



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:08 PM UTC

PDB ID : 9LA3 / pdb_00009la3
EMDB ID : EMD-62918
Title : Arabidopsis GORK WT3
Authors : Yamanashi, T.; Kume, T.; Sekido, N.; Muraoka, Y.; Yokoyama, T.; Tanaka, Y.; Uozumi, N.
Deposited on : 2025-01-01
Resolution : 3.19 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

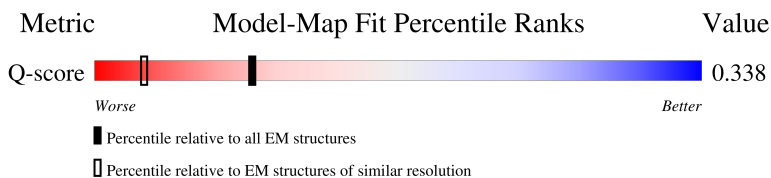
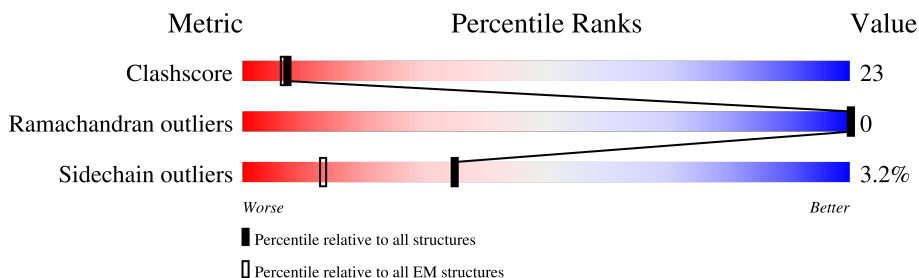
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.19 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	14455 (2.69 - 3.69)

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	
1	B	834	
1	C	834	
1	D	834	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21944 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	676	Total	C	N	O	S	0	0
			5486	3559	914	988	25		
1	B	676	Total	C	N	O	S	0	0
			5486	3559	914	988	25		
1	C	676	Total	C	N	O	S	0	0
			5486	3559	914	988	25		
1	D	676	Total	C	N	O	S	0	0
			5486	3559	914	988	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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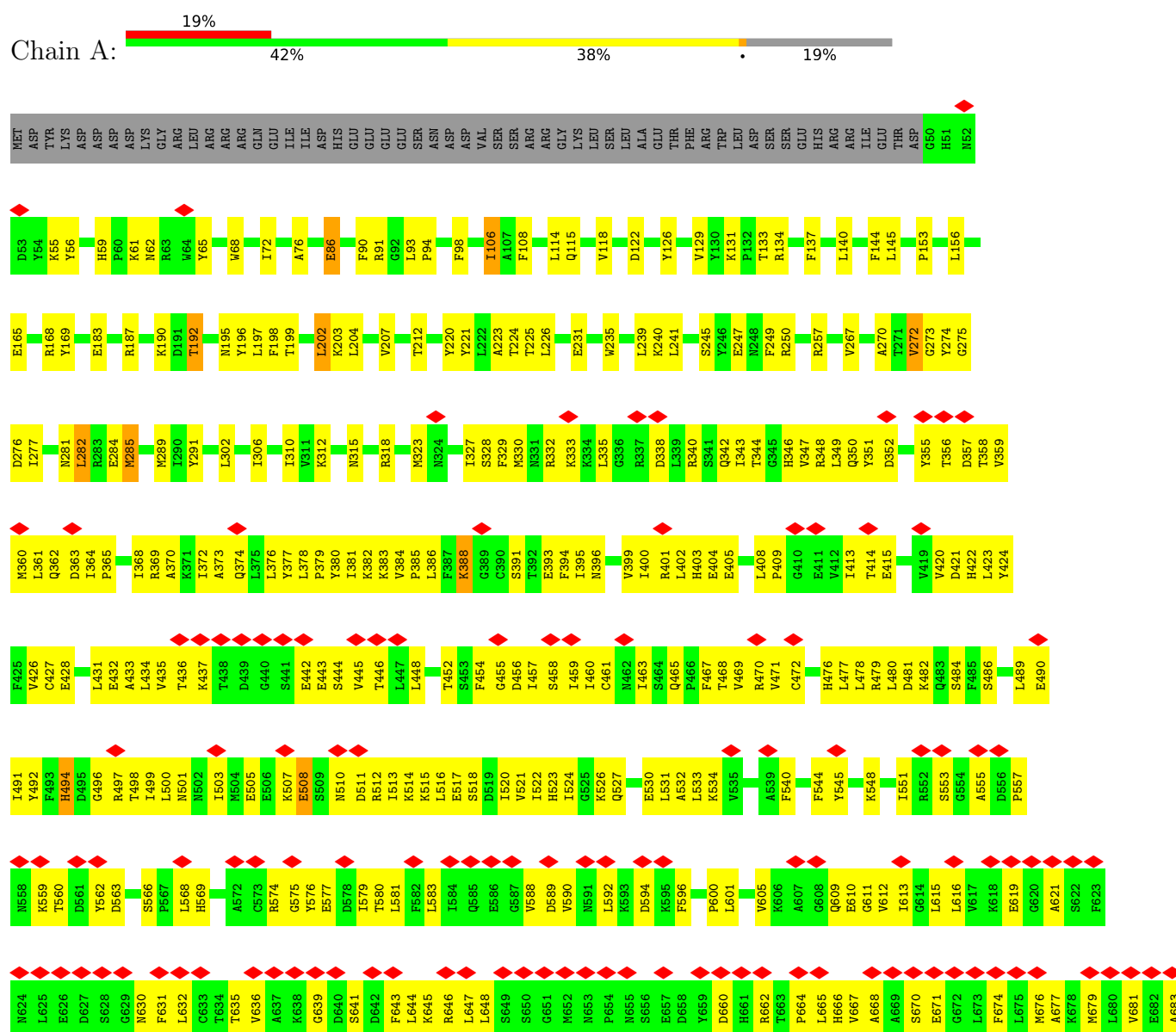
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ASP	-	expression tag	UNP Q94A76
B	1	LYS	-	expression tag	UNP Q94A76
B	821	HIS	-	expression tag	UNP Q94A76
B	822	HIS	-	expression tag	UNP Q94A76
B	823	HIS	-	expression tag	UNP Q94A76
B	824	HIS	-	expression 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.

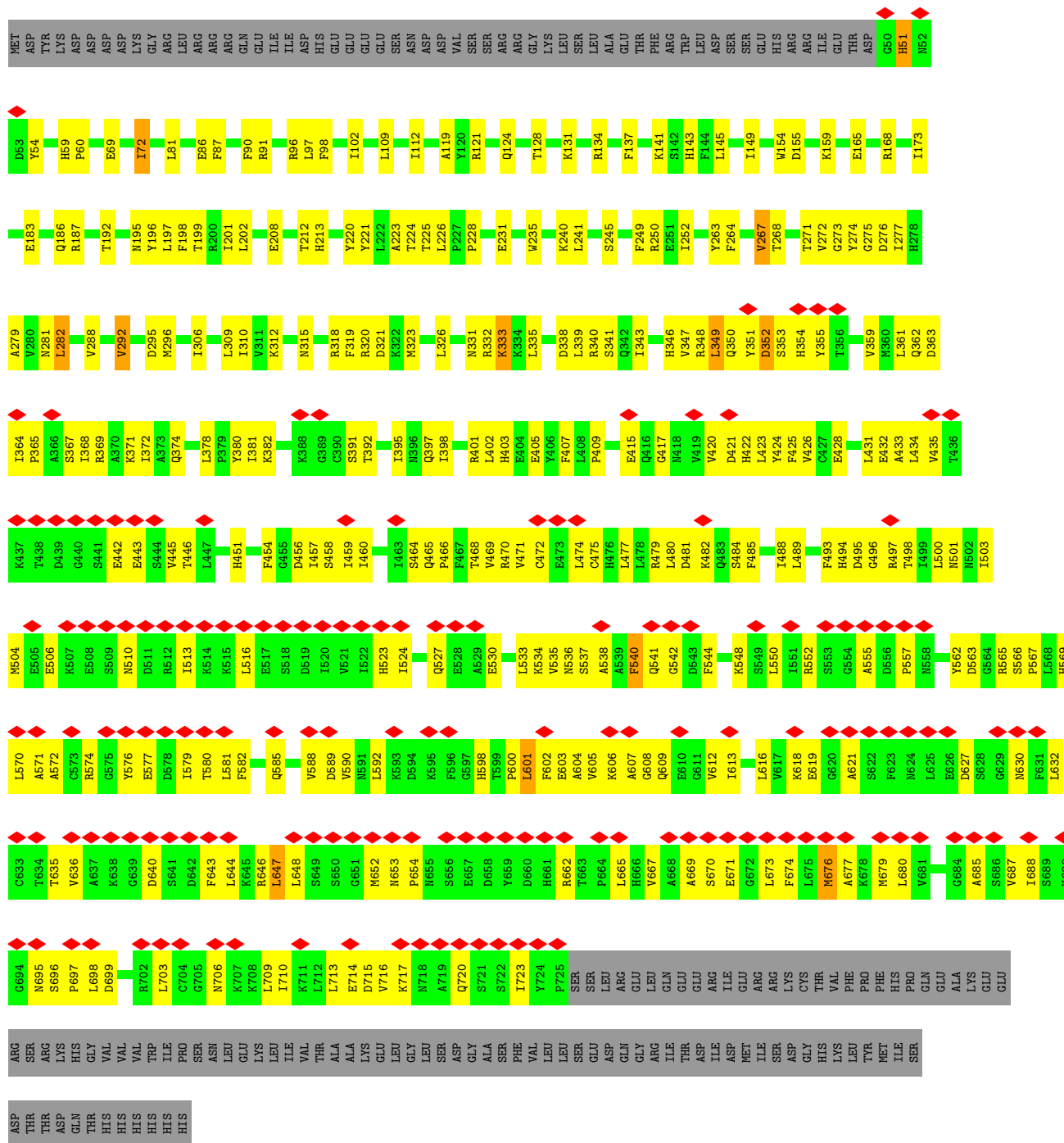
• Molecule 1: Potassium channel GORK



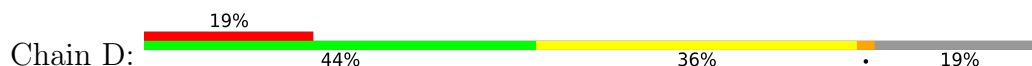


MET
ILE
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• Molecule 1: Potassium channel GORK



• Molecule 1: Potassium channel GORK





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23670	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	0.559	Depositor
Minimum map value	-0.301	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	315.19998, 315.19998, 315.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.27	0/5615	0.48	0/7596
1	B	0.28	0/5615	0.49	0/7596
1	C	0.30	0/5615	0.50	0/7596
1	D	0.33	0/5615	0.53	0/7596
All	All	0.30	0/22460	0.50	0/30384

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	5486	0	5502	297	0
1	B	5486	0	5502	280	0
1	C	5486	0	5502	253	0
1	D	5486	0	5502	267	0
All	All	21944	0	22008	1026	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 23.

All (1026) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:PRO:HB2	1:C:588:VAL:HG22	1.49	0.94
1:D:556:ASP:HB3	1:D:559:LYS:HG2	1.57	0.87
1:D:459:ILE:HG23	1:D:482:LYS:HG2	1.55	0.86
1:A:348:ARG:O	1:A:352:ASP:HB2	1.77	0.85
1:A:272:VAL:O	1:C:273:GLY:HA3	1.78	0.84
1:D:510:ASN:HD22	1:D:512:ARG:HG2	1.44	0.83
1:B:533:LEU:HD11	1:C:533:LEU:HD22	1.61	0.83
1:B:275:GLY:HA3	1:C:274:TYR:O	1.79	0.82
1:A:273:GLY:HA3	1:D:272:VAL:O	1.80	0.81
1:A:455:GLY:HA2	1:A:465:GLN:HE22	1.46	0.81
1:C:524:ILE:HA	1:C:527:GLN:HB2	1.63	0.81
1:A:358:THR:HA	1:A:361:LEU:HB2	1.63	0.80
1:B:503:ILE:HB	1:B:507:LYS:HE2	1.62	0.80
1:D:575:GLY:HA3	1:D:609:GLN:HG3	1.64	0.80
1:B:416:GLN:HE22	1:B:436:THR:HB	1.48	0.79
1:A:401:ARG:HD3	1:A:484:SER:HB3	1.64	0.79
1:D:470:ARG:NH1	1:D:472:CYS:SG	2.57	0.78
1:D:355:TYR:HA	1:D:358:THR:HG23	1.65	0.78
1:A:434:LEU:HA	1:A:444:SER:HA	1.65	0.78
1:B:332:ARG:HH12	1:D:354:HIS:CD2	2.00	0.78
1:D:428:GLU:HB3	1:D:476:HIS:HB3	1.67	0.77
1:A:636:VAL:HG22	1:A:644:LEU:HD22	1.68	0.76
1:B:371:LYS:HE3	1:B:375:LEU:HD23	1.68	0.75
1:B:436:THR:HG23	1:B:440:GLY:H	1.51	0.75
1:C:417:GLY:HA2	1:C:464:SER:HB2	1.68	0.75
1:B:329:PHE:HA	1:B:332:ARG:HD3	1.67	0.74
1:B:433:ALA:HA	1:B:469:VAL:HA	1.67	0.74
1:D:431:LEU:HG	1:D:471:VAL:HG13	1.67	0.74
1:A:431:LEU:HD12	1:A:432:GLU:H	1.52	0.74
1:B:131:LYS:HB3	1:B:134:ARG:HB2	1.70	0.74
1:B:273:GLY:HA3	1:C:272:VAL:O	1.88	0.73
1:B:640:ASP:HB3	1:B:643:PHE:HB3	1.70	0.73
1:A:370:ALA:HB1	1:A:400:ILE:HG12	1.70	0.73
1:D:87:PHE:O	1:D:168:ARG:NH2	2.22	0.73
1:B:330:MET:HE2	1:B:340:ARG:HA	1.69	0.72
1:A:421:ASP:HA	1:A:482:LYS:HD2	1.70	0.72
1:B:194:ILE:O	1:C:320:ARG:NH2	2.22	0.72
1:B:706:ASN:HD22	1:B:709:LEU:HB3	1.54	0.72
1:B:661:HIS:HB3	1:B:691:ASP:HA	1.71	0.72
1:C:350:GLN:HA	1:C:353:SER:HB2	1.71	0.72
1:C:603:GLU:HA	1:C:606:LYS:HG2	1.71	0.72
1:B:536:ASN:HA	1:B:567:PRO:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLY:HA3	1:D:274:TYR:O	1.89	0.71
1:D:350:GLN:HB3	1:D:356:THR:HG23	1.72	0.71
1:D:484:SER:HA	1:D:487:ASN:HD22	1.55	0.71
1:A:267:VAL:HG13	1:A:272:VAL:HG13	1.73	0.71
1:B:433:ALA:HB1	1:B:467:PHE:HB2	1.72	0.71
1:C:378:LEU:HD11	1:C:382:LYS:HE3	1.72	0.71
1:B:394:PHE:CE1	1:B:398:ILE:HD11	2.25	0.71
1:C:600:PRO:HB2	1:C:616:LEU:HD11	1.71	0.71
1:A:361:LEU:HA	1:A:364:ILE:HG12	1.72	0.71
1:A:457:ILE:HG21	1:A:516:LEU:HD23	1.73	0.71
1:A:360:MET:HB2	1:D:326:LEU:HD21	1.72	0.71
1:A:522:ILE:HG22	1:A:526:LYS:HE2	1.71	0.70
1:D:674:PHE:HB2	1:D:706:ASN:HD21	1.56	0.70
1:A:369:ARG:HA	1:A:372:ILE:HD12	1.72	0.70
1:B:484:SER:O	1:B:488:ILE:HG12	1.92	0.70
1:A:374:GLN:HE22	1:A:396:ASN:HB3	1.55	0.70
1:A:386:LEU:HB3	1:A:499:ILE:HG23	1.74	0.69
1:C:380:TYR:HA	1:C:451:HIS:HE1	1.57	0.69
1:C:87:PHE:O	1:C:168:ARG:NH2	2.24	0.69
1:D:331:ASN:OD1	1:D:340:ARG:NH1	2.25	0.69
1:A:59:HIS:HE1	1:A:61:LYS:HE2	1.56	0.69
1:A:323:MET:HE1	1:A:344:THR:HG22	1.74	0.69
1:B:526:LYS:HD2	1:C:541:GLN:HE22	1.55	0.69
1:D:377:TYR:HB2	1:D:399:VAL:HG13	1.74	0.69
1:A:380:TYR:CE1	1:A:427:CYS:HB2	2.27	0.69
1:A:687:VAL:HG13	1:A:713:LEU:HD22	1.75	0.69
1:C:434:LEU:HB2	1:C:468:THR:HB	1.75	0.69
1:B:648:LEU:HD11	1:B:680:LEU:HD23	1.74	0.69
1:C:644:LEU:HD22	1:C:676:MET:HE2	1.75	0.69
1:D:436:THR:HA	1:D:442:GLU:HA	1.74	0.69
1:C:398:ILE:HD11	1:C:480:LEU:HD22	1.74	0.69
1:D:560:THR:HB	1:D:564:GLY:HA2	1.74	0.68
1:A:421:ASP:HB2	1:A:482:LYS:HB2	1.74	0.68
1:A:601:LEU:HA	1:A:616:LEU:HD13	1.74	0.68
1:B:421:ASP:HB3	1:B:482:LYS:HG2	1.74	0.68
1:B:275:GLY:CA	1:C:274:TYR:O	2.41	0.68
1:D:471:VAL:HG11	1:D:475:CYS:SG	2.34	0.68
1:C:576:TYR:HB3	1:C:579:ILE:HB	1.75	0.68
1:D:461:CYS:HB2	1:D:463:ILE:HG22	1.76	0.68
1:A:436:THR:HA	1:A:442:GLU:HA	1.76	0.68
1:C:431:LEU:HA	1:C:471:VAL:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:LEU:HB3	1:B:676:MET:HE3	1.76	0.68
1:D:557:PRO:HB2	1:D:588:VAL:HG22	1.76	0.68
1:D:374:GLN:HG2	1:D:396:ASN:OD1	1.95	0.67
1:D:546:GLN:OE1	1:D:550:LEU:HG	1.95	0.67
1:A:577:GLU:O	1:A:581:LEU:HB2	1.94	0.67
1:C:145:LEU:O	1:C:149:ILE:HG12	1.93	0.67
1:D:358:THR:HA	1:D:361:LEU:HD23	1.76	0.67
1:A:409:PRO:HA	1:A:471:VAL:HG12	1.76	0.67
1:B:601:LEU:HB2	1:B:621:ALA:HB1	1.77	0.67
1:C:90:PHE:O	1:C:168:ARG:NH2	2.27	0.66
1:C:281:ASN:OD1	1:C:282:LEU:N	2.26	0.66
1:A:590:VAL:HG11	1:A:619:GLU:HB2	1.78	0.66
1:A:281:ASN:ND2	1:A:284:GLU:OE2	2.28	0.66
1:B:369:ARG:HA	1:B:372:ILE:HD12	1.77	0.65
1:A:681:VAL:HG23	1:A:685:ALA:HB3	1.79	0.65
1:B:323:MET:O	1:B:327:ILE:HG12	1.96	0.65
1:B:431:LEU:HB2	1:B:448:LEU:HB2	1.78	0.65
1:D:179:ARG:O	1:D:183:GLU:HG2	1.97	0.65
1:A:381:ILE:HG21	1:A:399:VAL:HG22	1.78	0.65
1:A:454:PHE:CE2	1:A:469:VAL:HG21	2.31	0.65
1:B:91:ARG:NH1	1:B:165:GLU:OE2	2.30	0.65
1:A:395:ILE:O	1:A:399:VAL:HG23	1.96	0.65
1:C:392:THR:HA	1:C:395:ILE:HD12	1.78	0.64
1:D:362:GLN:HA	1:D:369:ARG:HD3	1.79	0.64
1:A:357:ASP:O	1:A:361:LEU:N	2.29	0.64
1:D:418:ASN:HB2	1:D:465:GLN:HG3	1.79	0.64
1:A:435:VAL:N	1:A:443:GLU:O	2.29	0.64
1:A:496:GLY:HA2	1:A:499:ILE:HG12	1.79	0.64
1:A:557:PRO:HB2	1:A:588:VAL:HG23	1.79	0.64
1:C:662:ARG:HH22	1:C:670:SER:HB3	1.61	0.64
1:D:60:PRO:HD3	1:D:119:ALA:HB3	1.80	0.64
1:D:408:LEU:HD12	1:D:409:PRO:HD2	1.78	0.64
1:A:500:LEU:HA	1:A:503:ILE:HD12	1.79	0.64
1:D:145:LEU:O	1:D:149:ILE:HG12	1.98	0.64
1:B:382:LYS:O	1:B:388:LYS:NZ	2.31	0.64
1:A:327:ILE:HG21	1:C:192:THR:HG21	1.79	0.64
1:A:460:ILE:O	1:A:523:HIS:NE2	2.29	0.64
1:C:423:LEU:HD23	1:C:480:LEU:HD23	1.79	0.64
1:D:458:SER:HB2	1:D:466:PRO:HD3	1.80	0.64
1:D:707:LYS:HD3	1:D:710:ILE:HD12	1.79	0.64
1:A:90:PHE:O	1:A:168:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:TYR:HA	1:A:548:LYS:HE2	1.79	0.63
1:B:75:TRP:HZ3	1:B:104:GLY:HA2	1.63	0.63
1:B:385:PRO:HA	1:B:388:LYS:HE2	1.80	0.63
1:B:599:THR:HG21	1:B:624:ASN:HB2	1.80	0.63
1:A:590:VAL:HB	1:A:616:LEU:HD23	1.81	0.63
1:C:601:LEU:HD13	1:C:621:ALA:HB3	1.81	0.63
1:B:398:ILE:HG22	1:B:402:LEU:HD21	1.81	0.63
1:D:551:ILE:HG21	1:D:586:GLU:HG3	1.81	0.63
1:A:500:LEU:HD21	1:A:527:GLN:HE22	1.63	0.63
1:B:360:MET:HB2	1:C:326:LEU:HD21	1.81	0.63
1:D:523:HIS:O	1:D:526:LYS:N	2.32	0.63
1:B:496:GLY:O	1:B:500:LEU:HD12	1.99	0.62
1:A:346:HIS:CD2	1:C:365:PRO:HD3	2.34	0.62
1:A:434:LEU:HD13	1:A:442:GLU:HB2	1.81	0.62
1:A:517:GLU:O	1:A:521:VAL:HG23	1.98	0.62
1:D:499:ILE:O	1:D:503:ILE:HG12	1.98	0.62
1:C:109:LEU:HA	1:C:112:ILE:HD12	1.82	0.62
1:D:401:ARG:HH12	1:D:487:ASN:HB2	1.64	0.62
1:D:699:ASP:HA	1:D:702:ARG:HD2	1.82	0.62
1:B:327:ILE:HD13	1:B:330:MET:SD	2.40	0.62
1:B:698:LEU:HD23	1:B:717:LYS:HD3	1.80	0.62
1:B:540:PHE:HB2	1:B:570:LEU:HD23	1.82	0.62
1:A:511:ASP:HA	1:A:514:LYS:HB3	1.82	0.62
1:A:131:LYS:HG2	1:A:134:ARG:H	1.64	0.61
1:B:435:VAL:HG22	1:B:467:PHE:HB3	1.82	0.61
1:A:122:ASP:O	1:A:126:TYR:N	2.32	0.61
1:C:605:VAL:HG11	1:C:647:LEU:HD12	1.81	0.61
1:A:372:ILE:HG12	1:D:339:LEU:HD21	1.83	0.61
1:D:688:ILE:HA	1:D:717:LYS:HE3	1.82	0.61
1:B:565:ARG:NH1	1:C:563:ASP:OD2	2.34	0.61
1:A:665:LEU:HG	1:A:697:PRO:HB3	1.82	0.61
1:D:548:LYS:HG2	1:D:582:PHE:CE2	2.36	0.61
1:C:480:LEU:HD21	1:C:485:PHE:HB2	1.81	0.61
1:B:434:LEU:HA	1:B:444:SER:HA	1.83	0.61
1:B:487:ASN:OD1	1:B:488:ILE:N	2.34	0.61
1:D:339:LEU:O	1:D:343:ILE:HG13	2.00	0.61
1:B:326:LEU:O	1:B:330:MET:HG3	2.01	0.61
1:C:426:VAL:HG22	1:C:477:LEU:HD22	1.83	0.61
1:D:513:ILE:O	1:D:517:GLU:N	2.34	0.61
1:C:241:LEU:HD21	1:C:276:ASP:HB2	1.83	0.60
1:C:535:VAL:HG22	1:C:550:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:MET:O	1:A:289:MET:HG3	2.01	0.60
1:A:306:ILE:O	1:A:310:ILE:HG13	2.02	0.60
1:B:605:VAL:HG22	1:B:643:PHE:HE1	1.66	0.60
1:D:507:LYS:HE2	1:D:517:GLU:HG3	1.83	0.60
1:D:547:LEU:HD22	1:D:579:ILE:HD12	1.84	0.60
1:C:60:PRO:HD3	1:C:119:ALA:HB3	1.83	0.60
1:D:431:LEU:HD22	1:D:454:PHE:HE2	1.67	0.60
1:A:435:VAL:HG23	1:A:445:VAL:HB	1.84	0.60
1:D:511:ASP:OD2	1:D:512:ARG:N	2.34	0.60
1:D:523:HIS:O	1:D:527:GLN:HG2	2.02	0.60
1:B:671:GLU:HA	1:C:692:ARG:NH2	2.17	0.60
1:C:652:MET:SD	1:C:653:ASN:N	2.75	0.60
1:B:424:TYR:HB2	1:B:454:PHE:CE1	2.37	0.59
1:D:90:PHE:O	1:D:168:ARG:NH2	2.34	0.59
1:D:149:ILE:HG13	1:D:173:ILE:HG21	1.84	0.59
1:A:241:LEU:HD11	1:A:277:ILE:HD11	1.84	0.59
1:C:674:PHE:HB2	1:C:709:LEU:HB2	1.84	0.59
1:A:365:PRO:HD3	1:D:346:HIS:NE2	2.17	0.59
1:A:555:ALA:HB1	1:A:559:LYS:HZ1	1.67	0.59
1:B:457:ILE:HG23	1:B:520:ILE:HD11	1.83	0.59
1:B:517:GLU:O	1:B:521:VAL:HG23	2.02	0.59
1:D:392:THR:O	1:D:396:ASN:HB2	2.02	0.59
1:C:365:PRO:HB2	1:C:368:ILE:HG12	1.85	0.59
1:A:641:SER:HB3	1:A:676:MET:HG2	1.84	0.58
1:B:231:GLU:HB2	1:B:249:PHE:HE1	1.67	0.58
1:B:673:LEU:HD22	1:B:676:MET:HG2	1.85	0.58
1:A:510:ASN:HB2	1:A:513:ILE:HG12	1.84	0.58
1:A:605:VAL:HG13	1:A:646:ARG:HB3	1.85	0.58
1:B:416:GLN:NE2	1:B:436:THR:HB	2.18	0.58
1:D:533:LEU:HD11	1:D:562:TYR:CE1	2.38	0.58
1:D:543:ASP:HB3	1:D:546:GLN:HB3	1.85	0.58
1:B:692:ARG:NH1	1:C:671:GLU:OE2	2.36	0.58
1:C:618:LYS:NZ	1:C:619:GLU:OE2	2.30	0.58
1:A:568:LEU:HG	1:A:600:PRO:HB3	1.85	0.58
1:D:598:HIS:HB3	1:D:603:GLU:OE2	2.02	0.58
1:A:420:VAL:HG23	1:A:465:GLN:HB2	1.85	0.58
1:B:346:HIS:ND1	1:D:365:PRO:HD3	2.17	0.58
1:A:445:VAL:HG13	1:A:446:THR:HG22	1.86	0.58
1:B:701:ALA:HB1	1:B:706:ASN:HD21	1.68	0.58
1:B:75:TRP:CZ3	1:B:104:GLY:HA2	2.38	0.58
1:B:354:HIS:O	1:C:332:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:LEU:HD22	1:B:654:PRO:HG3	1.84	0.58
1:C:506:GLU:O	1:C:510:ASN:N	2.37	0.58
1:A:459:ILE:HA	1:A:482:LYS:HE3	1.85	0.58
1:A:517:GLU:HA	1:A:520:ILE:HG12	1.86	0.58
1:D:319:PHE:HE2	1:D:347:VAL:HG22	1.68	0.58
1:D:435:VAL:HG22	1:D:445:VAL:HG22	1.85	0.57
1:D:430:LEU:HB3	1:D:473:GLU:HB2	1.86	0.57
1:B:332:ARG:HH12	1:D:354:HIS:HD2	1.47	0.57
1:C:149:ILE:HG13	1:C:173:ILE:HG21	1.86	0.57
1:A:343:ILE:O	1:A:347:VAL:HG23	2.03	0.57
1:C:121:ARG:NE	1:C:128:THR:OG1	2.34	0.57
1:A:199:THR:HG22	1:A:203:LYS:HE3	1.87	0.57
1:A:274:TYR:O	1:C:275:GLY:HA3	2.04	0.57
1:A:315:ASN:HA	1:A:318:ARG:HD2	1.85	0.57
1:A:670:SER:HB3	1:A:700:GLU:HB3	1.86	0.57
1:B:364:ILE:HA	1:C:346:HIS:CD2	2.40	0.57
1:B:499:ILE:O	1:B:503:ILE:HG23	2.04	0.57
1:A:91:ARG:NH1	1:A:165:GLU:OE2	2.38	0.57
1:C:350:GLN:HB3	1:C:355:TYR:HB3	1.86	0.57
1:B:485:PHE:HA	1:B:488:ILE:HD11	1.86	0.57
1:B:642:ASP:O	1:B:646:ARG:HG3	2.05	0.57
1:D:531:LEU:HD11	1:D:555:ALA:HB2	1.87	0.57
1:A:381:ILE:HG23	1:A:395:ILE:HD11	1.87	0.57
1:A:687:VAL:HG11	1:A:717:LYS:HB2	1.87	0.56
1:B:93:LEU:HB2	1:B:155:ASP:OD2	2.05	0.56
1:D:415:GLU:CD	1:D:416:GLN:H	2.13	0.56
1:D:720:GLN:HA	1:D:723:ILE:HB	1.87	0.56
1:A:364:ILE:HG21	1:D:343:ILE:HG23	1.87	0.56
1:A:499:ILE:O	1:A:503:ILE:HG13	2.05	0.56
1:B:456:ASP:OD1	1:B:456:ASP:N	2.38	0.56
1:D:594:ASP:OD1	1:D:598:HIS:N	2.38	0.56
1:C:433:ALA:HB3	1:C:446:THR:H	1.69	0.56
1:C:435:VAL:HG22	1:C:445:VAL:HG22	1.87	0.56
1:C:662:ARG:HG2	1:C:691:ASP:HB2	1.87	0.56
1:D:532:ALA:HB2	1:D:559:LYS:HD2	1.87	0.56
1:B:560:THR:HG22	1:B:566:SER:HB3	1.88	0.56
1:A:644:LEU:O	1:A:648:LEU:HG	2.05	0.56
1:A:662:ARG:HH12	1:A:700:GLU:CD	2.13	0.56
1:B:272:VAL:O	1:D:273:GLY:HA3	2.05	0.56
1:B:281:ASN:ND2	1:B:284:GLU:OE2	2.39	0.56
1:B:349:LEU:HD22	1:B:408:LEU:HG	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ILE:O	1:B:376:LEU:HG	2.04	0.56
1:C:457:ILE:HB	1:C:466:PRO:HG3	1.88	0.56
1:B:533:LEU:HD21	1:C:533:LEU:HB3	1.88	0.56
1:D:590:VAL:HG11	1:D:619:GLU:HB3	1.87	0.56
1:A:275:GLY:CA	1:D:274:TYR:O	2.53	0.56
1:B:601:LEU:O	1:B:605:VAL:HG12	2.06	0.56
1:B:630:ASN:O	1:B:634:THR:HG23	2.05	0.56
1:C:577:GLU:HG2	1:C:612:VAL:HG23	1.88	0.56
1:A:424:TYR:HB2	1:A:454:PHE:CE1	2.40	0.56
1:B:409:PRO:HG3	1:B:473:GLU:HA	1.88	0.56
1:C:226:LEU:O	1:C:250:ARG:NH2	2.33	0.56
1:C:349:LEU:HD21	1:C:474:LEU:HD11	1.87	0.56
1:C:484:SER:O	1:C:488:ILE:HG13	2.06	0.56
1:C:121:ARG:HA	1:C:128:THR:HA	1.87	0.56
1:D:223:ALA:HB2	1:D:235:TRP:NE1	2.19	0.56
1:D:632:LEU:O	1:D:636:VAL:HG23	2.05	0.56
1:A:501:ASN:O	1:A:505:GLU:HG2	2.06	0.55
1:A:665:LEU:HD11	1:A:713:LEU:HD21	1.86	0.55
1:D:319:PHE:CZ	1:D:348:ARG:HA	2.42	0.55
1:B:524:ILE:O	1:B:527:GLN:HG3	2.06	0.55
1:A:428:GLU:HB2	1:A:476:HIS:HB3	1.88	0.55
1:B:90:PHE:O	1:B:168:ARG:NH1	2.39	0.55
1:B:557:PRO:HG3	1:B:586:GLU:HB3	1.88	0.55
1:B:604:ALA:HB2	1:B:616:LEU:HD22	1.88	0.55
1:D:517:GLU:O	1:D:521:VAL:HG13	2.06	0.55
1:B:252:ILE:O	1:B:257:ARG:NH1	2.39	0.55
1:D:60:PRO:HD2	1:D:61:LYS:HZ2	1.72	0.55
1:C:600:PRO:HB2	1:C:616:LEU:CD1	2.36	0.55
1:C:603:GLU:H	1:C:603:GLU:CD	2.13	0.55
1:A:405:GLU:O	1:A:476:HIS:ND1	2.36	0.55
1:C:540:PHE:HD1	1:C:570:LEU:HB3	1.72	0.55
1:D:395:ILE:HA	1:D:398:ILE:HG12	1.89	0.55
1:D:601:LEU:HD11	1:D:650:SER:HB3	1.87	0.55
1:D:627:ASP:HB3	1:D:630:ASN:HB3	1.88	0.55
1:C:51:HIS:CD2	1:C:51:HIS:H	2.24	0.55
1:D:146:MET:HA	1:D:146:MET:HE2	1.89	0.55
1:A:709:LEU:O	1:A:713:LEU:HB2	2.07	0.55
1:C:494:HIS:O	1:C:498:THR:OG1	2.22	0.55
1:B:416:GLN:H	1:B:468:THR:HG22	1.71	0.55
1:B:660:ASP:HB2	1:B:662:ARG:HG2	1.89	0.55
1:C:195:ASN:OD1	1:C:196:TYR:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:HA	1:A:90:PHE:HD2	1.72	0.55
1:A:220:TYR:O	1:A:224:THR:HG23	2.07	0.55
1:A:377:TYR:HB3	1:A:402:LEU:HD12	1.89	0.55
1:B:645:LYS:HB2	1:B:679:MET:SD	2.47	0.55
1:C:434:LEU:O	1:C:468:THR:N	2.38	0.55
1:A:378:LEU:O	1:A:381:ILE:HG22	2.06	0.54
1:A:467:PHE:HE2	1:A:516:LEU:HD21	1.72	0.54
1:B:136:ALA:O	1:B:140:LEU:HD12	2.07	0.54
1:B:315:ASN:HA	1:B:318:ARG:HE	1.70	0.54
1:B:430:LEU:HB3	1:B:473:GLU:OE1	2.06	0.54
1:B:500:LEU:O	1:B:503:ILE:HG13	2.07	0.54
1:B:526:LYS:HD2	1:C:541:GLN:NE2	2.22	0.54
1:D:583:LEU:HB3	1:D:588:VAL:HG21	1.89	0.54
1:A:413:ILE:HD13	1:A:477:LEU:HD11	1.90	0.54
1:B:654:PRO:HB2	1:B:685:ALA:HB2	1.90	0.54
1:D:119:ALA:HA	1:D:135:ILE:HD11	1.89	0.54
1:A:648:LEU:HD13	1:A:683:ALA:HB3	1.88	0.54
1:B:55:LYS:HD3	1:B:56:TYR:HD1	1.71	0.54
1:C:195:ASN:O	1:C:199:THR:HG22	2.07	0.54
1:C:432:GLU:N	1:C:470:ARG:O	2.40	0.54
1:D:165:GLU:OE1	1:D:168:ARG:NH1	2.38	0.54
1:A:346:HIS:NE2	1:C:363:ASP:O	2.41	0.54
1:B:665:LEU:HD22	1:B:685:ALA:HB1	1.90	0.54
1:C:431:LEU:HD23	1:C:471:VAL:HG12	1.89	0.54
1:C:315:ASN:OD1	1:C:318:ARG:NH2	2.40	0.54
1:A:527:GLN:HA	1:A:530:GLU:OE1	2.07	0.54
1:B:716:VAL:O	1:B:720:GLN:HG2	2.07	0.54
1:A:361:LEU:HB3	1:A:369:ARG:HH11	1.73	0.54
1:A:534:LYS:HD2	1:A:534:LYS:N	2.22	0.54
1:B:605:VAL:HG22	1:B:643:PHE:CE1	2.42	0.54
1:B:636:VAL:HG13	1:B:676:MET:SD	2.47	0.54
1:C:535:VAL:HG21	1:C:555:ALA:HB1	1.89	0.54
1:C:542:GLY:HA2	1:C:579:ILE:HD11	1.88	0.54
1:D:565:ARG:NE	1:D:569:HIS:HB3	2.22	0.54
1:A:338:ASP:O	1:A:342:GLN:HG2	2.08	0.54
1:A:514:LYS:O	1:A:517:GLU:HG3	2.07	0.54
1:C:395:ILE:HA	1:C:398:ILE:HG22	1.88	0.54
1:C:635:THR:HG23	1:C:640:ASP:HB2	1.89	0.54
1:D:604:ALA:HB2	1:D:616:LEU:HD12	1.89	0.54
1:A:533:LEU:HD22	1:D:533:LEU:HD22	1.90	0.53
1:C:432:GLU:O	1:C:469:VAL:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:PHE:CE1	1:D:398:ILE:HD11	2.43	0.53
1:A:507:LYS:HZ1	1:A:516:LEU:HD22	1.72	0.53
1:B:431:LEU:CD2	1:B:471:VAL:HA	2.38	0.53
1:B:322:LYS:O	1:B:326:LEU:HG	2.07	0.53
1:B:543:ASP:HB3	1:B:546:GLN:HB2	1.90	0.53
1:D:350:GLN:HG2	1:D:355:TYR:CE2	2.44	0.53
1:A:346:HIS:O	1:A:350:GLN:HG2	2.08	0.53
1:A:690:LYS:HB3	1:A:694:GLY:HA2	1.91	0.53
1:D:153:PRO:HB2	1:D:156:LEU:HB2	1.90	0.53
1:D:544:PHE:CZ	1:D:548:LYS:HE3	2.44	0.53
1:A:496:GLY:O	1:A:500:LEU:HD22	2.07	0.53
1:B:201:ILE:HG22	1:B:305:ASN:HB3	1.90	0.53
1:C:195:ASN:HD21	1:C:312:LYS:HE2	1.74	0.53
1:D:362:GLN:OE1	1:D:362:GLN:N	2.33	0.53
1:A:507:LYS:HD3	1:A:517:GLU:HG2	1.90	0.53
1:B:512:ARG:H	1:B:512:ARG:HD2	1.73	0.53
1:C:536:ASN:ND2	1:C:565:ARG:O	2.42	0.53
1:D:386:LEU:HD13	1:D:456:ASP:OD2	2.08	0.53
1:C:605:VAL:HA	1:C:613:ILE:HD11	1.90	0.53
1:D:488:ILE:HA	1:D:491:ILE:HD12	1.89	0.53
1:B:560:THR:HA	1:B:566:SER:HA	1.91	0.53
1:C:405:GLU:OE2	1:C:479:ARG:NE	2.42	0.53
1:A:454:PHE:HE2	1:A:469:VAL:HG21	1.73	0.53
1:B:424:TYR:HA	1:B:478:LEU:O	2.09	0.53
1:B:425:PHE:O	1:B:477:LEU:HA	2.08	0.53
1:B:627:ASP:HB3	1:B:630:ASN:HB3	1.90	0.53
1:C:223:ALA:HB2	1:C:235:TRP:NE1	2.24	0.53
1:A:520:ILE:HG22	1:A:524:ILE:HD11	1.90	0.53
1:A:532:ALA:HB2	1:A:559:LYS:HB3	1.91	0.53
1:C:368:ILE:O	1:C:372:ILE:HG22	2.09	0.53
1:A:632:LEU:O	1:A:636:VAL:HG23	2.09	0.52
1:B:328:SER:O	1:B:332:ARG:HG3	2.09	0.52
1:D:423:LEU:HB2	1:D:459:ILE:HD12	1.90	0.52
1:A:422:HIS:CE1	1:A:479:ARG:HD2	2.43	0.52
1:A:533:LEU:HB3	1:D:533:LEU:HD22	1.91	0.52
1:B:271:THR:HA	1:C:272:VAL:HG23	1.92	0.52
1:C:434:LEU:HD22	1:C:442:GLU:HB2	1.90	0.52
1:D:528:GLU:OE1	1:D:559:LYS:NZ	2.29	0.52
1:D:565:ARG:O	1:D:569:HIS:ND1	2.43	0.52
1:A:706:ASN:HB3	1:A:709:LEU:HB2	1.91	0.52
1:B:121:ARG:HA	1:B:128:THR:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:O	1:B:201:ILE:HG23	2.09	0.52
1:C:456:ASP:O	1:C:460:ILE:HG12	2.09	0.52
1:D:531:LEU:HD12	1:D:550:LEU:HD13	1.91	0.52
1:A:359:VAL:O	1:A:362:GLN:HB2	2.09	0.52
1:B:172:TRP:O	1:B:175:LEU:HB2	2.09	0.52
1:C:367:SER:O	1:C:371:LYS:HG3	2.09	0.52
1:D:115:GLN:HB3	1:D:139:TYR:CE1	2.44	0.52
1:A:423:LEU:HD13	1:A:456:ASP:N	2.23	0.52
1:A:687:VAL:O	1:A:697:PRO:HD2	2.10	0.52
1:A:402:LEU:HA	1:A:479:ARG:O	2.10	0.52
1:B:377:TYR:CD1	1:B:478:LEU:HD11	2.44	0.52
1:B:658:ASP:OD1	1:B:659:TYR:N	2.38	0.52
1:D:120:TYR:HD2	1:D:135:ILE:HG12	1.73	0.52
1:D:365:PRO:HD2	1:D:368:ILE:HD12	1.92	0.52
1:A:249:PHE:O	1:A:257:ARG:HD2	2.10	0.52
1:A:434:LEU:HB2	1:A:468:THR:O	2.10	0.52
1:B:448:LEU:HD13	1:B:454:PHE:CD2	2.45	0.52
1:D:208:GLU:O	1:D:212:THR:HG23	2.10	0.52
1:D:483:GLN:HE22	1:D:487:ASN:HD21	1.58	0.52
1:A:357:ASP:OD2	1:D:329:PHE:HB2	2.10	0.52
1:A:610:GLU:HA	1:A:613:ILE:HD12	1.92	0.52
1:B:428:GLU:HG2	1:B:476:HIS:HB2	1.92	0.52
1:B:457:ILE:HG21	1:B:516:LEU:HB3	1.91	0.52
1:B:623:PHE:CE1	1:B:628:SER:HB3	2.44	0.52
1:B:666:HIS:CD2	1:B:697:PRO:HG3	2.45	0.52
1:C:695:ASN:HB3	1:C:699:ASP:HB2	1.92	0.52
1:D:396:ASN:O	1:D:400:ILE:HG13	2.10	0.52
1:A:199:THR:O	1:A:203:LYS:HG3	2.10	0.52
1:A:415:GLU:HA	1:A:468:THR:HA	1.91	0.52
1:A:437:LYS:NZ	1:A:443:GLU:HB2	2.24	0.52
1:B:436:THR:HG23	1:B:440:GLY:N	2.24	0.52
1:C:220:TYR:O	1:C:224:THR:HG23	2.10	0.52
1:C:435:VAL:HG23	1:C:443:GLU:HB2	1.91	0.52
1:D:204:LEU:HD11	1:D:301:TYR:HB3	1.92	0.52
1:A:347:VAL:HG13	1:A:350:GLN:HE21	1.75	0.52
1:B:403:HIS:HB2	1:B:479:ARG:HE	1.74	0.52
1:B:131:LYS:HA	1:B:131:LYS:HE2	1.92	0.51
1:C:644:LEU:O	1:C:648:LEU:HG	2.09	0.51
1:D:485:PHE:HA	1:D:488:ILE:HD11	1.92	0.51
1:D:705:GLY:O	1:D:707:LYS:HE2	2.10	0.51
1:B:346:HIS:HA	1:B:408:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LEU:O	1:D:213:HIS:NE2	2.43	0.51
1:A:532:ALA:HA	1:A:559:LYS:HE2	1.92	0.51
1:B:340:ARG:O	1:B:344:THR:HG23	2.10	0.51
1:C:654:PRO:HB2	1:C:685:ALA:HB2	1.92	0.51
1:D:516:LEU:O	1:D:520:ILE:HG13	2.10	0.51
1:A:145:LEU:HD23	1:A:145:LEU:H	1.76	0.51
1:A:458:SER:HA	1:A:463:ILE:HG13	1.91	0.51
1:C:228:PRO:O	1:C:231:GLU:HB3	2.10	0.51
1:A:467:PHE:CE2	1:A:516:LEU:HD21	2.46	0.51
1:B:671:GLU:CD	1:C:692:ARG:HH22	2.19	0.51
1:A:433:ALA:HA	1:A:469:VAL:HA	1.93	0.51
1:A:688:ILE:HG22	1:A:717:LYS:HE3	1.93	0.51
1:A:223:ALA:HB2	1:A:235:TRP:NE1	2.26	0.51
1:A:476:HIS:O	1:A:477:LEU:HD23	2.10	0.51
1:A:517:GLU:HA	1:A:520:ILE:CG1	2.41	0.51
1:B:454:PHE:CE2	1:B:469:VAL:HG11	2.45	0.51
1:A:432:GLU:HB2	1:A:472:CYS:SG	2.51	0.51
1:A:494:HIS:O	1:A:498:THR:HG23	2.11	0.51
1:B:358:THR:HA	1:B:361:LEU:HD12	1.93	0.51
1:D:431:LEU:HD22	1:D:454:PHE:CE2	2.46	0.51
1:A:98:PHE:CE1	1:A:156:LEU:HD21	2.45	0.51
1:A:605:VAL:HG11	1:A:647:LEU:HD23	1.93	0.51
1:A:643:PHE:HA	1:A:646:ARG:HE	1.76	0.51
1:D:415:GLU:OE1	1:D:416:GLN:N	2.44	0.51
1:D:487:ASN:O	1:D:490:GLU:HG2	2.11	0.51
1:A:668:ALA:HB1	1:A:677:ALA:HB2	1.93	0.51
1:B:433:ALA:O	1:B:445:VAL:N	2.44	0.51
1:C:409:PRO:HB3	1:C:472:CYS:O	2.11	0.51
1:C:698:LEU:HA	1:C:713:LEU:HD13	1.92	0.51
1:A:65:TYR:CE1	1:A:118:VAL:HG11	2.47	0.50
1:B:306:ILE:O	1:B:310:ILE:HG12	2.11	0.50
1:B:706:ASN:ND2	1:B:709:LEU:HB3	2.25	0.50
1:C:208:GLU:O	1:C:212:THR:HG23	2.11	0.50
1:C:326:LEU:HD12	1:C:347:VAL:HG21	1.92	0.50
1:C:339:LEU:O	1:C:343:ILE:HG12	2.10	0.50
1:C:395:ILE:O	1:C:398:ILE:HG22	2.11	0.50
1:C:580:THR:HG21	1:C:612:VAL:HG13	1.93	0.50
1:D:610:GLU:HA	1:D:613:ILE:HB	1.92	0.50
1:A:415:GLU:HA	1:A:468:THR:HG23	1.93	0.50
1:B:644:LEU:O	1:B:648:LEU:HG	2.12	0.50
1:C:240:LYS:HD2	1:C:245:SER:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:PHE:HB2	1:D:475:CYS:SG	2.51	0.50
1:C:197:LEU:HB3	1:C:309:LEU:HB3	1.93	0.50
1:A:459:ILE:HG12	1:A:482:LYS:HE3	1.93	0.50
1:D:568:LEU:HB3	1:D:588:VAL:HG11	1.93	0.50
1:A:153:PRO:HB2	1:A:156:LEU:HB2	1.93	0.50
1:A:281:ASN:HD22	1:A:284:GLU:CD	2.20	0.50
1:A:361:LEU:HB3	1:A:369:ARG:NH1	2.27	0.50
1:A:378:LEU:HD11	1:A:382:LYS:HE2	1.94	0.50
1:C:98:PHE:O	1:C:102:ILE:HG12	2.11	0.50
1:C:566:SER:HB3	1:C:592:LEU:HD22	1.93	0.50
1:A:605:VAL:HG12	1:A:643:PHE:HE1	1.77	0.50
1:B:315:ASN:OD1	1:B:315:ASN:N	2.43	0.50
1:A:379:PRO:O	1:A:383:LYS:HE2	2.12	0.50
1:D:249:PHE:O	1:D:257:ARG:HD2	2.12	0.50
1:D:393:GLU:O	1:D:397:GLN:HG2	2.12	0.50
1:D:632:LEU:HB3	1:D:664:PRO:HG3	1.94	0.50
1:D:665:LEU:HG	1:D:697:PRO:HB2	1.94	0.50
1:B:213:HIS:ND1	1:B:258:TYR:OH	2.42	0.50
1:C:155:ASP:O	1:C:159:LYS:HG2	2.12	0.50
1:C:706:ASN:O	1:C:710:ILE:HG13	2.12	0.50
1:D:666:HIS:CE1	1:D:697:PRO:HD3	2.47	0.50
1:D:707:LYS:HA	1:D:710:ILE:HD12	1.94	0.50
1:A:494:HIS:HD1	1:A:494:HIS:H	1.60	0.50
1:A:560:THR:HG22	1:A:566:SER:HA	1.93	0.50
1:A:699:ASP:HA	1:A:702:ARG:HD2	1.93	0.50
1:B:272:VAL:HA	1:D:271:THR:O	2.12	0.50
1:C:380:TYR:HA	1:C:451:HIS:CE1	2.43	0.50
1:C:687:VAL:HG12	1:C:717:LYS:HD2	1.94	0.49
1:C:398:ILE:O	1:C:402:LEU:HG	2.12	0.49
1:A:241:LEU:HD21	1:A:276:ASP:HB2	1.95	0.49
1:A:393:GLU:HG3	1:A:394:PHE:N	2.27	0.49
1:B:358:THR:HG22	1:B:361:LEU:HD12	1.92	0.49
1:C:249:PHE:HA	1:C:252:ILE:HG13	1.94	0.49
1:C:698:LEU:HD11	1:C:714:GLU:OE2	2.12	0.49
1:D:105:GLN:OE1	1:D:177:ARG:NH2	2.42	0.49
1:D:690:LYS:HD3	1:D:696:SER:HB3	1.94	0.49
1:A:231:GLU:HB2	1:A:249:PHE:HE1	1.76	0.49
1:A:328:SER:O	1:A:332:ARG:HG2	2.11	0.49
1:A:631:PHE:O	1:A:635:THR:HG22	2.11	0.49
1:B:346:HIS:NE2	1:B:350:GLN:OE1	2.45	0.49
1:B:405:GLU:HB3	1:B:407:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:PHE:HD1	1:B:570:LEU:HB3	1.77	0.49
1:C:51:HIS:H	1:C:51:HIS:HD2	1.60	0.49
1:D:504:MET:HA	1:D:507:LYS:HD3	1.94	0.49
1:D:509:SER:HB3	1:D:513:ILE:HG21	1.94	0.49
1:A:192:THR:HA	1:D:320:ARG:HH22	1.78	0.49
1:B:377:TYR:HB2	1:B:399:VAL:HG13	1.95	0.49
1:C:687:VAL:CG1	1:C:713:LEU:HD22	2.42	0.49
1:A:129:VAL:HG22	1:A:131:LYS:H	1.77	0.49
1:A:446:THR:HA	1:A:512:ARG:NH2	2.27	0.49
1:A:569:HIS:CE1	1:A:594:ASP:HB3	2.47	0.49
1:A:605:VAL:HG12	1:A:643:PHE:CE1	2.48	0.49
1:D:437:LYS:HE3	1:D:443:GLU:HB2	1.95	0.49
1:A:403:HIS:HB2	1:A:479:ARG:HB3	1.95	0.49
1:A:76:ALA:HA	1:A:108:PHE:HZ	1.78	0.49
1:B:223:ALA:HB2	1:B:235:TRP:NE1	2.28	0.49
1:C:407:PHE:HB2	1:C:475:CYS:SG	2.52	0.49
1:D:565:ARG:HE	1:D:569:HIS:HB3	1.78	0.49
1:D:657:GLU:HB3	1:D:661:HIS:HA	1.94	0.49
1:D:669:ALA:HB1	1:D:701:ALA:HB2	1.95	0.49
1:A:363:ASP:HB3	1:D:350:GLN:HE22	1.78	0.49
1:B:497:ARG:HH22	1:B:554:GLY:C	2.20	0.49
1:A:357:ASP:OD1	1:D:325:ASP:HB3	2.13	0.49
1:C:149:ILE:O	1:C:154:TRP:NE1	2.45	0.49
1:C:674:PHE:HD1	1:C:709:LEU:HA	1.77	0.49
1:A:644:LEU:HA	1:A:647:LEU:HG	1.94	0.48
1:B:119:ALA:HA	1:B:135:ILE:HD11	1.94	0.48
1:C:667:VAL:O	1:C:671:GLU:HG2	2.12	0.48
1:B:427:CYS:O	1:B:450:PRO:HB3	2.13	0.48
1:B:569:HIS:HA	1:B:603:GLU:HG3	1.95	0.48
1:C:81:LEU:O	1:C:213:HIS:NE2	2.46	0.48
1:C:608:GLY:HA3	1:C:646:ARG:HH11	1.78	0.48
1:D:496:GLY:O	1:D:499:ILE:HG13	2.12	0.48
1:A:396:ASN:HA	1:A:399:VAL:HG23	1.96	0.48
1:A:497:ARG:HA	1:A:500:LEU:HD23	1.94	0.48
1:B:544:PHE:O	1:B:548:LYS:HG3	2.13	0.48
1:C:51:HIS:HB2	1:C:54:TYR:HD2	1.76	0.48
1:C:378:LEU:HA	1:C:381:ILE:HG22	1.95	0.48
1:A:414:THR:HB	1:A:420:VAL:HG21	1.94	0.48
1:C:479:ARG:HH11	1:C:479:ARG:HG2	1.77	0.48
1:D:653:ASN:OD1	1:D:655:ASN:ND2	2.47	0.48
1:A:685:ALA:O	1:A:720:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:SER:OG	1:B:541:GLN:NE2	2.46	0.48
1:B:609:GLN:HG3	1:B:612:VAL:H	1.79	0.48
1:D:338:ASP:OD1	1:D:338:ASP:N	2.45	0.48
1:D:339:LEU:HD23	1:D:343:ILE:HD11	1.95	0.48
1:D:454:PHE:CG	1:D:469:VAL:HG21	2.49	0.48
1:D:533:LEU:HD11	1:D:562:TYR:HE1	1.76	0.48
1:D:714:GLU:O	1:D:718:ASN:ND2	2.46	0.48
1:C:590:VAL:HG12	1:C:621:ALA:HB2	1.95	0.48
1:C:605:VAL:HG13	1:C:646:ARG:HB3	1.96	0.48
1:A:330:MET:SD	1:A:340:ARG:HG2	2.53	0.48
1:B:365:PRO:HD3	1:C:346:HIS:CE1	2.49	0.48
1:C:131:LYS:HB3	1:C:134:ARG:HD2	1.94	0.48
1:C:361:LEU:HB3	1:C:369:ARG:HD3	1.95	0.48
1:D:565:ARG:HH21	1:D:569:HIS:C	2.22	0.48
1:A:660:ASP:OD2	1:D:662:ARG:NH1	2.47	0.48
1:B:516:LEU:O	1:B:520:ILE:HG13	2.14	0.48
1:B:580:THR:O	1:B:584:ILE:HG12	2.13	0.48
1:C:500:LEU:HA	1:C:503:ILE:HG22	1.95	0.48
1:C:569:HIS:HE1	1:C:592:LEU:HD23	1.78	0.48
1:D:424:TYR:HB2	1:D:454:PHE:CE1	2.49	0.48
1:D:712:LEU:O	1:D:716:VAL:HG23	2.14	0.48
1:A:568:LEU:HB2	1:A:588:VAL:HG11	1.95	0.47
1:B:384:VAL:C	1:B:388:LYS:HZ3	2.22	0.47
1:C:423:LEU:HB2	1:C:459:ILE:HD12	1.96	0.47
1:D:53:ASP:OD1	1:D:53:ASP:N	2.47	0.47
1:D:598:HIS:CG	1:D:602:PHE:HE1	2.31	0.47
1:A:192:THR:HA	1:D:320:ARG:HH12	1.79	0.47
1:A:368:ILE:HD12	1:A:368:ILE:H	1.77	0.47
1:B:357:ASP:HA	1:B:360:MET:HG2	1.97	0.47
1:C:544:PHE:CE2	1:C:582:PHE:HD2	2.32	0.47
1:D:366:ALA:N	1:D:369:ARG:HH21	2.12	0.47
1:A:140:LEU:HA	1:A:144:PHE:HB3	1.95	0.47
1:D:183:GLU:O	1:D:187:ARG:HG3	2.14	0.47
1:D:503:ILE:O	1:D:507:LYS:HG3	2.15	0.47
1:A:404:GLU:HG2	1:A:476:HIS:CE1	2.50	0.47
1:B:511:ASP:HA	1:B:514:LYS:HB2	1.96	0.47
1:D:520:ILE:O	1:D:524:ILE:HG13	2.14	0.47
1:A:674:PHE:CD2	1:A:708:LYS:HE3	2.49	0.47
1:B:157:ILE:HG22	1:B:167:VAL:HG21	1.97	0.47
1:B:641:SER:HB3	1:B:679:MET:HE1	1.97	0.47
1:C:86:GLU:HA	1:C:90:PHE:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:PRO:HA	1:C:471:VAL:HG23	1.96	0.47
1:C:548:LYS:O	1:C:552:ARG:HG2	2.15	0.47
1:C:687:VAL:O	1:C:696:SER:HB2	2.15	0.47
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.77	0.47
1:A:497:ARG:NH1	1:A:553:SER:O	2.48	0.47
1:A:632:LEU:HB3	1:A:664:PRO:HG3	1.95	0.47
1:C:348:ARG:O	1:C:351:TYR:HB3	2.15	0.47
1:C:640:ASP:HB3	1:C:643:PHE:HB3	1.97	0.47
1:D:511:ASP:OD2	1:D:515:LYS:NZ	2.47	0.47
1:A:670:SER:C	1:D:692:ARG:HH21	2.23	0.47
1:A:692:ARG:HG3	1:A:693:TRP:CE3	2.49	0.47
1:B:356:THR:O	1:B:360:MET:HE2	2.14	0.47
1:D:86:GLU:HA	1:D:90:PHE:CD1	2.50	0.47
1:D:547:LEU:O	1:D:551:ILE:HG13	2.14	0.47
1:B:482:LYS:HG3	1:B:483:GLN:H	1.79	0.47
1:C:279:ALA:HB2	1:C:288:VAL:HG21	1.96	0.47
1:A:579:ILE:O	1:A:583:LEU:HD23	2.15	0.47
1:A:630:ASN:ND2	1:D:634:THR:OG1	2.48	0.47
1:B:688:ILE:HG22	1:B:717:LYS:HG3	1.97	0.47
1:C:69:GLU:OE2	1:C:187:ARG:NH1	2.48	0.47
1:D:363:ASP:N	1:D:363:ASP:OD1	2.45	0.47
1:B:573:CYS:SG	1:B:603:GLU:HB3	2.54	0.47
1:B:633:CYS:SG	1:B:667:VAL:HG21	2.55	0.47
1:B:634:THR:HG22	1:C:630:ASN:ND2	2.30	0.47
1:C:627:ASP:HB3	1:C:630:ASN:HB3	1.96	0.47
1:D:698:LEU:HD21	1:D:714:GLU:HG3	1.97	0.47
1:A:312:LYS:HE2	1:A:312:LYS:HB3	1.71	0.46
1:A:523:HIS:HA	1:A:526:LYS:HE3	1.96	0.46
1:B:398:ILE:HD13	1:B:398:ILE:N	2.30	0.46
1:D:220:TYR:O	1:D:224:THR:HG23	2.15	0.46
1:B:274:TYR:HB3	1:D:275:GLY:HA2	1.97	0.46
1:C:331:ASN:HA	1:C:340:ARG:NH2	2.30	0.46
1:D:417:GLY:H	1:D:465:GLN:HB2	1.81	0.46
1:B:446:THR:HG22	1:B:512:ARG:HG3	1.96	0.46
1:C:598:HIS:HB3	1:C:602:PHE:HD2	1.80	0.46
1:C:632:LEU:HD11	1:C:652:MET:HG3	1.97	0.46
1:D:405:GLU:HB3	1:D:407:PHE:CE1	2.51	0.46
1:D:431:LEU:CD2	1:D:471:VAL:HG22	2.46	0.46
1:D:706:ASN:O	1:D:710:ILE:HG13	2.14	0.46
1:B:240:LYS:HE3	1:B:240:LYS:HB3	1.75	0.46
1:B:414:THR:OG1	1:B:469:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:LEU:HD13	1:B:454:PHE:HD2	1.79	0.46
1:A:115:GLN:HA	1:A:118:VAL:HG22	1.97	0.46
1:A:426:VAL:HG21	1:A:448:LEU:HB3	1.96	0.46
1:A:691:ASP:OD1	1:A:695:ASN:N	2.48	0.46
1:B:327:ILE:HA	1:B:330:MET:SD	2.55	0.46
1:B:386:LEU:HD12	1:B:503:ILE:HG22	1.96	0.46
1:C:501:ASN:O	1:C:504:MET:HE3	2.15	0.46
1:D:408:LEU:HB3	1:D:411:GLU:HB2	1.98	0.46
1:C:137:PHE:O	1:C:141:LYS:HG2	2.15	0.46
1:C:197:LEU:HD13	1:C:309:LEU:HA	1.97	0.46
1:D:149:ILE:HA	1:D:152:PHE:CD2	2.50	0.46
1:A:240:LYS:HD2	1:A:245:SER:HB3	1.97	0.46
1:A:374:GLN:NE2	1:A:396:ASN:HB3	2.28	0.46
1:B:312:LYS:NZ	1:C:321:ASP:OD1	2.47	0.46
1:B:503:ILE:HD13	1:B:520:ILE:HD12	1.96	0.46
1:B:600:PRO:HA	1:B:603:GLU:HG2	1.97	0.46
1:C:374:GLN:O	1:C:378:LEU:HB3	2.16	0.46
1:D:319:PHE:O	1:D:323:MET:HG3	2.16	0.46
1:D:652:MET:O	1:D:653:ASN:C	2.58	0.46
1:A:437:LYS:HZ2	1:A:443:GLU:HB2	1.80	0.46
1:A:596:PHE:CD1	1:A:596:PHE:N	2.84	0.46
1:B:521:VAL:HA	1:B:524:ILE:HD12	1.97	0.46
1:B:655:ASN:HA	1:B:663:THR:HB	1.98	0.46
1:B:698:LEU:HD11	1:B:714:GLU:HG3	1.98	0.46
1:C:716:VAL:O	1:C:720:GLN:HG2	2.16	0.46
1:D:207:VAL:HG12	1:D:298:LEU:HD21	1.97	0.46
1:C:306:ILE:O	1:C:309:LEU:HG	2.16	0.46
1:C:415:GLU:HA	1:C:468:THR:HG23	1.97	0.46
1:C:421:ASP:HA	1:C:482:LYS:HG2	1.97	0.46
1:C:679:MET:SD	1:C:679:MET:N	2.89	0.46
1:A:662:ARG:NH1	1:A:700:GLU:OE2	2.46	0.46
1:B:390:CYS:HB3	1:B:394:PHE:CD2	2.51	0.46
1:B:602:PHE:HB2	1:B:625:LEU:HD21	1.97	0.46
1:A:282:LEU:HD22	1:A:282:LEU:HA	1.83	0.45
1:A:343:ILE:HG23	1:C:364:ILE:HD12	1.98	0.45
1:A:698:LEU:HD13	1:A:713:LEU:HB3	1.96	0.45
1:A:719:ALA:O	1:A:722:SER:OG	2.29	0.45
1:B:108:PHE:O	1:B:112:ILE:HG12	2.16	0.45
1:B:512:ARG:HG2	1:B:513:ILE:HD12	1.99	0.45
1:C:240:LYS:HG3	1:C:240:LYS:O	2.15	0.45
1:C:569:HIS:HD2	1:C:603:GLU:OE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:HG3	1:A:169:TYR:HE1	1.81	0.45
1:B:57:ILE:HD11	1:B:132:PRO:HG3	1.98	0.45
1:B:87:PHE:O	1:B:168:ARG:NH2	2.48	0.45
1:C:391:SER:HB3	1:C:494:HIS:CD2	2.50	0.45
1:D:231:GLU:O	1:D:237:GLY:HA3	2.16	0.45
1:D:488:ILE:HA	1:D:491:ILE:CD1	2.46	0.45
1:D:565:ARG:CZ	1:D:569:HIS:HB3	2.47	0.45
1:B:584:ILE:HD12	1:B:619:GLU:HG3	1.98	0.45
1:B:688:ILE:HA	1:B:696:SER:HB2	1.99	0.45
1:D:59:HIS:CE1	1:D:62:ASN:HB2	2.51	0.45
1:D:404:GLU:HG2	1:D:476:HIS:NE2	2.31	0.45
1:D:466:PRO:HB2	1:D:467:PHE:CD1	2.51	0.45
1:D:665:LEU:HD12	1:D:665:LEU:O	2.16	0.45
1:A:239:LEU:HD11	1:A:277:ILE:HG13	1.98	0.45
1:A:357:ASP:CG	1:D:329:PHE:HB2	2.42	0.45
1:A:360:MET:CB	1:D:326:LEU:HD21	2.41	0.45
1:B:655:ASN:ND2	1:B:686:SER:H	2.13	0.45
1:B:698:LEU:CD2	1:B:717:LYS:HD3	2.46	0.45
1:C:359:VAL:O	1:C:362:GLN:HG2	2.16	0.45
1:C:710:ILE:O	1:C:714:GLU:HG2	2.17	0.45
1:A:183:GLU:O	1:A:187:ARG:HG3	2.16	0.45
1:A:373:ALA:HA	1:A:377:TYR:CD2	2.52	0.45
1:A:384:VAL:HG13	1:A:385:PRO:HD2	1.98	0.45
1:A:403:HIS:CD2	1:A:479:ARG:HE	2.34	0.45
1:B:108:PHE:CZ	1:B:177:ARG:HD3	2.52	0.45
1:B:507:LYS:HD2	1:B:517:GLU:HB2	1.98	0.45
1:B:575:GLY:HA2	1:B:609:GLN:HG2	1.99	0.45
1:C:264:PHE:O	1:C:268:THR:HG23	2.16	0.45
1:C:350:GLN:C	1:C:352:ASP:N	2.71	0.45
1:C:601:LEU:CD1	1:C:616:LEU:HB3	2.46	0.45
1:D:695:ASN:N	1:D:695:ASN:HD22	2.12	0.45
1:A:431:LEU:HB3	1:A:448:LEU:HB2	1.98	0.45
1:B:568:LEU:HD21	1:B:590:VAL:HG22	1.99	0.45
1:B:677:ALA:HB3	1:B:709:LEU:HD11	1.98	0.45
1:C:496:GLY:O	1:C:500:LEU:HG	2.17	0.45
1:D:458:SER:OG	1:D:463:ILE:O	2.32	0.45
1:A:609:GLN:O	1:A:613:ILE:HG13	2.17	0.45
1:C:267:VAL:HG13	1:C:273:GLY:H	1.82	0.45
1:D:86:GLU:HA	1:D:90:PHE:HD1	1.81	0.45
1:D:97:LEU:HD23	1:D:97:LEU:H	1.81	0.45
1:D:249:PHE:HA	1:D:252:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:GLY:O	1:D:459:ILE:HG13	2.16	0.45
1:B:520:ILE:O	1:B:524:ILE:N	2.41	0.45
1:C:415:GLU:OE1	1:C:468:THR:OG1	2.31	0.45
1:C:669:ALA:HA	1:C:709:LEU:HD11	1.98	0.45
1:D:643:PHE:O	1:D:647:LEU:HB2	2.17	0.45
1:A:133:THR:O	1:A:137:PHE:HD2	2.00	0.45
1:A:544:PHE:O	1:A:548:LYS:HG3	2.17	0.45
1:C:458:SER:HB2	1:C:465:GLN:HA	1.99	0.45
1:B:367:SER:OG	1:C:424:TYR:OH	2.32	0.45
1:B:461:CYS:SG	1:B:520:ILE:HG12	2.57	0.45
1:B:605:VAL:HG23	1:B:646:ARG:HB2	1.99	0.45
1:D:183:GLU:O	1:D:186:GLN:HG3	2.17	0.45
1:D:194:ILE:HD11	1:D:198:PHE:HD2	1.82	0.45
1:D:373:ALA:HB1	1:D:399:VAL:HG12	1.99	0.45
1:D:611:GLY:O	1:D:615:LEU:HG	2.16	0.45
1:D:666:HIS:NE2	1:D:697:PRO:HD3	2.32	0.45
1:A:426:VAL:HG21	1:A:448:LEU:CB	2.48	0.44
1:A:660:ASP:HA	1:A:692:ARG:HD2	2.00	0.44
1:B:375:LEU:HD12	1:B:376:LEU:CD2	2.47	0.44
1:B:687:VAL:HG21	1:B:716:VAL:HB	1.99	0.44
1:C:364:ILE:HG22	1:C:368:ILE:HB	1.99	0.44
1:C:501:ASN:HA	1:C:504:MET:HB3	1.99	0.44
1:C:533:LEU:HD21	1:C:562:TYR:CE2	2.52	0.44
1:C:589:ASP:CG	1:C:592:LEU:HB2	2.41	0.44
1:D:121:ARG:HD2	1:D:128:THR:HG22	1.98	0.44
1:D:201:ILE:HD13	1:D:306:ILE:HG12	2.00	0.44
1:D:540:PHE:HB2	1:D:570:LEU:HD13	1.98	0.44
1:A:347:VAL:HA	1:A:350:GLN:HG2	1.99	0.44
1:A:534:LYS:NZ	1:D:530:GLU:HB3	2.32	0.44
1:C:571:ALA:HA	1:C:576:TYR:HB2	1.98	0.44
1:D:579:ILE:O	1:D:583:LEU:HG	2.17	0.44
1:A:507:LYS:O	1:A:514:LYS:HB2	2.17	0.44
1:A:507:LYS:NZ	1:A:513:ILE:HB	2.33	0.44
1:A:671:GLU:HG3	1:D:692:ARG:HH22	1.82	0.44
1:B:57:ILE:H	1:B:57:ILE:HD12	1.82	0.44
1:B:339:LEU:HD11	1:D:371:LYS:HB2	1.98	0.44
1:B:414:THR:HG1	1:B:469:VAL:HG23	1.83	0.44
1:B:496:GLY:O	1:B:499:ILE:HB	2.18	0.44
1:B:687:VAL:O	1:B:697:PRO:HD2	2.18	0.44
1:C:687:VAL:O	1:C:697:PRO:HD2	2.16	0.44
1:D:223:ALA:HB2	1:D:235:TRP:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:GLN:HE22	1:D:487:ASN:ND2	2.15	0.44
1:D:559:LYS:HA	1:D:559:LYS:HD3	1.72	0.44
1:A:540:PHE:CD2	1:D:562:TYR:HB3	2.53	0.44
1:A:674:PHE:HA	1:A:709:LEU:HD21	1.98	0.44
1:A:698:LEU:HA	1:A:713:LEU:HD13	1.99	0.44
1:B:712:LEU:O	1:B:716:VAL:HG23	2.17	0.44
1:D:172:TRP:HE3	1:D:175:LEU:HG	1.82	0.44
1:D:496:GLY:HA2	1:D:499:ILE:CG1	2.47	0.44
1:A:346:HIS:O	1:A:346:HIS:ND1	2.51	0.44
1:A:358:THR:O	1:A:362:GLN:HG3	2.18	0.44
1:A:445:VAL:O	1:A:512:ARG:HB2	2.17	0.44
1:A:589:ASP:OD1	1:A:592:LEU:HD22	2.17	0.44
1:A:688:ILE:O	1:A:690:LYS:HD2	2.17	0.44
1:B:203:LYS:O	1:B:207:VAL:HG23	2.18	0.44
1:B:336:GLY:O	1:B:340:ARG:HG3	2.18	0.44
1:B:407:PHE:CE1	1:B:477:LEU:HD12	2.53	0.44
1:B:563:ASP:HB3	1:B:596:PHE:CE2	2.53	0.44
1:C:323:MET:HG3	1:C:347:VAL:HG11	2.00	0.44
1:C:537:SER:O	1:C:541:GLN:HG2	2.18	0.44
1:D:606:LYS:HA	1:D:643:PHE:HE1	1.83	0.44
1:B:376:LEU:HD13	1:C:333:LYS:CE	2.48	0.44
1:B:513:ILE:HG22	1:B:516:LEU:HB2	1.99	0.44
1:B:666:HIS:ND1	1:B:691:ASP:HB3	2.33	0.44
1:C:338:ASP:O	1:C:341:SER:OG	2.32	0.44
1:C:503:ILE:HG12	1:C:513:ILE:HG21	1.99	0.44
1:C:665:LEU:HD21	1:C:687:VAL:HG22	2.00	0.44
1:C:677:ALA:HA	1:C:680:LEU:HD12	1.99	0.44
1:A:203:LYS:O	1:A:207:VAL:HG23	2.17	0.44
1:A:544:PHE:CD1	1:A:579:ILE:HG23	2.52	0.44
1:B:375:LEU:HD11	1:C:335:LEU:HD12	2.00	0.44
1:C:424:TYR:HD2	1:C:454:PHE:CE1	2.35	0.44
1:C:535:VAL:HG21	1:C:555:ALA:CB	2.47	0.44
1:C:607:ALA:HB1	1:C:609:GLN:HE21	1.83	0.44
1:D:524:ILE:O	1:D:528:GLU:HG2	2.18	0.44
1:A:190:LYS:NZ	1:D:348:ARG:HH22	2.16	0.44
1:A:611:GLY:O	1:A:615:LEU:HG	2.17	0.44
1:B:58:ILE:HD12	1:B:65:TYR:HB2	2.00	0.44
1:C:540:PHE:O	1:C:574:ARG:NH1	2.51	0.44
1:D:51:HIS:HB3	1:D:130:TYR:CD2	2.52	0.44
1:D:431:LEU:HD23	1:D:471:VAL:HG22	2.00	0.44
1:D:665:LEU:HG	1:D:697:PRO:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:HIS:CE1	1:A:61:LYS:HE2	2.45	0.43
1:A:202:LEU:HD22	1:A:202:LEU:HA	1.88	0.43
1:A:330:MET:HG2	1:A:335:LEU:HD22	1.99	0.43
1:A:486:SER:O	1:A:490:GLU:HG3	2.18	0.43
1:A:665:LEU:HD21	1:A:713:LEU:HD21	2.00	0.43
1:B:81:LEU:O	1:B:213:HIS:NE2	2.50	0.43
1:B:332:ARG:NH2	1:D:354:HIS:HB2	2.32	0.43
1:B:425:PHE:HB2	1:B:478:LEU:HB2	2.00	0.43
1:B:576:TYR:CD2	1:B:579:ILE:HD12	2.53	0.43
1:D:118:VAL:O	1:D:135:ILE:HD13	2.17	0.43
1:D:165:GLU:HG3	1:D:169:TYR:HE1	1.82	0.43
1:A:574:ARG:NH1	1:A:576:TYR:OH	2.50	0.43
1:A:667:VAL:O	1:A:671:GLU:HG3	2.18	0.43
1:D:578:ASP:HA	1:D:581:LEU:HG	1.99	0.43
1:D:671:GLU:HB2	1:D:673:LEU:HG	2.00	0.43
1:A:518:SER:O	1:A:522:ILE:HG13	2.17	0.43
1:B:106:ILE:HD13	1:B:106:ILE:HA	1.89	0.43
1:B:632:LEU:O	1:B:636:VAL:HG23	2.18	0.43
1:C:698:LEU:HD13	1:C:713:LEU:HB3	2.00	0.43
1:D:189:GLU:HG3	1:D:196:TYR:CD1	2.52	0.43
1:D:663:THR:O	1:D:666:HIS:HB2	2.19	0.43
1:B:339:LEU:O	1:B:343:ILE:HG13	2.19	0.43
1:B:378:LEU:HG	1:B:382:LYS:HD3	2.00	0.43
1:C:433:ALA:O	1:C:445:VAL:N	2.50	0.43
1:D:565:ARG:NH2	1:D:569:HIS:HB3	2.34	0.43
1:B:89:PHE:HA	1:B:220:TYR:CE2	2.53	0.43
1:B:345:GLY:HA2	1:B:348:ARG:NH2	2.33	0.43
1:B:364:ILE:H	1:B:364:ILE:HG13	1.62	0.43
1:B:431:LEU:HD23	1:B:471:VAL:HA	1.99	0.43
1:C:572:ALA:HB1	1:C:604:ALA:HA	2.00	0.43
1:D:518:SER:O	1:D:521:VAL:HG22	2.18	0.43
1:D:590:VAL:C	1:D:600:PRO:HG2	2.43	0.43
1:A:645:LYS:HB2	1:A:679:MET:HE2	2.01	0.43
1:B:435:VAL:HG13	1:B:466:PRO:O	2.18	0.43
1:B:598:HIS:HB3	1:B:603:GLU:OE2	2.18	0.43
1:B:688:ILE:HD11	1:B:724:TYR:HB2	2.01	0.43
1:C:350:GLN:HE21	1:C:355:TYR:HB3	1.83	0.43
1:C:530:GLU:O	1:C:534:LYS:HG3	2.18	0.43
1:D:600:PRO:HA	1:D:603:GLU:HG2	2.00	0.43
1:B:221:TYR:O	1:B:225:THR:HG23	2.18	0.43
1:B:468:THR:O	1:B:468:THR:OG1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:LYS:O	1:B:517:GLU:HB3	2.19	0.43
1:B:557:PRO:HB2	1:B:588:VAL:HG22	2.01	0.43
1:C:603:GLU:OE2	1:C:603:GLU:N	2.29	0.43
1:C:636:VAL:HG11	1:C:667:VAL:HG23	2.01	0.43
1:C:699:ASP:O	1:C:703:LEU:HG	2.18	0.43
1:D:434:LEU:HA	1:D:444:SER:HA	2.01	0.43
1:D:605:VAL:HG12	1:D:643:PHE:CE1	2.54	0.43
1:A:226:LEU:O	1:A:250:ARG:NH2	2.51	0.43
1:A:355:TYR:HA	1:A:358:THR:HG23	2.00	0.43
1:A:530:GLU:HA	1:A:533:LEU:HD12	2.01	0.43
1:A:616:LEU:HB3	1:A:621:ALA:HB3	2.01	0.43
1:B:394:PHE:HE1	1:B:398:ILE:HD11	1.82	0.43
1:B:551:ILE:HD12	1:B:582:PHE:CE2	2.54	0.43
1:C:124:GLN:OE1	1:C:124:GLN:N	2.48	0.43
1:D:326:LEU:HB3	1:D:330:MET:HE3	2.00	0.43
1:D:483:GLN:NE2	1:D:487:ASN:HD21	2.17	0.43
1:A:461:CYS:HA	1:A:523:HIS:CD2	2.53	0.43
1:A:605:VAL:HA	1:A:613:ILE:HD11	2.00	0.43
1:B:561:ASP:OD2	1:B:565:ARG:NH2	2.51	0.43
1:C:422:HIS:HA	1:C:480:LEU:O	2.18	0.43
1:C:671:GLU:HB2	1:C:673:LEU:HG	2.01	0.43
1:D:559:LYS:O	1:D:566:SER:HA	2.18	0.43
1:A:196:TYR:CE2	1:D:317:GLU:HB2	2.54	0.43
1:B:558:ASN:HA	1:B:588:VAL:HG13	1.99	0.43
1:C:420:VAL:HG21	1:C:465:GLN:OE1	2.19	0.43
1:A:423:LEU:HD23	1:A:480:LEU:HD23	2.01	0.42
1:B:681:VAL:HG11	1:B:716:VAL:HG21	2.01	0.42
1:C:485:PHE:CZ	1:C:489:LEU:HD11	2.54	0.42
1:A:68:TRP:CD1	1:A:114:LEU:HD12	2.54	0.42
1:A:391:SER:O	1:A:395:ILE:HG22	2.19	0.42
1:A:515:LYS:HG2	1:A:516:LEU:HD12	2.01	0.42
1:A:666:HIS:CE1	1:A:697:PRO:HD3	2.54	0.42
1:A:688:ILE:HD11	1:A:724:TYR:CE2	2.54	0.42
1:B:206:PHE:CE1	1:B:210:TYR:HE1	2.37	0.42
1:B:231:GLU:O	1:B:234:THR:OG1	2.36	0.42
1:C:581:LEU:O	1:C:585:GLN:HG2	2.19	0.42
1:D:65:TYR:OH	1:D:115:GLN:OE1	2.36	0.42
1:A:93:LEU:HD23	1:A:94:PRO:HD2	2.01	0.42
1:A:636:VAL:HG11	1:A:668:ALA:HB2	2.01	0.42
1:B:430:LEU:HD11	1:B:447:LEU:HB3	2.01	0.42
1:C:96:ARG:HA	1:C:96:ARG:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:ASP:O	1:C:481:ASP:HA	2.19	0.42
1:A:385:PRO:O	1:A:388:LYS:HE2	2.20	0.42
1:A:496:GLY:CA	1:A:499:ILE:HG12	2.48	0.42
1:A:568:LEU:HD13	1:A:580:THR:OG1	2.19	0.42
1:A:575:GLY:HA2	1:A:612:VAL:HG21	2.02	0.42
1:B:544:PHE:CD1	1:B:579:ILE:HG12	2.55	0.42
1:D:322:LYS:O	1:D:326:LEU:HG	2.19	0.42
1:D:536:ASN:HB3	1:D:570:LEU:HD12	2.01	0.42
1:D:698:LEU:HD23	1:D:717:LYS:HD3	2.01	0.42
1:A:270:ALA:HB2	1:C:292:VAL:HG13	2.02	0.42
1:A:426:VAL:HB	1:A:452:THR:OG1	2.19	0.42
1:B:409:PRO:HB3	1:B:472:CYS:O	2.19	0.42
1:B:431:LEU:O	1:B:448:LEU:N	2.44	0.42
1:B:546:GLN:O	1:B:550:LEU:HG	2.19	0.42
1:C:616:LEU:HD23	1:C:616:LEU:HA	1.77	0.42
1:C:713:LEU:HD23	1:C:713:LEU:HA	1.67	0.42
1:D:432:GLU:HA	1:D:447:LEU:HA	2.02	0.42
1:B:293:SER:O	1:B:297:VAL:HG23	2.19	0.42
1:B:391:SER:O	1:B:395:ILE:HG12	2.19	0.42
1:B:454:PHE:CD1	1:B:454:PHE:C	2.97	0.42
1:C:221:TYR:O	1:C:225:THR:HG23	2.20	0.42
1:C:397:GLN:O	1:C:401:ARG:HG3	2.19	0.42
1:D:219:PHE:HE1	1:D:284:GLU:HB3	1.84	0.42
1:D:582:PHE:CD1	1:D:582:PHE:C	2.97	0.42
1:D:656:SER:O	1:D:664:PRO:HD3	2.20	0.42
1:A:481:ASP:OD1	1:A:482:LYS:N	2.52	0.42
1:B:109:LEU:HD13	1:B:109:LEU:HA	1.85	0.42
1:B:655:ASN:HD21	1:B:686:SER:H	1.67	0.42
1:C:353:SER:O	1:C:354:HIS:C	2.62	0.42
1:C:402:LEU:HD21	1:C:425:PHE:CE2	2.55	0.42
1:C:456:ASP:OD1	1:C:456:ASP:N	2.53	0.42
1:C:569:HIS:HE1	1:C:592:LEU:CD2	2.32	0.42
1:C:688:ILE:H	1:C:688:ILE:HG13	1.64	0.42
1:C:698:LEU:HD11	1:C:714:GLU:CD	2.44	0.42
1:D:93:LEU:HB2	1:D:155:ASP:OD2	2.20	0.42
1:D:344:THR:HA	1:D:347:VAL:HG12	2.02	0.42
1:A:347:VAL:HA	1:A:350:GLN:CG	2.50	0.42
1:A:434:LEU:HD22	1:A:442:GLU:O	2.19	0.42
1:A:523:HIS:ND1	1:A:527:GLN:OE1	2.52	0.42
1:A:688:ILE:HD11	1:A:724:TYR:CD2	2.54	0.42
1:B:527:GLN:O	1:B:530:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:ASP:O	1:C:482:LYS:N	2.51	0.42
1:C:428:GLU:OE2	1:C:428:GLU:N	2.52	0.42
1:B:470:ARG:HB2	1:B:470:ARG:NH1	2.34	0.42
1:B:644:LEU:HD11	1:B:680:LEU:HD21	2.01	0.42
1:C:137:PHE:O	1:C:141:LYS:HE3	2.20	0.42
1:C:538:ALA:HA	1:C:541:GLN:HG3	2.02	0.42
1:C:544:PHE:CZ	1:C:579:ILE:HG12	2.54	0.42
1:D:180:LYS:HD3	1:D:180:LYS:HA	1.78	0.42
1:A:349:LEU:HB2	1:A:408:LEU:HD21	2.01	0.42
1:B:411:GLU:O	1:B:471:VAL:HG23	2.20	0.42
1:B:433:ALA:HB3	1:B:445:VAL:HB	2.01	0.42
1:D:657:GLU:OE1	1:D:661:HIS:ND1	2.53	0.42
1:A:378:LEU:N	1:A:379:PRO:HD2	2.35	0.41
1:C:424:TYR:HE1	1:C:479:ARG:HB2	1.85	0.41
1:A:687:VAL:HG12	1:A:717:LYS:HD2	2.01	0.41
1:A:195:ASN:HB3	1:A:198:PHE:HB3	2.01	0.41
1:A:424:TYR:HA	1:A:478:LEU:O	2.21	0.41
1:A:433:ALA:CB	1:A:469:VAL:HG22	2.50	0.41
1:A:531:LEU:HD21	1:A:555:ALA:HB2	2.01	0.41
1:B:567:PRO:HA	1:B:570:LEU:HD13	2.01	0.41
1:B:675:LEU:HA	1:B:678:LYS:HE3	2.02	0.41
1:C:544:PHE:CE1	1:C:579:ILE:HG12	2.55	0.41
1:C:647:LEU:HD23	1:C:652:MET:HG2	2.02	0.41
1:D:58:ILE:HD12	1:D:58:ILE:HA	1.89	0.41
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.90	0.41
1:A:221:TYR:O	1:A:225:THR:HG23	2.20	0.41
1:A:376:LEU:HD11	1:D:335:LEU:HD11	2.02	0.41
1:A:548:LYS:HA	1:A:551:ILE:HG12	2.02	0.41
1:A:701:ALA:O	1:A:705:GLY:N	2.53	0.41
1:B:164:HIS:O	1:B:164:HIS:ND1	2.51	0.41
1:B:431:LEU:HD11	1:B:477:LEU:HD11	2.03	0.41
1:C:391:SER:N	1:C:495:ASP:OD2	2.54	0.41
1:A:470:ARG:HH12	1:C:367:SER:HB3	1.85	0.41
1:B:88:GLY:HA2	1:B:221:TYR:HB2	2.02	0.41
1:C:589:ASP:OD2	1:C:589:ASP:C	2.63	0.41
1:D:423:LEU:HB3	1:D:480:LEU:HB3	2.02	0.41
1:D:487:ASN:O	1:D:491:ILE:HG13	2.20	0.41
1:D:520:ILE:HA	1:D:523:HIS:ND1	2.35	0.41
1:A:55:LYS:NZ	1:A:56:TYR:H	2.18	0.41
1:A:272:VAL:HG23	1:C:271:THR:HA	2.01	0.41
1:A:272:VAL:HA	1:C:271:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LYS:HA	1:A:333:LYS:HD3	1.91	0.41
1:A:388:LYS:HA	1:A:388:LYS:HD3	1.88	0.41
1:B:150:GLY:O	1:B:177:ARG:NH2	2.53	0.41
1:B:365:PRO:HB3	1:C:405:GLU:OE1	2.21	0.41
1:C:403:HIS:CG	1:C:479:ARG:HH22	2.38	0.41
1:D:526:LYS:O	1:D:530:GLU:HG2	2.20	0.41
1:A:62:ASN:ND2	1:A:65:TYR:H	2.19	0.41
1:B:285:MET:HG2	1:C:263:TYR:CG	2.55	0.41
1:B:332:ARG:NH1	1:D:354:HIS:CD2	2.79	0.41
1:B:457:ILE:HG21	1:B:516:LEU:HD13	2.02	0.41
1:C:91:ARG:NE	1:C:165:GLU:OE2	2.54	0.41
1:C:198:PHE:O	1:C:202:LEU:HG	2.20	0.41
1:C:497:ARG:H	1:C:497:ARG:HG2	1.68	0.41
1:C:709:LEU:O	1:C:713:LEU:HB2	2.20	0.41
1:D:495:ASP:O	1:D:499:ILE:HG12	2.20	0.41
1:D:604:ALA:HB1	1:D:613:ILE:HG12	2.03	0.41
1:A:365:PRO:HG2	1:A:368:ILE:HD12	2.03	0.41
1:B:388:LYS:O	1:B:502:ASN:ND2	2.49	0.41
1:B:666:HIS:NE2	1:B:697:PRO:HD3	2.36	0.41
1:C:723:ILE:HG22	1:C:723:ILE:O	2.21	0.41
1:D:351:TYR:O	1:D:354:HIS:ND1	2.54	0.41
1:A:459:ILE:HG23	1:A:482:LYS:HG3	2.02	0.41
1:A:665:LEU:HG	1:A:697:PRO:CB	2.49	0.41
1:B:140:LEU:HA	1:B:144:PHE:HB3	2.02	0.41
1:B:263:TYR:CG	1:D:285:MET:HG2	2.56	0.41
1:B:266:ILE:HG21	1:D:289:MET:HA	2.03	0.41
1:B:390:CYS:HB3	1:B:394:PHE:HD2	1.85	0.41
1:B:415:GLU:HB3	1:B:418:ASN:ND2	2.35	0.41
1:B:487:ASN:O	1:B:491:ILE:HG12	2.21	0.41
1:B:665:LEU:HD22	1:B:685:ALA:CB	2.49	0.41
1:C:493:PHE:CD2	1:C:524:ILE:HD13	2.56	0.41
1:C:566:SER:HB2	1:C:567:PRO:HD2	2.02	0.41
1:C:687:VAL:HG13	1:C:713:LEU:HD22	2.03	0.41
1:D:398:ILE:CD1	1:D:488:ILE:HD12	2.50	0.41
1:D:474:LEU:HD12	1:D:474:LEU:HA	1.75	0.41
1:D:592:LEU:O	1:D:600:PRO:HD3	2.20	0.41
1:A:212:THR:HG22	1:A:291:TYR:OH	2.21	0.41
1:B:415:GLU:HA	1:B:468:THR:HA	2.03	0.41
1:C:59:HIS:ND1	1:C:60:PRO:HD2	2.36	0.41
1:C:69:GLU:HA	1:C:72:ILE:HG22	2.03	0.41
1:C:97:LEU:HD12	1:C:97:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:LEU:HA	1:C:282:LEU:HD22	1.85	0.41
1:C:288:VAL:O	1:C:292:VAL:HB	2.20	0.41
1:C:306:ILE:O	1:C:310:ILE:HG13	2.20	0.41
1:D:183:GLU:HA	1:D:186:GLN:HG3	2.03	0.41
1:D:489:LEU:HD11	1:D:499:ILE:HD11	2.03	0.41
1:D:657:GLU:HA	1:D:662:ARG:O	2.21	0.41
1:B:198:PHE:O	1:B:201:ILE:HG13	2.21	0.40
1:B:498:THR:O	1:B:502:ASN:ND2	2.54	0.40
1:D:514:LYS:O	1:D:517:GLU:HB3	2.21	0.40
1:D:576:TYR:HB3	1:D:579:ILE:HG12	2.03	0.40
1:A:106:ILE:HD12	1:A:106:ILE:HA	1.90	0.40
1:C:339:LEU:HD23	1:C:339:LEU:HA	1.86	0.40
1:A:380:TYR:O	1:A:384:VAL:HG23	2.21	0.40
1:A:639:GLY:HA2	1:A:676:MET:CE	2.51	0.40
1:A:674:PHE:CD1	1:A:674:PHE:C	2.99	0.40
1:B:220:TYR:O	1:B:224:THR:HG23	2.21	0.40
1:B:461:CYS:SG	1:B:520:ILE:HA	2.62	0.40
1:B:670:SER:HB2	1:C:692:ARG:HD3	2.04	0.40
1:C:183:GLU:O	1:C:187:ARG:HG3	2.22	0.40
1:C:540:PHE:CD1	1:C:570:LEU:HB3	2.52	0.40
1:D:59:HIS:HA	1:D:119:ALA:HB3	2.03	0.40
1:D:96:ARG:C	1:D:96:ARG:HD3	2.46	0.40
1:D:381:ILE:HD11	1:D:478:LEU:HD12	2.02	0.40
1:A:486:SER:O	1:A:489:LEU:HG	2.22	0.40
1:A:491:ILE:HG22	1:A:492:TYR:CD1	2.57	0.40
1:A:505:GLU:O	1:A:508:GLU:HB2	2.21	0.40
1:C:523:HIS:O	1:C:527:GLN:N	2.54	0.40
1:D:100:LEU:HD13	1:D:100:LEU:HA	1.90	0.40
1:D:654:PRO:HG3	1:D:683:ALA:O	2.22	0.40
1:A:356:THR:O	1:A:359:VAL:HB	2.22	0.40
1:B:329:PHE:CA	1:B:332:ARG:HD3	2.45	0.40
1:B:431:LEU:HD23	1:B:431:LEU:HA	1.83	0.40
1:B:431:LEU:HD11	1:B:477:LEU:HD21	2.04	0.40
1:B:665:LEU:HD12	1:B:665:LEU:HA	1.69	0.40
1:B:678:LYS:HD3	1:B:682:GLU:OE2	2.21	0.40
1:B:689:SER:O	1:B:696:SER:HA	2.21	0.40
1:B:699:ASP:HA	1:B:702:ARG:HD2	2.04	0.40
1:D:190:LYS:HD3	1:D:190:LYS:HA	1.82	0.40
1:D:377:TYR:HA	1:D:380:TYR:CE2	2.56	0.40
1:D:420:VAL:HG11	1:D:458:SER:HB3	2.03	0.40
1:D:697:PRO:HA	1:D:700:GLU:HB2	2.03	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	674/834 (81%)	649 (96%)	25 (4%)	0	100	100
1	B	674/834 (81%)	651 (97%)	23 (3%)	0	100	100
1	C	674/834 (81%)	649 (96%)	25 (4%)	0	100	100
1	D	674/834 (81%)	653 (97%)	21 (3%)	0	100	100
All	All	2696/3336 (81%)	2602 (96%)	94 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	597/743 (80%)	580 (97%)	17 (3%)	38	68
1	B	597/743 (80%)	578 (97%)	19 (3%)	34	65
1	C	597/743 (80%)	576 (96%)	21 (4%)	32	64
1	D	597/743 (80%)	577 (97%)	20 (3%)	32	64
All	All	2388/2972 (80%)	2311 (97%)	77 (3%)	35	65

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ILE
1	A	86	GLU
1	A	106	ILE
1	A	192	THR
1	A	202	LEU
1	A	247	GLU
1	A	272	VAL
1	A	282	LEU
1	A	285	MET
1	A	302	LEU
1	A	329	PHE
1	A	351	TYR
1	A	388	LYS
1	A	494	HIS
1	A	508	GLU
1	A	562	TYR
1	A	563	ASP
1	B	55	LYS
1	B	97	LEU
1	B	109	LEU
1	B	126	TYR
1	B	170	LEU
1	B	201	ILE
1	B	204	LEU
1	B	269	MET
1	B	272	VAL
1	B	277	ILE
1	B	306	ILE
1	B	315	ASN
1	B	319	PHE
1	B	413	ILE
1	B	465	GLN
1	B	467	PHE
1	B	512	ARG
1	B	513	ILE
1	B	706	ASN
1	C	51	HIS
1	C	72	ILE
1	C	143	HIS
1	C	186	GLN
1	C	201	ILE
1	C	267	VAL
1	C	277	ILE

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Mol	Chain	Res	Type
1	C	282	LEU
1	C	292	VAL
1	C	295	ASP
1	C	296	MET
1	C	319	PHE
1	C	333	LYS
1	C	349	LEU
1	C	352	ASP
1	C	516	LEU
1	C	540	PHE
1	C	601	LEU
1	C	647	LEU
1	C	676	MET
1	C	715	ASP
1	D	97	LEU
1	D	120	TYR
1	D	123	THR
1	D	126	TYR
1	D	204	LEU
1	D	272	VAL
1	D	277	ILE
1	D	339	LEU
1	D	363	ASP
1	D	364	ILE
1	D	380	TYR
1	D	386	LEU
1	D	413	ILE
1	D	445	VAL
1	D	446	THR
1	D	474	LEU
1	D	475	CYS
1	D	488	ILE
1	D	501	ASN
1	D	562	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	342	GLN
1	A	350	GLN
1	A	374	GLN

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Mol	Chain	Res	Type
1	A	403	HIS
1	A	422	HIS
1	A	465	GLN
1	A	510	ASN
1	A	585	GLN
1	A	630	ASN
1	A	718	ASN
1	B	278	HIS
1	B	465	GLN
1	B	502	ASN
1	B	523	HIS
1	B	541	GLN
1	B	558	ASN
1	B	585	GLN
1	B	609	GLN
1	B	630	ASN
1	B	655	ASN
1	B	695	ASN
1	B	706	ASN
1	B	718	ASN
1	C	51	HIS
1	C	143	HIS
1	C	451	HIS
1	C	494	HIS
1	C	541	GLN
1	C	630	ASN
1	C	661	HIS
1	D	305	ASN
1	D	354	HIS
1	D	403	HIS
1	D	418	ASN
1	D	451	HIS
1	D	465	GLN
1	D	483	GLN
1	D	487	ASN
1	D	510	ASN
1	D	630	ASN
1	D	695	ASN
1	D	706	ASN
1	D	718	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 [i](#)

There are no chain breaks in this entry.

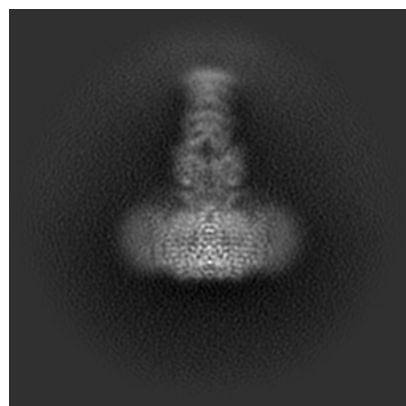
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62918. These allow visual inspection of the internal detail of the map and identification of artifacts.

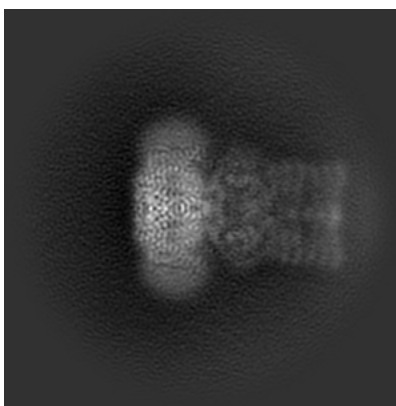
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

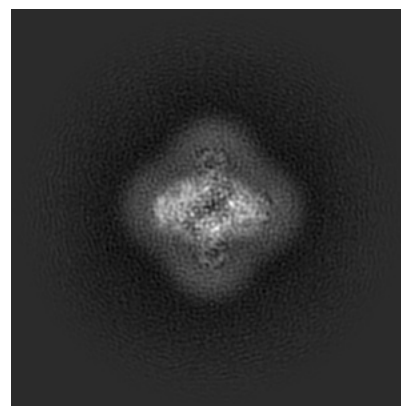
6.1.1 Primary map



X

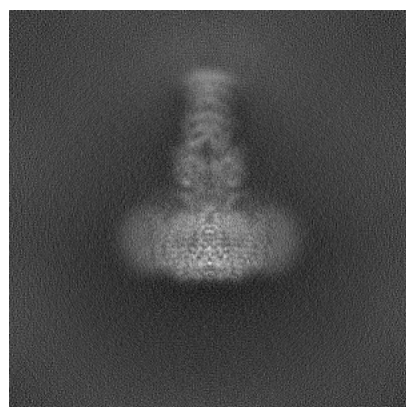


Y

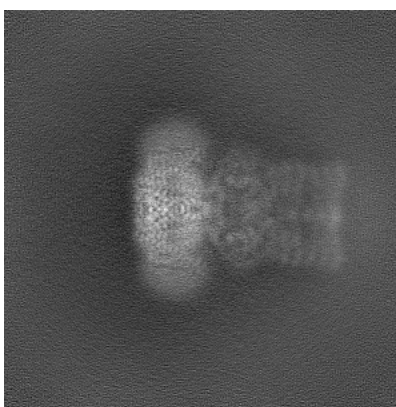


Z

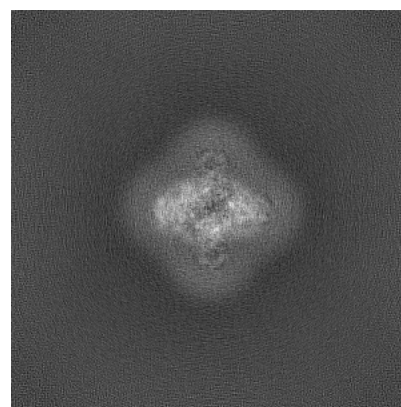
6.1.2 Raw map



X



Y

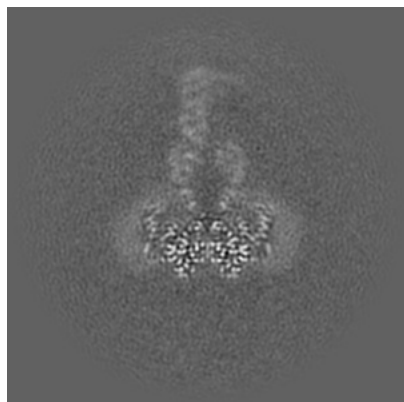


Z

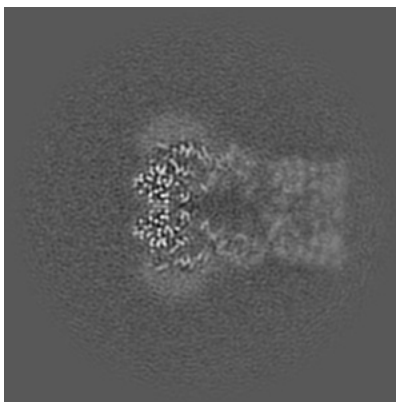
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

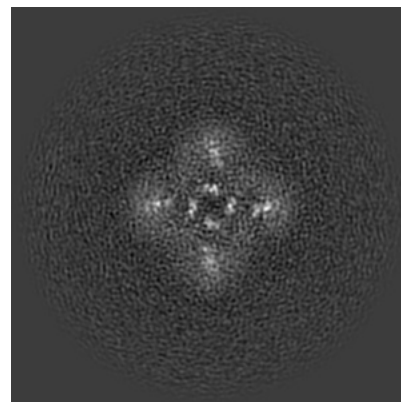
6.2.1 Primary map



X Index: 200

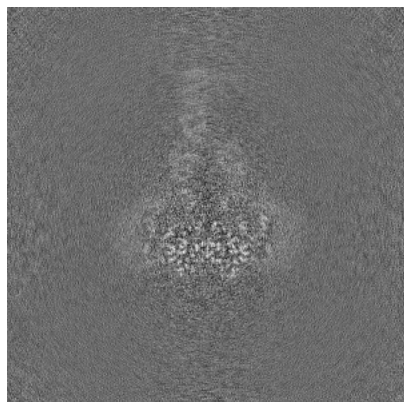


Y Index: 200

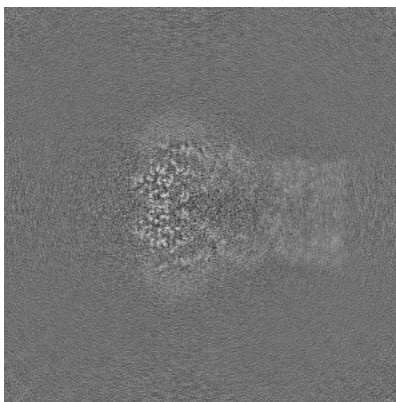


Z Index: 200

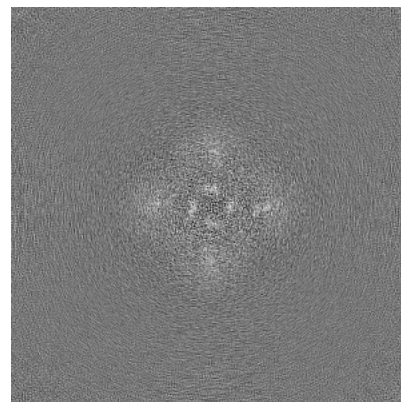
6.2.2 Raw map



X Index: 200



Y Index: 200

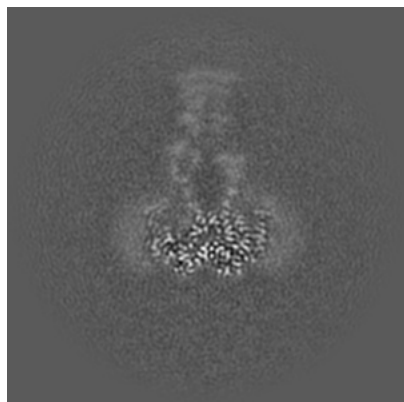


Z Index: 200

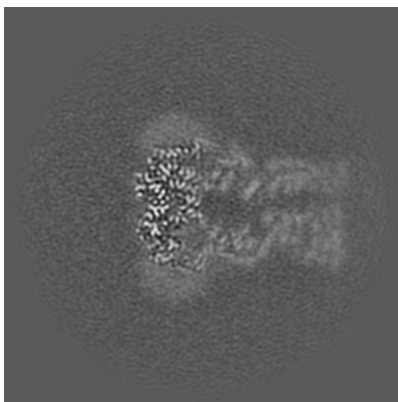
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

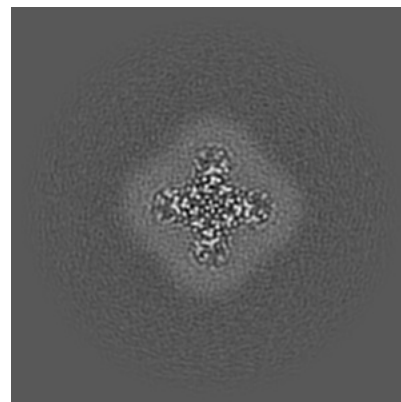
6.3.1 Primary map



X Index: 196

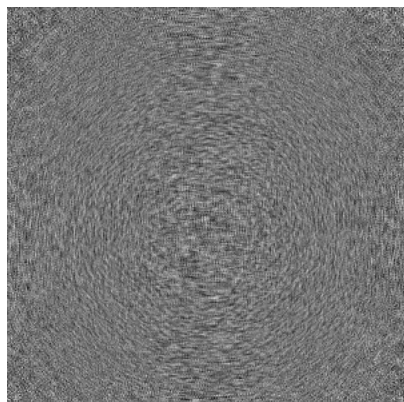


Y Index: 205

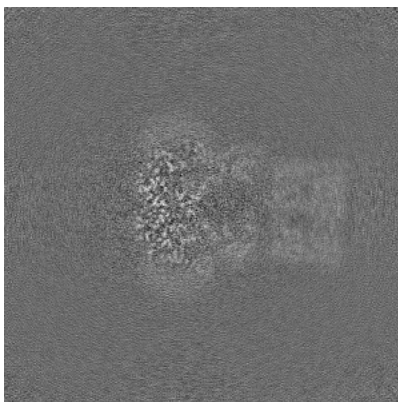


Z Index: 154

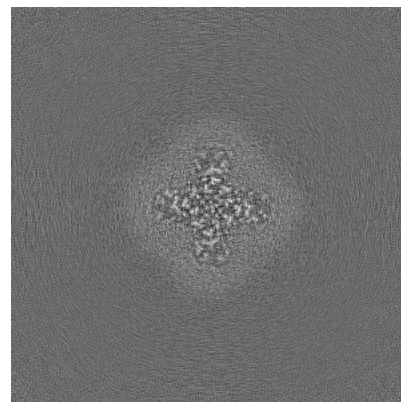
6.3.2 Raw map



X Index: 0



Y Index: 196

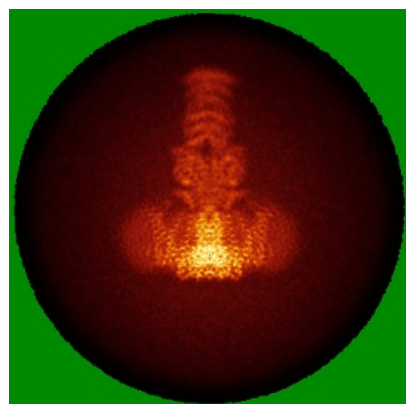


Z Index: 154

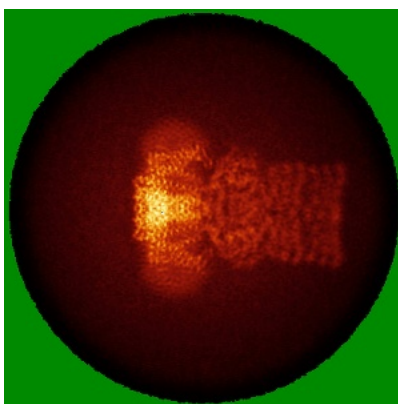
The images above show the largest variance slices of the map in three orthogonal directions.

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

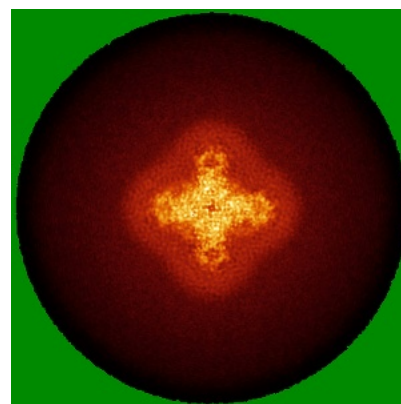
6.4.1 Primary map



X

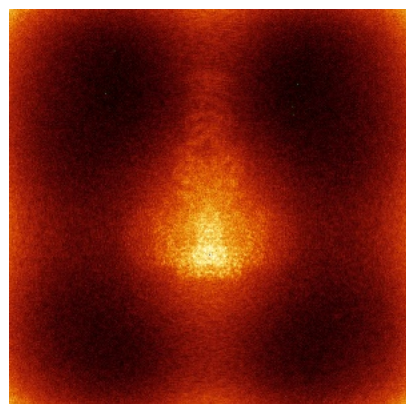


Y

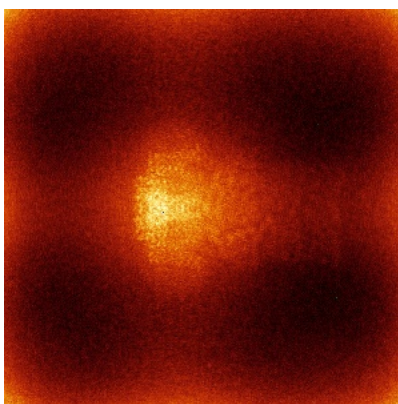


Z

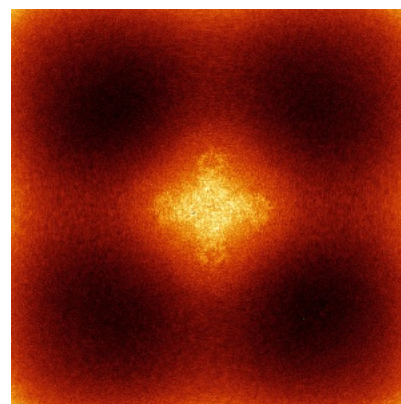
6.4.2 Raw map



X



Y

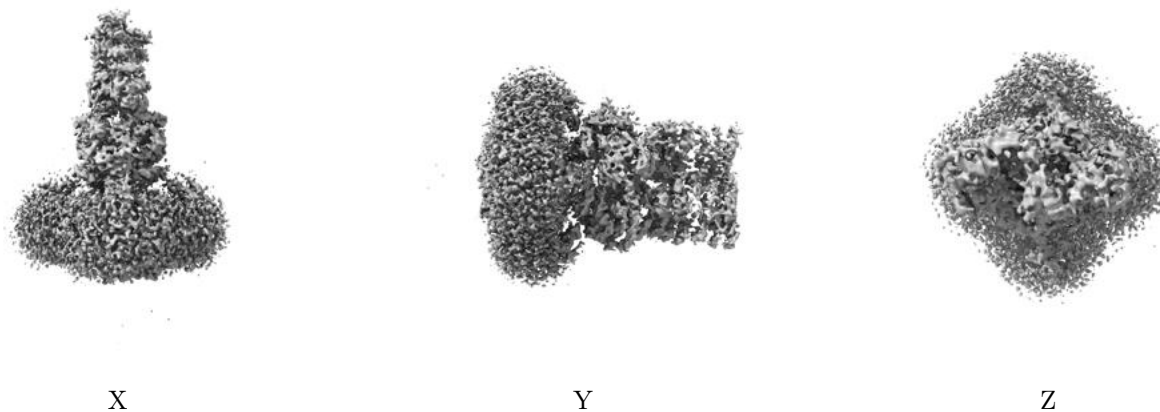


Z

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.

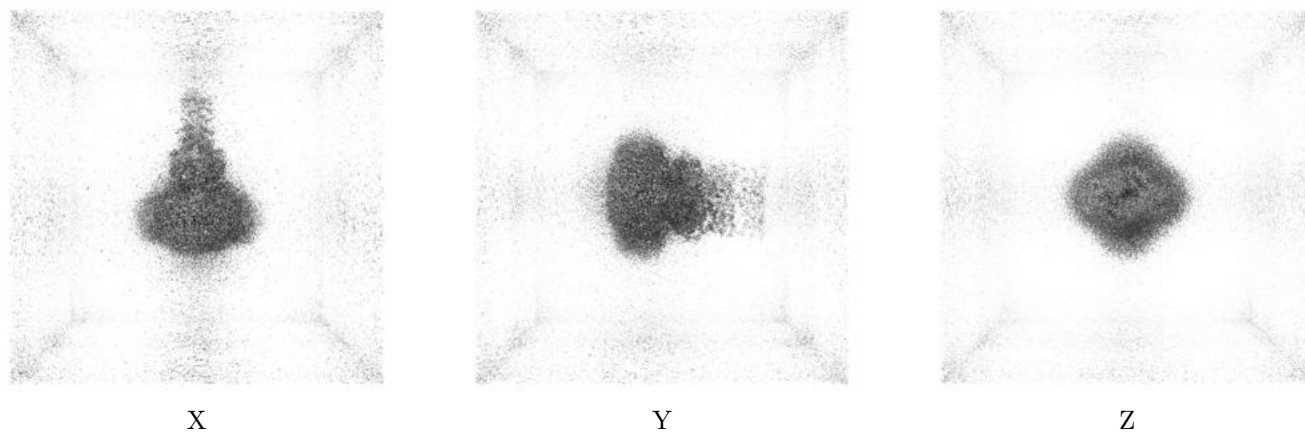
6.5 Orthogonal surface views [i](#)

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.

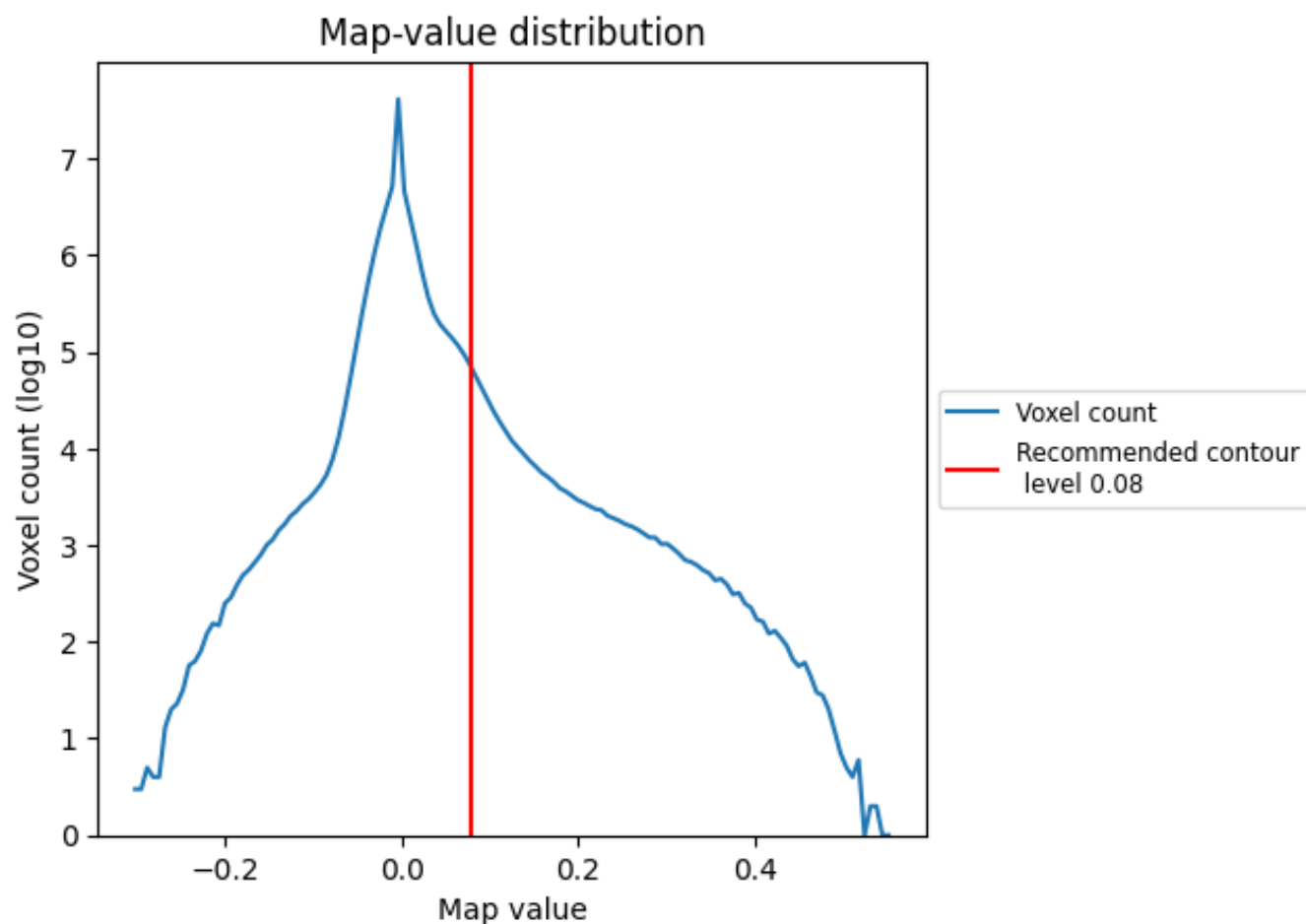
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

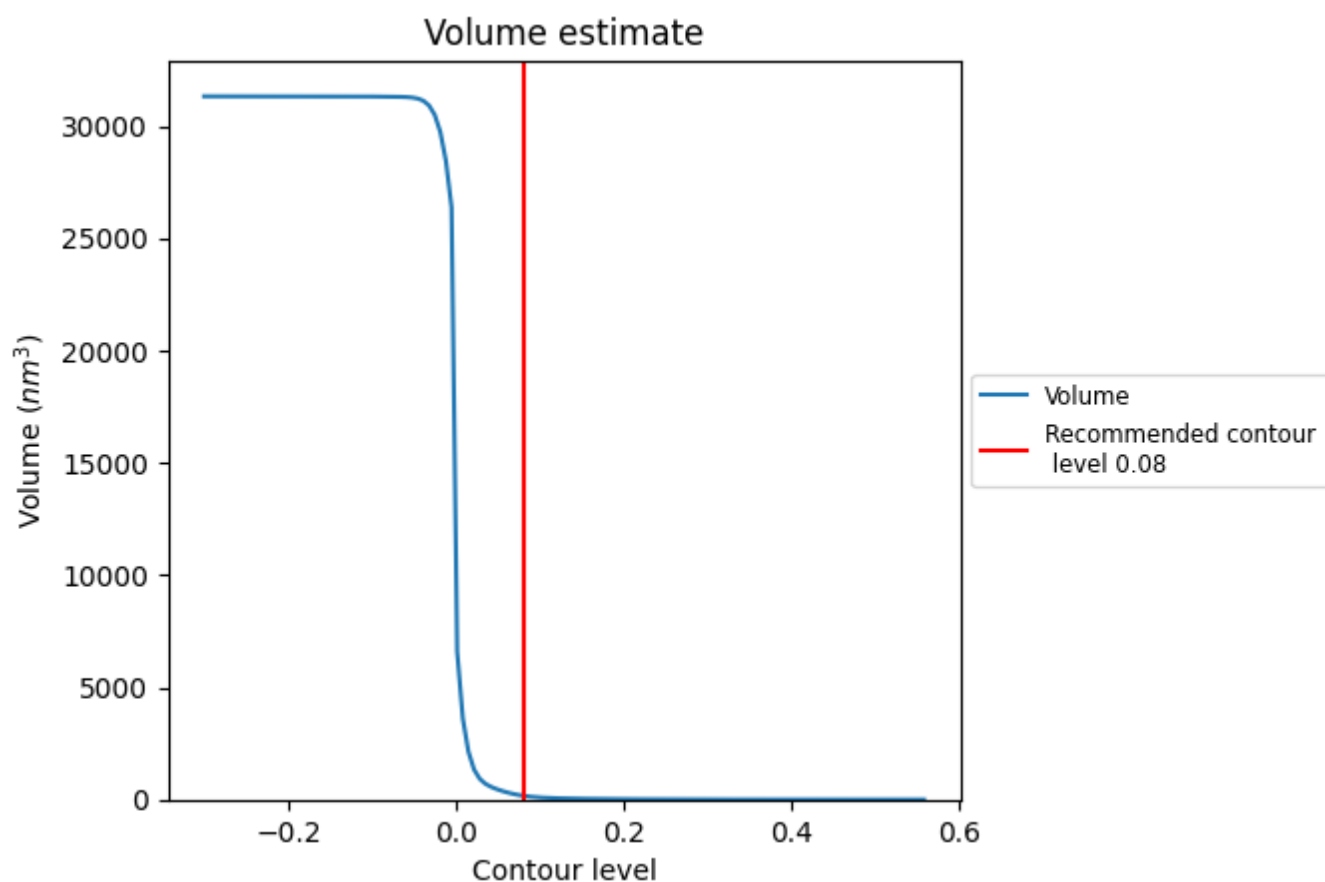
This section contains the results of statistical analysis of the map.

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.

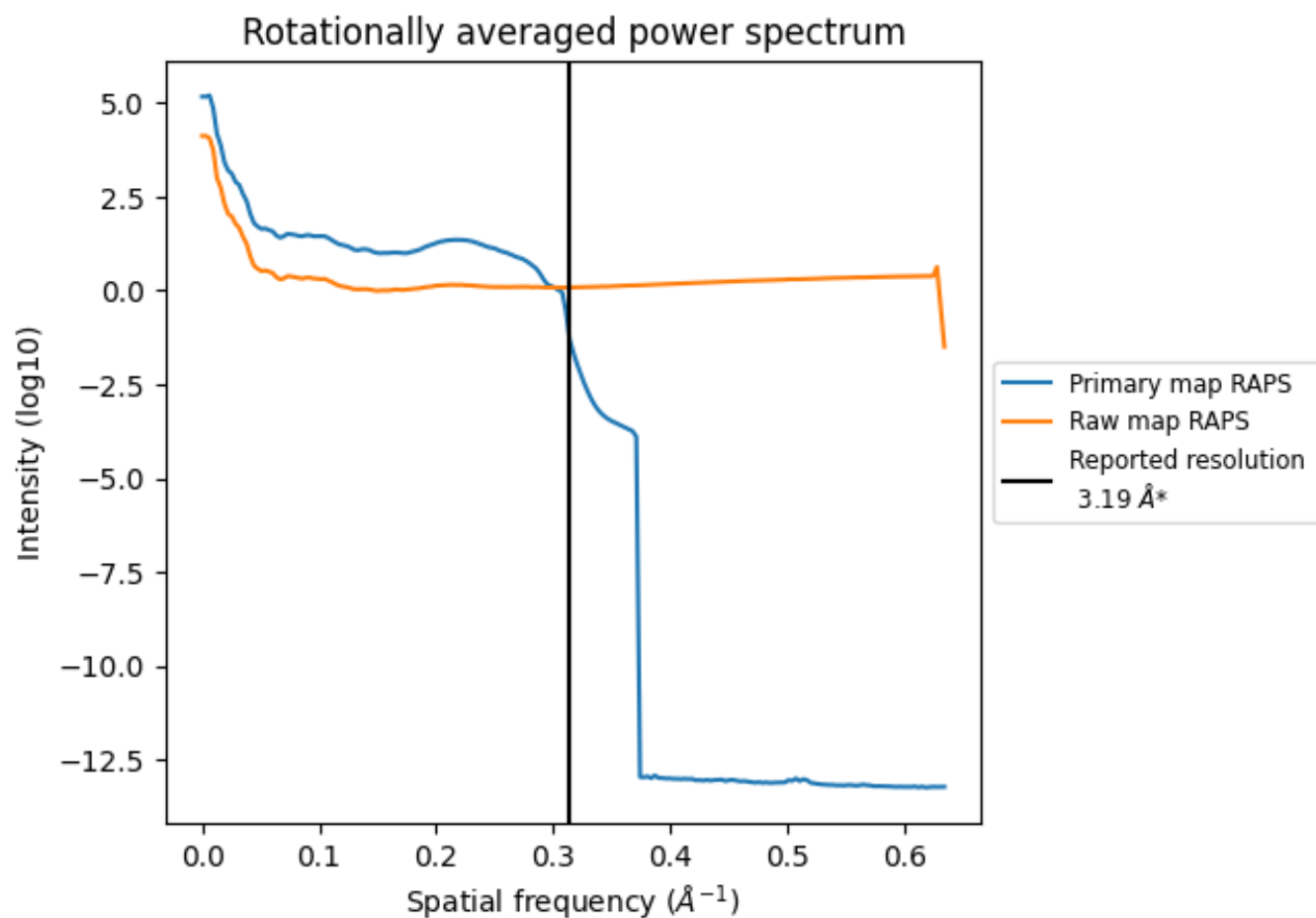
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm³; this corresponds to an approximate mass of 152 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 ⓘ

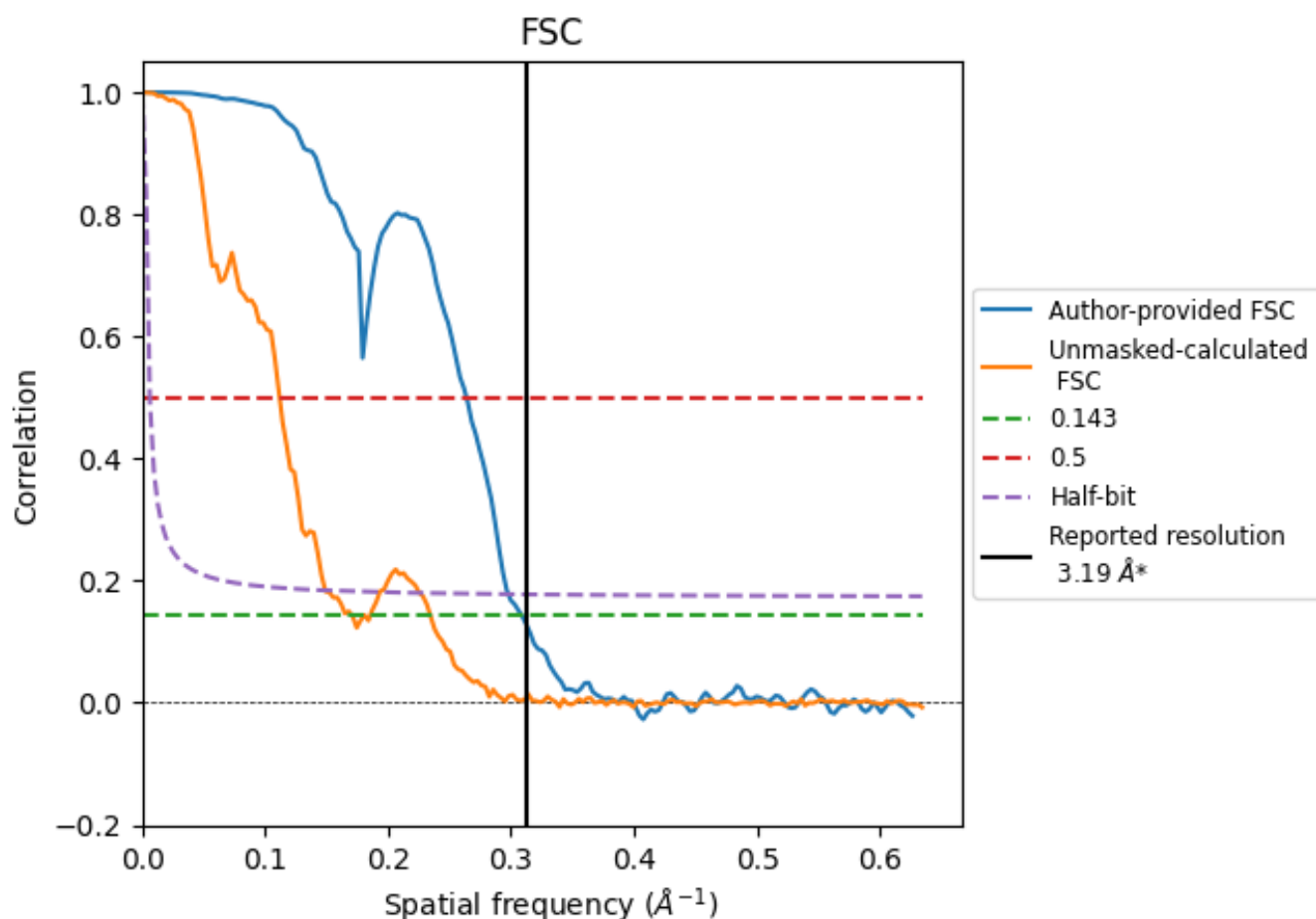


*Reported resolution corresponds to spatial frequency of 0.313 $\text{\AA}^{-1}$

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 0.313 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	3.24	3.79	3.36
Unmasked-calculated*	5.86	8.95	6.72

*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 5.86 differs from the reported value 3.19 by more than 10 %

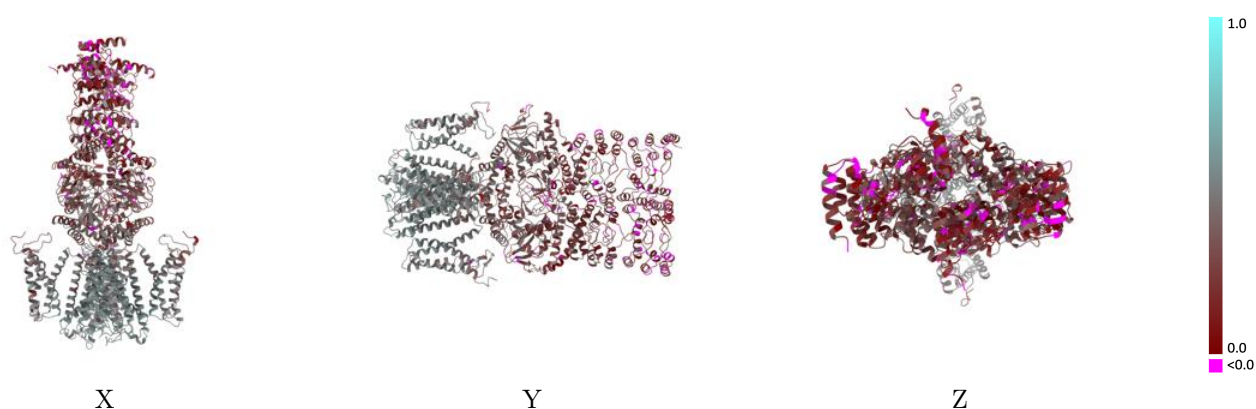
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62918 and PDB model 9LA3. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

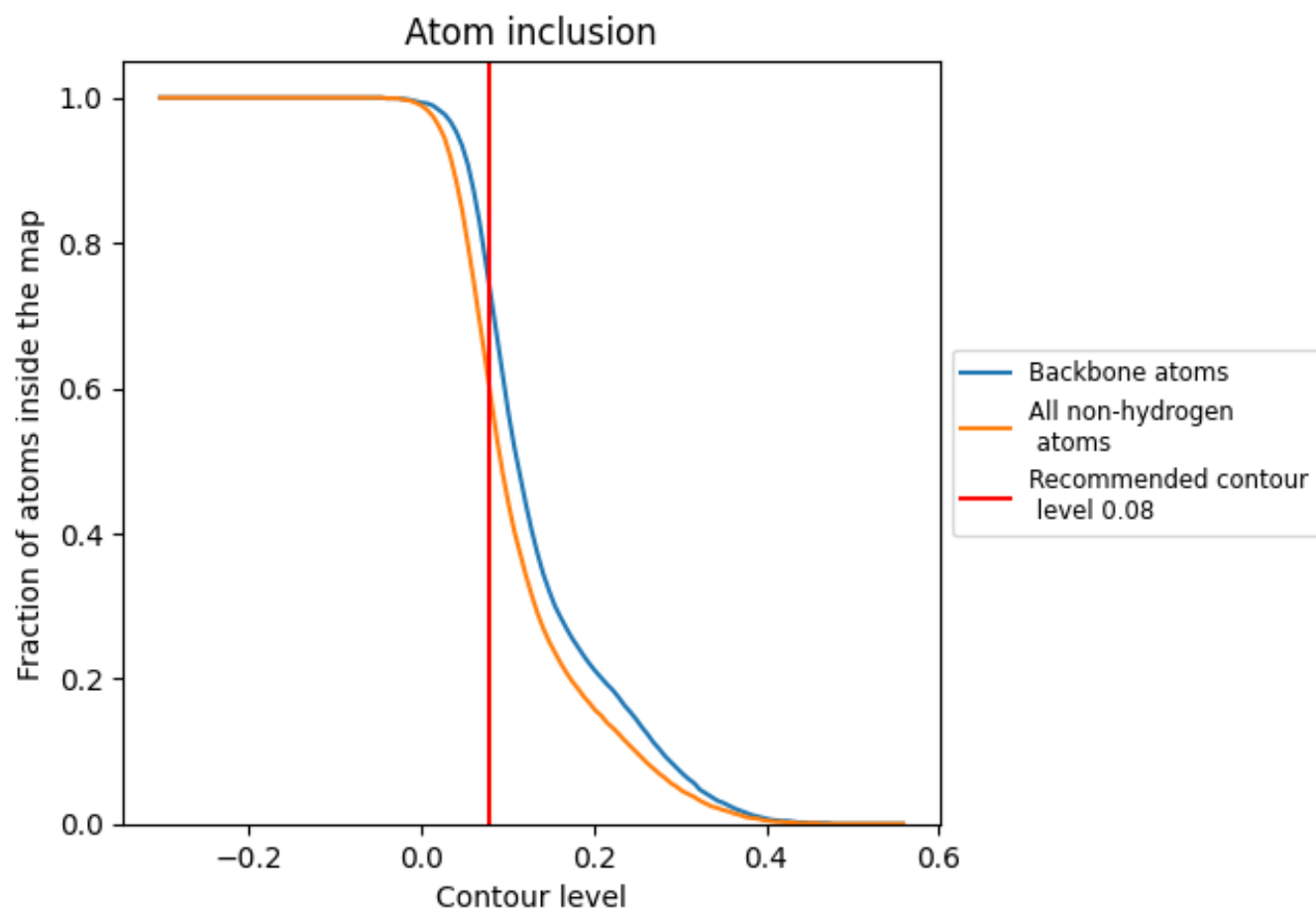


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 74% of all backbone atoms, 60% 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	0.5960	0.3380
A	0.6110	0.3430
B	0.5780	0.3280
C	0.5930	0.3430
D	0.6040	0.3370

