Full wwPDB EM Validation Report (i)

Sep 21, 2026 – 07:18 pm BST

PDB ID	:	9T5P / pdb_00009t5p
EMDB ID	:	EMD-55592
Title	:	Structure of heteromeric mouse LRRC8A/D Volume-Regulated Anion Channel in complex with synthetic nanobody Sb4
Authors	:	Lehmann, E.F.; Deneka, D.; Stierli, F.; Rutz, S.; Dutzler, R.
Deposited on	:	2025-11-05
Resolution	:	3.97 Å(reported)
Based on initial model	:	.

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 (i) 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 (1)) were used in the production of this report:

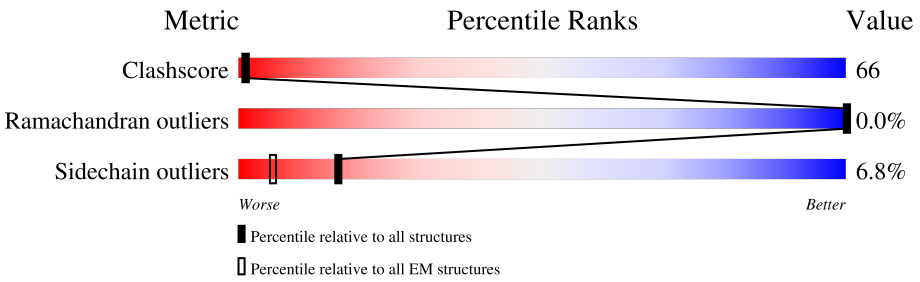
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

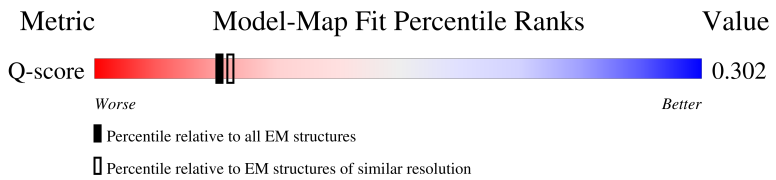
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.97 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	7578 (3.47 - 4.47)

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 <=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	806	6% 11% 26% • 60%
1	B	806	8% 21% 64% • 13%
1	C	806	6% 12% 25% • 60%
1	D	806	13% 12% 26% • 60%

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Mol	Chain	Length	Quality of chain
2	E	458	18% 16% 47% 33%
2	F	458	10% 22% 39% 6% 33%
3	J	128	47% 27% 70%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19794 atoms, of which 12 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 Volume-regulated anion channel subunit LRRC8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	319	2669	1759	429	464	17	0	0
1	B	701	5778	3765	973	1015	25	0	0
1	C	320	2678	1764	430	467	17	0	0
1	D	319	2669	1759	429	464	17	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q80WG5
A	1	SER	-	expression tag	UNP Q80WG5
B	0	MET	-	initiating methionine	UNP Q80WG5
B	1	SER	-	expression tag	UNP Q80WG5
C	0	MET	-	initiating methionine	UNP Q80WG5
C	1	SER	-	expression tag	UNP Q80WG5
D	0	MET	-	initiating methionine	UNP Q80WG5
D	1	SER	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Volume-regulated anion channel subunit LRRC8D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	307	2516	1672	391	435	18	0	0
2	F	305	2495	1657	388	432	18	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP A0A6P5PKE4

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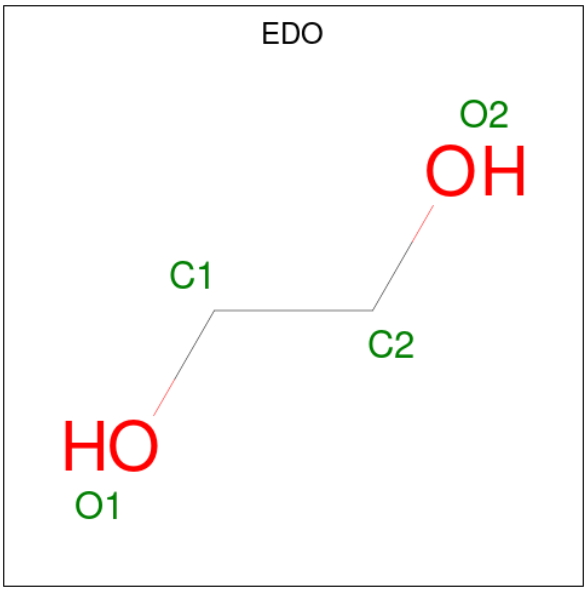
Chain	Residue	Modelled	Actual	Comment	Reference
E	1	SER	-	expression tag	UNP A0A6P5PKE4
E	61L	LEU	PHE	conflict	UNP A0A6P5PKE4
E	61Q	VAL	ALA	conflict	UNP A0A6P5PKE4
E	313	VAL	LEU	conflict	UNP A0A6P5PKE4
E	347	ILE	THR	conflict	UNP A0A6P5PKE4
F	0	MET	-	initiating methionine	UNP A0A6P5PKE4
F	1	SER	-	expression tag	UNP A0A6P5PKE4
F	61L	LEU	PHE	conflict	UNP A0A6P5PKE4
F	61Q	VAL	ALA	conflict	UNP A0A6P5PKE4
F	313	VAL	LEU	conflict	UNP A0A6P5PKE4
F	347	ILE	THR	conflict	UNP A0A6P5PKE4

- Molecule 3 is a protein called Volume-regulated anion channel subunit LRRC8D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	126	969	613	158	195	3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



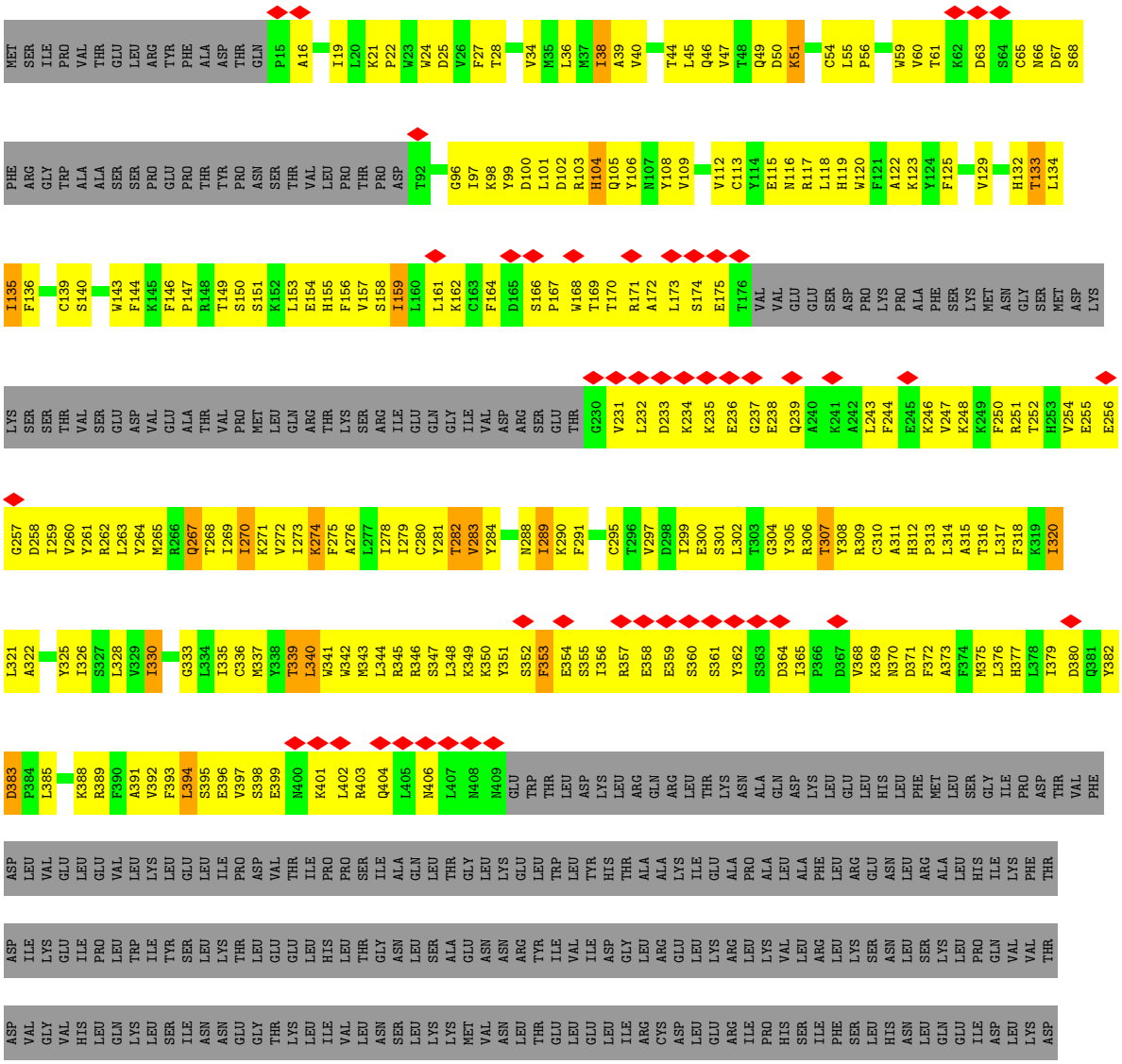
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
4	B	1	10	2	6	2	0
4	B	1	10	2	6	2	0

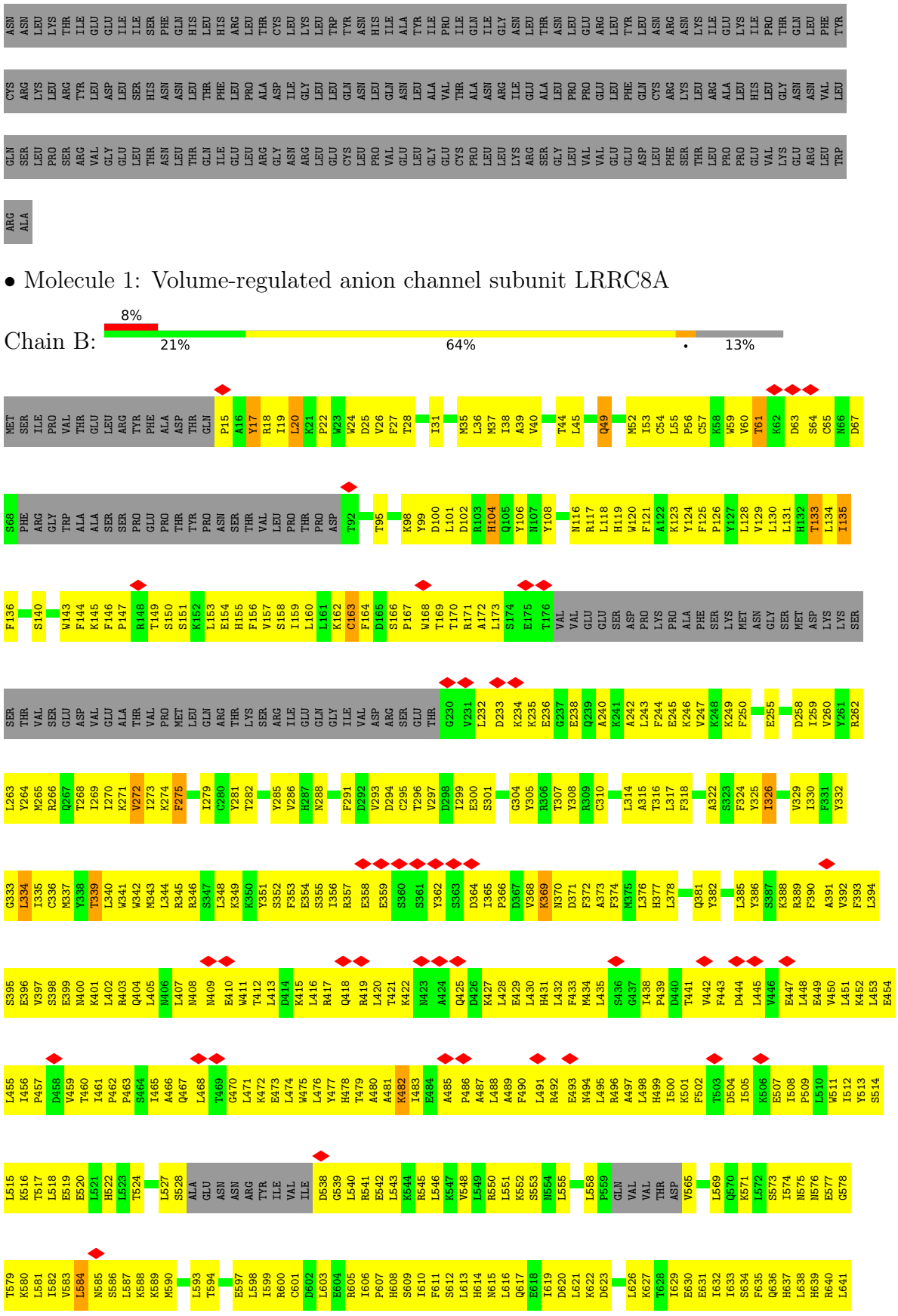
3 Residue-property plots (i)

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: Volume-regulated anion channel subunit LRRC8A

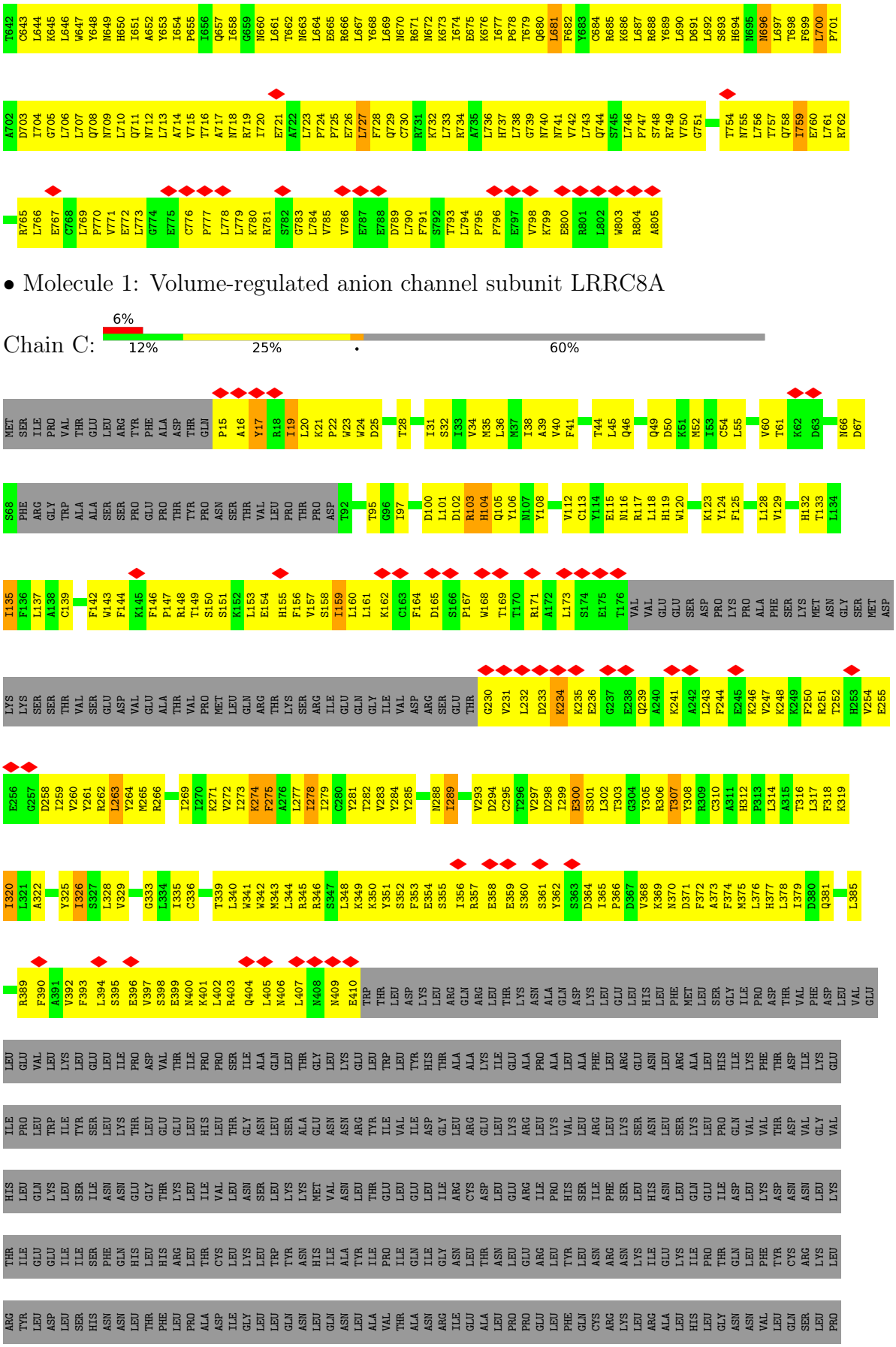
Chain A:





- Molecule 1: Volume-regulated anion channel subunit LRRC8A

Chain B: 8% 21% 64% • 13%

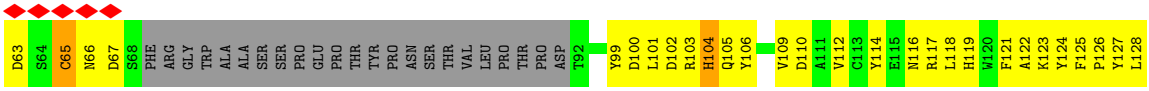


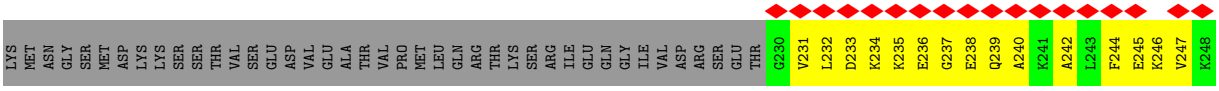
• Molecule 1: Volume-regulated anion channel subunit LRRC8A

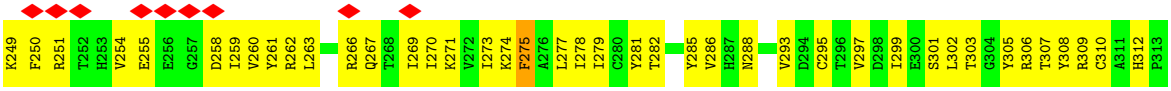
Chain C: 6% 12% 25% 60%

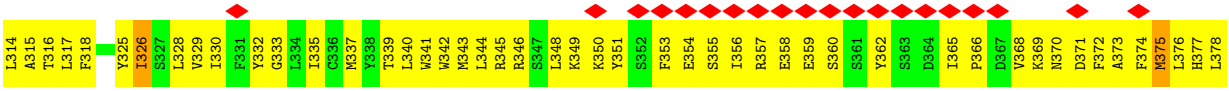
• Molecule 1: Volume-regulated anion channel subunit LRRC8A

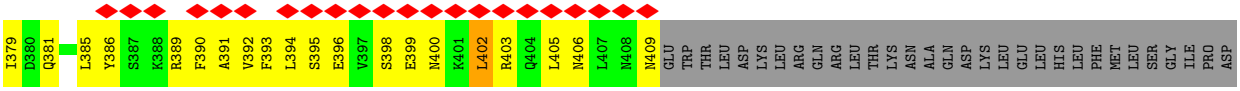
Chain D:

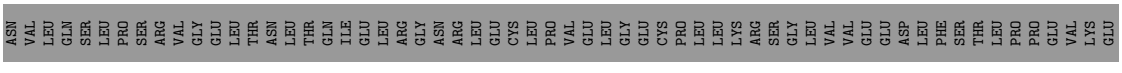






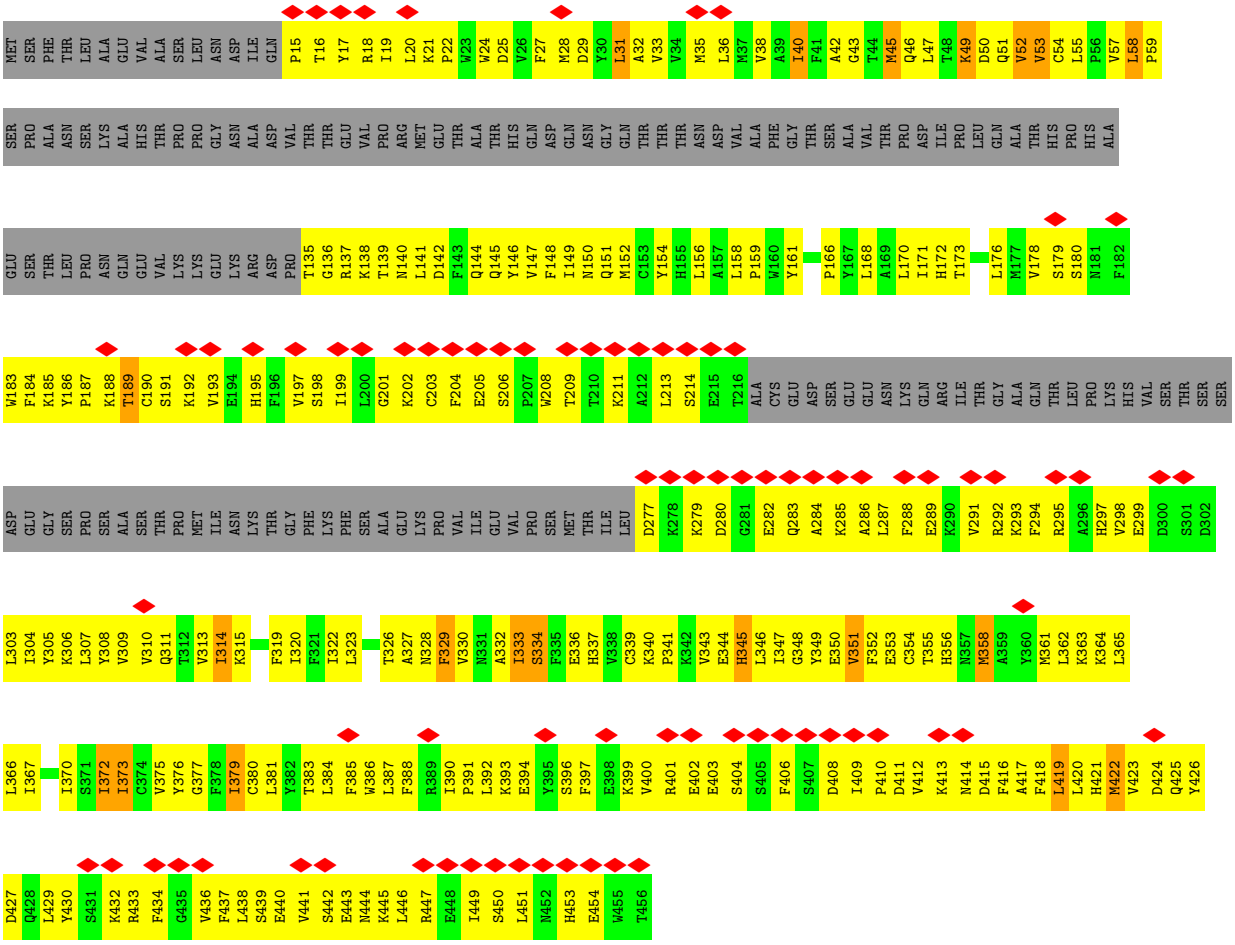






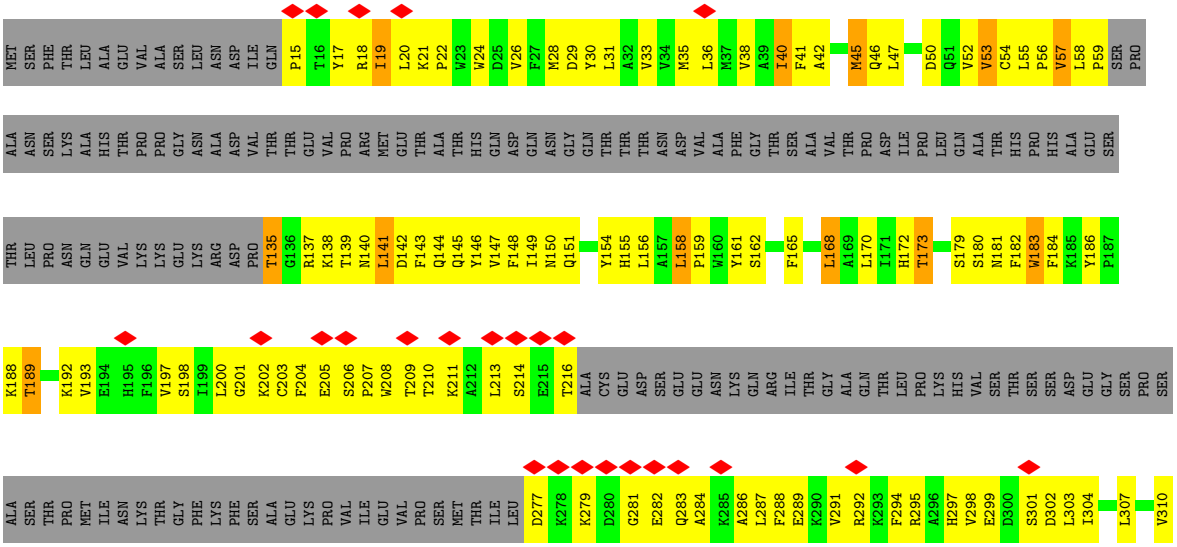
• Molecule 2: Volume-regulated anion channel subunit LRRC8D

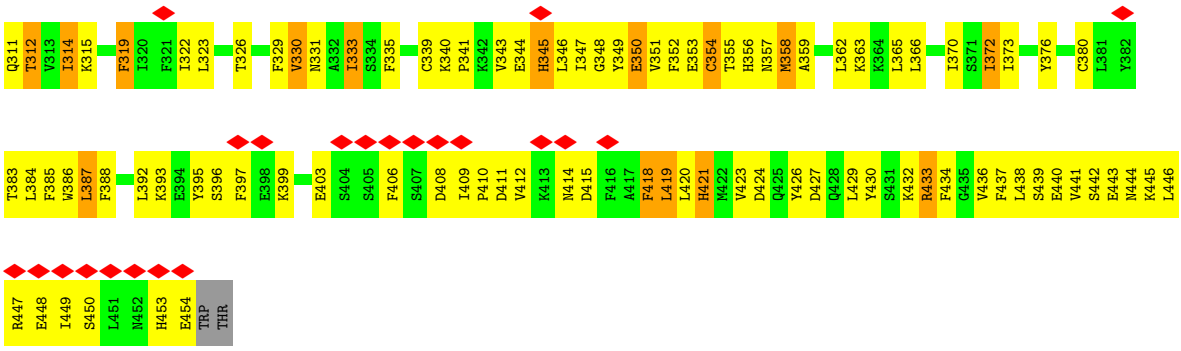
Chain E:



• Molecule 2: Volume-regulated anion channel subunit LRRC8D

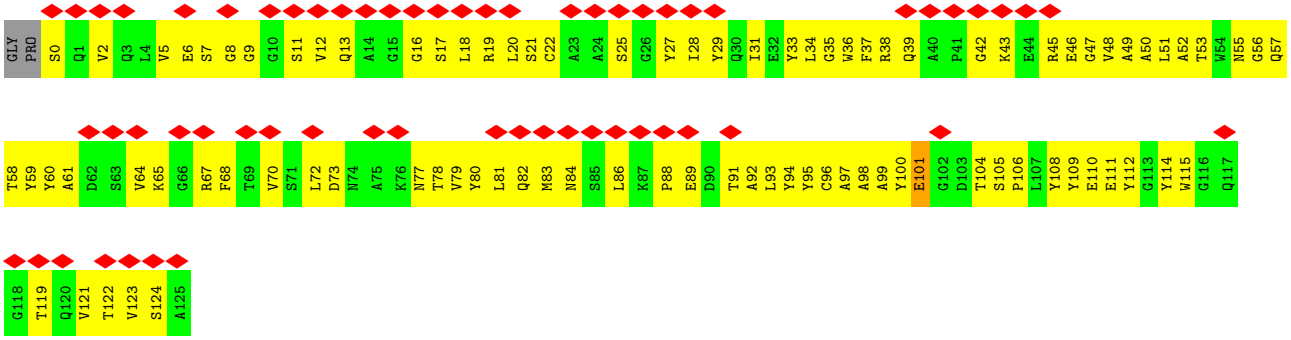
Chain F:





• Molecule 3: Volume-regulated anion channel subunit LRRC8D

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111259	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	61.39	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.044	Depositor
Minimum map value	-0.359	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.232	Depositor
Map size (Å)	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.44, 1.44, 1.44	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.23	0/2744	0.33	0/3716
1	B	0.19	0/5908	0.35	0/8004
1	C	0.21	0/2753	0.32	0/3728
1	D	0.19	0/2744	0.31	0/3716
2	E	0.20	0/2589	0.38	0/3514
2	F	0.23	0/2566	0.39	0/3481
3	J	0.13	0/992	0.28	0/1349
All	All	0.20	0/20296	0.35	0/27508

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	2669	0	2661	329	0
1	B	5778	0	5939	906	0
1	C	2678	0	2667	341	0
1	D	2669	0	2661	339	0
2	E	2516	0	2481	328	0
2	F	2495	0	2464	319	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	969	0	908	140	0
4	B	8	12	12	0	0
All	All	19782	12	19793	2605	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 66.

All (2605) 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:641:LEU:HG	1:B:664:LEU:HD21	1.29	1.14
1:B:517:THR:HA	1:B:545:ARG:HD2	1.21	1.14
1:B:700:LEU:HD12	1:B:724:PRO:HD2	1.20	1.14
1:B:650:HIS:HB3	1:B:673:LYS:HE2	1.19	1.11
1:B:527:LEU:HB2	1:B:555:LEU:HD21	1.36	1.08
3:J:51:LEU:HD21	3:J:56:GLY:HA2	1.34	1.06
1:B:473:GLU:HG2	1:B:497:ALA:HB3	1.37	1.06
2:E:404:SER:HB3	2:E:410:PRO:HA	1.39	1.04
1:A:67:ASP:HA	2:F:346:LEU:HD11	1.40	1.04
2:F:183:TRP:HA	2:F:307:LEU:HD21	1.40	1.04
1:C:31:ILE:HG22	1:C:35:MET:HE2	1.40	1.03
1:B:413:LEU:HD13	1:B:444:ASP:HB2	1.41	1.02
1:B:366:PRO:HD2	1:B:394:LEU:HB3	1.40	1.01
1:B:454:GLU:HG2	1:B:477:TYR:HB2	1.37	1.01
1:B:614:HIS:HA	1:B:638:LEU:HD22	1.42	1.01
1:A:39:ALA:HB2	1:A:129:VAL:HG12	1.42	1.00
3:J:91:THR:HG23	3:J:122:THR:HA	1.42	1.00
1:B:665:GLU:HA	1:B:687:LEU:HA	1.40	1.00
1:A:385:LEU:HD11	2:F:297:HIS:HE2	1.27	0.99
1:B:755:ASN:HA	1:B:778:LEU:HD12	1.44	0.99
1:B:450:VAL:HG22	1:B:473:GLU:HB2	1.44	0.99
1:B:569:LEU:HD23	1:B:590:MET:HE1	1.43	0.99
1:D:39:ALA:HB2	1:D:129:VAL:HG22	1.44	0.99
1:B:420:LEU:HD11	1:B:445:LEU:HD13	1.44	0.98
3:J:104:THR:HG23	3:J:111:GLU:HB3	1.43	0.98
1:C:243:LEU:HD12	1:C:246:LYS:HZ3	1.27	0.98
1:A:164:PHE:HA	1:A:389:ARG:HH12	1.28	0.97
1:B:629:ILE:HG21	1:B:646:LEU:HD13	1.47	0.97
1:B:619:ILE:HB	1:B:644:LEU:HD13	1.46	0.97
1:C:39:ALA:HB2	1:C:129:VAL:HG12	1.45	0.96
2:E:52:VAL:HG12	2:E:356:HIS:HA	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LYS:HE3	1:B:409:ASN:HB3	1.47	0.96
1:B:293:VAL:HG13	1:B:310:CYS:HB2	1.46	0.96
1:C:16:ALA:HB1	1:C:157:VAL:HG21	1.45	0.95
1:D:37:MET:HA	1:D:37:MET:HE2	1.47	0.95
1:A:269:ILE:HD12	1:A:340:LEU:HD21	1.46	0.95
1:B:63:ASP:HA	1:B:307:THR:HG21	1.48	0.95
1:C:401:LYS:HG3	1:C:402:LEU:HD12	1.49	0.94
1:B:430:LEU:HG	1:B:432:LEU:HD21	1.48	0.94
2:E:387:LEU:HD11	2:E:422:MET:HE1	1.49	0.94
1:B:606:ILE:HD12	1:B:631:GLU:HB2	1.50	0.93
2:E:147:VAL:HA	2:E:150:ASN:HD21	1.33	0.93
1:B:399:GLU:HB3	1:B:403:ARG:HH12	1.31	0.92
1:B:463:PRO:HB3	1:B:486:PRO:HB2	1.51	0.92
1:A:282:THR:HG22	1:A:326:ILE:HD11	1.50	0.92
1:C:258:ASP:HA	1:C:371:ASP:HB2	1.50	0.92
1:D:306:ARG:HA	1:D:306:ARG:HH11	1.35	0.91
2:E:213:LEU:HD11	2:E:436:VAL:HG21	1.53	0.91
1:D:149:THR:HB	1:D:260:VAL:HG22	1.51	0.91
1:D:63:ASP:HA	1:D:307:THR:HG21	1.50	0.90
2:E:19:ILE:HG23	2:E:426:TYR:HD2	1.35	0.90
1:C:117:ARG:HG3	1:C:295:CYS:HA	1.51	0.90
2:E:422:MET:HE2	2:E:422:MET:HA	1.52	0.90
2:F:19:ILE:HG21	2:F:423:VAL:HG13	1.54	0.89
1:B:126:PRO:HD3	1:B:318:PHE:HE2	1.37	0.89
1:A:264:TYR:HD2	1:A:343:MET:HE1	1.37	0.89
1:D:52:MET:HE3	1:D:118:LEU:HB2	1.52	0.89
1:D:232:LEU:HG	1:D:405:LEU:HD22	1.52	0.88
2:E:52:VAL:HG22	2:E:154:TYR:HD1	1.38	0.88
3:J:39:GLN:HB2	3:J:45:ARG:HA	1.54	0.88
1:C:354:GLU:HA	1:C:357:ARG:HH11	1.38	0.88
2:F:323:LEU:HD12	2:F:373:ILE:HG22	1.55	0.88
1:B:650:HIS:CB	1:B:673:LYS:HE2	2.04	0.87
1:A:354:GLU:HA	1:A:357:ARG:HH11	1.39	0.87
1:B:700:LEU:CD1	1:B:724:PRO:HD2	2.04	0.87
1:D:143:TRP:HB3	1:D:263:LEU:HD22	1.57	0.87
1:B:667:LEU:HB3	1:B:690:LEU:HD13	1.57	0.87
2:E:288:PHE:HE2	2:E:446:LEU:HD13	1.37	0.87
2:F:288:PHE:HE2	2:F:446:LEU:HD13	1.40	0.86
1:B:135:ILE:HG21	1:B:274:LYS:HZ2	1.37	0.86
1:D:354:GLU:HA	1:D:357:ARG:HD3	1.57	0.86
1:D:399:GLU:HA	1:D:402:LEU:HD11	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:VAL:HG13	1:C:310:CYS:HB2	1.58	0.86
3:J:20:LEU:HD22	3:J:119:THR:HG21	1.58	0.85
2:E:22:PRO:HG2	2:E:24:TRP:CZ2	2.11	0.85
1:C:398:SER:HA	1:C:401:LYS:HE3	1.57	0.85
2:F:52:VAL:HG12	2:F:356:HIS:HA	1.56	0.85
1:B:465:ILE:CD1	1:B:491:LEU:HD21	2.07	0.85
2:E:147:VAL:HA	2:E:150:ASN:ND2	1.91	0.85
2:F:330:VAL:HB	2:F:366:LEU:HD21	1.59	0.85
1:B:397:VAL:HA	1:B:400:ASN:OD1	1.76	0.85
1:A:258:ASP:H	1:A:371:ASP:HB2	1.39	0.85
1:A:243:LEU:HD23	1:A:246:LYS:HZ3	1.42	0.84
1:C:234:LYS:HD2	1:C:409:ASN:HB2	1.59	0.84
1:B:770:PRO:O	1:B:773:LEU:HG	1.78	0.84
2:F:292:ARG:HA	2:F:295:ARG:HB3	1.59	0.84
1:B:619:ILE:HB	1:B:644:LEU:CD1	2.07	0.83
1:B:622:LYS:HG3	1:B:648:TYR:HB2	1.60	0.83
2:E:394:GLU:HA	2:E:417:ALA:CA	2.08	0.83
1:B:548:VAL:HG22	1:B:571:LYS:HB3	1.57	0.83
1:B:650:HIS:HB3	1:B:673:LYS:CE	2.06	0.83
1:A:112:VAL:HG13	1:A:297:VAL:HG11	1.59	0.83
2:E:172:HIS:CE1	2:E:322:ILE:HG21	2.13	0.83
2:E:403:GLU:HG3	2:E:432:LYS:HE2	1.61	0.83
1:B:452:LYS:HA	1:B:475:TRP:HB2	1.59	0.83
1:B:700:LEU:HD11	1:B:723:LEU:HD22	1.61	0.83
1:B:425:GLN:HB3	1:B:427:LYS:HE3	1.61	0.82
1:B:769:LEU:HB3	1:B:773:LEU:HD11	1.60	0.82
1:A:51:LYS:H	1:A:51:LYS:HD3	1.41	0.82
1:B:646:LEU:HB2	1:B:669:LEU:HD22	1.61	0.82
1:C:366:PRO:HG2	1:C:394:LEU:HD21	1.58	0.82
2:F:409:ILE:HG21	2:F:442:SER:HB2	1.61	0.82
1:B:700:LEU:HD21	1:B:720:ILE:HD13	1.60	0.82
2:E:344:GLU:OE2	2:E:348:GLY:HA2	1.80	0.82
2:E:394:GLU:HA	2:E:417:ALA:HA	1.60	0.82
1:B:527:LEU:CB	1:B:555:LEU:HD21	2.10	0.82
1:B:725:PRO:HB2	1:B:749:ARG:HH11	1.45	0.81
1:B:599:ILE:HD12	1:B:622:LYS:HB3	1.62	0.81
2:F:399:LYS:CD	2:F:421:HIS:HB3	2.11	0.81
1:B:297:VAL:HG23	1:B:299:ILE:HG12	1.63	0.81
1:C:156:PHE:HA	1:C:159:ILE:HD11	1.61	0.81
1:B:355:SER:O	1:B:359:GLU:HG3	1.79	0.81
1:D:18:ARG:HG3	1:D:19:ILE:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:68:PHE:HB3	3:J:81:LEU:HD11	1.61	0.81
1:B:685:ARG:HA	1:B:707:LEU:CD2	2.11	0.81
3:J:33:TYR:CD2	3:J:104:THR:HB	2.15	0.81
1:B:282:THR:HG22	1:B:326:ILE:HD11	1.61	0.81
1:D:372:PHE:HA	1:D:375:MET:SD	2.21	0.81
1:B:645:LYS:HD3	1:B:647:TRP:CH2	2.16	0.81
1:C:169:THR:HG22	1:C:392:VAL:HG21	1.62	0.80
2:E:339:CYS:SG	2:E:341:PRO:HD3	2.21	0.80
1:B:641:LEU:HG	1:B:664:LEU:CD2	2.09	0.80
1:C:289:ILE:HG22	1:C:319:LYS:HE2	1.64	0.80
1:C:385:LEU:H	1:C:385:LEU:HD12	1.46	0.80
2:F:165:PHE:CE1	2:F:366:LEU:HD13	2.16	0.80
1:B:671:ARG:H	1:B:694:HIS:HB2	1.47	0.80
1:C:149:THR:HG21	1:C:263:LEU:CD2	2.12	0.80
3:J:22:CYS:HB3	3:J:79:VAL:HG12	1.64	0.80
1:B:550:ARG:NH2	1:B:552:LYS:HB2	1.97	0.79
1:B:600:ARG:HA	1:B:623:ASP:O	1.82	0.79
1:B:710:LEU:HG	1:B:733:LEU:HD21	1.62	0.79
1:B:297:VAL:CG2	1:B:299:ILE:HG12	2.12	0.79
2:F:444:ASN:O	2:F:447:ARG:HG2	1.81	0.79
1:B:746:LEU:HD23	1:B:770:PRO:HD2	1.65	0.79
1:B:607:PRO:HG2	1:B:610:ILE:HD11	1.63	0.79
2:E:58:LEU:HD12	2:E:137:ARG:HH12	1.45	0.79
2:E:294:PHE:HA	2:E:297:HIS:HB3	1.63	0.79
3:J:37:PHE:HA	3:J:48:VAL:HG23	1.63	0.79
3:J:83:MET:HB3	3:J:86:LEU:HD21	1.65	0.79
2:F:57:VAL:HG21	2:F:351:VAL:HG13	1.63	0.79
2:F:339:CYS:SG	2:F:341:PRO:HD3	2.22	0.79
1:B:685:ARG:HA	1:B:707:LEU:HD22	1.65	0.79
2:E:393:LYS:O	2:E:417:ALA:HA	1.83	0.78
1:A:233:ASP:HB3	1:A:236:GLU:HG3	1.65	0.78
2:E:38:VAL:HG13	2:E:365:LEU:HD11	1.64	0.78
2:F:172:HIS:NE2	2:F:322:ILE:HG12	1.98	0.78
1:B:438:ILE:HD12	1:B:460:THR:O	1.82	0.78
1:B:645:LYS:HG2	1:B:668:TYR:HD1	1.48	0.78
1:B:365:ILE:HA	1:B:394:LEU:O	1.83	0.78
1:A:269:ILE:CD1	1:A:340:LEU:HD21	2.13	0.78
1:A:34:VAL:O	1:A:38:ILE:HG23	1.83	0.78
1:B:502:PHE:HA	1:B:507:GLU:OE1	1.82	0.78
1:A:392:VAL:HG23	1:A:393:PHE:HD1	1.47	0.78
1:B:509:PRO:HB2	1:B:512:ILE:HG23	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LEU:HD21	1:C:260:VAL:HG21	1.64	0.78
1:A:291:PHE:HA	1:A:315:ALA:HB3	1.64	0.78
1:B:129:VAL:O	1:B:133:THR:HG22	1.84	0.77
1:B:481:ALA:HB1	1:B:511:TRP:HZ2	1.49	0.77
1:C:364:ASP:HB3	1:C:397:VAL:HG23	1.66	0.77
1:D:375:MET:O	1:D:379:ILE:HG12	1.85	0.77
2:E:19:ILE:HG13	2:E:426:TYR:HE2	1.49	0.77
1:C:164:PHE:HA	1:C:389:ARG:HH12	1.49	0.77
1:B:541:ARG:HA	1:B:565:VAL:CG1	2.13	0.77
1:D:147:PRO:HA	1:D:150:SER:OG	1.85	0.77
2:E:57:VAL:CG1	2:E:353:GLU:HG2	2.15	0.77
1:D:168:TRP:CD2	1:D:402:LEU:HD23	2.18	0.77
2:F:22:PRO:HG2	2:F:24:TRP:CZ2	2.19	0.77
1:B:746:LEU:HB3	1:B:770:PRO:HD3	1.66	0.77
1:C:374:PHE:O	1:C:378:LEU:HD13	1.85	0.77
1:C:364:ASP:O	1:C:395:SER:HA	1.83	0.77
1:A:234:LYS:HE2	1:A:406:ASN:O	1.85	0.77
1:B:354:GLU:HA	1:B:357:ARG:HD3	1.67	0.77
1:C:46:GLN:HB2	1:C:318:PHE:HZ	1.50	0.77
1:C:400:ASN:HB3	1:C:403:ARG:HH21	1.50	0.77
2:E:159:PRO:HB3	2:E:161:TYR:CZ	2.19	0.77
1:A:22:PRO:HG2	1:A:24:TRP:CZ2	2.20	0.77
1:A:135:ILE:HG21	1:A:274:LYS:HD2	1.66	0.77
1:D:343:MET:HA	1:D:348:LEU:CD2	2.14	0.77
1:B:736:LEU:HD11	1:B:738:LEU:HD21	1.67	0.76
2:F:403:GLU:HG3	2:F:432:LYS:HE2	1.66	0.76
1:D:369:LYS:HG2	1:D:370:ASN:H	1.49	0.76
1:B:345:ARG:HG3	1:B:346:ARG:HG2	1.67	0.76
1:D:163:CYS:HB2	1:D:393:PHE:CE1	2.21	0.76
1:B:60:VAL:HG21	1:B:307:THR:HG21	1.66	0.76
2:F:159:PRO:HB3	2:F:161:TYR:CZ	2.21	0.76
1:A:149:THR:HG21	1:A:263:LEU:HD22	1.67	0.76
1:B:675:GLU:HG2	1:B:696:ASN:HB2	1.66	0.76
1:B:724:PRO:HB2	1:B:726:GLU:OE1	1.86	0.76
2:F:42:ALA:HB2	2:F:365:LEU:HD21	1.68	0.76
1:B:665:GLU:HA	1:B:687:LEU:HD23	1.67	0.76
1:B:757:THR:HG22	1:B:778:LEU:HB3	1.68	0.76
1:B:665:GLU:CA	1:B:687:LEU:HD23	2.15	0.76
1:B:666:ARG:HG2	1:B:689:TYR:HB2	1.68	0.76
2:E:46:GLN:O	2:E:50:ASP:HB2	1.86	0.76
1:B:448:LEU:HD11	1:B:450:VAL:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ILE:HD13	1:B:491:LEU:HD21	1.67	0.75
1:B:502:PHE:HB2	1:B:507:GLU:HB2	1.68	0.75
2:E:18:ARG:HA	2:E:21:LYS:HE3	1.68	0.75
2:F:17:TYR:O	2:F:21:LYS:HE3	1.86	0.75
3:J:2:VAL:HA	3:J:25:SER:OG	1.87	0.75
2:E:288:PHE:CE2	2:E:446:LEU:HD13	2.19	0.75
1:B:129:VAL:HG23	1:B:325:TYR:CE1	2.21	0.75
1:D:354:GLU:HG2	1:D:357:ARG:HH11	1.51	0.75
2:E:19:ILE:H	2:E:19:ILE:HD12	1.50	0.75
2:E:58:LEU:HD12	2:E:137:ARG:NH1	2.02	0.75
1:B:654:ILE:HG13	1:B:674:ILE:HD13	1.67	0.75
1:B:413:LEU:CD1	1:B:444:ASP:HB2	2.16	0.75
1:C:102:ASP:H	1:C:105:GLN:HE21	1.34	0.75
1:B:429:GLU:HA	1:B:448:LEU:HD11	1.69	0.75
1:B:728:PHE:HZ	1:B:747:PRO:HG2	1.50	0.75
1:D:158:SER:O	1:D:162:LYS:HG2	1.86	0.75
2:F:279:LYS:O	2:F:283:GLN:HG2	1.87	0.75
1:C:40:VAL:O	1:C:44:THR:HG22	1.87	0.74
1:C:156:PHE:HB2	1:C:250:PHE:CZ	2.22	0.74
1:D:168:TRP:CE2	1:D:402:LEU:HD23	2.22	0.74
1:C:289:ILE:HG21	1:C:319:LYS:HB2	1.69	0.74
2:E:415:ASP:OD1	2:E:418:PHE:HB2	1.87	0.74
1:A:264:TYR:CD2	1:A:343:MET:HE1	2.23	0.74
1:B:146:PHE:HD1	1:B:147:PRO:HD2	1.51	0.74
1:D:235:LYS:NZ	1:D:239:GLN:HB2	2.02	0.74
1:B:143:TRP:HB3	1:B:263:LEU:CD2	2.17	0.74
1:B:451:LEU:HD11	1:B:453:LEU:HD21	1.69	0.74
1:D:377:HIS:O	1:D:381:GLN:HG2	1.86	0.74
3:J:37:PHE:O	3:J:94:TYR:HA	1.87	0.74
1:B:552:LYS:HG3	1:B:575:ASN:HB3	1.70	0.74
1:C:32:SER:HA	1:C:35:MET:HE3	1.68	0.74
1:C:392:VAL:HG23	1:C:393:PHE:HD1	1.51	0.74
1:D:251:ARG:HA	1:D:372:PHE:CE2	2.22	0.74
1:C:156:PHE:CZ	1:C:375:MET:HB3	2.23	0.74
1:A:156:PHE:HA	1:A:159:ILE:HD11	1.69	0.73
2:F:31:LEU:HD22	2:F:376:TYR:CD2	2.23	0.73
2:F:344:GLU:HB3	2:F:350:GLU:HA	1.69	0.73
1:A:364:ASP:O	1:A:395:SER:HA	1.88	0.73
1:D:398:SER:O	1:D:402:LEU:HG	1.88	0.73
2:F:45:MET:HE2	2:F:358:MET:HG3	1.70	0.73
2:F:346:LEU:C	2:F:347:ILE:HD12	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:187:PRO:HA	2:E:190:CYS:HB3	1.71	0.73
1:B:460:THR:HA	1:B:482:LYS:HB2	1.69	0.73
1:B:665:GLU:CA	1:B:687:LEU:HA	2.17	0.73
1:B:264:TYR:CD1	1:B:343:MET:HE1	2.23	0.73
1:C:398:SER:O	1:C:401:LYS:HG2	1.88	0.73
2:E:433:ARG:HH22	2:E:434:PHE:HB2	1.52	0.73
1:A:39:ALA:HB2	1:A:129:VAL:CG1	2.19	0.73
1:A:243:LEU:HA	1:A:246:LYS:HG2	1.70	0.73
1:B:452:LYS:O	1:B:453:LEU:HD23	1.89	0.73
1:B:553:SER:O	1:B:576:ASN:HA	1.88	0.73
2:E:396:SER:HA	2:E:399:LYS:HE2	1.71	0.73
3:J:108:TYR:HB2	3:J:111:GLU:HG2	1.70	0.73
1:A:295:CYS:SG	1:A:297:VAL:HG13	2.27	0.73
2:E:19:ILE:HG13	2:E:426:TYR:CE2	2.24	0.73
1:B:19:ILE:H	1:B:19:ILE:HD12	1.54	0.72
1:D:146:PHE:HD1	1:D:147:PRO:HD2	1.54	0.72
1:D:149:THR:O	1:D:153:LEU:HG	1.89	0.72
2:E:45:MET:HE2	2:E:358:MET:HE2	1.71	0.72
2:F:54:CYS:HB2	2:F:150:ASN:HB3	1.71	0.72
2:F:448:GLU:OE1	2:F:449:ILE:HD12	1.89	0.72
1:B:574:ILE:HB	1:B:598:LEU:HD23	1.72	0.72
1:D:39:ALA:HB2	1:D:129:VAL:CG2	2.17	0.72
1:A:171:ARG:HD2	1:A:232:LEU:HD12	1.72	0.72
1:B:645:LYS:HG2	1:B:668:TYR:CD1	2.24	0.72
2:F:444:ASN:HA	2:F:447:ARG:NE	2.03	0.72
1:A:49:GLN:HB2	1:A:51:LYS:HE3	1.70	0.72
1:B:54:CYS:O	1:B:55:LEU:HD23	1.90	0.72
1:B:244:PHE:CD2	1:B:399:GLU:HG3	2.24	0.72
2:E:42:ALA:HB2	2:E:365:LEU:HD21	1.71	0.72
2:E:444:ASN:HA	2:E:447:ARG:NE	2.04	0.72
1:A:36:LEU:HB2	1:A:133:THR:HG21	1.71	0.72
1:A:167:PRO:O	1:A:171:ARG:HG3	1.90	0.72
1:B:416:LEU:HB2	1:B:445:LEU:HD11	1.71	0.72
1:B:433:PHE:HA	1:B:454:GLU:O	1.90	0.72
1:B:498:LEU:HD12	1:B:499:HIS:H	1.55	0.72
1:C:17:TYR:HB3	1:C:144:PHE:CZ	2.25	0.72
3:J:22:CYS:HB2	3:J:36:TRP:CZ2	2.25	0.72
3:J:31:ILE:HD13	3:J:98:ALA:HB1	1.71	0.72
1:A:100:ASP:HB3	1:B:98:LYS:HE3	1.70	0.72
1:C:265:MET:O	1:C:269:ILE:HD13	1.89	0.72
1:B:704:ILE:HD13	1:B:727:LEU:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:144:GLN:HB2	2:F:146:TYR:CD2	2.23	0.72
2:E:403:GLU:HA	2:E:406:PHE:CZ	2.23	0.72
1:B:432:LEU:HB2	1:B:453:LEU:HD22	1.72	0.72
1:D:36:LEU:HG	1:D:133:THR:OG1	1.90	0.72
2:E:444:ASN:O	2:E:447:ARG:HG2	1.89	0.72
1:B:574:ILE:HG21	1:B:581:LEU:HD22	1.72	0.71
1:B:760:GLU:HA	1:B:785:VAL:HB	1.71	0.71
1:D:244:PHE:CD2	1:D:399:GLU:HG3	2.25	0.71
2:E:159:PRO:HB3	2:E:161:TYR:CE1	2.25	0.71
1:A:268:THR:HG22	1:A:340:LEU:HD23	1.70	0.71
2:F:38:VAL:HG13	2:F:365:LEU:HD11	1.72	0.71
2:F:165:PHE:HE1	2:F:366:LEU:HD13	1.53	0.71
2:F:189:THR:HG23	2:F:304:ILE:HD12	1.70	0.71
2:F:399:LYS:HD2	2:F:421:HIS:HB3	1.71	0.71
1:A:261:TYR:CE2	1:A:349:LYS:HE3	2.24	0.71
2:E:402:GLU:HG3	2:E:406:PHE:HE2	1.55	0.71
1:C:356:ILE:HG21	1:C:365:ILE:HG13	1.73	0.71
1:D:244:PHE:CE2	1:D:393:PHE:HA	2.25	0.71
1:C:375:MET:O	1:C:379:ILE:HG12	1.90	0.71
1:D:40:VAL:O	1:D:44:THR:HG22	1.91	0.71
1:B:474:LEU:HD11	1:B:476:LEU:HD21	1.72	0.71
2:F:46:GLN:O	2:F:50:ASP:HB2	1.91	0.71
3:J:20:LEU:O	3:J:80:TYR:HA	1.90	0.71
1:B:147:PRO:HG3	1:C:23:TRP:HB3	1.72	0.71
1:B:717:ALA:HA	1:B:740:ASN:HB2	1.72	0.71
1:C:45:LEU:HD21	1:C:317:LEU:HD23	1.72	0.71
2:E:387:LEU:HD11	2:E:422:MET:CE	2.21	0.71
3:J:73:ASP:HB2	3:J:80:TYR:CE2	2.26	0.71
1:B:60:VAL:HG21	1:B:307:THR:CG2	2.21	0.71
1:B:538:ASP:HB2	1:B:541:ARG:HH12	1.56	0.71
1:B:622:LYS:HE2	1:B:623:ASP:OD2	1.90	0.71
1:D:270:ILE:O	1:D:273:ILE:HG12	1.89	0.71
2:F:403:GLU:HA	2:F:406:PHE:CE1	2.26	0.71
3:J:11:SER:HA	3:J:122:THR:O	1.91	0.71
1:B:492:ARG:HG3	1:B:516:LYS:H	1.55	0.71
1:B:606:ILE:CD1	1:B:631:GLU:HB2	2.21	0.71
1:B:685:ARG:NH1	1:B:706:LEU:HB3	2.06	0.71
2:F:340:LYS:HG2	2:F:351:VAL:HG23	1.70	0.71
1:B:682:PHE:CD2	1:B:703:ASP:HB2	2.26	0.70
1:A:136:PHE:CE1	1:A:274:LYS:HG2	2.25	0.70
1:C:149:THR:O	1:C:153:LEU:HG	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:THR:HG22	1:C:326:ILE:HD11	1.74	0.70
1:D:164:PHE:CD1	1:D:389:ARG:HG3	2.25	0.70
2:F:396:SER:O	2:F:399:LYS:HG2	1.90	0.70
1:B:449:GLU:O	1:B:471:LEU:HD12	1.92	0.70
1:C:258:ASP:CA	1:C:371:ASP:HB2	2.22	0.70
1:D:343:MET:O	1:D:344:LEU:HD23	1.90	0.70
2:E:204:PHE:HA	2:E:433:ARG:CD	2.21	0.70
2:F:29:ASP:O	2:F:33:VAL:HG23	1.92	0.70
1:C:341:TRP:CG	1:C:345:ARG:HH21	2.10	0.70
1:D:343:MET:HA	1:D:348:LEU:HD22	1.74	0.70
1:A:158:SER:O	1:A:161:LEU:HG	1.91	0.70
1:A:239:GLN:O	1:A:243:LEU:HG	1.91	0.70
1:B:449:GLU:HA	1:B:470:GLY:O	1.90	0.70
1:B:671:ARG:N	1:B:694:HIS:HB2	2.06	0.70
1:B:714:ALA:HA	1:B:737:HIS:HB2	1.73	0.70
1:C:354:GLU:O	1:C:357:ARG:HG2	1.90	0.70
1:B:420:LEU:HB3	1:B:428:LEU:HD11	1.72	0.70
1:C:345:ARG:HG3	1:C:346:ARG:HD3	1.74	0.70
1:C:362:TYR:HB3	1:C:364:ASP:OD1	1.90	0.70
1:D:368:VAL:CG1	1:D:372:PHE:HB3	2.22	0.70
2:E:392:LEU:HD23	2:E:392:LEU:O	1.92	0.70
2:F:19:ILE:HD12	2:F:19:ILE:H	1.56	0.70
1:D:129:VAL:O	1:D:133:THR:HG22	1.92	0.70
1:A:244:PHE:HB3	1:A:248:LYS:NZ	2.07	0.70
1:B:399:GLU:O	1:B:402:LEU:HG	1.92	0.70
2:E:141:LEU:HD23	2:E:146:TYR:CE1	2.27	0.70
2:F:281:GLY:O	2:F:446:LEU:HD21	1.91	0.70
1:C:168:TRP:CE2	1:C:402:LEU:HD22	2.27	0.70
1:C:260:VAL:HG12	1:C:371:ASP:OD1	1.92	0.70
1:D:19:ILE:HD12	1:D:19:ILE:H	1.56	0.70
1:D:242:ALA:O	1:D:245:GLU:HG3	1.92	0.70
1:A:297:VAL:HG23	1:A:299:ILE:HG12	1.74	0.70
1:B:143:TRP:HB3	1:B:263:LEU:HD22	1.72	0.70
1:B:365:ILE:HG12	1:B:395:SER:HA	1.73	0.70
1:B:614:HIS:HA	1:B:638:LEU:CD2	2.21	0.70
1:B:622:LYS:CE	3:J:105:SER:HB2	2.22	0.70
2:E:189:THR:O	2:E:193:VAL:HG23	1.92	0.70
1:B:487:ALA:O	1:B:491:LEU:HG	1.92	0.69
1:B:632:ILE:HA	1:B:635:PHE:CD2	2.27	0.69
1:D:163:CYS:O	1:D:169:THR:HG21	1.91	0.69
1:B:576:ASN:HB3	1:B:579:THR:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:PRO:HG2	1:B:610:ILE:CD1	2.21	0.69
1:C:345:ARG:HD2	1:C:346:ARG:CZ	2.22	0.69
1:D:129:VAL:HG23	1:D:325:TYR:CE1	2.27	0.69
1:B:430:LEU:HG	1:B:432:LEU:CD2	2.22	0.69
1:B:627:LYS:O	1:B:651:ILE:HA	1.92	0.69
1:A:34:VAL:HG12	1:A:328:LEU:HD11	1.74	0.69
1:A:168:TRP:CZ2	1:A:399:GLU:HA	2.27	0.69
1:C:46:GLN:HB2	1:C:318:PHE:CZ	2.27	0.69
2:E:444:ASN:HA	2:E:447:ARG:HE	1.55	0.69
3:J:101:GLU:HB2	3:J:104:THR:OG1	1.92	0.69
1:A:169:THR:HG22	1:A:393:PHE:HE1	1.58	0.69
1:B:430:LEU:CG	1:B:432:LEU:HD21	2.23	0.69
1:B:643:CYS:SG	1:B:666:ARG:HB2	2.33	0.69
1:C:231:VAL:HG23	1:C:409:ASN:CG	2.18	0.69
1:C:352:SER:HB3	1:C:354:GLU:HG2	1.74	0.69
3:J:9:GLY:HA2	3:J:121:VAL:HG22	1.73	0.69
2:F:19:ILE:CG2	2:F:423:VAL:HG13	2.21	0.69
2:F:19:ILE:HG22	2:F:20:LEU:H	1.57	0.69
1:B:585:ASN:HA	1:B:588:LYS:HB2	1.75	0.69
1:C:243:LEU:HA	1:C:246:LYS:HG2	1.73	0.69
1:D:295:CYS:SG	1:D:297:VAL:HG13	2.32	0.69
2:E:52:VAL:HG22	2:E:154:TYR:CD1	2.24	0.69
3:J:22:CYS:HB3	3:J:79:VAL:CG1	2.23	0.69
1:A:385:LEU:HD11	2:F:297:HIS:NE2	2.06	0.69
1:A:393:PHE:O	1:A:394:LEU:HD13	1.91	0.69
1:B:262:ARG:HD2	1:B:266:ARG:NH2	2.07	0.69
1:B:728:PHE:CZ	1:B:747:PRO:HG2	2.27	0.69
1:C:251:ARG:HA	1:C:254:VAL:HG12	1.75	0.69
1:D:143:TRP:HB3	1:D:263:LEU:CD2	2.21	0.69
1:D:350:LYS:HD3	1:D:351:TYR:H	1.57	0.69
2:F:19:ILE:HG13	2:F:426:TYR:CD2	2.28	0.69
2:F:397:PHE:CB	2:F:415:ASP:H	2.06	0.69
3:J:51:LEU:HG	3:J:57:GLN:O	1.92	0.69
1:A:316:THR:O	1:A:320:ILE:HG23	1.93	0.69
1:B:349:LYS:O	1:B:373:ALA:HB3	1.93	0.69
1:B:402:LEU:HD12	1:B:403:ARG:N	2.07	0.69
1:B:475:TRP:O	1:B:476:LEU:HD23	1.93	0.69
1:B:692:LEU:HD13	1:B:697:LEU:HD11	1.75	0.69
1:D:131:LEU:O	1:D:135:ILE:HG13	1.93	0.69
1:D:164:PHE:HE1	1:D:385:LEU:HG	1.56	0.69
2:E:31:LEU:HD22	2:E:376:TYR:CD2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:294:PHE:O	2:F:298:VAL:HG22	1.92	0.69
3:J:51:LEU:HD12	3:J:58:THR:HG22	1.74	0.69
1:B:144:PHE:C	1:B:145:LYS:HE2	2.17	0.69
2:E:19:ILE:HG21	2:E:423:VAL:HG13	1.75	0.69
2:E:168:LEU:O	2:E:168:LEU:HD13	1.93	0.69
2:E:344:GLU:CD	2:E:348:GLY:HA2	2.18	0.69
1:B:585:ASN:HA	1:B:588:LYS:CB	2.24	0.68
1:B:688:ARG:HA	1:B:710:LEU:HA	1.73	0.68
1:C:366:PRO:HD2	1:C:394:LEU:HG	1.74	0.68
1:D:399:GLU:HA	1:D:402:LEU:CD1	2.22	0.68
2:F:411:ASP:HA	2:F:439:SER:CB	2.22	0.68
1:B:100:ASP:O	1:B:101:LEU:HD23	1.93	0.68
1:B:465:ILE:HD11	1:B:491:LEU:HD21	1.74	0.68
1:B:527:LEU:HB2	1:B:555:LEU:CD2	2.19	0.68
1:C:377:HIS:O	1:C:381:GLN:HG2	1.93	0.68
2:F:58:LEU:HB3	2:F:59:PRO:HD3	1.75	0.68
2:F:392:LEU:HD13	2:F:395:TYR:CB	2.23	0.68
1:A:301:SER:CB	1:B:67:ASP:HA	2.22	0.68
1:A:352:SER:HB3	1:A:354:GLU:HG2	1.76	0.68
1:C:108:TYR:CG	1:D:55:LEU:HD11	2.28	0.68
1:C:368:VAL:HG13	1:C:372:PHE:HB3	1.74	0.68
1:D:27:PHE:O	1:D:31:ILE:HG12	1.93	0.68
3:J:38:ARG:O	3:J:46:GLU:HG2	1.93	0.68
1:A:278:ILE:HD11	1:A:325:TYR:OH	1.93	0.68
2:E:411:ASP:HA	2:E:439:SER:CB	2.22	0.68
2:F:186:TYR:HE2	2:F:188:LYS:HB3	1.58	0.68
1:B:588:LYS:HE3	1:B:612:SER:OG	1.94	0.68
1:B:692:LEU:HB3	1:B:697:LEU:CD1	2.24	0.68
1:C:357:ARG:O	1:C:361:SER:HA	1.93	0.68
3:J:12:VAL:O	3:J:123:VAL:HA	1.93	0.68
1:B:147:PRO:HA	1:B:150:SER:OG	1.94	0.68
1:B:688:ARG:HD3	1:B:711:GLN:HE22	1.58	0.68
1:D:368:VAL:HG21	1:D:376:LEU:CD1	2.23	0.68
3:J:51:LEU:HD21	3:J:56:GLY:CA	2.20	0.68
1:B:692:LEU:HB3	1:B:697:LEU:HD12	1.76	0.68
1:B:630:GLU:O	1:B:633:ILE:HG22	1.94	0.68
1:B:677:ILE:HD11	1:B:697:LEU:HD13	1.75	0.68
1:C:371:ASP:O	1:C:375:MET:HE1	1.94	0.68
1:D:356:ILE:HA	1:D:359:GLU:HG2	1.77	0.68
2:E:198:SER:O	2:E:202:LYS:HG2	1.93	0.67
2:F:344:GLU:CB	2:F:350:GLU:HB2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:O	1:B:246:LYS:HG2	1.94	0.67
1:B:723:LEU:HD21	1:B:743:LEU:HD11	1.76	0.67
1:C:150:SER:O	1:C:154:GLU:HG2	1.94	0.67
1:B:700:LEU:HB2	1:B:724:PRO:CD	2.25	0.67
1:D:150:SER:O	1:D:154:GLU:HG3	1.95	0.67
2:E:403:GLU:HA	2:E:406:PHE:CE1	2.30	0.67
2:F:19:ILE:HG13	2:F:426:TYR:CE2	2.29	0.67
2:F:139:THR:HA	2:F:349:TYR:OH	1.94	0.67
2:F:159:PRO:HB3	2:F:161:TYR:CE1	2.29	0.67
2:F:323:LEU:HD12	2:F:373:ILE:CG2	2.24	0.67
1:A:356:ILE:HA	1:A:359:GLU:HG3	1.76	0.67
1:B:343:MET:O	1:B:344:LEU:HD23	1.93	0.67
1:B:349:LYS:HD2	1:B:370:ASN:CB	2.24	0.67
1:B:413:LEU:O	1:B:417:ARG:HG3	1.94	0.67
1:B:613:LEU:HD12	1:B:616:LEU:HD11	1.75	0.67
1:C:104:HIS:CD2	1:D:106:TYR:HB3	2.29	0.67
1:C:275:PHE:O	1:C:279:ILE:HG22	1.95	0.67
1:C:342:TRP:HA	1:C:345:ARG:CZ	2.24	0.67
1:A:392:VAL:HG23	1:A:393:PHE:CD1	2.29	0.67
1:D:353:PHE:CE1	1:D:365:ILE:HG21	2.30	0.67
2:F:424:ASP:HA	2:F:427:ASP:O	1.94	0.67
1:A:346:ARG:HB2	1:A:348:LEU:CD2	2.24	0.67
1:B:356:ILE:HA	1:B:359:GLU:OE2	1.95	0.67
1:B:691:ASP:O	1:B:692:LEU:HD23	1.94	0.67
1:B:629:ILE:CG2	1:B:646:LEU:HD13	2.24	0.67
1:C:143:TRP:HA	1:C:263:LEU:HD21	1.77	0.67
2:E:396:SER:O	2:E:400:VAL:HG23	1.95	0.67
1:B:399:GLU:HA	1:B:402:LEU:CD2	2.24	0.67
1:B:588:LYS:NZ	1:B:609:SER:HA	2.09	0.67
1:C:158:SER:HA	1:C:161:LEU:HD21	1.77	0.67
2:E:42:ALA:HB2	2:E:365:LEU:CD2	2.25	0.67
2:F:52:VAL:HG22	2:F:154:TYR:HB2	1.77	0.67
2:F:450:SER:O	2:F:454:GLU:HG2	1.95	0.67
1:A:108:TYR:HA	1:B:53:ILE:HG21	1.77	0.67
1:B:688:ARG:HB3	1:B:711:GLN:CD	2.20	0.67
1:B:769:LEU:HD21	1:B:790:LEU:HB3	1.76	0.67
1:C:244:PHE:O	1:C:248:LYS:HG3	1.94	0.67
1:D:234:LYS:O	1:D:238:GLU:HG2	1.95	0.67
2:E:21:LYS:HB2	2:E:25:ASP:OD2	1.95	0.67
2:F:180:SER:HA	2:F:315:LYS:HZ1	1.59	0.67
1:B:473:GLU:CG	1:B:497:ALA:HB3	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:83:MET:HE2	3:J:86:LEU:CD2	2.24	0.66
1:A:129:VAL:HG13	1:A:325:TYR:CE1	2.29	0.66
1:B:166:SER:O	1:B:170:THR:HG23	1.94	0.66
1:B:420:LEU:CD2	1:B:430:LEU:HB2	2.26	0.66
1:D:343:MET:HG3	1:D:348:LEU:HD22	1.77	0.66
2:F:15:PRO:HD2	2:F:17:TYR:CE2	2.30	0.66
1:A:354:GLU:O	1:A:357:ARG:HG2	1.94	0.66
1:A:365:ILE:HD11	1:A:395:SER:HB3	1.77	0.66
1:B:590:MET:O	1:B:613:LEU:HD22	1.95	0.66
1:B:685:ARG:HD3	1:B:707:LEU:HD23	1.77	0.66
1:B:693:SER:HA	1:B:718:ASN:ND2	2.10	0.66
1:B:717:ALA:H	1:B:740:ASN:HB2	1.60	0.66
1:C:349:LYS:O	1:C:370:ASN:HA	1.96	0.66
2:E:433:ARG:NH2	2:E:434:PHE:HB2	2.10	0.66
2:F:155:HIS:O	2:F:156:LEU:HD23	1.96	0.66
2:F:203:CYS:SG	2:F:434:PHE:HA	2.35	0.66
1:B:234:LYS:HE3	1:B:409:ASN:CB	2.22	0.66
1:B:474:LEU:HD12	1:B:475:TRP:H	1.59	0.66
1:B:633:ILE:HB	1:B:657:GLN:HG2	1.78	0.66
1:B:755:ASN:HA	1:B:778:LEU:CD1	2.23	0.66
2:E:411:ASP:HA	2:E:439:SER:OG	1.95	0.66
1:A:291:PHE:HA	1:A:315:ALA:CB	2.25	0.66
1:A:349:LYS:HD2	1:A:370:ASN:HB3	1.78	0.66
1:B:234:LYS:HG3	1:B:409:ASN:HB3	1.78	0.66
1:A:170:THR:HA	1:A:173:LEU:HD21	1.77	0.66
1:A:267:GLN:HE21	1:A:271:LYS:HZ1	1.44	0.66
1:B:416:LEU:O	1:B:419:ARG:HB2	1.94	0.66
1:C:34:VAL:HG12	1:C:328:LEU:HD11	1.77	0.66
1:C:116:ASN:HB3	1:C:117:ARG:NH1	2.10	0.66
1:C:158:SER:O	1:C:162:LYS:HG3	1.96	0.66
1:D:254:VAL:HB	1:D:372:PHE:HD2	1.59	0.66
2:E:285:LYS:HD3	2:E:446:LEU:HD22	1.78	0.66
1:B:578:GLY:N	1:B:600:ARG:HG2	2.11	0.66
1:B:744:GLN:O	1:B:766:LEU:HA	1.96	0.66
1:C:34:VAL:CG1	1:C:328:LEU:HD11	2.26	0.66
3:J:83:MET:CB	3:J:86:LEU:HD21	2.25	0.66
1:B:38:ILE:HD11	1:B:324:PHE:HD2	1.60	0.66
1:B:769:LEU:HB3	1:B:773:LEU:CD1	2.26	0.66
1:C:239:GLN:O	1:C:243:LEU:HD13	1.95	0.66
2:F:277:ASP:HB2	2:F:453:HIS:NE2	2.11	0.66
3:J:7:SER:HB3	3:J:21:SER:OG	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LYS:HA	1:B:249:LYS:HG2	1.78	0.66
1:B:698:THR:O	1:B:720:ILE:HA	1.95	0.66
1:B:760:GLU:O	1:B:761:LEU:HD23	1.96	0.66
1:C:164:PHE:HA	1:C:389:ARG:NH1	2.09	0.66
1:D:112:VAL:O	1:D:116:ASN:HB2	1.95	0.66
3:J:22:CYS:HB2	3:J:36:TRP:CH2	2.31	0.66
1:B:168:TRP:CZ3	1:B:398:SER:HB3	2.31	0.66
1:B:513:TYR:HA	1:B:543:LEU:HD21	1.78	0.66
1:C:275:PHE:CE1	1:C:333:GLY:HA3	2.31	0.66
1:A:368:VAL:HG13	1:A:372:PHE:HB3	1.77	0.65
1:C:38:ILE:HD11	1:C:325:TYR:HD1	1.60	0.65
2:E:402:GLU:HG3	2:E:406:PHE:CE2	2.30	0.65
2:F:144:GLN:O	2:F:147:VAL:HG22	1.95	0.65
1:A:106:TYR:HB3	2:F:144:GLN:NE2	2.10	0.65
1:B:169:THR:O	1:B:173:LEU:HD23	1.96	0.65
1:B:679:THR:HA	1:B:682:PHE:CD2	2.31	0.65
1:C:61:THR:HG23	1:C:66:ASN:HB2	1.76	0.65
2:E:422:MET:HA	2:E:422:MET:CE	2.26	0.65
2:F:58:LEU:HD12	2:F:137:ARG:HH22	1.61	0.65
2:F:323:LEU:O	2:F:323:LEU:HD23	1.96	0.65
1:B:116:ASN:HB3	1:B:117:ARG:CZ	2.25	0.65
1:B:300:GLU:O	1:B:304:GLY:HA2	1.96	0.65
1:B:479:THR:HG22	1:B:480:ALA:O	1.96	0.65
2:E:204:PHE:HA	2:E:433:ARG:NE	2.12	0.65
2:F:208:TRP:CZ2	2:F:446:LEU:HB2	2.32	0.65
1:A:368:VAL:CG1	1:A:372:PHE:HB3	2.26	0.65
1:B:771:VAL:HG12	1:B:795:PRO:CD	2.26	0.65
1:C:117:ARG:HB2	1:C:295:CYS:HB3	1.77	0.65
1:C:153:LEU:HD21	1:C:260:VAL:CG2	2.25	0.65
1:D:159:ILE:HG23	1:D:247:VAL:HG22	1.79	0.65
1:D:354:GLU:HG2	1:D:357:ARG:NH1	2.12	0.65
1:D:372:PHE:O	1:D:375:MET:HG3	1.96	0.65
2:F:53:VAL:HG22	2:F:355:THR:CG2	2.26	0.65
1:A:173:LEU:HD12	1:A:174:SER:N	2.11	0.65
1:B:147:PRO:CG	1:C:23:TRP:HB3	2.26	0.65
1:B:573:SER:HA	1:B:597:GLU:HB2	1.79	0.65
1:B:645:LYS:HD3	1:B:647:TRP:CZ2	2.32	0.65
1:A:396:GLU:OE2	1:A:397:VAL:HG23	1.97	0.65
1:B:233:ASP:OD1	1:B:235:LYS:HG2	1.96	0.65
1:B:495:LEU:HD11	1:B:497:ALA:O	1.97	0.65
2:F:312:THR:HG21	2:F:384:LEU:HG	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:68:PHE:CD1	3:J:83:MET:HA	2.32	0.65
3:J:108:TYR:HB3	3:J:110:GLU:OE2	1.97	0.65
1:A:116:ASN:HB3	1:A:117:ARG:NH1	2.12	0.65
3:J:12:VAL:HG21	3:J:86:LEU:CD1	2.26	0.65
3:J:33:TYR:O	3:J:34:LEU:HD23	1.96	0.65
1:B:456:ILE:O	1:B:479:THR:HG23	1.96	0.65
1:C:167:PRO:O	1:C:171:ARG:HG3	1.97	0.65
1:D:254:VAL:HB	1:D:372:PHE:CD2	2.32	0.65
2:F:279:LYS:HA	2:F:282:GLU:OE2	1.97	0.65
2:F:393:LYS:HA	2:F:421:HIS:NE2	2.12	0.65
3:J:39:GLN:HB2	3:J:45:ARG:CA	2.24	0.65
1:B:726:GLU:HA	1:B:729:GLN:CD	2.22	0.65
1:C:243:LEU:O	1:C:247:VAL:HG23	1.96	0.65
1:C:354:GLU:HA	1:C:357:ARG:NH1	2.08	0.65
2:E:55:LEU:O	2:E:352:PHE:HB3	1.97	0.65
1:B:703:ASP:HB3	1:B:706:LEU:HD12	1.79	0.65
1:D:173:LEU:HD22	1:D:392:VAL:HG11	1.79	0.65
2:E:208:TRP:CD2	2:E:446:LEU:HD12	2.31	0.65
2:E:397:PHE:CB	2:E:415:ASP:H	2.10	0.65
2:F:186:TYR:CE2	2:F:188:LYS:HB3	2.31	0.65
2:F:284:ALA:HB3	2:F:446:LEU:HD11	1.78	0.65
1:A:19:ILE:HA	1:A:382:TYR:CD1	2.33	0.64
1:B:478:HIS:HA	1:B:507:GLU:OE1	1.97	0.64
1:B:608:HIS:CD2	1:B:631:GLU:HG2	2.32	0.64
1:B:623:ASP:OD1	1:B:648:TYR:HB3	1.97	0.64
1:C:372:PHE:HA	1:C:375:MET:CE	2.27	0.64
2:F:345:HIS:C	2:F:346:LEU:HD12	2.22	0.64
1:A:301:SER:HB3	1:B:67:ASP:HA	1.79	0.64
1:B:688:ARG:HD3	1:B:711:GLN:NE2	2.12	0.64
1:B:692:LEU:HD13	1:B:697:LEU:CD1	2.27	0.64
3:J:28:ILE:HD12	3:J:77:ASN:C	2.23	0.64
1:B:164:PHE:CE1	1:B:385:LEU:HG	2.32	0.64
1:B:412:THR:O	1:B:416:LEU:HG	1.96	0.64
1:C:31:ILE:HG22	1:C:35:MET:CE	2.21	0.64
2:E:285:LYS:HA	2:E:288:PHE:HD2	1.62	0.64
3:J:31:ILE:HG21	3:J:98:ALA:HB1	1.79	0.64
1:B:249:LYS:HZ3	1:B:250:PHE:N	1.94	0.64
1:B:501:LYS:HA	1:B:524:THR:HB	1.80	0.64
1:C:161:LEU:HD12	1:C:162:LYS:N	2.13	0.64
1:C:316:THR:O	1:C:320:ILE:HG23	1.98	0.64
2:E:18:ARG:HD3	2:E:21:LYS:NZ	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:THR:HB	1:B:617:GLN:OE1	1.97	0.64
2:F:322:ILE:HD12	2:F:323:LEU:N	2.13	0.64
1:C:156:PHE:HA	1:C:159:ILE:CD1	2.27	0.64
1:B:293:VAL:CG1	1:B:310:CYS:HB2	2.24	0.64
1:B:452:LYS:HG3	1:B:475:TRP:CB	2.27	0.64
1:B:710:LEU:HG	1:B:733:LEU:CD2	2.27	0.64
1:B:780:LYS:HD2	1:B:805:ALA:C	2.22	0.64
2:E:287:LEU:O	2:E:287:LEU:HD23	1.97	0.64
2:F:277:ASP:HB2	2:F:453:HIS:CE1	2.32	0.64
1:B:679:THR:HA	1:B:682:PHE:CE2	2.32	0.64
1:D:22:PRO:HD2	1:D:25:ASP:CG	2.22	0.64
1:D:157:VAL:O	1:D:161:LEU:HG	1.98	0.64
2:E:54:CYS:SG	2:E:150:ASN:HA	2.38	0.64
1:B:171:ARG:HH11	1:B:232:LEU:HD13	1.63	0.64
1:B:399:GLU:HA	1:B:402:LEU:HD21	1.79	0.64
1:B:420:LEU:HD23	1:B:430:LEU:HD13	1.78	0.64
1:B:736:LEU:CD1	1:B:738:LEU:HD21	2.28	0.64
1:B:671:ARG:HD3	1:B:694:HIS:HB3	1.80	0.64
3:J:91:THR:CG2	3:J:122:THR:HA	2.25	0.64
1:B:39:ALA:CB	1:B:129:VAL:HG13	2.28	0.63
1:B:488:LEU:HD11	1:B:514:SER:OG	1.97	0.63
1:B:755:ASN:CA	1:B:778:LEU:HD12	2.25	0.63
1:D:354:GLU:HA	1:D:357:ARG:CD	2.28	0.63
1:B:164:PHE:HD1	1:B:386:TYR:HA	1.63	0.63
1:B:473:GLU:HA	1:B:497:ALA:O	1.97	0.63
1:C:350:LYS:HD3	1:C:350:LYS:H	1.64	0.63
1:D:232:LEU:HD23	1:D:405:LEU:HD13	1.80	0.63
2:E:29:ASP:O	2:E:33:VAL:HG23	1.98	0.63
2:E:447:ARG:O	2:E:451:LEU:HG	1.98	0.63
1:B:717:ALA:CA	1:B:740:ASN:HB2	2.28	0.63
1:B:725:PRO:HA	1:B:728:PHE:CD2	2.33	0.63
1:B:770:PRO:HB2	1:B:772:GLU:OE1	1.98	0.63
1:C:368:VAL:CG1	1:C:372:PHE:HB3	2.27	0.63
1:D:124:TYR:O	1:D:128:LEU:HG	1.98	0.63
1:D:149:THR:CB	1:D:260:VAL:HG22	2.26	0.63
2:E:399:LYS:HZ1	2:E:420:LEU:HB3	1.62	0.63
2:F:289:GLU:O	2:F:292:ARG:HD2	1.97	0.63
2:F:366:LEU:HD12	2:F:366:LEU:O	1.97	0.63
1:A:34:VAL:CG1	1:A:328:LEU:HD11	2.28	0.63
1:A:164:PHE:HA	1:A:389:ARG:NH1	2.09	0.63
1:B:746:LEU:CD2	1:B:773:LEU:HD21	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:9:GLY:CA	3:J:121:VAL:HG22	2.28	0.63
1:B:781:ARG:O	1:B:781:ARG:HD3	1.98	0.63
1:B:583:VAL:HG21	1:B:607:PRO:CB	2.29	0.63
1:A:297:VAL:CG2	1:A:299:ILE:HG12	2.29	0.63
1:B:723:LEU:HD11	1:B:738:LEU:HD13	1.81	0.63
1:B:769:LEU:HB2	1:B:794:LEU:HD21	1.80	0.63
1:A:164:PHE:CA	1:A:389:ARG:HH12	2.08	0.63
1:A:257:GLY:HA3	1:A:371:ASP:OD2	1.99	0.63
1:A:401:LYS:HG3	1:A:402:LEU:HD12	1.79	0.63
1:B:519:GLU:O	1:B:546:LEU:HD12	1.98	0.63
1:B:539:GLY:O	1:B:542:GLU:HG2	1.99	0.63
1:B:676:LYS:HE2	1:B:676:LYS:HA	1.81	0.63
1:B:784:LEU:HD23	1:B:791:PHE:CD1	2.34	0.63
1:D:262:ARG:O	1:D:266:ARG:HG3	1.98	0.63
2:F:344:GLU:HB3	2:F:350:GLU:HB2	1.81	0.63
3:J:61:ALA:O	3:J:65:LYS:HG3	1.99	0.63
1:B:126:PRO:HD3	1:B:318:PHE:CE2	2.27	0.63
1:B:769:LEU:HB2	1:B:794:LEU:CD2	2.29	0.63
1:D:109:VAL:HG11	1:D:308:TYR:CE2	2.34	0.63
1:D:36:LEU:O	1:D:40:VAL:HG12	1.99	0.62
1:D:159:ILE:CG2	1:D:247:VAL:HG22	2.29	0.62
1:D:171:ARG:NH1	1:D:232:LEU:HB3	2.14	0.62
2:E:291:VAL:O	2:E:295:ARG:HB3	1.99	0.62
2:F:201:GLY:O	2:F:205:GLU:HG3	1.99	0.62
3:J:31:ILE:HG12	3:J:100:TYR:CE1	2.34	0.62
1:A:155:HIS:O	1:A:159:ILE:HG12	1.99	0.62
1:B:246:LYS:O	1:B:249:LYS:HG3	1.99	0.62
1:B:264:TYR:HD1	1:B:343:MET:HE1	1.63	0.62
1:B:407:LEU:HD12	1:B:408:ASN:N	2.15	0.62
1:B:422:LYS:HA	1:B:427:LYS:O	1.99	0.62
1:B:620:ASP:O	1:B:621:LEU:HD23	1.97	0.62
1:D:101:LEU:HD12	1:D:106:TYR:CE1	2.34	0.62
2:F:430:TYR:HA	2:F:433:ARG:NH2	2.14	0.62
1:A:19:ILE:HD11	1:A:379:ILE:HD12	1.80	0.62
1:B:151:SER:HA	1:B:154:GLU:OE2	1.99	0.62
1:B:451:LEU:HD12	1:B:452:LYS:N	2.13	0.62
1:B:452:LYS:HG3	1:B:475:TRP:HB2	1.80	0.62
1:B:615:ASN:HA	1:B:640:ARG:HD3	1.80	0.62
1:B:666:ARG:HA	1:B:689:TYR:O	1.99	0.62
1:C:17:TYR:HB3	1:C:144:PHE:CE2	2.34	0.62
1:A:46:GLN:HG2	1:A:50:ASP:OD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:PHE:CZ	1:B:378:LEU:HD11	2.35	0.62
1:B:654:ILE:HD11	1:B:669:LEU:HD12	1.80	0.62
2:E:396:SER:HA	2:E:399:LYS:HG2	1.81	0.62
2:F:19:ILE:HD12	2:F:19:ILE:N	2.15	0.62
2:F:444:ASN:HA	2:F:447:ARG:HE	1.62	0.62
1:B:416:LEU:HD11	1:B:441:THR:OG1	1.99	0.62
1:B:717:ALA:N	1:B:740:ASN:HB2	2.14	0.62
1:C:302:LEU:HD21	1:D:65:CYS:SG	2.39	0.62
1:A:356:ILE:HA	1:A:359:GLU:CG	2.29	0.62
1:B:27:PHE:O	1:B:31:ILE:HG12	1.99	0.62
1:B:393:PHE:C	1:B:394:LEU:HD22	2.24	0.62
1:B:459:VAL:O	1:B:482:LYS:HB2	1.99	0.62
1:C:155:HIS:O	1:C:159:ILE:HG12	2.00	0.62
3:J:28:ILE:HB	3:J:77:ASN:HA	1.81	0.62
1:A:106:TYR:CD2	2:F:144:GLN:HB2	2.35	0.62
1:B:59:TRP:O	1:B:65:CYS:HA	1.99	0.62
1:B:401:LYS:O	1:B:405:LEU:HD23	1.99	0.62
1:B:688:ARG:O	1:B:710:LEU:HD12	1.99	0.62
1:B:693:SER:HA	1:B:718:ASN:HD21	1.65	0.62
2:F:412:VAL:CG2	2:F:438:LEU:HG	2.29	0.62
3:J:31:ILE:O	3:J:53:THR:HG21	2.00	0.62
1:A:265:MET:O	1:A:269:ILE:HD13	1.99	0.62
1:B:411:TRP:HB3	1:B:416:LEU:HD21	1.79	0.62
1:B:641:LEU:O	1:B:664:LEU:HD23	2.00	0.62
1:B:667:LEU:O	1:B:690:LEU:HD12	2.00	0.62
2:E:364:LYS:O	2:E:367:ILE:HG12	1.99	0.62
1:A:16:ALA:O	1:A:19:ILE:HG22	1.98	0.62
1:B:795:PRO:HG2	1:B:798:VAL:HG23	1.81	0.62
1:D:145:LYS:HE2	1:D:145:LYS:HA	1.82	0.62
2:F:172:HIS:CE1	2:F:322:ILE:HG21	2.35	0.62
1:B:682:PHE:O	1:B:707:LEU:HD21	1.99	0.62
1:C:24:TRP:O	1:C:28:THR:HG23	2.00	0.62
1:D:144:PHE:C	1:D:145:LYS:HE2	2.25	0.62
1:D:168:TRP:CZ3	1:D:398:SER:HB3	2.34	0.62
1:D:235:LYS:HA	1:D:238:GLU:OE2	2.00	0.62
1:A:112:VAL:CG1	1:A:297:VAL:HG11	2.30	0.61
1:B:718:ASN:O	1:B:741:ASN:HA	1.99	0.61
1:C:301:SER:HB3	1:D:67:ASP:HA	1.82	0.61
2:E:304:ILE:HG21	2:E:419:LEU:HG	1.80	0.61
3:J:105:SER:HB3	3:J:111:GLU:HG3	1.82	0.61
1:C:353:PHE:HA	1:C:356:ILE:HD13	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:VAL:HG21	1:D:376:LEU:HD12	1.80	0.61
2:F:287:LEU:O	2:F:291:VAL:HG23	2.00	0.61
1:B:354:GLU:HA	1:B:357:ARG:CD	2.29	0.61
1:B:439:PRO:HB2	1:B:442:VAL:HG23	1.82	0.61
1:C:398:SER:HA	1:C:401:LYS:CE	2.28	0.61
1:B:449:GLU:O	1:B:471:LEU:HA	2.00	0.61
2:F:204:PHE:HA	2:F:433:ARG:NE	2.15	0.61
1:B:576:ASN:CB	1:B:579:THR:HB	2.30	0.61
1:B:622:LYS:HB2	1:B:647:TRP:CD1	2.36	0.61
1:B:700:LEU:HB2	1:B:724:PRO:CG	2.30	0.61
1:B:713:LEU:HD11	1:B:715:VAL:HG12	1.83	0.61
1:C:289:ILE:HG22	1:C:319:LYS:CE	2.30	0.61
1:C:348:LEU:HD22	1:C:377:HIS:CG	2.35	0.61
1:D:255:GLU:CD	1:D:369:LYS:HB3	2.25	0.61
1:D:342:TRP:O	1:D:348:LEU:HD11	1.99	0.61
2:E:31:LEU:CD2	2:E:376:TYR:HB2	2.30	0.61
3:J:93:LEU:HD23	3:J:95:TYR:OH	2.00	0.61
1:A:341:TRP:O	1:A:345:ARG:HG2	2.00	0.61
1:B:38:ILE:HD11	1:B:324:PHE:CD2	2.35	0.61
1:B:587:LEU:HD11	1:B:613:LEU:HD11	1.82	0.61
1:B:736:LEU:CD2	1:B:738:LEU:HD11	2.30	0.61
1:B:771:VAL:HG12	1:B:795:PRO:HD3	1.81	0.61
1:C:146:PHE:CE2	1:C:148:ARG:HB3	2.35	0.61
1:C:272:VAL:HG22	1:C:336:CYS:HB3	1.80	0.61
1:D:58:LYS:HG2	1:D:99:TYR:HE1	1.65	0.61
2:F:298:VAL:O	2:F:299:GLU:HG2	2.01	0.61
1:C:355:SER:HA	1:C:358:GLU:OE2	2.01	0.61
2:E:161:TYR:HE2	2:E:332:ALA:O	1.84	0.61
2:E:424:ASP:HA	2:E:427:ASP:O	2.01	0.61
3:J:97:ALA:HB1	3:J:112:TYR:HB3	1.83	0.61
1:A:154:GLU:HA	1:A:157:VAL:HG12	1.83	0.61
1:A:250:PHE:O	1:A:254:VAL:HG22	2.01	0.61
1:B:131:LEU:C	1:B:131:LEU:HD23	2.26	0.61
1:B:164:PHE:CD1	1:B:386:TYR:HA	2.35	0.61
2:E:19:ILE:HA	2:E:426:TYR:CD2	2.36	0.61
2:E:142:ASP:H	2:E:145:GLN:NE2	1.98	0.61
1:A:300:GLU:HA	1:A:304:GLY:HA2	1.83	0.61
1:B:474:LEU:HD21	1:B:476:LEU:HD21	1.81	0.61
1:B:588:LYS:HZ2	1:B:609:SER:HA	1.65	0.61
1:B:717:ALA:HA	1:B:740:ASN:CB	2.31	0.61
1:D:306:ARG:HA	1:D:306:ARG:NH1	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:208:TRP:HB2	2:E:280:ASP:OD2	2.00	0.61
2:F:287:LEU:HD22	2:F:437:PHE:CE1	2.36	0.61
1:B:232:LEU:HD11	1:B:236:GLU:HB3	1.82	0.61
1:B:724:PRO:O	1:B:727:LEU:HB3	2.01	0.61
1:C:164:PHE:CE1	1:C:389:ARG:HD3	2.36	0.61
1:D:362:TYR:O	1:D:365:ILE:HG13	2.01	0.61
1:A:156:PHE:CD1	1:A:375:MET:HG2	2.35	0.60
1:C:169:THR:HG22	1:C:392:VAL:CG2	2.30	0.60
1:C:301:SER:CB	1:D:67:ASP:HA	2.31	0.60
1:D:261:TYR:CE1	1:D:349:LYS:HE3	2.36	0.60
1:D:353:PHE:O	1:D:357:ARG:HG2	2.00	0.60
1:A:234:LYS:O	1:A:238:GLU:HG3	2.00	0.60
1:A:401:LYS:HG3	1:A:402:LEU:CD1	2.32	0.60
1:B:429:GLU:HA	1:B:448:LEU:CD1	2.31	0.60
1:B:478:HIS:HA	1:B:507:GLU:CD	2.26	0.60
1:B:667:LEU:O	1:B:690:LEU:HA	2.02	0.60
1:B:737:HIS:O	1:B:738:LEU:HD23	2.00	0.60
1:D:156:PHE:HB2	1:D:250:PHE:CZ	2.36	0.60
3:J:67:ARG:HB3	3:J:84:ASN:O	2.01	0.60
1:B:258:ASP:HB2	1:B:370:ASN:OD1	2.00	0.60
1:B:498:LEU:HD12	1:B:499:HIS:N	2.15	0.60
1:D:22:PRO:HG2	1:D:24:TRP:CZ2	2.37	0.60
1:D:156:PHE:HE2	1:D:379:ILE:HD11	1.65	0.60
1:D:232:LEU:HG	1:D:405:LEU:CD2	2.29	0.60
1:D:366:PRO:HD2	1:D:394:LEU:O	2.01	0.60
2:E:31:LEU:HD23	2:E:35:MET:HE3	1.82	0.60
1:B:744:GLN:C	1:B:766:LEU:HD23	2.26	0.60
2:F:172:HIS:CD2	2:F:322:ILE:HG21	2.37	0.60
1:A:355:SER:O	1:A:359:GLU:HG3	2.01	0.60
1:B:235:LYS:O	1:B:238:GLU:HG2	2.01	0.60
1:B:240:ALA:O	1:B:244:PHE:HD1	1.84	0.60
1:B:629:ILE:O	1:B:632:ILE:HG23	2.01	0.60
2:E:397:PHE:CB	2:E:414:ASN:HA	2.31	0.60
3:J:12:VAL:HG21	3:J:86:LEU:HD12	1.84	0.60
1:B:580:LYS:HA	1:B:601:CYS:O	2.02	0.60
1:B:589:LYS:O	1:B:589:LYS:HD3	2.02	0.60
1:B:679:THR:HB	1:B:703:ASP:OD2	2.02	0.60
1:D:46:GLN:OE1	1:D:123:LYS:HA	2.02	0.60
1:D:46:GLN:HB2	1:D:318:PHE:HZ	1.65	0.60
1:D:233:ASP:OD2	1:D:235:LYS:HB3	2.02	0.60
1:D:351:TYR:HB2	1:D:373:ALA:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:CYS:O	1:C:55:LEU:HD23	2.02	0.60
1:C:234:LYS:HA	1:C:406:ASN:OD1	2.01	0.60
1:D:372:PHE:HA	1:D:375:MET:CG	2.32	0.60
2:E:323:LEU:O	2:E:323:LEU:HD23	2.00	0.60
2:E:396:SER:CA	2:E:399:LYS:HE2	2.31	0.60
1:A:342:TRP:HA	1:A:345:ARG:HE	1.65	0.60
1:B:269:ILE:O	1:B:273:ILE:HG12	2.02	0.60
1:B:443:PHE:C	1:B:468:LEU:HD21	2.27	0.60
1:B:748:SER:O	1:B:772:GLU:HG2	2.01	0.60
1:D:125:PHE:O	1:D:129:VAL:HG12	2.02	0.60
2:E:19:ILE:CG2	2:E:423:VAL:HG13	2.31	0.60
2:F:208:TRP:CE2	2:F:446:LEU:HB2	2.36	0.60
2:F:213:LEU:HD21	2:F:436:VAL:HG21	1.83	0.60
1:B:392:VAL:HG23	1:B:393:PHE:CD1	2.37	0.60
1:B:546:LEU:HD11	1:B:548:VAL:O	2.02	0.60
1:B:633:ILE:O	1:B:636:GLN:HG2	2.02	0.60
3:J:51:LEU:HA	3:J:57:GLN:O	2.02	0.60
1:B:410:GLU:O	1:B:415:LYS:HD2	2.02	0.59
1:B:721:GLU:HG2	1:B:742:VAL:CG2	2.32	0.59
1:C:129:VAL:HG22	1:C:325:TYR:CE2	2.37	0.59
1:D:145:LYS:HE2	1:D:145:LYS:CA	2.32	0.59
2:E:58:LEU:HD23	2:E:59:PRO:N	2.16	0.59
2:E:409:ILE:HG23	2:E:441:VAL:HG13	1.83	0.59
2:F:162:SER:OG	2:F:333:ILE:HG12	2.01	0.59
2:F:419:LEU:HD13	2:F:419:LEU:O	2.02	0.59
1:A:346:ARG:HB2	1:A:348:LEU:HD21	1.82	0.59
1:B:670:ASN:HA	1:B:693:SER:O	2.02	0.59
1:C:102:ASP:H	1:C:105:GLN:NE2	1.99	0.59
1:C:147:PRO:CG	1:D:23:TRP:HB3	2.32	0.59
2:F:57:VAL:CG2	2:F:351:VAL:HG13	2.31	0.59
3:J:12:VAL:HG11	3:J:18:LEU:HD21	1.83	0.59
1:B:124:TYR:O	1:B:128:LEU:HG	2.03	0.59
1:B:408:ASN:OD1	1:B:439:PRO:HA	2.02	0.59
1:B:489:ALA:O	1:B:493:GLU:HG2	2.02	0.59
1:B:583:VAL:HG21	1:B:607:PRO:HB3	1.84	0.59
1:D:277:LEU:HD12	1:D:278:ILE:N	2.17	0.59
2:E:32:ALA:O	2:E:35:MET:HG2	2.03	0.59
1:C:171:ARG:HD2	1:C:232:LEU:HD12	1.84	0.59
1:C:258:ASP:OD1	1:C:370:ASN:HB2	2.02	0.59
1:D:235:LYS:HZ3	1:D:239:GLN:HB2	1.67	0.59
2:E:403:GLU:OE2	2:E:432:LYS:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:LEU:HD23	1:B:543:LEU:HD13	1.84	0.59
2:F:288:PHE:CE2	2:F:446:LEU:HD13	2.31	0.59
2:F:399:LYS:CE	2:F:421:HIS:HB3	2.33	0.59
2:F:409:ILE:CG2	2:F:441:VAL:HG13	2.32	0.59
2:F:433:ARG:HH12	2:F:434:PHE:HB2	1.65	0.59
1:B:456:ILE:O	1:B:459:VAL:HG23	2.02	0.59
1:B:633:ILE:HD12	1:B:657:GLN:HG2	1.82	0.59
1:B:703:ASP:HB3	1:B:706:LEU:CD1	2.32	0.59
1:C:385:LEU:O	1:C:389:ARG:HG3	2.02	0.59
1:D:240:ALA:O	1:D:244:PHE:HD1	1.86	0.59
2:E:285:LYS:HA	2:E:288:PHE:CD2	2.37	0.59
1:A:260:VAL:HG22	1:A:371:ASP:OD1	2.03	0.59
1:C:160:LEU:HA	1:C:390:PHE:CE1	2.38	0.59
1:D:121:PHE:HD2	1:D:285:TYR:HB3	1.67	0.59
1:D:343:MET:O	1:D:348:LEU:HD13	2.03	0.59
2:F:54:CYS:SG	2:F:150:ASN:HA	2.43	0.59
2:F:142:ASP:H	2:F:145:GLN:NE2	2.00	0.59
2:F:211:LYS:HA	2:F:214:SER:OG	2.01	0.59
1:B:431:HIS:C	1:B:432:LEU:HD23	2.27	0.59
1:B:726:GLU:HA	1:B:729:GLN:HG3	1.85	0.59
1:C:169:THR:O	1:C:173:LEU:HD23	2.02	0.59
2:E:396:SER:CB	2:E:399:LYS:HE2	2.33	0.59
3:J:33:TYR:HB2	3:J:99:ALA:HB3	1.83	0.59
1:B:713:LEU:HD11	1:B:715:VAL:CG1	2.33	0.59
1:C:158:SER:O	1:C:161:LEU:HG	2.02	0.59
1:D:117:ARG:HA	1:D:117:ARG:NE	2.18	0.59
1:A:40:VAL:O	1:A:44:THR:HG22	2.03	0.59
1:B:685:ARG:HA	1:B:707:LEU:HD23	1.83	0.59
1:B:725:PRO:HB2	1:B:749:ARG:NH1	2.18	0.59
1:B:790:LEU:HA	1:B:793:THR:HG23	1.84	0.59
1:D:333:GLY:O	1:D:337:MET:HG3	2.03	0.59
2:E:204:PHE:HA	2:E:433:ARG:HD2	1.84	0.59
2:E:204:PHE:HE1	2:E:429:LEU:HG	1.67	0.59
2:E:385:PHE:HD1	2:E:386:TRP:HD1	1.51	0.59
3:J:38:ARG:HB3	3:J:94:TYR:CE2	2.38	0.59
1:A:115:GLU:HG2	1:B:291:PHE:CG	2.37	0.58
1:D:168:TRP:HA	1:D:171:ARG:HG2	1.84	0.58
2:E:322:ILE:HD12	2:E:323:LEU:N	2.18	0.58
1:B:358:GLU:HG3	1:B:359:GLU:N	2.17	0.58
1:B:472:LYS:O	1:B:495:LEU:HD12	2.02	0.58
1:B:715:VAL:HG22	1:B:738:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ASP:O	1:C:101:LEU:HD23	2.03	0.58
1:D:34:VAL:O	1:D:38:ILE:HG12	2.03	0.58
2:E:289:GLU:HA	2:E:292:ARG:CD	2.33	0.58
1:A:101:LEU:HD12	1:A:106:TYR:CE1	2.38	0.58
1:B:63:ASP:HA	1:B:307:THR:CG2	2.28	0.58
1:B:617:GLN:HA	1:B:640:ARG:O	2.03	0.58
1:B:746:LEU:HB3	1:B:770:PRO:CD	2.31	0.58
1:C:129:VAL:HG13	1:C:325:TYR:CE1	2.38	0.58
1:B:349:LYS:HD2	1:B:370:ASN:HB2	1.85	0.58
1:B:404:GLN:NE2	1:B:407:LEU:HD11	2.17	0.58
1:B:713:LEU:HD12	1:B:714:ALA:N	2.18	0.58
1:C:171:ARG:NH2	1:C:405:LEU:HD21	2.19	0.58
1:D:270:ILE:O	1:D:274:LYS:HG2	2.03	0.58
1:A:155:HIS:CE1	1:A:159:ILE:HD13	2.38	0.58
1:B:39:ALA:HB2	1:B:129:VAL:HG13	1.84	0.58
1:B:279:ILE:HD11	1:B:329:VAL:HG12	1.85	0.58
1:B:513:TYR:CE1	1:B:540:LEU:HD23	2.39	0.58
1:D:345:ARG:C	1:D:346:ARG:HD3	2.29	0.58
2:F:161:TYR:CD2	2:F:329:PHE:HB3	2.38	0.58
2:F:170:LEU:C	2:F:170:LEU:HD23	2.29	0.58
1:B:451:LEU:HD12	1:B:452:LYS:H	1.68	0.58
1:B:452:LYS:C	1:B:453:LEU:HD23	2.28	0.58
1:B:517:THR:HA	1:B:545:ARG:CD	2.14	0.58
1:B:685:ARG:HD3	1:B:707:LEU:CD2	2.32	0.58
1:D:29:ASP:O	1:D:33:ILE:HG12	2.04	0.58
1:D:104:HIS:HB2	2:E:146:TYR:CD2	2.38	0.58
1:D:342:TRP:HZ3	1:D:343:MET:HE2	1.68	0.58
1:D:372:PHE:C	1:D:375:MET:HG3	2.29	0.58
2:E:330:VAL:HG23	2:E:366:LEU:HD23	1.85	0.58
1:B:416:LEU:HD13	1:B:442:VAL:HA	1.86	0.58
1:C:366:PRO:CG	1:C:394:LEU:HD21	2.29	0.58
1:D:119:HIS:CD2	1:D:288:ASN:HB3	2.38	0.58
1:D:160:LEU:HD11	1:D:386:TYR:HB3	1.85	0.58
2:E:19:ILE:HD12	2:E:19:ILE:N	2.19	0.58
2:E:204:PHE:HA	2:E:433:ARG:CZ	2.34	0.58
2:E:279:LYS:HA	2:E:282:GLU:OE2	2.03	0.58
2:F:287:LEU:HB3	2:F:437:PHE:CZ	2.39	0.58
1:A:168:TRP:CZ2	1:A:402:LEU:HB2	2.38	0.58
1:B:670:ASN:HB3	1:B:691:ASP:OD1	2.03	0.58
1:B:721:GLU:HA	1:B:742:VAL:HG23	1.86	0.58
1:D:250:PHE:CZ	1:D:254:VAL:HG21	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:VAL:CG2	1:B:307:THR:HG21	2.33	0.58
1:B:416:LEU:CB	1:B:445:LEU:HD11	2.34	0.58
1:B:725:PRO:HA	1:B:728:PHE:CE2	2.39	0.58
1:C:149:THR:HG21	1:C:263:LEU:HD22	1.84	0.58
1:C:158:SER:HA	1:C:161:LEU:CD2	2.34	0.58
1:C:372:PHE:HA	1:C:375:MET:HE1	1.86	0.58
2:E:149:ILE:HD12	2:E:352:PHE:CZ	2.39	0.58
2:E:445:LYS:O	2:E:449:ILE:HD13	2.04	0.58
2:F:141:LEU:HG	2:F:145:GLN:HE21	1.68	0.58
1:B:452:LYS:CA	1:B:475:TRP:HB2	2.32	0.58
1:B:492:ARG:HB3	1:B:492:ARG:CZ	2.33	0.58
1:C:21:LYS:HG3	1:C:25:ASP:HB3	1.85	0.58
1:C:151:SER:HA	1:C:154:GLU:OE2	2.03	0.58
1:C:243:LEU:HB3	1:C:393:PHE:HE2	1.68	0.58
2:F:287:LEU:O	2:F:287:LEU:HD23	2.03	0.58
2:F:366:LEU:CD1	2:F:370:ILE:HG12	2.34	0.58
3:J:31:ILE:HG12	3:J:100:TYR:CZ	2.39	0.58
1:B:489:ALA:HA	1:B:492:ARG:NH1	2.19	0.57
1:B:758:GLN:HE22	1:B:783:GLY:HA2	1.70	0.57
1:D:59:TRP:CZ3	1:D:66:ASN:HB2	2.39	0.57
1:D:245:GLU:OE2	1:D:246:LYS:HG2	2.04	0.57
2:E:18:ARG:HA	2:E:21:LYS:CE	2.34	0.57
2:E:180:SER:HB3	2:E:315:LYS:HZ1	1.68	0.57
1:B:140:SER:HA	1:B:271:LYS:HZ1	1.69	0.57
1:B:513:TYR:HE1	1:B:540:LEU:HD23	1.69	0.57
1:D:301:SER:C	1:D:302:LEU:HD23	2.29	0.57
2:E:419:LEU:O	2:E:419:LEU:HD13	2.03	0.57
1:A:171:ARG:HD2	1:A:232:LEU:CD1	2.34	0.57
1:B:117:ARG:NE	1:B:117:ARG:HA	2.19	0.57
1:B:349:LYS:HD2	1:B:370:ASN:HB3	1.85	0.57
2:E:18:ARG:HD3	2:E:21:LYS:HZ1	1.69	0.57
2:F:344:GLU:HG3	2:F:345:HIS:ND1	2.19	0.57
1:A:65:CYS:HB3	2:F:346:LEU:HD21	1.85	0.57
1:A:301:SER:OG	1:B:67:ASP:HA	2.03	0.57
1:C:299:ILE:O	1:C:299:ILE:HG13	2.04	0.57
2:E:18:ARG:CA	2:E:21:LYS:HE3	2.34	0.57
2:E:287:LEU:HD22	2:E:437:PHE:CE1	2.40	0.57
2:F:24:TRP:CH2	2:F:387:LEU:HD13	2.39	0.57
2:F:399:LYS:HE2	2:F:421:HIS:HB3	1.87	0.57
1:A:118:LEU:HD12	1:A:119:HIS:N	2.19	0.57
1:A:140:SER:HA	1:A:271:LYS:HZ1	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:ILE:HA	1:D:359:GLU:CG	2.33	0.57
2:F:18:ARG:HA	2:F:21:LYS:HE3	1.85	0.57
3:J:28:ILE:HG22	3:J:77:ASN:OD1	2.04	0.57
1:A:65:CYS:SG	2:F:346:LEU:HD23	2.45	0.57
1:A:258:ASP:OD1	1:A:349:LYS:HE2	2.05	0.57
1:A:274:LYS:O	1:A:278:ILE:HG22	2.03	0.57
1:A:354:GLU:HA	1:A:357:ARG:NH1	2.13	0.57
1:B:168:TRP:O	1:B:171:ARG:HG2	2.04	0.57
1:B:420:LEU:CB	1:B:428:LEU:HD11	2.34	0.57
1:B:699:PHE:CE1	1:B:721:GLU:HB2	2.39	0.57
1:D:126:PRO:O	1:D:129:VAL:HG13	2.05	0.57
1:D:389:ARG:O	1:D:392:VAL:HG22	2.05	0.57
2:F:172:HIS:NE2	2:F:322:ILE:HG21	2.19	0.57
2:F:344:GLU:HB3	2:F:350:GLU:CA	2.34	0.57
1:A:161:LEU:HD12	1:A:162:LYS:N	2.19	0.57
1:A:235:LYS:HA	1:A:238:GLU:OE1	2.04	0.57
1:B:166:SER:HB3	1:B:169:THR:HG22	1.85	0.57
1:B:550:ARG:HD2	1:B:551:LEU:N	2.19	0.57
1:C:366:PRO:HD2	1:C:394:LEU:CG	2.35	0.57
2:F:399:LYS:NZ	2:F:420:LEU:HG	2.19	0.57
3:J:97:ALA:HB2	3:J:115:TRP:CE3	2.39	0.57
1:B:232:LEU:HD11	1:B:236:GLU:OE1	2.05	0.57
2:E:57:VAL:HG12	2:E:353:GLU:HG2	1.86	0.57
2:F:291:VAL:HG21	2:F:437:PHE:CD1	2.40	0.57
3:J:68:PHE:HA	3:J:82:GLN:O	2.05	0.57
1:B:149:THR:O	1:B:153:LEU:HG	2.04	0.57
1:B:435:LEU:O	1:B:457:PRO:HD2	2.05	0.57
2:E:280:ASP:O	2:E:284:ALA:HB3	2.05	0.57
2:E:408:ASP:C	2:E:409:ILE:HD12	2.29	0.57
1:B:255:GLU:CD	1:B:369:LYS:HG3	2.29	0.57
2:F:330:VAL:HG23	2:F:366:LEU:HD23	1.87	0.57
3:J:33:TYR:HD2	3:J:104:THR:HB	1.64	0.57
1:B:164:PHE:CZ	1:B:385:LEU:HG	2.40	0.56
1:B:578:GLY:CA	1:B:600:ARG:HG2	2.35	0.56
1:B:721:GLU:HG2	1:B:742:VAL:HG21	1.85	0.56
1:C:241:LYS:HA	1:C:244:PHE:CD2	2.40	0.56
1:D:100:ASP:O	1:D:101:LEU:HD23	2.04	0.56
2:E:141:LEU:HD11	2:E:347:ILE:HG23	1.87	0.56
2:F:19:ILE:HG22	2:F:20:LEU:N	2.20	0.56
2:F:200:LEU:HD21	2:F:430:TYR:HB3	1.87	0.56
1:A:171:ARG:CZ	1:A:232:LEU:HG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:PHE:CD1	1:C:333:GLY:HA3	2.40	0.56
2:E:19:ILE:HG23	2:E:426:TYR:CD2	2.27	0.56
2:E:170:LEU:HD23	2:E:170:LEU:C	2.29	0.56
2:F:52:VAL:CG2	2:F:154:TYR:HB2	2.34	0.56
3:J:72:LEU:HD12	3:J:73:ASP:N	2.20	0.56
3:J:83:MET:HE2	3:J:86:LEU:HD21	1.87	0.56
1:A:156:PHE:CE1	1:A:375:MET:HG2	2.40	0.56
1:A:234:LYS:HD3	1:A:406:ASN:OD1	2.05	0.56
1:B:19:ILE:HG23	1:B:382:TYR:CE2	2.40	0.56
1:B:234:LYS:CE	1:B:409:ASN:HB3	2.28	0.56
1:B:449:GLU:C	1:B:471:LEU:HD12	2.29	0.56
1:B:496:ARG:O	1:B:518:LEU:HD12	2.06	0.56
1:B:611:PHE:CE1	1:B:634:SER:HB2	2.41	0.56
1:B:677:ILE:HG23	1:B:681:LEU:HD13	1.88	0.56
1:B:689:TYR:CD2	1:B:712:ASN:HB3	2.40	0.56
1:B:696:ASN:HB3	1:B:719:ARG:NH2	2.21	0.56
1:C:39:ALA:HB2	1:C:129:VAL:CG1	2.28	0.56
1:C:143:TRP:CB	1:C:263:LEU:HD21	2.35	0.56
1:D:117:ARG:HG3	1:D:295:CYS:HA	1.87	0.56
1:D:126:PRO:HA	1:D:129:VAL:CG1	2.36	0.56
1:A:120:TRP:HA	1:A:123:LYS:HE2	1.86	0.56
1:B:443:PHE:CZ	1:B:462:PRO:HG2	2.41	0.56
1:B:448:LEU:HD12	1:B:449:GLU:H	1.70	0.56
1:C:243:LEU:HD12	1:C:246:LYS:NZ	2.12	0.56
1:D:168:TRP:O	1:D:171:ARG:HG2	2.05	0.56
1:D:372:PHE:HA	1:D:375:MET:HG3	1.87	0.56
2:E:183:TRP:NE1	2:E:308:TYR:HB2	2.20	0.56
2:F:365:LEU:O	2:F:365:LEU:HD12	2.05	0.56
3:J:7:SER:O	3:J:20:LEU:HA	2.05	0.56
1:A:393:PHE:C	1:A:394:LEU:HD13	2.30	0.56
1:B:746:LEU:HG	1:B:770:PRO:HG3	1.87	0.56
1:D:354:GLU:O	1:D:358:GLU:HG3	2.06	0.56
2:E:36:LEU:HB2	2:E:173:THR:HG21	1.86	0.56
2:E:346:LEU:C	2:E:347:ILE:HD12	2.31	0.56
2:F:31:LEU:CD2	2:F:376:TYR:HB2	2.36	0.56
1:A:108:TYR:CA	1:B:53:ILE:HG21	2.35	0.56
1:B:258:ASP:H	1:B:371:ASP:HB2	1.70	0.56
1:B:429:GLU:HA	1:B:450:VAL:O	2.05	0.56
1:B:622:LYS:NZ	3:J:105:SER:HB2	2.20	0.56
1:C:269:ILE:O	1:C:273:ILE:HG12	2.06	0.56
1:C:343:MET:C	1:C:344:LEU:HD22	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ASP:CB	1:C:397:VAL:HG23	2.33	0.56
1:D:37:MET:HA	1:D:37:MET:CE	2.26	0.56
1:D:357:ARG:HA	1:D:365:ILE:HD12	1.86	0.56
2:E:52:VAL:CG2	2:E:154:TYR:HD1	2.16	0.56
2:E:309:VAL:O	2:E:313:VAL:HG22	2.05	0.56
2:F:179:SER:OG	2:F:315:LYS:HE2	2.05	0.56
3:J:73:ASP:HB2	3:J:80:TYR:HE2	1.69	0.56
1:B:626:LEU:HG	1:B:649:ASN:OD1	2.05	0.56
1:B:682:PHE:CE2	1:B:701:PRO:HB2	2.41	0.56
1:B:700:LEU:O	1:B:724:PRO:HG3	2.03	0.56
1:C:401:LYS:CG	1:C:402:LEU:HD12	2.31	0.56
1:D:232:LEU:O	1:D:232:LEU:HD12	2.05	0.56
1:A:244:PHE:O	1:A:248:LYS:HG3	2.06	0.56
1:B:54:CYS:C	1:B:55:LEU:HD23	2.30	0.56
1:B:135:ILE:HD12	1:B:274:LYS:HZ1	1.71	0.56
1:B:404:GLN:O	1:B:407:LEU:HG	2.06	0.56
1:D:168:TRP:CH2	1:D:398:SER:HB3	2.41	0.56
2:E:180:SER:HB3	2:E:315:LYS:NZ	2.21	0.56
2:F:47:LEU:HD23	2:F:47:LEU:C	2.31	0.56
2:F:396:SER:OG	2:F:399:LYS:HE3	2.06	0.56
3:J:97:ALA:HB1	3:J:112:TYR:CB	2.35	0.56
1:A:118:LEU:HD12	1:A:119:HIS:H	1.70	0.56
1:A:268:THR:HG22	1:A:340:LEU:CD2	2.36	0.56
1:B:159:ILE:HG22	1:B:390:PHE:HE2	1.70	0.56
1:B:232:LEU:HD11	1:B:236:GLU:CG	2.36	0.56
1:B:746:LEU:HD12	1:B:747:PRO:HD2	1.88	0.56
1:C:32:SER:HA	1:C:35:MET:CE	2.35	0.56
2:E:297:HIS:ND1	2:E:298:VAL:HG13	2.21	0.56
2:F:298:VAL:O	2:F:298:VAL:HG23	2.06	0.56
1:A:301:SER:O	1:A:302:LEU:HD23	2.05	0.56
1:B:541:ARG:HA	1:B:565:VAL:HG13	1.87	0.56
1:B:575:ASN:HD21	1:B:600:ARG:NH2	2.04	0.56
1:C:353:PHE:CA	1:C:356:ILE:HD13	2.35	0.56
1:D:130:LEU:HD23	1:D:130:LEU:C	2.31	0.56
2:E:31:LEU:HD23	2:E:31:LEU:C	2.30	0.56
2:E:345:HIS:C	2:E:346:LEU:HD12	2.31	0.56
2:F:291:VAL:HG21	2:F:437:PHE:HD1	1.70	0.56
1:B:164:PHE:CD1	1:B:389:ARG:HG3	2.41	0.55
1:C:293:VAL:CG1	1:C:310:CYS:HB2	2.33	0.55
1:D:350:LYS:HD3	1:D:351:TYR:N	2.21	0.55
2:F:183:TRP:CA	2:F:307:LEU:HD21	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LYS:HE2	1:B:145:LYS:N	2.21	0.55
1:D:136:PHE:HE1	1:D:274:LYS:HB2	1.70	0.55
2:E:291:VAL:HG12	2:E:438:LEU:HD13	1.89	0.55
2:E:294:PHE:CA	2:E:297:HIS:HB3	2.35	0.55
2:F:57:VAL:HG13	2:F:352:PHE:HA	1.88	0.55
2:F:58:LEU:HD23	2:F:58:LEU:C	2.31	0.55
1:A:61:THR:HG23	1:A:66:ASN:HB2	1.87	0.55
1:B:143:TRP:HB3	1:B:263:LEU:HD21	1.88	0.55
1:B:550:ARG:O	1:B:551:LEU:HD23	2.07	0.55
1:A:132:HIS:CG	1:A:278:ILE:HD12	2.41	0.55
1:B:40:VAL:O	1:B:44:THR:HG22	2.07	0.55
1:D:255:GLU:OE2	1:D:369:LYS:HB3	2.07	0.55
1:D:353:PHE:HZ	1:D:391:ALA:HA	1.71	0.55
1:D:400:ASN:HA	1:D:403:ARG:NH2	2.21	0.55
2:E:170:LEU:O	2:E:173:THR:HB	2.06	0.55
2:F:445:LYS:O	2:F:449:ILE:HD13	2.07	0.55
3:J:38:ARG:HB2	3:J:92:ALA:HB3	1.88	0.55
1:A:24:TRP:O	1:A:28:THR:HG23	2.06	0.55
1:A:267:GLN:NE2	1:A:271:LYS:HZ1	2.03	0.55
1:B:492:ARG:HB3	1:B:492:ARG:NH1	2.21	0.55
1:B:505:ILE:HA	1:B:508:ILE:HD12	1.89	0.55
1:B:633:ILE:CG1	1:B:657:GLN:HG2	2.36	0.55
1:B:716:THR:HG23	1:B:739:GLY:O	2.06	0.55
1:D:171:ARG:O	1:D:175:GLU:HG2	2.07	0.55
1:B:736:LEU:HD21	1:B:738:LEU:HD11	1.89	0.55
1:C:272:VAL:CG2	1:C:336:CYS:HB3	2.36	0.55
1:C:366:PRO:HD2	1:C:394:LEU:CD2	2.37	0.55
1:C:406:ASN:HA	1:C:409:ASN:ND2	2.21	0.55
1:D:168:TRP:CE3	1:D:402:LEU:HD23	2.41	0.55
1:D:345:ARG:HG3	1:D:346:ARG:NE	2.21	0.55
2:E:346:LEU:HD21	2:F:353:GLU:OE1	2.07	0.55
1:A:243:LEU:HD23	1:A:246:LYS:NZ	2.19	0.55
1:B:671:ARG:HD2	3:J:108:TYR:CE1	2.41	0.55
1:B:688:ARG:HB3	1:B:711:GLN:OE1	2.07	0.55
1:D:250:PHE:O	1:D:254:VAL:HG23	2.07	0.55
2:E:52:VAL:O	2:E:150:ASN:HB2	2.06	0.55
2:F:31:LEU:CD2	2:F:35:MET:HE3	2.37	0.55
3:J:18:LEU:HD12	3:J:121:VAL:HG13	1.88	0.55
1:A:140:SER:HA	1:A:267:GLN:NE2	2.21	0.55
1:B:22:PRO:HD2	1:B:25:ASP:OD2	2.06	0.55
1:B:263:LEU:HD23	1:B:263:LEU:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:TYR:O	1:B:365:ILE:HG13	2.06	0.55
1:B:451:LEU:HD11	1:B:453:LEU:CD2	2.36	0.55
2:E:19:ILE:HG22	2:E:20:LEU:N	2.22	0.55
2:F:346:LEU:O	2:F:347:ILE:HD12	2.07	0.55
3:J:18:LEU:CD1	3:J:121:VAL:HG13	2.37	0.55
1:A:97:ILE:HD11	2:F:346:LEU:O	2.07	0.55
1:A:156:PHE:HA	1:A:159:ILE:CD1	2.37	0.55
1:B:474:LEU:O	1:B:498:LEU:HD12	2.07	0.55
1:C:251:ARG:HA	1:C:254:VAL:CG1	2.37	0.55
1:C:400:ASN:CB	1:C:403:ARG:HH21	2.16	0.55
1:D:342:TRP:HA	1:D:345:ARG:CD	2.37	0.55
1:D:355:SER:O	1:D:359:GLU:HG2	2.07	0.55
2:E:28:MET:CE	2:E:379:ILE:HG22	2.37	0.55
2:E:31:LEU:CD2	2:E:35:MET:HE3	2.37	0.55
2:F:193:VAL:O	2:F:197:VAL:HG23	2.07	0.55
1:B:758:GLN:NE2	1:B:783:GLY:HA2	2.22	0.55
1:D:28:THR:HG23	1:D:335:ILE:HG21	1.89	0.55
1:D:155:HIS:NE2	1:D:159:ILE:HD11	2.21	0.55
1:D:341:TRP:O	1:D:345:ARG:HG2	2.07	0.55
2:F:54:CYS:HA	2:F:354:CYS:HA	1.89	0.55
2:F:286:ALA:HA	2:F:289:GLU:CD	2.32	0.55
2:F:344:GLU:O	2:F:348:GLY:HA2	2.06	0.55
2:F:403:GLU:OE2	2:F:432:LYS:HA	2.08	0.55
1:B:354:GLU:O	1:B:357:ARG:HG2	2.07	0.54
1:B:550:ARG:HH22	1:B:575:ASN:CB	2.19	0.54
1:B:616:LEU:O	1:B:640:ARG:HB2	2.06	0.54
1:C:248:LYS:O	1:C:252:THR:HG23	2.07	0.54
1:A:300:GLU:HA	1:A:300:GLU:OE1	2.07	0.54
1:C:117:ARG:CB	1:C:295:CYS:HB3	2.38	0.54
1:D:269:ILE:O	1:D:273:ILE:HG23	2.07	0.54
1:D:350:LYS:HD3	1:D:368:VAL:O	2.06	0.54
2:E:401:ARG:HA	2:E:413:LYS:CB	2.38	0.54
1:A:258:ASP:O	1:A:262:ARG:HD2	2.06	0.54
1:B:342:TRP:HE1	1:B:381:GLN:NE2	2.05	0.54
1:B:489:ALA:HA	1:B:492:ARG:HH12	1.73	0.54
1:B:574:ILE:HG21	1:B:581:LEU:CD2	2.36	0.54
1:B:622:LYS:HB2	1:B:647:TRP:NE1	2.21	0.54
1:B:796:PRO:HA	1:B:799:LYS:HE3	1.90	0.54
1:C:36:LEU:HB2	1:C:133:THR:HG21	1.89	0.54
1:D:309:ARG:HG3	1:D:309:ARG:O	2.07	0.54
2:E:31:LEU:HD21	2:E:376:TYR:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:58:LEU:HD23	2:E:59:PRO:CD	2.38	0.54
2:F:149:ILE:HG21	2:F:352:PHE:CE2	2.42	0.54
2:F:412:VAL:HG23	2:F:438:LEU:O	2.07	0.54
1:A:46:GLN:HB2	1:A:318:PHE:HZ	1.72	0.54
1:B:52:MET:HE3	1:B:118:LEU:HD22	1.89	0.54
1:B:474:LEU:HD12	1:B:475:TRP:N	2.23	0.54
1:B:646:LEU:HB2	1:B:669:LEU:CD2	2.34	0.54
1:B:670:ASN:HB2	1:B:694:HIS:HD2	1.71	0.54
1:C:52:MET:HE1	1:C:113:CYS:HB3	1.88	0.54
1:C:298:ASP:HA	1:C:306:ARG:NH1	2.22	0.54
1:D:36:LEU:HD23	1:D:133:THR:HG21	1.90	0.54
1:D:54:CYS:O	1:D:55:LEU:HD23	2.08	0.54
2:E:208:TRP:CZ2	2:E:446:LEU:HB2	2.42	0.54
2:E:433:ARG:O	2:E:433:ARG:HG2	2.08	0.54
1:B:492:ARG:HG2	1:B:492:ARG:O	2.07	0.54
1:B:538:ASP:HB2	1:B:541:ARG:NH1	2.22	0.54
1:B:578:GLY:HA2	1:B:600:ARG:HG2	1.90	0.54
1:B:652:ALA:O	1:B:674:ILE:HA	2.07	0.54
1:C:407:LEU:O	1:C:410:GLU:HB3	2.08	0.54
1:D:282:THR:HG22	1:D:326:ILE:HD11	1.88	0.54
1:D:342:TRP:HA	1:D:345:ARG:HG2	1.89	0.54
2:E:322:ILE:O	2:E:326:THR:HG23	2.07	0.54
1:A:166:SER:HB3	1:A:169:THR:HG23	1.90	0.54
1:A:276:ALA:O	1:A:279:ILE:HG22	2.08	0.54
1:A:348:LEU:HD22	1:A:377:HIS:ND1	2.22	0.54
1:A:364:ASP:OD2	1:A:397:VAL:HB	2.07	0.54
1:B:24:TRP:O	1:B:28:THR:HG23	2.08	0.54
1:B:622:LYS:HG3	1:B:648:TYR:CB	2.33	0.54
1:C:45:LEU:HD21	1:C:314:LEU:HD11	1.90	0.54
1:C:255:GLU:OE1	1:C:369:LYS:HB2	2.07	0.54
1:D:232:LEU:CD2	1:D:405:LEU:HD13	2.36	0.54
1:D:351:TYR:HB3	1:D:368:VAL:HB	1.90	0.54
2:F:168:LEU:O	2:F:172:HIS:HB3	2.07	0.54
3:J:38:ARG:HB3	3:J:94:TYR:CD2	2.43	0.54
1:B:52:MET:CE	1:B:118:LEU:HB2	2.38	0.54
1:B:63:ASP:OD2	1:B:296:THR:HG21	2.08	0.54
1:B:104:HIS:CD2	1:C:106:TYR:HB3	2.42	0.54
1:B:445:LEU:O	1:B:468:LEU:HD22	2.08	0.54
1:B:654:ILE:CD1	1:B:669:LEU:HD12	2.37	0.54
1:B:682:PHE:CZ	1:B:701:PRO:HB2	2.43	0.54
1:C:45:LEU:HG	1:C:314:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ILE:CG2	1:C:319:LYS:HB2	2.36	0.54
2:E:443:GLU:HG2	2:E:447:ARG:NH2	2.23	0.54
2:F:204:PHE:HA	2:F:433:ARG:HD3	1.90	0.54
1:B:159:ILE:HG22	1:B:390:PHE:CE2	2.43	0.54
1:B:171:ARG:NH1	1:B:232:LEU:HD13	2.22	0.54
1:B:607:PRO:O	1:B:610:ILE:HG13	2.08	0.54
1:B:800:GLU:O	1:B:804:ARG:HG3	2.07	0.54
1:C:168:TRP:CZ2	1:C:399:GLU:HA	2.42	0.54
1:D:400:ASN:HA	1:D:403:ARG:HH22	1.72	0.54
2:F:294:PHE:CZ	2:F:298:VAL:HG21	2.43	0.54
1:B:135:ILE:HD12	1:B:274:LYS:NZ	2.22	0.54
1:B:435:LEU:O	1:B:456:ILE:HA	2.08	0.54
1:A:135:ILE:HD13	1:A:274:LYS:NZ	2.23	0.54
1:B:297:VAL:HG21	1:B:299:ILE:HG12	1.89	0.54
1:B:404:GLN:HA	1:B:407:LEU:HG	1.90	0.54
1:B:431:HIS:O	1:B:432:LEU:HD23	2.07	0.54
1:B:645:LYS:HE2	1:B:668:TYR:CE1	2.43	0.54
1:C:231:VAL:HG23	1:C:409:ASN:CB	2.38	0.54
1:D:258:ASP:H	1:D:371:ASP:HB2	1.73	0.54
2:E:295:ARG:O	2:E:299:GLU:HG2	2.08	0.54
2:E:387:LEU:O	2:E:387:LEU:HG	2.07	0.54
2:F:31:LEU:C	2:F:31:LEU:HD23	2.32	0.54
2:F:180:SER:HA	2:F:311:GLN:NE2	2.23	0.54
1:B:600:ARG:HD2	3:J:59:TYR:CZ	2.42	0.53
1:B:726:GLU:H	1:B:726:GLU:CD	2.17	0.53
1:C:365:ILE:HD11	1:C:395:SER:HB3	1.90	0.53
2:F:18:ARG:HA	2:F:21:LYS:CE	2.37	0.53
2:F:18:ARG:CA	2:F:21:LYS:HE3	2.37	0.53
3:J:104:THR:HG23	3:J:111:GLU:CB	2.26	0.53
1:A:255:GLU:OE1	1:A:369:LYS:HB2	2.08	0.53
1:B:696:ASN:HB3	1:B:719:ARG:CZ	2.38	0.53
1:C:262:ARG:HH21	1:C:266:ARG:NH2	2.06	0.53
1:D:19:ILE:HD12	1:D:19:ILE:N	2.22	0.53
1:D:35:MET:HE1	1:D:329:VAL:HA	1.90	0.53
1:D:167:PRO:HG2	1:D:236:GLU:CD	2.33	0.53
1:D:275:PHE:CE1	1:D:333:GLY:HA3	2.43	0.53
2:E:141:LEU:HG	2:E:145:GLN:HE21	1.72	0.53
2:E:172:HIS:NE2	2:E:322:ILE:HG12	2.21	0.53
3:J:27:TYR:HB3	3:J:29:TYR:CD2	2.43	0.53
3:J:70:VAL:HA	3:J:80:TYR:O	2.08	0.53
1:C:243:LEU:HB3	1:C:393:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ASP:HB2	1:C:396:GLU:CD	2.33	0.53
1:D:145:LYS:HE2	1:D:145:LYS:N	2.23	0.53
1:D:254:VAL:HG11	1:D:375:MET:SD	2.49	0.53
1:D:275:PHE:CD1	1:D:333:GLY:HA3	2.44	0.53
1:A:51:LYS:HD3	1:A:51:LYS:N	2.18	0.53
1:A:353:PHE:CE1	1:A:391:ALA:HB2	2.44	0.53
1:B:130:LEU:C	1:B:130:LEU:HD23	2.34	0.53
1:B:145:LYS:HE2	1:B:145:LYS:CA	2.37	0.53
1:D:52:MET:CE	1:D:118:LEU:HB2	2.33	0.53
1:A:170:THR:HA	1:A:173:LEU:CD2	2.39	0.53
1:A:269:ILE:O	1:A:273:ILE:HG12	2.09	0.53
1:A:299:ILE:O	1:A:299:ILE:HG13	2.08	0.53
1:B:22:PRO:HG2	1:B:24:TRP:CZ2	2.44	0.53
1:B:37:MET:HA	1:B:40:VAL:HG12	1.91	0.53
1:B:45:LEU:HD21	1:B:317:LEU:HD23	1.90	0.53
1:B:342:TRP:HE1	1:B:381:GLN:HE21	1.56	0.53
1:B:443:PHE:HB3	1:B:467:GLN:OE1	2.07	0.53
1:B:746:LEU:HD21	1:B:773:LEU:HD21	1.90	0.53
1:B:784:LEU:HD23	1:B:791:PHE:HD1	1.71	0.53
1:C:129:VAL:HG22	1:C:325:TYR:CZ	2.44	0.53
1:C:305:TYR:HB2	1:C:308:TYR:OH	2.08	0.53
1:D:28:THR:CG2	1:D:335:ILE:HG21	2.38	0.53
1:D:164:PHE:HD1	1:D:386:TYR:HA	1.72	0.53
2:F:288:PHE:HB3	2:F:292:ARG:NH2	2.23	0.53
2:F:333:ILE:O	2:F:333:ILE:HG22	2.07	0.53
3:J:68:PHE:HB3	3:J:81:LEU:CD1	2.35	0.53
1:A:38:ILE:HD11	1:A:325:TYR:HD1	1.74	0.53
1:B:15:PRO:HD2	1:B:17:TYR:CE2	2.43	0.53
1:B:381:GLN:OE1	1:B:381:GLN:HA	2.08	0.53
1:B:662:THR:O	1:B:686:LYS:HD2	2.08	0.53
1:C:274:LYS:O	1:C:278:ILE:HG22	2.09	0.53
1:D:45:LEU:HG	1:D:314:LEU:HD13	1.89	0.53
2:E:148:PHE:CE2	2:F:355:THR:HG21	2.44	0.53
2:E:439:SER:HB3	2:E:442:SER:HB3	1.89	0.53
1:B:119:HIS:CD2	1:B:288:ASN:HB3	2.43	0.53
1:B:790:LEU:HA	1:B:793:THR:CG2	2.38	0.53
1:D:258:ASP:H	1:D:371:ASP:CB	2.22	0.53
2:E:53:VAL:O	2:E:355:THR:HG22	2.09	0.53
2:E:430:TYR:HA	2:E:433:ARG:HH21	1.73	0.53
2:F:31:LEU:HD22	2:F:376:TYR:HD2	1.70	0.53
1:A:28:THR:HG23	1:A:335:ILE:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HD2	2:F:143:PHE:HD2	1.74	0.53
1:A:158:SER:HA	1:A:161:LEU:CD2	2.39	0.53
1:A:305:TYR:OH	1:B:95:THR:HA	2.08	0.53
1:A:403:ARG:HH22	1:A:404:GLN:HB2	1.72	0.53
1:B:245:GLU:OE2	1:B:246:LYS:HE2	2.09	0.53
2:E:289:GLU:O	2:E:293:LYS:HB3	2.09	0.53
2:F:403:GLU:HG3	2:F:432:LYS:CE	2.36	0.53
3:J:97:ALA:HA	3:J:114:TYR:O	2.09	0.53
1:A:364:ASP:HB2	1:A:396:GLU:OE2	2.09	0.53
1:B:145:LYS:HE2	1:B:145:LYS:HA	1.91	0.53
1:C:234:LYS:CD	1:C:409:ASN:HB2	2.36	0.53
1:C:306:ARG:HA	1:C:306:ARG:HH11	1.73	0.53
2:E:206:SER:HB3	2:E:209:THR:OG1	2.09	0.53
2:E:380:CYS:O	2:E:384:LEU:HB2	2.09	0.53
2:F:19:ILE:HG21	2:F:423:VAL:CG1	2.35	0.53
3:J:22:CYS:C	3:J:78:THR:HG23	2.34	0.53
3:J:97:ALA:HB2	3:J:115:TRP:CD2	2.44	0.53
1:A:19:ILE:CD1	1:A:379:ILE:HD12	2.38	0.53
1:B:126:PRO:HA	1:B:129:VAL:HG12	1.91	0.53
1:B:492:ARG:N	1:B:515:LEU:HD22	2.24	0.53
1:C:125:PHE:CZ	1:C:322:ALA:HA	2.44	0.53
1:D:356:ILE:HD12	1:D:391:ALA:HB2	1.91	0.53
2:E:152:MET:SD	2:F:335:PHE:HE2	2.31	0.53
2:E:442:SER:O	2:E:445:LYS:HB2	2.08	0.53
1:A:259:ILE:HG23	1:A:260:VAL:N	2.24	0.52
1:A:403:ARG:NH2	1:A:404:GLN:HB2	2.23	0.52
1:B:466:ALA:HA	1:B:490:PHE:CZ	2.45	0.52
1:D:354:GLU:OE1	1:D:358:GLU:HG2	2.09	0.52
2:E:186:TYR:CE2	2:E:188:LYS:HB3	2.44	0.52
2:F:200:LEU:O	2:F:200:LEU:HD23	2.09	0.52
3:J:51:LEU:HD23	3:J:52:ALA:N	2.24	0.52
1:A:360:SER:HB3	1:A:362:TYR:CE2	2.44	0.52
1:B:435:LEU:O	1:B:456:ILE:HG23	2.09	0.52
1:B:580:LYS:HG2	1:B:582:ILE:CD1	2.39	0.52
1:B:680:GLN:H	1:B:680:GLN:CD	2.17	0.52
1:C:35:MET:HG3	1:C:328:LEU:HD13	1.92	0.52
1:C:49:GLN:HG3	1:C:49:GLN:O	2.08	0.52
1:D:104:HIS:CD2	2:E:146:TYR:HB3	2.45	0.52
1:D:365:ILE:HG12	1:D:395:SER:HA	1.91	0.52
2:E:31:LEU:HD21	2:E:372:ILE:HG23	1.90	0.52
2:F:340:LYS:HG2	2:F:351:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:73:ASP:CB	3:J:80:TYR:OH	2.57	0.52
1:A:168:TRP:HZ2	1:A:399:GLU:HA	1.74	0.52
1:B:671:ARG:CA	1:B:694:HIS:HB2	2.40	0.52
1:B:685:ARG:CD	1:B:707:LEU:HD23	2.39	0.52
1:B:751:GLY:H	1:B:772:GLU:HB3	1.74	0.52
1:C:251:ARG:CA	1:C:254:VAL:HG12	2.39	0.52
1:D:55:LEU:O	1:D:308:TYR:HA	2.09	0.52
1:D:343:MET:HA	1:D:348:LEU:HD21	1.90	0.52
2:E:170:LEU:HD23	2:E:171:ILE:N	2.24	0.52
2:F:141:LEU:HD23	2:F:146:TYR:CE1	2.44	0.52
2:F:277:ASP:C	2:F:279:LYS:H	2.17	0.52
2:F:411:ASP:HA	2:F:439:SER:HB2	1.89	0.52
1:B:700:LEU:HB2	1:B:724:PRO:HG3	1.91	0.52
1:B:751:GLY:N	1:B:772:GLU:HB3	2.25	0.52
1:C:120:TRP:HA	1:C:123:LYS:NZ	2.25	0.52
2:E:345:HIS:O	2:E:346:LEU:HD12	2.09	0.52
2:E:385:PHE:HD1	2:E:386:TRP:CD1	2.28	0.52
2:F:24:TRP:O	2:F:28:MET:HG3	2.10	0.52
1:A:251:ARG:HG2	1:A:255:GLU:CG	2.39	0.52
1:A:283:VAL:HG23	1:A:326:ILE:HD13	1.91	0.52
1:A:333:GLY:O	1:A:337:MET:HG2	2.09	0.52
1:B:171:ARG:NH1	1:B:232:LEU:HB2	2.25	0.52
1:B:629:ILE:CG2	1:B:651:ILE:HD13	2.39	0.52
1:B:718:ASN:H	1:B:741:ASN:ND2	2.07	0.52
1:D:31:ILE:O	1:D:35:MET:HG3	2.09	0.52
1:D:168:TRP:CE2	1:D:402:LEU:HB3	2.44	0.52
2:E:297:HIS:CE1	2:E:298:VAL:HG13	2.44	0.52
2:F:52:VAL:O	2:F:150:ASN:HB2	2.10	0.52
1:A:259:ILE:O	1:A:262:ARG:HG2	2.08	0.52
1:B:156:PHE:HB2	1:B:250:PHE:HZ	1.75	0.52
1:B:430:LEU:O	1:B:451:LEU:HD12	2.10	0.52
1:C:234:LYS:HD2	1:C:409:ASN:CB	2.34	0.52
2:E:347:ILE:HD12	2:E:347:ILE:N	2.23	0.52
1:A:149:THR:HG21	1:A:263:LEU:CD2	2.38	0.52
1:A:170:THR:O	1:A:173:LEU:HG	2.09	0.52
1:B:466:ALA:HA	1:B:490:PHE:CE2	2.45	0.52
1:B:725:PRO:O	1:B:728:PHE:HD2	1.93	0.52
1:D:17:TYR:O	1:D:21:LYS:HG3	2.09	0.52
1:D:112:VAL:HG12	1:D:297:VAL:HG11	1.91	0.52
1:D:312:HIS:HB3	1:D:315:ALA:HB2	1.92	0.52
1:D:356:ILE:HA	1:D:359:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:193:VAL:O	2:E:197:VAL:HG23	2.08	0.52
2:E:319:PHE:CE1	2:E:377:GLY:HA3	2.45	0.52
2:F:399:LYS:CE	2:F:420:LEU:HG	2.40	0.52
1:B:434:MET:SD	1:B:455:LEU:HD12	2.49	0.52
1:B:781:ARG:HD3	1:B:781:ARG:C	2.35	0.52
1:C:20:LEU:O	1:C:20:LEU:HD23	2.09	0.52
1:C:251:ARG:O	1:C:254:VAL:HG12	2.09	0.52
1:C:356:ILE:N	1:C:356:ILE:HD12	2.25	0.52
1:D:263:LEU:C	1:D:263:LEU:HD23	2.35	0.52
2:F:344:GLU:CB	2:F:350:GLU:HA	2.38	0.52
3:J:35:GLY:HA2	3:J:49:ALA:O	2.10	0.52
1:B:518:LEU:HD11	1:B:520:GLU:O	2.10	0.52
1:B:708:GLN:OE1	1:B:730:CYS:HA	2.10	0.52
1:C:139:CYS:HB2	1:C:271:LYS:HZ3	1.75	0.52
1:D:168:TRP:HA	1:D:171:ARG:CD	2.40	0.52
2:E:147:VAL:HA	2:E:150:ASN:CG	2.35	0.52
1:B:168:TRP:CZ3	1:B:172:ALA:HB2	2.45	0.52
1:B:571:LYS:HE3	1:B:597:GLU:OE2	2.10	0.52
1:C:146:PHE:HE2	1:C:148:ARG:HB3	1.75	0.52
2:E:319:PHE:CD1	2:E:377:GLY:HA3	2.45	0.52
3:J:37:PHE:CD2	3:J:47:GLY:HA2	2.45	0.52
3:J:38:ARG:HA	3:J:93:LEU:O	2.10	0.52
1:B:675:GLU:C	1:B:697:LEU:HD23	2.35	0.51
1:A:45:LEU:HG	1:A:314:LEU:HD21	1.91	0.51
1:A:54:CYS:O	1:A:55:LEU:HD23	2.10	0.51
1:A:155:HIS:ND1	1:A:159:ILE:HD13	2.24	0.51
1:B:246:LYS:HA	1:B:249:LYS:CG	2.39	0.51
1:B:265:MET:SD	1:B:344:LEU:HD21	2.51	0.51
1:B:490:PHE:O	1:B:494:ASN:HB2	2.10	0.51
1:B:509:PRO:HB2	1:B:512:ILE:CG2	2.37	0.51
1:B:668:TYR:C	1:B:669:LEU:HD23	2.34	0.51
1:B:746:LEU:HD23	1:B:770:PRO:CD	2.39	0.51
2:E:19:ILE:HG22	2:E:20:LEU:H	1.75	0.51
2:F:56:PRO:HB3	2:F:349:TYR:CD2	2.46	0.51
2:F:207:PRO:HA	2:F:210:THR:HG22	1.92	0.51
2:F:385:PHE:HD1	2:F:386:TRP:CD1	2.27	0.51
3:J:28:ILE:CB	3:J:77:ASN:HA	2.40	0.51
1:B:52:MET:C	1:B:53:ILE:HD12	2.36	0.51
1:C:364:ASP:CG	1:C:395:SER:HB2	2.35	0.51
1:C:376:LEU:H	1:C:376:LEU:HD22	1.75	0.51
1:D:127:TYR:HE2	2:E:361:MET:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:THR:CG2	2:E:437:PHE:HD2	2.23	0.51
2:E:294:PHE:O	2:E:297:HIS:HB3	2.10	0.51
2:E:333:ILE:HD11	2:E:362:LEU:HD22	1.92	0.51
1:A:306:ARG:HA	1:A:306:ARG:HH11	1.75	0.51
1:B:232:LEU:HD21	1:B:236:GLU:OE1	2.09	0.51
1:B:275:PHE:CE1	1:B:333:GLY:HA3	2.46	0.51
1:B:636:GLN:OE1	1:B:660:ASN:HB3	2.11	0.51
1:B:715:VAL:HG22	1:B:738:LEU:CD2	2.40	0.51
1:B:750:VAL:HG21	1:B:773:LEU:CD2	2.40	0.51
1:C:52:MET:HE3	1:C:54:CYS:SG	2.50	0.51
1:C:400:ASN:HB3	1:C:403:ARG:NH2	2.20	0.51
1:D:59:TRP:HZ3	1:D:66:ASN:HB2	1.76	0.51
1:D:168:TRP:NE1	1:D:402:LEU:HB3	2.25	0.51
1:D:297:VAL:CG2	1:D:299:ILE:HG12	2.41	0.51
2:E:287:LEU:HB3	2:E:437:PHE:CZ	2.46	0.51
2:E:441:VAL:O	2:E:445:LYS:HG2	2.11	0.51
2:F:319:PHE:HD1	2:F:373:ILE:HG23	1.75	0.51
1:B:19:ILE:HG23	1:B:382:TYR:CD2	2.46	0.51
1:B:443:PHE:HA	1:B:468:LEU:HD11	1.93	0.51
1:B:450:VAL:CG2	1:B:473:GLU:HB2	2.30	0.51
1:B:668:TYR:HA	1:B:691:ASP:HB3	1.93	0.51
1:D:112:VAL:HG12	1:D:297:VAL:CG1	2.41	0.51
2:E:403:GLU:HG3	2:E:432:LYS:CE	2.38	0.51
2:F:15:PRO:HD2	2:F:17:TYR:CZ	2.46	0.51
2:F:392:LEU:O	2:F:392:LEU:HD23	2.11	0.51
2:F:393:LYS:HA	2:F:421:HIS:CE1	2.45	0.51
1:A:109:VAL:HG11	1:A:308:TYR:CE2	2.45	0.51
1:A:243:LEU:CA	1:A:246:LYS:HG2	2.40	0.51
1:B:354:GLU:O	1:B:358:GLU:HG2	2.10	0.51
1:B:481:ALA:O	1:B:482:LYS:O	2.28	0.51
1:B:492:ARG:HG3	1:B:514:SER:O	2.11	0.51
1:B:663:ASN:HA	1:B:686:LYS:HD2	1.93	0.51
1:B:726:GLU:HA	1:B:729:GLN:CG	2.40	0.51
1:B:767:GLU:C	1:B:790:LEU:HD22	2.36	0.51
1:B:769:LEU:CD2	1:B:790:LEU:HB3	2.39	0.51
3:J:12:VAL:CG1	3:J:18:LEU:HD21	2.41	0.51
1:B:24:TRP:CD1	1:B:339:THR:HG1	2.28	0.51
1:B:118:LEU:HD23	1:B:123:LYS:HG2	1.93	0.51
1:B:746:LEU:HD23	1:B:773:LEU:HD21	1.91	0.51
1:C:132:HIS:CG	1:C:278:ILE:HD12	2.45	0.51
1:C:243:LEU:HA	1:C:246:LYS:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:PHE:HA	1:C:375:MET:HE2	1.92	0.51
1:D:351:TYR:HB2	1:D:373:ALA:HB1	1.92	0.51
1:A:356:ILE:HD12	1:A:356:ILE:N	2.26	0.51
1:B:351:TYR:HB2	1:B:373:ALA:CB	2.41	0.51
1:C:385:LEU:HD12	1:C:385:LEU:N	2.22	0.51
2:E:31:LEU:HD22	2:E:376:TYR:HD2	1.74	0.51
2:E:327:ALA:C	2:E:330:VAL:HG12	2.36	0.51
1:A:356:ILE:HA	1:A:359:GLU:OE2	2.11	0.51
1:B:377:HIS:O	1:B:381:GLN:HG2	2.11	0.51
1:B:629:ILE:HG23	1:B:651:ILE:HD13	1.93	0.51
1:C:351:TYR:HB2	1:C:373:ALA:CB	2.41	0.51
1:D:156:PHE:CE2	1:D:379:ILE:HD11	2.45	0.51
2:F:189:THR:HG23	2:F:304:ILE:CD1	2.38	0.51
3:J:28:ILE:HD13	3:J:72:LEU:HD11	1.92	0.51
1:B:600:ARG:HD2	3:J:59:TYR:CE1	2.46	0.51
1:D:101:LEU:HA	1:D:105:GLN:OE1	2.11	0.51
2:F:53:VAL:HG22	2:F:355:THR:HG23	1.92	0.51
2:F:189:THR:O	2:F:193:VAL:HG23	2.11	0.51
2:F:204:PHE:HA	2:F:433:ARG:CD	2.41	0.51
1:A:101:LEU:HA	1:A:105:GLN:HE22	1.76	0.50
1:A:243:LEU:HA	1:A:246:LYS:CG	2.40	0.50
1:A:355:SER:HA	1:A:358:GLU:OE2	2.11	0.50
1:B:235:LYS:HA	1:B:238:GLU:CD	2.36	0.50
1:B:368:VAL:CG1	1:B:372:PHE:HB3	2.41	0.50
1:B:474:LEU:HD11	1:B:476:LEU:CD2	2.40	0.50
1:D:118:LEU:HD23	1:D:123:LYS:HG3	1.93	0.50
1:D:274:LYS:O	1:D:278:ILE:HG13	2.12	0.50
2:E:399:LYS:HG3	2:E:400:VAL:N	2.26	0.50
3:J:22:CYS:O	3:J:78:THR:HA	2.11	0.50
3:J:99:ALA:CB	3:J:104:THR:HG21	2.41	0.50
1:A:259:ILE:HG23	1:A:260:VAL:H	1.77	0.50
1:B:593:LEU:O	1:B:616:LEU:HD23	2.11	0.50
1:B:668:TYR:O	1:B:669:LEU:HD23	2.11	0.50
1:D:354:GLU:CD	1:D:358:GLU:HG2	2.36	0.50
1:D:399:GLU:O	1:D:402:LEU:HD12	2.12	0.50
2:E:190:CYS:O	2:E:193:VAL:HB	2.11	0.50
2:E:289:GLU:O	2:E:292:ARG:HD2	2.11	0.50
2:E:366:LEU:HD12	2:E:366:LEU:O	2.10	0.50
2:F:288:PHE:O	2:F:291:VAL:HB	2.11	0.50
1:A:248:LYS:O	1:A:252:THR:HG23	2.12	0.50
1:B:232:LEU:CD1	1:B:236:GLU:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LYS:HA	1:B:238:GLU:OE2	2.09	0.50
1:B:509:PRO:O	1:B:512:ILE:HG12	2.10	0.50
1:B:585:ASN:HA	1:B:588:LYS:HB3	1.92	0.50
1:B:665:GLU:HA	1:B:687:LEU:CA	2.28	0.50
1:B:759:ILE:O	1:B:785:VAL:HB	2.11	0.50
1:C:230:GLY:O	1:C:405:LEU:HD11	2.12	0.50
1:C:301:SER:C	1:C:302:LEU:HD23	2.36	0.50
1:D:131:LEU:HD23	1:D:131:LEU:C	2.36	0.50
1:D:160:LEU:HD12	1:D:163:CYS:SG	2.52	0.50
1:D:244:PHE:CE1	1:D:402:LEU:HD21	2.46	0.50
2:E:47:LEU:HD23	2:E:47:LEU:C	2.36	0.50
3:J:28:ILE:HB	3:J:77:ASN:CA	2.41	0.50
1:A:117:ARG:HG3	1:A:295:CYS:HA	1.92	0.50
1:B:18:ARG:HD2	1:B:19:ILE:N	2.27	0.50
1:B:155:HIS:NE2	1:B:159:ILE:HD11	2.26	0.50
1:B:160:LEU:HD12	1:B:160:LEU:O	2.12	0.50
1:B:356:ILE:HD13	1:B:388:LYS:HA	1.93	0.50
1:B:399:GLU:HB3	1:B:403:ARG:NH1	2.13	0.50
1:B:626:LEU:O	1:B:651:ILE:HG13	2.10	0.50
1:B:690:LEU:HD12	1:B:691:ASP:N	2.26	0.50
1:B:769:LEU:HD21	1:B:790:LEU:CB	2.39	0.50
1:C:35:MET:O	1:C:38:ILE:HG12	2.10	0.50
1:C:117:ARG:HG3	1:C:295:CYS:CA	2.35	0.50
1:C:154:GLU:HA	1:C:157:VAL:HG12	1.94	0.50
1:C:236:GLU:HA	1:C:239:GLN:HE21	1.77	0.50
1:C:301:SER:HB3	1:D:67:ASP:CA	2.41	0.50
1:C:385:LEU:H	1:C:385:LEU:CD1	2.22	0.50
1:D:348:LEU:HA	1:D:377:HIS:CE1	2.47	0.50
2:F:366:LEU:HD11	2:F:370:ILE:HG12	1.92	0.50
1:A:343:MET:C	1:A:344:LEU:HD22	2.37	0.50
1:A:351:TYR:HB2	1:A:373:ALA:CB	2.41	0.50
1:B:158:SER:O	1:B:162:LYS:HG2	2.11	0.50
1:B:275:PHE:CD1	1:B:333:GLY:HA3	2.46	0.50
1:B:351:TYR:HD2	1:B:376:LEU:HD12	1.76	0.50
1:B:368:VAL:HG12	1:B:369:LYS:H	1.74	0.50
1:B:421:THR:O	1:B:428:LEU:HA	2.11	0.50
1:B:502:PHE:HZ	1:B:527:LEU:HD21	1.77	0.50
1:D:153:LEU:O	1:D:157:VAL:HG23	2.11	0.50
2:E:396:SER:OG	2:E:399:LYS:HE2	2.11	0.50
2:F:24:TRP:CE3	2:F:383:THR:HG21	2.47	0.50
2:F:31:LEU:HD23	2:F:35:MET:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:384:LEU:O	2:F:388:PHE:HB3	2.11	0.50
3:J:17:SER:HA	3:J:83:MET:O	2.11	0.50
1:A:258:ASP:N	1:A:371:ASP:HB2	2.18	0.50
1:B:713:LEU:HD12	1:B:714:ALA:H	1.77	0.50
1:C:346:ARG:HB2	1:C:348:LEU:CD2	2.41	0.50
2:E:323:LEU:HD23	2:E:323:LEU:C	2.37	0.50
2:F:344:GLU:HB3	2:F:350:GLU:CB	2.42	0.50
3:J:34:LEU:O	3:J:50:ALA:HA	2.10	0.50
1:A:356:ILE:HG22	1:A:362:TYR:HB2	1.92	0.50
1:A:394:LEU:HD22	1:A:394:LEU:N	2.25	0.50
1:B:653:TYR:HA	1:B:674:ILE:HG23	1.94	0.50
1:D:393:PHE:O	1:D:394:LEU:HD22	2.12	0.50
2:E:183:TRP:CE2	2:E:308:TYR:HD1	2.29	0.50
2:E:362:LEU:HD23	2:E:362:LEU:C	2.36	0.50
2:E:394:GLU:HA	2:E:417:ALA:N	2.26	0.50
1:A:56:PRO:HG2	1:A:99:TYR:CE1	2.46	0.50
1:B:358:GLU:HG3	1:B:359:GLU:H	1.76	0.50
1:B:541:ARG:HA	1:B:565:VAL:HG11	1.93	0.50
1:D:247:VAL:HG13	1:D:390:PHE:CZ	2.47	0.50
1:D:251:ARG:HD3	1:D:394:LEU:HD11	1.94	0.50
2:F:54:CYS:O	2:F:55:LEU:HG	2.11	0.50
1:A:317:LEU:HD12	1:A:317:LEU:O	2.12	0.50
1:A:359:GLU:HG2	1:A:388:LYS:HZ1	1.77	0.50
1:B:243:LEU:HD23	1:B:393:PHE:CZ	2.47	0.50
1:B:354:GLU:HA	1:B:357:ARG:CG	2.42	0.50
1:B:459:VAL:HG21	1:B:479:THR:HG21	1.94	0.50
1:B:769:LEU:HG	1:B:790:LEU:O	2.12	0.50
1:C:104:HIS:HB2	1:D:106:TYR:CD2	2.46	0.50
1:C:251:ARG:HD2	1:C:251:ARG:C	2.37	0.50
1:D:131:LEU:HD23	1:D:132:HIS:N	2.27	0.50
1:D:146:PHE:O	1:D:150:SER:HB3	2.12	0.50
1:D:348:LEU:N	1:D:348:LEU:HD12	2.27	0.50
2:E:31:LEU:CD2	2:E:372:ILE:HG23	2.42	0.50
2:F:380:CYS:C	2:F:384:LEU:HD23	2.37	0.50
2:F:409:ILE:HG22	2:F:441:VAL:HG13	1.94	0.50
3:J:22:CYS:O	3:J:78:THR:HG23	2.11	0.50
1:A:244:PHE:HB3	1:A:248:LYS:HZ1	1.74	0.49
1:A:300:GLU:CA	1:A:304:GLY:HA2	2.41	0.49
1:A:398:SER:HA	1:A:401:LYS:HG2	1.94	0.49
1:B:156:PHE:HB2	1:B:250:PHE:CZ	2.47	0.49
1:B:345:ARG:C	1:B:346:ARG:HE	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LYS:CG	1:B:575:ASN:HB3	2.38	0.49
1:B:670:ASN:HB3	1:B:691:ASP:CG	2.37	0.49
1:C:398:SER:HA	1:C:401:LYS:CD	2.42	0.49
1:D:263:LEU:HD23	1:D:263:LEU:O	2.11	0.49
1:D:297:VAL:HB	1:D:299:ILE:HG12	1.94	0.49
2:F:363:LYS:O	2:F:366:LEU:HB3	2.12	0.49
1:A:140:SER:HA	1:A:267:GLN:HE22	1.77	0.49
1:A:341:TRP:NE1	1:A:345:ARG:HD3	2.27	0.49
1:A:348:LEU:HA	1:A:377:HIS:CE1	2.47	0.49
1:B:243:LEU:O	1:B:247:VAL:HG23	2.12	0.49
1:B:576:ASN:CG	1:B:579:THR:HB	2.37	0.49
1:B:675:GLU:CG	1:B:696:ASN:HB2	2.38	0.49
1:B:718:ASN:H	1:B:741:ASN:HD21	1.60	0.49
2:E:279:LYS:O	2:E:283:GLN:HG2	2.12	0.49
3:J:37:PHE:CA	3:J:48:VAL:HG23	2.38	0.49
1:A:27:PHE:HZ	2:F:182:PHE:CE1	2.31	0.49
1:A:347:SER:HB3	1:A:350:LYS:HZ3	1.76	0.49
1:B:669:LEU:C	1:B:672:ASN:HD22	2.20	0.49
1:C:142:PHE:HE1	1:D:27:PHE:HZ	1.59	0.49
1:D:374:PHE:O	1:D:378:LEU:HD13	2.12	0.49
2:F:147:VAL:O	2:F:151:GLN:HB2	2.12	0.49
3:J:28:ILE:CG2	3:J:77:ASN:HA	2.41	0.49
1:A:236:GLU:O	1:A:239:GLN:HG3	2.13	0.49
1:B:234:LYS:N	1:B:234:LYS:HD2	2.27	0.49
1:B:258:ASP:H	1:B:371:ASP:CB	2.25	0.49
1:B:709:ASN:HA	1:B:732:LYS:HD2	1.93	0.49
1:B:751:GLY:HA3	1:B:772:GLU:HB3	1.94	0.49
1:C:45:LEU:CD2	1:C:317:LEU:HD23	2.42	0.49
1:D:104:HIS:NE2	2:E:146:TYR:HB3	2.27	0.49
1:D:368:VAL:HG21	1:D:376:LEU:HD11	1.92	0.49
2:E:22:PRO:HG2	2:E:24:TRP:CE2	2.46	0.49
2:E:27:PHE:O	2:E:28:MET:C	2.55	0.49
1:A:96:GLY:HA3	2:F:141:LEU:CD1	2.43	0.49
1:A:301:SER:C	1:A:302:LEU:HD23	2.38	0.49
1:B:448:LEU:HD12	1:B:449:GLU:N	2.27	0.49
1:B:679:THR:O	1:B:682:PHE:HD2	1.96	0.49
1:C:16:ALA:HB1	1:C:157:VAL:CG2	2.30	0.49
1:C:283:VAL:HG23	1:C:326:ILE:HD13	1.93	0.49
2:E:291:VAL:HG21	2:E:437:PHE:CD1	2.46	0.49
2:E:412:VAL:HG23	2:E:438:LEU:O	2.12	0.49
2:F:50:ASP:OD1	2:F:356:HIS:HE1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:HA	1:B:245:GLU:HG3	1.94	0.49
1:B:452:LYS:HE2	1:B:454:GLU:OE2	2.13	0.49
1:B:662:THR:HA	1:B:684:CYS:SG	2.53	0.49
1:C:255:GLU:OE2	1:C:368:VAL:HG13	2.12	0.49
1:D:20:LEU:O	1:D:22:PRO:HD3	2.12	0.49
1:D:176:THR:HG23	1:D:360:SER:O	2.11	0.49
1:D:354:GLU:HA	1:D:357:ARG:CG	2.41	0.49
2:E:429:LEU:HD12	2:E:429:LEU:O	2.12	0.49
2:F:45:MET:HE1	2:F:362:LEU:HD12	1.93	0.49
3:J:38:ARG:HD3	3:J:94:TYR:CE2	2.48	0.49
3:J:89:GLU:CD	3:J:89:GLU:H	2.20	0.49
1:A:356:ILE:CA	1:A:359:GLU:HG3	2.43	0.49
1:B:262:ARG:O	1:B:266:ARG:HG3	2.13	0.49
1:B:461:ILE:HD12	1:B:483:ILE:HD12	1.95	0.49
1:B:476:LEU:O	1:B:500:ILE:HA	2.12	0.49
1:B:489:ALA:CB	1:B:492:ARG:HH22	2.25	0.49
1:B:633:ILE:CB	1:B:657:GLN:HG2	2.42	0.49
1:B:716:THR:HA	1:B:739:GLY:O	2.13	0.49
1:C:139:CYS:CB	1:C:271:LYS:HZ3	2.26	0.49
1:D:52:MET:HE2	1:D:293:VAL:HG11	1.94	0.49
2:E:334:SER:O	2:E:337:HIS:HE1	1.96	0.49
2:E:387:LEU:HD21	2:E:422:MET:SD	2.51	0.49
1:A:171:ARG:O	1:A:175:GLU:HG2	2.13	0.49
1:B:368:VAL:HG11	1:B:372:PHE:HB3	1.92	0.49
1:B:550:ARG:HD3	1:B:573:SER:OG	2.13	0.49
1:B:643:CYS:HB2	1:B:666:ARG:HE	1.78	0.49
3:J:108:TYR:HB2	3:J:111:GLU:CG	2.41	0.49
1:A:98:LYS:HE2	2:F:140:ASN:HD21	1.78	0.49
1:A:154:GLU:HA	1:A:157:VAL:CG1	2.43	0.49
1:A:275:PHE:CD1	1:A:333:GLY:HA3	2.48	0.49
1:B:118:LEU:HD12	1:B:119:HIS:N	2.27	0.49
1:B:452:LYS:CB	1:B:475:TRP:HB2	2.42	0.49
1:B:548:VAL:HG13	1:B:571:LYS:CG	2.42	0.49
1:B:639:HIS:HA	1:B:663:ASN:HD22	1.76	0.49
1:C:244:PHE:HB3	1:C:248:LYS:NZ	2.28	0.49
2:E:148:PHE:CG	2:F:55:LEU:HD11	2.48	0.49
2:E:185:LYS:O	2:E:187:PRO:HD3	2.12	0.49
2:E:298:VAL:HG23	2:E:298:VAL:O	2.13	0.49
2:F:446:LEU:HD23	2:F:446:LEU:C	2.38	0.49
1:A:311:ALA:HB2	2:F:148:PHE:HE2	1.78	0.49
1:B:118:LEU:CD2	1:B:123:LYS:HG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:TYR:CD2	1:B:376:LEU:HD12	2.48	0.49
1:B:496:ARG:C	1:B:518:LEU:HD12	2.37	0.49
1:C:143:TRP:CA	1:C:263:LEU:HD21	2.41	0.49
1:C:389:ARG:NH1	1:C:389:ARG:HB3	2.28	0.49
1:D:28:THR:O	1:D:332:TYR:HE2	1.96	0.49
3:J:18:LEU:O	3:J:83:MET:HG3	2.13	0.49
3:J:61:ALA:HB3	3:J:64:VAL:HG22	1.94	0.49
1:A:97:ILE:HD11	2:F:347:ILE:HA	1.94	0.48
1:A:109:VAL:O	1:A:112:VAL:HG12	2.13	0.48
1:A:398:SER:O	1:A:401:LYS:HG2	2.13	0.48
1:B:682:PHE:CD1	1:B:704:ILE:HA	2.48	0.48
1:C:28:THR:CG2	1:C:335:ILE:HG21	2.42	0.48
1:D:45:LEU:HD21	1:D:317:LEU:HD23	1.95	0.48
1:D:58:LYS:HG2	1:D:99:TYR:CE1	2.46	0.48
1:D:156:PHE:HD1	1:D:250:PHE:HE2	1.61	0.48
1:A:159:ILE:HA	1:A:162:LYS:NZ	2.28	0.48
1:D:342:TRP:HA	1:D:345:ARG:HD3	1.95	0.48
1:D:372:PHE:CA	1:D:375:MET:HG3	2.43	0.48
2:F:323:LEU:HA	2:F:326:THR:OG1	2.14	0.48
1:C:156:PHE:HA	1:C:159:ILE:CG1	2.43	0.48
1:C:349:LYS:HE2	1:C:370:ASN:HB3	1.95	0.48
2:E:172:HIS:CE1	2:E:322:ILE:HG12	2.49	0.48
2:E:409:ILE:CG2	2:E:441:VAL:HG13	2.43	0.48
1:B:550:ARG:HA	1:B:573:SER:HB3	1.95	0.48
1:B:769:LEU:O	1:B:794:LEU:HD23	2.13	0.48
1:C:236:GLU:O	1:C:239:GLN:HG3	2.12	0.48
1:D:36:LEU:HG	1:D:133:THR:HG1	1.79	0.48
2:E:138:LYS:C	2:E:140:ASN:H	2.22	0.48
2:E:191:SER:HB2	2:F:427:ASP:OD2	2.14	0.48
2:E:282:GLU:HG2	2:E:283:GLN:N	2.28	0.48
1:A:108:TYR:HD1	1:B:53:ILE:HG22	1.78	0.48
1:A:357:ARG:O	1:A:361:SER:HA	2.12	0.48
1:B:20:LEU:O	1:B:22:PRO:HD3	2.13	0.48
1:B:38:ILE:CD1	1:B:324:PHE:HD2	2.25	0.48
1:B:52:MET:CE	1:B:118:LEU:HD13	2.43	0.48
1:B:130:LEU:HD23	1:B:130:LEU:O	2.14	0.48
1:B:243:LEU:HD23	1:B:393:PHE:HZ	1.78	0.48
1:B:270:ILE:HA	1:B:273:ILE:HD11	1.96	0.48
1:B:459:VAL:HB	1:B:480:ALA:O	2.13	0.48
1:B:481:ALA:HB1	1:B:511:TRP:CZ2	2.40	0.48
1:C:132:HIS:CD2	1:C:278:ILE:HD12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:PRO:O	2:E:441:VAL:HG12	2.12	0.48
2:F:180:SER:CA	2:F:315:LYS:HZ1	2.27	0.48
1:A:108:TYR:HB2	1:B:53:ILE:CG2	2.43	0.48
1:A:357:ARG:HG3	1:A:358:GLU:OE1	2.13	0.48
1:B:243:LEU:HG	1:B:393:PHE:CE2	2.48	0.48
1:B:295:CYS:SG	1:B:297:VAL:HG13	2.53	0.48
1:B:502:PHE:HZ	1:B:527:LEU:CD2	2.26	0.48
1:B:548:VAL:CG1	1:B:571:LYS:HD3	2.44	0.48
1:B:675:GLU:HG2	1:B:696:ASN:CB	2.39	0.48
1:C:265:MET:HB2	1:C:343:MET:HE1	1.95	0.48
1:C:350:LYS:HD3	1:C:350:LYS:N	2.28	0.48
2:E:201:GLY:O	2:E:205:GLU:HG3	2.13	0.48
2:F:326:THR:HB	2:F:370:ILE:HD11	1.94	0.48
2:F:410:PRO:O	2:F:441:VAL:HG12	2.14	0.48
1:B:242:ALA:HA	1:B:245:GLU:CG	2.44	0.48
1:B:483:ILE:HG21	1:B:511:TRP:CD2	2.47	0.48
1:B:548:VAL:HG11	1:B:571:LYS:HD3	1.94	0.48
1:B:633:ILE:CD1	1:B:657:GLN:HG2	2.44	0.48
1:C:404:GLN:HA	1:C:404:GLN:HE21	1.78	0.48
1:D:254:VAL:O	1:D:371:ASP:HB3	2.13	0.48
2:E:35:MET:HE2	2:E:372:ILE:CG2	2.44	0.48
2:F:58:LEU:HD12	2:F:137:ARG:HH12	1.79	0.48
1:A:359:GLU:HG2	1:A:388:LYS:NZ	2.29	0.48
1:B:166:SER:CB	1:B:169:THR:HG22	2.43	0.48
1:B:475:TRP:C	1:B:476:LEU:HD23	2.38	0.48
1:B:528:SER:O	1:B:555:LEU:HA	2.13	0.48
1:B:582:ILE:HD12	1:B:582:ILE:N	2.29	0.48
1:B:608:HIS:NE2	1:B:631:GLU:HG2	2.28	0.48
1:B:725:PRO:HA	1:B:728:PHE:HD2	1.79	0.48
1:B:751:GLY:CA	1:B:772:GLU:HB3	2.44	0.48
1:C:353:PHE:C	1:C:356:ILE:HD13	2.39	0.48
2:E:28:MET:CE	2:E:380:CYS:HA	2.44	0.48
2:E:203:CYS:HB3	2:E:434:PHE:HD2	1.79	0.48
2:E:299:GLU:HA	2:E:299:GLU:OE1	2.14	0.48
2:F:216:THR:HG22	2:F:408:ASP:HB3	1.95	0.48
2:F:287:LEU:HD22	2:F:437:PHE:CZ	2.49	0.48
3:J:5:VAL:O	3:J:22:CYS:HA	2.14	0.48
3:J:6:GLU:HG3	3:J:96:CYS:SG	2.54	0.48
3:J:12:VAL:HG21	3:J:86:LEU:HD13	1.95	0.48
1:A:103:ARG:HD2	2:F:143:PHE:CD2	2.49	0.48
1:B:404:GLN:HA	1:B:407:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:GLN:HB3	1:B:427:LYS:CE	2.40	0.48
1:B:430:LEU:CD2	1:B:432:LEU:HD21	2.44	0.48
1:B:432:LEU:O	1:B:453:LEU:HA	2.14	0.48
1:B:789:ASP:O	1:B:793:THR:HG23	2.13	0.48
1:D:116:ASN:HB3	1:D:117:ARG:CZ	2.44	0.48
2:F:141:LEU:HA	2:F:141:LEU:HD12	1.64	0.48
1:A:365:ILE:CD1	1:A:395:SER:HB3	2.43	0.48
1:B:125:PHE:CE1	1:B:322:ALA:HA	2.48	0.48
1:B:452:LYS:HG3	1:B:475:TRP:HB3	1.94	0.48
1:B:483:ILE:CD1	1:B:491:LEU:HD12	2.44	0.48
1:B:710:LEU:CG	1:B:733:LEU:HD21	2.41	0.48
1:C:147:PRO:HG3	1:D:23:TRP:N	2.29	0.48
1:D:293:VAL:HG13	1:D:310:CYS:HB2	1.95	0.48
1:D:343:MET:C	1:D:348:LEU:HD13	2.39	0.48
2:E:28:MET:HE2	2:E:380:CYS:HB2	1.95	0.48
2:E:412:VAL:CG2	2:E:438:LEU:HG	2.44	0.48
1:A:288:ASN:O	1:A:290:LYS:HG3	2.14	0.47
1:B:400:ASN:ND2	1:B:403:ARG:HH21	2.12	0.47
1:C:61:THR:CG2	1:C:66:ASN:HB2	2.44	0.47
1:D:301:SER:O	1:D:302:LEU:HD23	2.14	0.47
2:E:57:VAL:HG11	2:E:353:GLU:HG2	1.93	0.47
2:F:433:ARG:O	2:F:433:ARG:HD2	2.14	0.47
1:A:27:PHE:HZ	2:F:182:PHE:HE1	1.62	0.47
1:B:121:PHE:CD2	1:B:285:TYR:HB3	2.49	0.47
1:B:744:GLN:HA	1:B:765:ARG:O	2.15	0.47
1:C:171:ARG:CZ	1:C:232:LEU:HG	2.44	0.47
1:C:231:VAL:HG23	1:C:409:ASN:HB3	1.95	0.47
2:E:409:ILE:HD12	2:E:409:ILE:N	2.29	0.47
2:F:397:PHE:CB	2:F:414:ASN:HA	2.45	0.47
1:A:272:VAL:HG22	1:A:336:CYS:HB3	1.97	0.47
1:B:116:ASN:HB3	1:B:117:ARG:NH1	2.29	0.47
1:B:698:THR:HA	1:B:720:ILE:HA	1.96	0.47
1:B:754:THR:HA	1:B:777:PRO:HD2	1.95	0.47
1:C:160:LEU:HD12	1:C:160:LEU:O	2.14	0.47
1:D:164:PHE:CE1	1:D:385:LEU:HG	2.43	0.47
1:D:169:THR:O	1:D:173:LEU:HD23	2.13	0.47
1:D:340:LEU:HD11	1:D:344:LEU:HD11	1.95	0.47
1:D:345:ARG:HG3	1:D:346:ARG:HD3	1.94	0.47
2:E:291:VAL:HG21	2:E:437:PHE:CE1	2.49	0.47
2:F:31:LEU:HD21	2:F:372:ILE:HG23	1.96	0.47
2:F:399:LYS:HE2	2:F:421:HIS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HD13	1:A:274:LYS:HZ2	1.79	0.47
1:B:282:THR:HG22	1:B:326:ILE:CD1	2.39	0.47
1:B:552:LYS:HG3	1:B:575:ASN:CB	2.43	0.47
1:B:555:LEU:O	1:B:581:LEU:HD13	2.13	0.47
1:B:558:LEU:HD21	1:B:581:LEU:HD21	1.97	0.47
2:E:19:ILE:O	2:E:20:LEU:HB2	2.13	0.47
1:A:289:ILE:O	1:A:289:ILE:HG22	2.13	0.47
1:B:130:LEU:O	1:B:133:THR:HG23	2.15	0.47
1:B:153:LEU:O	1:B:157:VAL:HG23	2.14	0.47
1:C:243:LEU:CA	1:C:246:LYS:HG2	2.43	0.47
2:E:35:MET:HE1	2:E:373:ILE:CD1	2.45	0.47
2:F:209:THR:O	2:F:213:LEU:HD23	2.15	0.47
1:A:169:THR:CG2	1:A:393:PHE:HE1	2.24	0.47
1:A:259:ILE:HA	1:A:262:ARG:HG2	1.96	0.47
1:B:52:MET:HE3	1:B:118:LEU:HB2	1.94	0.47
1:B:590:MET:HE2	1:B:593:LEU:HD21	1.97	0.47
1:B:598:LEU:O	1:B:621:LEU:HA	2.14	0.47
1:B:736:LEU:CG	1:B:738:LEU:HD21	2.44	0.47
1:B:757:THR:HG22	1:B:778:LEU:CB	2.42	0.47
1:C:364:ASP:OD2	1:C:395:SER:HB2	2.15	0.47
1:D:156:PHE:HB2	1:D:250:PHE:HZ	1.77	0.47
1:D:156:PHE:HD1	1:D:250:PHE:CE2	2.32	0.47
2:E:58:LEU:HB3	2:E:59:PRO:HD3	1.96	0.47
2:E:144:GLN:HA	2:E:147:VAL:HG22	1.97	0.47
2:E:349:TYR:CE1	2:F:135:THR:HA	2.50	0.47
2:E:381:LEU:HD23	2:E:381:LEU:C	2.39	0.47
2:F:142:ASP:H	2:F:145:GLN:HE22	1.63	0.47
2:F:181:ASN:O	2:F:184:PHE:HB3	2.14	0.47
3:J:13:GLN:HA	3:J:124:SER:O	2.15	0.47
1:A:106:TYR:HE2	2:F:142:ASP:OD2	1.98	0.47
1:A:231:VAL:O	1:A:232:LEU:HD23	2.15	0.47
1:A:251:ARG:HG2	1:A:255:GLU:HG3	1.96	0.47
1:A:347:SER:HB3	1:A:350:LYS:NZ	2.30	0.47
1:B:416:LEU:CD1	1:B:442:VAL:HA	2.45	0.47
1:B:583:VAL:HG21	1:B:607:PRO:HB2	1.96	0.47
1:B:590:MET:HE2	1:B:593:LEU:CG	2.45	0.47
1:B:776:CYS:HB2	1:B:779:LEU:HB3	1.96	0.47
1:C:143:TRP:NE1	1:C:144:PHE:HD1	2.12	0.47
1:C:143:TRP:CD1	1:C:144:PHE:H	2.32	0.47
1:C:300:GLU:OE1	1:C:300:GLU:HA	2.15	0.47
1:C:345:ARG:HG3	1:C:346:ARG:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:49:LYS:O	2:E:358:MET:HE1	2.14	0.47
2:E:286:ALA:HA	2:E:289:GLU:OE1	2.14	0.47
2:F:162:SER:HA	2:F:333:ILE:HD11	1.96	0.47
2:F:441:VAL:O	2:F:445:LYS:HG2	2.15	0.47
3:J:45:ARG:HD3	3:J:115:TRP:CZ3	2.50	0.47
3:J:99:ALA:HB2	3:J:112:TYR:CD2	2.50	0.47
1:A:129:VAL:HG22	1:A:325:TYR:CE1	2.50	0.47
1:A:316:THR:HG21	2:F:155:HIS:CD2	2.50	0.47
1:B:301:SER:CB	1:C:67:ASP:HA	2.45	0.47
1:B:478:HIS:NE2	1:B:501:LYS:HG2	2.30	0.47
1:C:159:ILE:HA	1:C:162:LYS:HD2	1.97	0.47
1:D:48:THR:HG22	1:D:49:GLN:OE1	2.15	0.47
1:D:130:LEU:O	1:D:133:THR:HG23	2.15	0.47
2:E:32:ALA:HA	2:E:35:MET:HG2	1.95	0.47
2:E:344:GLU:OE2	2:E:348:GLY:CA	2.59	0.47
2:E:427:ASP:HB2	2:E:430:TYR:HD2	1.80	0.47
1:B:291:PHE:HA	1:B:315:ALA:HB3	1.95	0.47
1:B:483:ILE:HD12	1:B:491:LEU:HD12	1.96	0.47
1:B:550:ARG:HH22	1:B:575:ASN:HB3	1.79	0.47
1:D:368:VAL:HG13	1:D:372:PHE:HB3	1.96	0.47
2:E:183:TRP:HB3	2:E:311:GLN:HG3	1.96	0.47
2:E:343:VAL:HG23	2:E:343:VAL:O	2.14	0.47
2:F:18:ARG:C	2:F:21:LYS:HE3	2.40	0.47
2:F:347:ILE:O	2:F:347:ILE:HG22	2.14	0.47
3:J:55:ASN:HD21	3:J:57:GLN:HB2	1.79	0.47
1:A:112:VAL:HA	1:B:291:PHE:CZ	2.50	0.47
1:A:139:CYS:CB	1:A:271:LYS:HE3	2.45	0.47
1:A:234:LYS:HG3	1:A:238:GLU:OE2	2.15	0.47
1:B:18:ARG:NH1	1:B:19:ILE:HG13	2.30	0.47
1:B:588:LYS:CD	1:B:609:SER:HA	2.44	0.47
1:B:643:CYS:SG	1:B:668:TYR:HE1	2.38	0.47
1:B:781:ARG:HG3	1:B:803:TRP:CE2	2.50	0.47
1:C:38:ILE:HG13	1:C:39:ALA:N	2.30	0.47
1:C:52:MET:HE1	1:C:113:CYS:C	2.39	0.47
1:C:251:ARG:C	1:C:254:VAL:HG12	2.40	0.47
1:C:364:ASP:HB2	1:C:396:GLU:OE1	2.15	0.47
2:F:58:LEU:HD12	2:F:137:ARG:NH2	2.30	0.47
2:F:288:PHE:N	2:F:437:PHE:HE1	2.13	0.47
2:F:297:HIS:ND1	2:F:298:VAL:HG13	2.30	0.47
2:F:411:ASP:HA	2:F:439:SER:HA	1.96	0.47
1:B:135:ILE:CG2	1:B:274:LYS:HZ2	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:O	1:B:245:GLU:HG3	2.16	0.46
1:B:451:LEU:CD1	1:B:453:LEU:HD21	2.42	0.46
1:B:667:LEU:CB	1:B:690:LEU:HD13	2.37	0.46
1:C:398:SER:HA	1:C:401:LYS:HG2	1.97	0.46
1:D:162:LYS:HA	1:D:165:ASP:OD1	2.15	0.46
1:D:259:ILE:HA	1:D:262:ARG:HG2	1.97	0.46
2:E:285:LYS:CD	2:E:446:LEU:HD22	2.44	0.46
2:F:188:LYS:O	2:F:192:LYS:HE3	2.15	0.46
3:J:31:ILE:HD13	3:J:98:ALA:CB	2.43	0.46
3:J:73:ASP:HB2	3:J:80:TYR:CZ	2.50	0.46
1:A:68:SER:C	2:F:345:HIS:HB2	2.40	0.46
1:A:108:TYR:HB3	1:B:55:LEU:HD11	1.97	0.46
1:A:342:TRP:CD1	1:A:346:ARG:HG3	2.51	0.46
1:B:417:ARG:C	1:B:419:ARG:H	2.22	0.46
1:B:450:VAL:HA	1:B:471:LEU:CD1	2.45	0.46
1:B:654:ILE:CG1	1:B:674:ILE:HD13	2.42	0.46
1:C:171:ARG:HD2	1:C:232:LEU:CD1	2.44	0.46
1:C:372:PHE:HD1	1:C:375:MET:HE2	1.79	0.46
1:C:395:SER:O	1:C:399:GLU:HG3	2.16	0.46
1:D:24:TRP:O	1:D:28:THR:HG23	2.15	0.46
1:D:132:HIS:NE2	1:D:278:ILE:HG12	2.31	0.46
2:E:54:CYS:O	2:E:55:LEU:HD23	2.15	0.46
3:J:58:THR:HB	3:J:60:TYR:CZ	2.50	0.46
3:J:83:MET:HB3	3:J:86:LEU:CD2	2.40	0.46
1:B:675:GLU:O	1:B:697:LEU:HA	2.14	0.46
1:C:259:ILE:O	1:C:262:ARG:HG2	2.15	0.46
2:F:433:ARG:NH1	2:F:434:PHE:HB2	2.30	0.46
1:B:471:LEU:HD11	1:B:473:GLU:O	2.15	0.46
1:C:168:TRP:HZ2	1:C:399:GLU:HA	1.79	0.46
2:E:15:PRO:HD2	2:E:17:TYR:CD2	2.50	0.46
2:F:384:LEU:HD22	2:F:384:LEU:N	2.31	0.46
1:A:117:ARG:HA	1:A:117:ARG:HD3	1.63	0.46
1:B:262:ARG:HD2	1:B:266:ARG:HH21	1.80	0.46
1:B:485:ALA:HB3	1:B:486:PRO:HD3	1.98	0.46
1:B:637:HIS:CD2	1:B:638:LEU:HD23	2.50	0.46
1:C:156:PHE:CD2	1:C:375:MET:HG2	2.50	0.46
1:C:265:MET:CA	1:C:343:MET:HE1	2.45	0.46
1:C:341:TRP:NE1	1:C:345:ARG:HE	2.13	0.46
1:D:104:HIS:HB2	2:E:146:TYR:CE2	2.50	0.46
2:E:349:TYR:O	2:E:350:GLU:C	2.59	0.46
2:F:31:LEU:HD21	2:F:372:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:VAL:HA	2:F:150:ASN:OD1	2.15	0.46
2:F:182:PHE:CE1	2:F:186:TYR:HD1	2.33	0.46
1:A:354:GLU:OE1	1:A:357:ARG:HD2	2.16	0.46
1:B:39:ALA:HB1	1:B:130:LEU:HB2	1.97	0.46
1:B:136:PHE:HE1	1:B:274:LYS:HG2	1.80	0.46
1:B:353:PHE:HZ	1:B:391:ALA:HA	1.81	0.46
1:C:236:GLU:HA	1:C:239:GLN:CG	2.45	0.46
1:D:130:LEU:HA	1:D:133:THR:CG2	2.46	0.46
1:D:396:GLU:OE1	1:D:396:GLU:HA	2.16	0.46
2:F:31:LEU:CD1	2:F:376:TYR:HB2	2.46	0.46
1:A:28:THR:CG2	1:A:335:ILE:HG21	2.46	0.46
1:B:477:TYR:CG	1:B:501:LYS:HB3	2.51	0.46
1:B:502:PHE:HD1	1:B:504:ASP:C	2.23	0.46
1:B:569:LEU:HD23	1:B:590:MET:CE	2.30	0.46
1:B:671:ARG:HA	1:B:694:HIS:HB2	1.96	0.46
1:B:690:LEU:HD12	1:B:691:ASP:H	1.79	0.46
1:B:720:ILE:O	1:B:743:LEU:HD23	2.16	0.46
1:B:727:LEU:O	1:B:727:LEU:HD12	2.16	0.46
1:B:795:PRO:HG2	1:B:798:VAL:CG2	2.45	0.46
1:C:21:LYS:CG	1:C:25:ASP:HB3	2.44	0.46
1:C:283:VAL:CG2	1:C:326:ILE:HD13	2.46	0.46
1:C:374:PHE:CE2	1:C:378:LEU:HD11	2.51	0.46
1:D:16:ALA:O	1:D:19:ILE:HD13	2.16	0.46
1:D:261:TYR:HD2	1:D:374:PHE:HB2	1.80	0.46
1:D:277:LEU:CD1	1:D:278:ILE:HG13	2.46	0.46
1:D:400:ASN:HA	1:D:403:ARG:NH1	2.30	0.46
2:E:179:SER:OG	2:E:315:LYS:HE3	2.16	0.46
2:F:204:PHE:HE2	2:F:429:LEU:HD21	1.81	0.46
1:A:143:TRP:NE1	1:A:144:PHE:HD1	2.14	0.46
1:B:24:TRP:HB2	1:B:335:ILE:HG23	1.97	0.46
1:B:450:VAL:HA	1:B:471:LEU:HD12	1.97	0.46
1:B:452:LYS:CG	1:B:475:TRP:HB2	2.45	0.46
1:B:466:ALA:HA	1:B:490:PHE:CE1	2.51	0.46
1:B:528:SER:O	1:B:555:LEU:HD23	2.15	0.46
1:C:21:LYS:CD	1:C:25:ASP:HB3	2.46	0.46
1:C:351:TYR:N	1:C:373:ALA:HB2	2.31	0.46
2:E:50:ASP:OD1	2:E:356:HIS:HE1	1.99	0.46
2:E:299:GLU:OE1	2:E:416:PHE:HB3	2.16	0.46
2:F:294:PHE:CE1	2:F:298:VAL:HG21	2.50	0.46
1:A:154:GLU:O	1:A:157:VAL:HG12	2.15	0.46
1:B:349:LYS:O	1:B:370:ASN:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:LEU:HD12	1:B:408:ASN:OD1	2.16	0.46
1:B:412:THR:OG1	1:B:415:LYS:HG3	2.15	0.46
1:B:420:LEU:HB3	1:B:428:LEU:CD1	2.45	0.46
1:B:684:CYS:O	1:B:707:LEU:HD22	2.16	0.46
1:C:168:TRP:CZ2	1:C:402:LEU:HD13	2.51	0.46
1:C:278:ILE:HD11	1:C:325:TYR:OH	2.15	0.46
1:C:364:ASP:O	1:C:365:ILE:HD13	2.16	0.46
1:C:404:GLN:HA	1:C:404:GLN:NE2	2.31	0.46
1:D:142:PHE:HB3	1:D:267:GLN:OE1	2.16	0.46
2:E:279:LYS:HG3	2:E:283:GLN:HG3	1.97	0.46
2:E:384:LEU:HD22	2:E:384:LEU:N	2.31	0.46
2:F:141:LEU:HG	2:F:145:GLN:NE2	2.31	0.46
2:F:162:SER:CB	2:F:333:ILE:HG12	2.46	0.46
2:F:294:PHE:HE2	2:F:418:PHE:HZ	1.64	0.46
2:F:403:GLU:OE2	2:F:432:LYS:HD3	2.15	0.46
1:A:122:ALA:HA	1:A:289:ILE:HD11	1.98	0.46
1:B:168:TRP:CH2	1:B:398:SER:HB3	2.50	0.46
1:B:396:GLU:HA	1:B:396:GLU:OE1	2.15	0.46
1:B:495:LEU:HD21	1:B:498:LEU:HB2	1.96	0.46
1:B:629:ILE:O	1:B:632:ILE:HG12	2.15	0.46
1:C:243:LEU:CB	1:C:393:PHE:HE2	2.28	0.46
1:D:22:PRO:HB2	1:D:24:TRP:CE2	2.50	0.46
2:E:19:ILE:H	2:E:19:ILE:CD1	2.25	0.46
2:E:158:LEU:HD23	2:E:159:PRO:N	2.31	0.46
2:E:333:ILE:HG23	2:E:333:ILE:O	2.16	0.46
2:F:206:SER:HB3	2:F:209:THR:HG23	1.97	0.46
1:A:151:SER:O	1:A:154:GLU:HG2	2.16	0.45
1:B:118:LEU:HD12	1:B:119:HIS:H	1.82	0.45
1:B:780:LYS:HG2	1:B:805:ALA:HB1	1.98	0.45
1:C:302:LEU:HD23	1:C:302:LEU:N	2.31	0.45
1:C:398:SER:CA	1:C:401:LYS:HE3	2.35	0.45
2:E:36:LEU:HD23	2:E:36:LEU:C	2.41	0.45
2:E:287:LEU:HB3	2:E:437:PHE:HZ	1.80	0.45
2:E:346:LEU:CB	2:E:347:ILE:HD12	2.46	0.45
2:F:204:PHE:HD2	2:F:433:ARG:HE	1.62	0.45
3:J:72:LEU:HD12	3:J:73:ASP:H	1.79	0.45
1:A:313:PRO:HB3	2:F:151:GLN:NE2	2.31	0.45
1:B:49:GLN:O	1:B:314:LEU:HD11	2.17	0.45
1:D:399:GLU:H	1:D:399:GLU:CD	2.24	0.45
2:F:409:ILE:HG23	2:F:441:VAL:HG13	1.97	0.45
1:A:112:VAL:HG13	1:A:113:CYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:SER:O	1:B:154:GLU:HG2	2.16	0.45
1:B:341:TRP:NE1	1:B:345:ARG:HD2	2.30	0.45
1:B:688:ARG:C	1:B:710:LEU:HD12	2.41	0.45
1:C:118:LEU:HD21	1:C:312:HIS:CE1	2.51	0.45
1:C:356:ILE:HA	1:C:359:GLU:HG3	1.98	0.45
1:D:37:MET:HE2	1:D:37:MET:CA	2.32	0.45
1:D:342:TRP:HA	1:D:345:ARG:CG	2.46	0.45
1:D:354:GLU:OE2	1:D:358:GLU:HG2	2.16	0.45
2:E:138:LYS:C	2:E:139:THR:HG23	2.41	0.45
2:E:195:HIS:CE1	2:E:199:ILE:HD11	2.51	0.45
2:E:204:PHE:HD1	2:E:433:ARG:HE	1.63	0.45
1:A:300:GLU:HA	1:A:304:GLY:CA	2.46	0.45
1:A:356:ILE:HG13	1:A:388:LYS:HZ2	1.82	0.45
1:B:232:LEU:HD11	1:B:236:GLU:CB	2.45	0.45
1:B:249:LYS:HZ3	1:B:250:PHE:CA	2.29	0.45
1:B:263:LEU:HD23	1:B:263:LEU:O	2.16	0.45
1:B:354:GLU:OE2	1:B:358:GLU:HB3	2.15	0.45
1:B:463:PRO:HB3	1:B:486:PRO:CB	2.35	0.45
1:B:784:LEU:HG	1:B:786:VAL:HG12	1.99	0.45
1:D:117:ARG:HA	1:D:117:ARG:HE	1.79	0.45
1:D:140:SER:HB3	1:D:271:LYS:HZ3	1.81	0.45
1:D:168:TRP:HA	1:D:171:ARG:CG	2.45	0.45
2:E:385:PHE:CD1	2:E:386:TRP:HD1	2.33	0.45
2:F:19:ILE:O	2:F:20:LEU:HB2	2.17	0.45
2:F:198:SER:O	2:F:202:LYS:HG2	2.16	0.45
2:F:436:VAL:O	2:F:439:SER:HB3	2.16	0.45
3:J:0:SER:HA	3:J:114:TYR:OH	2.16	0.45
1:A:146:PHE:CD1	1:A:147:PRO:HD2	2.51	0.45
1:A:270:ILE:HA	1:A:273:ILE:HD11	1.98	0.45
1:B:613:LEU:HB2	1:B:616:LEU:CD1	2.46	0.45
1:B:641:LEU:CG	1:B:664:LEU:HD21	2.21	0.45
1:B:671:ARG:HD3	1:B:694:HIS:CB	2.46	0.45
1:B:676:LYS:NZ	1:B:699:PHE:H	2.15	0.45
1:B:698:THR:HG22	1:B:699:PHE:CE2	2.51	0.45
1:B:739:GLY:HA2	1:B:762:ARG:O	2.17	0.45
1:C:135:ILE:HG21	1:C:274:LYS:HD2	1.97	0.45
2:E:288:PHE:HB3	2:E:292:ARG:HH21	1.80	0.45
2:E:327:ALA:HA	2:E:330:VAL:HG11	1.99	0.45
2:F:149:ILE:HD11	2:F:343:VAL:HG21	1.98	0.45
2:F:303:LEU:O	2:F:307:LEU:N	2.49	0.45
3:J:28:ILE:HD13	3:J:72:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:THR:HG23	1:A:317:LEU:N	2.31	0.45
1:B:420:LEU:CD1	1:B:445:LEU:HD13	2.30	0.45
1:B:451:LEU:H	1:B:471:LEU:HD11	1.81	0.45
1:B:548:VAL:HG13	1:B:571:LYS:HB3	1.97	0.45
1:B:700:LEU:CD2	1:B:720:ILE:HD13	2.37	0.45
1:D:56:PRO:HG3	1:D:305:TYR:CD2	2.51	0.45
1:D:118:LEU:CD2	1:D:123:LYS:HG3	2.47	0.45
1:D:153:LEU:HD21	1:D:260:VAL:HG11	1.99	0.45
2:E:209:THR:O	2:E:213:LEU:HD23	2.16	0.45
2:E:370:ILE:HD13	2:E:370:ILE:HA	1.83	0.45
3:J:88:PRO:HA	3:J:123:VAL:HB	1.99	0.45
1:B:117:ARG:HA	1:B:117:ARG:HE	1.80	0.45
1:B:548:VAL:CG2	1:B:571:LYS:HB3	2.39	0.45
1:C:158:SER:HB2	1:C:162:LYS:HE3	1.99	0.45
1:C:353:PHE:O	1:C:356:ILE:HD13	2.17	0.45
1:D:121:PHE:CD2	1:D:285:TYR:HB3	2.48	0.45
1:D:279:ILE:HD11	1:D:329:VAL:HG12	1.98	0.45
2:E:327:ALA:HA	2:E:330:VAL:CG1	2.47	0.45
2:E:333:ILE:HG23	2:E:363:LYS:HE2	1.98	0.45
1:A:151:SER:HA	1:A:154:GLU:HG2	1.98	0.45
1:B:577:GLU:OE2	3:J:52:ALA:HB2	2.16	0.45
1:B:678:PRO:HB2	1:B:680:GLN:OE1	2.16	0.45
2:F:42:ALA:HB2	2:F:365:LEU:CD2	2.45	0.45
3:J:51:LEU:HD23	3:J:52:ALA:C	2.42	0.45
3:J:98:ALA:HB3	3:J:114:TYR:HB2	1.98	0.45
1:A:135:ILE:CG2	1:A:274:LYS:HD2	2.43	0.45
1:A:330:ILE:HD13	1:A:330:ILE:HA	1.81	0.45
1:B:28:THR:HB	1:B:332:TYR:CZ	2.52	0.45
1:B:353:PHE:O	1:B:353:PHE:HD1	1.99	0.45
1:B:368:VAL:HG12	1:B:369:LYS:N	2.32	0.45
1:B:577:GLU:OE1	1:B:577:GLU:HA	2.17	0.45
1:B:767:GLU:O	1:B:790:LEU:HD22	2.17	0.45
1:C:341:TRP:CD1	1:C:345:ARG:HE	2.34	0.45
1:D:168:TRP:CZ2	1:D:402:LEU:HD23	2.50	0.45
2:E:396:SER:HA	2:E:399:LYS:CE	2.45	0.45
2:F:55:LEU:HB3	2:F:56:PRO:HD2	1.97	0.45
3:J:108:TYR:HB3	3:J:110:GLU:CD	2.42	0.45
1:A:104:HIS:HB2	1:B:106:TYR:CD2	2.52	0.45
1:A:125:PHE:CE1	1:A:322:ALA:HA	2.52	0.45
1:A:155:HIS:C	1:A:155:HIS:HD1	2.25	0.45
1:A:251:ARG:O	1:A:255:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:ARG:HA	1:B:515:LEU:HA	1.99	0.45
1:B:551:LEU:O	1:B:574:ILE:HA	2.16	0.45
1:B:681:LEU:HD23	1:B:681:LEU:C	2.41	0.45
1:C:31:ILE:C	1:C:35:MET:HE2	2.42	0.45
1:D:345:ARG:HG3	1:D:346:ARG:CD	2.46	0.45
2:E:40:ILE:HD13	2:E:40:ILE:HA	1.85	0.45
2:F:366:LEU:HD12	2:F:370:ILE:HG12	1.99	0.45
3:J:20:LEU:HD22	3:J:119:THR:CG2	2.39	0.45
3:J:60:TYR:CE1	3:J:70:VAL:HG12	2.51	0.45
1:A:45:LEU:HG	1:A:314:LEU:CD2	2.47	0.44
1:A:100:ASP:HB3	1:B:98:LYS:CE	2.43	0.44
1:A:268:THR:HG21	1:A:339:THR:HG22	1.98	0.44
1:A:353:PHE:CD1	1:A:356:ILE:HD13	2.51	0.44
1:B:128:LEU:N	1:B:128:LEU:HD23	2.32	0.44
1:B:130:LEU:HD23	1:B:134:LEU:HG	1.99	0.44
1:B:428:LEU:CD2	1:B:447:GLU:HG2	2.46	0.44
1:B:705:GLY:HA3	1:B:729:GLN:OE1	2.18	0.44
1:B:736:LEU:HG	1:B:738:LEU:HG	1.99	0.44
1:B:773:LEU:HD12	1:B:794:LEU:HD11	1.99	0.44
1:C:35:MET:HA	1:C:38:ILE:HG12	1.99	0.44
1:C:277:LEU:HD23	1:C:277:LEU:O	2.16	0.44
1:D:52:MET:SD	1:D:114:TYR:HA	2.57	0.44
1:D:232:LEU:HD12	1:D:232:LEU:C	2.41	0.44
2:E:288:PHE:HA	2:E:437:PHE:HE1	1.82	0.44
2:F:58:LEU:CB	2:F:59:PRO:HD3	2.46	0.44
1:A:115:GLU:OE2	1:B:316:THR:HB	2.17	0.44
1:A:129:VAL:HG13	1:A:325:TYR:HE1	1.79	0.44
1:B:245:GLU:OE1	1:B:246:LYS:HD3	2.18	0.44
1:B:580:LYS:HG2	1:B:582:ILE:HD12	2.00	0.44
1:C:259:ILE:HD12	1:C:262:ARG:HD3	1.98	0.44
1:C:348:LEU:HA	1:C:377:HIS:CE1	2.52	0.44
1:D:345:ARG:HG3	1:D:346:ARG:HE	1.82	0.44
1:A:279:ILE:HG23	1:A:280:CYS:N	2.31	0.44
1:A:403:ARG:HH22	1:A:404:GLN:HE21	1.65	0.44
1:B:466:ALA:HA	1:B:490:PHE:CD2	2.51	0.44
1:B:632:ILE:HG13	1:B:633:ILE:N	2.33	0.44
1:B:665:GLU:C	1:B:687:LEU:HD23	2.42	0.44
1:B:748:SER:HB2	1:B:772:GLU:CD	2.42	0.44
1:D:356:ILE:CA	1:D:359:GLU:HG2	2.45	0.44
2:E:28:MET:HE3	2:E:379:ILE:HG22	1.98	0.44
2:F:288:PHE:O	2:F:292:ARG:NE	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:288:PHE:CE1	2:F:443:GLU:HB2	2.51	0.44
1:A:21:LYS:HB3	1:A:25:ASP:CB	2.47	0.44
1:A:65:CYS:HB3	2:F:346:LEU:CD2	2.47	0.44
1:A:154:GLU:CA	1:A:157:VAL:HG12	2.47	0.44
1:A:158:SER:HA	1:A:161:LEU:HD21	1.99	0.44
1:A:356:ILE:HD12	1:A:356:ILE:H	1.82	0.44
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.85	0.44
1:B:272:VAL:HG23	1:B:336:CYS:HB3	1.99	0.44
1:B:611:PHE:HZ	1:B:631:GLU:HB3	1.81	0.44
1:B:655:PRO:O	1:B:658:ILE:HG22	2.17	0.44
1:B:666:ARG:HB3	1:B:668:TYR:CE1	2.52	0.44
1:B:711:GLN:HA	1:B:733:LEU:HA	1.99	0.44
1:C:342:TRP:HA	1:C:345:ARG:NH1	2.33	0.44
2:E:285:LYS:HD3	2:E:446:LEU:CD2	2.46	0.44
2:F:58:LEU:HD23	2:F:59:PRO:N	2.32	0.44
2:F:138:LYS:C	2:F:140:ASN:H	2.26	0.44
1:A:46:GLN:HB2	1:A:318:PHE:CZ	2.51	0.44
1:A:101:LEU:HA	1:A:105:GLN:NE2	2.32	0.44
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.81	0.44
1:A:306:ARG:HB3	1:A:306:ARG:CZ	2.47	0.44
1:B:19:ILE:HD12	1:B:19:ILE:N	2.29	0.44
1:B:167:PRO:HG2	1:B:236:GLU:OE2	2.17	0.44
1:B:438:ILE:CD1	1:B:460:THR:O	2.59	0.44
1:B:481:ALA:CB	1:B:511:TRP:HZ2	2.25	0.44
1:B:598:LEU:HB2	1:B:621:LEU:HD22	1.98	0.44
1:C:135:ILE:HG21	1:C:274:LYS:CD	2.48	0.44
1:C:251:ARG:O	1:C:255:GLU:HG2	2.17	0.44
1:C:355:SER:O	1:C:359:GLU:HG3	2.17	0.44
1:D:343:MET:C	1:D:344:LEU:HD23	2.41	0.44
1:D:348:LEU:HD12	1:D:348:LEU:H	1.81	0.44
1:D:368:VAL:HG12	1:D:373:ALA:N	2.32	0.44
2:E:159:PRO:CB	2:E:161:TYR:CZ	2.94	0.44
2:E:390:ILE:HB	2:E:391:PRO:HD3	2.00	0.44
3:J:16:GLY:O	3:J:86:LEU:HG	2.17	0.44
1:A:96:GLY:HA3	2:F:141:LEU:HD13	2.00	0.44
1:A:108:TYR:CB	1:B:55:LEU:HD11	2.47	0.44
1:B:22:PRO:HD2	1:B:25:ASP:CG	2.42	0.44
1:B:147:PRO:HA	1:B:150:SER:HG	1.82	0.44
1:B:474:LEU:CD1	1:B:476:LEU:HD21	2.43	0.44
1:B:611:PHE:CZ	1:B:634:SER:HB2	2.53	0.44
1:C:356:ILE:HA	1:C:359:GLU:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:GLU:OE1	1:D:369:LYS:HB3	2.17	0.44
2:E:180:SER:HA	2:E:311:GLN:NE2	2.33	0.44
2:F:56:PRO:HG3	2:F:139:THR:HB	2.00	0.44
2:F:358:MET:HE3	2:F:358:MET:HB3	1.64	0.44
1:A:36:LEU:HD13	1:A:133:THR:HG21	2.00	0.44
1:A:147:PRO:HA	1:A:150:SER:OG	2.18	0.44
1:B:150:SER:O	1:B:154:GLU:HG2	2.18	0.44
1:B:451:LEU:O	1:B:474:LEU:HD12	2.18	0.44
1:B:661:LEU:N	1:B:661:LEU:HD23	2.33	0.44
1:C:20:LEU:O	1:C:22:PRO:HD3	2.18	0.44
1:C:289:ILE:HG22	1:C:289:ILE:O	2.17	0.44
1:C:298:ASP:HA	1:C:306:ARG:HH12	1.81	0.44
1:C:366:PRO:CD	1:C:394:LEU:HD21	2.48	0.44
2:F:58:LEU:CD1	2:F:137:ARG:HH22	2.30	0.44
2:F:366:LEU:HD12	2:F:366:LEU:C	2.42	0.44
1:B:679:THR:HA	1:B:682:PHE:HD2	1.79	0.44
1:D:37:MET:HE2	1:D:40:VAL:HG11	1.98	0.44
2:E:141:LEU:HG	2:E:145:GLN:NE2	2.32	0.44
2:E:148:PHE:HD2	2:F:53:VAL:CG2	2.30	0.44
2:E:156:LEU:N	2:E:156:LEU:HD23	2.33	0.44
2:E:289:GLU:HA	2:E:292:ARG:NE	2.32	0.44
2:E:399:LYS:HG3	2:E:400:VAL:H	1.83	0.44
1:A:56:PRO:HG2	1:A:99:TYR:CD1	2.53	0.44
1:B:657:GLN:CD	1:B:657:GLN:H	2.24	0.44
1:B:671:ARG:CZ	3:J:108:TYR:HD1	2.31	0.44
1:B:754:THR:O	1:B:778:LEU:HG	2.18	0.44
1:C:234:LYS:NZ	1:C:410:GLU:HA	2.32	0.44
1:C:265:MET:CB	1:C:343:MET:HE1	2.48	0.44
2:E:339:CYS:O	2:E:351:VAL:HB	2.17	0.44
3:J:51:LEU:HD23	3:J:52:ALA:O	2.18	0.44
1:A:316:THR:HB	2:F:155:HIS:NE2	2.32	0.43
1:B:428:LEU:O	1:B:448:LEU:HD12	2.18	0.43
1:B:512:ILE:HG13	1:B:513:TYR:N	2.32	0.43
1:B:784:LEU:HD23	1:B:791:PHE:CE1	2.53	0.43
1:C:372:PHE:CE1	1:C:376:LEU:HD21	2.53	0.43
1:C:406:ASN:HA	1:C:409:ASN:HD22	1.83	0.43
2:E:54:CYS:HA	2:E:354:CYS:HA	2.00	0.43
2:F:213:LEU:HD11	2:F:436:VAL:HG21	1.99	0.43
2:F:347:ILE:O	2:F:347:ILE:CG2	2.66	0.43
1:A:106:TYR:HB3	2:F:144:GLN:HE21	1.83	0.43
1:A:389:ARG:HB3	1:A:389:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:MET:HE2	1:B:337:MET:HB3	1.90	0.43
1:B:357:ARG:HB2	1:B:362:TYR:O	2.17	0.43
1:B:700:LEU:CG	1:B:724:PRO:HD2	2.47	0.43
1:B:757:THR:CG2	1:B:778:LEU:HB3	2.45	0.43
1:C:146:PHE:HD2	1:C:149:THR:HG22	1.83	0.43
1:C:366:PRO:HD2	1:C:394:LEU:HD21	2.00	0.43
1:D:102:ASP:H	1:D:105:GLN:CD	2.26	0.43
2:E:161:TYR:CE2	2:E:329:PHE:HB2	2.53	0.43
1:A:235:LYS:HA	1:A:238:GLU:CD	2.43	0.43
1:A:349:LYS:HD2	1:A:370:ASN:CB	2.48	0.43
1:B:28:THR:HG23	1:B:335:ILE:HG21	2.01	0.43
1:B:146:PHE:HD1	1:B:147:PRO:CD	2.26	0.43
1:B:339:THR:HG22	1:B:340:LEU:N	2.31	0.43
1:C:244:PHE:HB3	1:C:248:LYS:HZ2	1.81	0.43
1:C:349:LYS:HE2	1:C:370:ASN:CB	2.48	0.43
1:C:350:LYS:HA	1:C:368:VAL:O	2.18	0.43
1:C:356:ILE:HD12	1:C:356:ILE:H	1.83	0.43
1:D:167:PRO:HG2	1:D:236:GLU:OE2	2.18	0.43
1:D:297:VAL:HG23	1:D:299:ILE:HG12	2.00	0.43
2:F:19:ILE:H	2:F:19:ILE:CD1	2.29	0.43
3:J:42:GLY:O	3:J:43:LYS:HD2	2.19	0.43
3:J:50:ALA:HB3	3:J:106:PRO:HB3	1.99	0.43
1:A:115:GLU:HG2	1:B:291:PHE:CD2	2.54	0.43
1:A:156:PHE:CG	1:A:375:MET:HG2	2.53	0.43
1:B:173:LEU:CD2	1:B:392:VAL:HG11	2.48	0.43
1:B:394:LEU:HD22	1:B:394:LEU:N	2.33	0.43
1:B:675:GLU:HB3	1:B:719:ARG:HH21	1.83	0.43
1:B:759:ILE:HD11	1:B:761:LEU:HD21	2.01	0.43
1:C:21:LYS:HG3	1:C:25:ASP:CB	2.48	0.43
1:D:39:ALA:CB	1:D:129:VAL:HG13	2.48	0.43
1:D:104:HIS:CE1	2:E:146:TYR:HB3	2.54	0.43
1:D:149:THR:CG2	1:D:260:VAL:HG22	2.48	0.43
1:D:237:GLY:HA3	1:D:406:ASN:OD1	2.19	0.43
1:D:278:ILE:HA	1:D:281:TYR:CE1	2.53	0.43
2:E:170:LEU:HD23	2:E:171:ILE:HD13	2.00	0.43
2:F:419:LEU:O	2:F:419:LEU:HD22	2.17	0.43
1:A:100:ASP:CB	1:B:98:LYS:HE3	2.43	0.43
1:A:283:VAL:HG12	1:A:284:TYR:N	2.33	0.43
1:B:316:THR:HG23	1:B:317:LEU:N	2.34	0.43
1:B:701:PRO:O	1:B:704:ILE:HG22	2.16	0.43
1:C:340:LEU:HD13	1:C:340:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:SER:HB3	1:C:362:TYR:CD2	2.53	0.43
1:D:125:PHE:N	1:D:126:PRO:HD2	2.34	0.43
1:D:146:PHE:HD1	1:D:147:PRO:CD	2.27	0.43
2:E:17:TYR:O	2:E:21:LYS:HE3	2.18	0.43
2:E:31:LEU:CD1	2:E:375:VAL:HG12	2.48	0.43
2:E:353:GLU:HA	2:E:353:GLU:OE1	2.18	0.43
1:A:24:TRP:HB2	1:A:335:ILE:HG23	1.99	0.43
1:A:275:PHE:CE1	1:A:333:GLY:HA3	2.53	0.43
1:B:159:ILE:HD12	1:B:250:PHE:CD1	2.53	0.43
1:B:258:ASP:HA	1:B:371:ASP:HB2	2.01	0.43
1:B:353:PHE:O	1:B:357:ARG:HD2	2.19	0.43
1:B:364:ASP:OD2	1:B:397:VAL:HG13	2.18	0.43
1:C:232:LEU:HB3	1:C:236:GLU:OE1	2.18	0.43
1:D:118:LEU:HD11	1:D:122:ALA:HB3	2.00	0.43
2:E:277:ASP:HB2	2:E:453:HIS:CE1	2.53	0.43
2:E:305:TYR:O	2:E:309:VAL:HG23	2.19	0.43
2:E:394:GLU:HA	2:E:417:ALA:CB	2.49	0.43
2:E:451:LEU:O	2:E:454:GLU:HG2	2.17	0.43
2:F:411:ASP:HA	2:F:439:SER:CA	2.49	0.43
1:A:106:TYR:CE2	2:F:142:ASP:OD2	2.72	0.43
1:B:576:ASN:ND2	1:B:581:LEU:HB2	2.34	0.43
1:B:584:LEU:HD12	1:B:586:SER:H	1.83	0.43
1:D:349:LYS:O	1:D:373:ALA:HB3	2.19	0.43
2:E:28:MET:HE2	2:E:379:ILE:HG22	2.01	0.43
3:J:6:GLU:HA	3:J:21:SER:O	2.18	0.43
3:J:8:GLY:HA3	3:J:19:ARG:O	2.18	0.43
1:A:51:LYS:NZ	1:A:313:PRO:HG3	2.34	0.43
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.76	0.43
1:A:346:ARG:HB2	1:A:348:LEU:HD23	2.01	0.43
1:B:126:PRO:O	1:B:129:VAL:HG12	2.18	0.43
1:B:451:LEU:N	1:B:471:LEU:HD11	2.34	0.43
1:B:580:LYS:HG2	1:B:582:ILE:HD11	2.00	0.43
1:B:737:HIS:C	1:B:738:LEU:HD23	2.42	0.43
1:C:46:GLN:O	1:C:50:ASP:HB3	2.19	0.43
1:D:19:ILE:H	1:D:19:ILE:CD1	2.26	0.43
2:E:189:THR:O	2:E:192:LYS:HG2	2.19	0.43
2:E:450:SER:O	2:E:454:GLU:HG2	2.19	0.43
2:F:22:PRO:O	2:F:26:VAL:HG23	2.19	0.43
2:F:31:LEU:HD21	2:F:376:TYR:HB2	2.00	0.43
2:F:344:GLU:CB	2:F:350:GLU:CA	2.96	0.43
2:F:399:LYS:HZ3	2:F:420:LEU:HG	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:109:TYR:HB2	3:J:115:TRP:CH2	2.54	0.43
1:A:313:PRO:HB3	2:F:151:GLN:HE21	1.81	0.43
1:A:351:TYR:HB2	1:A:373:ALA:HB1	2.00	0.43
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.75	0.43
1:B:647:TRP:HA	1:B:672:ASN:HD21	1.84	0.43
1:D:242:ALA:C	1:D:245:GLU:HG3	2.44	0.43
1:D:368:VAL:HG11	1:D:372:PHE:HD1	1.84	0.43
1:D:369:LYS:HG2	1:D:370:ASN:N	2.27	0.43
2:E:15:PRO:HG2	2:E:16:THR:H	1.82	0.43
2:F:291:VAL:HG12	2:F:438:LEU:HD13	2.01	0.43
3:J:73:ASP:HB2	3:J:80:TYR:OH	2.18	0.43
1:A:36:LEU:CB	1:A:133:THR:HG21	2.45	0.43
1:A:243:LEU:O	1:A:246:LYS:HG2	2.19	0.43
1:B:235:LYS:HA	1:B:238:GLU:HG2	1.99	0.43
1:B:598:LEU:HB2	1:B:621:LEU:CD2	2.49	0.43
1:B:698:THR:C	1:B:720:ILE:HA	2.44	0.43
1:B:769:LEU:HB2	1:B:794:LEU:HG	2.00	0.43
1:D:242:ALA:HA	1:D:245:GLU:HG3	2.01	0.43
1:D:278:ILE:HA	1:D:281:TYR:CD1	2.54	0.43
2:E:148:PHE:CE2	2:F:355:THR:CG2	3.01	0.43
2:F:20:LEU:N	2:F:20:LEU:HD12	2.34	0.43
2:F:310:VAL:O	2:F:314:ILE:HG22	2.19	0.43
1:A:139:CYS:HB3	1:A:271:LYS:HE3	2.01	0.42
1:A:251:ARG:HG2	1:A:255:GLU:HG2	1.99	0.42
1:A:278:ILE:HG23	1:A:279:ILE:N	2.34	0.42
1:B:45:LEU:CD2	1:B:317:LEU:HD23	2.49	0.42
1:B:57:CYS:HB3	1:B:65:CYS:HB3	1.96	0.42
1:B:443:PHE:HD1	1:B:465:ILE:HA	1.84	0.42
1:B:590:MET:CE	1:B:593:LEU:HD21	2.48	0.42
1:B:606:ILE:HB	1:B:631:GLU:CG	2.49	0.42
1:C:164:PHE:CA	1:C:389:ARG:HH12	2.25	0.42
1:C:328:LEU:HA	1:C:328:LEU:HD23	1.71	0.42
2:E:285:LYS:HB2	2:E:446:LEU:CD2	2.48	0.42
2:E:399:LYS:HZ3	2:E:421:HIS:N	2.17	0.42
2:F:409:ILE:CG2	2:F:442:SER:HB2	2.41	0.42
3:J:83:MET:HE2	3:J:86:LEU:HD22	1.98	0.42
1:B:692:LEU:HB3	1:B:697:LEU:HD11	1.97	0.42
1:B:736:LEU:HG	1:B:738:LEU:CG	2.49	0.42
2:E:409:ILE:HG21	2:E:442:SER:HB2	2.00	0.42
2:F:168:LEU:HA	2:F:168:LEU:HD22	1.82	0.42
3:J:105:SER:O	3:J:111:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLU:OE1	1:A:300:GLU:CA	2.68	0.42
1:B:234:LYS:CG	1:B:409:ASN:HB3	2.47	0.42
1:B:593:LEU:C	1:B:616:LEU:HD23	2.44	0.42
1:B:716:THR:HG23	1:B:739:GLY:C	2.44	0.42
1:C:275:PHE:O	1:C:278:ILE:HG22	2.20	0.42
1:D:356:ILE:HG22	1:D:359:GLU:OE2	2.20	0.42
1:A:54:CYS:HA	1:A:310:CYS:HA	2.01	0.42
1:A:156:PHE:HA	1:A:159:ILE:CG1	2.50	0.42
1:A:159:ILE:HA	1:A:162:LYS:HZ3	1.83	0.42
1:A:269:ILE:HD12	1:A:340:LEU:CD2	2.34	0.42
1:B:108:TYR:CB	1:C:55:LEU:HD11	2.50	0.42
1:B:265:MET:HG2	1:B:343:MET:SD	2.59	0.42
1:B:493:GLU:OE1	1:B:493:GLU:HA	2.19	0.42
1:B:574:ILE:HB	1:B:598:LEU:CD2	2.47	0.42
1:B:723:LEU:CD1	1:B:738:LEU:HD13	2.49	0.42
1:C:289:ILE:HG22	1:C:319:LYS:NZ	2.34	0.42
1:C:398:SER:C	1:C:401:LYS:HG2	2.44	0.42
2:E:287:LEU:O	2:E:291:VAL:HG23	2.20	0.42
1:A:115:GLU:HB2	1:B:291:PHE:CE1	2.55	0.42
1:A:122:ALA:CB	1:A:289:ILE:HG12	2.49	0.42
1:B:49:GLN:O	1:B:49:GLN:HG2	2.19	0.42
1:B:445:LEU:HD22	1:B:447:GLU:OE2	2.18	0.42
1:B:450:VAL:HG22	1:B:473:GLU:CB	2.33	0.42
1:B:689:TYR:CE2	1:B:712:ASN:HB3	2.54	0.42
1:B:693:SER:CA	1:B:718:ASN:HD21	2.29	0.42
1:B:769:LEU:HB2	1:B:794:LEU:CG	2.49	0.42
1:C:34:VAL:O	1:C:38:ILE:HG23	2.19	0.42
1:C:119:HIS:CD2	1:C:288:ASN:HD22	2.38	0.42
1:D:274:LYS:O	1:D:277:LEU:HG	2.19	0.42
2:E:379:ILE:O	2:E:384:LEU:HD23	2.19	0.42
2:F:303:LEU:HD23	2:F:303:LEU:HA	1.86	0.42
2:F:344:GLU:CB	2:F:350:GLU:CB	2.97	0.42
3:J:93:LEU:HD23	3:J:95:TYR:HH	1.83	0.42
1:A:282:THR:HG22	1:A:326:ILE:CD1	2.37	0.42
1:B:28:THR:CG2	1:B:335:ILE:HG21	2.49	0.42
1:B:475:TRP:HE3	1:B:477:TYR:HH	1.61	0.42
1:B:723:LEU:HD11	1:B:743:LEU:CD1	2.50	0.42
1:C:38:ILE:HD12	1:C:325:TYR:HB2	2.01	0.42
1:C:259:ILE:HA	1:C:262:ARG:HG2	2.01	0.42
1:C:392:VAL:HG23	1:C:393:PHE:CD1	2.42	0.42
1:D:400:ASN:HA	1:D:403:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:31:LEU:HG	2:E:372:ILE:HG23	2.01	0.42
2:E:345:HIS:CD2	2:E:346:LEU:HD13	2.55	0.42
2:E:373:ILE:HD12	2:E:373:ILE:HA	1.79	0.42
2:E:380:CYS:HA	2:E:384:LEU:HD23	2.00	0.42
1:A:172:ALA:O	1:A:175:GLU:HB2	2.20	0.42
1:A:175:GLU:OE1	1:A:175:GLU:HA	2.19	0.42
1:A:275:PHE:O	1:A:279:ILE:HG22	2.20	0.42
1:D:351:TYR:CB	1:D:368:VAL:HB	2.48	0.42
2:F:22:PRO:HB2	2:F:24:TRP:CD2	2.55	0.42
1:A:364:ASP:OD2	1:A:395:SER:HB2	2.19	0.42
1:B:259:ILE:HG23	1:B:260:VAL:N	2.34	0.42
1:B:404:GLN:HA	1:B:407:LEU:CG	2.49	0.42
1:B:474:LEU:HD21	1:B:476:LEU:HD11	2.01	0.42
1:B:600:ARG:HD2	3:J:59:TYR:OH	2.18	0.42
1:B:780:LYS:HG2	1:B:805:ALA:CB	2.49	0.42
1:C:147:PRO:HG3	1:D:23:TRP:CA	2.50	0.42
1:C:234:LYS:HZ2	1:C:410:GLU:HA	1.85	0.42
1:D:22:PRO:HD2	1:D:25:ASP:OD2	2.19	0.42
1:D:101:LEU:HD21	2:E:136:GLY:HA3	2.01	0.42
2:F:55:LEU:O	2:F:352:PHE:HB3	2.20	0.42
3:J:93:LEU:HG	3:J:95:TYR:CZ	2.55	0.42
1:B:351:TYR:HD1	1:B:352:SER:N	2.17	0.42
1:B:615:ASN:CG	1:B:640:ARG:HH11	2.28	0.42
1:C:255:GLU:OE1	1:C:255:GLU:HA	2.20	0.42
1:D:15:PRO:HG2	1:D:16:ALA:H	1.85	0.42
1:D:127:TYR:CE2	2:E:361:MET:HE1	2.54	0.42
1:D:231:VAL:HA	1:D:405:LEU:HD21	2.02	0.42
2:E:289:GLU:HA	2:E:292:ARG:HD3	2.01	0.42
2:E:303:LEU:O	2:E:307:LEU:HB2	2.20	0.42
2:F:186:TYR:HE2	2:F:188:LYS:CB	2.30	0.42
2:F:287:LEU:HB3	2:F:437:PHE:HZ	1.82	0.42
2:F:412:VAL:HG12	2:F:414:ASN:H	1.85	0.42
1:A:104:HIS:CE1	1:B:106:TYR:HB3	2.55	0.42
1:B:116:ASN:HB3	1:B:117:ARG:NH2	2.33	0.42
1:B:120:TRP:HZ2	1:B:285:TYR:CE2	2.38	0.42
1:B:249:LYS:HG3	1:B:250:PHE:N	2.35	0.42
1:B:305:TYR:OH	1:C:95:THR:HA	2.20	0.42
1:B:345:ARG:HG3	1:B:346:ARG:HE	1.85	0.42
1:B:461:ILE:HB	1:B:483:ILE:HG13	2.01	0.42
1:B:587:LEU:HD12	1:B:587:LEU:O	2.20	0.42
1:B:636:GLN:HB3	1:B:660:ASN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ARG:HH22	1:D:103:ARG:HH21	1.66	0.42
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.73	0.42
1:C:258:ASP:N	1:C:371:ASP:HB2	2.35	0.42
1:C:370:ASN:O	1:C:371:ASP:HB3	2.20	0.42
1:D:118:LEU:HD23	1:D:123:LYS:CG	2.49	0.42
1:D:119:HIS:CE1	1:D:121:PHE:HB2	2.55	0.42
2:F:158:LEU:HD22	2:F:158:LEU:HA	1.74	0.42
1:A:371:ASP:OD1	1:A:371:ASP:O	2.38	0.41
1:B:126:PRO:O	1:B:129:VAL:CG1	2.68	0.41
1:B:259:ILE:HD13	1:B:262:ARG:HH21	1.85	0.41
1:B:665:GLU:HG2	1:B:686:LYS:O	2.20	0.41
1:B:666:ARG:HD2	1:B:668:TYR:OH	2.20	0.41
1:D:258:ASP:O	1:D:262:ARG:HG2	2.20	0.41
1:D:369:LYS:CG	1:D:370:ASN:H	2.26	0.41
2:E:186:TYR:HE2	2:E:188:LYS:HB3	1.83	0.41
2:E:211:LYS:HA	2:E:214:SER:OG	2.20	0.41
1:A:46:GLN:HA	1:A:50:ASP:HB3	2.02	0.41
1:B:404:GLN:HA	1:B:407:LEU:HD21	2.02	0.41
1:B:681:LEU:HD23	1:B:682:PHE:N	2.35	0.41
1:C:168:TRP:CE2	1:C:244:PHE:HZ	2.38	0.41
1:D:126:PRO:HA	1:D:129:VAL:HG12	2.01	0.41
1:D:259:ILE:HG23	1:D:260:VAL:N	2.35	0.41
2:E:142:ASP:OD2	2:F:146:TYR:HE2	2.02	0.41
2:E:306:LYS:O	2:E:310:VAL:HG12	2.20	0.41
2:F:301:SER:O	2:F:302:ASP:C	2.62	0.41
3:J:18:LEU:HD12	3:J:121:VAL:CG1	2.49	0.41
1:A:36:LEU:HD13	1:A:133:THR:CG2	2.50	0.41
1:A:38:ILE:HD11	1:A:325:TYR:HB2	2.01	0.41
1:A:302:LEU:HA	1:B:99:TYR:OH	2.20	0.41
1:B:36:LEU:C	1:B:36:LEU:HD23	2.44	0.41
1:B:163:CYS:O	1:B:169:THR:HG21	2.21	0.41
1:B:293:VAL:HG22	1:B:294:ASP:O	2.21	0.41
1:B:395:SER:O	1:B:396:GLU:HB3	2.20	0.41
1:B:552:LYS:HA	1:B:575:ASN:O	2.19	0.41
1:B:583:VAL:CG2	1:B:607:PRO:HB3	2.49	0.41
1:B:590:MET:HE2	1:B:593:LEU:HG	2.02	0.41
1:B:756:LEU:HD12	1:B:757:THR:N	2.34	0.41
1:C:162:LYS:HA	1:C:165:ASP:OD2	2.19	0.41
1:C:261:TYR:HB2	1:C:374:PHE:CD1	2.56	0.41
2:E:140:ASN:O	2:E:140:ASN:OD1	2.39	0.41
2:E:358:MET:O	2:E:362:LEU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:412:VAL:HG23	2:F:438:LEU:HG	2.00	0.41
3:J:2:VAL:HA	3:J:25:SER:HG	1.83	0.41
3:J:28:ILE:HG21	3:J:77:ASN:HA	2.01	0.41
1:A:59:TRP:HB2	1:A:66:ASN:HB3	2.02	0.41
1:A:250:PHE:HE2	1:A:372:PHE:CE1	2.37	0.41
1:A:312:HIS:HB3	1:A:315:ALA:HB2	2.02	0.41
1:B:28:THR:HB	1:B:332:TYR:CE2	2.55	0.41
1:B:56:PRO:HB3	1:B:308:TYR:CE2	2.56	0.41
1:B:232:LEU:HD11	1:B:236:GLU:CD	2.44	0.41
1:B:432:LEU:HD12	1:B:453:LEU:HD22	2.03	0.41
1:B:443:PHE:CD1	1:B:465:ILE:HA	2.55	0.41
1:B:502:PHE:CB	1:B:507:GLU:HB2	2.45	0.41
1:C:150:SER:HA	1:C:153:LEU:HD12	2.02	0.41
1:C:235:LYS:O	1:C:239:GLN:HG3	2.20	0.41
1:C:378:LEU:O	1:C:381:GLN:HB2	2.20	0.41
2:E:340:LYS:HG2	2:E:351:VAL:CG1	2.50	0.41
2:E:358:MET:HE3	2:E:358:MET:HB3	1.84	0.41
2:E:394:GLU:CB	2:E:417:ALA:HB2	2.51	0.41
2:F:53:VAL:O	2:F:355:THR:HG22	2.20	0.41
2:F:288:PHE:HA	2:F:291:VAL:CG2	2.50	0.41
2:F:307:LEU:O	2:F:310:VAL:HG12	2.20	0.41
2:F:326:THR:O	2:F:330:VAL:HG12	2.21	0.41
1:A:38:ILE:HD11	1:A:325:TYR:CD1	2.53	0.41
1:B:130:LEU:HD21	1:B:134:LEU:HD11	2.03	0.41
1:B:696:ASN:C	1:B:719:ARG:HE	2.27	0.41
1:B:734:ARG:HA	1:B:756:LEU:HA	2.03	0.41
1:C:20:LEU:CD2	1:C:378:LEU:HD23	2.51	0.41
1:D:22:PRO:HG2	1:D:24:TRP:CE2	2.56	0.41
1:D:168:TRP:C	1:D:171:ARG:HG2	2.46	0.41
1:D:263:LEU:HD23	1:D:267:GLN:HG3	2.03	0.41
1:D:349:LYS:O	1:D:370:ASN:HA	2.21	0.41
2:E:422:MET:CE	2:E:425:GLN:HG3	2.50	0.41
2:F:149:ILE:HD12	2:F:352:PHE:CZ	2.54	0.41
2:F:385:PHE:HD1	2:F:386:TRP:HD1	1.68	0.41
2:F:433:ARG:CZ	2:F:433:ARG:HB3	2.49	0.41
1:A:60:VAL:CG2	1:A:307:THR:HG21	2.50	0.41
1:A:140:SER:HA	1:A:271:LYS:NZ	2.34	0.41
1:A:237:GLY:HA3	1:A:406:ASN:OD1	2.21	0.41
1:B:522:HIS:HA	1:B:550:ARG:O	2.21	0.41
1:B:576:ASN:HB3	1:B:579:THR:O	2.20	0.41
1:B:622:LYS:HG2	1:B:623:ASP:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:LEU:C	1:B:664:LEU:HD23	2.45	0.41
1:B:693:SER:HA	1:B:716:THR:O	2.20	0.41
1:C:112:VAL:CG2	1:C:297:VAL:HG11	2.50	0.41
1:C:376:LEU:HD22	1:C:376:LEU:N	2.34	0.41
1:D:354:GLU:C	1:D:357:ARG:HG2	2.46	0.41
1:D:368:VAL:HG12	1:D:372:PHE:HB3	1.98	0.41
2:E:58:LEU:HD12	2:E:137:ARG:CZ	2.49	0.41
2:E:148:PHE:HE2	2:F:355:THR:CG2	2.32	0.41
2:E:151:GLN:OE1	2:E:151:GLN:HA	2.20	0.41
2:E:158:LEU:HD23	2:E:159:PRO:O	2.21	0.41
2:F:415:ASP:OD2	2:F:418:PHE:HD2	2.03	0.41
3:J:27:TYR:HB3	3:J:29:TYR:HD2	1.83	0.41
1:A:311:ALA:HB2	2:F:148:PHE:CE2	2.54	0.41
1:A:356:ILE:HG23	1:A:359:GLU:OE2	2.19	0.41
1:B:149:THR:CG2	1:B:260:VAL:HG22	2.50	0.41
1:B:249:LYS:HG3	1:B:250:PHE:H	1.86	0.41
1:B:348:LEU:HG	1:B:377:HIS:ND1	2.35	0.41
1:B:605:ARG:HA	1:B:605:ARG:HD2	1.86	0.41
1:B:750:VAL:HG11	1:B:773:LEU:HD23	2.01	0.41
1:C:233:ASP:CG	1:C:235:LYS:HG2	2.45	0.41
1:C:264:TYR:CD1	1:C:374:PHE:HZ	2.39	0.41
1:D:274:LYS:HA	1:D:277:LEU:HD21	2.03	0.41
2:E:315:LYS:HZ2	2:E:315:LYS:HG3	1.71	0.41
2:F:45:MET:O	2:F:45:MET:HG2	2.20	0.41
1:B:629:ILE:HG23	1:B:651:ILE:CD1	2.50	0.41
1:C:34:VAL:HG12	1:C:328:LEU:CD1	2.49	0.41
1:C:124:TYR:O	1:C:128:LEU:HG	2.21	0.41
1:C:147:PRO:CD	1:D:23:TRP:HB3	2.51	0.41
1:C:369:LYS:HE2	1:C:369:LYS:HB3	1.87	0.41
1:D:282:THR:HG21	1:D:326:ILE:HG13	2.03	0.41
2:E:294:PHE:C	2:E:297:HIS:HB3	2.45	0.41
2:F:294:PHE:CE2	2:F:418:PHE:HZ	2.38	0.41
1:A:243:LEU:O	1:A:247:VAL:HG23	2.21	0.41
1:A:351:TYR:HB3	1:A:368:VAL:HB	2.02	0.41
1:B:117:ARG:NE	1:B:117:ARG:CA	2.83	0.41
1:B:235:LYS:C	1:B:238:GLU:HG2	2.46	0.41
1:B:428:LEU:H	1:B:449:GLU:CD	2.28	0.41
1:B:474:LEU:CG	1:B:476:LEU:HD21	2.51	0.41
1:B:633:ILE:HB	1:B:657:GLN:CG	2.48	0.41
1:C:19:ILE:O	1:C:19:ILE:HG12	2.20	0.41
1:C:115:GLU:HA	1:C:115:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ILE:HG23	1:C:279:ILE:N	2.35	0.41
1:C:284:TYR:HD2	1:C:285:TYR:CD1	2.39	0.41
1:D:53:ILE:HA	1:D:110:ASP:OD2	2.20	0.41
1:D:249:LYS:HD2	1:D:249:LYS:O	2.20	0.41
1:D:400:ASN:HA	1:D:403:ARG:CZ	2.51	0.41
2:E:15:PRO:HD2	2:E:184:PHE:HZ	1.86	0.41
2:E:24:TRP:CE3	2:E:383:THR:HG21	2.55	0.41
2:E:43:GLY:N	2:E:166:PRO:HB3	2.35	0.41
2:E:441:VAL:HG22	2:E:445:LYS:NZ	2.36	0.41
2:F:40:ILE:HG22	2:F:41:PHE:N	2.35	0.41
2:F:155:HIS:C	2:F:156:LEU:HD23	2.46	0.41
2:F:303:LEU:O	2:F:307:LEU:HB3	2.21	0.41
2:F:356:HIS:HB3	2:F:359:ALA:HB2	2.02	0.41
1:B:35:MET:HE1	1:B:329:VAL:HA	2.03	0.41
1:B:108:TYR:HB3	1:C:55:LEU:HD11	2.03	0.41
1:B:411:TRP:CD1	1:B:439:PRO:HG3	2.56	0.41
1:B:598:LEU:CD1	1:B:603:LEU:HD11	2.50	0.41
1:C:263:LEU:HD12	1:C:263:LEU:O	2.21	0.41
1:C:356:ILE:CG2	1:C:365:ILE:HG13	2.47	0.41
2:E:15:PRO:HD2	2:E:17:TYR:CE2	2.55	0.41
2:F:183:TRP:CZ3	2:F:184:PHE:HD2	2.39	0.41
1:B:619:ILE:O	1:B:644:LEU:HD12	2.21	0.40
1:B:671:ARG:HD2	3:J:108:TYR:CD1	2.56	0.40
1:D:168:TRP:HZ3	1:D:398:SER:HB3	1.84	0.40
1:D:258:ASP:HA	1:D:371:ASP:HB2	2.03	0.40
1:D:339:THR:O	1:D:342:TRP:HE3	2.04	0.40
2:F:36:LEU:HB2	2:F:173:THR:HG21	2.03	0.40
1:B:279:ILE:CD1	1:B:329:VAL:HG12	2.50	0.40
1:B:502:PHE:CZ	1:B:527:LEU:HD21	2.55	0.40
1:B:569:LEU:HB3	1:B:590:MET:HE3	2.04	0.40
1:B:613:LEU:HB3	1:B:616:LEU:HG	2.04	0.40
1:B:721:GLU:HG2	1:B:742:VAL:HG23	2.01	0.40
1:C:15:PRO:HG2	1:C:16:ALA:H	1.85	0.40
1:C:234:LYS:HG3	1:C:406:ASN:OD1	2.21	0.40
2:E:307:LEU:HA	2:E:310:VAL:HG12	2.03	0.40
2:E:314:ILE:HG22	2:E:315:LYS:N	2.35	0.40
2:F:45:MET:CE	2:F:358:MET:HG3	2.46	0.40
2:F:311:GLN:O	2:F:314:ILE:HG23	2.21	0.40
1:A:155:HIS:CD2	1:A:250:PHE:HD1	2.39	0.40
1:A:161:LEU:HD12	1:A:161:LEU:C	2.45	0.40
1:B:143:TRP:CZ2	1:B:144:PHE:HE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:ARG:HH22	1:B:575:ASN:HB2	1.85	0.40
1:B:679:THR:HA	1:B:682:PHE:HE2	1.84	0.40
1:B:696:ASN:CB	1:B:719:ARG:NH2	2.84	0.40
1:D:132:HIS:CD2	1:D:278:ILE:HD13	2.56	0.40
1:D:258:ASP:H	1:D:371:ASP:CG	2.29	0.40
2:E:158:LEU:HD23	2:E:158:LEU:C	2.47	0.40
2:E:322:ILE:HD12	2:E:322:ILE:C	2.46	0.40
1:A:46:GLN:OE1	1:A:47:VAL:HG23	2.21	0.40
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.72	0.40
1:A:256:GLU:HA	1:A:256:GLU:OE1	2.22	0.40
1:B:425:GLN:O	1:B:427:LYS:HG3	2.22	0.40
1:B:483:ILE:CD1	1:B:488:LEU:HA	2.52	0.40
1:C:60:VAL:HB	1:C:307:THR:HG21	2.02	0.40
1:C:154:GLU:O	1:C:157:VAL:HG12	2.21	0.40
1:C:231:VAL:HG23	1:C:409:ASN:OD1	2.20	0.40
1:C:255:GLU:CD	1:C:369:LYS:HB2	2.46	0.40
1:C:351:TYR:HB2	1:C:373:ALA:HA	2.03	0.40
1:C:392:VAL:HG23	1:C:393:PHE:N	2.37	0.40
1:D:143:TRP:N	1:D:143:TRP:CD1	2.90	0.40
1:D:305:TYR:CE1	2:E:135:THR:N	2.89	0.40
1:A:22:PRO:HD2	1:A:25:ASP:CG	2.47	0.40
1:A:383:ASP:OD1	1:A:385:LEU:HB2	2.22	0.40
1:B:61:THR:HG23	1:B:64:SER:O	2.22	0.40
1:B:126:PRO:HA	1:B:129:VAL:CG1	2.52	0.40
1:B:489:ALA:HA	1:B:492:ARG:NH2	2.36	0.40
1:C:41:PHE:O	1:C:44:THR:HG23	2.22	0.40
1:C:351:TYR:N	1:C:373:ALA:CB	2.85	0.40
1:D:234:LYS:HD3	1:D:409:ASN:HB2	2.02	0.40
1:D:244:PHE:CZ	1:D:402:LEU:HD21	2.56	0.40
2:E:172:HIS:NE2	2:E:322:ILE:CG1	2.85	0.40
2:E:183:TRP:CD1	2:E:307:LEU:HD23	2.56	0.40
3:J:28:ILE:HB	3:J:77:ASN:CB	2.51	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	313/806 (39%)	303 (97%)	10 (3%)	0	100	100
1	B	691/806 (86%)	659 (95%)	31 (4%)	1 (0%)	48	80
1	C	314/806 (39%)	304 (97%)	10 (3%)	0	100	100
1	D	313/806 (39%)	300 (96%)	13 (4%)	0	100	100
2	E	301/458 (66%)	273 (91%)	28 (9%)	0	100	100
2	F	299/458 (65%)	269 (90%)	30 (10%)	0	100	100
3	J	124/128 (97%)	123 (99%)	1 (1%)	0	100	100
All	All	2355/4268 (55%)	2231 (95%)	123 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	LYS

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	296/746 (40%)	271 (92%)	25 (8%)	10	33
1	B	649/746 (87%)	622 (96%)	27 (4%)	26	49
1	C	297/746 (40%)	275 (93%)	22 (7%)	13	36
1	D	296/746 (40%)	281 (95%)	15 (5%)	21	44
2	E	275/417 (66%)	247 (90%)	28 (10%)	7	25
2	F	273/417 (66%)	242 (89%)	31 (11%)	5	21
3	J	97/98 (99%)	96 (99%)	1 (1%)	68	76
All	All	2183/3916 (56%)	2034 (93%)	149 (7%)	16	39

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ILE
1	A	51	LYS
1	A	63	ASP
1	A	102	ASP
1	A	104	HIS
1	A	133	THR
1	A	135	ILE
1	A	159	ILE
1	A	267	GLN
1	A	270	ILE
1	A	274	LYS
1	A	281	TYR
1	A	282	THR
1	A	283	VAL
1	A	289	ILE
1	A	307	THR
1	A	309	ARG
1	A	320	ILE
1	A	330	ILE
1	A	339	THR
1	A	340	LEU
1	A	353	PHE
1	A	380	ASP
1	A	383	ASP
1	A	394	LEU
1	B	17	TYR
1	B	20	LEU
1	B	26	VAL
1	B	49	GLN
1	B	61	THR
1	B	102	ASP
1	B	104	HIS
1	B	133	THR
1	B	135	ILE
1	B	163	CYS
1	B	268	THR
1	B	272	VAL
1	B	275	PHE
1	B	281	TYR
1	B	286	VAL
1	B	326	ILE
1	B	330	ILE
1	B	334	LEU

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Mol	Chain	Res	Type
1	B	339	THR
1	B	369	LYS
1	B	418	GLN
1	B	584	LEU
1	B	681	LEU
1	B	696	ASN
1	B	700	LEU
1	B	727	LEU
1	B	759	ILE
1	C	17	TYR
1	C	19	ILE
1	C	97	ILE
1	C	103	ARG
1	C	104	HIS
1	C	135	ILE
1	C	159	ILE
1	C	234	LYS
1	C	263	LEU
1	C	274	LYS
1	C	275	PHE
1	C	278	ILE
1	C	281	TYR
1	C	289	ILE
1	C	294	ASP
1	C	300	GLU
1	C	303	THR
1	C	307	THR
1	C	320	ILE
1	C	326	ILE
1	C	329	VAL
1	C	339	THR
1	D	55	LEU
1	D	65	CYS
1	D	104	HIS
1	D	129	VAL
1	D	131	LEU
1	D	133	THR
1	D	275	PHE
1	D	286	VAL
1	D	303	THR
1	D	316	THR
1	D	326	ILE

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Mol	Chain	Res	Type
1	D	328	LEU
1	D	330	ILE
1	D	375	MET
1	D	402	LEU
2	E	31	LEU
2	E	40	ILE
2	E	45	MET
2	E	49	LYS
2	E	51	GLN
2	E	52	VAL
2	E	53	VAL
2	E	58	LEU
2	E	176	LEU
2	E	178	VAL
2	E	189	THR
2	E	314	ILE
2	E	320	ILE
2	E	328	ASN
2	E	329	PHE
2	E	333	ILE
2	E	334	SER
2	E	336	GLU
2	E	345	HIS
2	E	351	VAL
2	E	358	MET
2	E	372	ILE
2	E	373	ILE
2	E	379	ILE
2	E	388	PHE
2	E	419	LEU
2	E	422	MET
2	E	440	GLU
2	F	19	ILE
2	F	30	TYR
2	F	40	ILE
2	F	45	MET
2	F	53	VAL
2	F	57	VAL
2	F	135	THR
2	F	141	LEU
2	F	158	LEU
2	F	168	LEU

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Mol	Chain	Res	Type
2	F	173	THR
2	F	183	TRP
2	F	189	THR
2	F	312	THR
2	F	314	ILE
2	F	319	PHE
2	F	330	VAL
2	F	331	ASN
2	F	333	ILE
2	F	345	HIS
2	F	350	GLU
2	F	354	CYS
2	F	357	ASN
2	F	358	MET
2	F	372	ILE
2	F	387	LEU
2	F	418	PHE
2	F	419	LEU
2	F	421	HIS
2	F	433	ARG
2	F	440	GLU
3	J	101	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	132	HIS
1	A	267	GLN
1	A	381	GLN
1	A	404	GLN
1	B	46	GLN
1	B	155	HIS
1	B	253	HIS
1	B	406	ASN
1	B	409	ASN
1	B	499	HIS
1	B	576	ASN
1	B	592	ASN
1	B	625	ASN
1	B	694	HIS
1	B	696	ASN

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Mol	Chain	Res	Type
1	C	105	GLN
1	C	253	HIS
1	C	312	HIS
1	C	381	GLN
1	C	404	GLN
1	D	377	HIS
2	E	145	GLN
2	E	151	GLN
2	E	283	GLN
2	E	311	GLN
2	E	328	ASN
2	E	337	HIS
2	E	345	HIS
2	E	357	ASN
2	E	428	GLN
2	F	145	GLN
2	F	195	HIS
2	F	283	GLN
2	F	357	ASN
2	F	428	GLN
3	J	1	GLN
3	J	13	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	B	902	-	3,3,3	0.27	0	2,2,2	0.27	0
4	EDO	B	901	-	3,3,3	0.24	0	2,2,2	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	902	-	-	0/1/1/1	-
4	EDO	B	901	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

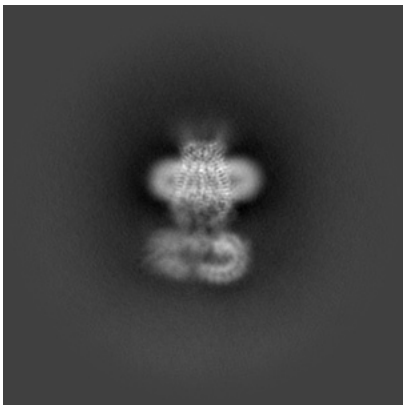
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55592. These allow visual inspection of the internal detail of the map and identification of artifacts.

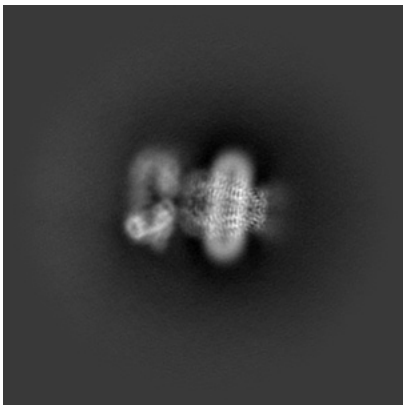
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

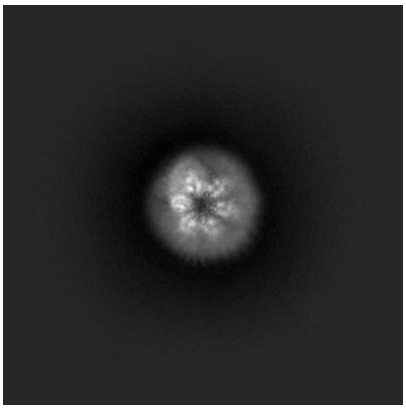
6.1.1 Primary map



X

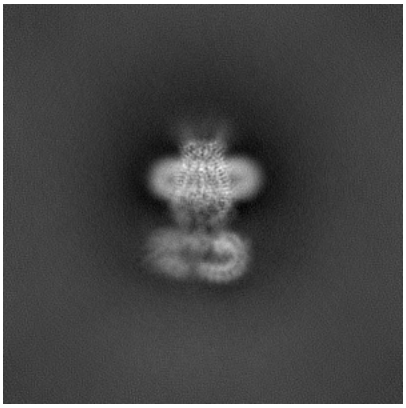


Y

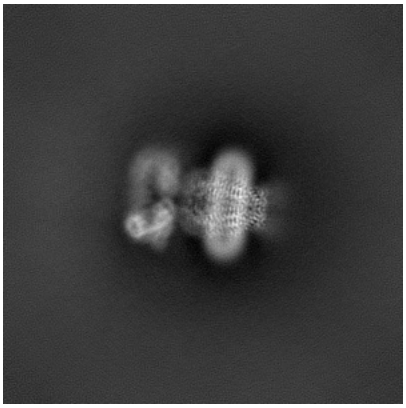


Z

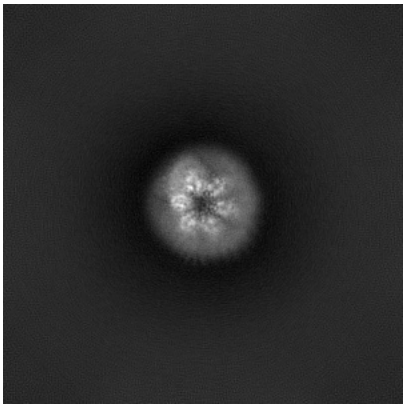
6.1.2 Raw map



X



Y



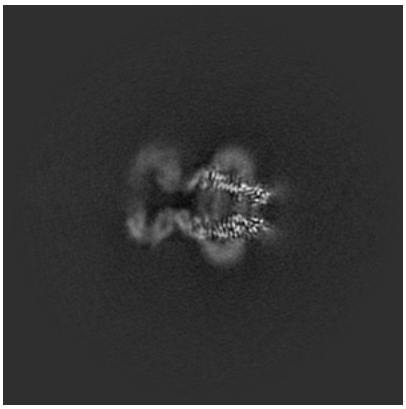
Z

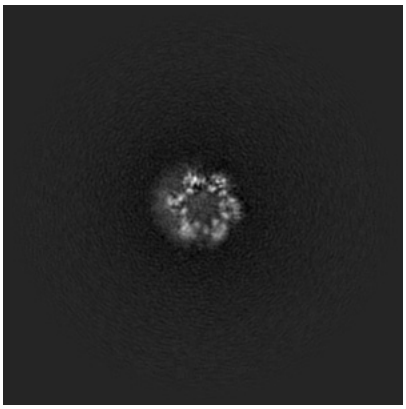
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

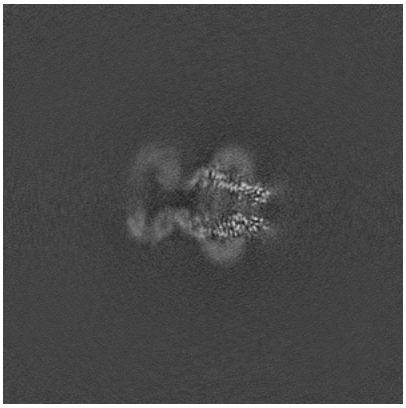
X Index: 168

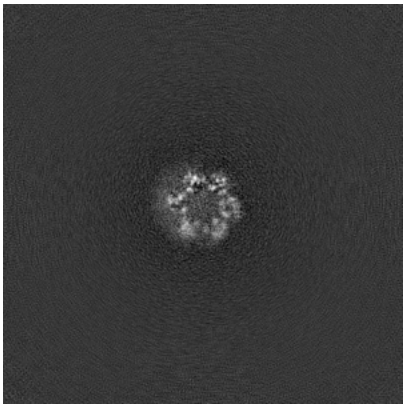

Y Index: 168


Z Index: 168

6.2.2 Raw map

X Index: 168

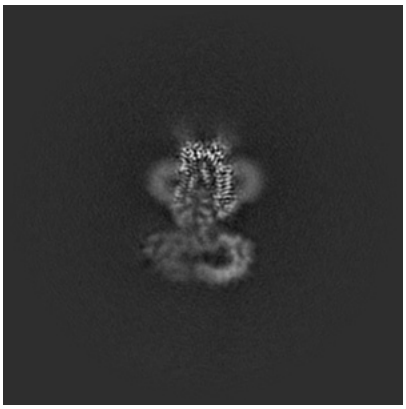

Y Index: 168

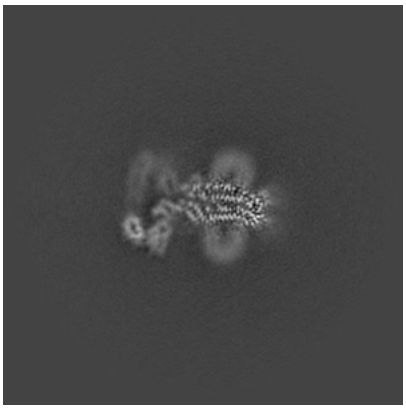

Z Index: 168

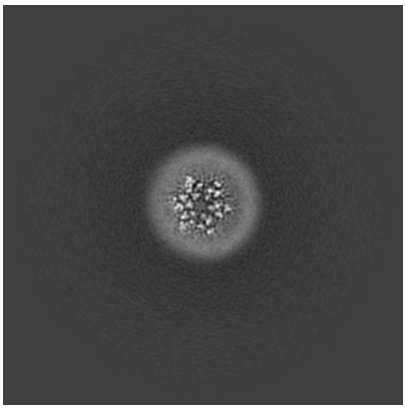
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

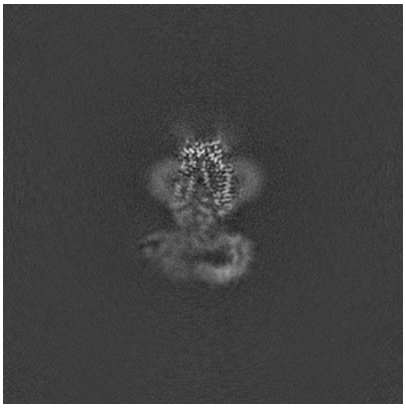
6.3.1 Primary map

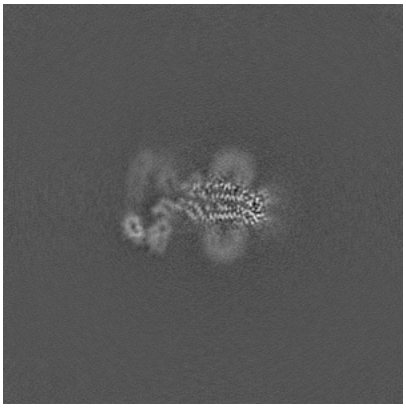

X Index: 156

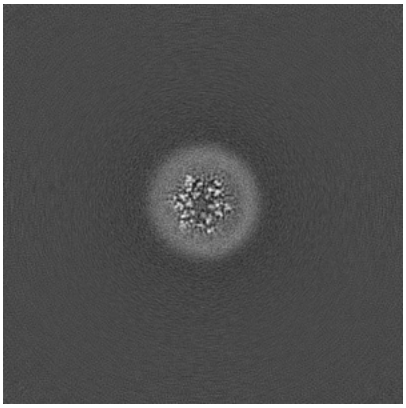

Y Index: 181


Z Index: 196

6.3.2 Raw map


X Index: 155

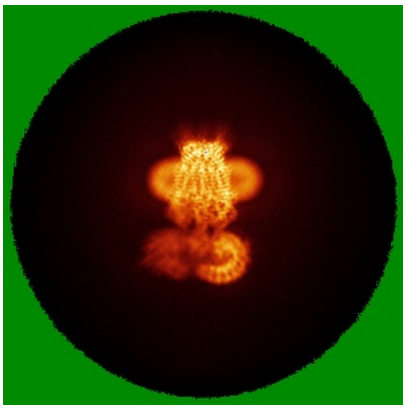

Y Index: 181

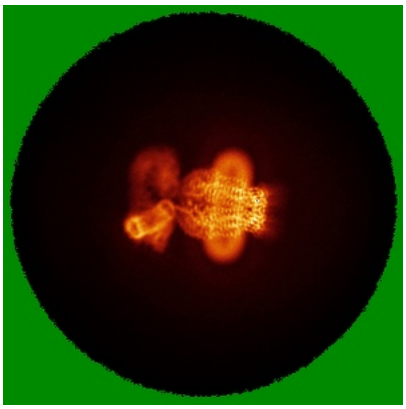

Z Index: 196

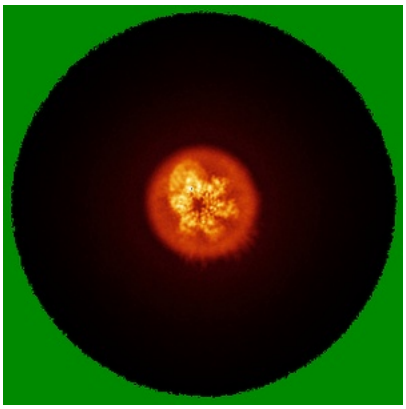
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

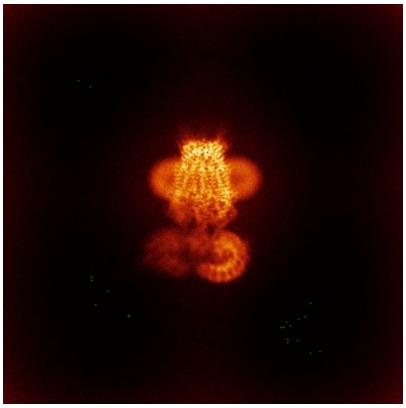
6.4.1 Primary map

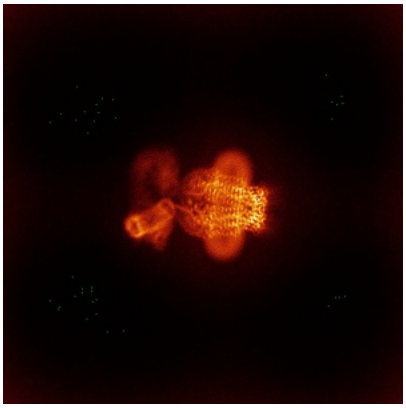

X

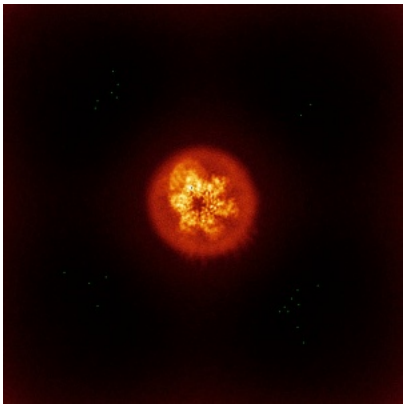

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.232. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

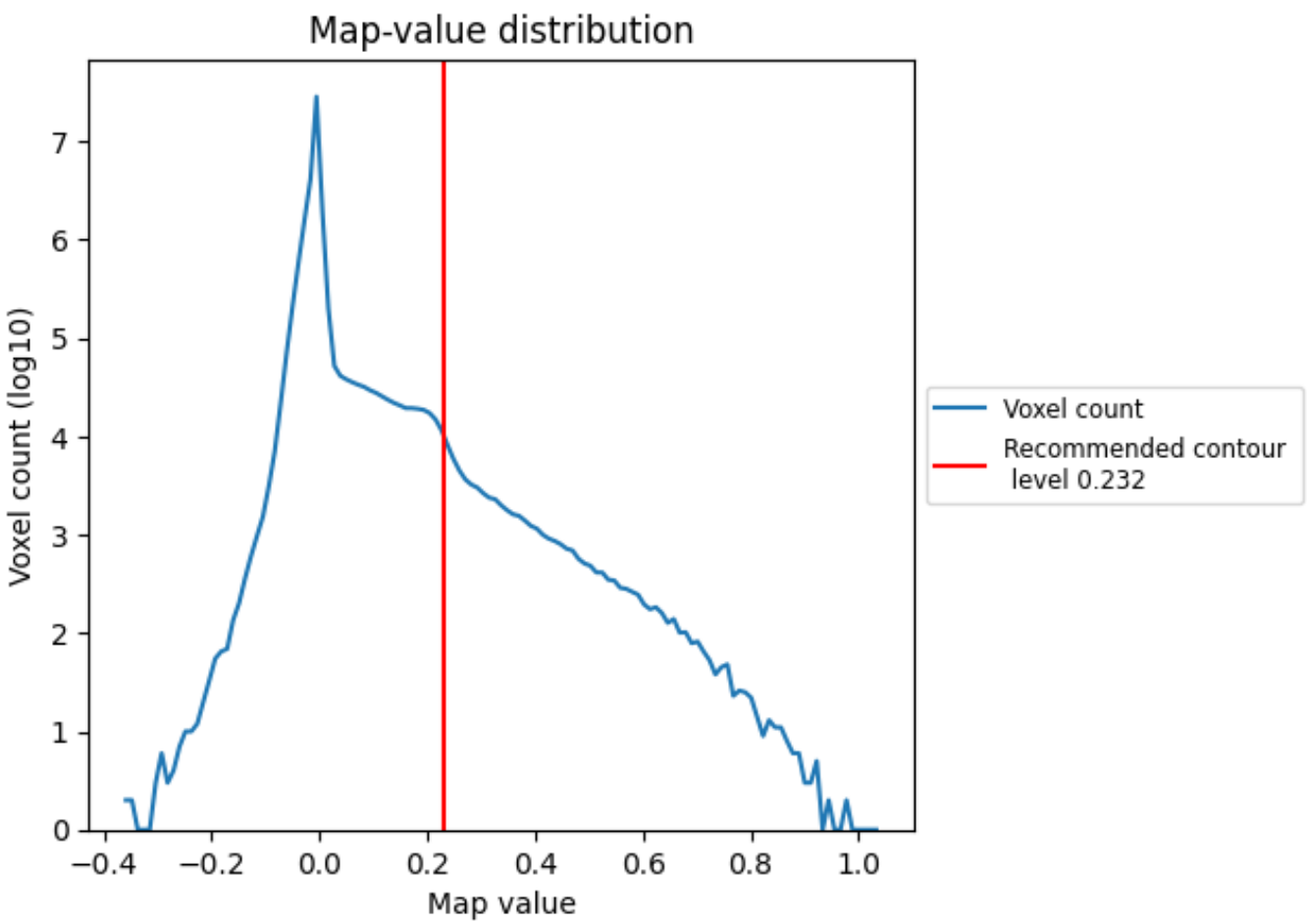
6.6 Mask visualisation (i)

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

7 Map analysis (i)

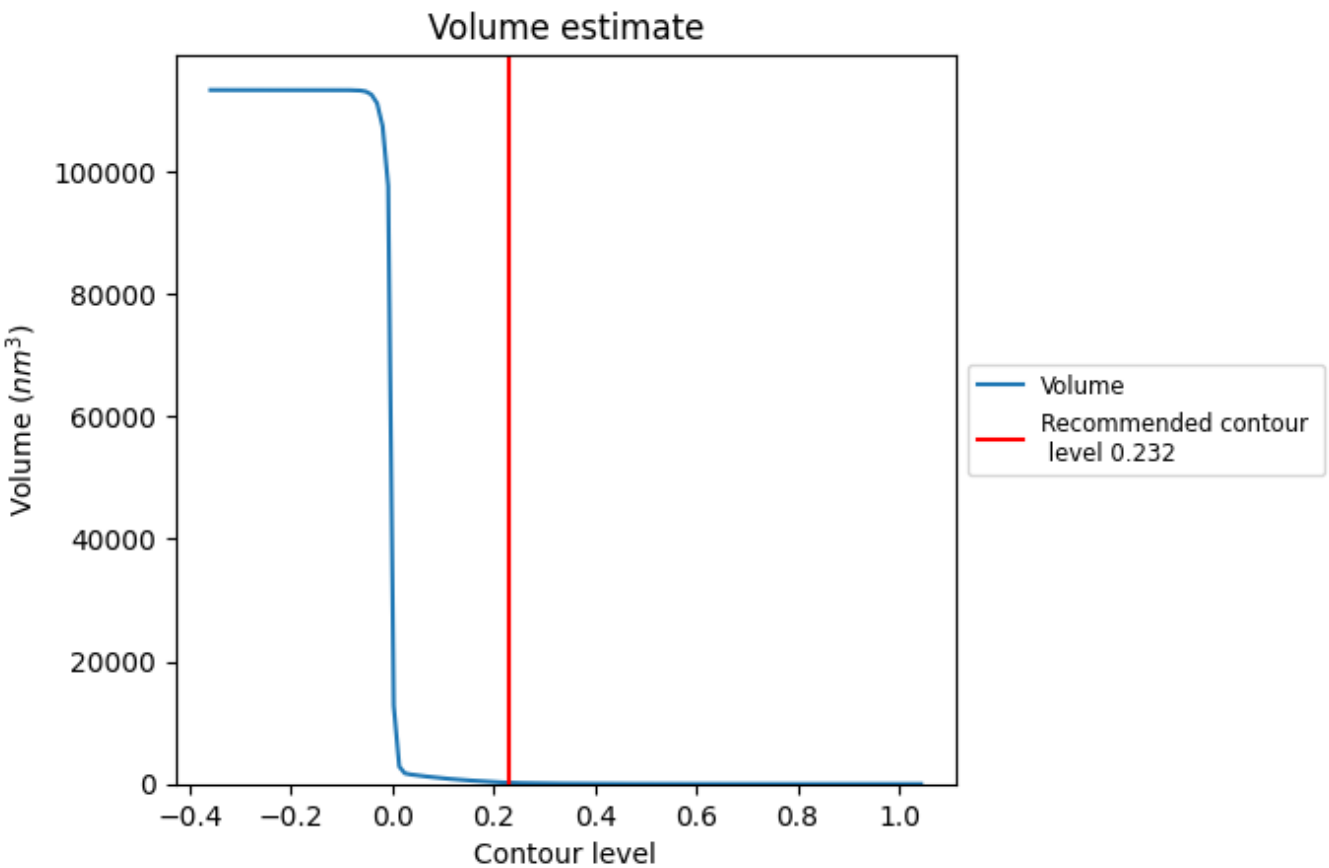
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

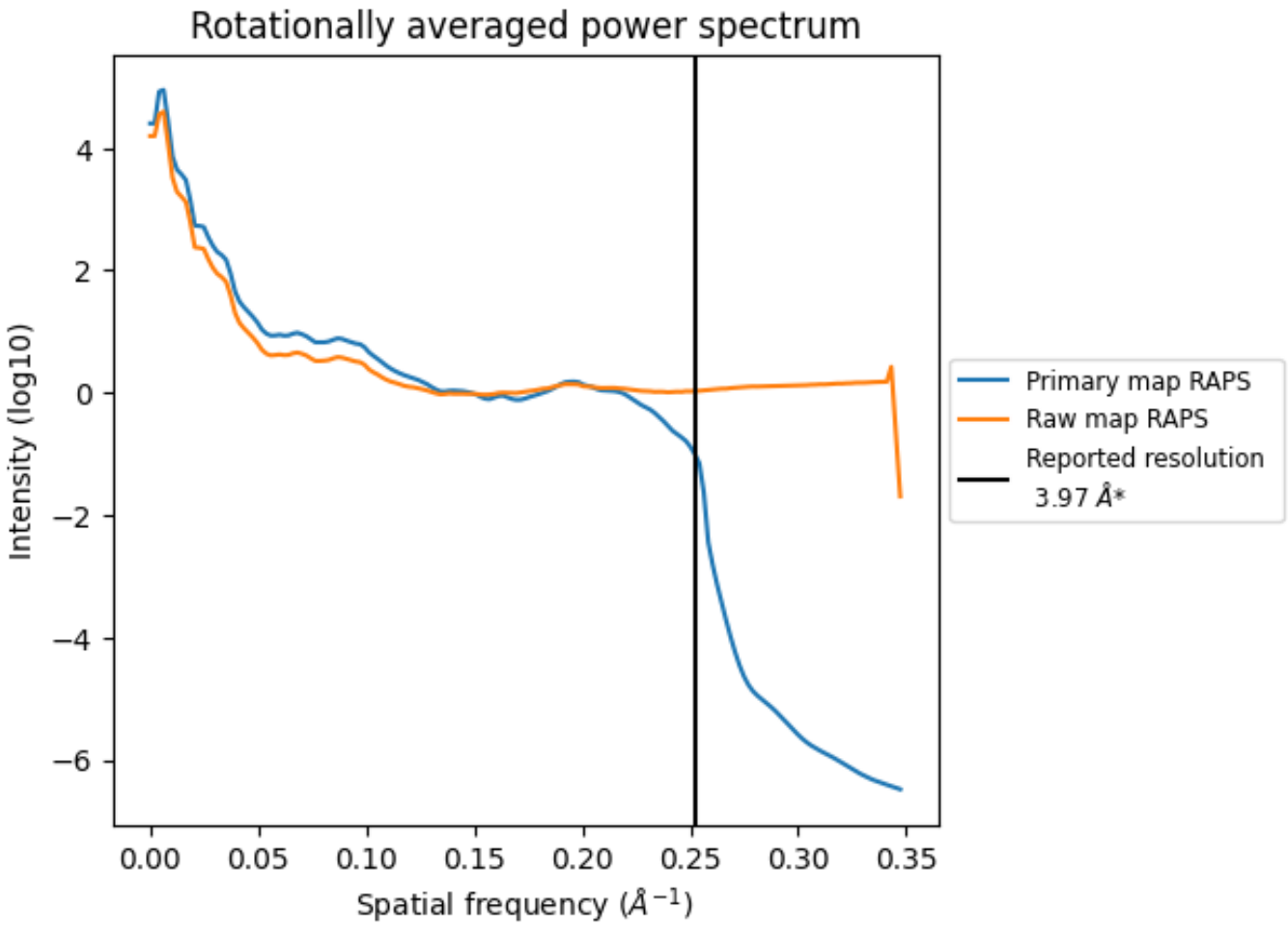
7.2 Volume estimate (i)



The volume at the recommended contour level is 188 nm^3; this corresponds to an approximate mass of 170 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

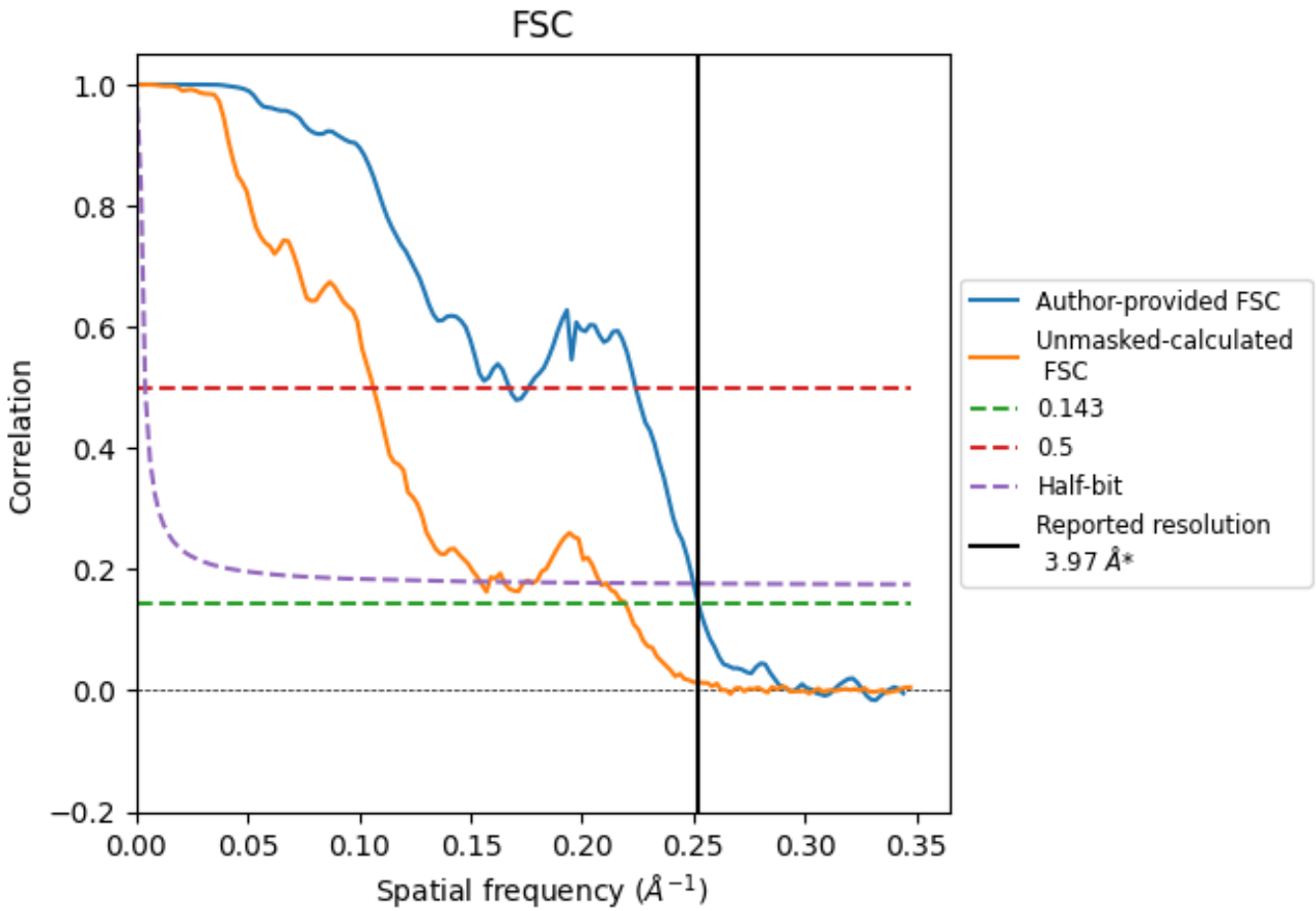


*Reported resolution corresponds to spatial frequency of 0.252 Å^{-1}

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 0.252 Å^{-1}

8.2 Resolution estimates (i)

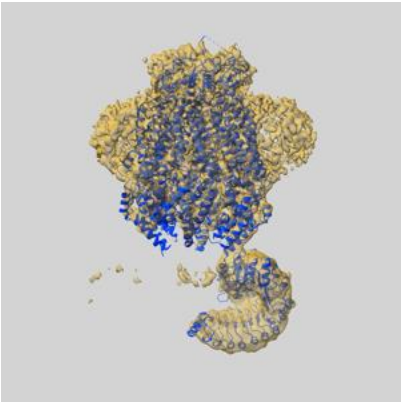
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.97	-	-
Author-provided FSC curve	3.97	5.98	4.00
Unmasked-calculated*	4.56	9.40	6.48

*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 4.56 differs from the reported value 3.97 by more than 10 %

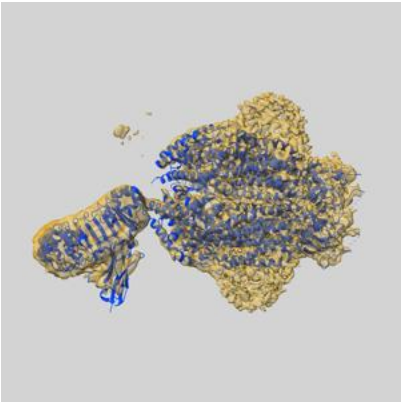
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55592 and PDB model 9T5P. Per-residue inclusion information can be found in section 3 on page 6.

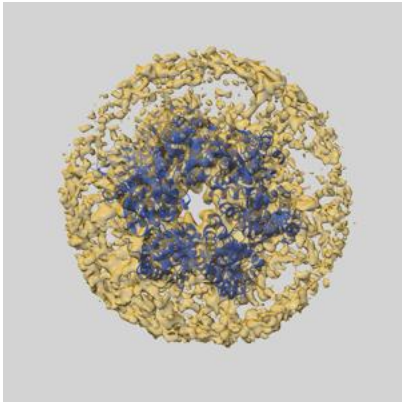
9.1 Map-model overlay (i)



X



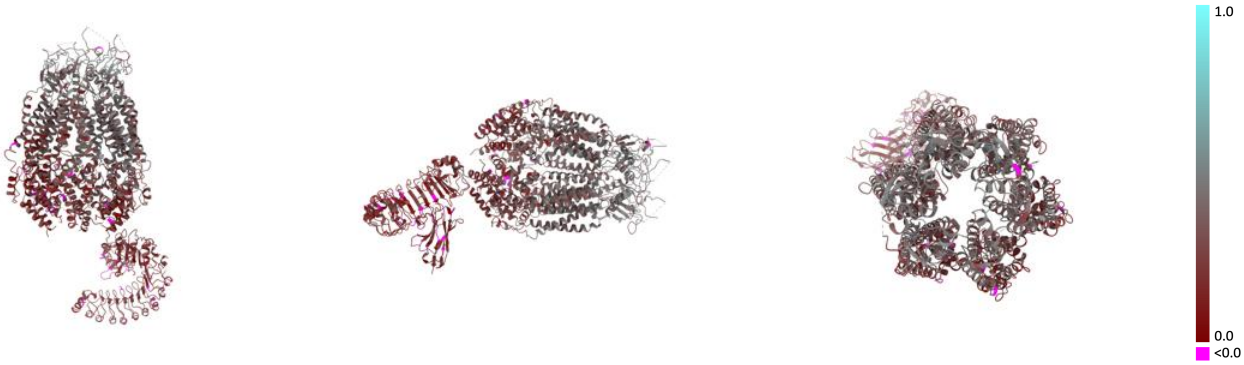
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.232 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.

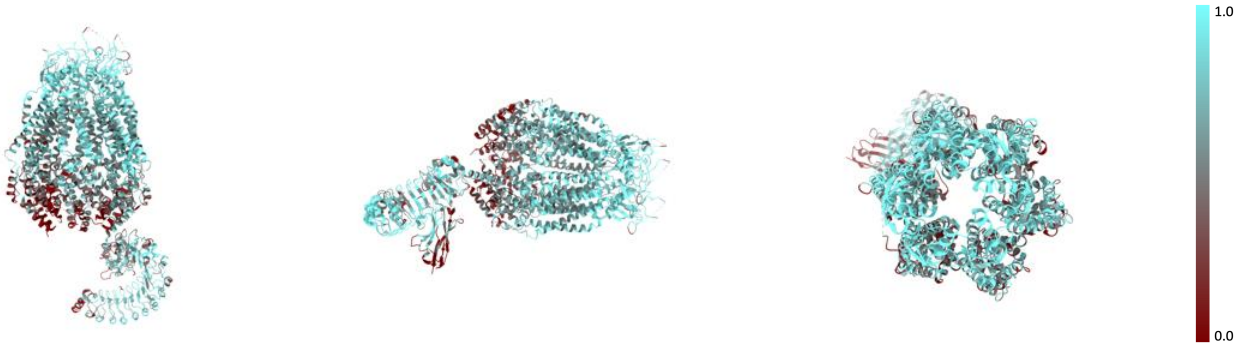
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

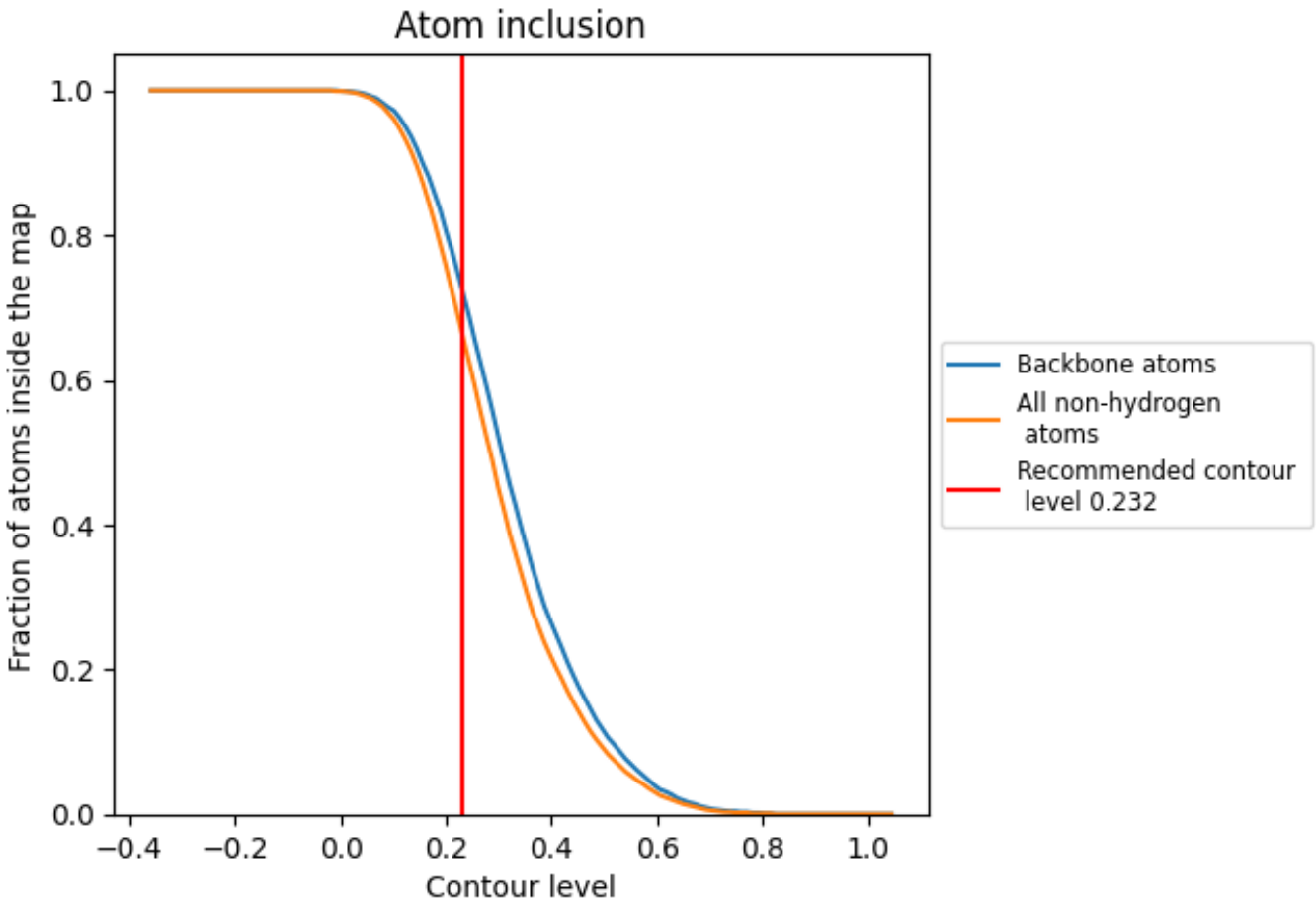
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.232).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.232) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6610	0.3020
A	0.7000	0.3660
B	0.7380	0.2700
C	0.6920	0.3440
D	0.5640	0.2950
E	0.6120	0.2990
F	0.6770	0.3320
J	0.4700	0.1590