



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:39 PM UTC

PDB ID : 3J09 / pdb_00003j09
EMDB ID : EMD-5004
Title : High resolution helical reconstruction of the bacterial p-type ATPase copper transporter CopA
Authors : Wu, C.; Allen, G.S.; Cardozo, T.; Stokes, D.L.
Deposited on : 2011-05-09
Resolution : 10.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

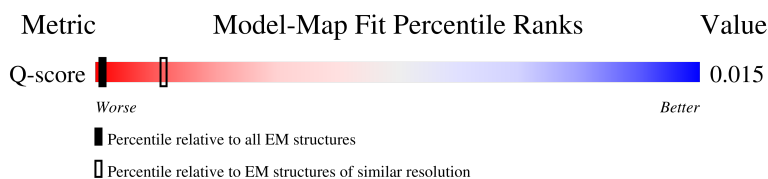
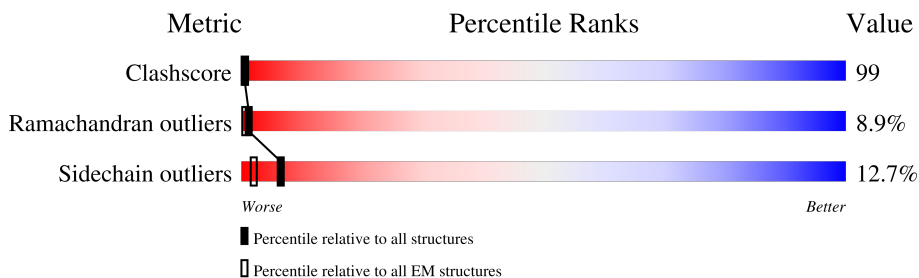
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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	45 (17.00 - 18.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	723	37% 49% 33% 12% 7%
1	B	723	34% 48% 34% 12% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

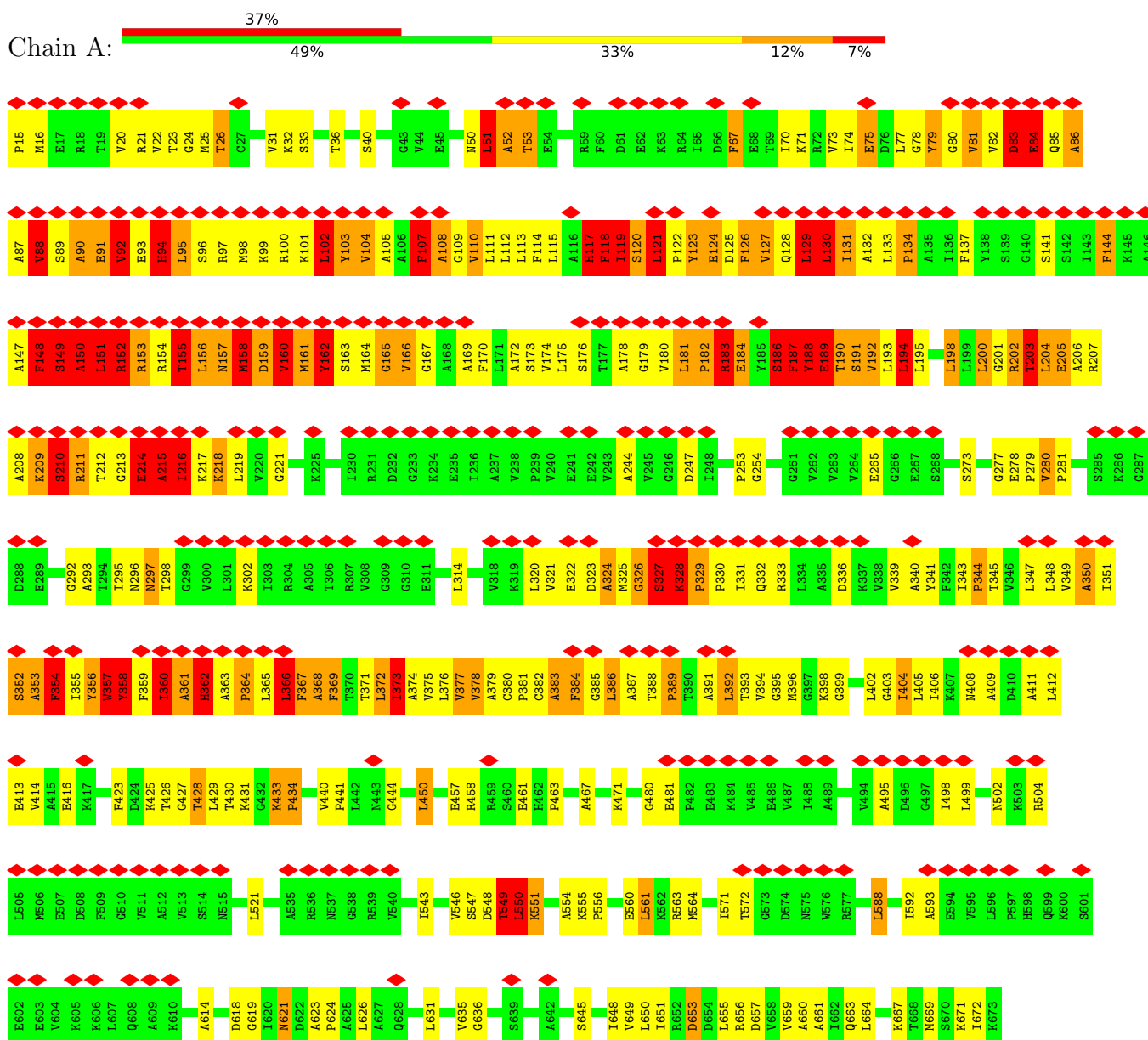
- Molecule 1 is a protein called copper-exporting P-type ATPase A.

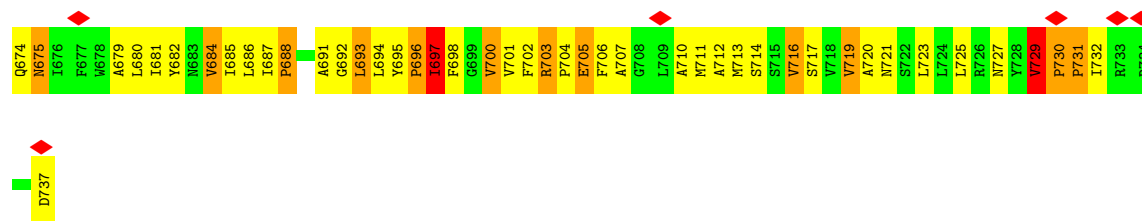
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	723	Total	C	N	O	S	0	0
			5466	3511	920	1015	20		
1	B	723	Total	C	N	O	S	0	0
			5466	3511	920	1015	20		

3 Residue-property plots

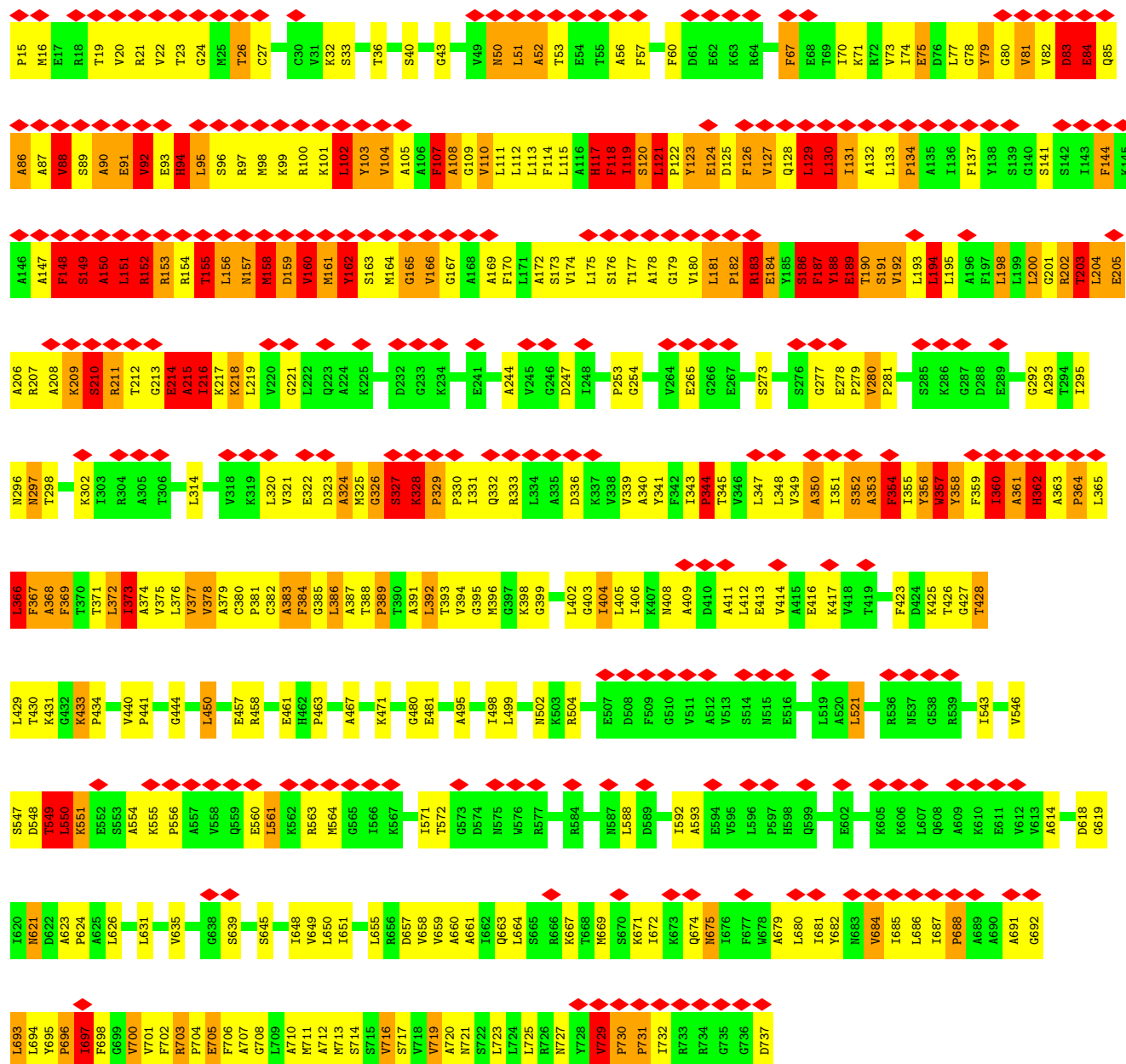
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: copper-exporting P-type ATPase A





• Molecule 1: copper-exporting P-type ATPase A



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	OTHER	Depositor
CTF correction method	each tube-crystal	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	75.388	Depositor
Minimum map value	-48.614	Depositor
Average map value	0.529	Depositor
Map value standard deviation	4.943	Depositor
Recommended contour level	10	Depositor
Map size (Å)	202, 202, 202	wwPDB
Map dimensions	101, 101, 101	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2, 2, 2	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.30	45/5545 (0.8%)	1.49	79/7515 (1.1%)
1	B	1.25	48/5545 (0.9%)	1.50	78/7515 (1.0%)
All	All	1.27	93/11090 (0.8%)	1.50	157/15030 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	9
All	All	0	18

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	ALA	CA-CB	38.53	2.18	1.53
1	B	356	TYR	CG-CD1	24.78	1.91	1.39
1	A	356	TYR	CG-CD1	23.61	1.89	1.39
1	B	51	LEU	CB-CG	20.72	1.94	1.53
1	A	356	TYR	CG-CD2	19.25	1.79	1.39
1	B	356	TYR	CE1-CZ	18.45	1.82	1.38
1	A	356	TYR	CE1-CZ	18.02	1.81	1.38
1	A	356	TYR	CA-CB	-17.14	1.19	1.53
1	B	356	TYR	CA-CB	-16.75	1.20	1.53
1	B	51	LEU	CA-CB	15.24	1.77	1.53
1	B	52	ALA	CA-CB	14.86	1.77	1.53
1	B	51	LEU	CG-CD1	14.74	2.01	1.52
1	A	51	LEU	CA-CB	14.58	1.76	1.53
1	B	356	TYR	CG-CD2	13.05	1.66	1.39
1	B	404	ILE	CA-CB	-11.87	1.39	1.54
1	A	404	ILE	CA-CB	-11.65	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	356	TYR	CD1-CE1	11.61	1.73	1.38
1	A	119	ILE	C-O	-11.39	1.10	1.24
1	B	119	ILE	C-O	-11.34	1.10	1.24
1	A	356	TYR	CD1-CE1	11.14	1.72	1.38
1	B	356	TYR	CE2-CZ	10.59	1.63	1.38
1	A	356	TYR	CE2-CZ	10.46	1.63	1.38
1	A	120	SER	CA-CB	-10.30	1.32	1.53
1	B	120	SER	CA-CB	-10.17	1.33	1.53
1	A	697	ILE	CA-CB	-9.68	1.41	1.54
1	B	697	ILE	CA-CB	-9.65	1.41	1.54
1	A	189	GLU	CA-CB	-9.29	1.37	1.53
1	B	189	GLU	CA-CB	-9.24	1.37	1.53
1	B	389	PRO	N-CD	-9.23	1.34	1.47
1	A	389	PRO	N-CD	-9.21	1.34	1.47
1	A	117	HIS	CE1-NE2	8.39	1.41	1.32
1	B	362	HIS	CA-CB	8.38	1.70	1.53
1	A	362	HIS	CA-CB	8.35	1.70	1.53
1	B	117	HIS	CE1-NE2	8.30	1.40	1.32
1	A	117	HIS	CB-CG	-8.23	1.38	1.50
1	B	117	HIS	CB-CG	-8.12	1.38	1.50
1	B	688	PRO	N-CD	-7.77	1.36	1.47
1	A	688	PRO	N-CD	-7.67	1.37	1.47
1	B	81	VAL	C-O	-7.29	1.16	1.24
1	A	81	VAL	C-O	-7.21	1.16	1.24
1	A	729	VAL	C-O	-7.20	1.15	1.24
1	B	155	THR	CA-CB	-7.11	1.35	1.54
1	B	729	VAL	C-O	-7.11	1.15	1.24
1	A	155	THR	CA-CB	-7.06	1.35	1.54
1	A	373	ILE	CA-CB	-7.04	1.45	1.54
1	A	151	LEU	C-O	-6.78	1.15	1.24
1	B	151	LEU	C-O	-6.74	1.15	1.24
1	B	373	ILE	CA-CB	-6.63	1.46	1.54
1	B	354	PHE	CA-CB	6.53	1.64	1.53
1	B	327	SER	CA-CB	-6.44	1.42	1.53
1	B	121	LEU	C-O	-6.38	1.16	1.24
1	A	327	SER	CA-CB	-6.34	1.42	1.53
1	B	166	VAL	CA-CB	-6.33	1.46	1.54
1	A	354	PHE	CA-CB	6.30	1.64	1.53
1	A	121	LEU	C-O	-6.29	1.16	1.24
1	A	166	VAL	CA-CB	-6.20	1.46	1.54
1	A	117	HIS	ND1-CE1	-6.11	1.26	1.32
1	B	356	TYR	CD2-CE2	6.02	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	HIS	ND1-CE1	-6.01	1.26	1.32
1	A	356	TYR	CD2-CE2	5.94	1.56	1.38
1	B	91	GLU	CA-CB	5.88	1.65	1.53
1	A	91	GLU	CA-CB	5.84	1.65	1.53
1	A	352	SER	CA-CB	5.84	1.62	1.53
1	B	50	ASN	CA-CB	5.72	1.60	1.53
1	B	352	SER	CA-CB	5.68	1.62	1.53
1	B	50	ASN	CB-CG	5.64	1.66	1.52
1	B	118	PHE	C-O	-5.61	1.17	1.24
1	A	434	PRO	N-CD	-5.44	1.40	1.47
1	B	117	HIS	CD2-NE2	-5.40	1.31	1.37
1	A	117	HIS	CD2-NE2	-5.37	1.31	1.37
1	B	360	ILE	CA-CB	-5.31	1.47	1.54
1	A	118	PHE	C-O	-5.28	1.17	1.24
1	A	352	SER	C-O	5.28	1.30	1.24
1	B	134	PRO	N-CD	-5.26	1.40	1.47
1	A	215	ALA	CA-CB	-5.22	1.44	1.53
1	B	123	TYR	CA-CB	5.22	1.61	1.53
1	B	130	LEU	CG-CD1	-5.21	1.35	1.52
1	A	130	LEU	C-O	-5.21	1.17	1.24
1	A	130	LEU	CG-CD1	-5.21	1.35	1.52
1	A	134	PRO	N-CD	-5.20	1.40	1.47
1	B	684	VAL	C-O	-5.18	1.18	1.24
1	A	684	VAL	C-O	-5.16	1.18	1.24
1	A	344	PRO	N-CD	-5.15	1.40	1.47
1	A	123	TYR	CA-CB	5.15	1.61	1.53
1	A	129	LEU	C-O	-5.14	1.17	1.23
1	B	130	LEU	C-O	-5.13	1.17	1.24
1	A	150	ALA	C-O	-5.12	1.17	1.24
1	B	352	SER	C-O	5.12	1.29	1.24
1	B	150	ALA	C-O	-5.11	1.17	1.24
1	A	360	ILE	CA-CB	-5.11	1.47	1.54
1	B	344	PRO	N-CD	-5.09	1.40	1.47
1	B	129	LEU	C-O	-5.08	1.17	1.23
1	B	215	ALA	CA-CB	-5.07	1.45	1.53

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	SER	O-C-N	26.31	149.39	122.03
1	A	352	SER	O-C-N	26.16	149.24	122.03
1	B	352	SER	CA-C-O	-24.08	95.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	SER	CA-C-O	-24.03	95.77	121.00
1	A	51	LEU	N-CA-CB	-16.45	85.68	110.20
1	B	50	ASN	CB-CA-C	14.32	133.70	110.78
1	A	731	PRO	CA-N-CD	-13.65	92.89	112.00
1	B	731	PRO	CA-N-CD	-13.57	93.00	112.00
1	B	51	LEU	CB-CA-C	12.06	131.35	110.85
1	B	52	ALA	N-CA-CB	11.88	129.14	109.78
1	B	51	LEU	N-CA-CB	-11.84	92.64	110.16
1	A	67	PHE	CA-CB-CG	-11.38	102.42	113.80
1	B	67	PHE	CA-CB-CG	-11.35	102.45	113.80
1	A	731	PRO	N-CD-CG	10.95	119.62	103.20
1	B	731	PRO	N-CD-CG	10.90	119.56	103.20
1	B	364	PRO	CA-N-CD	-10.53	97.26	112.00
1	A	364	PRO	CA-N-CD	-10.48	97.33	112.00
1	B	134	PRO	CA-N-CD	-10.40	97.44	112.00
1	A	134	PRO	CA-N-CD	-10.37	97.48	112.00
1	B	84	GLU	N-CA-CB	10.32	128.05	110.50
1	B	364	PRO	N-CA-CB	9.87	112.69	103.41
1	A	364	PRO	N-CA-CB	9.74	112.57	103.41
1	A	84	GLU	N-CA-CB	9.61	126.83	110.50
1	A	352	SER	CB-CA-C	9.33	125.33	110.96
1	B	352	SER	CB-CA-C	9.33	125.33	110.96
1	A	366	LEU	N-CA-CB	9.11	125.82	110.71
1	A	731	PRO	N-CA-CB	8.92	113.43	103.44
1	B	366	LEU	N-CA-CB	8.88	125.44	110.71
1	A	189	GLU	CB-CG-CD	8.83	127.61	112.60
1	B	731	PRO	N-CA-CB	8.83	113.33	103.44
1	B	189	GLU	CB-CG-CD	8.82	127.60	112.60
1	B	50	ASN	OD1-CG-ND2	-8.67	113.93	122.60
1	A	155	THR	N-CA-CB	8.53	125.99	111.50
1	A	117	HIS	ND1-CG-CD2	8.52	114.62	106.10
1	B	155	THR	N-CA-CB	8.52	125.99	111.50
1	B	117	HIS	ND1-CG-CD2	8.50	114.60	106.10
1	B	326	GLY	CA-C-O	-8.48	115.06	120.91
1	A	326	GLY	CA-C-O	-8.42	115.10	120.91
1	A	51	LEU	CA-C-O	8.35	129.51	120.24
1	A	53	THR	CB-CA-C	-8.26	97.72	111.02
1	A	83	ASP	N-CA-CB	8.23	124.41	110.49
1	A	51	LEU	CB-CA-C	8.23	125.76	110.70
1	B	129	LEU	O-C-N	8.22	132.81	123.27
1	B	83	ASP	N-CA-CB	8.11	124.20	110.49
1	A	129	LEU	O-C-N	8.11	132.68	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	PRO	CA-N-CD	-8.05	100.73	112.00
1	B	688	PRO	CA-N-CD	-7.96	100.85	112.00
1	A	194	LEU	CB-CA-C	7.96	124.38	110.85
1	A	389	PRO	CA-N-CD	-7.72	101.19	112.00
1	B	194	LEU	CB-CA-C	7.72	123.97	110.85
1	A	350	ALA	O-C-N	7.72	130.02	122.07
1	B	327	SER	CB-CA-C	7.69	125.71	110.42
1	B	389	PRO	CA-N-CD	-7.67	101.25	112.00
1	B	84	GLU	CB-CA-C	-7.66	95.54	110.10
1	A	327	SER	CB-CA-C	7.65	125.65	110.42
1	B	350	ALA	O-C-N	7.65	129.95	122.07
1	B	129	LEU	CA-C-O	-7.64	112.20	121.06
1	B	696	PRO	CA-N-CD	-7.60	101.35	112.00
1	A	369	PHE	CA-CB-CG	-7.58	106.22	113.80
1	A	129	LEU	CA-C-O	-7.57	112.28	121.06
1	A	696	PRO	CA-N-CD	-7.54	101.44	112.00
1	A	84	GLU	CB-CA-C	-7.49	95.87	110.10
1	B	369	PHE	CA-CB-CG	-7.45	106.35	113.80
1	A	50	ASN	CA-CB-CG	-7.33	105.27	112.60
1	B	50	ASN	N-CA-CB	-7.31	98.31	110.37
1	A	52	ALA	N-CA-CB	7.27	122.77	110.49
1	A	389	PRO	N-CD-CG	7.23	114.05	103.20
1	B	389	PRO	N-CD-CG	7.19	113.99	103.20
1	B	327	SER	N-CA-CB	-7.13	98.44	110.49
1	A	327	SER	N-CA-CB	-7.09	98.50	110.49
1	A	104	VAL	N-CA-CB	7.03	119.33	110.05
1	B	203	THR	O-C-N	7.01	131.92	122.59
1	B	104	VAL	N-CA-CB	7.00	119.29	110.05
1	B	621	ASN	CA-CB-CG	-6.99	105.61	112.60
1	A	203	THR	O-C-N	6.98	131.87	122.59
1	A	280	VAL	CB-CA-C	-6.98	103.35	110.89
1	A	621	ASN	CA-CB-CG	-6.92	105.68	112.60
1	A	92	VAL	N-CA-CB	6.84	123.13	111.50
1	A	117	HIS	CG-CD2-NE2	-6.84	100.36	107.20
1	B	92	VAL	N-CA-CB	6.83	123.11	111.50
1	B	134	PRO	N-CD-CG	6.83	113.44	103.20
1	A	134	PRO	N-CD-CG	6.83	113.44	103.20
1	B	117	HIS	CG-CD2-NE2	-6.81	100.39	107.20
1	B	280	VAL	CB-CA-C	-6.81	103.54	110.89
1	B	696	PRO	N-CD-CG	6.78	113.37	103.20
1	A	353	ALA	CA-C-O	6.70	127.66	120.55
1	B	353	ALA	CA-C-O	6.68	127.63	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	PRO	N-CD-CG	6.59	113.09	103.20
1	B	356	TYR	CB-CG-CD2	-6.49	111.06	120.80
1	A	188	TYR	O-C-N	6.49	131.22	122.59
1	B	188	TYR	O-C-N	6.48	131.21	122.59
1	A	357	TRP	CB-CA-C	6.48	121.13	110.90
1	B	357	TRP	CB-CA-C	6.45	121.10	110.90
1	A	329	PRO	CA-N-CD	-6.36	103.10	112.00
1	B	329	PRO	CA-N-CD	-6.32	103.15	112.00
1	A	328	LYS	CB-CA-C	-6.31	97.73	110.17
1	B	328	LYS	CB-CA-C	-6.29	97.79	110.17
1	B	51	LEU	CD1-CG-CD2	-6.26	97.03	110.80
1	B	384	PHE	N-CA-CB	-6.22	100.98	110.01
1	A	134	PRO	N-CA-CB	6.22	110.41	103.44
1	B	697	ILE	CB-CA-C	-6.21	101.11	111.29
1	B	92	VAL	CB-CA-C	-6.21	99.61	111.40
1	A	92	VAL	CB-CA-C	-6.19	99.64	111.40
1	B	134	PRO	N-CA-CB	6.17	110.35	103.44
1	A	384	PHE	N-CA-CB	-6.14	101.10	110.01
1	A	364	PRO	CB-CA-C	6.08	120.62	111.44
1	B	364	PRO	CB-CA-C	6.01	120.52	111.44
1	A	697	ILE	CB-CA-C	-6.01	101.44	111.29
1	A	26	THR	O-C-N	5.95	130.33	122.36
1	B	353	ALA	O-C-N	-5.93	115.84	122.12
1	B	389	PRO	N-CA-CB	5.93	109.47	103.25
1	A	353	ALA	O-C-N	-5.92	115.84	122.12
1	A	389	PRO	N-CA-CB	5.91	109.46	103.25
1	A	350	ALA	CA-C-O	-5.90	114.63	120.82
1	B	50	ASN	CB-CG-OD1	5.85	132.50	120.80
1	B	350	ALA	CA-C-O	-5.84	114.68	120.82
1	A	356	TYR	CB-CG-CD1	5.82	129.53	120.80
1	A	550	LEU	O-C-N	5.80	130.30	122.59
1	B	550	LEU	O-C-N	5.78	130.28	122.59
1	A	653	ASP	CA-CB-CG	-5.74	106.86	112.60
1	B	104	VAL	CB-CA-C	-5.68	102.74	111.71
1	A	344	PRO	CA-N-CD	-5.63	104.11	112.00
1	A	104	VAL	CB-CA-C	-5.63	102.82	111.71
1	B	356	TYR	CB-CG-CD1	5.62	129.23	120.80
1	B	344	PRO	CA-N-CD	-5.60	104.16	112.00
1	A	688	PRO	N-CD-CG	5.59	111.59	103.20
1	B	361	ALA	CB-CA-C	-5.59	102.11	110.50
1	B	688	PRO	N-CD-CG	5.59	111.59	103.20
1	A	356	TYR	CB-CG-CD2	-5.58	112.43	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	SER	O-C-N	5.56	129.99	122.59
1	A	160	VAL	N-CA-CB	-5.52	102.12	111.23
1	A	361	ALA	CB-CA-C	-5.52	102.22	110.50
1	B	160	VAL	N-CA-CB	-5.52	102.13	111.23
1	A	149	SER	O-C-N	5.50	129.91	122.59
1	B	102	LEU	CB-CA-C	5.48	121.33	110.42
1	A	102	LEU	CB-CA-C	5.46	121.29	110.42
1	A	51	LEU	O-C-N	-5.41	115.19	122.23
1	B	362	HIS	CA-CB-CG	5.37	119.17	113.80
1	A	357	TRP	N-CA-CB	-5.29	102.39	110.07
1	B	357	TRP	N-CA-CB	-5.26	102.44	110.07
1	A	51	LEU	CD1-CG-CD2	-5.24	99.27	110.80
1	A	203	THR	CA-C-O	-5.23	113.03	120.51
1	B	203	THR	CA-C-O	-5.23	113.03	120.51
1	B	26	THR	O-C-N	5.19	128.76	122.48
1	B	75	GLU	N-CA-CB	5.18	117.82	110.16
1	B	183	ARG	CB-CA-C	-5.16	109.64	117.07
1	A	362	HIS	CA-CB-CG	5.15	118.95	113.80
1	A	183	ARG	CB-CA-C	-5.11	109.72	117.07
1	A	730	PRO	C-N-CD	5.11	145.93	125.00
1	A	75	GLU	N-CA-CB	5.10	117.71	110.16
1	B	730	PRO	C-N-CD	5.09	145.86	125.00
1	B	57	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	189	GLU	CB-CA-C	-5.07	100.32	110.42
1	B	57	PHE	CB-CA-C	-5.05	102.00	110.19
1	A	696	PRO	N-CA-CB	5.04	108.54	103.25
1	A	189	GLU	CB-CA-C	-5.03	100.42	110.42
1	A	358	TYR	N-CA-CB	-5.01	101.99	110.50

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PHE	Peptide
1	A	121	LEU	Peptide
1	A	186	SER	Peptide
1	A	209	LYS	Peptide
1	A	210	SER	Peptide
1	A	211	ARG	Peptide
1	A	213	GLY	Peptide
1	A	297	ASN	Peptide
1	A	327	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	107	PHE	Peptide
1	B	121	LEU	Peptide
1	B	186	SER	Peptide
1	B	209	LYS	Peptide
1	B	210	SER	Peptide
1	B	211	ARG	Peptide
1	B	213	GLY	Peptide
1	B	297	ASN	Peptide
1	B	327	SER	Peptide

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	5466	0	5715	1130	0
1	B	5466	0	5715	1117	0
All	All	10932	0	11430	2203	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 99.

All (2203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:TYR:CD2	1:A:356:TYR:CG	1.79	1.64
1:B:356:TYR:CE1	1:B:356:TYR:CZ	1.82	1.62
1:A:353:ALA:C	1:A:356:TYR:CG	1.76	1.60
1:A:354:PHE:N	1:A:356:TYR:CD1	1.68	1.59
1:A:51:LEU:CB	1:A:51:LEU:CA	1.77	1.59
1:B:52:ALA:CB	1:B:52:ALA:CA	1.77	1.59
1:B:352:SER:N	1:B:356:TYR:CE1	1.70	1.58
1:B:51:LEU:CB	1:B:51:LEU:CA	1.77	1.56
1:B:351:ILE:C	1:B:356:TYR:CE1	1.84	1.55
1:B:354:PHE:N	1:B:356:TYR:CD1	1.73	1.54
1:B:353:ALA:C	1:B:356:TYR:CG	1.79	1.52
1:B:363:ALA:C	1:B:365:LEU:HA	1.29	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:SER:N	1:A:356:TYR:CE1	1.81	1.48
1:A:363:ALA:C	1:A:365:LEU:HA	1.29	1.48
1:B:51:LEU:CB	1:B:51:LEU:CG	1.94	1.44
1:B:51:LEU:CG	1:B:51:LEU:CD1	2.01	1.39
1:A:360:ILE:H	1:A:361:ALA:CA	1.37	1.38
1:B:71:LYS:HE3	1:B:75:GLU:CG	1.54	1.38
1:A:351:ILE:C	1:A:356:TYR:CE1	2.04	1.36
1:B:360:ILE:H	1:B:361:ALA:CA	1.36	1.35
1:A:71:LYS:HE3	1:A:75:GLU:CG	1.53	1.34
1:A:360:ILE:HG21	1:A:697:ILE:CG2	1.57	1.33
1:B:160:VAL:HA	1:B:161:MET:C	1.49	1.33
1:B:360:ILE:HG21	1:B:697:ILE:CG2	1.58	1.32
1:B:160:VAL:HA	1:B:162:TYR:N	1.41	1.32
1:A:160:VAL:HA	1:A:162:TYR:N	1.41	1.32
1:A:160:VAL:HA	1:A:161:MET:C	1.50	1.26
1:A:363:ALA:C	1:A:365:LEU:CA	2.09	1.24
1:A:51:LEU:O	1:B:52:ALA:HA	1.36	1.24
1:A:352:SER:C	1:A:356:TYR:CD2	2.01	1.23
1:B:363:ALA:C	1:B:365:LEU:CA	2.09	1.23
1:A:119:ILE:O	1:A:187:PHE:N	1.71	1.22
1:B:119:ILE:O	1:B:187:PHE:N	1.72	1.22
1:B:353:ALA:HA	1:B:356:TYR:CD2	1.63	1.21
1:A:52:ALA:CA	1:A:52:ALA:CB	2.18	1.20
1:B:353:ALA:C	1:B:356:TYR:CB	2.14	1.20
1:A:353:ALA:C	1:A:356:TYR:CB	2.15	1.18
1:B:364:PRO:N	1:B:365:LEU:C	2.02	1.18
1:A:364:PRO:N	1:A:365:LEU:C	2.02	1.17
1:B:95:LEU:HB3	1:B:96:SER:C	1.68	1.17
1:A:95:LEU:HB3	1:A:96:SER:C	1.68	1.17
1:B:120:SER:HB3	1:B:123:TYR:CA	1.73	1.17
1:A:130:LEU:HD13	1:A:354:PHE:CB	1.76	1.16
1:B:215:ALA:HB2	1:B:645:SER:HA	1.25	1.16
1:A:153:ARG:HB2	1:A:155:THR:CB	1.76	1.15
1:A:120:SER:HB3	1:A:123:TYR:CA	1.73	1.15
1:A:51:LEU:C	1:B:52:ALA:HB2	1.69	1.15
1:B:130:LEU:HD13	1:B:354:PHE:CB	1.76	1.15
1:B:153:ARG:HB2	1:B:155:THR:CB	1.77	1.15
1:A:91:GLU:HA	1:A:92:VAL:HG13	1.28	1.15
1:A:404:ILE:HD11	1:A:657:ASP:O	1.47	1.15
1:A:71:LYS:HE3	1:A:75:GLU:HG3	1.28	1.14
1:A:353:ALA:CA	1:A:356:TYR:CD2	2.18	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ILE:H	1:A:361:ALA:HA	1.09	1.13
1:A:150:ALA:C	1:A:153:ARG:HB3	1.74	1.12
1:B:86:ALA:HB1	1:B:87:ALA:HB2	1.21	1.12
1:A:153:ARG:HB2	1:A:155:THR:HB	1.29	1.12
1:A:353:ALA:HA	1:A:356:TYR:CD2	1.67	1.12
1:A:349:VAL:O	1:A:356:TYR:CZ	2.02	1.11
1:B:91:GLU:HA	1:B:92:VAL:HG13	1.28	1.11
1:B:130:LEU:O	1:B:134:PRO:HD2	1.50	1.11
1:A:203:THR:O	1:A:205:GLU:N	1.83	1.11
1:B:188:TYR:O	1:B:189:GLU:HB3	1.51	1.11
1:A:130:LEU:O	1:A:134:PRO:HD2	1.50	1.10
1:B:404:ILE:HD11	1:B:657:ASP:O	1.51	1.10
1:A:215:ALA:HB2	1:A:645:SER:HA	1.24	1.10
1:B:150:ALA:C	1:B:153:ARG:HB3	1.74	1.10
1:A:86:ALA:HB1	1:A:87:ALA:HB2	1.20	1.10
1:B:203:THR:O	1:B:205:GLU:N	1.83	1.10
1:B:71:LYS:HE3	1:B:75:GLU:HG3	1.29	1.09
1:B:189:GLU:CG	1:B:193:LEU:H	1.64	1.09
1:A:120:SER:HB3	1:A:123:TYR:HA	1.33	1.09
1:A:189:GLU:CG	1:A:193:LEU:H	1.64	1.09
1:B:352:SER:N	1:B:356:TYR:CZ	2.02	1.09
1:A:150:ALA:O	1:A:153:ARG:HB3	1.51	1.09
1:B:360:ILE:N	1:B:361:ALA:HA	1.60	1.08
1:A:353:ALA:O	1:A:356:TYR:CB	2.01	1.08
1:B:154:ARG:HA	1:B:155:THR:O	1.53	1.08
1:A:684:VAL:O	1:A:688:PRO:HD2	1.54	1.08
1:B:363:ALA:HA	1:B:365:LEU:O	1.52	1.07
1:A:353:ALA:C	1:A:356:TYR:CD1	2.08	1.07
1:A:363:ALA:HA	1:A:365:LEU:O	1.52	1.07
1:A:189:GLU:CD	1:A:189:GLU:C	2.23	1.07
1:A:656:ARG:HH12	1:B:82:VAL:CG1	1.65	1.07
1:A:181:LEU:N	1:A:182:PRO:HA	1.69	1.07
1:B:353:ALA:O	1:B:356:TYR:CB	2.01	1.07
1:A:360:ILE:N	1:A:361:ALA:HA	1.60	1.06
1:B:118:PHE:O	1:B:187:PHE:N	1.88	1.06
1:B:150:ALA:O	1:B:153:ARG:HB3	1.51	1.06
1:B:353:ALA:CA	1:B:356:TYR:CD2	2.10	1.06
1:A:83:ASP:N	1:A:84:GLU:HB3	1.70	1.06
1:B:115:LEU:HD22	1:B:174:VAL:HG13	1.35	1.06
1:B:120:SER:HB3	1:B:123:TYR:HA	1.33	1.06
1:B:684:VAL:O	1:B:688:PRO:HD2	1.54	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ILE:HG21	1:A:697:ILE:HG23	1.09	1.05
1:B:153:ARG:HB2	1:B:155:THR:HB	1.29	1.05
1:B:360:ILE:H	1:B:361:ALA:HA	1.09	1.05
1:B:189:GLU:C	1:B:189:GLU:CD	2.23	1.05
1:A:51:LEU:CB	1:A:51:LEU:N	2.20	1.05
1:A:151:LEU:O	1:A:153:ARG:CA	2.05	1.05
1:B:129:LEU:O	1:B:130:LEU:HG	1.55	1.05
1:B:151:LEU:O	1:B:153:ARG:CA	2.05	1.05
1:B:181:LEU:N	1:B:182:PRO:HA	1.69	1.05
1:A:188:TYR:O	1:A:189:GLU:HB3	1.51	1.04
1:A:360:ILE:H	1:A:361:ALA:CB	1.70	1.04
1:A:129:LEU:HD22	1:A:368:ALA:HB3	1.38	1.04
1:A:154:ARG:HA	1:A:155:THR:O	1.53	1.04
1:B:129:LEU:HD22	1:B:368:ALA:HB3	1.38	1.04
1:B:354:PHE:CA	1:B:356:TYR:CD1	2.39	1.04
1:B:360:ILE:HG21	1:B:697:ILE:HG23	1.06	1.04
1:A:115:LEU:HD22	1:A:174:VAL:HG13	1.35	1.04
1:A:118:PHE:O	1:A:187:PHE:N	1.89	1.04
1:A:360:ILE:HG22	1:A:362:HIS:O	1.56	1.04
1:A:384:PHE:CE2	1:A:679:ALA:HB1	1.91	1.04
1:B:349:VAL:O	1:B:356:TYR:CZ	2.11	1.04
1:A:129:LEU:O	1:A:130:LEU:HG	1.56	1.03
1:B:83:ASP:HB2	1:B:84:GLU:HA	1.38	1.03
1:B:360:ILE:H	1:B:361:ALA:CB	1.70	1.03
1:B:384:PHE:CE2	1:B:679:ALA:HB1	1.91	1.03
1:A:51:LEU:C	1:B:52:ALA:CB	2.32	1.03
1:A:354:PHE:CA	1:A:356:TYR:HD1	1.71	1.03
1:B:160:VAL:CA	1:B:161:MET:C	2.32	1.02
1:B:360:ILE:N	1:B:361:ALA:CA	2.13	1.02
1:A:94:HIS:C	1:A:95:LEU:HD23	1.84	1.02
1:A:692:GLY:O	1:A:696:PRO:HD2	1.60	1.02
1:B:94:HIS:C	1:B:95:LEU:HD23	1.84	1.02
1:B:354:PHE:CA	1:B:356:TYR:HD1	1.72	1.02
1:A:160:VAL:CA	1:A:161:MET:C	2.32	1.02
1:A:360:ILE:N	1:A:361:ALA:CA	2.13	1.02
1:B:83:ASP:N	1:B:84:GLU:HB3	1.73	1.02
1:A:360:ILE:HG23	1:A:363:ALA:H	1.22	1.02
1:A:364:PRO:N	1:A:365:LEU:CA	2.21	1.02
1:B:360:ILE:HG22	1:B:362:HIS:O	1.59	1.02
1:A:83:ASP:HB2	1:A:84:GLU:HA	1.41	1.01
1:A:354:PHE:CA	1:A:356:TYR:CD1	2.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:HD11	1:B:158:MET:CA	1.90	1.01
1:B:120:SER:CB	1:B:123:TYR:HA	1.90	1.01
1:A:352:SER:N	1:A:356:TYR:CZ	2.18	1.01
1:B:360:ILE:HG23	1:B:363:ALA:H	1.23	1.01
1:B:364:PRO:N	1:B:365:LEU:CA	2.21	1.01
1:A:215:ALA:CB	1:A:645:SER:HA	1.90	1.01
1:A:364:PRO:HG2	1:A:366:LEU:C	1.85	1.01
1:A:349:VAL:C	1:A:356:TYR:OH	2.04	1.01
1:B:352:SER:CB	1:B:356:TYR:CE2	2.44	1.01
1:A:94:HIS:O	1:A:95:LEU:HD23	1.59	1.01
1:A:363:ALA:O	1:A:365:LEU:HA	1.58	1.01
1:A:433:LYS:HD2	1:A:433:LYS:O	1.59	1.00
1:B:94:HIS:O	1:B:95:LEU:HD23	1.60	1.00
1:B:363:ALA:O	1:B:365:LEU:HA	1.58	1.00
1:B:364:PRO:HG2	1:B:366:LEU:C	1.85	1.00
1:B:215:ALA:CB	1:B:645:SER:HA	1.91	1.00
1:A:52:ALA:HB3	1:B:51:LEU:CG	1.90	1.00
1:B:120:SER:CB	1:B:123:TYR:CA	2.39	1.00
1:A:120:SER:CB	1:A:123:TYR:HA	1.90	1.00
1:B:95:LEU:CD1	1:B:158:MET:HA	1.92	1.00
1:A:120:SER:CB	1:A:123:TYR:CA	2.39	1.00
1:B:129:LEU:O	1:B:130:LEU:CG	2.10	1.00
1:A:51:LEU:CA	1:B:52:ALA:HB2	1.92	0.99
1:A:83:ASP:HB2	1:A:84:GLU:CA	1.92	0.99
1:B:91:GLU:HA	1:B:92:VAL:CG1	1.92	0.99
1:B:692:GLY:O	1:B:696:PRO:HD2	1.60	0.99
1:A:350:ALA:C	1:A:356:TYR:HE1	1.69	0.99
1:B:350:ALA:O	1:B:356:TYR:CE1	2.16	0.99
1:B:353:ALA:C	1:B:356:TYR:CD1	2.20	0.99
1:B:729:VAL:O	1:B:731:PRO:CD	2.11	0.99
1:A:91:GLU:HA	1:A:92:VAL:CG1	1.92	0.99
1:A:95:LEU:HD11	1:A:158:MET:CA	1.92	0.99
1:B:83:ASP:HB2	1:B:84:GLU:CA	1.90	0.98
1:B:151:LEU:O	1:B:153:ARG:CB	2.11	0.98
1:A:95:LEU:CD1	1:A:158:MET:HA	1.92	0.98
1:B:95:LEU:HD11	1:B:158:MET:CB	1.92	0.98
1:A:150:ALA:O	1:A:153:ARG:CB	2.11	0.98
1:A:189:GLU:CG	1:A:192:VAL:N	2.26	0.98
1:A:189:GLU:HB2	1:A:191:SER:N	1.78	0.98
1:A:428:THR:HG23	1:A:655:LEU:CD2	1.94	0.98
1:B:189:GLU:CG	1:B:192:VAL:N	2.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:O	1:B:52:ALA:CA	2.12	0.98
1:A:129:LEU:O	1:A:130:LEU:CG	2.10	0.98
1:B:354:PHE:CB	1:B:356:TYR:HD1	1.77	0.98
1:A:215:ALA:O	1:A:217:LYS:N	1.97	0.97
1:A:350:ALA:O	1:A:356:TYR:CE1	2.17	0.97
1:A:357:TRP:CB	1:A:695:TYR:HA	1.94	0.97
1:B:189:GLU:HB2	1:B:191:SER:N	1.78	0.97
1:B:355:ILE:N	1:B:356:TYR:CD1	2.32	0.97
1:A:151:LEU:O	1:A:153:ARG:CB	2.12	0.97
1:A:729:VAL:O	1:A:731:PRO:CD	2.11	0.97
1:B:357:TRP:CB	1:B:695:TYR:HA	1.94	0.97
1:B:95:LEU:HB3	1:B:96:SER:CA	1.95	0.97
1:A:95:LEU:HB3	1:A:96:SER:CA	1.95	0.97
1:A:83:ASP:CA	1:A:84:GLU:HB3	1.95	0.96
1:B:215:ALA:O	1:B:217:LYS:N	1.97	0.96
1:A:349:VAL:O	1:A:356:TYR:OH	1.82	0.96
1:A:95:LEU:HD11	1:A:158:MET:CB	1.95	0.96
1:B:23:THR:N	1:B:80:GLY:O	1.99	0.96
1:A:130:LEU:HD13	1:A:354:PHE:HB2	1.47	0.96
1:A:352:SER:CB	1:A:356:TYR:CE2	2.49	0.96
1:B:150:ALA:O	1:B:153:ARG:CB	2.11	0.96
1:B:428:THR:HG23	1:B:655:LEU:CD2	1.95	0.96
1:B:189:GLU:CB	1:B:192:VAL:N	2.29	0.95
1:A:52:ALA:CB	1:B:51:LEU:CG	2.44	0.95
1:B:350:ALA:C	1:B:356:TYR:HE1	1.75	0.95
1:A:189:GLU:CB	1:A:192:VAL:N	2.29	0.95
1:B:130:LEU:HD13	1:B:354:PHE:HB2	1.47	0.94
1:B:150:ALA:O	1:B:153:ARG:CG	2.15	0.94
1:A:327:SER:HB2	1:A:328:LYS:CG	1.97	0.94
1:A:23:THR:N	1:A:80:GLY:O	2.00	0.94
1:B:90:ALA:HA	1:B:91:GLU:HB2	1.50	0.94
1:A:360:ILE:HG21	1:A:697:ILE:HG21	1.48	0.94
1:B:83:ASP:CA	1:B:84:GLU:HB3	1.98	0.94
1:A:351:ILE:C	1:A:356:TYR:HE1	1.74	0.94
1:A:52:ALA:HB2	1:B:51:LEU:CB	1.42	0.94
1:A:90:ALA:HA	1:A:91:GLU:HB2	1.50	0.94
1:B:71:LYS:HE3	1:B:75:GLU:HG2	1.49	0.94
1:B:327:SER:HB2	1:B:328:LYS:CG	1.97	0.94
1:A:150:ALA:O	1:A:153:ARG:CG	2.15	0.93
1:B:550:LEU:O	1:B:551:LYS:O	1.87	0.93
1:B:349:VAL:C	1:B:356:TYR:OH	2.11	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ALA:HB2	1:A:723:LEU:HD13	1.51	0.92
1:A:189:GLU:CB	1:A:192:VAL:H	1.82	0.92
1:B:121:LEU:O	1:B:183:ARG:O	1.88	0.92
1:B:354:PHE:C	1:B:356:TYR:HB2	1.93	0.92
1:A:78:GLY:O	1:A:79:TYR:CG	2.23	0.92
1:B:429:LEU:O	1:B:550:LEU:C	2.11	0.92
1:B:189:GLU:CB	1:B:192:VAL:H	1.82	0.92
1:B:391:ALA:HB2	1:B:723:LEU:HD13	1.52	0.92
1:A:95:LEU:HA	1:A:96:SER:HB2	1.52	0.91
1:A:121:LEU:O	1:A:183:ARG:O	1.88	0.91
1:A:209:LYS:O	1:A:211:ARG:N	2.04	0.91
1:A:117:HIS:HB3	1:A:191:SER:HB2	1.52	0.91
1:A:189:GLU:HB2	1:A:191:SER:CA	2.01	0.91
1:B:81:VAL:O	1:B:84:GLU:CD	2.14	0.91
1:A:404:ILE:HD13	1:A:661:ALA:N	1.86	0.91
1:A:429:LEU:O	1:A:550:LEU:C	2.12	0.91
1:B:117:HIS:HB3	1:B:191:SER:HB2	1.51	0.91
1:B:120:SER:HB3	1:B:123:TYR:N	1.85	0.91
1:B:360:ILE:CG2	1:B:697:ILE:CG2	2.49	0.91
1:A:71:LYS:CE	1:A:75:GLU:HG3	2.01	0.91
1:B:189:GLU:HG3	1:B:192:VAL:CA	2.01	0.91
1:B:209:LYS:O	1:B:211:ARG:N	2.03	0.91
1:B:350:ALA:C	1:B:356:TYR:CE1	2.49	0.91
1:B:404:ILE:HD13	1:B:661:ALA:N	1.85	0.91
1:A:90:ALA:CA	1:A:91:GLU:HB2	2.01	0.91
1:B:95:LEU:HD11	1:B:158:MET:HA	1.51	0.91
1:B:189:GLU:CB	1:B:191:SER:N	2.34	0.90
1:A:189:GLU:CB	1:A:191:SER:N	2.34	0.90
1:B:78:GLY:O	1:B:79:TYR:CG	2.24	0.90
1:B:354:PHE:HB3	1:B:356:TYR:HD1	1.34	0.90
1:B:696:PRO:O	1:B:698:PHE:N	2.05	0.90
1:A:189:GLU:HG3	1:A:192:VAL:CA	2.01	0.90
1:A:360:ILE:HB	1:A:697:ILE:HG12	1.53	0.90
1:A:550:LEU:O	1:A:551:LYS:O	1.87	0.90
1:A:360:ILE:CG2	1:A:697:ILE:CG2	2.48	0.90
1:B:83:ASP:CB	1:B:84:GLU:CB	2.49	0.90
1:B:360:ILE:HB	1:B:697:ILE:HG12	1.53	0.90
1:A:81:VAL:O	1:A:84:GLU:CD	2.15	0.90
1:B:353:ALA:O	1:B:356:TYR:HB3	1.70	0.90
1:A:423:PHE:CD1	1:A:428:THR:HG21	2.07	0.90
1:B:90:ALA:CA	1:B:91:GLU:HB2	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ALA:CB	1:B:51:LEU:HB2	1.39	0.90
1:A:120:SER:HB3	1:A:123:TYR:N	1.85	0.90
1:A:189:GLU:HG2	1:A:190:THR:C	1.97	0.90
1:A:71:LYS:HE3	1:A:75:GLU:HG2	1.49	0.89
1:A:352:SER:CB	1:A:356:TYR:CZ	2.45	0.89
1:B:360:ILE:HG21	1:B:697:ILE:HG21	1.52	0.89
1:A:21:ARG:O	1:A:81:VAL:HA	1.72	0.89
1:A:696:PRO:O	1:A:698:PHE:N	2.05	0.89
1:B:51:LEU:CB	1:B:51:LEU:N	2.34	0.89
1:B:95:LEU:HA	1:B:96:SER:HB2	1.52	0.89
1:A:95:LEU:HD11	1:A:158:MET:HA	1.51	0.89
1:B:326:GLY:O	1:B:327:SER:O	1.90	0.89
1:B:189:GLU:HB2	1:B:191:SER:CA	2.01	0.89
1:A:326:GLY:O	1:A:327:SER:O	1.90	0.89
1:A:354:PHE:C	1:A:356:TYR:HB2	1.95	0.89
1:A:83:ASP:CB	1:A:84:GLU:CB	2.51	0.89
1:B:160:VAL:HG22	1:B:162:TYR:HA	1.53	0.89
1:B:189:GLU:HG2	1:B:190:THR:C	1.97	0.89
1:B:71:LYS:CE	1:B:75:GLU:HG3	2.02	0.88
1:A:350:ALA:C	1:A:356:TYR:CE1	2.50	0.88
1:A:354:PHE:CB	1:A:356:TYR:HD1	1.85	0.88
1:B:360:ILE:CG2	1:B:697:ILE:HG23	2.00	0.88
1:A:111:LEU:HD22	1:A:198:LEU:HD11	1.55	0.88
1:B:189:GLU:HG2	1:B:191:SER:C	1.99	0.88
1:A:129:LEU:C	1:A:129:LEU:HD23	1.98	0.88
1:B:149:SER:O	1:B:153:ARG:HB3	1.74	0.88
1:B:352:SER:CB	1:B:356:TYR:CZ	2.40	0.88
1:B:428:THR:HG23	1:B:655:LEU:HD22	1.56	0.88
1:A:91:GLU:HB3	1:A:92:VAL:HG22	1.55	0.88
1:A:350:ALA:O	1:A:356:TYR:HE1	1.53	0.88
1:B:111:LEU:HD22	1:B:198:LEU:HD11	1.55	0.88
1:B:129:LEU:HD23	1:B:129:LEU:C	1.99	0.88
1:B:360:ILE:CG1	1:B:697:ILE:HG12	2.04	0.88
1:A:51:LEU:O	1:B:52:ALA:CB	2.22	0.87
1:A:119:ILE:O	1:A:186:SER:C	2.17	0.87
1:A:357:TRP:HB3	1:A:695:TYR:HA	1.54	0.87
1:B:119:ILE:O	1:B:186:SER:C	2.17	0.87
1:A:160:VAL:HG22	1:A:162:TYR:HA	1.53	0.87
1:A:51:LEU:C	1:B:52:ALA:CA	2.42	0.87
1:B:349:VAL:O	1:B:356:TYR:OH	1.91	0.87
1:A:355:ILE:N	1:A:356:TYR:CD1	2.41	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:SER:O	1:A:153:ARG:HB3	1.74	0.87
1:B:429:LEU:O	1:B:551:LYS:N	2.06	0.87
1:B:21:ARG:O	1:B:81:VAL:HA	1.74	0.87
1:B:352:SER:HB3	1:B:356:TYR:CE2	2.09	0.87
1:B:385:GLY:O	1:B:389:PRO:CD	2.23	0.87
1:B:423:PHE:CD1	1:B:428:THR:HG21	2.09	0.87
1:B:430:THR:O	1:B:551:LYS:CG	2.22	0.87
1:A:189:GLU:HG2	1:A:191:SER:C	1.99	0.86
1:A:429:LEU:O	1:A:551:LYS:N	2.08	0.86
1:B:111:LEU:HB3	1:B:170:PHE:CE1	2.10	0.86
1:B:122:PRO:HB2	1:B:125:ASP:HB2	1.57	0.86
1:B:154:ARG:HA	1:B:155:THR:C	2.01	0.86
1:A:385:GLY:O	1:A:389:PRO:CD	2.23	0.86
1:A:428:THR:HG23	1:A:655:LEU:HD22	1.55	0.86
1:B:91:GLU:HB3	1:B:92:VAL:HG22	1.55	0.86
1:A:111:LEU:HB3	1:A:170:PHE:CE1	2.10	0.86
1:A:113:LEU:HD11	1:A:376:LEU:HB3	1.58	0.86
1:A:126:PHE:CD1	1:A:129:LEU:HB2	2.10	0.86
1:A:352:SER:HB3	1:A:356:TYR:CE2	2.11	0.86
1:A:353:ALA:O	1:A:356:TYR:HB2	1.75	0.86
1:A:353:ALA:O	1:A:356:TYR:HB3	1.74	0.86
1:A:656:ARG:HH12	1:B:82:VAL:HG11	1.37	0.86
1:B:160:VAL:CA	1:B:162:TYR:N	2.35	0.86
1:A:360:ILE:CG2	1:A:697:ILE:HG23	2.01	0.86
1:B:126:PHE:CD1	1:B:129:LEU:HB2	2.10	0.86
1:B:189:GLU:HG3	1:B:193:LEU:H	1.41	0.86
1:B:130:LEU:HD13	1:B:354:PHE:CG	2.10	0.85
1:B:357:TRP:HB3	1:B:695:TYR:HA	1.55	0.85
1:B:430:THR:O	1:B:551:LYS:HG3	1.75	0.85
1:A:360:ILE:CG1	1:A:697:ILE:HG12	2.06	0.85
1:A:362:HIS:HB3	1:A:363:ALA:HB2	1.57	0.85
1:A:189:GLU:HB2	1:A:192:VAL:N	1.92	0.85
1:B:94:HIS:O	1:B:95:LEU:CD2	2.24	0.85
1:B:129:LEU:O	1:B:130:LEU:CD2	2.24	0.85
1:A:53:THR:HG22	1:B:51:LEU:HD11	1.58	0.85
1:A:129:LEU:O	1:A:130:LEU:CD2	2.24	0.85
1:A:189:GLU:HG3	1:A:192:VAL:HB	1.58	0.85
1:A:404:ILE:HG21	1:A:661:ALA:CB	2.06	0.85
1:A:52:ALA:HB3	1:B:51:LEU:HB2	0.96	0.85
1:A:151:LEU:O	1:A:153:ARG:N	2.10	0.85
1:B:328:LYS:H	1:B:329:PRO:CD	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ALA:C	1:A:365:LEU:C	2.40	0.85
1:A:696:PRO:C	1:A:698:PHE:H	1.85	0.85
1:A:101:LYS:C	1:A:103:TYR:H	1.85	0.85
1:B:121:LEU:N	1:B:122:PRO:O	2.10	0.85
1:A:100:ARG:O	1:A:104:VAL:HB	1.77	0.85
1:A:328:LYS:H	1:A:329:PRO:CD	1.89	0.85
1:A:360:ILE:HG23	1:A:363:ALA:N	1.91	0.85
1:B:100:ARG:O	1:B:104:VAL:HB	1.77	0.85
1:B:189:GLU:HB2	1:B:192:VAL:N	1.91	0.85
1:A:111:LEU:O	1:A:115:LEU:HG	1.77	0.84
1:A:154:ARG:HA	1:A:155:THR:C	2.01	0.84
1:B:113:LEU:HD11	1:B:376:LEU:HB3	1.59	0.84
1:B:151:LEU:O	1:B:153:ARG:N	2.10	0.84
1:A:52:ALA:CA	1:B:51:LEU:CB	2.55	0.84
1:A:130:LEU:HD13	1:A:354:PHE:CG	2.12	0.84
1:B:181:LEU:N	1:B:182:PRO:CA	2.40	0.84
1:A:181:LEU:N	1:A:182:PRO:CA	2.40	0.84
1:A:430:THR:O	1:A:551:LYS:HG3	1.77	0.84
1:A:121:LEU:N	1:A:122:PRO:O	2.10	0.84
1:A:357:TRP:N	1:A:358:TYR:HA	1.92	0.84
1:B:111:LEU:O	1:B:115:LEU:HG	1.77	0.84
1:B:327:SER:HB2	1:B:328:LYS:CB	2.07	0.84
1:A:94:HIS:O	1:A:95:LEU:CD2	2.24	0.84
1:A:127:VAL:O	1:A:366:LEU:HB2	1.78	0.84
1:A:189:GLU:HG3	1:A:193:LEU:H	1.41	0.84
1:B:101:LYS:C	1:B:103:TYR:H	1.85	0.84
1:B:362:HIS:HB3	1:B:363:ALA:HB2	1.57	0.84
1:B:357:TRP:HB3	1:B:694:LEU:O	1.77	0.83
1:B:684:VAL:O	1:B:688:PRO:CD	2.26	0.83
1:A:101:LYS:HA	1:A:104:VAL:HG12	1.60	0.83
1:B:95:LEU:CB	1:B:96:SER:C	2.50	0.83
1:B:363:ALA:C	1:B:365:LEU:C	2.40	0.83
1:A:160:VAL:CA	1:A:162:TYR:N	2.35	0.83
1:A:357:TRP:HB3	1:A:694:LEU:O	1.77	0.83
1:B:360:ILE:HG23	1:B:363:ALA:N	1.93	0.83
1:A:684:VAL:O	1:A:688:PRO:CD	2.26	0.83
1:B:84:GLU:CD	1:B:84:GLU:O	2.21	0.83
1:B:101:LYS:HA	1:B:104:VAL:HG12	1.60	0.83
1:B:696:PRO:C	1:B:698:PHE:H	1.85	0.83
1:A:189:GLU:CG	1:A:193:LEU:N	2.42	0.83
1:B:355:ILE:N	1:B:356:TYR:CG	2.47	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:CE	1:A:75:GLU:CG	2.48	0.83
1:A:122:PRO:HB2	1:A:125:ASP:HB2	1.58	0.83
1:A:327:SER:HB2	1:A:328:LYS:CB	2.07	0.83
1:B:127:VAL:O	1:B:366:LEU:HB2	1.78	0.83
1:A:86:ALA:CB	1:A:87:ALA:HB2	2.07	0.83
1:B:189:GLU:CG	1:B:193:LEU:N	2.42	0.83
1:B:95:LEU:CD1	1:B:158:MET:CA	2.54	0.83
1:B:156:LEU:HB3	1:B:163:SER:HA	1.61	0.83
1:B:353:ALA:O	1:B:356:TYR:HB2	1.78	0.83
1:B:357:TRP:N	1:B:358:TYR:HA	1.92	0.83
1:B:189:GLU:HG3	1:B:192:VAL:HB	1.58	0.82
1:B:327:SER:HB2	1:B:328:LYS:HG2	1.61	0.82
1:A:83:ASP:H	1:A:84:GLU:HB3	1.43	0.82
1:A:656:ARG:NH1	1:B:82:VAL:HG11	1.94	0.82
1:B:181:LEU:H	1:B:182:PRO:HA	1.42	0.82
1:A:181:LEU:H	1:A:182:PRO:HA	1.43	0.82
1:A:368:ALA:O	1:A:371:THR:N	2.12	0.82
1:B:86:ALA:CB	1:B:87:ALA:HB2	2.07	0.82
1:B:729:VAL:O	1:B:731:PRO:HD2	1.79	0.82
1:A:428:THR:O	1:A:655:LEU:HD11	1.78	0.82
1:B:385:GLY:O	1:B:389:PRO:HD3	1.78	0.82
1:A:385:GLY:O	1:A:389:PRO:HD3	1.79	0.82
1:B:83:ASP:HB2	1:B:84:GLU:CB	2.10	0.82
1:B:121:LEU:O	1:B:183:ARG:C	2.23	0.82
1:B:357:TRP:N	1:B:358:TYR:CA	2.43	0.82
1:B:729:VAL:O	1:B:731:PRO:HD3	1.77	0.82
1:A:95:LEU:CB	1:A:96:SER:C	2.51	0.82
1:A:729:VAL:O	1:A:731:PRO:HD2	1.79	0.82
1:B:117:HIS:NE2	1:B:373:ILE:HG21	1.94	0.82
1:B:368:ALA:O	1:B:371:THR:N	2.12	0.82
1:A:51:LEU:HA	1:B:52:ALA:HB2	1.60	0.81
1:B:428:THR:O	1:B:655:LEU:HD11	1.80	0.81
1:A:121:LEU:O	1:A:183:ARG:C	2.23	0.81
1:A:150:ALA:O	1:A:151:LEU:O	1.97	0.81
1:A:357:TRP:N	1:A:358:TYR:CA	2.43	0.81
1:B:81:VAL:HG12	1:B:83:ASP:OD1	1.79	0.81
1:B:95:LEU:HB3	1:B:96:SER:CB	2.11	0.81
1:B:190:THR:O	1:B:194:LEU:HD12	1.79	0.81
1:B:404:ILE:HG21	1:B:661:ALA:CB	2.10	0.81
1:B:429:LEU:HA	1:B:655:LEU:HD11	1.63	0.81
1:A:156:LEU:HB3	1:A:163:SER:HA	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:CD	1:A:190:THR:N	2.37	0.81
1:B:189:GLU:CD	1:B:190:THR:N	2.38	0.81
1:A:117:HIS:NE2	1:A:373:ILE:HG21	1.94	0.81
1:A:189:GLU:CG	1:A:190:THR:C	2.53	0.81
1:A:729:VAL:O	1:A:731:PRO:HD3	1.77	0.81
1:A:130:LEU:CD1	1:A:354:PHE:CG	2.64	0.81
1:A:52:ALA:HB1	1:B:51:LEU:CB	1.30	0.81
1:A:95:LEU:HB3	1:A:96:SER:CB	2.10	0.81
1:A:428:THR:HG23	1:A:655:LEU:HD21	1.63	0.81
1:B:151:LEU:C	1:B:153:ARG:HA	2.06	0.81
1:B:360:ILE:CB	1:B:697:ILE:HG12	2.08	0.81
1:B:352:SER:HB2	1:B:356:TYR:OH	1.81	0.81
1:A:83:ASP:HB2	1:A:84:GLU:CB	2.09	0.81
1:B:130:LEU:CD1	1:B:354:PHE:CG	2.63	0.81
1:A:51:LEU:O	1:B:52:ALA:HB2	1.79	0.80
1:B:83:ASP:H	1:B:84:GLU:HB3	1.45	0.80
1:B:95:LEU:CA	1:B:96:SER:HB2	2.12	0.80
1:B:351:ILE:O	1:B:356:TYR:CE1	2.34	0.80
1:B:354:PHE:HB3	1:B:356:TYR:CD1	2.15	0.80
1:A:95:LEU:CB	1:A:96:SER:HB2	2.11	0.80
1:A:151:LEU:C	1:A:153:ARG:HA	2.06	0.80
1:A:340:ALA:O	1:A:344:PRO:CD	2.29	0.80
1:A:362:HIS:HA	1:A:365:LEU:O	1.81	0.80
1:B:52:ALA:CB	1:B:52:ALA:HA	2.09	0.80
1:B:120:SER:OG	1:B:123:TYR:CB	2.29	0.80
1:B:340:ALA:O	1:B:344:PRO:CD	2.30	0.80
1:B:189:GLU:CG	1:B:190:THR:C	2.53	0.80
1:A:208:ALA:O	1:A:210:SER:HB3	1.82	0.80
1:B:102:LEU:HB2	1:B:156:LEU:HD12	1.63	0.80
1:B:150:ALA:O	1:B:151:LEU:O	1.97	0.80
1:A:327:SER:HB2	1:A:328:LYS:HG2	1.62	0.80
1:A:360:ILE:CB	1:A:697:ILE:HG12	2.10	0.80
1:B:95:LEU:CD1	1:B:158:MET:CB	2.60	0.80
1:A:190:THR:O	1:A:194:LEU:HD12	1.82	0.80
1:A:95:LEU:CD1	1:A:158:MET:CA	2.55	0.80
1:A:189:GLU:HG3	1:A:192:VAL:CB	2.12	0.80
1:A:189:GLU:OE1	1:A:189:GLU:O	2.00	0.80
1:B:189:GLU:OE2	1:B:193:LEU:HB2	1.82	0.80
1:A:95:LEU:CA	1:A:96:SER:HB2	2.12	0.79
1:B:371:THR:O	1:B:374:ALA:N	2.15	0.79
1:A:51:LEU:C	1:B:52:ALA:HA	2.04	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD12	1:A:369:PHE:CD1	2.17	0.79
1:A:189:GLU:HG2	1:A:190:THR:O	1.82	0.79
1:A:404:ILE:HG21	1:A:661:ALA:HB2	1.64	0.79
1:B:95:LEU:CB	1:B:96:SER:HB2	2.12	0.79
1:B:71:LYS:CE	1:B:75:GLU:CG	2.49	0.79
1:B:114:PHE:HA	1:B:117:HIS:HB2	1.64	0.79
1:B:119:ILE:C	1:B:186:SER:O	2.26	0.79
1:B:186:SER:CB	1:B:187:PHE:HA	2.12	0.79
1:B:189:GLU:OE1	1:B:189:GLU:O	2.00	0.79
1:A:81:VAL:O	1:A:84:GLU:CG	2.31	0.79
1:A:356:TYR:C	1:A:358:TYR:HB2	2.08	0.79
1:A:153:ARG:HG3	1:A:157:ASN:HB2	1.65	0.79
1:B:189:GLU:HB2	1:B:192:VAL:H	1.46	0.79
1:B:392:LEU:HG	1:B:412:LEU:HD12	1.64	0.79
1:A:120:SER:OG	1:A:123:TYR:CB	2.30	0.79
1:B:392:LEU:O	1:B:396:MET:N	2.15	0.79
1:A:51:LEU:HD12	1:B:52:ALA:HB3	1.65	0.79
1:A:102:LEU:HB2	1:A:156:LEU:HD12	1.63	0.79
1:B:696:PRO:C	1:B:698:PHE:N	2.40	0.79
1:A:340:ALA:O	1:A:344:PRO:HD2	1.82	0.79
1:A:368:ALA:O	1:A:372:LEU:N	2.15	0.79
1:A:392:LEU:O	1:A:396:MET:N	2.15	0.79
1:B:362:HIS:HA	1:B:365:LEU:O	1.81	0.79
1:A:327:SER:CB	1:A:328:LYS:CG	2.61	0.79
1:B:277:GLY:HA2	1:B:621:ASN:OD1	1.83	0.79
1:B:356:TYR:C	1:B:358:TYR:HB2	2.08	0.79
1:A:84:GLU:CD	1:A:84:GLU:O	2.26	0.79
1:A:277:GLY:HA2	1:A:621:ASN:OD1	1.83	0.79
1:A:186:SER:CB	1:A:187:PHE:HA	2.12	0.78
1:A:189:GLU:OE2	1:A:193:LEU:HB2	1.82	0.78
1:A:696:PRO:C	1:A:698:PHE:N	2.40	0.78
1:B:129:LEU:HD12	1:B:369:PHE:CD1	2.18	0.78
1:B:189:GLU:HG3	1:B:192:VAL:CB	2.12	0.78
1:A:115:LEU:HD13	1:A:174:VAL:HA	1.63	0.78
1:A:395:GLY:O	1:A:398:LYS:N	2.16	0.78
1:B:189:GLU:HG2	1:B:190:THR:O	1.82	0.78
1:B:340:ALA:O	1:B:344:PRO:HD2	1.82	0.78
1:A:153:ARG:CB	1:A:155:THR:HB	2.13	0.78
1:B:327:SER:CB	1:B:328:LYS:CG	2.61	0.78
1:A:113:LEU:HD11	1:A:376:LEU:CB	2.14	0.78
1:A:352:SER:O	1:A:355:ILE:HB	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:THR:O	1:A:374:ALA:N	2.15	0.78
1:A:404:ILE:HD13	1:A:661:ALA:CA	2.14	0.78
1:A:119:ILE:C	1:A:186:SER:O	2.26	0.78
1:A:564:MET:CG	1:A:732:ILE:HG23	2.14	0.78
1:B:149:SER:O	1:B:153:ARG:CB	2.32	0.78
1:A:392:LEU:HG	1:A:412:LEU:HD12	1.65	0.78
1:B:280:VAL:HG13	1:B:461:GLU:HB3	1.65	0.78
1:A:114:PHE:HA	1:A:117:HIS:HB2	1.65	0.78
1:A:363:ALA:CA	1:A:365:LEU:O	2.31	0.78
1:A:430:THR:O	1:A:551:LYS:CG	2.31	0.78
1:A:95:LEU:CD1	1:A:158:MET:CB	2.61	0.78
1:B:208:ALA:O	1:B:210:SER:HB3	1.82	0.78
1:A:189:GLU:HG3	1:A:192:VAL:N	1.97	0.78
1:B:153:ARG:C	1:B:155:THR:HB	2.09	0.78
1:A:280:VAL:HG13	1:A:461:GLU:HB3	1.65	0.77
1:B:156:LEU:HD13	1:B:163:SER:O	1.83	0.77
1:B:363:ALA:CA	1:B:365:LEU:O	2.31	0.77
1:B:395:GLY:O	1:B:398:LYS:N	2.16	0.77
1:A:91:GLU:CA	1:A:92:VAL:HG13	2.12	0.77
1:A:429:LEU:HA	1:A:655:LEU:HD11	1.64	0.77
1:B:115:LEU:HD13	1:B:174:VAL:HA	1.65	0.77
1:B:368:ALA:O	1:B:372:LEU:N	2.15	0.77
1:A:149:SER:O	1:A:153:ARG:CB	2.32	0.77
1:A:159:ASP:O	1:A:160:VAL:O	2.01	0.77
1:B:153:ARG:HG3	1:B:157:ASN:HB2	1.65	0.77
1:B:327:SER:CB	1:B:328:LYS:CB	2.63	0.77
1:B:352:SER:O	1:B:355:ILE:HB	1.82	0.77
1:B:355:ILE:N	1:B:356:TYR:HB2	1.98	0.77
1:B:189:GLU:HG3	1:B:192:VAL:N	1.97	0.77
1:B:83:ASP:CB	1:B:84:GLU:HB3	2.14	0.77
1:B:564:MET:CG	1:B:732:ILE:HG23	2.14	0.77
1:B:355:ILE:N	1:B:356:TYR:CB	2.48	0.77
1:A:130:LEU:HD11	1:A:354:PHE:HA	1.65	0.77
1:A:156:LEU:HD13	1:A:163:SER:O	1.83	0.77
1:A:656:ARG:NH1	1:B:82:VAL:CG1	2.46	0.77
1:B:159:ASP:O	1:B:160:VAL:O	2.01	0.77
1:A:153:ARG:C	1:A:155:THR:HB	2.09	0.77
1:A:189:GLU:HB2	1:A:192:VAL:H	1.46	0.77
1:A:83:ASP:CB	1:A:84:GLU:HB3	2.14	0.77
1:A:329:PRO:O	1:A:333:ARG:N	2.17	0.77
1:A:354:PHE:HB3	1:A:356:TYR:HD1	1.46	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:SER:H	1:B:356:TYR:HH	1.29	0.76
1:B:563:ARG:O	1:B:732:ILE:O	2.02	0.76
1:B:428:THR:HG23	1:B:655:LEU:HD21	1.65	0.76
1:A:355:ILE:N	1:A:356:TYR:HB2	2.00	0.76
1:B:355:ILE:HB	1:B:356:TYR:HA	1.67	0.76
1:B:130:LEU:HD11	1:B:354:PHE:HA	1.67	0.76
1:A:355:ILE:N	1:A:356:TYR:CG	2.53	0.76
1:B:150:ALA:O	1:B:153:ARG:CD	2.34	0.76
1:B:189:GLU:CD	1:B:193:LEU:H	1.92	0.76
1:A:81:VAL:HG12	1:A:83:ASP:OD1	1.85	0.76
1:A:327:SER:CB	1:A:328:LYS:CB	2.63	0.76
1:A:384:PHE:CE2	1:A:679:ALA:CB	2.68	0.76
1:B:113:LEU:HD11	1:B:376:LEU:CB	2.15	0.76
1:B:564:MET:HA	1:B:732:ILE:O	1.86	0.76
1:B:51:LEU:CB	1:B:51:LEU:HG	2.13	0.76
1:B:108:ALA:O	1:B:111:LEU:N	2.19	0.76
1:A:149:SER:C	1:A:155:THR:OG1	2.29	0.76
1:A:563:ARG:O	1:A:732:ILE:O	2.02	0.76
1:B:118:PHE:O	1:B:186:SER:C	2.29	0.76
1:A:207:ARG:O	1:A:210:SER:CB	2.34	0.75
1:A:564:MET:HA	1:A:732:ILE:O	1.85	0.75
1:B:84:GLU:O	1:B:84:GLU:CG	2.32	0.75
1:B:688:PRO:HA	1:B:691:ALA:HB3	1.69	0.75
1:A:189:GLU:CD	1:A:193:LEU:H	1.92	0.75
1:A:189:GLU:HG3	1:A:193:LEU:N	1.99	0.75
1:B:360:ILE:N	1:B:361:ALA:CB	2.47	0.75
1:B:384:PHE:CE2	1:B:679:ALA:CB	2.68	0.75
1:B:22:VAL:HA	1:B:80:GLY:O	1.86	0.75
1:B:329:PRO:O	1:B:333:ARG:N	2.17	0.75
1:A:130:LEU:CD1	1:A:354:PHE:HA	2.16	0.75
1:A:215:ALA:CB	1:A:645:SER:CA	2.65	0.75
1:A:360:ILE:N	1:A:361:ALA:CB	2.47	0.75
1:B:149:SER:C	1:B:155:THR:OG1	2.30	0.75
1:B:215:ALA:CB	1:B:645:SER:CA	2.65	0.75
1:A:150:ALA:O	1:A:153:ARG:CD	2.34	0.75
1:B:81:VAL:O	1:B:84:GLU:OE1	2.03	0.75
1:B:277:GLY:HA3	1:B:621:ASN:CG	2.11	0.75
1:B:404:ILE:HG21	1:B:661:ALA:HB2	1.69	0.75
1:A:120:SER:CB	1:A:123:TYR:HB3	2.17	0.74
1:A:277:GLY:HA3	1:A:621:ASN:CG	2.11	0.74
1:A:688:PRO:HA	1:A:691:ALA:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:O	1:B:84:GLU:CG	2.35	0.74
1:B:129:LEU:O	1:B:130:LEU:HD23	1.87	0.74
1:B:351:ILE:C	1:B:356:TYR:HE1	1.53	0.74
1:A:51:LEU:O	1:A:52:ALA:C	2.26	0.74
1:A:81:VAL:O	1:A:84:GLU:OE1	2.05	0.74
1:A:91:GLU:HA	1:A:92:VAL:CB	2.12	0.74
1:B:186:SER:HB2	1:B:187:PHE:HA	1.68	0.74
1:A:355:ILE:HB	1:A:356:TYR:HA	1.66	0.74
1:A:360:ILE:CG2	1:A:362:HIS:O	2.34	0.74
1:B:130:LEU:CD1	1:B:354:PHE:HA	2.17	0.74
1:B:351:ILE:O	1:B:356:TYR:CD1	2.40	0.74
1:B:356:TYR:N	1:B:358:TYR:HB2	2.02	0.74
1:B:23:THR:H	1:B:80:GLY:C	1.95	0.74
1:A:404:ILE:CD1	1:A:661:ALA:N	2.49	0.74
1:A:404:ILE:CD1	1:A:657:ASP:O	2.33	0.74
1:B:154:ARG:N	1:B:155:THR:HB	2.03	0.74
1:B:189:GLU:HG3	1:B:193:LEU:N	1.99	0.74
1:B:90:ALA:CA	1:B:91:GLU:CB	2.66	0.74
1:B:91:GLU:HA	1:B:92:VAL:CB	2.11	0.74
1:A:90:ALA:CA	1:A:91:GLU:CB	2.66	0.74
1:A:107:PHE:C	1:A:109:GLY:H	1.93	0.74
1:B:120:SER:CB	1:B:123:TYR:HB3	2.17	0.74
1:A:71:LYS:HE3	1:A:75:GLU:CD	2.12	0.74
1:A:186:SER:HB2	1:A:187:PHE:HA	1.68	0.74
1:B:280:VAL:CG1	1:B:461:GLU:HB3	2.18	0.74
1:A:51:LEU:HB3	1:A:51:LEU:H	1.52	0.74
1:A:396:MET:HE1	1:A:406:ILE:O	1.88	0.74
1:A:405:LEU:HB2	1:A:649:VAL:O	1.88	0.74
1:B:350:ALA:O	1:B:356:TYR:HE1	1.62	0.74
1:A:52:ALA:HB3	1:B:51:LEU:HB3	0.80	0.73
1:A:110:VAL:HA	1:A:113:LEU:HD12	1.70	0.73
1:B:207:ARG:O	1:B:210:SER:CB	2.35	0.73
1:B:360:ILE:CG2	1:B:362:HIS:O	2.36	0.73
1:B:404:ILE:HD13	1:B:661:ALA:CA	2.16	0.73
1:B:405:LEU:HB2	1:B:649:VAL:O	1.87	0.73
1:A:352:SER:H	1:A:356:TYR:HH	1.35	0.73
1:B:22:VAL:HG22	1:B:81:VAL:HG13	1.70	0.73
1:B:71:LYS:HE3	1:B:75:GLU:CD	2.13	0.73
1:B:353:ALA:C	1:B:356:TYR:HB3	2.12	0.73
1:B:354:PHE:CB	1:B:356:TYR:CD1	2.66	0.73
1:A:84:GLU:CG	1:A:84:GLU:O	2.31	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD11	1:A:158:MET:CG	2.19	0.73
1:A:358:TYR:CG	1:A:358:TYR:O	2.42	0.73
1:B:122:PRO:HB2	1:B:125:ASP:CB	2.18	0.73
1:A:280:VAL:CG1	1:A:461:GLU:HB3	2.17	0.73
1:B:110:VAL:HA	1:B:113:LEU:HD12	1.71	0.73
1:A:118:PHE:O	1:A:186:SER:C	2.30	0.73
1:A:154:ARG:N	1:A:155:THR:HB	2.02	0.73
1:A:71:LYS:HD3	1:A:85:GLN:N	2.04	0.73
1:A:353:ALA:C	1:A:356:TYR:HB2	2.12	0.73
1:A:356:TYR:N	1:A:358:TYR:HB2	2.03	0.73
1:B:91:GLU:CA	1:B:92:VAL:HG13	2.12	0.73
1:B:153:ARG:HG3	1:B:157:ASN:CB	2.18	0.73
1:A:355:ILE:N	1:A:356:TYR:CB	2.52	0.73
1:A:153:ARG:HG3	1:A:157:ASN:CB	2.18	0.73
1:A:423:PHE:HD1	1:A:428:THR:HG21	1.52	0.73
1:B:358:TYR:CG	1:B:358:TYR:O	2.41	0.73
1:A:155:THR:C	1:A:157:ASN:H	1.96	0.73
1:A:157:ASN:O	1:A:158:MET:CB	2.37	0.73
1:B:95:LEU:HD11	1:B:158:MET:CG	2.18	0.73
1:A:399:GLY:CA	1:A:664:LEU:HD22	2.19	0.73
1:B:215:ALA:HB1	1:B:645:SER:OG	1.89	0.73
1:B:352:SER:HB2	1:B:356:TYR:CZ	2.23	0.73
1:A:189:GLU:HB2	1:A:191:SER:CB	2.19	0.72
1:A:203:THR:C	1:A:205:GLU:N	2.47	0.72
1:A:327:SER:OG	1:A:328:LYS:HG3	1.89	0.72
1:B:102:LEU:O	1:B:166:VAL:HG21	1.89	0.72
1:B:157:ASN:O	1:B:158:MET:CB	2.37	0.72
1:A:129:LEU:HD22	1:A:368:ALA:CB	2.18	0.72
1:A:129:LEU:O	1:A:130:LEU:HD23	1.87	0.72
1:B:402:LEU:HB3	1:B:660:ALA:HB1	1.71	0.72
1:A:125:ASP:O	1:A:126:PHE:HB2	1.88	0.72
1:B:151:LEU:C	1:B:153:ARG:CA	2.61	0.72
1:B:406:ILE:HD13	1:B:412:LEU:HD23	1.71	0.72
1:B:551:LYS:HD2	1:B:655:LEU:HG	1.71	0.72
1:A:362:HIS:HB3	1:A:363:ALA:CB	2.20	0.72
1:B:203:THR:C	1:B:205:GLU:N	2.47	0.72
1:B:404:ILE:HA	1:B:650:LEU:HD23	1.72	0.72
1:A:90:ALA:HA	1:A:91:GLU:CB	2.14	0.72
1:A:277:GLY:CA	1:A:621:ASN:OD1	2.38	0.72
1:A:130:LEU:CD1	1:A:354:PHE:CB	2.63	0.72
1:A:328:LYS:O	1:A:328:LYS:HE3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:TYR:CD2	1:A:356:TYR:CB	2.68	0.72
1:B:327:SER:OG	1:B:328:LYS:HG3	1.89	0.72
1:A:122:PRO:HB2	1:A:125:ASP:CB	2.19	0.72
1:A:130:LEU:HD13	1:A:354:PHE:CA	2.20	0.72
1:A:189:GLU:CA	1:A:191:SER:N	2.52	0.72
1:B:107:PHE:C	1:B:109:GLY:H	1.95	0.72
1:B:125:ASP:O	1:B:126:PHE:HB2	1.88	0.72
1:B:396:MET:HE1	1:B:406:ILE:O	1.88	0.72
1:A:51:LEU:CB	1:A:51:LEU:H	2.00	0.72
1:A:551:LYS:HD2	1:A:655:LEU:HG	1.71	0.72
1:B:113:LEU:HD21	1:B:376:LEU:HD12	1.72	0.72
1:B:155:THR:C	1:B:157:ASN:H	1.96	0.72
1:A:102:LEU:O	1:A:166:VAL:HG21	1.90	0.72
1:B:189:GLU:HA	1:B:190:THR:CB	2.19	0.72
1:A:189:GLU:HA	1:A:190:THR:CB	2.20	0.72
1:A:352:SER:HB2	1:A:356:TYR:OH	1.89	0.72
1:A:360:ILE:CG2	1:A:697:ILE:HG21	2.15	0.72
1:B:153:ARG:CB	1:B:155:THR:HB	2.13	0.72
1:B:189:GLU:HB2	1:B:191:SER:CB	2.19	0.72
1:B:277:GLY:CA	1:B:621:ASN:OD1	2.38	0.72
1:A:120:SER:CB	1:A:123:TYR:CB	2.68	0.71
1:A:189:GLU:CG	1:A:191:SER:C	2.62	0.71
1:B:189:GLU:CA	1:B:191:SER:N	2.53	0.71
1:B:399:GLY:CA	1:B:664:LEU:HD22	2.19	0.71
1:B:51:LEU:CD1	1:B:51:LEU:CD2	2.68	0.71
1:B:71:LYS:HD3	1:B:85:GLN:N	2.04	0.71
1:B:215:ALA:C	1:B:217:LYS:N	2.48	0.71
1:B:696:PRO:C	1:B:697:ILE:HD12	2.15	0.71
1:A:23:THR:H	1:A:80:GLY:C	1.98	0.71
1:B:430:THR:HA	1:B:550:LEU:HA	1.72	0.71
1:B:406:ILE:CD1	1:B:412:LEU:HD23	2.21	0.71
1:A:108:ALA:O	1:A:111:LEU:N	2.23	0.71
1:A:126:PHE:CD1	1:A:128:GLN:O	2.43	0.71
1:B:103:TYR:CD2	1:B:166:VAL:HG21	2.26	0.71
1:B:362:HIS:HB3	1:B:363:ALA:CB	2.19	0.71
1:A:404:ILE:HD13	1:A:661:ALA:HB2	1.72	0.71
1:B:129:LEU:HD22	1:B:368:ALA:CB	2.19	0.71
1:B:351:ILE:CA	1:B:356:TYR:HE1	2.03	0.71
1:B:404:ILE:CD1	1:B:657:ASP:O	2.36	0.71
1:A:90:ALA:N	1:A:91:GLU:HB2	2.04	0.71
1:A:215:ALA:HB1	1:A:645:SER:OG	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:O	1:B:84:GLU:OE2	2.09	0.71
1:A:151:LEU:C	1:A:153:ARG:CA	2.61	0.71
1:A:696:PRO:C	1:A:697:ILE:HD12	2.16	0.71
1:A:404:ILE:HG12	1:A:650:LEU:HD22	1.71	0.71
1:B:90:ALA:N	1:B:91:GLU:HB2	2.04	0.71
1:B:120:SER:CB	1:B:123:TYR:CB	2.68	0.71
1:A:430:THR:HA	1:A:550:LEU:HA	1.72	0.71
1:B:130:LEU:HD13	1:B:354:PHE:CA	2.20	0.71
1:A:402:LEU:HB3	1:A:660:ALA:HB1	1.72	0.70
1:B:122:PRO:CB	1:B:125:ASP:HB2	2.21	0.70
1:B:126:PHE:CD1	1:B:128:GLN:O	2.43	0.70
1:A:113:LEU:HD21	1:A:376:LEU:HD12	1.73	0.70
1:A:103:TYR:CD2	1:A:166:VAL:HG21	2.26	0.70
1:B:357:TRP:H	1:B:358:TYR:HA	1.56	0.70
1:B:391:ALA:O	1:B:395:GLY:N	2.22	0.70
1:B:117:HIS:HB3	1:B:191:SER:CB	2.22	0.70
1:B:189:GLU:HA	1:B:191:SER:H	1.57	0.70
1:B:328:LYS:O	1:B:328:LYS:HE3	1.90	0.70
1:A:406:ILE:HD13	1:A:412:LEU:HD23	1.72	0.70
1:A:352:SER:HB2	1:A:356:TYR:CZ	2.25	0.70
1:B:133:LEU:HD13	1:B:372:LEU:HG	1.74	0.70
1:B:191:SER:OG	1:B:192:VAL:N	2.25	0.70
1:A:349:VAL:CA	1:A:356:TYR:OH	2.40	0.69
1:A:406:ILE:CD1	1:A:412:LEU:HD23	2.22	0.69
1:B:189:GLU:CG	1:B:191:SER:C	2.62	0.69
1:B:430:THR:O	1:B:551:LYS:HG2	1.90	0.69
1:B:329:PRO:HB2	1:B:330:PRO:HD2	1.74	0.69
1:B:360:ILE:O	1:B:363:ALA:N	2.22	0.69
1:B:433:LYS:O	1:B:433:LYS:HD2	1.92	0.69
1:B:160:VAL:HG13	1:B:161:MET:O	1.93	0.69
1:B:564:MET:HG2	1:B:732:ILE:HG12	1.74	0.69
1:A:26:THR:O	1:B:53:THR:CG2	2.41	0.69
1:A:31:VAL:CG2	1:A:51:LEU:HD13	2.23	0.69
1:A:52:ALA:CB	1:B:51:LEU:HB3	1.31	0.69
1:A:133:LEU:HD13	1:A:372:LEU:HG	1.73	0.69
1:A:404:ILE:HA	1:A:650:LEU:HD23	1.73	0.69
1:A:160:VAL:HG13	1:A:161:MET:O	1.93	0.69
1:A:189:GLU:HA	1:A:191:SER:H	1.56	0.69
1:A:357:TRP:H	1:A:358:TYR:HA	1.56	0.69
1:B:95:LEU:CD1	1:B:158:MET:HB2	2.22	0.69
1:B:404:ILE:CD1	1:B:661:ALA:N	2.53	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ILE:HG12	1:B:650:LEU:HD22	1.74	0.69
1:B:95:LEU:HB3	1:B:96:SER:O	1.93	0.69
1:B:67:PHE:CZ	1:B:83:ASP:OD2	2.46	0.69
1:A:114:PHE:CD2	1:A:198:LEU:HD12	2.28	0.68
1:A:194:LEU:HD23	1:A:377:VAL:HG11	1.75	0.68
1:A:83:ASP:CA	1:A:84:GLU:CB	2.65	0.68
1:A:329:PRO:HB2	1:A:330:PRO:HD2	1.75	0.68
1:B:21:ARG:O	1:B:82:VAL:N	2.27	0.68
1:A:81:VAL:O	1:A:84:GLU:HG3	1.92	0.68
1:A:360:ILE:O	1:A:363:ALA:N	2.22	0.68
1:B:130:LEU:CD1	1:B:354:PHE:CB	2.63	0.68
1:B:362:HIS:CB	1:B:363:ALA:HB2	2.23	0.68
1:A:95:LEU:HA	1:A:96:SER:CB	2.24	0.68
1:A:101:LYS:HA	1:A:104:VAL:CG1	2.23	0.68
1:A:122:PRO:CB	1:A:125:ASP:HB2	2.22	0.68
1:A:215:ALA:C	1:A:217:LYS:N	2.48	0.68
1:B:83:ASP:CG	1:B:84:GLU:CB	2.67	0.68
1:A:95:LEU:CD1	1:A:158:MET:HB2	2.24	0.68
1:B:78:GLY:O	1:B:79:TYR:CD2	2.47	0.68
1:B:108:ALA:HA	1:B:111:LEU:HG	1.76	0.68
1:A:95:LEU:HB3	1:A:96:SER:O	1.93	0.68
1:A:108:ALA:HA	1:A:111:LEU:HG	1.74	0.68
1:A:117:HIS:HB3	1:A:191:SER:CB	2.22	0.68
1:A:692:GLY:O	1:A:694:LEU:N	2.27	0.68
1:A:67:PHE:CZ	1:A:83:ASP:OD2	2.47	0.68
1:A:434:PRO:CG	1:A:463:PRO:O	2.41	0.68
1:B:152:ARG:CB	1:B:153:ARG:HA	2.23	0.68
1:A:22:VAL:HG22	1:A:81:VAL:HG13	1.76	0.67
1:A:102:LEU:O	1:A:166:VAL:HG11	1.94	0.67
1:B:101:LYS:HA	1:B:104:VAL:CG1	2.23	0.67
1:B:328:LYS:HE3	1:B:333:ARG:HG3	1.75	0.67
1:B:423:PHE:HD1	1:B:428:THR:HG21	1.54	0.67
1:A:104:VAL:HG13	1:A:104:VAL:O	1.94	0.67
1:A:328:LYS:HE3	1:A:333:ARG:HG3	1.75	0.67
1:A:404:ILE:HD13	1:A:661:ALA:CB	2.24	0.67
1:B:32:LYS:HG3	1:B:461:GLU:CD	2.20	0.67
1:B:71:LYS:NZ	1:B:75:GLU:OE1	2.27	0.67
1:B:194:LEU:HD23	1:B:377:VAL:HG11	1.76	0.67
1:B:101:LYS:HE2	1:B:104:VAL:HG11	1.76	0.67
1:B:635:VAL:HG22	1:B:650:LEU:HD12	1.76	0.67
1:A:354:PHE:HB3	1:A:356:TYR:CD1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ALA:O	1:B:88:VAL:HG23	1.94	0.67
1:A:327:SER:HB2	1:A:328:LYS:CA	2.24	0.67
1:A:71:LYS:NZ	1:A:75:GLU:OE1	2.27	0.67
1:A:189:GLU:HA	1:A:191:SER:N	2.10	0.67
1:A:363:ALA:HA	1:A:365:LEU:C	2.19	0.67
1:A:382:CYS:O	1:A:383:ALA:HB3	1.95	0.67
1:B:189:GLU:HA	1:B:191:SER:N	2.10	0.67
1:B:618:ASP:OD2	1:B:621:ASN:ND2	2.27	0.67
1:A:429:LEU:O	1:A:550:LEU:CA	2.43	0.67
1:B:151:LEU:O	1:B:153:ARG:HB3	1.94	0.67
1:B:327:SER:HB2	1:B:328:LYS:CA	2.24	0.67
1:B:363:ALA:HA	1:B:365:LEU:C	2.19	0.67
1:A:78:GLY:O	1:A:79:TYR:CD2	2.47	0.67
1:A:153:ARG:HG3	1:A:157:ASN:CG	2.20	0.67
1:B:153:ARG:HG3	1:B:157:ASN:CG	2.20	0.67
1:A:128:GLN:HA	1:A:366:LEU:HD13	1.77	0.66
1:A:564:MET:HG2	1:A:732:ILE:HG12	1.75	0.66
1:A:618:ASP:OD2	1:A:621:ASN:ND2	2.27	0.66
1:B:102:LEU:O	1:B:166:VAL:HG11	1.94	0.66
1:B:114:PHE:CD2	1:B:198:LEU:HD12	2.30	0.66
1:B:360:ILE:HB	1:B:697:ILE:CG1	2.24	0.66
1:B:406:ILE:HG12	1:B:648:ILE:HG12	1.77	0.66
1:B:429:LEU:O	1:B:550:LEU:CA	2.43	0.66
1:B:386:LEU:C	1:B:389:PRO:HD2	2.21	0.66
1:B:692:GLY:O	1:B:694:LEU:N	2.28	0.66
1:A:130:LEU:CD1	1:A:354:PHE:CA	2.74	0.66
1:A:280:VAL:HG13	1:A:461:GLU:CB	2.25	0.66
1:A:360:ILE:HB	1:A:697:ILE:CG1	2.25	0.66
1:A:656:ARG:HH12	1:B:82:VAL:HG13	1.57	0.66
1:B:102:LEU:HB3	1:B:166:VAL:HB	1.77	0.66
1:A:32:LYS:HG3	1:A:461:GLU:CD	2.20	0.66
1:A:394:VAL:O	1:A:398:LYS:N	2.29	0.66
1:A:688:PRO:O	1:A:692:GLY:N	2.29	0.66
1:B:147:ALA:O	1:B:148:PHE:C	2.39	0.66
1:B:386:LEU:O	1:B:389:PRO:HG2	1.96	0.66
1:A:87:ALA:O	1:A:88:VAL:HG23	1.94	0.66
1:A:352:SER:O	1:A:356:TYR:CD2	2.49	0.66
1:B:104:VAL:HG13	1:B:104:VAL:O	1.94	0.66
1:B:280:VAL:HG22	1:B:461:GLU:HB3	1.77	0.66
1:A:156:LEU:O	1:A:158:MET:N	2.28	0.66
1:A:191:SER:OG	1:A:192:VAL:N	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASP:O	1:A:324:ALA:CB	2.44	0.66
1:A:362:HIS:CB	1:A:363:ALA:HB2	2.24	0.66
1:A:386:LEU:O	1:A:389:PRO:HG2	1.96	0.66
1:A:635:VAL:HG22	1:A:650:LEU:HD12	1.75	0.66
1:B:120:SER:HB3	1:B:122:PRO:C	2.20	0.66
1:B:156:LEU:O	1:B:158:MET:N	2.28	0.66
1:A:404:ILE:CG2	1:A:661:ALA:HB2	2.24	0.66
1:B:90:ALA:HA	1:B:91:GLU:O	1.96	0.66
1:B:154:ARG:CA	1:B:155:THR:C	2.69	0.66
1:A:101:LYS:HE2	1:A:104:VAL:HG11	1.78	0.66
1:B:128:GLN:HA	1:B:366:LEU:HD13	1.78	0.66
1:B:156:LEU:HD11	1:B:166:VAL:H	1.60	0.66
1:A:156:LEU:HD11	1:A:166:VAL:H	1.60	0.65
1:A:280:VAL:HG22	1:A:461:GLU:HB3	1.77	0.65
1:B:148:PHE:O	1:B:149:SER:CB	2.44	0.65
1:A:108:ALA:CA	1:A:111:LEU:HG	2.26	0.65
1:B:108:ALA:CA	1:B:111:LEU:HG	2.26	0.65
1:B:404:ILE:CG2	1:B:661:ALA:HB2	2.27	0.65
1:A:102:LEU:HB3	1:A:166:VAL:HB	1.78	0.65
1:A:129:LEU:HD23	1:A:130:LEU:N	2.11	0.65
1:A:406:ILE:HG12	1:A:648:ILE:HG12	1.78	0.65
1:B:111:LEU:CB	1:B:170:PHE:CE1	2.79	0.65
1:B:129:LEU:HD23	1:B:130:LEU:N	2.11	0.65
1:A:86:ALA:HB1	1:A:87:ALA:CB	2.12	0.65
1:A:111:LEU:CB	1:A:170:PHE:CE1	2.79	0.65
1:A:148:PHE:O	1:A:149:SER:CB	2.44	0.65
1:A:151:LEU:O	1:A:153:ARG:HB3	1.95	0.65
1:A:187:PHE:CG	1:A:187:PHE:O	2.49	0.65
1:B:95:LEU:HA	1:B:96:SER:CB	2.24	0.65
1:B:189:GLU:HB2	1:B:191:SER:C	2.21	0.65
1:B:394:VAL:O	1:B:398:LYS:N	2.29	0.65
1:A:152:ARG:CB	1:A:153:ARG:HA	2.24	0.65
1:A:178:ALA:O	1:A:182:PRO:C	2.40	0.65
1:B:363:ALA:CA	1:B:365:LEU:C	2.69	0.65
1:B:382:CYS:O	1:B:383:ALA:HB3	1.95	0.65
1:A:129:LEU:HD13	1:A:369:PHE:CA	2.27	0.65
1:B:85:GLN:O	1:B:86:ALA:CB	2.44	0.65
1:B:101:LYS:C	1:B:103:TYR:N	2.53	0.65
1:B:178:ALA:O	1:B:182:PRO:C	2.40	0.65
1:B:280:VAL:HG13	1:B:461:GLU:CB	2.25	0.65
1:B:129:LEU:HD13	1:B:369:PHE:CA	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:SER:HB3	1:A:122:PRO:C	2.20	0.65
1:A:154:ARG:CA	1:A:155:THR:C	2.69	0.65
1:A:85:GLN:O	1:A:86:ALA:CB	2.44	0.65
1:A:153:ARG:HB2	1:A:155:THR:OG1	1.97	0.65
1:A:685:ILE:O	1:A:688:PRO:HG2	1.96	0.65
1:B:130:LEU:CD1	1:B:354:PHE:CA	2.75	0.65
1:B:187:PHE:CG	1:B:187:PHE:O	2.49	0.65
1:B:189:GLU:HA	1:B:190:THR:HB	1.79	0.65
1:A:90:ALA:HA	1:A:91:GLU:O	1.96	0.64
1:A:280:VAL:CG2	1:A:461:GLU:HB3	2.27	0.64
1:B:152:ARG:CB	1:B:153:ARG:CA	2.75	0.64
1:B:153:ARG:HB2	1:B:155:THR:OG1	1.97	0.64
1:B:685:ILE:O	1:B:688:PRO:HG2	1.96	0.64
1:A:189:GLU:HB2	1:A:191:SER:C	2.21	0.64
1:A:189:GLU:HA	1:A:190:THR:HB	1.79	0.64
1:A:431:LYS:HB2	1:A:548:ASP:O	1.97	0.64
1:A:129:LEU:HD13	1:A:369:PHE:N	2.12	0.64
1:A:210:SER:OG	1:A:211:ARG:HB2	1.97	0.64
1:A:354:PHE:CB	1:A:356:TYR:CD1	2.76	0.64
1:A:434:PRO:HB2	1:A:546:VAL:CG1	2.27	0.64
1:B:107:PHE:C	1:B:109:GLY:N	2.53	0.64
1:B:280:VAL:CG2	1:B:461:GLU:HB3	2.27	0.64
1:A:21:ARG:O	1:A:82:VAL:N	2.28	0.64
1:A:125:ASP:O	1:A:126:PHE:CB	2.46	0.64
1:A:147:ALA:O	1:A:148:PHE:C	2.39	0.64
1:A:386:LEU:C	1:A:389:PRO:HD2	2.21	0.64
1:B:86:ALA:HB1	1:B:87:ALA:CB	2.13	0.64
1:B:153:ARG:HG2	1:B:327:SER:HB3	1.80	0.64
1:B:210:SER:OG	1:B:211:ARG:HB2	1.97	0.64
1:B:323:ASP:O	1:B:324:ALA:CB	2.44	0.64
1:A:189:GLU:HG2	1:A:193:LEU:H	1.59	0.64
1:A:434:PRO:HG2	1:A:463:PRO:O	1.97	0.64
1:B:22:VAL:HG13	1:B:81:VAL:HG22	1.79	0.64
1:B:189:GLU:CB	1:B:190:THR:C	2.71	0.64
1:A:129:LEU:HD21	1:A:133:LEU:CD1	2.28	0.64
1:B:130:LEU:CD1	1:B:354:PHE:CD1	2.81	0.64
1:A:328:LYS:N	1:A:329:PRO:CD	2.59	0.64
1:B:129:LEU:HD13	1:B:369:PHE:N	2.12	0.64
1:B:207:ARG:O	1:B:210:SER:HB3	1.97	0.64
1:A:51:LEU:CD1	1:B:52:ALA:HB3	2.28	0.64
1:A:129:LEU:HD11	1:A:133:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:O	1:A:210:SER:HB3	1.97	0.64
1:A:353:ALA:C	1:A:356:TYR:HB3	2.18	0.64
1:B:354:PHE:C	1:B:356:TYR:CD1	2.76	0.64
1:A:351:ILE:O	1:A:354:PHE:HB3	1.98	0.63
1:B:20:VAL:CG1	1:B:83:ASP:OD1	2.45	0.63
1:B:81:VAL:O	1:B:84:GLU:HG3	1.98	0.63
1:B:120:SER:OG	1:B:123:TYR:CA	2.46	0.63
1:A:153:ARG:HG2	1:A:327:SER:HB3	1.79	0.63
1:A:391:ALA:O	1:A:395:GLY:N	2.22	0.63
1:B:120:SER:OG	1:B:123:TYR:HA	1.99	0.63
1:B:352:SER:O	1:B:355:ILE:N	2.30	0.63
1:A:53:THR:CG2	1:B:51:LEU:HD11	2.27	0.63
1:B:83:ASP:CA	1:B:84:GLU:CB	2.67	0.63
1:B:404:ILE:HA	1:B:650:LEU:CD2	2.27	0.63
1:A:341:TYR:O	1:A:344:PRO:HG2	1.98	0.63
1:A:363:ALA:CA	1:A:365:LEU:C	2.70	0.63
1:B:83:ASP:CB	1:B:84:GLU:CA	2.62	0.63
1:B:328:LYS:H	1:B:329:PRO:HD2	1.63	0.63
1:B:399:GLY:HA3	1:B:664:LEU:HD22	1.81	0.63
1:A:360:ILE:N	1:A:361:ALA:HB2	2.13	0.63
1:A:404:ILE:HA	1:A:650:LEU:CD2	2.28	0.63
1:B:108:ALA:HB1	1:B:111:LEU:HD12	1.81	0.63
1:B:125:ASP:O	1:B:126:PHE:CB	2.46	0.63
1:B:151:LEU:O	1:B:152:ARG:C	2.42	0.63
1:A:107:PHE:C	1:A:109:GLY:N	2.52	0.63
1:A:153:ARG:CD	1:A:155:THR:HG21	2.29	0.63
1:A:352:SER:O	1:A:355:ILE:N	2.30	0.63
1:B:131:ILE:O	1:B:134:PRO:HG2	1.99	0.63
1:A:91:GLU:CB	1:A:92:VAL:HG22	2.29	0.63
1:A:155:THR:O	1:A:157:ASN:N	2.32	0.63
1:B:52:ALA:CB	1:B:52:ALA:C	2.67	0.63
1:B:126:PHE:CE1	1:B:129:LEU:HB2	2.33	0.63
1:B:153:ARG:CD	1:B:155:THR:HG21	2.29	0.63
1:B:328:LYS:N	1:B:329:PRO:CD	2.59	0.63
1:B:360:ILE:H	1:B:361:ALA:HB2	1.62	0.63
1:A:115:LEU:HD22	1:A:174:VAL:CG1	2.22	0.63
1:A:117:HIS:CG	1:A:191:SER:HA	2.33	0.63
1:A:152:ARG:CB	1:A:153:ARG:CA	2.76	0.63
1:B:20:VAL:HB	1:B:83:ASP:OD1	1.98	0.63
1:B:94:HIS:C	1:B:95:LEU:CD2	2.66	0.63
1:B:129:LEU:HD21	1:B:133:LEU:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ILE:N	1:B:361:ALA:HB2	2.13	0.63
1:A:84:GLU:O	1:A:84:GLU:OE2	2.16	0.63
1:A:189:GLU:CB	1:A:190:THR:C	2.71	0.63
1:B:129:LEU:HD11	1:B:133:LEU:HD21	1.80	0.63
1:A:126:PHE:CE1	1:A:129:LEU:HB2	2.33	0.62
1:A:355:ILE:CB	1:A:356:TYR:HA	2.28	0.62
1:A:373:ILE:O	1:A:377:VAL:HG22	1.99	0.62
1:B:129:LEU:HD13	1:B:369:PHE:H	1.64	0.62
1:B:402:LEU:HB3	1:B:660:ALA:CB	2.29	0.62
1:A:671:LYS:CD	1:A:723:LEU:O	2.47	0.62
1:B:126:PHE:HA	1:B:127:VAL:C	2.24	0.62
1:B:215:ALA:O	1:B:216:ILE:C	2.42	0.62
1:B:360:ILE:HG13	1:B:697:ILE:HG21	1.82	0.62
1:B:376:LEU:O	1:B:379:ALA:N	2.32	0.62
1:A:368:ALA:O	1:A:369:PHE:C	2.42	0.62
1:B:115:LEU:HD22	1:B:174:VAL:CG1	2.21	0.62
1:B:118:PHE:C	1:B:186:SER:C	2.67	0.62
1:B:353:ALA:C	1:B:356:TYR:HB2	2.14	0.62
1:B:671:LYS:CD	1:B:723:LEU:O	2.48	0.62
1:A:95:LEU:CB	1:A:96:SER:CB	2.73	0.62
1:A:151:LEU:O	1:A:152:ARG:C	2.42	0.62
1:A:154:ARG:N	1:A:155:THR:CB	2.61	0.62
1:A:215:ALA:O	1:A:216:ILE:C	2.42	0.62
1:B:89:SER:OG	1:B:91:GLU:HG3	1.99	0.62
1:B:120:SER:OG	1:B:123:TYR:HB3	1.99	0.62
1:A:22:VAL:HG13	1:A:81:VAL:HG22	1.81	0.62
1:A:129:LEU:HD13	1:A:369:PHE:H	1.65	0.62
1:A:351:ILE:O	1:A:356:TYR:CD1	2.52	0.62
1:A:376:LEU:O	1:A:379:ALA:N	2.33	0.62
1:A:383:ALA:HB3	1:A:711:MET:O	2.00	0.62
1:A:405:LEU:O	1:A:649:VAL:N	2.29	0.62
1:B:154:ARG:N	1:B:155:THR:CB	2.61	0.62
1:B:355:ILE:CB	1:B:356:TYR:HA	2.30	0.62
1:A:113:LEU:HD21	1:A:376:LEU:HB2	1.81	0.62
1:A:402:LEU:HB3	1:A:660:ALA:CB	2.30	0.62
1:B:102:LEU:HD23	1:B:102:LEU:N	2.15	0.62
1:B:113:LEU:HD21	1:B:376:LEU:HB2	1.82	0.62
1:B:357:TRP:HB2	1:B:695:TYR:HA	1.80	0.62
1:A:130:LEU:CD1	1:A:354:PHE:CD1	2.82	0.62
1:A:395:GLY:O	1:A:398:LYS:HB2	2.00	0.62
1:B:351:ILE:O	1:B:354:PHE:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ILE:O	1:B:377:VAL:HG22	1.99	0.62
1:A:53:THR:HG22	1:B:51:LEU:CD1	2.28	0.62
1:A:131:ILE:O	1:A:134:PRO:HG2	1.99	0.62
1:A:328:LYS:H	1:A:329:PRO:HD2	1.63	0.62
1:A:549:THR:O	1:A:551:LYS:N	2.33	0.62
1:B:368:ALA:O	1:B:369:PHE:C	2.42	0.62
1:A:191:SER:O	1:A:192:VAL:C	2.43	0.62
1:B:91:GLU:CB	1:B:92:VAL:HG22	2.29	0.62
1:B:155:THR:O	1:B:157:ASN:N	2.31	0.62
1:B:191:SER:O	1:B:192:VAL:C	2.43	0.62
1:B:395:GLY:O	1:B:398:LYS:HB2	2.00	0.62
1:A:115:LEU:HD13	1:A:174:VAL:CA	2.30	0.62
1:A:710:ALA:C	1:A:712:ALA:H	2.08	0.62
1:B:360:ILE:CG2	1:B:697:ILE:HG21	2.19	0.62
1:B:383:ALA:HB3	1:B:711:MET:O	1.99	0.62
1:B:404:ILE:HD13	1:B:661:ALA:H	1.63	0.62
1:A:120:SER:OG	1:A:123:TYR:CA	2.47	0.61
1:A:357:TRP:HB2	1:A:695:TYR:HA	1.82	0.61
1:B:117:HIS:CG	1:B:191:SER:HA	2.34	0.61
1:B:121:LEU:O	1:B:184:GLU:HB2	2.00	0.61
1:B:149:SER:O	1:B:150:ALA:C	2.42	0.61
1:A:89:SER:OG	1:A:91:GLU:HG3	1.99	0.61
1:A:144:PHE:CZ	1:A:340:ALA:HB1	2.36	0.61
1:B:688:PRO:O	1:B:692:GLY:N	2.29	0.61
1:A:126:PHE:HA	1:A:127:VAL:C	2.24	0.61
1:A:360:ILE:HG13	1:A:697:ILE:HG21	1.81	0.61
1:A:120:SER:OG	1:A:123:TYR:HA	1.99	0.61
1:A:121:LEU:O	1:A:184:GLU:HB2	1.99	0.61
1:A:186:SER:CB	1:A:187:PHE:CA	2.78	0.61
1:A:349:VAL:HA	1:A:356:TYR:OH	2.00	0.61
1:A:399:GLY:HA3	1:A:664:LEU:HD22	1.81	0.61
1:B:20:VAL:HG11	1:B:83:ASP:OD1	2.00	0.61
1:B:83:ASP:CG	1:B:84:GLU:HB3	2.26	0.61
1:B:83:ASP:CG	1:B:84:GLU:HB2	2.25	0.61
1:A:33:SER:OG	1:A:279:PRO:HB3	2.01	0.61
1:B:341:TYR:O	1:B:344:PRO:HG2	1.98	0.61
1:B:352:SER:O	1:B:355:ILE:CB	2.49	0.61
1:A:149:SER:O	1:A:150:ALA:C	2.42	0.61
1:B:129:LEU:HD23	1:B:130:LEU:HD23	1.82	0.61
1:B:144:PHE:CZ	1:B:340:ALA:HB1	2.35	0.61
1:A:102:LEU:N	1:A:102:LEU:HD23	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:HB1	1:A:111:LEU:HD12	1.80	0.61
1:B:33:SER:OG	1:B:279:PRO:HB3	2.00	0.61
1:B:710:ALA:C	1:B:712:ALA:H	2.08	0.61
1:A:113:LEU:CD2	1:A:376:LEU:HB2	2.31	0.61
1:B:156:LEU:C	1:B:158:MET:N	2.56	0.61
1:B:351:ILE:N	1:B:356:TYR:HE1	1.99	0.61
1:A:83:ASP:CB	1:A:84:GLU:CA	2.64	0.60
1:A:129:LEU:HD23	1:A:130:LEU:HD23	1.82	0.60
1:B:549:THR:O	1:B:551:LYS:N	2.33	0.60
1:A:31:VAL:HG23	1:A:51:LEU:HD13	1.82	0.60
1:A:118:PHE:C	1:A:186:SER:C	2.68	0.60
1:A:129:LEU:HD21	1:A:133:LEU:HG	1.82	0.60
1:A:148:PHE:O	1:A:149:SER:HB3	2.00	0.60
1:A:155:THR:C	1:A:157:ASN:N	2.59	0.60
1:B:156:LEU:HD13	1:B:163:SER:C	2.26	0.60
1:A:384:PHE:CE2	1:A:680:LEU:HD23	2.37	0.60
1:A:564:MET:HG2	1:A:732:ILE:HG23	1.83	0.60
1:A:352:SER:O	1:A:355:ILE:CB	2.49	0.60
1:B:357:TRP:HE1	1:B:361:ALA:C	2.10	0.60
1:B:404:ILE:HD13	1:B:661:ALA:HB2	1.84	0.60
1:B:431:LYS:HB2	1:B:548:ASP:O	2.00	0.60
1:A:26:THR:O	1:B:53:THR:HG22	2.00	0.60
1:A:327:SER:CB	1:A:328:LYS:HB2	2.32	0.60
1:B:155:THR:C	1:B:157:ASN:N	2.59	0.60
1:A:186:SER:HB2	1:A:187:PHE:CA	2.32	0.60
1:B:129:LEU:HD21	1:B:133:LEU:HG	1.82	0.60
1:B:23:THR:HB	1:B:80:GLY:HA3	1.83	0.60
1:B:154:ARG:CA	1:B:155:THR:O	2.41	0.60
1:A:23:THR:HB	1:A:80:GLY:HA3	1.84	0.60
1:A:94:HIS:C	1:A:95:LEU:CD2	2.67	0.60
1:A:156:LEU:HD13	1:A:163:SER:C	2.26	0.60
1:B:148:PHE:O	1:B:149:SER:HB3	2.00	0.60
1:B:156:LEU:HD22	1:B:163:SER:HA	1.84	0.60
1:B:352:SER:CA	1:B:356:TYR:CE2	2.40	0.60
1:A:95:LEU:CA	1:A:96:SER:CB	2.76	0.60
1:A:352:SER:CA	1:A:356:TYR:CE2	2.52	0.60
1:A:357:TRP:HA	1:A:695:TYR:HD1	1.67	0.60
1:B:16:MET:HA	1:B:16:MET:HE2	1.83	0.60
1:A:194:LEU:HD21	1:A:704:PRO:HB2	1.84	0.60
1:B:403:GLY:C	1:B:404:ILE:HG13	2.27	0.60
1:A:154:ARG:CA	1:A:155:THR:O	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLY:HA3	1:A:621:ASN:CB	2.32	0.59
1:A:277:GLY:HA3	1:A:621:ASN:HB3	1.83	0.59
1:A:357:TRP:HE1	1:A:361:ALA:C	2.10	0.59
1:A:156:LEU:HD22	1:A:163:SER:HA	1.84	0.59
1:B:32:LYS:CG	1:B:461:GLU:HG3	2.32	0.59
1:B:349:VAL:C	1:B:356:TYR:HH	2.09	0.59
1:B:113:LEU:CD2	1:B:376:LEU:HB2	2.32	0.59
1:B:126:PHE:HA	1:B:127:VAL:HB	1.83	0.59
1:B:129:LEU:C	1:B:130:LEU:CG	2.75	0.59
1:B:349:VAL:CA	1:B:356:TYR:OH	2.50	0.59
1:B:384:PHE:CE2	1:B:680:LEU:HD23	2.36	0.59
1:A:156:LEU:C	1:A:158:MET:N	2.56	0.59
1:A:404:ILE:HD13	1:A:661:ALA:H	1.62	0.59
1:B:405:LEU:O	1:B:649:VAL:N	2.27	0.59
1:B:429:LEU:O	1:B:550:LEU:HA	2.02	0.59
1:A:351:ILE:O	1:A:356:TYR:CE1	2.53	0.59
1:B:151:LEU:O	1:B:153:ARG:CG	2.50	0.59
1:B:178:ALA:O	1:B:183:ARG:N	2.36	0.59
1:B:357:TRP:HA	1:B:695:TYR:HD1	1.67	0.59
1:A:161:MET:C	1:A:162:TYR:CG	2.80	0.59
1:B:364:PRO:N	1:B:366:LEU:N	2.50	0.59
1:B:692:GLY:C	1:B:694:LEU:H	2.10	0.59
1:B:692:GLY:C	1:B:694:LEU:N	2.57	0.59
1:A:129:LEU:C	1:A:130:LEU:CG	2.76	0.59
1:A:450:LEU:HD11	1:A:471:LYS:HG3	1.84	0.59
1:A:178:ALA:O	1:A:183:ARG:N	2.36	0.59
1:A:433:LYS:O	1:A:433:LYS:CD	2.45	0.59
1:A:692:GLY:C	1:A:694:LEU:N	2.57	0.59
1:B:95:LEU:CB	1:B:96:SER:CB	2.74	0.59
1:A:126:PHE:HA	1:A:127:VAL:HB	1.84	0.59
1:A:189:GLU:OE2	1:A:190:THR:N	2.35	0.59
1:A:720:ALA:HA	1:A:723:LEU:HD12	1.84	0.59
1:B:21:ARG:HB3	1:B:82:VAL:CG2	2.33	0.59
1:B:81:VAL:HG12	1:B:83:ASP:CG	2.28	0.59
1:A:20:VAL:HG12	1:A:82:VAL:O	2.03	0.59
1:A:181:LEU:HB3	1:A:182:PRO:O	2.03	0.59
1:A:692:GLY:HA2	1:A:695:TYR:CD2	2.38	0.59
1:B:32:LYS:HG2	1:B:461:GLU:HG3	1.85	0.59
1:B:161:MET:C	1:B:162:TYR:CG	2.81	0.59
1:B:201:GLY:O	1:B:202:ARG:C	2.46	0.59
1:B:277:GLY:HA3	1:B:621:ASN:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:TYR:H	1:B:358:TYR:HB2	1.68	0.59
1:A:32:LYS:CG	1:A:461:GLU:HG3	2.33	0.58
1:A:292:GLY:O	1:A:293:ALA:HB3	2.03	0.58
1:A:364:PRO:N	1:A:366:LEU:N	2.50	0.58
1:B:327:SER:CB	1:B:328:LYS:HB2	2.32	0.58
1:A:71:LYS:HZ3	1:A:84:GLU:HG2	1.67	0.58
1:A:151:LEU:O	1:A:153:ARG:CG	2.50	0.58
1:B:115:LEU:HD13	1:B:174:VAL:CA	2.32	0.58
1:B:156:LEU:C	1:B:158:MET:H	2.11	0.58
1:B:277:GLY:HA3	1:B:621:ASN:HB3	1.84	0.58
1:B:564:MET:HG2	1:B:732:ILE:HG23	1.83	0.58
1:A:357:TRP:HA	1:A:695:TYR:CD1	2.39	0.58
1:B:71:LYS:HD2	1:B:84:GLU:CG	2.34	0.58
1:B:189:GLU:OE2	1:B:190:THR:N	2.35	0.58
1:B:194:LEU:HD21	1:B:704:PRO:HB2	1.83	0.58
1:B:692:GLY:HA2	1:B:695:TYR:CD2	2.38	0.58
1:A:83:ASP:CG	1:A:84:GLU:CB	2.76	0.58
1:A:113:LEU:HB3	1:A:373:ILE:HG13	1.86	0.58
1:A:692:GLY:C	1:A:694:LEU:H	2.10	0.58
1:A:729:VAL:HB	1:A:730:PRO:CD	2.34	0.58
1:B:88:VAL:O	1:B:89:SER:HB2	2.04	0.58
1:A:201:GLY:O	1:A:202:ARG:C	2.47	0.58
1:B:292:GLY:O	1:B:293:ALA:HB3	2.03	0.58
1:A:32:LYS:HG2	1:A:461:GLU:HG3	1.85	0.58
1:A:102:LEU:CB	1:A:166:VAL:HB	2.34	0.58
1:A:141:SER:HB3	1:A:343:ILE:CG2	2.34	0.58
1:B:357:TRP:HA	1:B:695:TYR:CD1	2.39	0.58
1:B:357:TRP:CD1	1:B:358:TYR:HA	2.39	0.58
1:B:731:PRO:HG2	1:B:732:ILE:HG13	1.86	0.58
1:A:120:SER:OG	1:A:123:TYR:HB3	1.99	0.58
1:A:156:LEU:C	1:A:158:MET:H	2.11	0.58
1:A:194:LEU:CD2	1:A:377:VAL:HG11	2.32	0.58
1:A:280:VAL:HG22	1:A:461:GLU:HG2	1.86	0.58
1:A:619:GLY:HA2	1:A:626:LEU:CD1	2.33	0.58
1:B:328:LYS:CE	1:B:333:ARG:HG3	2.33	0.58
1:B:696:PRO:HB2	1:B:698:PHE:CD1	2.38	0.58
1:A:696:PRO:HB2	1:A:698:PHE:CD1	2.38	0.58
1:B:113:LEU:HB3	1:B:373:ILE:HG13	1.85	0.58
1:B:170:PHE:O	1:B:173:SER:N	2.37	0.58
1:B:15:PRO:O	1:B:16:MET:HG2	2.04	0.58
1:B:141:SER:HB3	1:B:343:ILE:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:CD2	1:B:377:VAL:HG11	2.34	0.58
1:A:117:HIS:C	1:A:191:SER:HB2	2.29	0.57
1:A:126:PHE:CA	1:A:127:VAL:HB	2.34	0.57
1:A:371:THR:O	1:A:372:LEU:C	2.47	0.57
1:A:429:LEU:O	1:A:550:LEU:HA	2.02	0.57
1:B:144:PHE:O	1:B:148:PHE:O	2.22	0.57
1:B:181:LEU:HB3	1:B:182:PRO:O	2.03	0.57
1:B:189:GLU:HG2	1:B:193:LEU:H	1.59	0.57
1:A:170:PHE:O	1:A:173:SER:N	2.37	0.57
1:A:354:PHE:C	1:A:356:TYR:CD1	2.82	0.57
1:A:357:TRP:HB3	1:A:694:LEU:C	2.29	0.57
1:B:102:LEU:CB	1:B:166:VAL:HB	2.33	0.57
1:B:186:SER:CB	1:B:187:PHE:CA	2.78	0.57
1:B:404:ILE:HD13	1:B:661:ALA:CB	2.34	0.57
1:B:619:GLY:HA2	1:B:626:LEU:CD1	2.33	0.57
1:A:164:MET:O	1:A:165:GLY:C	2.46	0.57
1:A:360:ILE:CG2	1:A:362:HIS:C	2.77	0.57
1:B:126:PHE:H	1:B:127:VAL:HB	1.69	0.57
1:B:164:MET:O	1:B:165:GLY:C	2.47	0.57
1:B:280:VAL:HG22	1:B:461:GLU:HG2	1.86	0.57
1:B:357:TRP:HB3	1:B:694:LEU:C	2.29	0.57
1:B:729:VAL:HB	1:B:730:PRO:HD3	1.87	0.57
1:A:203:THR:O	1:A:204:LEU:C	2.48	0.57
1:A:360:ILE:CG2	1:A:363:ALA:N	2.66	0.57
1:A:731:PRO:HG2	1:A:732:ILE:HG13	1.86	0.57
1:A:81:VAL:HG12	1:A:83:ASP:CG	2.28	0.57
1:A:357:TRP:CD1	1:A:358:TYR:HA	2.38	0.57
1:B:371:THR:O	1:B:372:LEU:C	2.47	0.57
1:A:67:PHE:CE2	1:A:83:ASP:OD2	2.58	0.57
1:A:84:GLU:O	1:A:84:GLU:HG2	1.92	0.57
1:A:104:VAL:CG1	1:A:104:VAL:O	2.53	0.57
1:A:144:PHE:O	1:A:148:PHE:O	2.22	0.57
1:A:364:PRO:HG2	1:A:367:PHE:N	2.20	0.57
1:A:385:GLY:O	1:A:389:PRO:HD2	2.05	0.57
1:B:141:SER:CB	1:B:343:ILE:CG2	2.82	0.57
1:A:88:VAL:O	1:A:89:SER:HB2	2.04	0.57
1:A:121:LEU:HG	1:A:369:PHE:CZ	2.39	0.57
1:A:636:GLY:HA3	1:A:653:ASP:OD1	2.05	0.57
1:B:71:LYS:HZ3	1:B:84:GLU:HG2	1.70	0.57
1:B:450:LEU:HD11	1:B:471:LYS:HG3	1.86	0.57
1:B:126:PHE:CA	1:B:127:VAL:HB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:HD12	1:B:354:PHE:CD1	2.40	0.57
1:B:364:PRO:HG2	1:B:367:PHE:N	2.20	0.57
1:B:729:VAL:HB	1:B:730:PRO:CD	2.34	0.57
1:A:20:VAL:HB	1:A:83:ASP:OD1	2.04	0.57
1:A:36:THR:HG21	1:A:281:PRO:HD2	1.86	0.57
1:A:695:TYR:C	1:A:697:ILE:H	2.13	0.57
1:B:117:HIS:C	1:B:191:SER:HB2	2.29	0.57
1:B:215:ALA:C	1:B:217:LYS:H	2.12	0.57
1:B:326:GLY:O	1:B:327:SER:C	2.48	0.57
1:B:360:ILE:CG2	1:B:363:ALA:N	2.67	0.57
1:A:67:PHE:C	1:A:67:PHE:CD2	2.82	0.57
1:A:103:TYR:CE2	1:A:166:VAL:CG2	2.88	0.57
1:A:416:GLU:OE1	1:A:737:ASP:HB2	2.04	0.57
1:B:36:THR:HG21	1:B:281:PRO:HD2	1.86	0.57
1:B:121:LEU:HG	1:B:369:PHE:CZ	2.40	0.57
1:B:363:ALA:CA	1:B:365:LEU:HA	2.27	0.57
1:A:216:ILE:C	1:A:218:LYS:H	2.13	0.56
1:A:323:ASP:O	1:A:324:ALA:HB3	2.04	0.56
1:A:328:LYS:CE	1:A:333:ARG:HG3	2.33	0.56
1:B:20:VAL:CB	1:B:83:ASP:OD1	2.53	0.56
1:B:104:VAL:CG1	1:B:104:VAL:O	2.53	0.56
1:A:26:THR:C	1:B:53:THR:HG22	2.30	0.56
1:A:112:LEU:HD23	1:A:173:SER:HB3	1.86	0.56
1:A:126:PHE:H	1:A:127:VAL:HB	1.69	0.56
1:A:194:LEU:CD2	1:A:704:PRO:HB2	2.35	0.56
1:A:358:TYR:C	1:A:358:TYR:CD2	2.84	0.56
1:B:88:VAL:CG1	1:B:89:SER:N	2.69	0.56
1:B:112:LEU:HD23	1:B:173:SER:HB3	1.86	0.56
1:B:321:VAL:O	1:B:323:ASP:N	2.37	0.56
1:B:327:SER:OG	1:B:328:LYS:CG	2.53	0.56
1:B:721:ASN:C	1:B:723:LEU:H	2.13	0.56
1:A:121:LEU:HD13	1:A:178:ALA:HB2	1.87	0.56
1:A:356:TYR:H	1:A:358:TYR:HB2	1.68	0.56
1:B:209:LYS:C	1:B:211:ARG:H	2.13	0.56
1:B:385:GLY:O	1:B:389:PRO:HD2	2.05	0.56
1:B:71:LYS:CD	1:B:84:GLU:HG2	2.35	0.56
1:B:152:ARG:HB3	1:B:153:ARG:C	2.30	0.56
1:B:323:ASP:O	1:B:324:ALA:HB3	2.04	0.56
1:A:130:LEU:HD12	1:A:354:PHE:CD1	2.40	0.56
1:A:141:SER:CB	1:A:343:ILE:CG2	2.83	0.56
1:A:153:ARG:NE	1:A:155:THR:HG21	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:TYR:C	1:B:358:TYR:CD2	2.83	0.56
1:B:695:TYR:C	1:B:697:ILE:H	2.13	0.56
1:A:327:SER:OG	1:A:328:LYS:CG	2.53	0.56
1:A:564:MET:HG3	1:A:732:ILE:HG23	1.87	0.56
1:B:153:ARG:NE	1:B:155:THR:HG21	2.20	0.56
1:B:186:SER:HB2	1:B:187:PHE:CA	2.32	0.56
1:A:214:GLU:HG2	1:A:215:ALA:N	2.21	0.56
1:B:130:LEU:O	1:B:133:LEU:N	2.39	0.56
1:A:151:LEU:O	1:A:153:ARG:HG2	2.05	0.56
1:B:189:GLU:CD	1:B:189:GLU:O	2.41	0.56
1:A:152:ARG:HB3	1:A:153:ARG:C	2.30	0.56
1:B:103:TYR:CE2	1:B:166:VAL:CG2	2.88	0.56
1:B:560:GLU:O	1:B:564:MET:HG3	2.06	0.56
1:A:215:ALA:C	1:A:217:LYS:H	2.12	0.55
1:A:326:GLY:O	1:A:327:SER:C	2.48	0.55
1:B:151:LEU:O	1:B:153:ARG:HG2	2.05	0.55
1:B:203:THR:O	1:B:204:LEU:C	2.48	0.55
1:B:360:ILE:CG2	1:B:362:HIS:C	2.79	0.55
1:A:130:LEU:O	1:A:133:LEU:N	2.39	0.55
1:B:67:PHE:CE2	1:B:83:ASP:OD2	2.59	0.55
1:B:360:ILE:HG13	1:B:697:ILE:HG12	1.85	0.55
1:B:720:ALA:HA	1:B:723:LEU:HD12	1.87	0.55
1:A:88:VAL:CG1	1:A:89:SER:N	2.69	0.55
1:A:211:ARG:O	1:A:211:ARG:HD3	2.06	0.55
1:A:721:ASN:C	1:A:723:LEU:H	2.13	0.55
1:A:729:VAL:HB	1:A:730:PRO:HD3	1.87	0.55
1:B:194:LEU:CD2	1:B:704:PRO:HB2	2.36	0.55
1:B:327:SER:OG	1:B:328:LYS:HB2	2.06	0.55
1:B:396:MET:CE	1:B:406:ILE:O	2.55	0.55
1:A:85:GLN:O	1:A:86:ALA:HB2	2.06	0.55
1:B:67:PHE:C	1:B:67:PHE:CD2	2.82	0.55
1:B:216:ILE:C	1:B:218:LYS:H	2.13	0.55
1:A:22:VAL:HA	1:A:80:GLY:O	2.05	0.55
1:A:189:GLU:CA	1:A:190:THR:C	2.79	0.55
1:A:430:THR:O	1:A:551:LYS:HG2	2.03	0.55
1:B:22:VAL:CA	1:B:80:GLY:O	2.53	0.55
1:B:157:ASN:O	1:B:158:MET:HB2	2.05	0.55
1:A:425:LYS:C	1:A:427:GLY:H	2.15	0.55
1:A:157:ASN:O	1:A:158:MET:HB2	2.05	0.55
1:A:349:VAL:C	1:A:356:TYR:HH	2.13	0.55
1:B:51:LEU:CB	1:B:51:LEU:H	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:CG1	1:B:161:MET:O	2.55	0.55
1:B:216:ILE:C	1:B:218:LYS:N	2.64	0.55
1:A:15:PRO:O	1:A:16:MET:HG2	2.07	0.55
1:B:84:GLU:O	1:B:84:GLU:HG2	1.96	0.55
1:B:416:GLU:OE1	1:B:737:ASP:HB2	2.07	0.55
1:A:696:PRO:O	1:A:697:ILE:HD12	2.06	0.55
1:A:411:ALA:C	1:A:413:GLU:H	2.15	0.54
1:B:85:GLN:O	1:B:86:ALA:HB2	2.06	0.54
1:A:265:GLU:HB3	1:A:302:LYS:HB2	1.89	0.54
1:A:280:VAL:HG22	1:A:461:GLU:CG	2.37	0.54
1:A:327:SER:OG	1:A:328:LYS:HB2	2.06	0.54
1:A:560:GLU:O	1:A:564:MET:HG3	2.06	0.54
1:B:111:LEU:CD2	1:B:198:LEU:HD11	2.34	0.54
1:B:129:LEU:C	1:B:129:LEU:CD2	2.71	0.54
1:B:211:ARG:O	1:B:211:ARG:HD3	2.06	0.54
1:B:360:ILE:O	1:B:363:ALA:CB	2.54	0.54
1:B:696:PRO:O	1:B:697:ILE:HD12	2.06	0.54
1:A:160:VAL:CG1	1:A:161:MET:O	2.55	0.54
1:A:166:VAL:O	1:A:169:ALA:N	2.41	0.54
1:A:360:ILE:O	1:A:363:ALA:CB	2.55	0.54
1:B:130:LEU:O	1:B:131:ILE:C	2.51	0.54
1:B:280:VAL:HG22	1:B:461:GLU:CG	2.37	0.54
1:B:429:LEU:HA	1:B:655:LEU:CD1	2.35	0.54
1:B:564:MET:HG3	1:B:732:ILE:HG23	1.87	0.54
1:A:129:LEU:CD2	1:A:368:ALA:HB3	2.26	0.54
1:A:130:LEU:O	1:A:131:ILE:C	2.51	0.54
1:A:326:GLY:C	1:A:327:SER:O	2.51	0.54
1:A:396:MET:CE	1:A:406:ILE:O	2.54	0.54
1:B:121:LEU:HD13	1:B:178:ALA:HB2	1.87	0.54
1:B:214:GLU:O	1:B:217:LYS:HB2	2.08	0.54
1:B:214:GLU:HG2	1:B:215:ALA:N	2.21	0.54
1:B:326:GLY:C	1:B:327:SER:O	2.51	0.54
1:B:382:CYS:O	1:B:383:ALA:CB	2.55	0.54
1:B:411:ALA:C	1:B:413:GLU:H	2.15	0.54
1:B:671:LYS:HD3	1:B:723:LEU:O	2.08	0.54
1:A:130:LEU:HD12	1:A:354:PHE:CG	2.43	0.54
1:A:151:LEU:HD23	1:A:328:LYS:HZ3	1.72	0.54
1:A:321:VAL:O	1:A:323:ASP:N	2.37	0.54
1:A:364:PRO:HG3	1:A:367:PHE:CD1	2.43	0.54
1:A:382:CYS:O	1:A:383:ALA:CB	2.54	0.54
1:B:364:PRO:HG3	1:B:367:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ALA:C	1:B:413:GLU:N	2.65	0.54
1:B:425:LYS:C	1:B:427:GLY:H	2.15	0.54
1:A:53:THR:HG23	1:B:51:LEU:CG	2.38	0.54
1:A:111:LEU:CD2	1:A:198:LEU:HD11	2.34	0.54
1:A:209:LYS:C	1:A:211:ARG:H	2.14	0.54
1:B:189:GLU:CA	1:B:190:THR:C	2.80	0.54
1:A:131:ILE:O	1:A:134:PRO:CD	2.56	0.54
1:A:215:ALA:CB	1:A:645:SER:CB	2.86	0.54
1:A:216:ILE:C	1:A:218:LYS:N	2.64	0.54
1:B:83:ASP:OD2	1:B:84:GLU:HB2	2.07	0.54
1:B:88:VAL:HG13	1:B:89:SER:H	1.73	0.54
1:A:113:LEU:O	1:A:373:ILE:HD11	2.08	0.54
1:B:131:ILE:O	1:B:134:PRO:CD	2.56	0.54
1:B:357:TRP:O	1:B:695:TYR:HB3	2.07	0.54
1:B:357:TRP:O	1:B:695:TYR:CD1	2.61	0.54
1:B:363:ALA:CA	1:B:365:LEU:CA	2.85	0.54
1:A:214:GLU:O	1:A:217:LYS:HB2	2.08	0.54
1:A:105:ALA:O	1:A:339:VAL:HG11	2.08	0.54
1:A:254:GLY:N	1:A:296:ASN:O	2.33	0.54
1:A:119:ILE:O	1:A:186:SER:O	2.23	0.53
1:A:357:TRP:O	1:A:695:TYR:CD1	2.61	0.53
1:A:560:GLU:OE1	1:A:732:ILE:HG21	2.08	0.53
1:A:671:LYS:HD3	1:A:723:LEU:O	2.07	0.53
1:B:215:ALA:CB	1:B:645:SER:CB	2.86	0.53
1:B:440:VAL:HB	1:B:543:ILE:HG12	1.90	0.53
1:A:151:LEU:HA	1:A:328:LYS:CG	2.39	0.53
1:A:360:ILE:HG13	1:A:697:ILE:HG12	1.86	0.53
1:A:367:PHE:O	1:A:368:ALA:HB3	2.07	0.53
1:B:166:VAL:O	1:B:169:ALA:N	2.40	0.53
1:B:203:THR:C	1:B:205:GLU:H	2.13	0.53
1:B:279:PRO:HB2	1:B:461:GLU:OE2	2.08	0.53
1:B:381:PRO:C	1:B:384:PHE:CD1	2.86	0.53
1:B:384:PHE:CD2	1:B:679:ALA:HB1	2.41	0.53
1:B:395:GLY:C	1:B:398:LYS:H	2.15	0.53
1:B:550:LEU:O	1:B:554:ALA:HB3	2.07	0.53
1:A:52:ALA:O	1:B:52:ALA:HA	2.04	0.53
1:A:88:VAL:HG13	1:A:89:SER:H	1.73	0.53
1:A:277:GLY:CA	1:A:621:ASN:CG	2.78	0.53
1:A:351:ILE:C	1:A:356:TYR:CD1	2.85	0.53
1:A:357:TRP:O	1:A:695:TYR:HB3	2.08	0.53
1:A:395:GLY:C	1:A:398:LYS:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:O	1:B:373:ILE:HD11	2.08	0.53
1:B:373:ILE:HG22	1:B:704:PRO:HB3	1.90	0.53
1:B:560:GLU:OE1	1:B:732:ILE:HG21	2.08	0.53
1:A:125:ASP:OD2	1:A:126:PHE:N	2.42	0.53
1:B:164:MET:O	1:B:167:GLY:N	2.41	0.53
1:A:279:PRO:HB2	1:A:461:GLU:OE2	2.09	0.53
1:A:434:PRO:HG3	1:A:463:PRO:O	2.07	0.53
1:B:130:LEU:HD12	1:B:354:PHE:CG	2.43	0.53
1:B:209:LYS:C	1:B:211:ARG:N	2.67	0.53
1:A:117:HIS:O	1:A:118:PHE:C	2.51	0.53
1:B:125:ASP:OD2	1:B:126:PHE:N	2.42	0.53
1:B:151:LEU:HA	1:B:328:LYS:CG	2.39	0.53
1:A:71:LYS:HG3	1:A:75:GLU:HG2	1.91	0.53
1:A:181:LEU:CB	1:A:182:PRO:O	2.57	0.53
1:A:550:LEU:O	1:A:554:ALA:HB3	2.08	0.53
1:A:571:ILE:HA	1:A:592:ILE:O	2.09	0.53
1:B:108:ALA:HB1	1:B:111:LEU:CD1	2.39	0.53
1:B:376:LEU:C	1:B:378:VAL:N	2.66	0.53
1:B:396:MET:HG2	1:B:412:LEU:HD11	1.91	0.53
1:B:406:ILE:HG12	1:B:648:ILE:CG1	2.39	0.53
1:A:117:HIS:O	1:A:119:ILE:N	2.42	0.53
1:A:129:LEU:C	1:A:130:LEU:HG	2.30	0.53
1:A:164:MET:O	1:A:167:GLY:N	2.41	0.53
1:A:201:GLY:O	1:A:203:THR:N	2.42	0.53
1:A:373:ILE:HG22	1:A:704:PRO:HB3	1.90	0.53
1:A:396:MET:HG2	1:A:412:LEU:HD11	1.91	0.53
1:A:434:PRO:HG3	1:A:463:PRO:C	2.33	0.53
1:B:108:ALA:HB1	1:B:111:LEU:CG	2.39	0.53
1:B:117:HIS:O	1:B:118:PHE:C	2.51	0.53
1:A:363:ALA:CA	1:A:365:LEU:CA	2.85	0.53
1:A:381:PRO:C	1:A:384:PHE:CD1	2.87	0.53
1:B:129:LEU:CD2	1:B:368:ALA:HB3	2.26	0.53
1:B:273:SER:O	1:B:277:GLY:HA2	2.09	0.53
1:A:83:ASP:CG	1:A:84:GLU:HB2	2.34	0.53
1:A:564:MET:CA	1:A:732:ILE:HG23	2.39	0.53
1:B:147:ALA:O	1:B:149:SER:N	2.42	0.53
1:B:265:GLU:HB3	1:B:302:LYS:HB2	1.90	0.53
1:B:373:ILE:N	1:B:373:ILE:CD1	2.72	0.53
1:A:351:ILE:N	1:A:356:TYR:HE1	2.06	0.52
1:B:36:THR:HG21	1:B:281:PRO:CD	2.39	0.52
1:B:117:HIS:CE1	1:B:373:ILE:HG21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LYS:H	1:B:329:PRO:HD3	1.74	0.52
1:B:434:PRO:HB2	1:B:546:VAL:CG1	2.38	0.52
1:A:102:LEU:HD12	1:A:163:SER:O	2.09	0.52
1:A:363:ALA:CA	1:A:365:LEU:HA	2.27	0.52
1:A:403:GLY:C	1:A:404:ILE:HG13	2.30	0.52
1:A:406:ILE:HG12	1:A:648:ILE:CG1	2.39	0.52
1:B:172:ALA:O	1:B:176:SER:HB2	2.10	0.52
1:B:367:PHE:O	1:B:368:ALA:HB3	2.07	0.52
1:A:36:THR:HG21	1:A:281:PRO:CD	2.39	0.52
1:A:172:ALA:O	1:A:176:SER:HB2	2.10	0.52
1:A:273:SER:O	1:A:277:GLY:HA2	2.08	0.52
1:A:328:LYS:CE	1:A:333:ARG:CG	2.88	0.52
1:A:364:PRO:HG2	1:A:366:LEU:CA	2.40	0.52
1:B:191:SER:O	1:B:194:LEU:N	2.42	0.52
1:A:373:ILE:CD1	1:A:373:ILE:N	2.72	0.52
1:A:440:VAL:HB	1:A:543:ILE:HG12	1.90	0.52
1:B:152:ARG:N	1:B:153:ARG:HA	2.18	0.52
1:B:571:ILE:HA	1:B:592:ILE:O	2.10	0.52
1:A:83:ASP:CG	1:A:84:GLU:HB3	2.35	0.52
1:A:667:LYS:HD2	1:A:727:ASN:OD1	2.10	0.52
1:B:664:LEU:HD12	1:B:667:LYS:HE2	1.92	0.52
1:A:156:LEU:CB	1:A:163:SER:HA	2.38	0.52
1:B:117:HIS:O	1:B:119:ILE:N	2.42	0.52
1:B:201:GLY:O	1:B:203:THR:N	2.42	0.52
1:B:388:THR:N	1:B:389:PRO:HD2	2.25	0.52
1:A:351:ILE:CA	1:A:356:TYR:HE1	2.23	0.52
1:A:388:THR:N	1:A:389:PRO:HD2	2.25	0.52
1:A:429:LEU:HA	1:A:655:LEU:CD1	2.36	0.52
1:A:671:LYS:HD2	1:A:723:LEU:O	2.10	0.52
1:B:90:ALA:HA	1:B:91:GLU:C	2.34	0.52
1:B:126:PHE:N	1:B:127:VAL:HB	2.25	0.52
1:B:434:PRO:HB2	1:B:467:ALA:HB2	1.92	0.52
1:A:97:ARG:O	1:A:100:ARG:HG3	2.10	0.52
1:A:117:HIS:CG	1:A:373:ILE:HG12	2.45	0.52
1:A:117:HIS:CD2	1:A:191:SER:HA	2.45	0.52
1:A:126:PHE:N	1:A:127:VAL:HB	2.25	0.52
1:B:19:THR:HG23	1:B:56:ALA:O	2.09	0.52
1:B:101:LYS:HG3	1:B:205:GLU:HB2	1.92	0.52
1:B:181:LEU:CB	1:B:182:PRO:O	2.57	0.52
1:B:214:GLU:CG	1:B:215:ALA:N	2.73	0.52
1:B:564:MET:CA	1:B:732:ILE:HG23	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD12	1:A:369:PHE:HD1	1.73	0.52
1:A:147:ALA:O	1:A:149:SER:N	2.42	0.52
1:A:189:GLU:HG2	1:A:193:LEU:N	2.21	0.52
1:A:209:LYS:C	1:A:211:ARG:N	2.67	0.52
1:A:434:PRO:HB2	1:A:467:ALA:HB2	1.92	0.52
1:B:378:VAL:HG13	1:B:686:LEU:HB3	1.92	0.52
1:A:117:HIS:O	1:A:191:SER:HB3	2.10	0.52
1:A:712:ALA:O	1:A:716:VAL:HB	2.10	0.52
1:B:125:ASP:O	1:B:126:PHE:CD2	2.62	0.52
1:A:378:VAL:HG13	1:A:686:LEU:HB3	1.93	0.51
1:B:71:LYS:HG3	1:B:75:GLU:HG2	1.91	0.51
1:B:117:HIS:CG	1:B:373:ILE:HG12	2.44	0.51
1:B:130:LEU:O	1:B:134:PRO:CD	2.41	0.51
1:B:190:THR:O	1:B:194:LEU:CD1	2.56	0.51
1:B:349:VAL:HA	1:B:356:TYR:OH	2.10	0.51
1:A:117:HIS:CE1	1:A:373:ILE:HG21	2.45	0.51
1:A:191:SER:O	1:A:194:LEU:N	2.43	0.51
1:A:280:VAL:HG22	1:A:461:GLU:CB	2.40	0.51
1:A:664:LEU:HD12	1:A:667:LYS:HE2	1.92	0.51
1:A:108:ALA:HB1	1:A:111:LEU:CD1	2.40	0.51
1:A:112:LEU:CD2	1:A:173:SER:HB3	2.41	0.51
1:A:150:ALA:O	1:A:153:ARG:HG2	2.08	0.51
1:A:384:PHE:CD2	1:A:679:ALA:HB1	2.43	0.51
1:A:720:ALA:O	1:A:723:LEU:HB2	2.11	0.51
1:B:388:THR:O	1:B:392:LEU:HD13	2.10	0.51
1:A:125:ASP:O	1:A:126:PHE:CD2	2.62	0.51
1:A:561:LEU:HD13	1:A:659:VAL:HG22	1.91	0.51
1:B:102:LEU:HD12	1:B:163:SER:O	2.10	0.51
1:B:364:PRO:HG2	1:B:366:LEU:CA	2.40	0.51
1:B:381:PRO:HB2	1:B:384:PHE:CD2	2.46	0.51
1:A:156:LEU:HD22	1:A:162:TYR:O	2.10	0.51
1:A:356:TYR:H	1:A:358:TYR:CB	2.24	0.51
1:A:434:PRO:HB2	1:A:546:VAL:HG13	1.92	0.51
1:A:126:PHE:CA	1:A:127:VAL:CB	2.89	0.51
1:A:180:VAL:C	1:A:182:PRO:HA	2.34	0.51
1:A:428:THR:CG2	1:A:655:LEU:HD21	2.39	0.51
1:B:117:HIS:CD2	1:B:191:SER:HA	2.46	0.51
1:B:328:LYS:CE	1:B:333:ARG:CG	2.87	0.51
1:B:667:LYS:HD2	1:B:727:ASN:OD1	2.10	0.51
1:B:671:LYS:HD2	1:B:723:LEU:O	2.10	0.51
1:A:53:THR:CG2	1:B:51:LEU:CD1	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CE2	1:A:166:VAL:HG21	2.46	0.51
1:A:428:THR:O	1:A:655:LEU:CD1	2.55	0.51
1:A:716:VAL:O	1:A:719:VAL:HB	2.11	0.51
1:B:97:ARG:O	1:B:100:ARG:HG3	2.10	0.51
1:B:356:TYR:H	1:B:358:TYR:CB	2.24	0.51
1:B:112:LEU:HA	1:B:115:LEU:HD12	1.93	0.51
1:A:214:GLU:CG	1:A:215:ALA:N	2.73	0.51
1:B:215:ALA:O	1:B:218:LYS:N	2.43	0.51
1:A:172:ALA:O	1:A:176:SER:CB	2.59	0.51
1:A:203:THR:C	1:A:205:GLU:H	2.13	0.51
1:A:215:ALA:CB	1:A:645:SER:OG	2.58	0.51
1:A:253:PRO:HB3	1:A:297:ASN:O	2.11	0.51
1:B:137:PHE:HB2	1:B:347:LEU:HD13	1.93	0.51
1:B:561:LEU:HD13	1:B:659:VAL:HG22	1.93	0.51
1:A:388:THR:O	1:A:392:LEU:HD13	2.11	0.50
1:B:151:LEU:HA	1:B:328:LYS:HG2	1.93	0.50
1:B:672:ILE:C	1:B:674:GLN:N	2.68	0.50
1:A:327:SER:HB2	1:A:328:LYS:HA	1.93	0.50
1:B:105:ALA:O	1:B:339:VAL:HG11	2.10	0.50
1:B:345:THR:O	1:B:348:LEU:N	2.43	0.50
1:A:710:ALA:C	1:A:712:ALA:N	2.69	0.50
1:B:117:HIS:O	1:B:191:SER:HB3	2.10	0.50
1:B:121:LEU:N	1:B:122:PRO:C	2.70	0.50
1:B:277:GLY:CA	1:B:621:ASN:CG	2.78	0.50
1:B:404:ILE:CD1	1:B:660:ALA:HB3	2.41	0.50
1:A:21:ARG:HB3	1:A:82:VAL:CG2	2.41	0.50
1:A:101:LYS:HG3	1:A:205:GLU:HB2	1.91	0.50
1:A:151:LEU:O	1:A:327:SER:HB3	2.11	0.50
1:B:254:GLY:N	1:B:296:ASN:O	2.34	0.50
1:B:434:PRO:CG	1:B:463:PRO:O	2.59	0.50
1:A:157:ASN:O	1:A:158:MET:HB3	2.10	0.50
1:A:381:PRO:HB2	1:A:384:PHE:CD2	2.47	0.50
1:B:51:LEU:O	1:B:52:ALA:C	2.51	0.50
1:B:172:ALA:O	1:B:176:SER:CB	2.60	0.50
1:B:180:VAL:C	1:B:182:PRO:HA	2.34	0.50
1:A:110:VAL:HA	1:A:113:LEU:CD1	2.40	0.50
1:A:411:ALA:C	1:A:413:GLU:N	2.65	0.50
1:B:110:VAL:HA	1:B:113:LEU:CD1	2.40	0.50
1:B:112:LEU:CD2	1:B:173:SER:HB3	2.41	0.50
1:B:129:LEU:C	1:B:130:LEU:HG	2.29	0.50
1:B:215:ALA:CB	1:B:645:SER:OG	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ALA:CB	1:B:51:LEU:CB	0.71	0.50
1:A:73:VAL:HG22	1:A:295:ILE:HG21	1.93	0.50
1:B:103:TYR:CE2	1:B:166:VAL:HG21	2.46	0.50
1:B:372:LEU:HD23	1:B:372:LEU:O	2.12	0.50
1:A:31:VAL:HG21	1:A:51:LEU:HD13	1.93	0.50
1:A:149:SER:CA	1:A:155:THR:OG1	2.60	0.50
1:A:189:GLU:HB2	1:A:191:SER:OG	2.12	0.50
1:A:364:PRO:CD	1:A:365:LEU:C	2.83	0.50
1:B:67:PHE:O	1:B:70:ILE:N	2.42	0.50
1:B:208:ALA:C	1:B:210:SER:N	2.70	0.50
1:A:118:PHE:HB3	1:A:186:SER:HA	1.94	0.50
1:A:189:GLU:HG3	1:A:192:VAL:C	2.36	0.50
1:B:121:LEU:HD13	1:B:178:ALA:CB	2.42	0.50
1:B:156:LEU:HD22	1:B:162:TYR:O	2.11	0.50
1:B:357:TRP:HB3	1:B:695:TYR:CA	2.35	0.50
1:B:564:MET:HA	1:B:732:ILE:HG23	1.93	0.50
1:A:51:LEU:CG	1:B:52:ALA:HB3	2.42	0.49
1:A:89:SER:OG	1:A:221:GLY:CA	2.60	0.49
1:A:101:LYS:HD2	1:A:205:GLU:HB3	1.94	0.49
1:A:170:PHE:O	1:A:173:SER:HB2	2.12	0.49
1:B:114:PHE:CE1	1:B:194:LEU:O	2.65	0.49
1:B:125:ASP:C	1:B:126:PHE:CD2	2.90	0.49
1:B:151:LEU:O	1:B:327:SER:HB3	2.11	0.49
1:B:170:PHE:O	1:B:173:SER:HB2	2.12	0.49
1:B:189:GLU:HG3	1:B:192:VAL:C	2.36	0.49
1:B:348:LEU:O	1:B:356:TYR:OH	2.29	0.49
1:A:95:LEU:HD12	1:A:158:MET:HB2	1.93	0.49
1:A:108:ALA:HB1	1:A:111:LEU:CG	2.42	0.49
1:A:121:LEU:N	1:A:122:PRO:C	2.70	0.49
1:B:73:VAL:HG22	1:B:295:ILE:HG21	1.94	0.49
1:B:131:ILE:O	1:B:134:PRO:CG	2.61	0.49
1:B:149:SER:CA	1:B:155:THR:OG1	2.60	0.49
1:B:357:TRP:CB	1:B:358:TYR:HA	2.41	0.49
1:A:125:ASP:C	1:A:126:PHE:CD2	2.90	0.49
1:B:189:GLU:HB2	1:B:191:SER:OG	2.12	0.49
1:B:710:ALA:C	1:B:712:ALA:N	2.69	0.49
1:A:170:PHE:CZ	1:A:174:VAL:HG22	2.47	0.49
1:A:354:PHE:O	1:A:355:ILE:C	2.54	0.49
1:B:170:PHE:CZ	1:B:174:VAL:HG22	2.47	0.49
1:B:253:PRO:HB3	1:B:297:ASN:O	2.11	0.49
1:B:364:PRO:CD	1:B:365:LEU:C	2.83	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:O	1:A:70:ILE:N	2.43	0.49
1:A:129:LEU:HD21	1:A:133:LEU:CG	2.42	0.49
1:A:130:LEU:C	1:A:134:PRO:HD2	2.31	0.49
1:A:137:PHE:HB2	1:A:347:LEU:HD13	1.93	0.49
1:A:149:SER:OG	1:A:155:THR:OG1	2.26	0.49
1:A:189:GLU:CB	1:A:191:SER:C	2.82	0.49
1:A:360:ILE:HG22	1:A:362:HIS:C	2.31	0.49
1:A:696:PRO:O	1:A:697:ILE:C	2.55	0.49
1:B:189:GLU:OE2	1:B:705:GLU:HG2	2.12	0.49
1:B:280:VAL:HG22	1:B:461:GLU:CB	2.40	0.49
1:A:83:ASP:H	1:A:84:GLU:CB	2.18	0.49
1:A:215:ALA:O	1:A:218:LYS:N	2.43	0.49
1:A:356:TYR:CA	1:A:358:TYR:HB2	2.42	0.49
1:A:357:TRP:N	1:A:358:TYR:HB2	2.28	0.49
1:A:376:LEU:C	1:A:378:VAL:N	2.66	0.49
1:A:716:VAL:HG12	1:A:717:SER:N	2.28	0.49
1:B:89:SER:OG	1:B:221:GLY:CA	2.60	0.49
1:B:118:PHE:HB3	1:B:186:SER:HA	1.93	0.49
1:A:52:ALA:HB3	1:B:51:LEU:CB	0.29	0.49
1:B:101:LYS:CA	1:B:104:VAL:HG12	2.38	0.49
1:B:108:ALA:HB1	1:B:111:LEU:HG	1.94	0.49
1:B:129:LEU:HD21	1:B:133:LEU:CG	2.43	0.49
1:B:189:GLU:HG2	1:B:193:LEU:N	2.21	0.49
1:B:712:ALA:O	1:B:716:VAL:CG2	2.61	0.49
1:A:564:MET:HA	1:A:732:ILE:HG23	1.93	0.49
1:B:126:PHE:CA	1:B:127:VAL:CB	2.89	0.49
1:B:356:TYR:CA	1:B:358:TYR:HB2	2.42	0.49
1:B:404:ILE:HD11	1:B:660:ALA:HB3	1.92	0.49
1:A:21:ARG:HB3	1:A:82:VAL:HG23	1.94	0.49
1:A:395:GLY:O	1:A:398:LYS:CA	2.61	0.49
1:A:706:PHE:O	1:A:707:ALA:C	2.55	0.49
1:A:721:ASN:C	1:A:723:LEU:N	2.71	0.49
1:B:692:GLY:O	1:B:696:PRO:CD	2.49	0.49
1:A:105:ALA:O	1:A:339:VAL:HG21	2.13	0.49
1:B:101:LYS:HD2	1:B:205:GLU:HB3	1.94	0.49
1:A:131:ILE:O	1:A:134:PRO:CG	2.60	0.48
1:A:357:TRP:CB	1:A:358:TYR:HA	2.41	0.48
1:A:357:TRP:NE1	1:A:361:ALA:O	2.43	0.48
1:A:360:ILE:CG1	1:A:697:ILE:HG21	2.42	0.48
1:A:550:LEU:O	1:A:551:LYS:C	2.56	0.48
1:B:354:PHE:C	1:B:356:TYR:HD1	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LEU:C	1:B:372:LEU:CD2	2.86	0.48
1:B:426:THR:O	1:B:426:THR:HG22	2.13	0.48
1:A:110:VAL:HG12	1:A:114:PHE:CZ	2.47	0.48
1:A:151:LEU:HA	1:A:328:LYS:HG2	1.93	0.48
1:A:183:ARG:O	1:A:184:GLU:HB2	2.13	0.48
1:A:372:LEU:C	1:A:372:LEU:CD2	2.86	0.48
1:B:149:SER:OG	1:B:155:THR:OG1	2.26	0.48
1:B:186:SER:OG	1:B:187:PHE:HA	2.12	0.48
1:B:194:LEU:HD11	1:B:704:PRO:HB2	1.95	0.48
1:B:712:ALA:O	1:B:716:VAL:HG21	2.13	0.48
1:A:71:LYS:HD2	1:A:84:GLU:CG	2.42	0.48
1:A:112:LEU:HA	1:A:115:LEU:HD12	1.94	0.48
1:A:121:LEU:HD13	1:A:178:ALA:CB	2.43	0.48
1:A:205:GLU:O	1:A:208:ALA:HB3	2.13	0.48
1:A:356:TYR:CD2	1:A:356:TYR:CA	2.97	0.48
1:A:372:LEU:O	1:A:372:LEU:HD23	2.11	0.48
1:A:426:THR:O	1:A:426:THR:HG22	2.14	0.48
1:A:695:TYR:HB2	1:A:696:PRO:HD3	1.95	0.48
1:B:480:GLY:O	1:B:481:GLU:C	2.57	0.48
1:B:695:TYR:HB2	1:B:696:PRO:HD3	1.96	0.48
1:A:101:LYS:C	1:A:103:TYR:N	2.53	0.48
1:A:126:PHE:HA	1:A:128:GLN:N	2.28	0.48
1:B:114:PHE:CA	1:B:117:HIS:HB2	2.39	0.48
1:B:354:PHE:O	1:B:355:ILE:C	2.55	0.48
1:B:357:TRP:N	1:B:358:TYR:HB2	2.28	0.48
1:B:720:ALA:O	1:B:723:LEU:HB2	2.13	0.48
1:A:16:MET:HE2	1:A:16:MET:HA	1.95	0.48
1:A:434:PRO:HB2	1:A:546:VAL:HG11	1.95	0.48
1:B:126:PHE:CD1	1:B:129:LEU:CB	2.92	0.48
1:B:327:SER:CB	1:B:328:LYS:HG3	2.40	0.48
1:A:114:PHE:CA	1:A:117:HIS:HB2	2.40	0.48
1:A:115:LEU:HD11	1:A:170:PHE:CE1	2.49	0.48
1:A:144:PHE:CD2	1:A:144:PHE:C	2.92	0.48
1:A:186:SER:OG	1:A:187:PHE:HA	2.12	0.48
1:B:129:LEU:CD2	1:B:368:ALA:CB	2.90	0.48
1:B:360:ILE:HG22	1:B:362:HIS:C	2.33	0.48
1:B:428:THR:O	1:B:655:LEU:CD1	2.56	0.48
1:B:685:ILE:O	1:B:688:PRO:CG	2.62	0.48
1:B:687:ILE:O	1:B:691:ALA:N	2.47	0.48
1:B:712:ALA:O	1:B:716:VAL:HB	2.13	0.48
1:A:404:ILE:CD1	1:A:661:ALA:H	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ALA:O	1:B:339:VAL:HG21	2.13	0.48
1:B:110:VAL:HG12	1:B:114:PHE:CZ	2.48	0.48
1:B:137:PHE:HB3	1:B:347:LEU:HB2	1.96	0.48
1:A:114:PHE:CE1	1:A:194:LEU:O	2.67	0.48
1:B:125:ASP:C	1:B:126:PHE:CG	2.92	0.48
1:B:126:PHE:HA	1:B:128:GLN:N	2.28	0.48
1:B:144:PHE:C	1:B:144:PHE:CD2	2.92	0.48
1:B:183:ARG:O	1:B:184:GLU:HB2	2.14	0.48
1:B:721:ASN:C	1:B:723:LEU:N	2.71	0.48
1:A:129:LEU:C	1:A:129:LEU:CD2	2.71	0.48
1:A:208:ALA:C	1:A:210:SER:N	2.70	0.48
1:B:92:VAL:HG11	1:B:217:LYS:HG2	1.96	0.48
1:B:108:ALA:CB	1:B:111:LEU:HG	2.43	0.48
1:B:550:LEU:C	1:B:551:LYS:O	2.55	0.48
1:A:550:LEU:C	1:A:551:LYS:O	2.55	0.48
1:A:664:LEU:HD12	1:A:667:LYS:CE	2.44	0.48
1:B:194:LEU:CD1	1:B:704:PRO:HB2	2.44	0.48
1:B:201:GLY:C	1:B:203:THR:N	2.71	0.48
1:B:360:ILE:CG1	1:B:697:ILE:HG21	2.43	0.48
1:B:635:VAL:CG2	1:B:650:LEU:HD12	2.44	0.48
1:B:671:LYS:CE	1:B:725:LEU:O	2.62	0.48
1:B:685:ILE:C	1:B:688:PRO:HD2	2.39	0.48
1:B:706:PHE:O	1:B:707:ALA:C	2.55	0.48
1:A:123:TYR:CE2	1:A:124:GLU:HB3	2.49	0.47
1:A:431:LYS:CE	1:A:549:THR:HB	2.44	0.47
1:B:98:MET:O	1:B:100:ARG:N	2.41	0.47
1:B:189:GLU:HB3	1:B:192:VAL:H	1.73	0.47
1:A:129:LEU:CD2	1:A:368:ALA:CB	2.90	0.47
1:A:152:ARG:HB3	1:A:153:ARG:CA	2.44	0.47
1:A:219:LEU:HB3	1:A:314:LEU:HD11	1.96	0.47
1:A:729:VAL:CB	1:A:730:PRO:CD	2.92	0.47
1:B:113:LEU:HD11	1:B:376:LEU:HB2	1.96	0.47
1:B:130:LEU:C	1:B:134:PRO:HD2	2.31	0.47
1:B:133:LEU:HD22	1:B:372:LEU:HD12	1.96	0.47
1:B:150:ALA:C	1:B:151:LEU:O	2.57	0.47
1:B:152:ARG:HB3	1:B:153:ARG:CA	2.43	0.47
1:A:74:ILE:HG21	1:A:81:VAL:HG21	1.94	0.47
1:A:98:MET:O	1:A:100:ARG:N	2.41	0.47
1:A:113:LEU:CD1	1:A:376:LEU:HB2	2.44	0.47
1:A:189:GLU:HB3	1:A:192:VAL:H	1.72	0.47
1:A:189:GLU:OE2	1:A:705:GLU:HG2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PHE:CD1	1:A:428:THR:CG2	2.92	0.47
1:A:687:ILE:O	1:A:691:ALA:N	2.46	0.47
1:B:36:THR:CG2	1:B:281:PRO:CD	2.92	0.47
1:B:71:LYS:CD	1:B:84:GLU:CG	2.92	0.47
1:B:157:ASN:O	1:B:158:MET:HB3	2.11	0.47
1:B:729:VAL:CB	1:B:730:PRO:CD	2.92	0.47
1:A:20:VAL:CB	1:A:83:ASP:OD1	2.62	0.47
1:A:101:LYS:CA	1:A:104:VAL:HG12	2.38	0.47
1:A:119:ILE:C	1:A:186:SER:C	2.74	0.47
1:A:125:ASP:C	1:A:126:PHE:CG	2.92	0.47
1:A:623:ALA:N	1:A:624:PRO:CD	2.78	0.47
1:B:114:PHE:O	1:B:117:HIS:HB2	2.14	0.47
1:B:141:SER:O	1:B:144:PHE:CD1	2.68	0.47
1:B:664:LEU:HD12	1:B:667:LYS:CE	2.44	0.47
1:A:137:PHE:HB3	1:A:347:LEU:HB2	1.96	0.47
1:A:328:LYS:H	1:A:329:PRO:HD3	1.74	0.47
1:A:685:ILE:C	1:A:688:PRO:HD2	2.39	0.47
1:B:129:LEU:HD12	1:B:369:PHE:HD1	1.73	0.47
1:B:151:LEU:HD23	1:B:328:LYS:HZ3	1.79	0.47
1:A:166:VAL:O	1:A:169:ALA:HB3	2.15	0.47
1:A:480:GLY:O	1:A:481:GLU:C	2.57	0.47
1:A:671:LYS:CE	1:A:725:LEU:O	2.62	0.47
1:B:387:ALA:C	1:B:389:PRO:HD2	2.40	0.47
1:A:36:THR:CG2	1:A:281:PRO:CD	2.92	0.47
1:A:92:VAL:HG11	1:A:217:LYS:HG2	1.96	0.47
1:A:428:THR:C	1:A:655:LEU:HD11	2.39	0.47
1:A:619:GLY:HA2	1:A:626:LEU:HD11	1.97	0.47
1:B:43:GLY:O	1:B:60:PHE:HA	2.15	0.47
1:B:166:VAL:O	1:B:169:ALA:HB3	2.15	0.47
1:B:219:LEU:HB3	1:B:314:LEU:HD11	1.96	0.47
1:B:327:SER:HB2	1:B:328:LYS:HA	1.93	0.47
1:B:395:GLY:O	1:B:398:LYS:CA	2.61	0.47
1:B:696:PRO:O	1:B:697:ILE:C	2.55	0.47
1:A:129:LEU:CD2	1:A:133:LEU:HG	2.44	0.47
1:A:392:LEU:O	1:A:396:MET:HG2	2.15	0.47
1:A:703:ARG:HB3	1:A:704:PRO:HD2	1.97	0.47
1:B:141:SER:CB	1:B:343:ILE:HG22	2.44	0.47
1:B:205:GLU:O	1:B:208:ALA:HB3	2.15	0.47
1:B:404:ILE:CD1	1:B:661:ALA:H	2.25	0.47
1:B:667:LYS:HG3	1:B:727:ASN:OD1	2.14	0.47
1:A:108:ALA:CB	1:A:111:LEU:HG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TYR:HB2	1:A:696:PRO:CD	2.45	0.47
1:A:712:ALA:O	1:A:716:VAL:HG21	2.15	0.47
1:B:113:LEU:CD1	1:B:376:LEU:CB	2.91	0.47
1:B:129:LEU:CD2	1:B:133:LEU:HG	2.44	0.47
1:B:703:ARG:HB3	1:B:704:PRO:HD2	1.97	0.47
1:A:126:PHE:HD1	1:A:128:GLN:O	1.97	0.47
1:A:156:LEU:HD22	1:A:163:SER:CA	2.45	0.47
1:A:161:MET:O	1:A:162:TYR:CB	2.63	0.47
1:A:194:LEU:CD1	1:A:704:PRO:HB2	2.45	0.47
1:A:357:TRP:HB3	1:A:695:TYR:CA	2.35	0.47
1:A:406:ILE:HD12	1:A:412:LEU:HD23	1.96	0.47
1:A:672:ILE:C	1:A:674:GLN:N	2.68	0.47
1:B:77:LEU:HD12	1:B:273:SER:OG	2.15	0.47
1:B:83:ASP:H	1:B:84:GLU:CB	2.21	0.47
1:B:113:LEU:CD1	1:B:376:LEU:HB2	2.45	0.47
1:B:156:LEU:O	1:B:157:ASN:C	2.58	0.47
1:B:392:LEU:O	1:B:396:MET:HG2	2.15	0.47
1:A:201:GLY:C	1:A:203:THR:N	2.72	0.46
1:B:156:LEU:HD22	1:B:163:SER:CA	2.44	0.46
1:A:141:SER:CB	1:A:343:ILE:HG22	2.46	0.46
1:A:431:LYS:HG3	1:A:549:THR:O	2.15	0.46
1:A:387:ALA:C	1:A:389:PRO:HD2	2.40	0.46
1:B:74:ILE:HG21	1:B:81:VAL:HG21	1.96	0.46
1:B:141:SER:HB2	1:B:343:ILE:HG22	1.98	0.46
1:A:71:LYS:CD	1:A:84:GLU:HG2	2.46	0.46
1:A:89:SER:OG	1:A:221:GLY:HA2	2.16	0.46
1:A:117:HIS:O	1:A:119:ILE:HB	2.15	0.46
1:A:133:LEU:HD22	1:A:372:LEU:HD12	1.96	0.46
1:A:404:ILE:HG12	1:A:650:LEU:CD2	2.44	0.46
1:B:92:VAL:HG11	1:B:217:LYS:CG	2.45	0.46
1:B:406:ILE:HD12	1:B:412:LEU:HD23	1.96	0.46
1:B:408:ASN:O	1:B:409:ALA:C	2.58	0.46
1:B:495:ALA:HB3	1:B:498:ILE:HB	1.98	0.46
1:A:205:GLU:CG	1:A:206:ALA:N	2.79	0.46
1:A:357:TRP:O	1:A:695:TYR:HD1	1.99	0.46
1:A:357:TRP:CA	1:A:695:TYR:HA	2.46	0.46
1:A:381:PRO:O	1:A:384:PHE:CD1	2.69	0.46
1:A:408:ASN:O	1:A:409:ALA:C	2.58	0.46
1:A:495:ALA:HB3	1:A:498:ILE:HB	1.98	0.46
1:A:667:LYS:HG3	1:A:727:ASN:OD1	2.15	0.46
1:B:623:ALA:N	1:B:624:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:ASN:O	1:B:679:ALA:HB2	2.16	0.46
1:A:20:VAL:HG11	1:A:83:ASP:OD1	2.16	0.46
1:A:685:ILE:O	1:A:688:PRO:CG	2.62	0.46
1:B:95:LEU:HD12	1:B:158:MET:HB2	1.94	0.46
1:B:117:HIS:CE1	1:B:373:ILE:HG12	2.51	0.46
1:B:344:PRO:O	1:B:345:THR:C	2.58	0.46
1:B:381:PRO:O	1:B:384:PHE:CD1	2.68	0.46
1:A:51:LEU:HG	1:B:52:ALA:HB3	1.96	0.46
1:A:114:PHE:O	1:A:117:HIS:HB2	2.15	0.46
1:B:428:THR:C	1:B:655:LEU:HD11	2.38	0.46
1:A:141:SER:O	1:A:144:PHE:CD1	2.68	0.46
1:A:345:THR:O	1:A:348:LEU:N	2.43	0.46
1:A:712:ALA:O	1:A:716:VAL:CG2	2.64	0.46
1:B:108:ALA:O	1:B:109:GLY:C	2.58	0.46
1:B:173:SER:O	1:B:177:THR:OG1	2.29	0.46
1:B:244:ALA:O	1:B:247:ASP:HB2	2.16	0.46
1:B:373:ILE:C	1:B:375:VAL:H	2.23	0.46
1:A:150:ALA:C	1:A:151:LEU:O	2.57	0.46
1:B:156:LEU:CB	1:B:163:SER:HA	2.38	0.46
1:B:161:MET:O	1:B:162:TYR:CB	2.63	0.46
1:B:214:GLU:CG	1:B:215:ALA:H	2.29	0.46
1:A:108:ALA:HB1	1:A:111:LEU:HG	1.98	0.46
1:A:130:LEU:O	1:A:134:PRO:CD	2.42	0.46
1:A:159:ASP:O	1:A:160:VAL:C	2.59	0.46
1:A:344:PRO:O	1:A:345:THR:C	2.59	0.46
1:A:502:ASN:OD1	1:A:504:ARG:HB2	2.16	0.46
1:B:113:LEU:HD22	1:B:373:ILE:HA	1.97	0.46
1:B:685:ILE:O	1:B:688:PRO:CD	2.64	0.46
1:B:716:VAL:HG12	1:B:717:SER:N	2.31	0.46
1:A:77:LEU:HD12	1:A:273:SER:OG	2.16	0.45
1:A:92:VAL:HG11	1:A:217:LYS:CG	2.46	0.45
1:A:113:LEU:CD2	1:A:376:LEU:HD12	2.45	0.45
1:A:675:ASN:O	1:A:679:ALA:HB2	2.16	0.45
1:B:88:VAL:HG13	1:B:89:SER:N	2.31	0.45
1:B:91:GLU:HB3	1:B:92:VAL:CG2	2.39	0.45
1:B:572:THR:O	1:B:593:ALA:HA	2.16	0.45
1:B:619:GLY:HA2	1:B:626:LEU:HD11	1.97	0.45
1:A:71:LYS:CE	1:A:75:GLU:OE1	2.65	0.45
1:A:94:HIS:O	1:A:95:LEU:HD22	2.13	0.45
1:A:214:GLU:CG	1:A:215:ALA:H	2.29	0.45
1:B:101:LYS:HA	1:B:104:VAL:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASP:O	1:B:160:VAL:C	2.59	0.45
1:B:330:PRO:CG	1:B:417:LYS:HD2	2.46	0.45
1:B:372:LEU:C	1:B:372:LEU:HD23	2.42	0.45
1:A:20:VAL:CG1	1:A:83:ASP:OD1	2.64	0.45
1:A:244:ALA:O	1:A:247:ASP:HB2	2.16	0.45
1:A:327:SER:CB	1:A:328:LYS:HG3	2.40	0.45
1:A:341:TYR:O	1:A:344:PRO:CG	2.65	0.45
1:A:416:GLU:CD	1:A:737:ASP:HB2	2.42	0.45
1:B:83:ASP:CB	1:B:84:GLU:HB2	2.42	0.45
1:B:117:HIS:O	1:B:119:ILE:HB	2.15	0.45
1:B:150:ALA:O	1:B:153:ARG:HG2	2.09	0.45
1:B:357:TRP:NE1	1:B:361:ALA:O	2.44	0.45
1:A:113:LEU:HD21	1:A:376:LEU:CD1	2.45	0.45
1:A:115:LEU:HD21	1:A:170:PHE:CZ	2.52	0.45
1:A:141:SER:HB2	1:A:343:ILE:HG22	1.99	0.45
1:B:71:LYS:CE	1:B:75:GLU:OE1	2.65	0.45
1:A:26:THR:C	1:B:53:THR:CG2	2.89	0.45
1:A:216:ILE:O	1:A:218:LYS:N	2.50	0.45
1:A:572:THR:O	1:A:593:ALA:HA	2.16	0.45
1:B:203:THR:O	1:B:205:GLU:CA	2.61	0.45
1:B:357:TRP:CA	1:B:695:TYR:HA	2.46	0.45
1:B:395:GLY:O	1:B:396:MET:C	2.60	0.45
1:B:428:THR:CG2	1:B:655:LEU:HD21	2.41	0.45
1:B:502:ASN:OD1	1:B:504:ARG:HB2	2.16	0.45
1:B:550:LEU:O	1:B:554:ALA:CB	2.65	0.45
1:A:113:LEU:HD22	1:A:373:ILE:HA	1.99	0.45
1:B:692:GLY:O	1:B:693:LEU:C	2.60	0.45
1:A:88:VAL:HG13	1:A:89:SER:N	2.31	0.45
1:A:101:LYS:HA	1:A:104:VAL:CB	2.47	0.45
1:A:161:MET:O	1:A:162:TYR:CG	2.70	0.45
1:A:685:ILE:O	1:A:688:PRO:CD	2.64	0.45
1:B:123:TYR:CE2	1:B:124:GLU:HB3	2.50	0.45
1:A:118:PHE:O	1:A:119:ILE:O	2.34	0.45
1:B:22:VAL:HA	1:B:81:VAL:HA	1.98	0.45
1:B:32:LYS:HG3	1:B:461:GLU:HG3	1.99	0.45
1:B:364:PRO:HG3	1:B:367:PHE:HD1	1.80	0.45
1:B:695:TYR:HB2	1:B:696:PRO:CD	2.47	0.45
1:A:83:ASP:CB	1:A:84:GLU:HB2	2.44	0.45
1:A:119:ILE:HA	1:A:120:SER:HA	1.62	0.45
1:A:635:VAL:CG2	1:A:650:LEU:HD12	2.44	0.45
1:B:111:LEU:CD2	1:B:198:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:HD11	1:B:133:LEU:HD11	1.98	0.45
1:B:198:LEU:O	1:B:198:LEU:HD23	2.17	0.45
1:A:51:LEU:HD12	1:B:52:ALA:CB	2.43	0.45
1:A:131:ILE:O	1:A:132:ALA:C	2.59	0.45
1:A:156:LEU:O	1:A:157:ASN:C	2.59	0.45
1:A:189:GLU:CD	1:A:189:GLU:O	2.41	0.45
1:A:200:LEU:O	1:A:203:THR:HB	2.16	0.45
1:A:404:ILE:CD1	1:A:660:ALA:HB3	2.47	0.45
1:A:700:VAL:HG12	1:A:702:PHE:O	2.18	0.45
1:B:87:ALA:O	1:B:88:VAL:CG2	2.65	0.45
1:B:341:TYR:C	1:B:344:PRO:HD2	2.42	0.45
1:B:700:VAL:HG12	1:B:702:PHE:O	2.17	0.45
1:A:357:TRP:CG	1:A:358:TYR:HA	2.52	0.44
1:A:373:ILE:C	1:A:375:VAL:H	2.23	0.44
1:A:22:VAL:HA	1:A:81:VAL:HA	1.99	0.44
1:A:131:ILE:O	1:A:134:PRO:HD2	2.18	0.44
1:A:152:ARG:HB2	1:A:153:ARG:HA	1.99	0.44
1:A:206:ALA:O	1:A:207:ARG:C	2.60	0.44
1:A:341:TYR:C	1:A:344:PRO:HD2	2.43	0.44
1:A:411:ALA:O	1:A:413:GLU:N	2.50	0.44
1:A:550:LEU:O	1:A:554:ALA:CB	2.65	0.44
1:A:710:ALA:O	1:A:712:ALA:N	2.51	0.44
1:B:110:VAL:HB	1:B:114:PHE:HE2	1.82	0.44
1:B:194:LEU:HD21	1:B:377:VAL:HG21	1.99	0.44
1:B:216:ILE:O	1:B:218:LYS:N	2.50	0.44
1:B:376:LEU:HD22	1:B:380:CYS:SG	2.57	0.44
1:B:395:GLY:O	1:B:398:LYS:CB	2.65	0.44
1:A:108:ALA:O	1:A:109:GLY:C	2.60	0.44
1:A:194:LEU:HD21	1:A:377:VAL:HG21	1.99	0.44
1:A:376:LEU:HD22	1:A:380:CYS:SG	2.57	0.44
1:B:89:SER:OG	1:B:221:GLY:HA2	2.16	0.44
1:B:129:LEU:CD2	1:B:130:LEU:N	2.80	0.44
1:B:152:ARG:HB2	1:B:153:ARG:HA	1.98	0.44
1:B:360:ILE:O	1:B:360:ILE:HD13	2.17	0.44
1:B:417:LYS:HG2	1:B:737:ASP:O	2.17	0.44
1:B:697:ILE:O	1:B:697:ILE:HG22	2.17	0.44
1:A:190:THR:O	1:A:194:LEU:CD1	2.58	0.44
1:A:194:LEU:HD11	1:A:704:PRO:HB2	1.98	0.44
1:A:404:ILE:HD11	1:A:660:ALA:HB3	1.98	0.44
1:B:131:ILE:O	1:B:132:ALA:C	2.59	0.44
1:B:161:MET:O	1:B:162:TYR:CG	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HG3	1:A:461:GLU:HG3	1.99	0.44
1:A:126:PHE:CD1	1:A:129:LEU:CB	2.92	0.44
1:A:209:LYS:O	1:A:210:SER:C	2.59	0.44
1:A:355:ILE:HD13	1:A:355:ILE:HA	1.88	0.44
1:A:357:TRP:N	1:A:358:TYR:CB	2.80	0.44
1:A:692:GLY:O	1:A:693:LEU:C	2.60	0.44
1:B:115:LEU:HD11	1:B:170:PHE:CE1	2.52	0.44
1:B:150:ALA:HA	1:B:153:ARG:HD2	2.00	0.44
1:B:357:TRP:O	1:B:695:TYR:HD1	1.99	0.44
1:B:357:TRP:CG	1:B:358:TYR:HA	2.52	0.44
1:B:360:ILE:HG13	1:B:697:ILE:CG1	2.48	0.44
1:A:129:LEU:HD11	1:A:133:LEU:HD11	1.98	0.44
1:A:198:LEU:HD23	1:A:198:LEU:O	2.18	0.44
1:B:102:LEU:O	1:B:166:VAL:CG2	2.64	0.44
1:B:117:HIS:C	1:B:191:SER:CB	2.91	0.44
1:B:129:LEU:CD1	1:B:369:PHE:CA	2.96	0.44
1:B:357:TRP:N	1:B:358:TYR:CB	2.80	0.44
1:A:117:HIS:C	1:A:191:SER:CB	2.91	0.44
1:B:392:LEU:O	1:B:393:THR:C	2.60	0.44
1:A:150:ALA:HA	1:A:153:ARG:HD2	2.00	0.44
1:A:358:TYR:O	1:A:358:TYR:CD2	2.70	0.44
1:A:360:ILE:O	1:A:360:ILE:HD13	2.18	0.44
1:A:383:ALA:HB1	1:A:716:VAL:CG2	2.47	0.44
1:A:712:ALA:O	1:A:716:VAL:CB	2.66	0.44
1:B:90:ALA:HA	1:B:91:GLU:CB	2.14	0.44
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.84	0.44
1:A:91:GLU:CA	1:A:92:VAL:HG22	2.48	0.44
1:A:117:HIS:NE2	1:A:373:ILE:CG2	2.75	0.44
1:A:372:LEU:C	1:A:372:LEU:HD23	2.42	0.44
1:A:395:GLY:O	1:A:396:MET:C	2.60	0.44
1:A:399:GLY:N	1:A:664:LEU:HD22	2.33	0.44
1:A:441:PRO:HG2	1:A:444:GLY:HA2	2.00	0.44
1:B:27:CYS:CA	1:B:51:LEU:HD11	2.48	0.44
1:B:692:GLY:O	1:B:695:TYR:N	2.35	0.44
1:B:716:VAL:O	1:B:719:VAL:HB	2.17	0.44
1:A:129:LEU:HD13	1:A:369:PHE:CB	2.48	0.43
1:A:327:SER:OG	1:A:328:LYS:CB	2.66	0.43
1:A:330:PRO:HD2	1:A:414:VAL:HG22	2.00	0.43
1:A:352:SER:N	1:A:356:TYR:OH	2.49	0.43
1:A:364:PRO:HG3	1:A:367:PHE:HD1	1.80	0.43
1:A:588:LEU:HD12	1:A:588:LEU:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ALA:O	1:B:210:SER:CB	2.60	0.43
1:B:209:LYS:O	1:B:210:SER:C	2.59	0.43
1:B:358:TYR:O	1:B:358:TYR:CD2	2.70	0.43
1:B:441:PRO:HG2	1:B:444:GLY:HA2	2.00	0.43
1:B:521:LEU:HD12	1:B:521:LEU:HA	1.87	0.43
1:B:564:MET:HG2	1:B:732:ILE:CG2	2.47	0.43
1:A:126:PHE:H	1:A:127:VAL:CB	2.30	0.43
1:A:161:MET:O	1:A:162:TYR:CD1	2.72	0.43
1:A:203:THR:O	1:A:205:GLU:CA	2.62	0.43
1:A:395:GLY:O	1:A:398:LYS:CB	2.65	0.43
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.92	0.43
1:B:126:PHE:HD1	1:B:128:GLN:C	2.26	0.43
1:B:129:LEU:CD1	1:B:369:PHE:HA	2.49	0.43
1:B:330:PRO:HG3	1:B:417:LYS:HD2	2.00	0.43
1:B:406:ILE:HD12	1:B:412:LEU:CD2	2.48	0.43
1:B:555:LYS:N	1:B:556:PRO:HD2	2.33	0.43
1:A:126:PHE:HD1	1:A:128:GLN:C	2.26	0.43
1:A:129:LEU:CD1	1:A:369:PHE:HA	2.48	0.43
1:A:215:ALA:HB1	1:A:645:SER:CA	2.48	0.43
1:A:392:LEU:O	1:A:393:THR:C	2.60	0.43
1:A:406:ILE:HD12	1:A:412:LEU:CD2	2.49	0.43
1:A:434:PRO:CB	1:A:467:ALA:HB2	2.49	0.43
1:B:115:LEU:HD21	1:B:170:PHE:CZ	2.53	0.43
1:A:32:LYS:HG3	1:A:461:GLU:CG	2.48	0.43
1:A:83:ASP:OD2	1:A:84:GLU:HB2	2.19	0.43
1:A:102:LEU:O	1:A:166:VAL:CG2	2.64	0.43
1:A:160:VAL:CG2	1:A:162:TYR:HA	2.38	0.43
1:A:328:LYS:HE2	1:A:333:ARG:CG	2.48	0.43
1:A:353:ALA:HB1	1:A:357:TRP:CZ3	2.54	0.43
1:A:434:PRO:O	1:A:467:ALA:CB	2.66	0.43
1:A:441:PRO:HB2	1:A:444:GLY:H	1.83	0.43
1:A:564:MET:HG2	1:A:732:ILE:CG1	2.47	0.43
1:A:667:LYS:O	1:A:671:LYS:HE3	2.19	0.43
1:A:713:MET:O	1:A:714:SER:C	2.62	0.43
1:B:119:ILE:O	1:B:186:SER:O	2.22	0.43
1:B:131:ILE:O	1:B:134:PRO:HD2	2.18	0.43
1:B:194:LEU:CD1	1:B:704:PRO:HG2	2.48	0.43
1:B:457:GLU:O	1:B:458:ARG:C	2.61	0.43
1:A:86:ALA:HA	1:A:87:ALA:HA	1.73	0.43
1:A:101:LYS:CG	1:A:205:GLU:HB2	2.49	0.43
1:A:341:TYR:O	1:A:344:PRO:CD	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:O	1:A:375:VAL:HB	2.19	0.43
1:A:376:LEU:O	1:A:378:VAL:N	2.52	0.43
1:A:402:LEU:HD13	1:A:660:ALA:HB1	2.01	0.43
1:A:440:VAL:HB	1:A:543:ILE:CG1	2.49	0.43
1:B:161:MET:O	1:B:162:TYR:CD1	2.72	0.43
1:B:411:ALA:O	1:B:413:GLU:N	2.51	0.43
1:A:71:LYS:HE3	1:A:75:GLU:OE1	2.18	0.43
1:A:103:TYR:CD2	1:A:155:THR:HA	2.54	0.43
1:A:360:ILE:HG13	1:A:697:ILE:CG1	2.48	0.43
1:A:429:LEU:CA	1:A:655:LEU:HD11	2.43	0.43
1:A:707:ALA:O	1:A:710:ALA:HB3	2.19	0.43
1:B:101:LYS:CG	1:B:205:GLU:HB2	2.49	0.43
1:B:205:GLU:CG	1:B:206:ALA:N	2.79	0.43
1:B:280:VAL:CB	1:B:461:GLU:HB3	2.48	0.43
1:B:327:SER:CB	1:B:328:LYS:CA	2.92	0.43
1:B:707:ALA:O	1:B:710:ALA:HB3	2.19	0.43
1:A:121:LEU:CD1	1:A:178:ALA:HB2	2.49	0.43
1:B:118:PHE:O	1:B:119:ILE:O	2.35	0.43
1:B:200:LEU:O	1:B:203:THR:HB	2.19	0.43
1:B:441:PRO:HB2	1:B:444:GLY:H	1.83	0.43
1:B:710:ALA:O	1:B:712:ALA:N	2.51	0.43
1:B:713:MET:O	1:B:714:SER:C	2.62	0.43
1:A:194:LEU:CD1	1:A:704:PRO:HG2	2.49	0.43
1:A:376:LEU:O	1:A:380:CYS:N	2.38	0.43
1:A:423:PHE:HB3	1:A:428:THR:HG21	2.01	0.43
1:A:729:VAL:CB	1:A:730:PRO:HD3	2.49	0.43
1:B:292:GLY:O	1:B:293:ALA:CB	2.66	0.43
1:B:330:PRO:HD2	1:B:414:VAL:HG22	2.00	0.43
1:B:376:LEU:O	1:B:378:VAL:N	2.52	0.43
1:B:423:PHE:CD1	1:B:428:THR:CG2	2.93	0.43
1:A:133:LEU:HD13	1:A:372:LEU:CG	2.45	0.43
1:B:121:LEU:CD1	1:B:178:ALA:HB2	2.48	0.43
1:B:131:ILE:C	1:B:134:PRO:HD2	2.43	0.43
1:B:328:LYS:N	1:B:329:PRO:HD3	2.33	0.43
1:B:329:PRO:HB2	1:B:330:PRO:CD	2.45	0.43
1:B:429:LEU:C	1:B:550:LEU:HA	2.43	0.43
1:B:440:VAL:HB	1:B:543:ILE:CG1	2.48	0.43
1:A:91:GLU:CA	1:A:92:VAL:CB	2.92	0.43
1:A:202:ARG:O	1:A:205:GLU:HB3	2.19	0.43
1:A:280:VAL:CB	1:A:461:GLU:HB3	2.48	0.43
1:A:329:PRO:HD2	1:A:332:GLN:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LEU:O	1:A:389:PRO:CG	2.66	0.43
1:A:555:LYS:N	1:A:556:PRO:HD2	2.33	0.43
1:B:32:LYS:HG3	1:B:461:GLU:CG	2.48	0.43
1:B:51:LEU:HB3	1:B:51:LEU:H	1.83	0.43
1:B:71:LYS:HE3	1:B:75:GLU:OE1	2.18	0.43
1:B:189:GLU:CA	1:B:190:THR:CB	2.95	0.43
1:A:327:SER:CB	1:A:328:LYS:CA	2.92	0.42
1:A:655:LEU:HD23	1:A:655:LEU:HA	1.79	0.42
1:B:24:GLY:O	1:B:26:THR:HG23	2.18	0.42
1:B:327:SER:OG	1:B:328:LYS:CB	2.66	0.42
1:B:362:HIS:HA	1:B:363:ALA:HA	1.71	0.42
1:B:402:LEU:HD13	1:B:660:ALA:HB1	2.00	0.42
1:A:129:LEU:CD1	1:A:369:PHE:CA	2.96	0.42
1:A:131:ILE:C	1:A:134:PRO:HD2	2.44	0.42
1:A:175:LEU:O	1:A:179:GLY:HA3	2.19	0.42
1:A:362:HIS:HB3	1:A:363:ALA:CA	2.50	0.42
1:A:457:GLU:O	1:A:458:ARG:C	2.61	0.42
1:B:118:PHE:C	1:B:186:SER:O	2.62	0.42
1:B:126:PHE:H	1:B:127:VAL:CB	2.30	0.42
1:B:214:GLU:O	1:B:217:LYS:CB	2.67	0.42
1:B:372:LEU:O	1:B:375:VAL:HB	2.18	0.42
1:B:383:ALA:CB	1:B:711:MET:O	2.66	0.42
1:B:564:MET:HG2	1:B:732:ILE:CG1	2.46	0.42
1:A:25:MET:HG2	1:A:79:TYR:CE1	2.54	0.42
1:A:95:LEU:HD13	1:A:96:SER:CB	2.49	0.42
1:B:90:ALA:N	1:B:91:GLU:CB	2.79	0.42
1:B:101:LYS:O	1:B:103:TYR:N	2.52	0.42
1:B:362:HIS:HB3	1:B:363:ALA:CA	2.49	0.42
1:B:655:LEU:HA	1:B:655:LEU:HD23	1.79	0.42
1:A:91:GLU:HB3	1:A:92:VAL:CG2	2.38	0.42
1:A:207:ARG:O	1:A:210:SER:HB2	2.17	0.42
1:A:564:MET:HG2	1:A:732:ILE:CG2	2.47	0.42
1:A:636:GLY:CA	1:A:653:ASP:OD1	2.67	0.42
1:B:40:SER:HB3	1:B:298:THR:HG22	2.02	0.42
1:B:91:GLU:CA	1:B:92:VAL:HG22	2.48	0.42
1:B:175:LEU:O	1:B:179:GLY:HA3	2.18	0.42
1:B:328:LYS:HE2	1:B:333:ARG:CG	2.48	0.42
1:B:355:ILE:CA	1:B:356:TYR:CB	2.96	0.42
1:B:399:GLY:N	1:B:664:LEU:HD22	2.33	0.42
1:A:114:PHE:O	1:A:117:HIS:N	2.49	0.42
1:A:152:ARG:N	1:A:153:ARG:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:PHE:C	1:A:354:PHE:CD1	2.97	0.42
1:B:117:HIS:C	1:B:119:ILE:N	2.78	0.42
1:B:119:ILE:HA	1:B:120:SER:HA	1.61	0.42
1:B:189:GLU:CG	1:B:192:VAL:HB	2.41	0.42
1:B:202:ARG:O	1:B:205:GLU:HB3	2.19	0.42
1:B:341:TYR:O	1:B:344:PRO:CD	2.66	0.42
1:A:101:LYS:O	1:A:103:TYR:N	2.52	0.42
1:A:117:HIS:CE1	1:A:373:ILE:HG12	2.55	0.42
1:A:126:PHE:H	1:A:127:VAL:CG2	2.32	0.42
1:B:117:HIS:NE2	1:B:373:ILE:CG2	2.74	0.42
1:B:206:ALA:O	1:B:207:ARG:C	2.61	0.42
1:B:215:ALA:HB1	1:B:645:SER:CA	2.48	0.42
1:A:51:LEU:CA	1:B:52:ALA:CB	2.79	0.42
1:A:95:LEU:HD12	1:A:158:MET:CA	2.48	0.42
1:A:429:LEU:C	1:A:550:LEU:HA	2.45	0.42
1:B:113:LEU:CD2	1:B:376:LEU:HD12	2.44	0.42
1:B:126:PHE:H	1:B:127:VAL:CG2	2.32	0.42
1:B:129:LEU:HD13	1:B:369:PHE:CB	2.48	0.42
1:B:170:PHE:CE1	1:B:174:VAL:HG22	2.55	0.42
1:B:198:LEU:C	1:B:198:LEU:CD2	2.93	0.42
1:B:354:PHE:C	1:B:354:PHE:CD1	2.98	0.42
1:A:24:GLY:O	1:A:26:THR:HG23	2.19	0.42
1:A:115:LEU:HD13	1:A:174:VAL:N	2.35	0.42
1:A:129:LEU:CD1	1:A:133:LEU:HD21	2.50	0.42
1:A:194:LEU:HD11	1:A:705:GLU:N	2.35	0.42
1:A:215:ALA:HB1	1:A:645:SER:CB	2.50	0.42
1:B:329:PRO:HD2	1:B:332:GLN:CB	2.49	0.42
1:B:386:LEU:O	1:B:389:PRO:CG	2.66	0.42
1:B:434:PRO:HG2	1:B:463:PRO:O	2.20	0.42
1:A:100:ARG:O	1:A:101:LYS:HG2	2.20	0.42
1:A:126:PHE:CE1	1:A:128:GLN:O	2.73	0.42
1:A:129:LEU:CD2	1:A:130:LEU:N	2.80	0.42
1:A:214:GLU:O	1:A:217:LYS:CB	2.67	0.42
1:B:364:PRO:HG2	1:B:366:LEU:N	2.34	0.42
1:B:381:PRO:HA	1:B:384:PHE:CE1	2.54	0.42
1:A:364:PRO:HG2	1:A:366:LEU:N	2.35	0.42
1:A:367:PHE:CD2	1:A:694:LEU:HD23	2.55	0.42
1:A:405:LEU:HD12	1:A:651:ILE:HD11	2.02	0.42
1:B:353:ALA:HB1	1:B:357:TRP:CZ3	2.54	0.42
1:B:117:HIS:HB3	1:B:191:SER:CA	2.50	0.41
1:B:357:TRP:CB	1:B:694:LEU:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:THR:O	1:B:396:MET:HB2	2.19	0.41
1:B:667:LYS:O	1:B:671:LYS:HE3	2.19	0.41
1:B:95:LEU:HD13	1:B:96:SER:CB	2.50	0.41
1:B:103:TYR:CD2	1:B:155:THR:HA	2.54	0.41
1:B:194:LEU:HD11	1:B:704:PRO:CB	2.49	0.41
1:A:71:LYS:CE	1:A:75:GLU:CD	2.90	0.41
1:A:110:VAL:HB	1:A:114:PHE:HE2	1.84	0.41
1:A:156:LEU:HB3	1:A:163:SER:CA	2.40	0.41
1:A:208:ALA:O	1:A:210:SER:CB	2.61	0.41
1:A:393:THR:O	1:A:396:MET:HB2	2.19	0.41
1:B:100:ARG:O	1:B:101:LYS:HG2	2.20	0.41
1:B:341:TYR:O	1:B:344:PRO:CG	2.65	0.41
1:A:40:SER:HB3	1:A:298:THR:HG22	2.02	0.41
1:A:67:PHE:HZ	1:A:83:ASP:OD2	2.01	0.41
1:A:111:LEU:HB2	1:A:170:PHE:CD1	2.56	0.41
1:A:292:GLY:O	1:A:293:ALA:CB	2.66	0.41
1:A:329:PRO:HB2	1:A:330:PRO:CD	2.45	0.41
1:A:340:ALA:O	1:A:344:PRO:HD3	2.19	0.41
1:A:672:ILE:C	1:A:674:GLN:H	2.29	0.41
1:A:672:ILE:O	1:A:674:GLN:N	2.54	0.41
1:B:657:ASP:O	1:B:658:VAL:C	2.64	0.41
1:B:712:ALA:O	1:B:716:VAL:CB	2.68	0.41
1:A:71:LYS:O	1:A:74:ILE:N	2.54	0.41
1:A:189:GLU:CA	1:A:190:THR:CB	2.95	0.41
1:A:328:LYS:N	1:A:329:PRO:HD3	2.33	0.41
1:A:381:PRO:HA	1:A:384:PHE:CE1	2.56	0.41
1:A:434:PRO:CB	1:A:546:VAL:CG1	2.95	0.41
1:A:697:ILE:O	1:A:697:ILE:HG22	2.21	0.41
1:B:202:ARG:O	1:B:203:THR:O	2.38	0.41
1:B:405:LEU:HD12	1:B:651:ILE:HD11	2.02	0.41
1:A:26:THR:O	1:B:53:THR:HG21	2.18	0.41
1:A:151:LEU:HA	1:A:328:LYS:CD	2.51	0.41
1:A:202:ARG:O	1:A:203:THR:O	2.38	0.41
1:A:388:THR:N	1:A:389:PRO:CD	2.84	0.41
1:B:21:ARG:HB3	1:B:82:VAL:HG23	2.01	0.41
1:B:27:CYS:N	1:B:51:LEU:CD1	2.84	0.41
1:B:91:GLU:CA	1:B:92:VAL:CB	2.92	0.41
1:B:357:TRP:NE1	1:B:361:ALA:C	2.78	0.41
1:B:367:PHE:CD2	1:B:694:LEU:HD23	2.56	0.41
1:A:614:ALA:HA	1:A:631:LEU:O	2.20	0.41
1:B:20:VAL:HG12	1:B:82:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PHE:O	1:B:117:HIS:N	2.49	0.41
1:B:384:PHE:CD1	1:B:384:PHE:N	2.89	0.41
1:B:404:ILE:HG12	1:B:650:LEU:CD2	2.46	0.41
1:B:729:VAL:CB	1:B:730:PRO:HD3	2.49	0.41
1:A:170:PHE:CE1	1:A:174:VAL:HG22	2.55	0.41
1:B:23:THR:HG22	1:B:639:SER:HB2	2.03	0.41
1:B:376:LEU:O	1:B:380:CYS:N	2.38	0.41
1:B:434:PRO:HB2	1:B:546:VAL:HG13	2.02	0.41
1:B:663:GLN:O	1:B:664:LEU:C	2.63	0.41
1:A:52:ALA:O	1:B:51:LEU:C	2.63	0.41
1:A:117:HIS:HB3	1:A:191:SER:CA	2.50	0.41
1:A:189:GLU:CA	1:A:191:SER:H	2.22	0.41
1:A:695:TYR:C	1:A:697:ILE:N	2.79	0.41
1:B:111:LEU:HB2	1:B:170:PHE:CD1	2.56	0.41
1:A:71:LYS:HD3	1:A:85:GLN:H	1.82	0.41
1:A:357:TRP:NE1	1:A:361:ALA:C	2.78	0.41
1:A:396:MET:HE1	1:A:406:ILE:C	2.46	0.41
1:B:94:HIS:O	1:B:95:LEU:HD22	2.13	0.41
1:B:129:LEU:C	1:B:130:LEU:HD23	2.45	0.41
1:B:189:GLU:CG	1:B:192:VAL:CA	2.78	0.41
1:B:672:ILE:O	1:B:674:GLN:N	2.54	0.41
1:A:87:ALA:O	1:A:88:VAL:CB	2.69	0.40
1:A:153:ARG:HD2	1:A:155:THR:HG21	2.03	0.40
1:A:428:THR:O	1:A:655:LEU:HD21	2.21	0.40
1:B:71:LYS:O	1:B:74:ILE:N	2.54	0.40
1:B:126:PHE:HD1	1:B:128:GLN:O	1.98	0.40
1:B:215:ALA:HB1	1:B:645:SER:CB	2.50	0.40
1:B:425:LYS:C	1:B:427:GLY:N	2.78	0.40
1:B:614:ALA:HA	1:B:631:LEU:O	2.20	0.40
1:A:118:PHE:C	1:A:186:SER:O	2.64	0.40
1:A:149:SER:C	1:A:153:ARG:HB3	2.44	0.40
1:A:190:THR:HB	1:A:191:SER:H	1.78	0.40
1:A:279:PRO:CB	1:A:461:GLU:OE2	2.69	0.40
1:A:408:ASN:O	1:A:411:ALA:N	2.44	0.40
1:B:27:CYS:HA	1:B:51:LEU:HD11	2.03	0.40
1:B:189:GLU:OE2	1:B:193:LEU:CB	2.62	0.40
1:B:381:PRO:O	1:B:384:PHE:HB2	2.21	0.40
1:B:396:MET:HE1	1:B:406:ILE:C	2.46	0.40
1:B:695:TYR:C	1:B:697:ILE:N	2.79	0.40
1:B:708:GLY:C	1:B:710:ALA:N	2.78	0.40
1:A:102:LEU:O	1:A:166:VAL:CG1	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:N	1:A:102:LEU:CD2	2.80	0.40
1:A:121:LEU:O	1:A:184:GLU:CB	2.69	0.40
1:A:387:ALA:HB1	1:A:719:VAL:CG1	2.52	0.40
1:A:685:ILE:O	1:A:688:PRO:HD2	2.22	0.40
1:A:688:PRO:C	1:A:691:ALA:H	2.29	0.40
1:A:692:GLY:O	1:A:695:TYR:N	2.35	0.40
1:B:86:ALA:HA	1:B:87:ALA:HA	1.73	0.40
1:B:95:LEU:HD12	1:B:96:SER:O	2.20	0.40
1:B:103:TYR:CD2	1:B:166:VAL:CG2	3.02	0.40
1:B:115:LEU:HD13	1:B:174:VAL:N	2.36	0.40
1:B:387:ALA:HB1	1:B:719:VAL:CG1	2.52	0.40
1:B:672:ILE:C	1:B:674:GLN:H	2.29	0.40
1:A:113:LEU:CD1	1:A:376:LEU:CB	2.90	0.40
1:A:356:TYR:N	1:A:358:TYR:CB	2.78	0.40
1:A:384:PHE:CD1	1:A:384:PHE:N	2.89	0.40
1:A:663:GLN:O	1:A:664:LEU:C	2.64	0.40
1:B:373:ILE:O	1:B:377:VAL:CG2	2.68	0.40
1:B:376:LEU:C	1:B:378:VAL:H	2.27	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	721/723 (100%)	576 (80%)	81 (11%)	64 (9%)	0	8
1	B	721/723 (100%)	576 (80%)	80 (11%)	65 (9%)	0	8
All	All	1442/1446 (100%)	1152 (80%)	161 (11%)	129 (9%)	1	8

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	86	ALA
1	A	88	VAL
1	A	102	LEU
1	A	119	ILE
1	A	130	LEU
1	A	148	PHE
1	A	149	SER
1	A	150	ALA
1	A	151	LEU
1	A	152	ARG
1	A	158	MET
1	A	160	VAL
1	A	162	TYR
1	A	184	GLU
1	A	187	PHE
1	A	203	THR
1	A	204	LEU
1	A	210	SER
1	A	216	ILE
1	A	324	ALA
1	A	327	SER
1	A	328	LYS
1	A	550	LEU
1	A	551	LYS
1	A	729	VAL
1	B	84	GLU
1	B	86	ALA
1	B	88	VAL
1	B	102	LEU
1	B	119	ILE
1	B	130	LEU
1	B	148	PHE
1	B	149	SER
1	B	150	ALA
1	B	151	LEU
1	B	152	ARG
1	B	158	MET
1	B	160	VAL
1	B	162	TYR
1	B	184	GLU
1	B	187	PHE
1	B	203	THR

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Mol	Chain	Res	Type
1	B	204	LEU
1	B	210	SER
1	B	216	ILE
1	B	324	ALA
1	B	327	SER
1	B	328	LYS
1	B	550	LEU
1	B	551	LYS
1	B	729	VAL
1	A	79	TYR
1	A	92	VAL
1	A	99	LYS
1	A	103	TYR
1	A	108	ALA
1	A	126	PHE
1	A	131	ILE
1	A	157	ASN
1	A	189	GLU
1	A	192	VAL
1	A	202	ARG
1	A	214	GLU
1	A	215	ALA
1	A	359	PHE
1	A	360	ILE
1	A	362	HIS
1	A	549	THR
1	A	693	LEU
1	A	697	ILE
1	B	79	TYR
1	B	92	VAL
1	B	99	LYS
1	B	103	TYR
1	B	108	ALA
1	B	126	PHE
1	B	131	ILE
1	B	157	ASN
1	B	189	GLU
1	B	192	VAL
1	B	202	ARG
1	B	214	GLU
1	B	215	ALA
1	B	359	PHE

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Mol	Chain	Res	Type
1	B	360	ILE
1	B	362	HIS
1	B	549	THR
1	B	693	LEU
1	B	697	ILE
1	A	107	PHE
1	A	121	LEU
1	A	127	VAL
1	A	155	THR
1	A	156	LEU
1	A	159	ASP
1	A	188	TYR
1	A	191	SER
1	A	212	THR
1	A	322	GLU
1	A	325	MET
1	A	368	ALA
1	B	121	LEU
1	B	127	VAL
1	B	155	THR
1	B	156	LEU
1	B	159	ASP
1	B	188	TYR
1	B	191	SER
1	B	212	THR
1	B	322	GLU
1	B	325	MET
1	B	368	ALA
1	A	90	ALA
1	A	118	PHE
1	A	161	MET
1	A	383	ALA
1	B	90	ALA
1	B	107	PHE
1	B	118	PHE
1	B	161	MET
1	B	383	ALA
1	A	94	HIS
1	B	94	HIS
1	A	165	GLY
1	B	165	GLY
1	B	344	PRO

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Mol	Chain	Res	Type
1	A	182	PRO
1	B	182	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	581/581 (100%)	507 (87%)	74 (13%)	4	16
1	B	581/581 (100%)	507 (87%)	74 (13%)	4	16
All	All	1162/1162 (100%)	1014 (87%)	148 (13%)	6	16

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	83	ASP
1	A	84	GLU
1	A	88	VAL
1	A	92	VAL
1	A	93	GLU
1	A	94	HIS
1	A	95	LEU
1	A	102	LEU
1	A	110	VAL
1	A	117	HIS
1	A	119	ILE
1	A	121	LEU
1	A	124	GLU
1	A	129	LEU
1	A	144	PHE
1	A	148	PHE
1	A	152	ARG
1	A	153	ARG
1	A	158	MET
1	A	162	TYR

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Mol	Chain	Res	Type
1	A	181	LEU
1	A	183	ARG
1	A	186	SER
1	A	187	PHE
1	A	189	GLU
1	A	190	THR
1	A	194	LEU
1	A	195	LEU
1	A	198	LEU
1	A	200	LEU
1	A	205	GLU
1	A	210	SER
1	A	214	GLU
1	A	216	ILE
1	A	218	LYS
1	A	278	GLU
1	A	320	LEU
1	A	328	LYS
1	A	331	ILE
1	A	336	ASP
1	A	354	PHE
1	A	357	TRP
1	A	358	TYR
1	A	360	ILE
1	A	366	LEU
1	A	367	PHE
1	A	372	LEU
1	A	373	ILE
1	A	377	VAL
1	A	378	VAL
1	A	386	LEU
1	A	392	LEU
1	A	428	THR
1	A	433	LYS
1	A	450	LEU
1	A	499	LEU
1	A	521	LEU
1	A	547	SER
1	A	549	THR
1	A	550	LEU
1	A	561	LEU
1	A	588	LEU

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Mol	Chain	Res	Type
1	A	669	MET
1	A	675	ASN
1	A	681	ILE
1	A	682	TYR
1	A	697	ILE
1	A	700	VAL
1	A	701	VAL
1	A	703	ARG
1	A	705	GLU
1	A	716	VAL
1	A	719	VAL
1	B	50	ASN
1	B	83	ASP
1	B	84	GLU
1	B	88	VAL
1	B	92	VAL
1	B	93	GLU
1	B	94	HIS
1	B	95	LEU
1	B	102	LEU
1	B	110	VAL
1	B	117	HIS
1	B	119	ILE
1	B	121	LEU
1	B	124	GLU
1	B	129	LEU
1	B	144	PHE
1	B	148	PHE
1	B	152	ARG
1	B	153	ARG
1	B	158	MET
1	B	162	TYR
1	B	181	LEU
1	B	183	ARG
1	B	186	SER
1	B	187	PHE
1	B	189	GLU
1	B	190	THR
1	B	194	LEU
1	B	195	LEU
1	B	198	LEU
1	B	200	LEU

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Mol	Chain	Res	Type
1	B	205	GLU
1	B	210	SER
1	B	214	GLU
1	B	216	ILE
1	B	218	LYS
1	B	278	GLU
1	B	320	LEU
1	B	328	LYS
1	B	331	ILE
1	B	336	ASP
1	B	354	PHE
1	B	357	TRP
1	B	358	TYR
1	B	360	ILE
1	B	366	LEU
1	B	367	PHE
1	B	372	LEU
1	B	373	ILE
1	B	377	VAL
1	B	378	VAL
1	B	386	LEU
1	B	392	LEU
1	B	428	THR
1	B	433	LYS
1	B	450	LEU
1	B	499	LEU
1	B	521	LEU
1	B	547	SER
1	B	549	THR
1	B	550	LEU
1	B	561	LEU
1	B	588	LEU
1	B	669	MET
1	B	675	ASN
1	B	681	ILE
1	B	682	TYR
1	B	697	ILE
1	B	700	VAL
1	B	701	VAL
1	B	703	ARG
1	B	705	GLU
1	B	716	VAL

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Mol	Chain	Res	Type
1	B	719	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	587	ASN
1	A	721	ASN
1	B	587	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

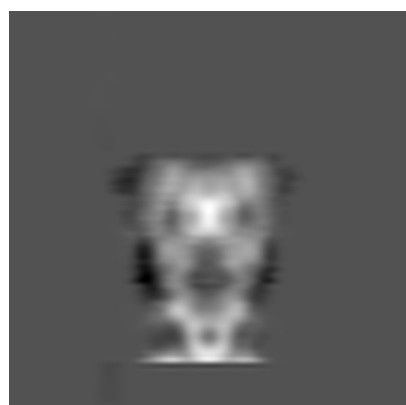
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5004. These allow visual inspection of the internal detail of the map and identification of artifacts.

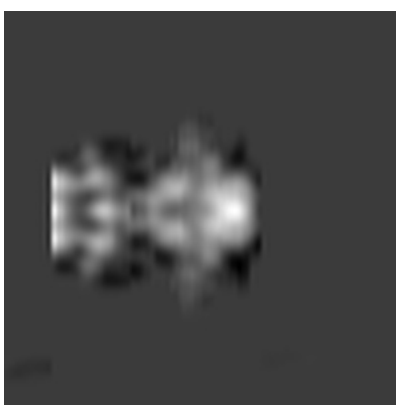
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

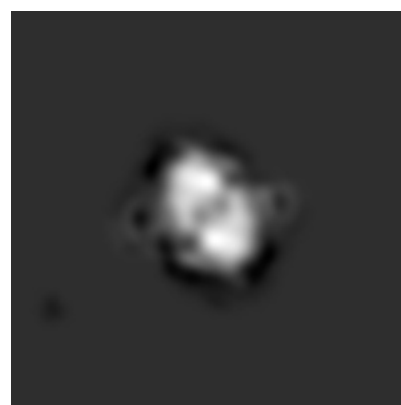
6.1.1 Primary map



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: 50



Y Index: 50



Z Index: 50

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: 50



Y Index: 47



Z Index: 57

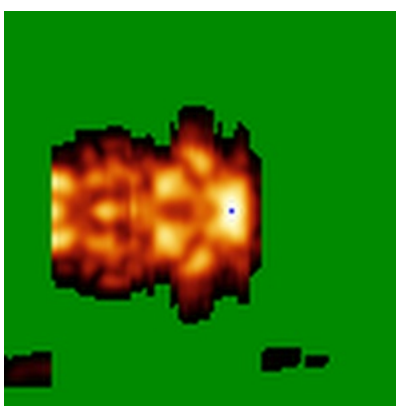
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

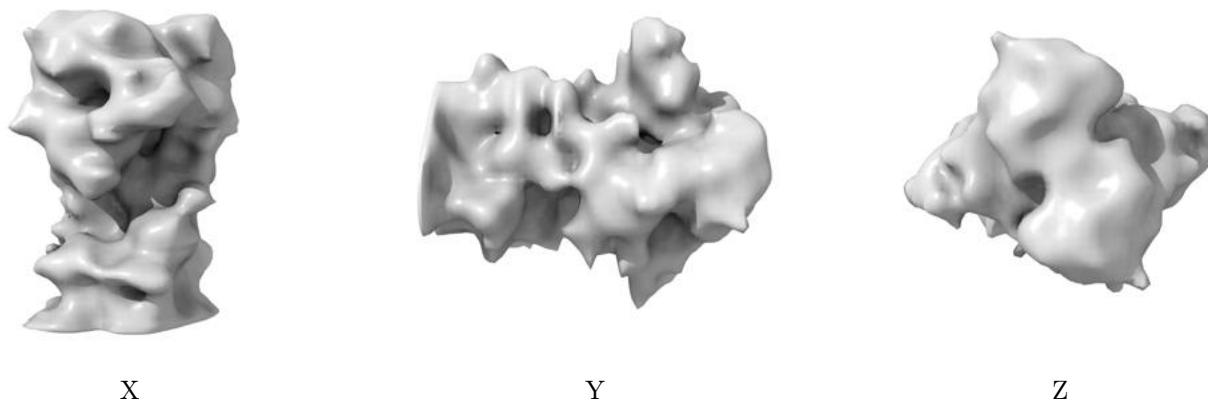


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

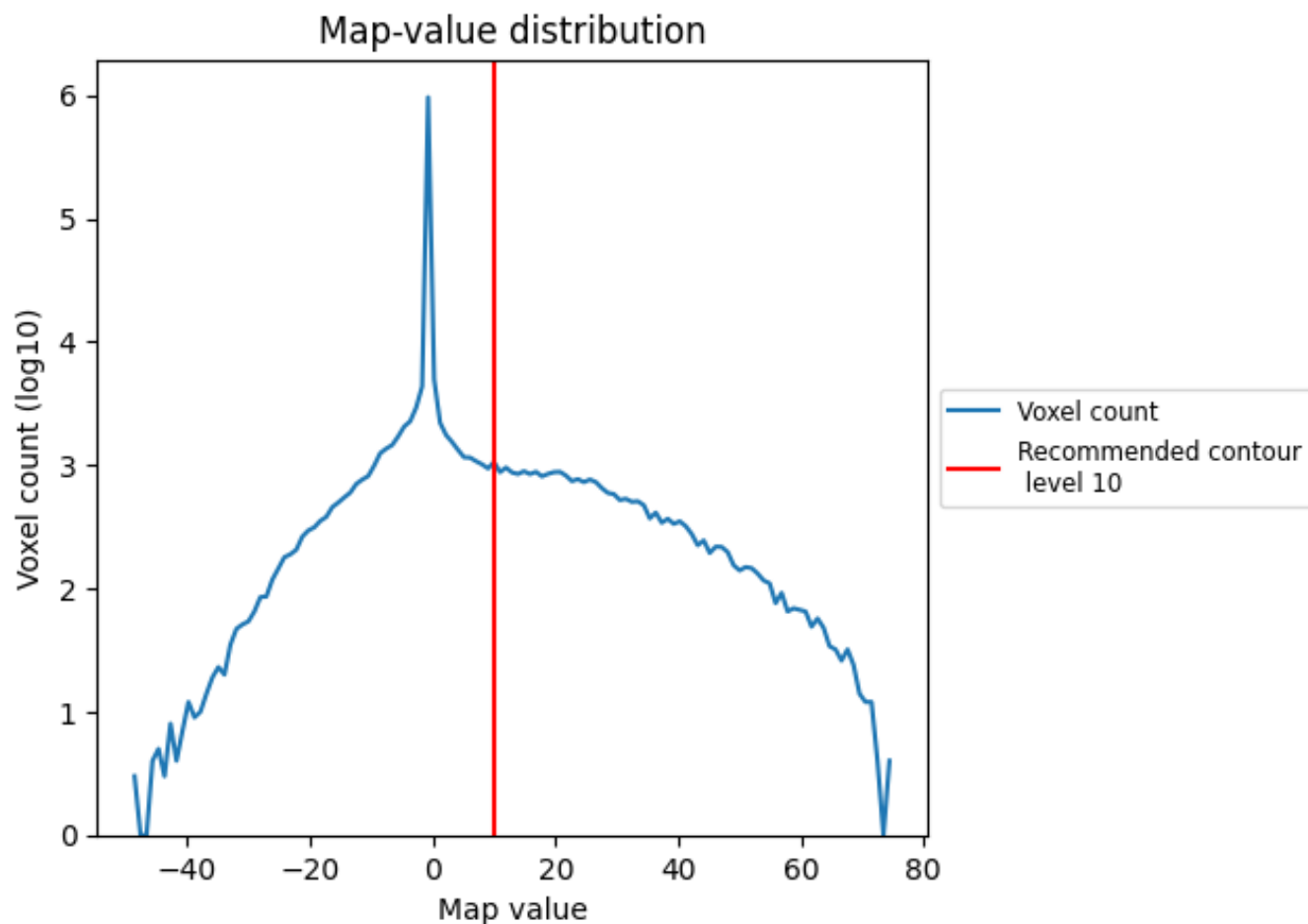
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

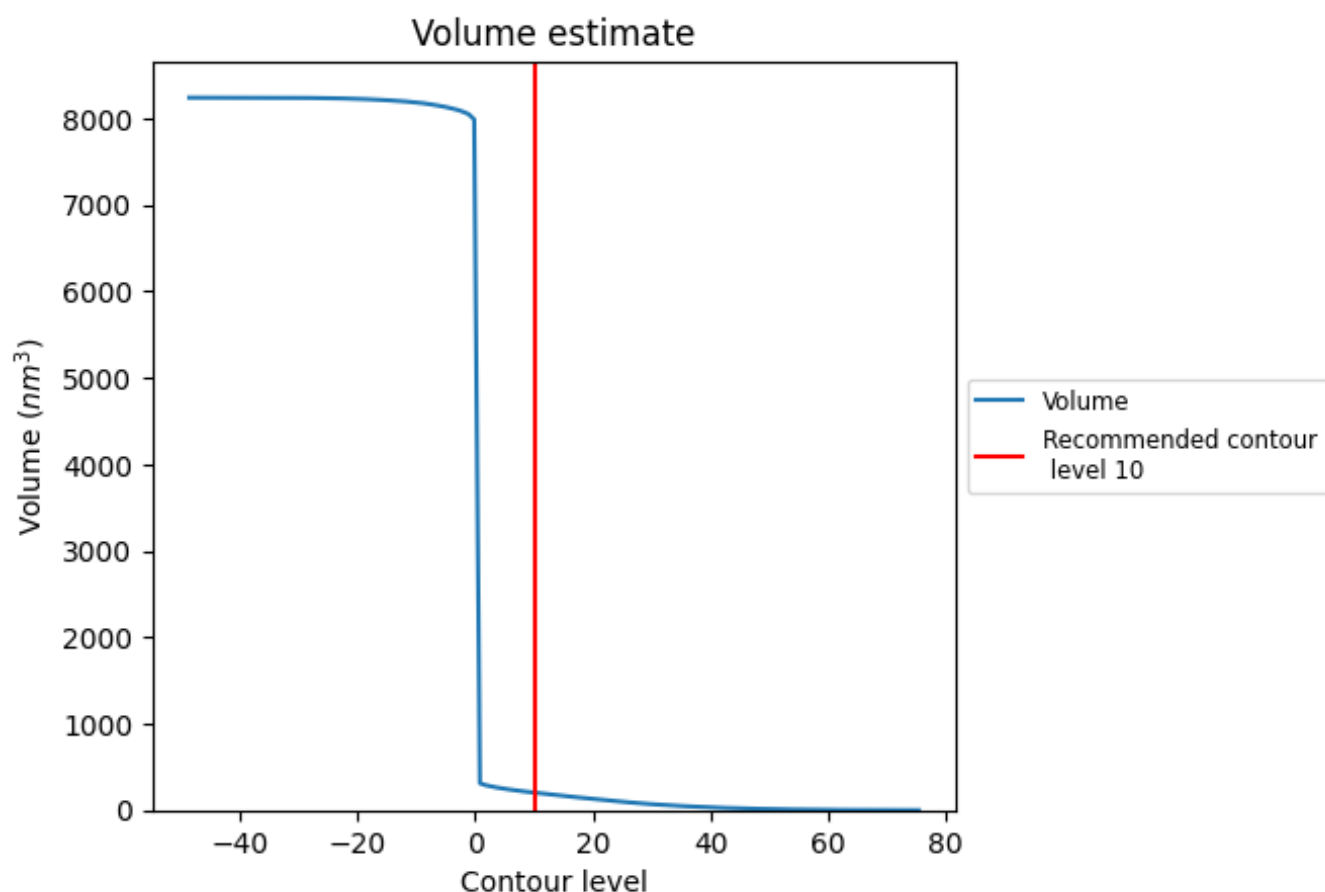
This section contains the results of statistical analysis of the map.

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.

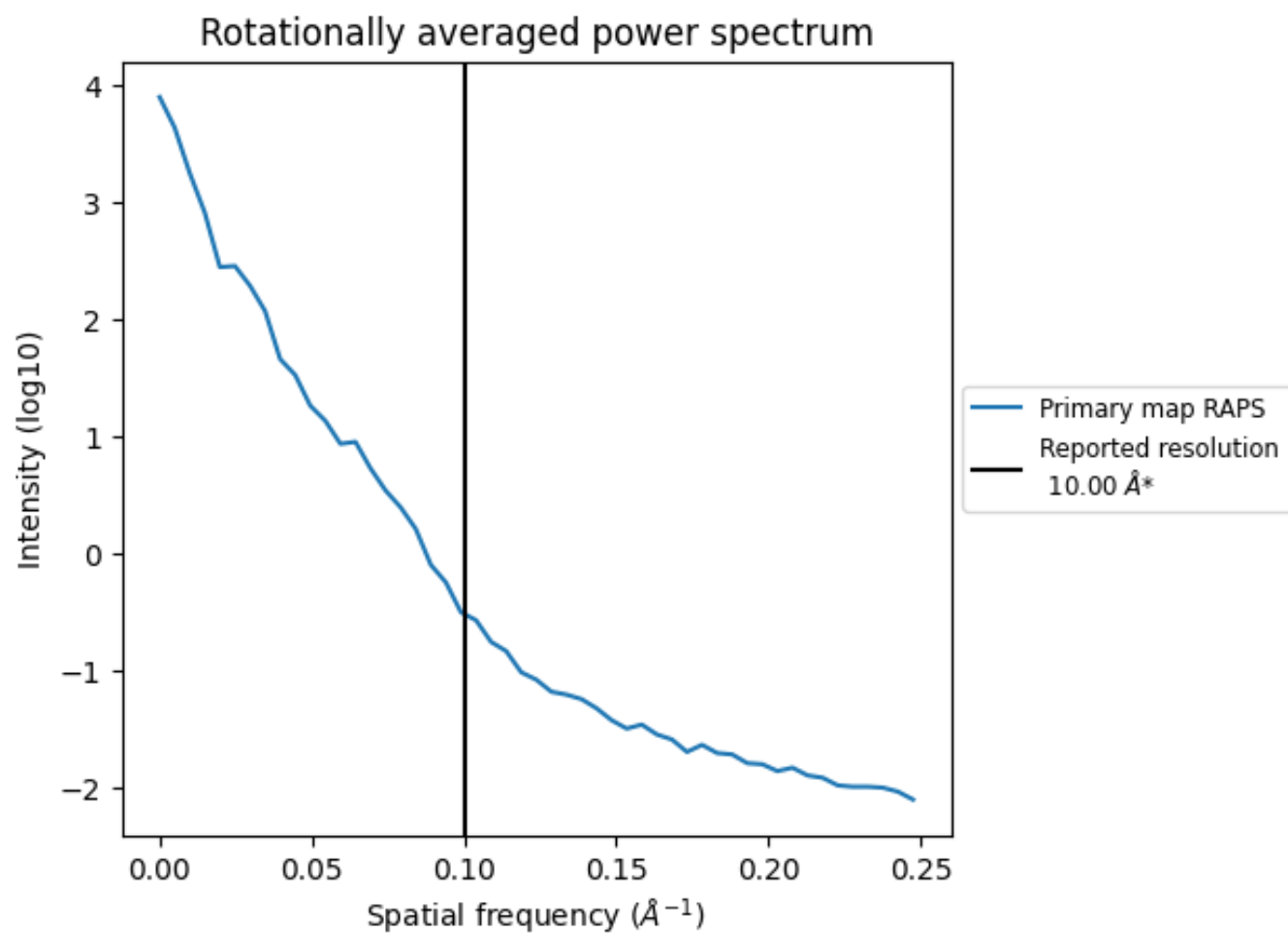
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

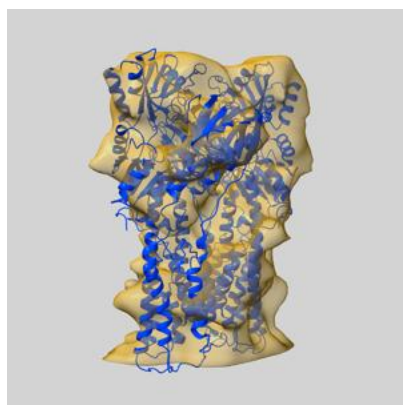
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

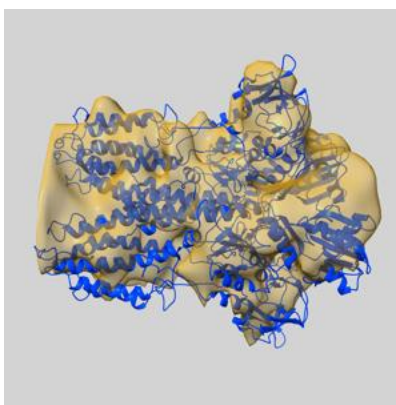
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5004 and PDB model 3J09. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

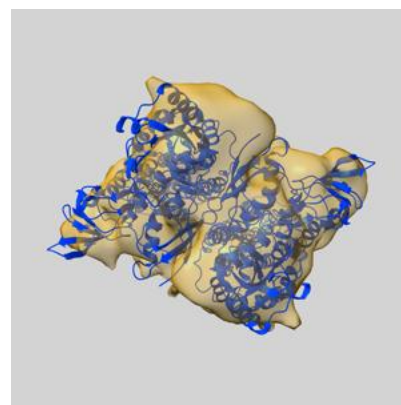
9.1 Map-model overlay [i](#)



X



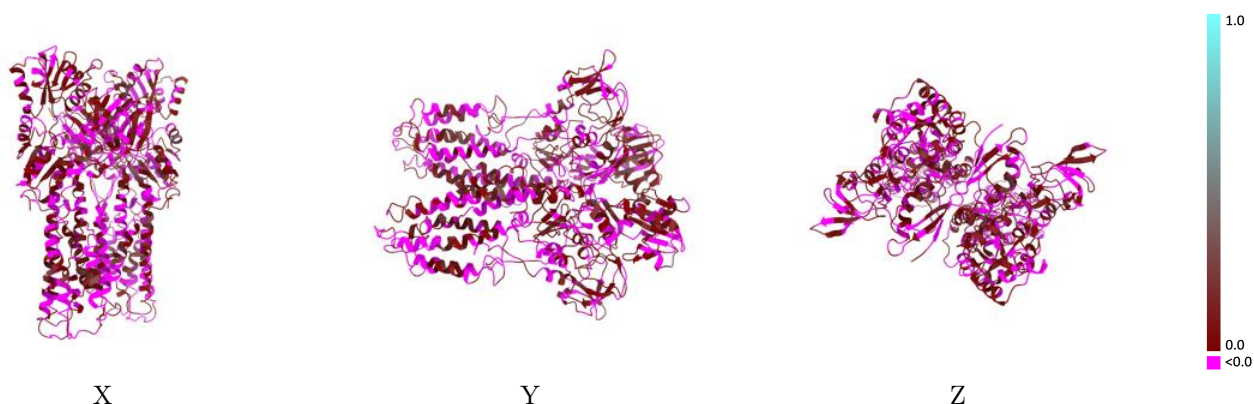
Y



Z

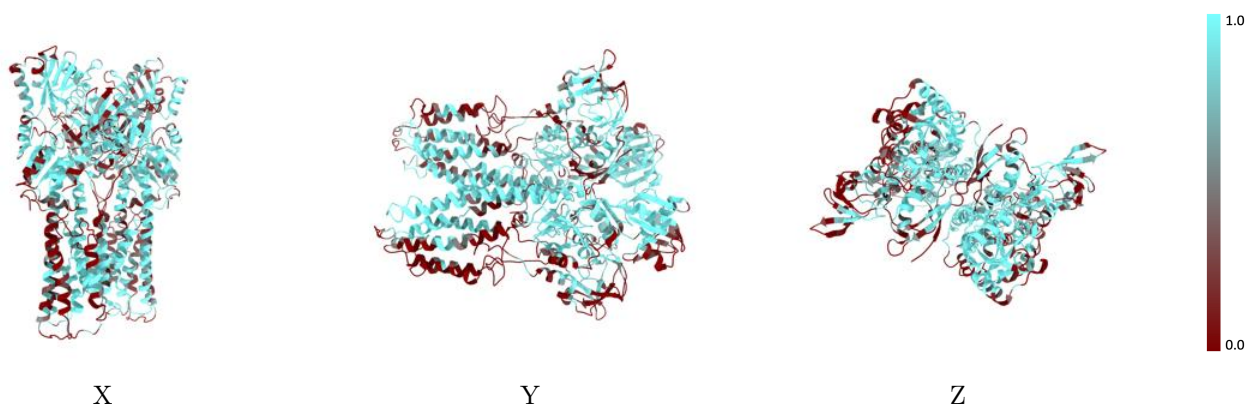
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



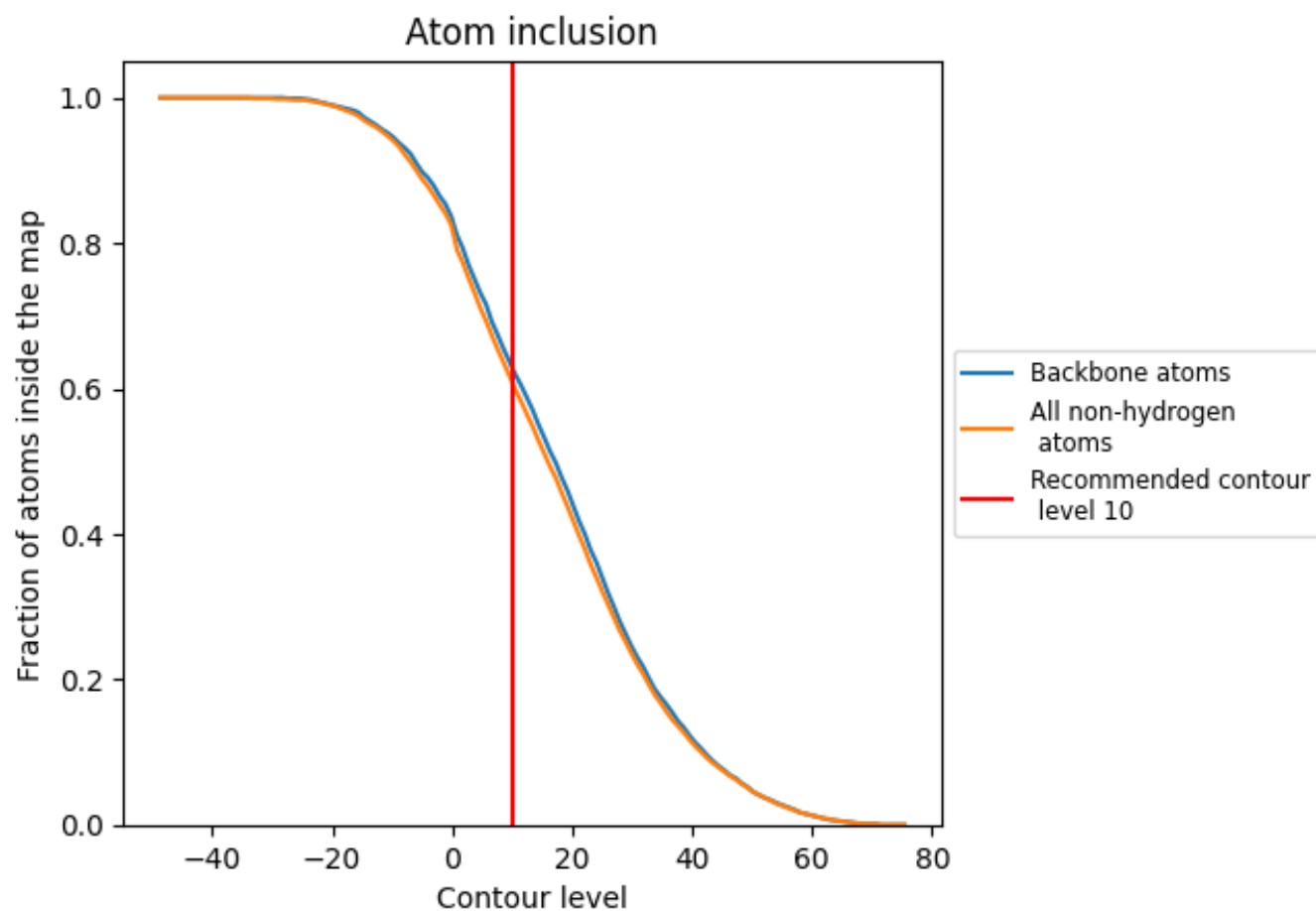
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (10).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6090	0.0150
A	0.5890	0.0150
B	0.6290	0.0150

