:TRP:HE3	1:D:175:LEU:HD22	1.77	0.49
1:A:662:ARG:HE	1:A:666:HIS:HB3	1.76	0.49
1:B:192:THR:HA	1:C:320:ARG:HH12	1.78	0.49
1:C:628:SER:OG	1:C:653:ASN:ND2	2.46	0.49
1:A:275:GLY:HA2	1:D:274:TYR:HB3	1.94	0.49
1:A:364:ILE:HG22	1:D:350:GLN:HE22	1.76	0.49
1:A:423:LEU:HD22	1:A:459:ILE:CD1	2.43	0.49
1:B:421:ASP:O	1:B:422:HIS:ND1	2.46	0.49
1:C:565:ARG:HH12	1:C:570:LEU:HD21	1.77	0.49
1:B:320:ARG:HD2	1:D:196:TYR:HB2	1.95	0.49
1:B:510:ASN:ND2	1:B:512:ARG:H	2.10	0.49
1:B:605:VAL:HG12	1:B:643:PHE:CD1	2.47	0.49
1:C:402:LEU:HA	1:C:479:ARG:O	2.13	0.49
1:C:498:THR:O	1:C:502:ASN:ND2	2.46	0.49
1:A:421:ASP:CG	1:A:422:HIS:N	2.71	0.48
1:D:435:VAL:O	1:D:512:ARG:NH2	2.46	0.48
1:D:551:ILE:HG21	1:D:582:PHE:CZ	2.48	0.48
1:A:374:GLN:HA	1:A:378:LEU:HG	1.94	0.48
1:A:377:TYR:HB2	1:A:399:VAL:CG2	2.43	0.48
1:A:507:LYS:HG3	1:A:513:ILE:HG22	1.94	0.48
1:A:330:MET:HE1	1:A:340:ARG:HA	1.96	0.48
1:A:419:VAL:HG12	1:A:421:ASP:H	1.79	0.48
1:A:565:ARG:CZ	1:A:569:HIS:HB3	2.43	0.48
1:B:393:GLU:O	1:B:397:GLN:HG2	2.13	0.48
1:D:404:GLU:HB3	1:D:476:HIS:NE2	2.28	0.48
1:D:411:GLU:O	1:D:470:ARG:HD2	2.14	0.48
1:D:644:LEU:HA	1:D:647:LEU:HD12	1.96	0.48
1:B:296:MET:HE1	1:C:269:MET:SD	2.53	0.48
1:B:487:ASN:HA	1:B:490:GLU:OE1	2.13	0.48
1:C:358:THR:HA	1:C:361:LEU:HG	1.94	0.48
1:C:409:PRO:HA	1:C:471:VAL:HG12	1.96	0.48
1:D:346:HIS:HE1	1:D:407:PHE:HA	1.78	0.48
1:D:386:LEU:HD11	1:D:456:ASP:HB3	1.96	0.48
1:A:662:ARG:HH22	1:A:670:SER:HB3	1.79	0.48
1:B:380:TYR:CD1	1:B:427:CYS:HB3	2.49	0.48
1:B:446:THR:H	1:B:512:ARG:HD3	1.78	0.48
1:B:544:PHE:CE1	1:B:548:LYS:HD2	2.49	0.48
1:C:188:LEU:HD23	1:C:199:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLY:O	1:C:340:ARG:N	2.36	0.48
1:A:379:PRO:O	1:A:383:LYS:HD3	2.13	0.48
1:A:496:GLY:HA2	1:A:499:ILE:HG13	1.95	0.48
1:C:431:LEU:HD11	1:C:471:VAL:HG22	1.96	0.48
1:D:658:ASP:OD1	1:D:662:ARG:N	2.45	0.48
1:D:363:ASP:OD1	1:D:364:ILE:N	2.46	0.48
1:D:394:PHE:CE1	1:D:488:ILE:HG22	2.48	0.48
1:D:714:GLU:HA	1:D:717:LYS:HE2	1.95	0.48
1:A:115:GLN:HB3	1:A:139:TYR:CE2	2.46	0.48
1:A:221:TYR:O	1:A:225:THR:HG23	2.14	0.48
1:B:269:MET:HE2	1:B:269:MET:HB3	1.77	0.48
1:B:433:ALA:HA	1:B:469:VAL:HA	1.96	0.48
1:B:436:THR:HG23	1:B:440:GLY:HA2	1.95	0.48
1:C:57:ILE:HD11	1:C:132:PRO:HB3	1.95	0.48
1:C:208:GLU:O	1:C:212:THR:HG23	2.14	0.48
1:D:474:LEU:H	1:D:474:LEU:HD23	1.79	0.48
1:A:397:GLN:OE1	1:D:419:VAL:HG12	2.12	0.48
1:A:558:ASN:OD1	1:A:588:VAL:HG23	2.13	0.48
1:A:560:THR:HG22	1:A:592:LEU:HD11	1.96	0.48
1:B:530:GLU:O	1:B:534:LYS:HG3	2.13	0.48
1:B:602:PHE:CE1	1:B:606:LYS:HE3	2.48	0.48
1:C:676:MET:SD	1:C:676:MET:N	2.86	0.48
1:D:394:PHE:HD1	1:D:492:TYR:CD1	2.31	0.48
1:B:422:HIS:CG	1:B:479:ARG:HD2	2.49	0.48
1:C:249:PHE:O	1:C:257:ARG:HD3	2.14	0.48
1:C:534:LYS:NZ	1:C:546:GLN:NE2	2.62	0.48
1:D:293:SER:O	1:D:297:VAL:HG23	2.14	0.48
1:A:460:ILE:HD12	1:A:489:LEU:HD11	1.96	0.47
1:D:51:HIS:HB2	1:D:54:TYR:HD2	1.79	0.47
1:D:311:VAL:C	1:D:313:GLY:H	2.22	0.47
1:A:201:ILE:HG22	1:A:305:ASN:HB3	1.96	0.47
1:A:427:CYS:HA	1:A:451:HIS:H	1.78	0.47
1:A:438:THR:HB	1:C:552:ARG:CZ	2.44	0.47
1:B:192:THR:HA	1:C:320:ARG:HH22	1.79	0.47
1:B:493:PHE:CD1	1:B:494:HIS:N	2.82	0.47
1:A:635:THR:HA	1:A:638:LYS:HD2	1.96	0.47
1:B:547:LEU:O	1:B:551:ILE:HG13	2.14	0.47
1:B:569:HIS:HD1	1:B:569:HIS:H	1.62	0.47
1:B:662:ARG:HE	1:B:666:HIS:HB3	1.76	0.47
1:C:706:ASN:HB2	1:C:709:LEU:HB3	1.95	0.47
1:D:660:ASP:HA	1:D:692:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:HIS:HB2	1:B:62:ASN:HB2	1.95	0.47
1:B:610:GLU:HA	1:B:613:ILE:HB	1.96	0.47
1:B:714:GLU:O	1:B:718:ASN:ND2	2.47	0.47
1:C:548:LYS:HB2	1:C:548:LYS:HZ2	1.80	0.47
1:D:359:VAL:O	1:D:362:GLN:HB2	2.15	0.47
1:D:610:GLU:HA	1:D:613:ILE:HD12	1.96	0.47
1:A:185:PHE:CG	1:A:203:LYS:HG2	2.49	0.47
1:C:402:LEU:HD13	1:C:478:LEU:HD13	1.96	0.47
1:A:212:THR:HG21	1:A:266:ILE:HG12	1.97	0.47
1:A:358:THR:HG22	1:A:361:LEU:HD12	1.96	0.47
1:A:461:CYS:HA	1:A:523:HIS:HB2	1.96	0.47
1:A:544:PHE:CE2	1:A:548:LYS:HD2	2.49	0.47
1:A:714:GLU:O	1:A:718:ASN:ND2	2.47	0.47
1:B:197:LEU:O	1:B:201:ILE:HG23	2.14	0.47
1:B:272:VAL:O	1:D:273:GLY:HA3	2.15	0.47
1:C:362:GLN:HA	1:C:369:ARG:HH21	1.78	0.47
1:C:417:GLY:HA2	1:C:464:SER:HB2	1.96	0.47
1:C:482:LYS:HG3	1:C:483:GLN:N	2.30	0.47
1:D:108:PHE:CE2	1:D:177:ARG:HD3	2.49	0.47
1:D:443:GLU:HB3	1:D:512:ARG:NH1	2.29	0.47
1:D:503:ILE:O	1:D:507:LYS:NZ	2.26	0.47
1:D:510:ASN:HD22	1:D:513:ILE:HD12	1.78	0.47
1:C:165:GLU:HG3	1:C:169:TYR:HE1	1.79	0.47
1:C:386:LEU:O	1:C:499:ILE:HG23	2.15	0.47
1:C:386:LEU:HD23	1:C:387:PHE:CE1	2.50	0.47
1:C:593:LYS:HG2	1:C:599:THR:HG22	1.96	0.47
1:D:540:PHE:CD1	1:D:574:ARG:HD3	2.46	0.47
1:A:109:LEU:HD22	1:A:151:CYS:HB3	1.95	0.47
1:A:511:ASP:HA	1:A:514:LYS:HG2	1.96	0.47
1:A:568:LEU:HD11	1:A:588:VAL:HG21	1.96	0.47
1:C:383:LYS:HD3	1:C:451:HIS:CE1	2.50	0.47
1:C:569:HIS:HD2	1:C:603:GLU:OE2	1.98	0.47
1:D:319:PHE:HD1	1:D:322:LYS:HE3	1.80	0.47
1:D:457:ILE:HG21	1:D:466:PRO:HG3	1.97	0.47
1:A:409:PRO:HB3	1:A:473:GLU:HA	1.96	0.47
1:A:454:PHE:CE1	1:A:469:VAL:HG11	2.50	0.46
1:A:615:LEU:O	1:A:619:GLU:HG2	2.15	0.46
1:C:255:TRP:O	1:C:259:THR:OG1	2.25	0.46
1:D:220:TYR:O	1:D:224:THR:HG23	2.15	0.46
1:B:212:THR:HG22	1:B:291:TYR:OH	2.16	0.46
1:B:601:LEU:O	1:B:605:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LEU:O	1:C:213:HIS:NE2	2.48	0.46
1:C:465:GLN:HE21	1:C:466:PRO:HD2	1.80	0.46
1:D:510:ASN:HB3	1:D:513:ILE:HD12	1.97	0.46
1:D:675:LEU:HD12	1:D:676:MET:H	1.80	0.46
1:B:115:GLN:HB3	1:B:139:TYR:CD2	2.50	0.46
1:B:183:GLU:O	1:B:187:ARG:HG3	2.15	0.46
1:B:661:HIS:O	1:B:691:ASP:HA	2.14	0.46
1:C:357:ASP:O	1:C:361:LEU:HG	2.15	0.46
1:A:368:ILE:HD12	1:A:369:ARG:N	2.30	0.46
1:B:221:TYR:O	1:B:225:THR:HG23	2.15	0.46
1:B:581:LEU:O	1:B:585:GLN:HG3	2.15	0.46
1:C:698:LEU:HD23	1:C:717:LYS:HD2	1.97	0.46
1:D:212:THR:HG22	1:D:291:TYR:OH	2.15	0.46
1:D:269:MET:HE2	1:D:269:MET:HB3	1.78	0.46
1:A:358:THR:CA	1:A:361:LEU:HB2	2.44	0.46
1:B:371:LYS:HD2	1:C:339:LEU:HD22	1.96	0.46
1:B:394:PHE:CZ	1:B:398:ILE:HD11	2.50	0.46
1:B:413:ILE:HG12	1:B:414:THR:HG23	1.96	0.46
1:B:413:ILE:HG23	1:B:414:THR:H	1.80	0.46
1:B:636:VAL:HA	1:B:676:MET:HE1	1.97	0.46
1:C:221:TYR:O	1:C:225:THR:HG23	2.14	0.46
1:C:314:SER:HA	1:C:318:ARG:HG3	1.96	0.46
1:D:197:LEU:HD23	1:D:197:LEU:HA	1.76	0.46
1:A:378:LEU:HG	1:A:399:VAL:HG11	1.98	0.46
1:A:384:VAL:HG12	1:A:386:LEU:H	1.80	0.46
1:A:385:PRO:HA	1:A:388:LYS:HG3	1.96	0.46
1:A:449:GLY:O	1:A:452:THR:OG1	2.31	0.46
1:B:279:ALA:HB2	1:B:288:VAL:HG21	1.98	0.46
1:C:660:ASP:HA	1:C:692:ARG:HE	1.80	0.46
1:D:690:LYS:NZ	1:D:696:SER:HB3	2.30	0.46
1:A:711:LYS:HG3	1:A:712:LEU:N	2.31	0.46
1:B:367:SER:HB3	1:C:413:ILE:O	2.16	0.46
1:B:698:LEU:HD23	1:B:717:LYS:HD3	1.97	0.46
1:D:68:TRP:O	1:D:72:ILE:HG22	2.16	0.46
1:D:623:PHE:HE2	1:D:650:SER:HB2	1.80	0.46
1:A:360:MET:SD	1:D:322:LYS:HG3	2.56	0.46
1:A:374:GLN:O	1:A:378:LEU:HB2	2.15	0.46
1:A:634:THR:O	1:A:638:LYS:HG3	2.15	0.46
1:B:605:VAL:HG12	1:B:643:PHE:CE1	2.51	0.46
1:C:348:ARG:NH1	1:C:352:ASP:HB2	2.25	0.46
1:A:263:TYR:CG	1:C:285:MET:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:TYR:HA	1:A:358:THR:CG2	2.43	0.46
1:B:185:PHE:CG	1:B:203:LYS:HG2	2.51	0.46
1:B:334:LYS:HD2	1:B:334:LYS:N	2.31	0.46
1:B:398:ILE:HD13	1:B:488:ILE:HG21	1.97	0.46
1:B:658:ASP:CG	1:B:659:TYR:N	2.74	0.46
1:C:85:MET:HE1	1:C:255:TRP:CZ3	2.51	0.46
1:C:110:VAL:O	1:C:114:LEU:N	2.39	0.46
1:C:236:ILE:HG12	1:C:249:PHE:HB2	1.98	0.46
1:C:306:ILE:O	1:C:310:ILE:HG13	2.16	0.46
1:D:424:TYR:CZ	1:D:479:ARG:HD3	2.50	0.46
1:D:448:LEU:HD13	1:D:454:PHE:HB3	1.98	0.46
1:D:530:GLU:HA	1:D:533:LEU:HG	1.98	0.46
1:B:333:LYS:HB3	1:D:376:LEU:HD21	1.98	0.46
1:B:471:VAL:HG13	1:B:475:CYS:SG	2.56	0.46
1:D:249:PHE:O	1:D:257:ARG:HD2	2.16	0.46
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.80	0.45
1:A:612:VAL:O	1:A:616:LEU:HG	2.15	0.45
1:B:625:LEU:HD23	1:B:625:LEU:HA	1.79	0.45
1:C:387:PHE:HE1	1:C:425:PHE:HE2	1.61	0.45
1:D:437:LYS:HG2	1:D:512:ARG:NH2	2.31	0.45
1:D:657:GLU:OE1	1:D:657:GLU:N	2.47	0.45
1:A:335:LEU:HB3	1:A:339:LEU:HD23	1.98	0.45
1:A:336:GLY:HA2	1:A:337:ARG:NH2	2.31	0.45
1:B:131:LYS:O	1:B:135:ILE:N	2.46	0.45
1:B:328:SER:O	1:B:332:ARG:HG2	2.17	0.45
1:B:371:LYS:CD	1:C:339:LEU:HD22	2.47	0.45
1:B:434:LEU:HA	1:B:443:GLU:O	2.16	0.45
1:C:108:PHE:CZ	1:C:177:ARG:HD2	2.51	0.45
1:D:394:PHE:O	1:D:398:ILE:HG23	2.16	0.45
1:D:691:ASP:OD1	1:D:695:ASN:N	2.40	0.45
1:A:568:LEU:CD2	1:A:588:VAL:HG21	2.46	0.45
1:B:662:ARG:HG2	1:B:691:ASP:HB2	1.98	0.45
1:C:663:THR:O	1:C:666:HIS:HB2	2.16	0.45
1:A:666:HIS:NE2	1:A:697:PRO:HD3	2.31	0.45
1:B:380:TYR:HD1	1:B:427:CYS:HB3	1.82	0.45
1:D:456:ASP:HA	1:D:459:ILE:HD11	1.98	0.45
1:A:678:LYS:HE2	1:A:682:GLU:HG3	1.99	0.45
1:C:289:MET:O	1:C:293:SER:OG	2.28	0.45
1:C:467:PHE:CE2	1:C:516:LEU:HD11	2.52	0.45
1:C:629:GLY:HA2	1:C:656:SER:CB	2.46	0.45
1:C:643:PHE:HA	1:C:646:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ASP:HA	1:D:360:MET:HE3	1.97	0.45
1:D:666:HIS:CE1	1:D:697:PRO:HD3	2.51	0.45
1:A:196:TYR:CD1	1:D:317:GLU:HB2	2.51	0.45
1:B:165:GLU:OE2	1:B:168:ARG:NH2	2.47	0.45
1:B:207:VAL:HG12	1:B:298:LEU:HD11	1.98	0.45
1:B:413:ILE:HD11	1:B:424:TYR:CE2	2.51	0.45
1:C:94:PRO:HD2	1:C:97:LEU:HD21	1.97	0.45
1:C:416:GLN:NE2	1:C:466:PRO:O	2.50	0.45
1:D:94:PRO:HD2	1:D:97:LEU:HD11	1.99	0.45
1:D:425:PHE:O	1:D:477:LEU:HB3	2.17	0.45
1:D:648:LEU:HD22	1:D:683:ALA:CB	2.47	0.45
1:A:384:VAL:HG12	1:A:386:LEU:HB3	1.99	0.45
1:B:84:PRO:HG2	1:B:214:THR:HG22	1.97	0.45
1:C:128:THR:O	1:C:128:THR:OG1	2.33	0.45
1:D:335:LEU:C	1:D:340:ARG:HE	2.24	0.45
1:D:507:LYS:HA	1:D:510:ASN:OD1	2.17	0.45
1:A:93:LEU:HB2	1:A:155:ASP:CG	2.41	0.45
1:A:565:ARG:HG3	1:A:565:ARG:HH11	1.82	0.45
1:A:657:GLU:OE1	1:A:658:ASP:N	2.50	0.45
1:D:311:VAL:C	1:D:313:GLY:N	2.72	0.45
1:D:660:ASP:O	1:D:692:ARG:HB2	2.17	0.45
1:A:584:ILE:HA	1:A:588:VAL:CG1	2.47	0.45
1:C:435:VAL:HG22	1:C:467:PHE:CD1	2.52	0.45
1:C:483:GLN:HE21	1:C:487:ASN:HD21	1.65	0.45
1:D:346:HIS:CE1	1:D:407:PHE:HA	2.51	0.45
1:A:446:THR:HG22	1:A:448:LEU:HD23	1.99	0.45
1:B:422:HIS:CD2	1:B:479:ARG:HD2	2.51	0.45
1:D:59:HIS:C	1:D:61:LYS:H	2.25	0.45
1:D:197:LEU:O	1:D:201:ILE:HG13	2.17	0.45
1:A:112:ILE:O	1:A:116:PHE:HB2	2.17	0.44
1:B:569:HIS:HA	1:B:600:PRO:HA	1.98	0.44
1:B:572:ALA:O	1:B:609:GLN:HG3	2.18	0.44
1:C:120:TYR:CZ	1:C:138:ARG:HG3	2.52	0.44
1:C:140:LEU:HA	1:C:144:PHE:HB3	1.99	0.44
1:C:501:ASN:O	1:C:505:GLU:HG2	2.17	0.44
1:D:423:LEU:HD22	1:D:424:TYR:N	2.31	0.44
1:D:687:VAL:O	1:D:697:PRO:HD2	2.17	0.44
1:A:632:LEU:HG	1:A:644:LEU:CD1	2.46	0.44
1:A:636:VAL:HG23	1:A:644:LEU:HD21	1.99	0.44
1:C:494:HIS:O	1:C:497:ARG:HG3	2.17	0.44
1:C:499:ILE:O	1:C:503:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PHE:HE1	1:A:156:LEU:HD21	1.82	0.44
1:A:131:LYS:HB3	1:A:134:ARG:HB2	1.98	0.44
1:A:549:SER:N	1:A:552:ARG:HH21	2.16	0.44
1:C:534:LYS:HZ2	1:C:546:GLN:HE22	1.63	0.44
1:C:674:PHE:HA	1:C:709:LEU:HD22	1.99	0.44
1:D:93:LEU:HD23	1:D:93:LEU:HA	1.86	0.44
1:D:565:ARG:HD2	1:D:569:HIS:HB3	1.99	0.44
1:D:662:ARG:HG2	1:D:691:ASP:HB2	1.99	0.44
1:A:197:LEU:O	1:A:201:ILE:HG23	2.16	0.44
1:A:563:ASP:CG	1:A:563:ASP:O	2.60	0.44
1:B:361:LEU:O	1:B:369:ARG:NE	2.31	0.44
1:C:416:GLN:HB2	1:C:468:THR:OG1	2.16	0.44
1:A:483:GLN:O	1:A:487:ASN:ND2	2.50	0.44
1:A:495:ASP:O	1:A:499:ILE:HG13	2.18	0.44
1:B:501:ASN:HA	1:B:504:MET:HE3	1.99	0.44
1:D:531:LEU:O	1:D:535:VAL:HG23	2.17	0.44
1:D:674:PHE:CE1	1:D:708:LYS:HG3	2.52	0.44
1:A:418:ASN:H	1:A:465:GLN:HG3	1.82	0.44
1:B:402:LEU:HD22	1:B:478:LEU:HG	1.99	0.44
1:B:572:ALA:HA	1:B:612:VAL:HG11	2.00	0.44
1:C:493:PHE:HD1	1:C:552:ARG:CZ	2.29	0.44
1:C:507:LYS:HZ1	1:C:516:LEU:HB2	1.82	0.44
1:C:640:ASP:O	1:C:644:LEU:HD23	2.18	0.44
1:D:488:ILE:HA	1:D:491:ILE:HG12	1.99	0.44
1:D:536:ASN:HB3	1:D:570:LEU:HD22	1.99	0.44
1:D:622:SER:OG	1:D:624:ASN:ND2	2.47	0.44
1:B:202:LEU:HD12	1:B:202:LEU:HA	1.73	0.44
1:C:383:LYS:HD3	1:C:451:HIS:NE2	2.33	0.44
1:C:406:TYR:CZ	1:C:476:HIS:CD2	3.06	0.44
1:C:527:GLN:OE1	1:C:531:LEU:HG	2.18	0.44
1:C:668:ALA:O	1:C:673:LEU:N	2.50	0.44
1:B:569:HIS:CE1	1:B:600:PRO:HG3	2.53	0.44
1:C:119:ALA:HA	1:C:135:ILE:HD11	2.00	0.44
1:C:263:TYR:HD2	1:C:277:ILE:HD13	1.82	0.44
1:C:480:LEU:HD12	1:C:480:LEU:HA	1.75	0.44
1:C:499:ILE:O	1:C:502:ASN:N	2.50	0.44
1:A:605:VAL:HG22	1:A:613:ILE:HD13	2.00	0.44
1:A:611:GLY:O	1:A:615:LEU:HG	2.17	0.44
1:B:601:LEU:HG	1:B:623:PHE:CE1	2.53	0.44
1:B:705:GLY:HA2	1:B:710:ILE:HD11	2.00	0.44
1:C:505:GLU:HG2	1:C:505:GLU:H	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:O	1:D:320:ARG:NH1	2.50	0.43
1:A:208:GLU:HB3	1:A:269:MET:HE2	2.00	0.43
1:C:563:ASP:HB3	1:C:596:PHE:HE1	1.83	0.43
1:A:93:LEU:HD22	1:A:97:LEU:HD12	2.00	0.43
1:A:380:TYR:HB3	1:A:427:CYS:SG	2.58	0.43
1:A:375:LEU:HD12	1:A:375:LEU:O	2.19	0.43
1:B:87:PHE:O	1:B:168:ARG:NH1	2.38	0.43
1:B:413:ILE:HD11	1:B:424:TYR:CD2	2.54	0.43
1:C:212:THR:HG22	1:C:291:TYR:OH	2.17	0.43
1:C:590:VAL:HB	1:C:621:ALA:HB2	2.01	0.43
1:A:86:GLU:HA	1:A:90:PHE:CD2	2.52	0.43
1:A:396:ASN:O	1:A:399:VAL:HG12	2.18	0.43
1:A:485:PHE:O	1:A:489:LEU:HG	2.19	0.43
1:D:574:ARG:HA	1:D:574:ARG:NE	2.34	0.43
1:D:605:VAL:HA	1:D:613:ILE:HD11	1.99	0.43
1:D:605:VAL:HG21	1:D:647:LEU:HD23	2.00	0.43
1:A:568:LEU:HG	1:A:583:LEU:CD2	2.49	0.43
1:C:486:SER:O	1:C:490:GLU:HG3	2.19	0.43
1:C:535:VAL:HG12	1:C:567:PRO:HG3	2.00	0.43
1:A:376:LEU:HD11	1:D:333:LYS:HD2	2.01	0.43
1:A:454:PHE:CZ	1:A:469:VAL:HG21	2.53	0.43
1:B:662:ARG:HH22	1:B:670:SER:CB	2.32	0.43
1:B:701:ALA:HB2	1:B:713:LEU:HD12	2.01	0.43
1:C:226:LEU:HD12	1:C:234:THR:HG22	2.00	0.43
1:C:264:PHE:O	1:C:268:THR:HG23	2.18	0.43
1:D:239:LEU:HD12	1:D:239:LEU:HA	1.89	0.43
1:A:364:ILE:HA	1:D:350:GLN:HE22	1.84	0.43
1:A:634:THR:HG22	1:A:638:LYS:HE3	2.01	0.43
1:B:58:ILE:HB	1:B:118:VAL:HG12	2.00	0.43
1:B:310:ILE:HD12	1:D:304:GLY:HA3	2.01	0.43
1:B:511:ASP:HA	1:B:514:LYS:HB2	2.01	0.43
1:B:599:THR:H	1:B:602:PHE:HB2	1.83	0.43
1:C:507:LYS:O	1:C:514:LYS:HB2	2.18	0.43
1:D:323:MET:O	1:D:327:ILE:HG13	2.19	0.43
1:D:415:GLU:O	1:D:418:ASN:HB2	2.18	0.43
1:D:557:PRO:HG3	1:D:586:GLU:HB3	2.01	0.43
1:D:590:VAL:HG21	1:D:619:GLU:HG2	2.01	0.43
1:D:601:LEU:HB2	1:D:621:ALA:HB1	2.00	0.43
1:D:693:TRP:HB2	1:D:695:ASN:ND2	2.33	0.43
1:C:364:ILE:HG22	1:C:368:ILE:HB	2.01	0.43
1:C:575:GLY:HA2	1:C:612:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:HB2	1:A:125:THR:HB	2.00	0.43
1:A:145:LEU:HD23	1:A:145:LEU:H	1.84	0.43
1:A:296:MET:HG2	1:A:297:VAL:N	2.32	0.43
1:A:448:LEU:HD12	1:A:454:PHE:HB2	2.01	0.43
1:A:658:ASP:CG	1:A:659:TYR:H	2.27	0.43
1:D:348:ARG:HH11	1:D:351:TYR:HE1	1.65	0.43
1:D:548:LYS:HE3	1:D:582:PHE:CD1	2.54	0.43
1:A:288:VAL:O	1:A:292:VAL:HB	2.18	0.43
1:A:326:LEU:HB3	1:A:343:ILE:HD11	2.00	0.43
1:A:423:LEU:HD12	1:A:425:PHE:CE1	2.54	0.43
1:B:339:LEU:O	1:B:343:ILE:HG13	2.19	0.43
1:B:348:ARG:HD2	1:B:348:ARG:HA	1.79	0.43
1:B:349:LEU:O	1:B:353:SER:N	2.43	0.43
1:B:353:SER:O	1:B:354:HIS:C	2.61	0.43
1:B:401:ARG:HG3	1:B:401:ARG:HH11	1.84	0.43
1:B:478:LEU:HD12	1:B:479:ARG:H	1.83	0.43
1:C:492:TYR:O	1:C:495:ASP:HB2	2.19	0.43
1:C:606:LYS:HA	1:C:606:LYS:HE2	2.01	0.43
1:D:226:LEU:HD13	1:D:227:PRO:HD2	2.00	0.43
1:D:335:LEU:HD23	1:D:336:GLY:N	2.33	0.43
1:D:377:TYR:HB3	1:D:478:LEU:HD21	2.01	0.43
1:A:403:HIS:CE1	1:A:479:ARG:HH22	2.36	0.42
1:A:502:ASN:O	1:A:506:GLU:HG3	2.19	0.42
1:C:241:LEU:HD21	1:C:276:ASP:HB2	2.01	0.42
1:C:434:LEU:HD23	1:C:443:GLU:C	2.44	0.42
1:C:458:SER:OG	1:C:463:ILE:O	2.37	0.42
1:D:455:GLY:O	1:D:459:ILE:HG12	2.19	0.42
1:D:458:SER:HB2	1:D:463:ILE:O	2.19	0.42
1:D:487:ASN:O	1:D:491:ILE:HG12	2.18	0.42
1:D:702:ARG:HA	1:D:710:ILE:HD11	2.01	0.42
1:B:228:PRO:O	1:B:231:GLU:HB3	2.18	0.42
1:B:687:VAL:O	1:B:696:SER:HB2	2.19	0.42
1:C:343:ILE:O	1:C:347:VAL:HG13	2.18	0.42
1:C:396:ASN:O	1:C:400:ILE:HG13	2.19	0.42
1:D:236:ILE:O	1:D:246:TYR:HB2	2.20	0.42
1:A:125:THR:HA	1:D:474:LEU:HD13	2.01	0.42
1:A:346:HIS:CE1	1:C:365:PRO:HD3	2.55	0.42
1:A:570:LEU:HA	1:A:573:CYS:SG	2.60	0.42
1:A:658:ASP:O	1:A:661:HIS:ND1	2.52	0.42
1:B:153:PRO:HB2	1:B:156:LEU:HB3	2.00	0.42
1:B:602:PHE:HA	1:B:623:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:VAL:HB	1:B:717:LYS:HB2	2.02	0.42
1:C:645:LYS:O	1:C:645:LYS:HD3	2.19	0.42
1:C:646:ARG:O	1:C:649:SER:OG	2.24	0.42
1:D:108:PHE:N	1:D:108:PHE:CD1	2.87	0.42
1:A:401:ARG:NH2	1:D:419:VAL:HG11	2.32	0.42
1:C:394:PHE:HD2	1:C:492:TYR:HB2	1.84	0.42
1:A:256:LYS:HA	1:C:282:LEU:HD21	2.00	0.42
1:A:264:PHE:O	1:A:268:THR:HG23	2.20	0.42
1:A:335:LEU:HD13	1:C:372:ILE:HD12	2.01	0.42
1:A:582:PHE:O	1:A:586:GLU:HG2	2.19	0.42
1:B:315:ASN:HA	1:B:318:ARG:NH1	2.35	0.42
1:C:197:LEU:HD23	1:C:197:LEU:HA	1.86	0.42
1:C:279:ALA:HB2	1:C:288:VAL:HG21	2.00	0.42
1:C:350:GLN:HB3	1:C:355:TYR:HB3	2.01	0.42
1:C:434:LEU:HD22	1:C:442:GLU:C	2.44	0.42
1:D:115:GLN:HA	1:D:118:VAL:CG1	2.49	0.42
1:D:294:PHE:CZ	1:D:298:LEU:HD22	2.55	0.42
1:D:350:GLN:O	1:D:355:TYR:HB2	2.19	0.42
1:D:431:LEU:HB2	1:D:448:LEU:HB2	2.02	0.42
1:D:529:ALA:O	1:D:533:LEU:HG	2.20	0.42
1:A:391:SER:O	1:A:395:ILE:HG13	2.20	0.42
1:A:398:ILE:O	1:A:402:LEU:HG	2.19	0.42
1:A:410:GLY:O	1:A:470:ARG:NH1	2.52	0.42
1:A:688:ILE:HG22	1:A:717:LYS:HE3	2.01	0.42
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.89	0.42
1:B:376:LEU:HG	1:C:333:LYS:HD2	2.01	0.42
1:B:504:MET:HE2	1:B:504:MET:HB3	1.84	0.42
1:C:632:LEU:HA	1:C:635:THR:OG1	2.20	0.42
1:D:565:ARG:NE	1:D:594:ASP:OD2	2.52	0.42
1:A:340:ARG:O	1:A:344:THR:HG23	2.20	0.42
1:A:712:LEU:O	1:A:716:VAL:HG23	2.19	0.42
1:D:706:ASN:OD1	1:D:708:LYS:HE3	2.19	0.42
1:B:529:ALA:O	1:B:533:LEU:HG	2.20	0.42
1:C:517:GLU:O	1:C:520:ILE:HG12	2.20	0.42
1:A:364:ILE:HB	1:A:368:ILE:HD11	2.01	0.42
1:A:438:THR:HA	1:C:491:ILE:HG22	2.02	0.42
1:B:407:PHE:HB3	1:B:471:VAL:HG21	2.02	0.42
1:C:59:HIS:ND1	1:C:60:PRO:HD2	2.35	0.42
1:C:557:PRO:HB3	1:C:567:PRO:HG2	2.01	0.42
1:D:108:PHE:N	1:D:108:PHE:HD1	2.18	0.42
1:D:561:ASP:OD1	1:D:561:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:O	1:A:213:HIS:NE2	2.53	0.42
1:A:120:TYR:CG	1:A:138:ARG:HD2	2.55	0.42
1:A:645:LYS:HZ2	1:A:645:LYS:HG2	1.62	0.42
1:B:329:PHE:HA	1:B:332:ARG:CZ	2.50	0.42
1:B:491:ILE:HG13	1:C:419:VAL:HG22	2.02	0.42
1:B:616:LEU:C	1:B:621:ALA:HB2	2.45	0.42
1:B:642:ASP:OD1	1:B:643:PHE:N	2.52	0.42
1:C:431:LEU:O	1:C:448:LEU:N	2.53	0.42
1:C:581:LEU:O	1:C:585:GLN:HG3	2.20	0.42
1:A:196:TYR:CE1	1:D:317:GLU:HB2	2.54	0.41
1:A:660:ASP:C	1:A:662:ARG:H	2.27	0.41
1:B:185:PHE:CD2	1:B:203:LYS:HG2	2.54	0.41
1:B:689:SER:O	1:B:697:PRO:HD3	2.20	0.41
1:C:75:TRP:CZ3	1:C:104:GLY:HA2	2.55	0.41
1:C:378:LEU:O	1:C:381:ILE:HG22	2.20	0.41
1:C:449:GLY:O	1:C:452:THR:OG1	2.24	0.41
1:D:204:LEU:HD23	1:D:204:LEU:HA	1.77	0.41
1:D:319:PHE:HE1	1:D:347:VAL:HG12	1.85	0.41
1:D:500:LEU:HD12	1:D:500:LEU:HA	1.79	0.41
1:A:459:ILE:HD12	1:A:482:LYS:HD3	2.02	0.41
1:C:393:GLU:O	1:C:397:GLN:HG2	2.20	0.41
1:D:62:ASN:HD21	1:D:64:TRP:HB2	1.83	0.41
1:D:437:LYS:HE2	1:D:512:ARG:NH1	2.32	0.41
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.89	0.41
1:A:411:GLU:HA	1:C:367:SER:HB3	2.03	0.41
1:A:698:LEU:O	1:A:702:ARG:HG3	2.20	0.41
1:B:403:HIS:C	1:B:403:HIS:CD2	2.98	0.41
1:B:671:GLU:HG3	1:C:659:TYR:CE2	2.56	0.41
1:C:93:LEU:HD23	1:C:93:LEU:HA	1.85	0.41
1:C:522:ILE:O	1:C:526:LYS:HG3	2.21	0.41
1:D:63:ARG:HH11	1:D:64:TRP:CD1	2.38	0.41
1:D:510:ASN:O	1:D:514:LYS:HB2	2.20	0.41
1:A:486:SER:O	1:A:490:GLU:HG3	2.20	0.41
1:A:691:ASP:OD1	1:A:695:ASN:N	2.54	0.41
1:B:507:LYS:O	1:B:514:LYS:HG3	2.20	0.41
1:B:647:LEU:HD22	1:B:652:MET:HE3	2.02	0.41
1:C:516:LEU:O	1:C:520:ILE:HG23	2.20	0.41
1:C:548:LYS:HA	1:C:582:PHE:CE2	2.56	0.41
1:D:63:ARG:HG3	1:D:64:TRP:HD1	1.84	0.41
1:D:337:ARG:HD2	1:D:337:ARG:C	2.45	0.41
1:A:336:GLY:HA2	1:A:337:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:GLU:HG3	1:D:365:PRO:HB3	2.02	0.41
1:C:496:GLY:HA2	1:C:499:ILE:HG12	2.01	0.41
1:C:695:ASN:OD1	1:C:695:ASN:N	2.54	0.41
1:A:127:ARG:HH21	1:D:473:GLU:HB2	1.85	0.41
1:A:305:ASN:ND2	1:D:310:ILE:HD13	2.35	0.41
1:A:370:ALA:HB3	1:A:371:LYS:NZ	2.35	0.41
1:C:165:GLU:HG3	1:C:169:TYR:CE1	2.55	0.41
1:C:320:ARG:HD2	1:C:320:ARG:HA	1.87	0.41
1:C:643:PHE:CD2	1:C:644:LEU:HD22	2.55	0.41
1:D:404:GLU:HG3	1:D:478:LEU:HD13	2.02	0.41
1:D:409:PRO:HB3	1:D:473:GLU:HA	2.02	0.41
1:D:548:LYS:O	1:D:551:ILE:HG22	2.21	0.41
1:A:219:PHE:HD1	1:A:287:PHE:CD2	2.37	0.41
1:A:524:ILE:HA	1:A:527:GLN:HB3	2.02	0.41
1:B:548:LYS:HE2	1:B:552:ARG:HH21	1.86	0.41
1:B:623:PHE:HB2	1:B:652:MET:HB3	2.02	0.41
1:C:374:GLN:O	1:C:378:LEU:HB2	2.20	0.41
1:C:402:LEU:HD13	1:C:478:LEU:HD22	2.02	0.41
1:C:408:LEU:HA	1:C:409:PRO:HD3	1.95	0.41
1:C:663:THR:OG1	1:C:666:HIS:N	2.48	0.41
1:C:716:VAL:O	1:C:720:GLN:HG3	2.20	0.41
1:D:416:GLN:OE1	1:D:436:THR:N	2.54	0.41
1:A:357:ASP:C	1:A:359:VAL:N	2.78	0.41
1:A:687:VAL:O	1:A:697:PRO:HD2	2.21	0.41
1:B:90:PHE:HZ	1:B:254:LEU:HD22	1.86	0.41
1:B:271:THR:HA	1:C:272:VAL:HG13	2.03	0.41
1:B:339:LEU:HD21	1:D:372:ILE:HG23	2.03	0.41
1:C:408:LEU:HD23	1:C:409:PRO:O	2.21	0.41
1:C:625:LEU:HD11	1:C:628:SER:HA	2.02	0.41
1:D:457:ILE:O	1:D:461:CYS:HB2	2.21	0.41
1:D:486:SER:O	1:D:490:GLU:HG2	2.21	0.41
1:D:516:LEU:O	1:D:520:ILE:HG13	2.21	0.41
1:D:613:ILE:CD1	1:D:646:ARG:HD2	2.50	0.41
1:A:109:LEU:HD13	1:A:109:LEU:HA	1.83	0.41
1:A:131:LYS:HD2	1:A:134:ARG:HG2	2.03	0.41
1:A:252:ILE:HG22	1:A:253:ASP:N	2.36	0.41
1:A:360:MET:O	1:A:364:ILE:HG12	2.21	0.41
1:A:401:ARG:NE	1:A:484:SER:HB3	2.33	0.41
1:A:450:PRO:C	1:A:451:HIS:ND1	2.79	0.41
1:A:492:TYR:HB3	1:A:495:ASP:OD2	2.20	0.41
1:A:501:ASN:O	1:A:504:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASP:CG	1:A:659:TYR:N	2.79	0.41
1:A:661:HIS:O	1:A:691:ASP:HA	2.21	0.41
1:A:692:ARG:NH2	1:D:670:SER:O	2.53	0.41
1:B:401:ARG:HG3	1:B:401:ARG:NH1	2.34	0.41
1:B:618:LYS:HG2	1:B:619:GLU:OE2	2.21	0.41
1:B:638:LYS:NZ	1:C:627:ASP:OD2	2.45	0.41
1:C:330:MET:SD	1:C:340:ARG:HG3	2.61	0.41
1:C:577:GLU:HG2	1:C:612:VAL:HG22	2.01	0.41
1:C:641:SER:HB3	1:C:676:MET:HE3	2.02	0.41
1:C:643:PHE:HB2	1:C:646:ARG:NH2	2.35	0.41
1:C:662:ARG:NH2	1:C:667:VAL:HA	2.35	0.41
1:D:435:VAL:HG22	1:D:467:PHE:HB3	2.02	0.41
1:D:511:ASP:C	1:D:514:LYS:H	2.28	0.41
1:D:569:HIS:NE2	1:D:600:PRO:HD3	2.36	0.41
1:A:141:LYS:HA	1:A:141:LYS:HD2	1.87	0.41
1:A:253:ASP:OD1	1:A:254:LEU:N	2.54	0.41
1:A:414:THR:HB	1:A:465:GLN:NE2	2.24	0.41
1:A:482:LYS:HD2	1:A:482:LYS:O	2.21	0.41
1:A:500:LEU:HD11	1:A:523:HIS:CD2	2.55	0.41
1:D:213:HIS:CE1	1:D:258:TYR:HH	2.32	0.41
1:D:503:ILE:HG12	1:D:503:ILE:H	1.64	0.41
1:A:226:LEU:HD13	1:A:234:THR:HG22	2.03	0.40
1:A:530:GLU:O	1:A:531:LEU:C	2.64	0.40
1:B:330:MET:O	1:B:334:LYS:N	2.54	0.40
1:B:674:PHE:CD2	1:B:708:LYS:HD2	2.57	0.40
1:C:53:ASP:OD1	1:C:53:ASP:N	2.52	0.40
1:C:354:HIS:HB2	1:C:357:ASP:CG	2.46	0.40
1:C:398:ILE:HG23	1:C:480:LEU:HD21	2.03	0.40
1:C:484:SER:O	1:C:488:ILE:HG13	2.21	0.40
1:D:603:GLU:HA	1:D:603:GLU:OE1	2.22	0.40
1:A:124:GLN:HE21	1:A:124:GLN:HB2	1.62	0.40
1:A:249:PHE:HA	1:A:252:ILE:HD12	2.04	0.40
1:A:450:PRO:O	1:A:452:THR:HG23	2.21	0.40
1:B:131:LYS:HB2	1:B:134:ARG:HB2	2.02	0.40
1:B:187:ARG:HA	1:B:190:LYS:HE2	2.02	0.40
1:B:360:MET:SD	1:C:326:LEU:HD12	2.61	0.40
1:B:375:LEU:HD23	1:C:335:LEU:CD2	2.51	0.40
1:B:692:ARG:HH22	1:C:671:GLU:HA	1.85	0.40
1:B:696:SER:O	1:B:700:GLU:HG2	2.20	0.40
1:C:409:PRO:HB3	1:C:472:CYS:O	2.21	0.40
1:C:433:ALA:HB3	1:C:445:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:TYR:O	1:D:214:THR:HG23	2.21	0.40
1:D:239:LEU:HB3	1:D:246:TYR:CD1	2.57	0.40
1:A:196:TYR:HD1	1:A:197:LEU:HD13	1.86	0.40
1:A:249:PHE:HA	1:A:252:ILE:CD1	2.51	0.40
1:A:396:ASN:O	1:A:400:ILE:HG13	2.21	0.40
1:A:547:LEU:HD21	1:A:583:LEU:CD1	2.51	0.40
1:A:669:ALA:HB3	1:A:700:GLU:HB2	2.03	0.40
1:B:65:TYR:CZ	1:B:118:VAL:HG11	2.56	0.40
1:C:434:LEU:HD22	1:C:442:GLU:CB	2.50	0.40
1:C:623:PHE:CZ	1:C:652:MET:HA	2.56	0.40
1:D:515:LYS:HG3	1:D:516:LEU:N	2.35	0.40
1:A:531:LEU:O	1:A:535:VAL:HG23	2.22	0.40
1:A:636:VAL:HG11	1:A:668:ALA:HA	2.03	0.40
1:B:381:ILE:HD13	1:B:381:ILE:HA	1.85	0.40
1:B:513:ILE:H	1:B:513:ILE:HG13	1.77	0.40
1:C:63:ARG:HA	1:C:63:ARG:HD3	1.97	0.40
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.88	0.40
1:C:421:ASP:HA	1:C:482:LYS:HG2	2.04	0.40
1:C:590:VAL:HG11	1:C:619:GLU:HG3	2.03	0.40
1:D:72:ILE:O	1:D:72:ILE:HG13	2.21	0.40
1:D:173:ILE:HD13	1:D:173:ILE:HA	1.84	0.40
1:D:563:ASP:HA	1:D:595:LYS:HD2	2.02	0.40
1:A:120:TYR:CD1	1:A:138:ARG:HD2	2.57	0.40
1:A:182:VAL:O	1:A:186:GLN:HG2	2.21	0.40
1:A:629:GLY:HA3	1:A:656:SER:O	2.21	0.40
1:B:425:PHE:N	1:B:425:PHE:CD1	2.89	0.40
1:B:505:GLU:HA	1:B:508:GLU:OE1	2.20	0.40
1:C:524:ILE:HA	1:C:527:GLN:HB3	2.03	0.40
1:C:648:LEU:C	1:C:651:GLY:H	2.30	0.40
1:D:127:ARG:HA	1:D:127:ARG:HD3	1.88	0.40
1:D:594:ASP:OD1	1:D:597:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	671/834 (80%)	640 (95%)	31 (5%)	0	100	100
1	B	674/834 (81%)	658 (98%)	16 (2%)	0	100	100
1	C	670/834 (80%)	647 (97%)	23 (3%)	0	100	100
1	D	669/834 (80%)	640 (96%)	29 (4%)	0	100	100
All	All	2684/3336 (80%)	2585 (96%)	99 (4%)	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	594/743 (80%)	570 (96%)	24 (4%)	27	56
1	B	595/743 (80%)	584 (98%)	11 (2%)	54	75
1	C	593/743 (80%)	581 (98%)	12 (2%)	50	72
1	D	592/743 (80%)	574 (97%)	18 (3%)	36	62
All	All	2374/2972 (80%)	2309 (97%)	65 (3%)	41	65

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	TYR
1	A	109	LEU
1	A	124	GLN
1	A	129	VAL
1	A	143	HIS
1	A	195	ASN
1	A	266	ILE
1	A	269	MET
1	A	272	VAL
1	A	276	ASP

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Mol	Chain	Res	Type
1	A	292	VAL
1	A	312	LYS
1	A	342	GLN
1	A	364	ILE
1	A	395	ILE
1	A	399	VAL
1	A	459	ILE
1	A	519	ASP
1	A	528	GLU
1	A	530	GLU
1	A	534	LYS
1	A	592	LEU
1	A	652	MET
1	A	657	GLU
1	B	126	TYR
1	B	205	LEU
1	B	354	HIS
1	B	368	ILE
1	B	467	PHE
1	B	520	ILE
1	B	565	ARG
1	B	625	LEU
1	B	652	MET
1	B	659	TYR
1	B	687	VAL
1	C	114	LEU
1	C	145	LEU
1	C	250	ARG
1	C	272	VAL
1	C	282	LEU
1	C	327	ILE
1	C	346	HIS
1	C	493	PHE
1	C	562	TYR
1	C	659	TYR
1	C	690	LYS
1	C	695	ASN
1	D	99	VAL
1	D	105	GLN
1	D	189	GLU
1	D	272	VAL
1	D	277	ILE

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Mol	Chain	Res	Type
1	D	282	LEU
1	D	284	GLU
1	D	329	PHE
1	D	357	ASP
1	D	398	ILE
1	D	406	TYR
1	D	423	LEU
1	D	477	LEU
1	D	507	LYS
1	D	515	LYS
1	D	517	GLU
1	D	644	LEU
1	D	678	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	305	ASN
1	A	350	GLN
1	A	396	ASN
1	A	422	HIS
1	A	465	GLN
1	A	487	ASN
1	A	502	ASN
1	A	718	ASN
1	B	143	HIS
1	B	346	HIS
1	B	350	GLN
1	B	397	GLN
1	B	462	ASN
1	B	483	GLN
1	B	487	ASN
1	B	501	ASN
1	B	510	ASN
1	B	558	ASN
1	B	585	GLN
1	B	591	ASN
1	B	630	ASN
1	B	661	HIS
1	B	695	ASN
1	B	706	ASN

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Mol	Chain	Res	Type
1	B	718	ASN
1	C	105	GLN
1	C	124	GLN
1	C	483	GLN
1	C	546	GLN
1	C	661	HIS
1	D	59	HIS
1	D	105	GLN
1	D	124	GLN
1	D	346	HIS
1	D	350	GLN
1	D	451	HIS
1	D	527	GLN
1	D	598	HIS
1	D	624	ASN
1	D	695	ASN

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 ⓘ

There are no chain breaks in this entry.

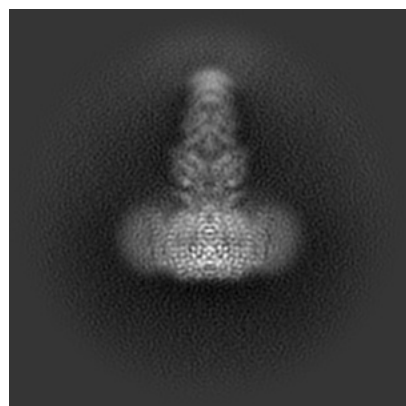
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62913. These allow visual inspection of the internal detail of the map and identification of artifacts.

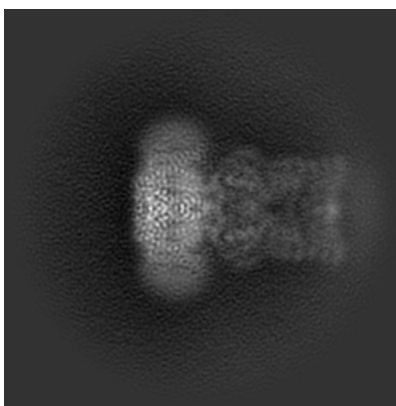
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

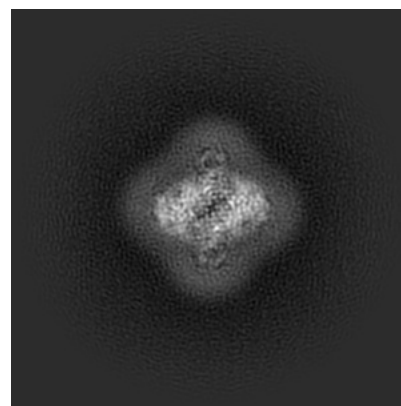
6.1.1 Primary map



X

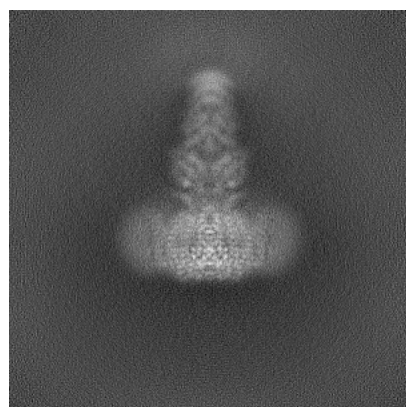


Y

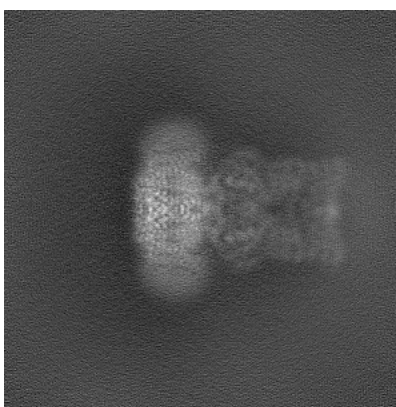


Z

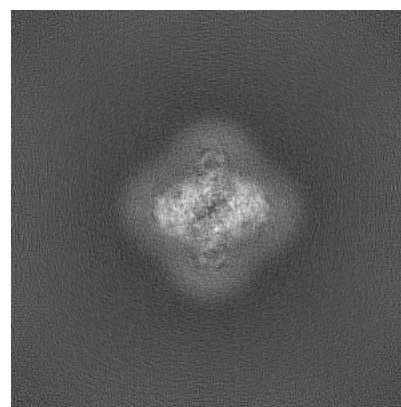
6.1.2 Raw map



X



Y

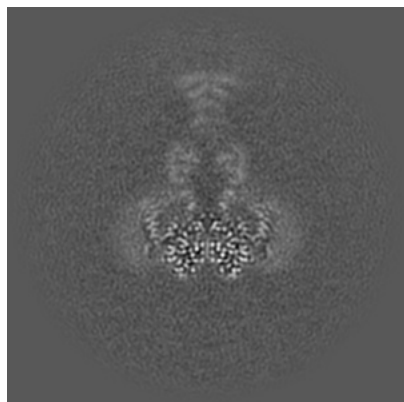


Z

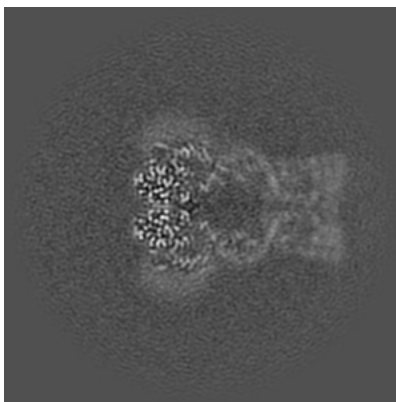
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

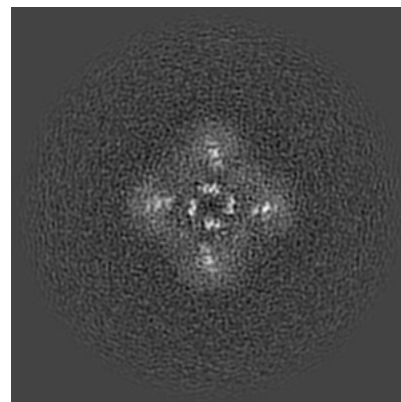
6.2.1 Primary map



X Index: 200

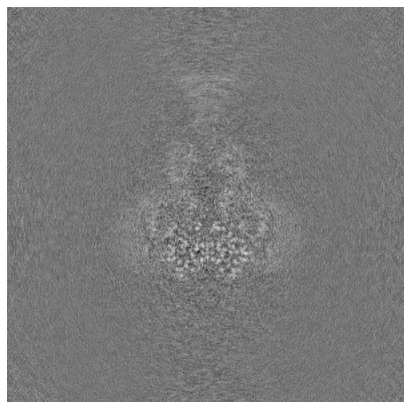


Y Index: 200

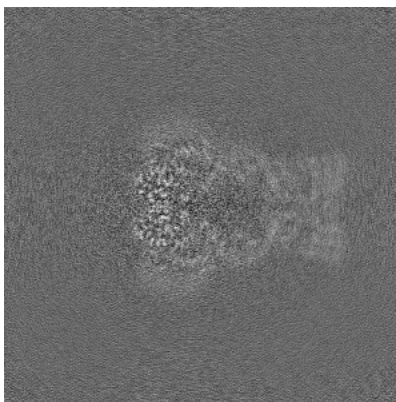


Z Index: 200

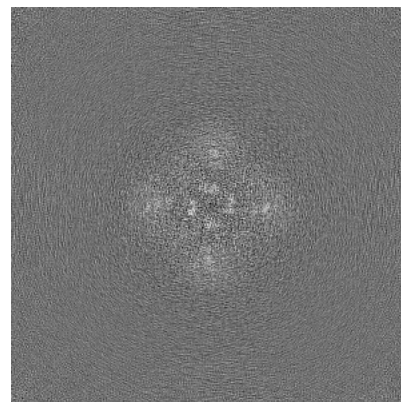
6.2.2 Raw map



X Index: 200



Y Index: 200

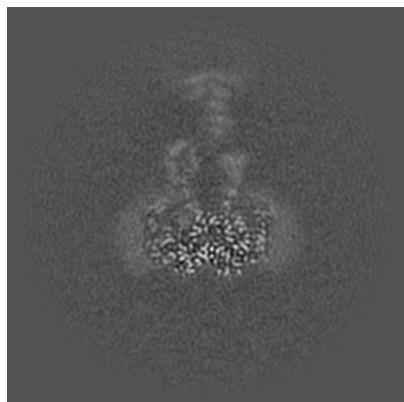


Z Index: 200

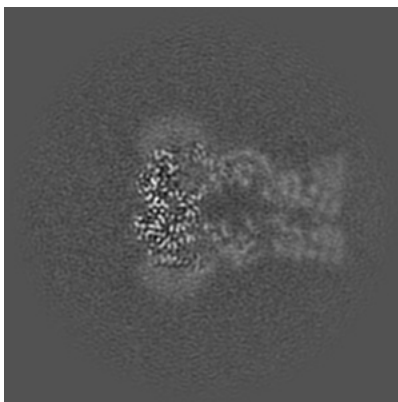
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

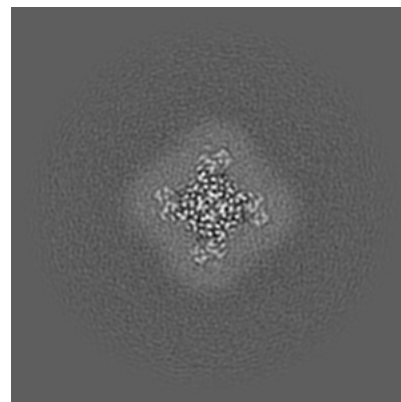
6.3.1 Primary map



X Index: 196

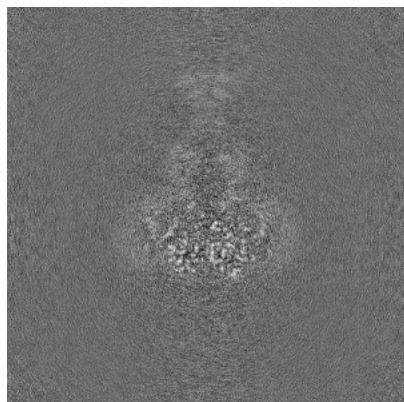


Y Index: 195

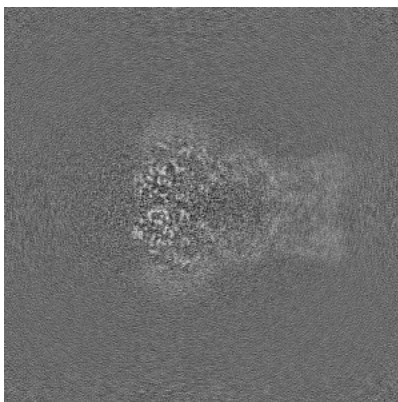


Z Index: 146

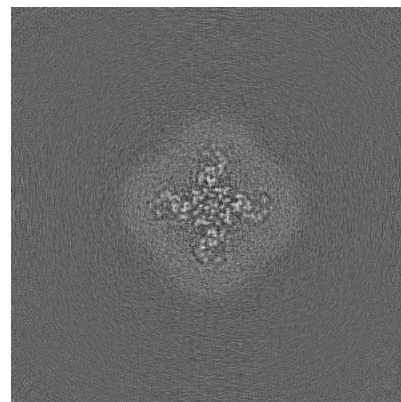
6.3.2 Raw map



X Index: 199



Y Index: 199

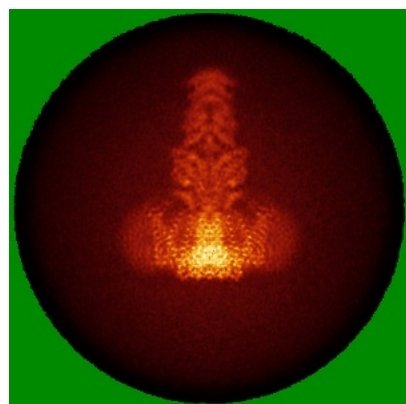


Z Index: 160

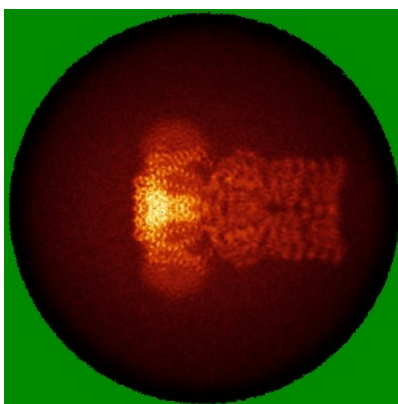
The images above show the largest variance slices of the map in three orthogonal directions.

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

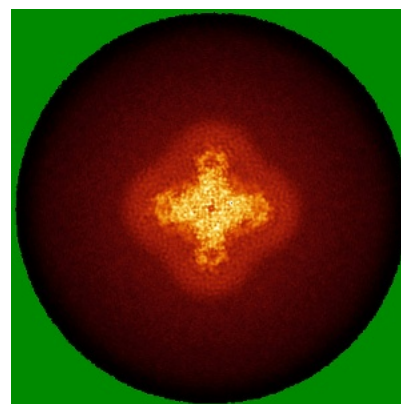
6.4.1 Primary map



X

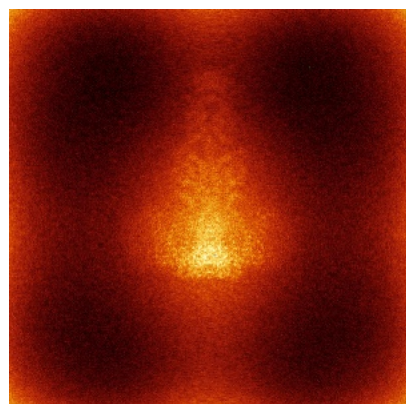


Y

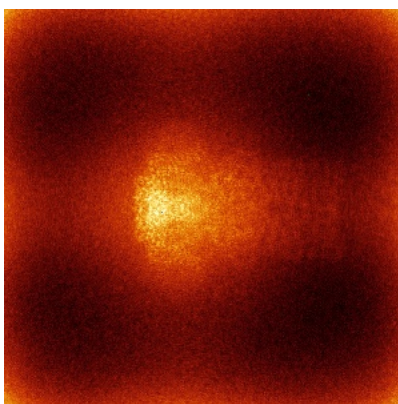


Z

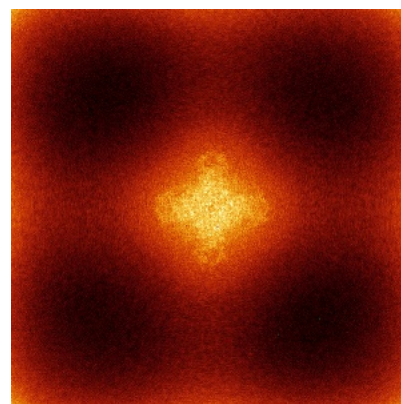
6.4.2 Raw map



X



Y

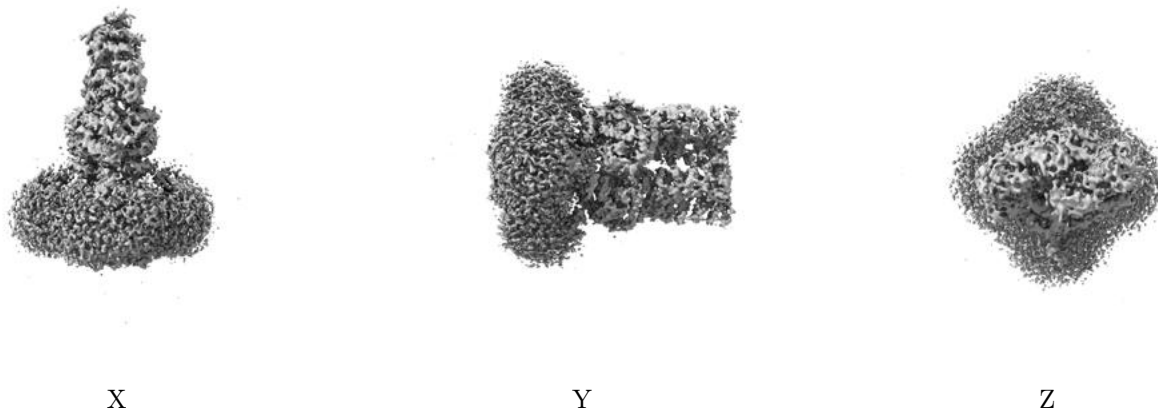


Z

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.

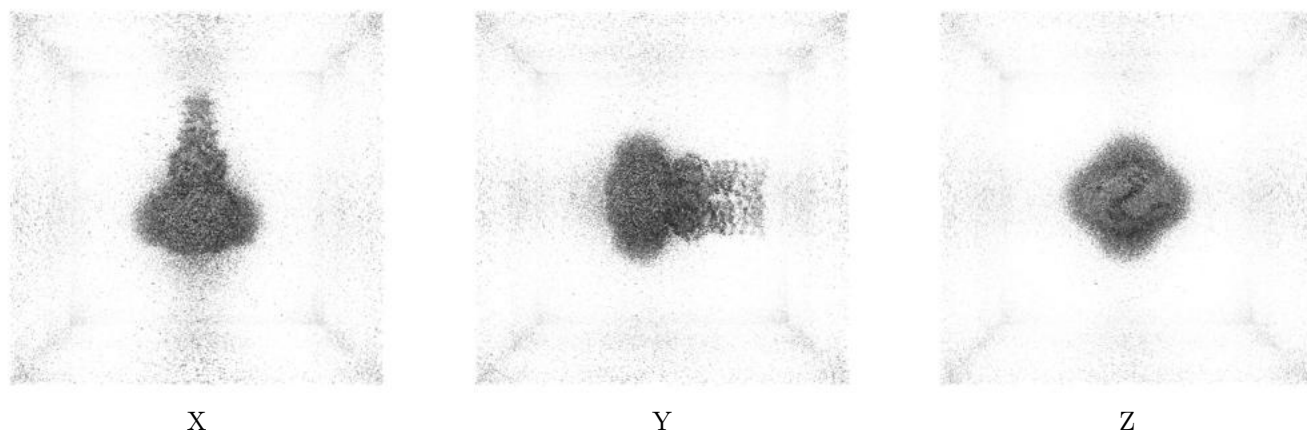
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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



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.

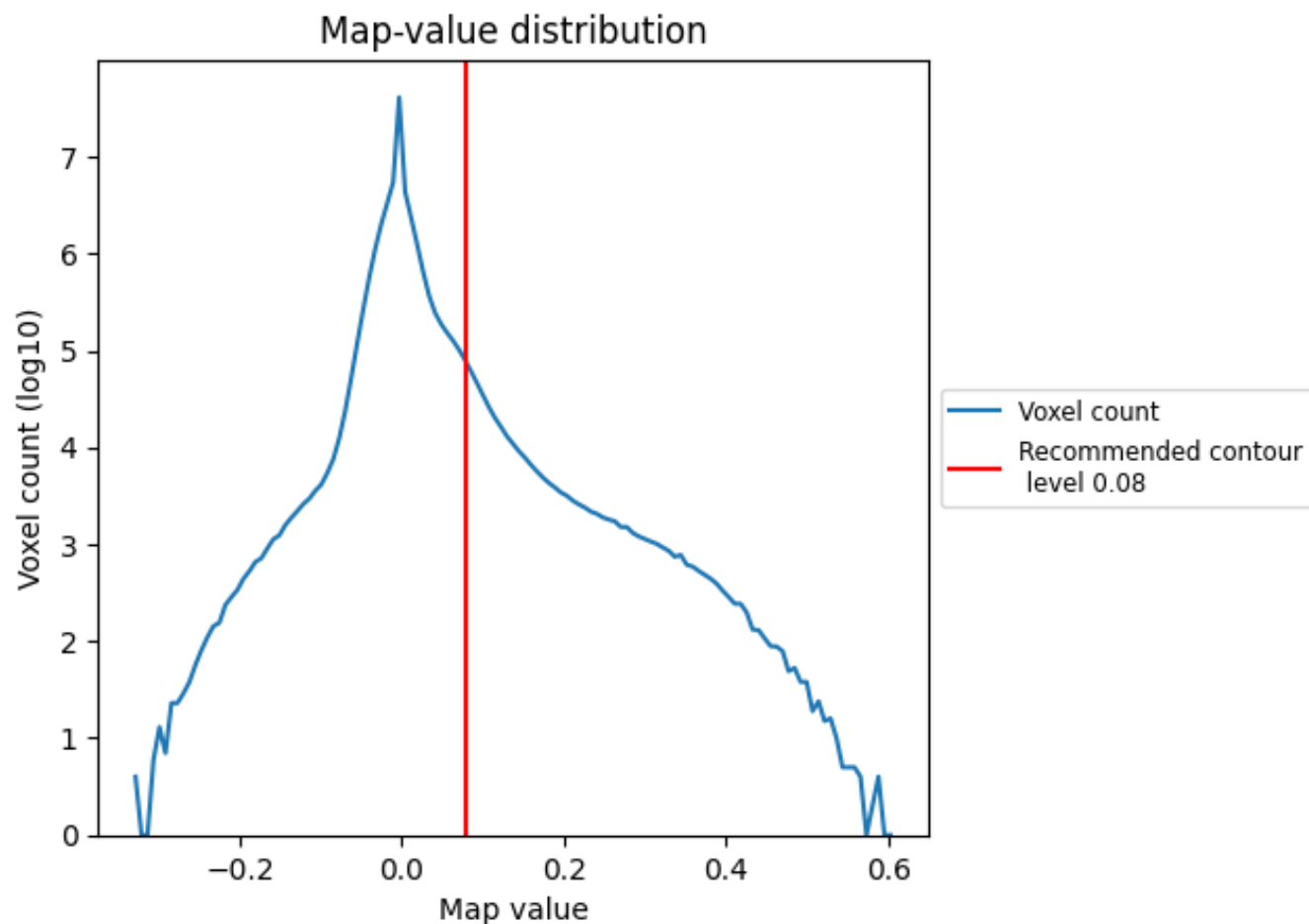
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

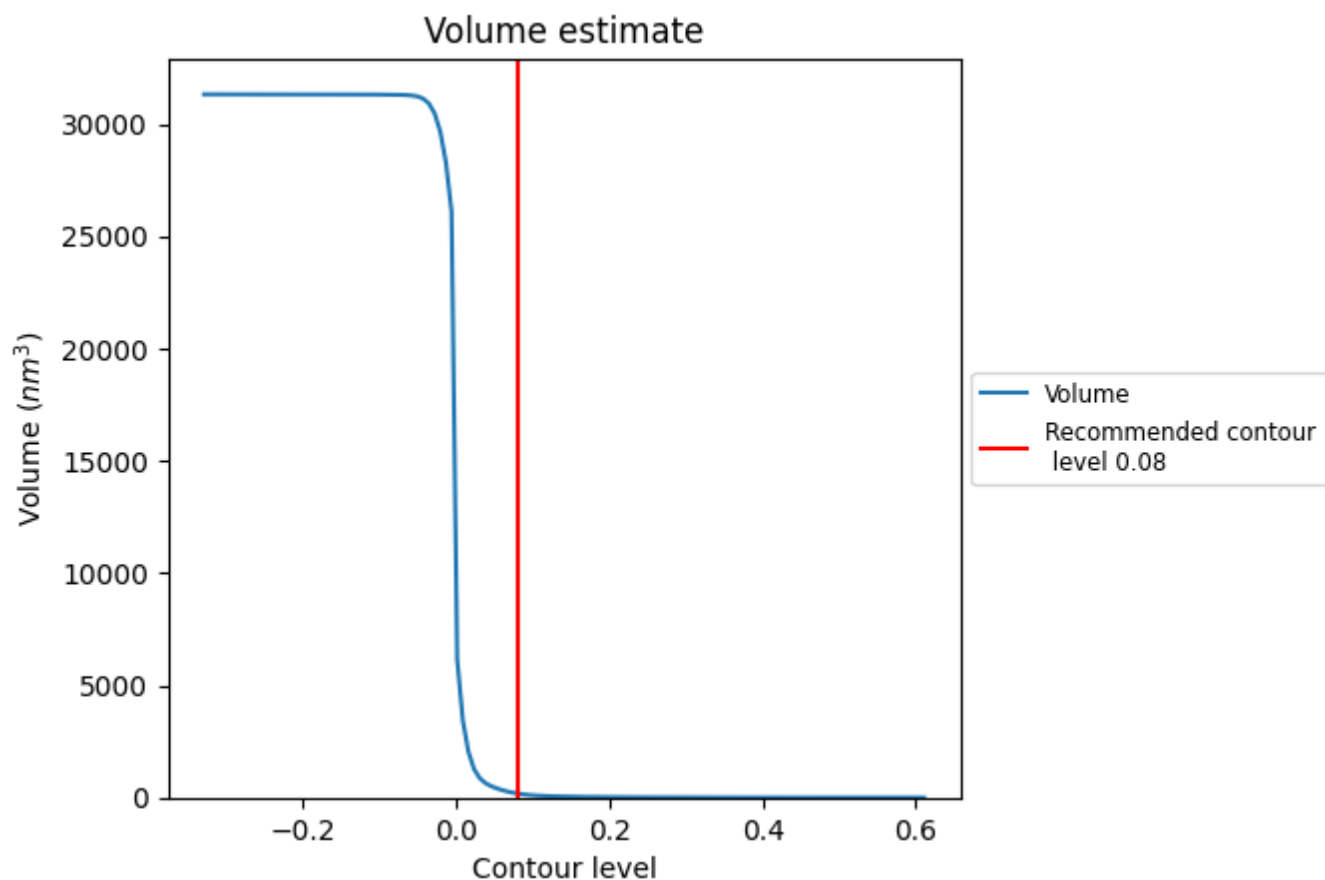
This section contains the results of statistical analysis of the map.

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.

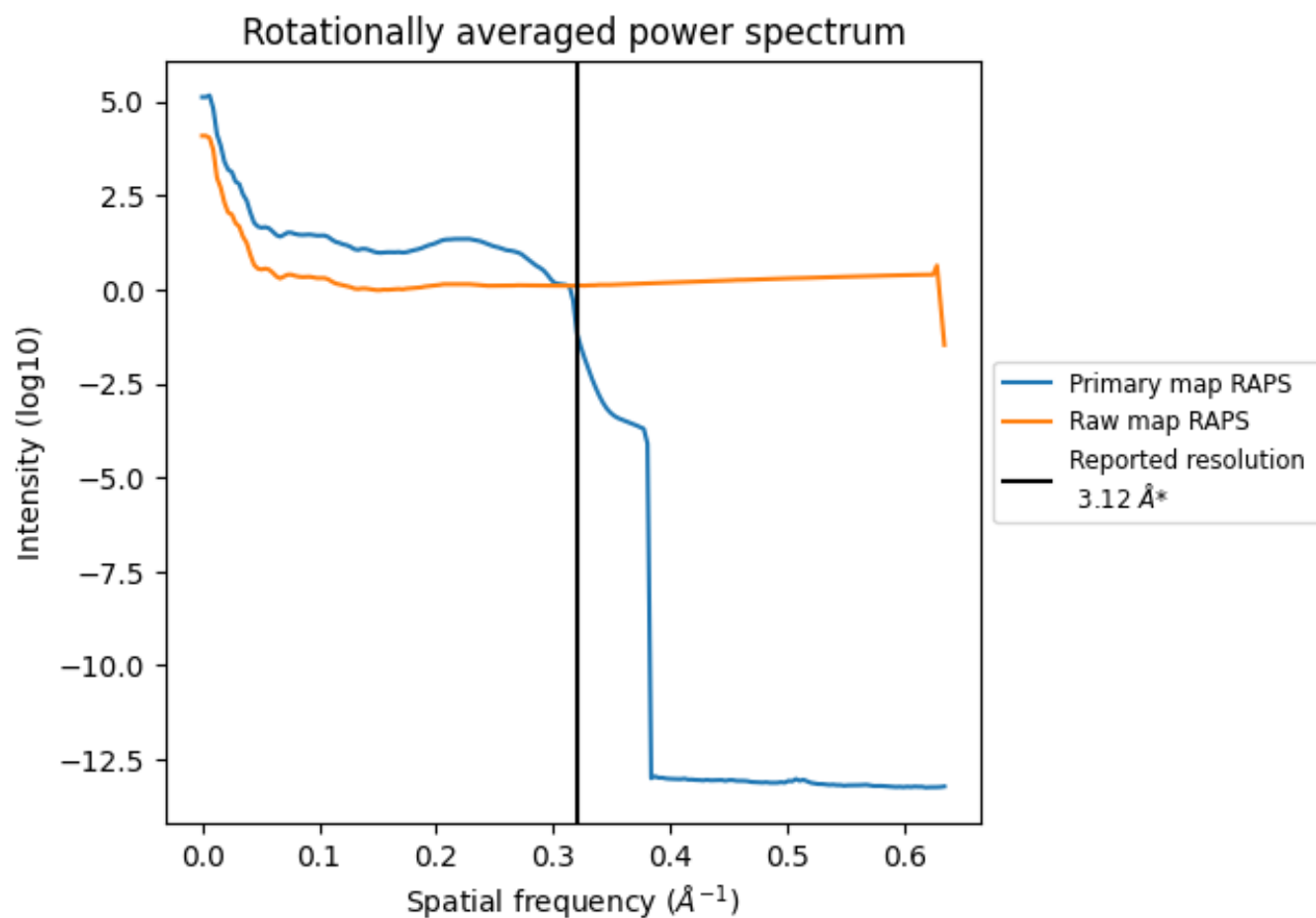
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183 nm³; this corresponds to an approximate mass of 165 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 ⓘ

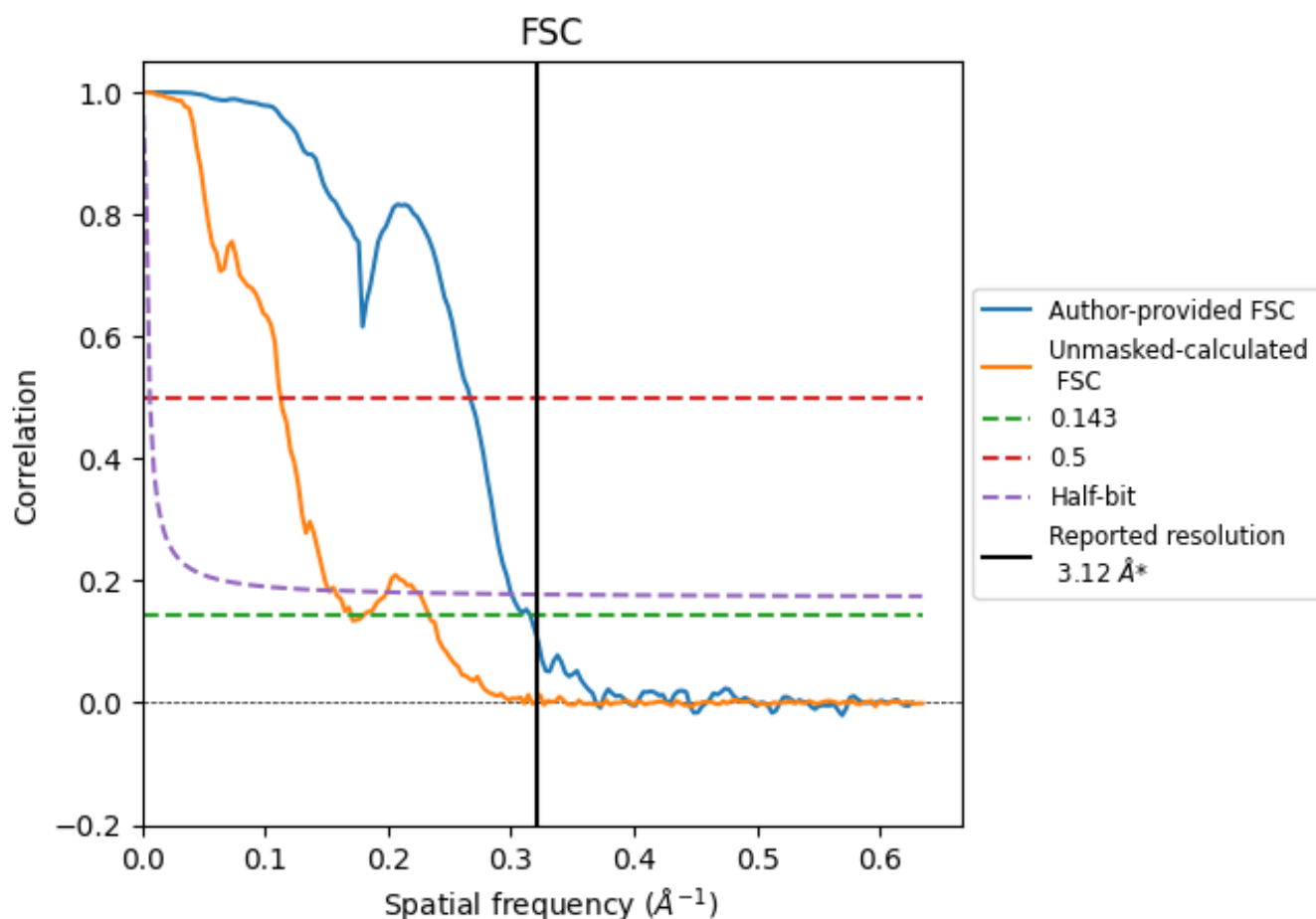


*Reported resolution corresponds to spatial frequency of 0.321 Å⁻¹

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 0.321 \AA^{-1}

8.2 Resolution estimates [i](#)

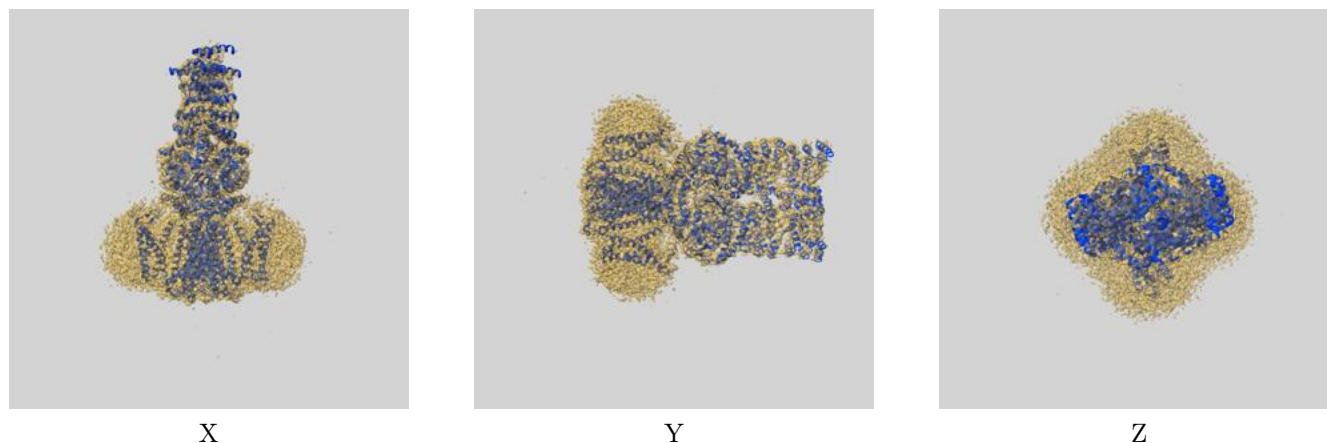
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.12	-	-
Author-provided FSC curve	3.17	3.75	3.33
Unmasked-calculated*	5.88	8.88	6.58

*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 5.88 differs from the reported value 3.12 by more than 10 %

9 Map-model fit [i](#)

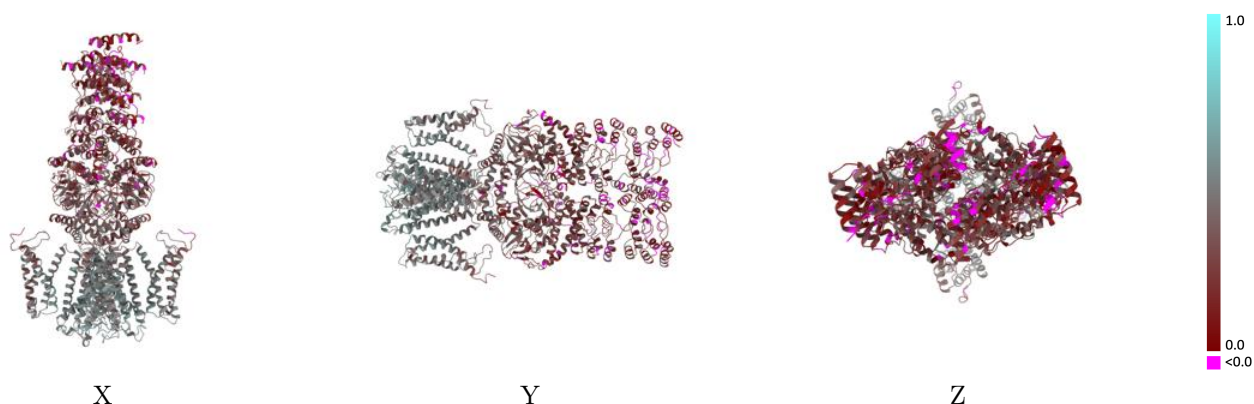
This section contains information regarding the fit between EMDB map EMD-62913 and PDB model 9L9U. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



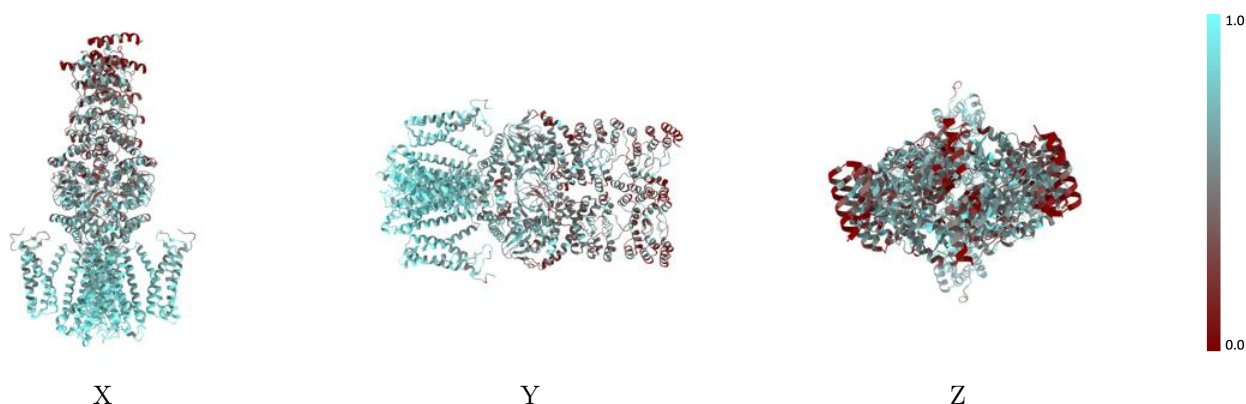
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



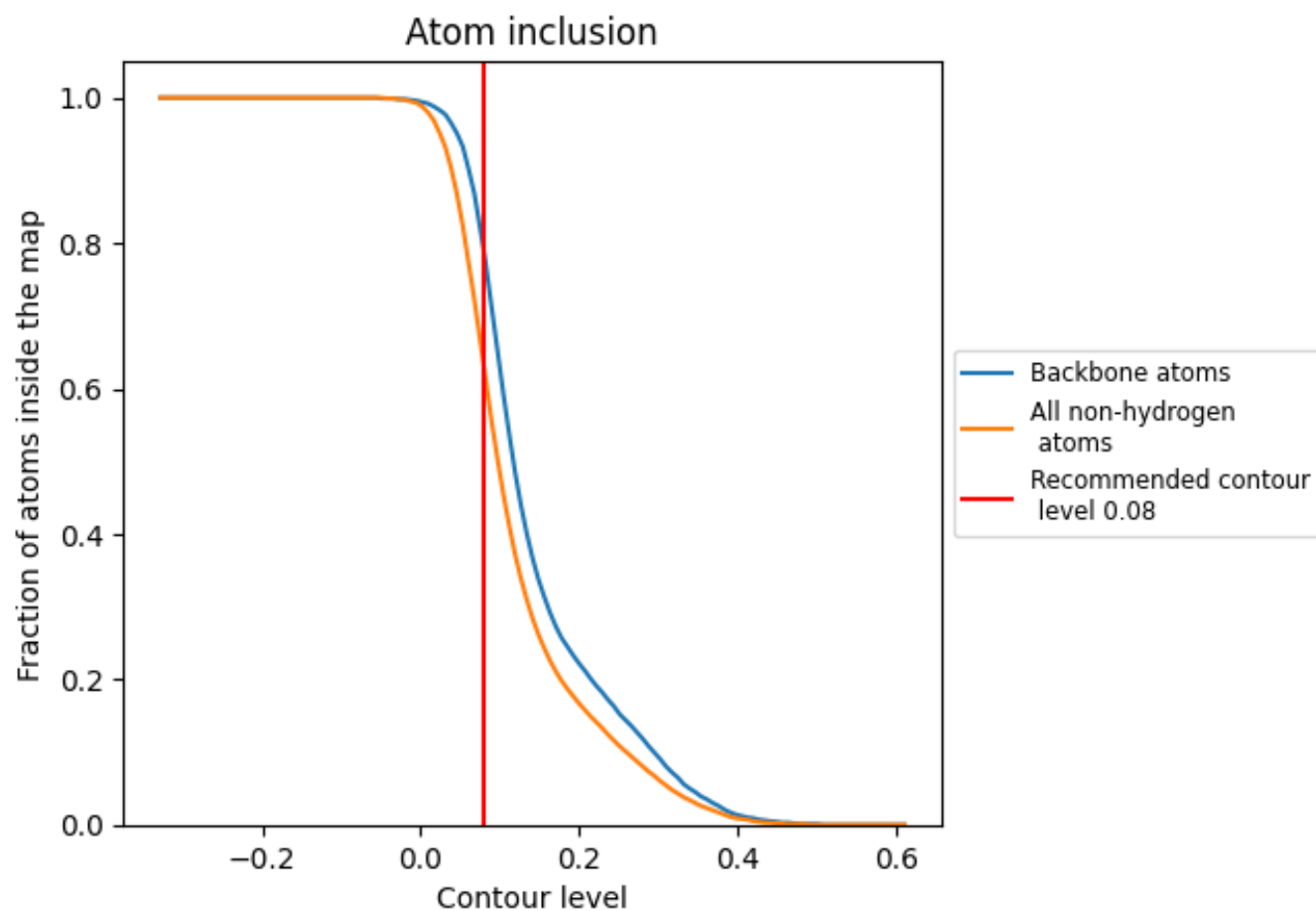
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 63% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6290	<div></div> 0.3360
A	<div></div> 0.6240	<div></div> 0.3350
B	<div></div> 0.6170	<div></div> 0.3300
C	<div></div> 0.6400	<div></div> 0.3410
D	<div></div> 0.6340	<div></div> 0.3400

