



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:01 am BST

PDB ID : 5UJ8
Title : Human Origin Recognition Complex subunits 2 and 3
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Deposited on : 2017-01-17
Resolution : 6.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

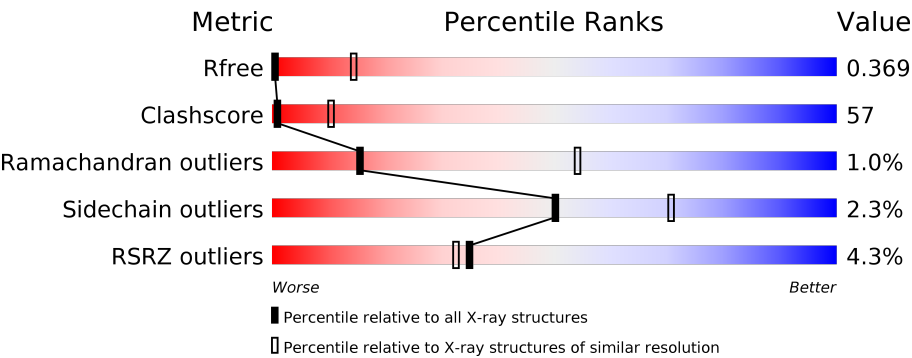
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)
RSRZ outliers	127900	1015 (8.20-3.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	712	<div><div>3%</div><div>24%</div><div>50%</div><div>22%</div></div>
1	B	712	<div><div>3%</div><div>25%</div><div>50%</div><div>22%</div></div>
1	C	712	<div><div>5%</div><div>23%</div><div>52%</div><div>22%</div></div>
1	D	712	<div><div>4%</div><div>26%</div><div>48%</div><div>22%</div></div>
2	E	347	<div><div>%</div><div>22%</div><div>29%</div><div>47%</div></div>
2	F	347	<div><div>2%</div><div>22%</div><div>29%</div><div>47%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	347	<div><div><div></div><div></div><div></div><div></div></div><div>3%22%29%47%</div></div>
2	H	347	<div><div><div></div><div></div><div></div><div></div></div><div>%21%31%47%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24144 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4524	2920	767	812	25			
1	B	553	Total	C	N	O	S	0	0	0
			4524	2920	767	812	25			
1	C	553	Total	C	N	O	S	0	0	0
			4524	2920	767	812	25			
1	D	553	Total	C	N	O	S	0	0	0
			4524	2920	767	812	25			

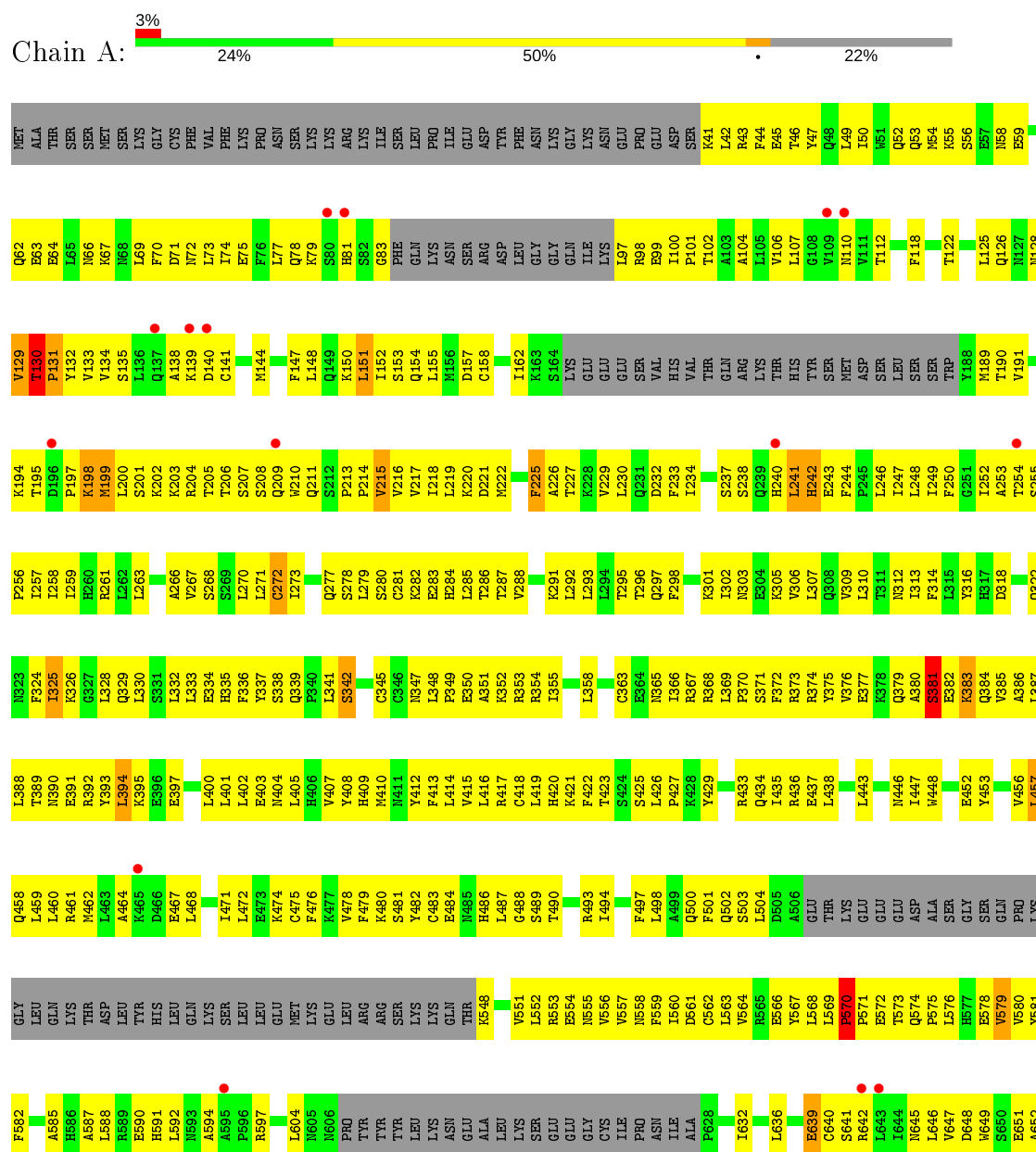
- Molecule 2 is a protein called Origin recognition complex subunit 2.

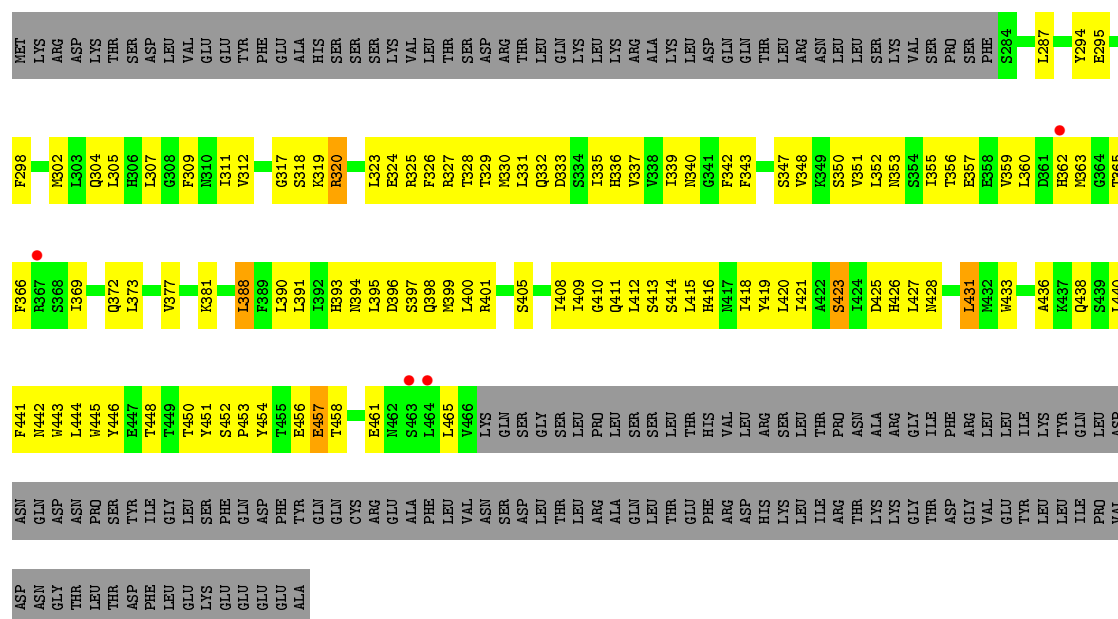
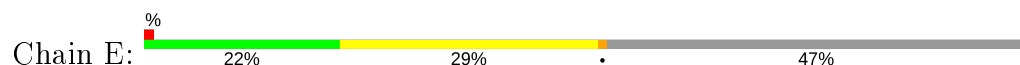
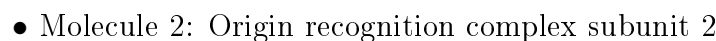
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	183	Total	C	N	O	S	0	0	0
			1512	978	249	280	5			
2	F	183	Total	C	N	O	S	0	0	0
			1512	978	249	280	5			
2	G	183	Total	C	N	O	S	0	0	0
			1512	978	249	280	5			
2	H	183	Total	C	N	O	S	0	0	0
			1512	978	249	280	5			

3 Residue-property plots [i](#)

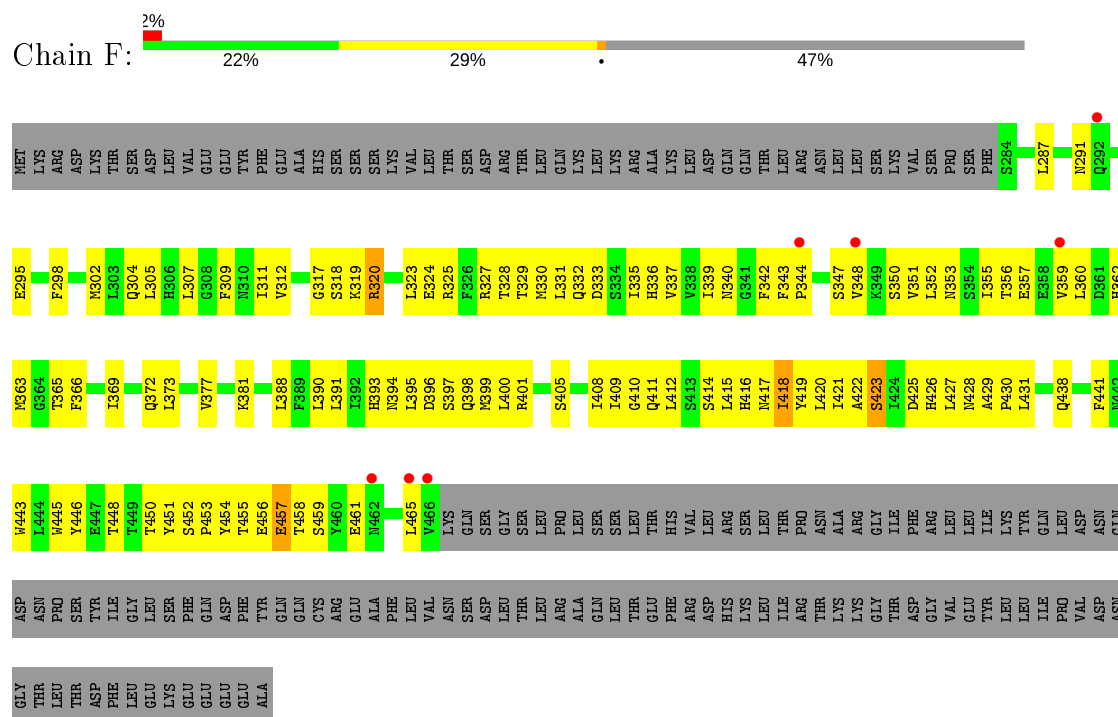
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Origin recognition complex subunit 3

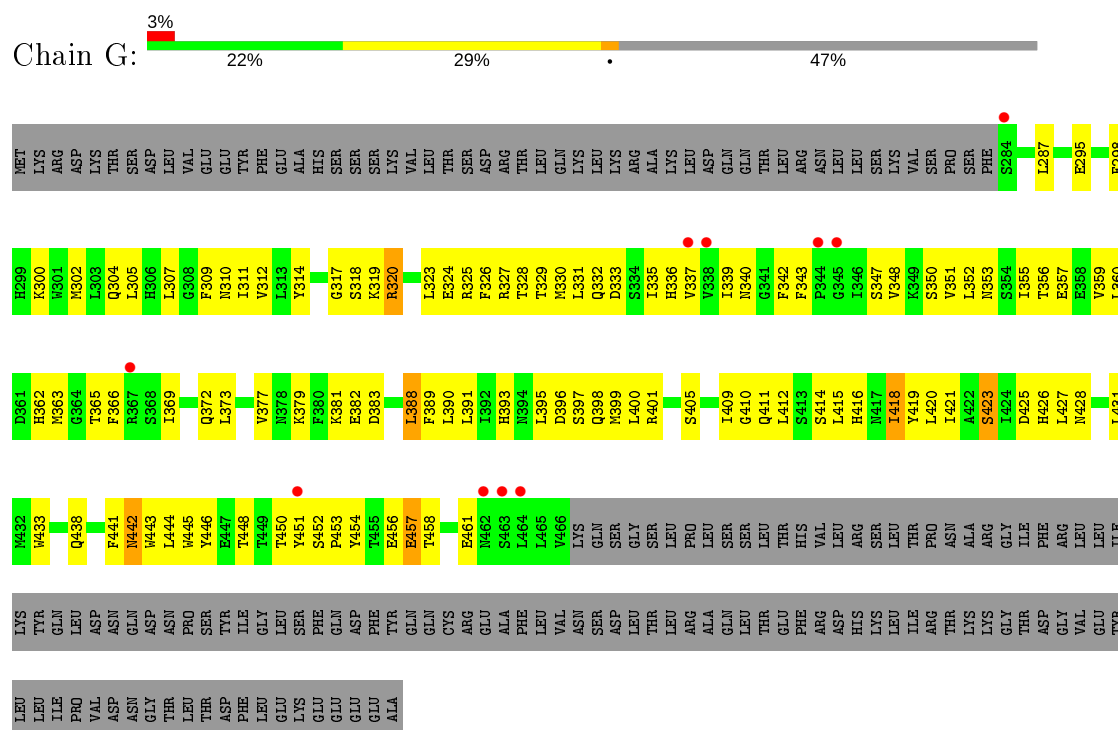




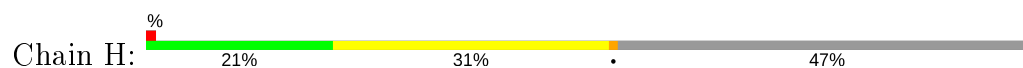
- Molecule 2: Origin recognition complex subunit 2



- Molecule 2: Origin recognition complex subunit 2



- Molecule 2: Origin recognition complex subunit 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.26Å 114.96Å 316.45Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	20.07 – 6.00 20.07 – 6.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (20.07-6.00) 94.2 (20.07-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 5.93Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.318 , 0.368 0.336 , 0.369	Depositor DCC
R_{free} test set	753 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	287.3	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 190.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.155 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	24144	wwPDB-VP
Average B, all atoms (Å ²)	303.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9421e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	0/4616	0.70	5/6244 (0.1%)
1	B	0.45	0/4616	0.69	4/6244 (0.1%)
1	C	1.12	9/4616 (0.2%)	0.75	7/6244 (0.1%)
1	D	0.48	0/4616	0.71	5/6244 (0.1%)
2	E	0.42	0/1548	0.70	2/2097 (0.1%)
2	F	0.39	0/1548	0.68	1/2097 (0.0%)
2	G	0.40	0/1548	0.69	2/2097 (0.1%)
2	H	0.41	0/1548	0.69	1/2097 (0.0%)
All	All	0.63	9/24656 (0.0%)	0.71	27/33364 (0.1%)

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	5
1	B	0	5
1	C	0	3
1	D	0	3
All	All	0	16

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	MET	CG-SD	38.31	2.80	1.81
1	C	244	PHE	CE1-CZ	28.73	1.92	1.37
1	C	244	PHE	CE2-CZ	27.23	1.89	1.37
1	C	244	PHE	CD2-CE2	25.67	1.90	1.39
1	C	244	PHE	CD1-CE1	23.71	1.86	1.39
1	C	244	PHE	CG-CD2	15.73	1.62	1.38
1	C	244	PHE	CG-CD1	14.13	1.59	1.38
1	C	199	MET	CB-CG	5.42	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	448	TRP	CB-CG	-5.25	1.40	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	MET	CG-SD-CE	16.48	126.57	100.20
1	C	151	LEU	CA-CB-CG	10.74	140.00	115.30
1	D	151	LEU	CA-CB-CG	10.43	139.29	115.30
1	B	151	LEU	CA-CB-CG	10.19	138.75	115.30
2	H	320	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	A	151	LEU	CA-CB-CG	10.17	138.70	115.30
2	F	320	ARG	NE-CZ-NH2	-10.04	115.28	120.30
2	E	320	ARG	NE-CZ-NH2	-10.00	115.30	120.30
2	G	320	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	C	199	MET	CB-CG-SD	6.70	132.51	112.40
1	C	198	LYS	CD-CE-NZ	6.60	126.89	111.70
1	A	241	LEU	CB-CG-CD1	-6.50	99.94	111.00
1	C	241	LEU	CB-CG-CD1	-6.44	100.05	111.00
1	B	241	LEU	CB-CG-CD1	-6.38	100.16	111.00
1	C	151	LEU	CB-CG-CD1	6.15	121.45	111.00
1	C	244	PHE	CB-CG-CD1	-6.02	116.59	120.80
1	D	241	LEU	CB-CG-CD1	-5.92	100.93	111.00
2	G	320	ARG	CG-CD-NE	-5.85	99.52	111.80
1	A	151	LEU	CB-CG-CD1	5.64	120.58	111.00
1	D	151	LEU	CB-CG-CD1	5.50	120.36	111.00
1	B	198	LYS	CD-CE-NZ	5.46	124.26	111.70
1	A	198	LYS	CD-CE-NZ	5.45	124.24	111.70
1	B	151	LEU	CB-CG-CD1	5.45	120.26	111.00
1	D	688	LEU	CB-CG-CD1	5.44	120.25	111.00
2	E	431	LEU	CA-CB-CG	5.41	127.74	115.30
1	D	198	LYS	CD-CE-NZ	5.34	123.98	111.70
1	A	215	VAL	CA-CB-CG2	-5.25	103.03	110.90

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	THR	Peptide
1	A	140	ASP	Peptide
1	A	240	HIS	Peptide
1	A	242	HIS	Peptide
1	A	639	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	140	ASP	Peptide
1	B	189	MET	Peptide
1	B	240	HIS	Peptide
1	B	242	HIS	Peptide
1	B	639	GLU	Peptide
1	C	140	ASP	Peptide
1	C	242	HIS	Peptide
1	C	639	GLU	Peptide
1	D	140	ASP	Peptide
1	D	242	HIS	Peptide
1	D	639	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4524	0	4619	564	0
1	B	4524	0	4619	544	0
1	C	4524	0	4619	578	0
1	D	4524	0	4619	547	0
2	E	1512	0	1495	153	0
2	F	1512	0	1495	150	0
2	G	1512	0	1495	157	0
2	H	1512	0	1495	163	0
All	All	24144	0	24456	2749	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 57.

All (2749) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:PHE:CD1	1:C:244:PHE:CE1	1.86	1.61
1:C:244:PHE:CE2	1:C:244:PHE:CD2	1.90	1.59
1:C:244:PHE:CZ	1:C:244:PHE:CE1	1.91	1.57
1:C:244:PHE:CD2	1:C:246:LEU:HG	1.41	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LYS:NZ	1:C:244:PHE:CE1	1.73	1.40
1:C:244:PHE:CD2	1:C:246:LEU:CG	2.12	1.30
1:C:202:LYS:NZ	1:C:244:PHE:CD1	2.07	1.22
1:C:381:SER:O	1:C:384:GLN:N	1.77	1.16
1:C:379:GLN:HG3	1:C:380:ALA:H	1.03	1.14
1:C:244:PHE:CD2	1:C:246:LEU:CD1	2.33	1.12
1:C:381:SER:O	1:C:383:LYS:N	1.84	1.11
1:D:379:GLN:HG3	1:D:380:ALA:H	1.02	1.11
1:D:381:SER:O	1:D:384:GLN:N	1.84	1.08
1:A:379:GLN:HG3	1:A:380:ALA:H	0.94	1.07
1:D:381:SER:O	1:D:383:LYS:N	1.89	1.03
1:C:244:PHE:CE1	1:C:246:LEU:HD21	1.93	1.03
1:A:394:LEU:O	1:A:397:GLU:N	1.93	1.02
1:C:379:GLN:HG3	1:C:380:ALA:N	1.76	1.01
1:D:379:GLN:HG3	1:D:380:ALA:N	1.76	0.99
1:B:394:LEU:O	1:B:397:GLU:N	1.98	0.96
1:A:379:GLN:HG3	1:A:380:ALA:N	1.77	0.96
1:D:394:LEU:O	1:D:397:GLU:N	1.99	0.96
1:C:394:LEU:O	1:C:397:GLU:N	1.99	0.95
1:A:379:GLN:CG	1:A:380:ALA:H	1.80	0.95
1:B:107:LEU:N	1:B:252:ILE:O	2.01	0.94
1:C:202:LYS:HZ1	1:C:244:PHE:HE1	1.08	0.94
1:D:645:ASN:O	1:D:649:TRP:N	2.03	0.92
1:A:645:ASN:O	1:A:649:TRP:N	2.01	0.92
2:H:317:GLY:N	2:H:450:THR:O	2.03	0.91
2:F:317:GLY:N	2:F:450:THR:O	2.04	0.91
1:C:645:ASN:O	1:C:649:TRP:N	2.03	0.91
2:G:347:SER:O	2:G:351:VAL:N	2.02	0.91
1:B:375:TYR:OH	1:B:397:GLU:OE1	1.88	0.90
1:B:645:ASN:O	1:B:649:TRP:N	2.04	0.90
2:G:317:GLY:N	2:G:450:THR:O	2.04	0.90
1:A:687:GLU:O	1:A:691:LEU:N	2.05	0.89
1:A:375:TYR:OH	1:A:397:GLU:OE1	1.90	0.89
1:A:200:LEU:O	1:A:204:ARG:N	2.06	0.89
1:D:201:SER:O	1:D:205:THR:OG1	1.90	0.88
1:B:43:ARG:NH2	1:B:339:GLN:O	2.07	0.88
1:D:695:LYS:HD2	1:D:707:LEU:HD11	1.54	0.87
2:E:317:GLY:N	2:E:450:THR:O	2.07	0.86
1:A:107:LEU:N	1:A:252:ILE:O	2.09	0.86
1:B:201:SER:O	1:B:205:THR:OG1	1.92	0.86
1:C:563:LEU:HA	1:C:567:TYR:CD2	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:O	1:D:81:HIS:ND1	2.08	0.86
1:B:200:LEU:O	1:B:204:ARG:N	2.09	0.86
2:E:347:SER:O	2:E:351:VAL:N	2.08	0.85
1:C:200:LEU:O	1:C:204:ARG:N	2.10	0.85
1:C:372:PHE:O	1:C:376:VAL:N	2.10	0.84
2:F:319:LYS:O	2:F:323:LEU:N	2.11	0.84
1:A:77:LEU:O	1:A:81:HIS:ND1	2.09	0.84
1:A:201:SER:O	1:A:205:THR:OG1	1.95	0.84
2:E:319:LYS:O	2:E:323:LEU:N	2.10	0.83
1:A:112:THR:OG1	1:A:322:GLN:OE1	1.96	0.83
2:H:347:SER:O	2:H:351:VAL:N	2.10	0.83
1:B:77:LEU:O	1:B:81:HIS:ND1	2.11	0.82
2:F:347:SER:O	2:F:351:VAL:N	2.11	0.82
1:C:562:CYS:HB3	1:C:567:TYR:CE2	2.14	0.82
1:C:563:LEU:HA	1:C:567:TYR:HD2	1.42	0.82
2:H:366:PHE:O	2:H:372:GLN:NE2	2.12	0.82
1:D:200:LEU:O	1:D:204:ARG:N	2.12	0.82
1:D:141:CYS:HB3	1:D:147:PHE:CZ	2.15	0.82
1:C:66:ASN:O	1:C:69:LEU:N	2.12	0.81
2:G:319:LYS:O	2:G:323:LEU:N	2.12	0.81
1:D:418:CYS:HG	1:D:422:PHE:HE2	1.28	0.81
2:G:320:ARG:NH1	2:G:457:GLU:OE1	2.13	0.81
1:C:587:ALA:O	1:C:591:HIS:ND1	2.13	0.81
2:H:319:LYS:O	2:H:323:LEU:N	2.14	0.81
1:A:691:LEU:O	2:G:427:LEU:N	2.12	0.81
1:A:384:GLN:HG2	1:A:388:LEU:HD11	1.63	0.81
1:C:77:LEU:O	1:C:81:HIS:ND1	2.14	0.81
1:A:141:CYS:HB3	1:A:147:PHE:CZ	2.17	0.80
2:F:366:PHE:O	2:F:372:GLN:NE2	2.14	0.80
2:E:318:SER:O	2:E:452:SER:OG	2.00	0.80
2:H:320:ARG:NH1	2:H:457:GLU:OE1	2.15	0.80
1:A:43:ARG:NH2	1:A:339:GLN:O	2.15	0.80
2:G:391:LEU:HD22	2:G:421:ILE:HB	1.64	0.80
1:D:683:ARG:NH1	2:F:458:THR:HA	1.97	0.79
1:C:43:ARG:NH2	1:C:339:GLN:O	2.14	0.79
1:C:201:SER:O	1:C:205:THR:OG1	1.99	0.79
1:A:66:ASN:O	1:A:69:LEU:N	2.15	0.79
1:C:202:LYS:CE	1:C:244:PHE:CE1	2.66	0.79
1:D:107:LEU:N	1:D:252:ILE:O	2.16	0.78
1:D:385:VAL:O	1:D:389:THR:N	2.16	0.78
2:E:391:LEU:HD22	2:E:421:ILE:HB	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LYS:O	1:A:207:SER:N	2.16	0.78
1:C:375:TYR:CE2	1:C:401:LEU:HD21	2.18	0.78
1:A:591:HIS:HA	2:G:445:TRP:O	1.84	0.77
1:A:202:LYS:HD2	1:A:244:PHE:CE1	2.19	0.77
2:G:366:PHE:O	2:G:372:GLN:NE2	2.16	0.77
1:B:199:MET:HA	1:B:244:PHE:CZ	2.19	0.77
2:H:328:THR:O	2:H:332:GLN:NE2	2.17	0.77
1:A:385:VAL:O	1:A:389:THR:N	2.18	0.77
2:E:320:ARG:NH1	2:E:457:GLU:OE1	2.18	0.77
1:A:202:LYS:HD2	1:A:244:PHE:HE1	1.49	0.76
1:C:141:CYS:HB3	1:C:147:PHE:CZ	2.20	0.76
1:C:433:ARG:N	1:C:437:GLU:OE1	2.17	0.76
1:B:302:ILE:CG2	1:B:306:VAL:HG22	2.16	0.76
1:B:687:GLU:O	1:B:691:LEU:N	2.18	0.76
1:C:415:VAL:HG12	1:C:567:TYR:CE1	2.20	0.76
1:C:102:THR:OG1	1:C:273:ILE:HG12	1.85	0.75
1:C:381:SER:O	1:C:383:LYS:CA	2.34	0.75
1:B:379:GLN:HE22	1:B:387:LEU:CD1	2.00	0.75
1:C:107:LEU:N	1:C:252:ILE:O	2.18	0.75
1:A:302:ILE:CG2	1:A:306:VAL:HG22	2.17	0.75
1:B:141:CYS:HB3	1:B:147:PHE:CE2	2.22	0.75
2:H:391:LEU:HD22	2:H:421:ILE:HB	1.68	0.75
1:B:382:GLU:O	1:B:384:GLN:N	2.17	0.75
1:C:563:LEU:CA	1:C:567:TYR:HD2	1.99	0.75
1:D:43:ARG:NH2	1:D:339:GLN:O	2.20	0.75
2:E:366:PHE:O	2:E:372:GLN:NE2	2.18	0.75
1:A:100:ILE:HG13	1:A:241:LEU:HD11	1.69	0.75
1:B:112:THR:OG1	1:B:322:GLN:OE1	2.03	0.74
1:D:687:GLU:O	1:D:691:LEU:N	2.19	0.74
1:B:347:ASN:OD1	1:D:350:GLU:N	2.20	0.74
1:A:382:GLU:O	1:A:383:LYS:C	2.25	0.74
1:B:202:LYS:HD2	1:B:244:PHE:CE1	2.22	0.74
1:D:66:ASN:O	1:D:69:LEU:N	2.19	0.74
2:F:391:LEU:HD22	2:F:421:ILE:HB	1.67	0.74
1:A:382:GLU:O	1:A:385:VAL:N	2.19	0.74
1:B:587:ALA:O	1:B:591:HIS:ND1	2.21	0.73
1:D:556:VAL:HA	1:D:559:PHE:HB2	1.70	0.73
1:A:199:MET:HA	1:A:244:PHE:CZ	2.23	0.73
1:B:132:TYR:O	1:B:215:VAL:HG22	1.87	0.73
1:B:133:VAL:N	1:B:158:CYS:SG	2.62	0.73
1:B:385:VAL:O	1:B:389:THR:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:GLU:OE1	1:B:452:GLU:N	2.21	0.73
1:B:66:ASN:O	1:B:69:LEU:N	2.20	0.73
1:D:326:LYS:O	1:D:330:LEU:HG	1.87	0.73
1:D:555:ASN:O	1:D:559:PHE:N	2.21	0.73
1:B:372:PHE:O	1:B:376:VAL:N	2.21	0.73
2:G:353:ASN:O	2:G:357:GLU:N	2.22	0.73
1:A:433:ARG:N	1:A:437:GLU:OE1	2.20	0.73
2:F:353:ASN:O	2:F:357:GLU:N	2.20	0.73
1:A:237:SER:O	1:A:241:LEU:HG	1.89	0.72
1:A:452:GLU:N	1:A:452:GLU:OE1	2.22	0.72
1:A:382:GLU:O	1:A:384:GLN:N	2.22	0.72
1:C:648:ASP:O	1:C:652:ALA:HB2	1.89	0.72
1:D:372:PHE:O	1:D:376:VAL:N	2.22	0.72
1:C:687:GLU:O	1:C:691:LEU:N	2.22	0.72
1:B:100:ILE:HG13	1:B:241:LEU:HD11	1.71	0.72
1:D:189:MET:O	1:D:191:VAL:N	2.23	0.72
1:D:569:LEU:HB3	1:D:571:PRO:HD2	1.71	0.72
1:A:372:PHE:O	1:A:376:VAL:N	2.23	0.71
1:D:102:THR:HG1	1:D:250:PHE:HE2	1.38	0.71
1:D:302:ILE:CG2	1:D:306:VAL:HG22	2.19	0.71
2:G:318:SER:O	2:G:452:SER:OG	2.08	0.71
1:C:151:LEU:HD12	1:C:198:LYS:NZ	2.04	0.71
1:D:112:THR:OG1	1:D:322:GLN:OE1	2.08	0.71
2:E:353:ASN:O	2:E:357:GLU:N	2.22	0.71
1:C:420:HIS:CD2	1:C:435:ILE:HA	2.25	0.71
2:H:353:ASN:O	2:H:357:GLU:N	2.21	0.71
1:C:244:PHE:CE1	1:C:246:LEU:CD2	2.72	0.71
1:C:385:VAL:O	1:C:389:THR:N	2.22	0.71
1:B:141:CYS:HB3	1:B:147:PHE:CZ	2.26	0.71
1:D:476:PHE:O	1:D:480:LYS:HB2	1.91	0.71
2:E:453:PRO:HA	2:E:454:TYR:HB2	1.73	0.71
1:D:587:ALA:O	1:D:591:HIS:ND1	2.23	0.71
1:A:556:VAL:HA	1:A:559:PHE:HB2	1.73	0.71
1:C:100:ILE:HG13	1:C:241:LEU:HD11	1.72	0.71
1:C:381:SER:C	1:C:383:LYS:N	2.40	0.71
1:D:203:LYS:O	1:D:207:SER:N	2.24	0.71
1:D:433:ARG:N	1:D:437:GLU:OE1	2.21	0.71
2:G:356:THR:HA	2:G:360:LEU:HB2	1.73	0.71
1:A:405:LEU:N	1:A:574:GLN:OE1	2.24	0.70
1:B:590:GLU:O	2:E:445:TRP:HB2	1.91	0.70
1:B:482:TYR:O	1:B:486:HIS:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ILE:HG13	1:D:241:LEU:HD11	1.72	0.70
1:D:375:TYR:CE2	1:D:401:LEU:HD21	2.26	0.70
1:A:556:VAL:HA	1:A:559:PHE:HD2	1.55	0.70
1:A:63:GLU:O	1:A:67:LYS:HG3	1.92	0.70
1:C:416:LEU:O	1:C:420:HIS:ND1	2.24	0.70
2:F:453:PRO:HA	2:F:454:TYR:HB2	1.73	0.70
1:C:302:ILE:CG2	1:C:306:VAL:HG22	2.21	0.70
1:B:683:ARG:NH1	2:E:458:THR:HA	2.06	0.70
2:H:453:PRO:HA	2:H:454:TYR:HB2	1.72	0.70
1:B:556:VAL:HA	1:B:559:PHE:HD2	1.56	0.70
1:D:648:ASP:O	1:D:652:ALA:HB2	1.91	0.70
1:A:202:LYS:HE2	1:A:213:PRO:HG2	1.73	0.70
1:D:420:HIS:CD2	1:D:435:ILE:HA	2.27	0.70
1:C:476:PHE:O	1:C:480:LYS:HB2	1.92	0.70
1:D:562:CYS:O	1:D:566:GLU:N	2.24	0.70
1:A:291:LYS:O	1:A:295:THR:HG23	1.92	0.69
1:C:556:VAL:HA	1:C:559:PHE:HB2	1.72	0.69
1:D:132:TYR:O	1:D:215:VAL:HG22	1.91	0.69
1:D:291:LYS:O	1:D:295:THR:HG23	1.92	0.69
1:B:556:VAL:HA	1:B:559:PHE:HB2	1.74	0.69
1:C:590:GLU:O	2:H:445:TRP:HB2	1.92	0.69
1:A:335:HIS:NE2	1:A:579:VAL:O	2.25	0.69
1:C:237:SER:O	1:C:241:LEU:HG	1.91	0.69
1:D:151:LEU:HD12	1:D:198:LYS:NZ	2.08	0.69
1:D:416:LEU:O	1:D:420:HIS:ND1	2.24	0.69
1:A:52:GLN:O	1:A:56:SER:OG	2.06	0.69
1:D:202:LYS:HB2	1:D:244:PHE:HE1	1.56	0.69
1:A:125:LEU:O	1:A:131:PRO:HD2	1.93	0.69
1:A:555:ASN:O	1:A:559:PHE:N	2.26	0.69
2:E:298:PHE:HB3	2:E:330:MET:SD	2.32	0.69
1:B:237:SER:O	1:B:241:LEU:HG	1.92	0.69
1:D:688:LEU:HG	1:D:693:PHE:HB2	1.74	0.69
2:E:352:LEU:HD23	2:E:372:GLN:OE1	1.93	0.69
2:F:320:ARG:NH1	2:F:457:GLU:OE1	2.25	0.69
2:F:356:THR:HA	2:F:360:LEU:HB2	1.73	0.69
1:B:203:LYS:O	1:B:207:SER:N	2.25	0.69
1:C:202:LYS:NZ	1:C:244:PHE:HE1	1.69	0.69
1:D:689:GLU:HG3	1:D:694:ILE:HD11	1.74	0.69
1:A:689:GLU:HG3	1:A:694:ILE:HD11	1.75	0.69
1:C:199:MET:SD	1:C:199:MET:CG	2.80	0.68
1:C:381:SER:O	1:C:383:LYS:C	2.32	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:SER:O	1:D:241:LEU:HG	1.92	0.68
2:F:318:SER:O	2:F:452:SER:OG	2.11	0.68
1:A:130:THR:OG1	1:A:131:PRO:HD3	1.92	0.68
1:C:209:GLN:N	1:C:210:TRP:HA	2.08	0.68
1:C:147:PHE:HB2	1:C:233:PHE:CZ	2.28	0.68
1:C:405:LEU:N	1:C:574:GLN:OE1	2.26	0.68
2:G:352:LEU:HD23	2:G:372:GLN:OE1	1.92	0.68
1:B:548:LYS:O	1:B:552:LEU:N	2.24	0.68
1:B:405:LEU:N	1:B:574:GLN:OE1	2.27	0.68
1:C:63:GLU:O	1:C:67:LYS:HG3	1.93	0.68
2:G:398:GLN:HB3	2:G:399:MET:HA	1.76	0.68
1:C:291:LYS:O	1:C:295:THR:HG23	1.94	0.68
1:D:457:LEU:HG	1:D:559:PHE:CZ	2.29	0.68
2:G:453:PRO:HA	2:G:454:TYR:HB2	1.75	0.68
1:C:381:SER:O	1:C:382:GLU:C	2.32	0.68
1:B:420:HIS:CD2	1:B:435:ILE:HA	2.29	0.68
1:A:132:TYR:O	1:A:215:VAL:HG22	1.93	0.67
1:B:476:PHE:O	1:B:480:LYS:HB2	1.93	0.67
1:C:562:CYS:O	1:C:566:GLU:N	2.26	0.67
1:A:45:GLU:O	1:A:49:LEU:HG	1.94	0.67
1:C:482:TYR:O	1:C:486:HIS:N	2.28	0.67
1:D:347:ASN:O	1:D:351:ALA:N	2.25	0.67
1:A:415:VAL:HG12	1:A:567:TYR:CZ	2.29	0.67
1:B:151:LEU:HD12	1:B:198:LYS:NZ	2.08	0.67
1:B:453:TYR:OH	1:B:563:LEU:HD13	1.94	0.67
1:C:335:HIS:NE2	1:C:579:VAL:O	2.26	0.67
2:H:398:GLN:HB3	2:H:399:MET:HA	1.77	0.67
1:B:433:ARG:N	1:B:437:GLU:OE1	2.22	0.67
1:B:416:LEU:O	1:B:420:HIS:ND1	2.28	0.67
1:B:648:ASP:O	1:B:652:ALA:HB2	1.93	0.67
2:E:337:VAL:HG22	2:E:359:VAL:HG21	1.76	0.67
2:H:411:GLN:O	2:H:415:LEU:N	2.25	0.67
1:C:125:LEU:O	1:C:131:PRO:CD	2.43	0.67
1:C:347:ASN:O	1:C:351:ALA:N	2.22	0.67
1:A:648:ASP:O	1:A:652:ALA:HB2	1.94	0.67
1:B:199:MET:HE2	1:B:244:PHE:HE2	1.59	0.67
1:C:47:TYR:OH	1:C:329:GLN:OE1	2.08	0.67
1:C:457:LEU:HG	1:C:559:PHE:CZ	2.29	0.67
1:A:151:LEU:HD12	1:A:198:LYS:NZ	2.09	0.67
1:D:475:CYS:O	1:D:479:PHE:HB2	1.93	0.67
1:D:63:GLU:O	1:D:67:LYS:HG3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:428:ASN:O	2:H:431:LEU:HB3	1.95	0.67
1:D:199:MET:HA	1:D:244:PHE:CZ	2.31	0.66
2:E:356:THR:HA	2:E:360:LEU:HB2	1.77	0.66
2:H:352:LEU:HD23	2:H:372:GLN:OE1	1.94	0.66
1:B:63:GLU:O	1:B:67:LYS:HG3	1.94	0.66
1:A:151:LEU:HG	1:A:198:LYS:HD2	1.77	0.66
1:A:102:THR:OG1	1:A:273:ILE:HG12	1.96	0.66
1:A:384:GLN:HG2	1:A:388:LEU:CD1	2.26	0.66
1:B:199:MET:HA	1:B:244:PHE:CE2	2.30	0.66
2:H:356:THR:HA	2:H:360:LEU:HB2	1.77	0.66
1:A:199:MET:HA	1:A:244:PHE:CE2	2.30	0.66
1:B:689:GLU:HG3	1:B:694:ILE:HD11	1.78	0.66
1:D:381:SER:C	1:D:383:LYS:N	2.48	0.66
2:E:398:GLN:HB3	2:E:399:MET:HA	1.77	0.66
1:C:429:TYR:HB3	1:C:433:ARG:HG2	1.78	0.66
1:C:569:LEU:HB3	1:C:571:PRO:HD2	1.77	0.66
1:B:688:LEU:HG	1:B:693:PHE:HB2	1.77	0.66
1:C:151:LEU:HG	1:C:198:LYS:HD2	1.76	0.66
1:C:415:VAL:HG12	1:C:567:TYR:CZ	2.30	0.66
1:C:689:GLU:HG3	1:C:694:ILE:HD11	1.77	0.66
1:A:475:CYS:O	1:A:479:PHE:HB2	1.96	0.66
1:D:415:VAL:HG12	1:D:567:TYR:CZ	2.30	0.66
1:D:147:PHE:HB2	1:D:233:PHE:CZ	2.31	0.65
1:B:151:LEU:HG	1:B:198:LYS:HD2	1.77	0.65
1:B:457:LEU:HG	1:B:559:PHE:CZ	2.31	0.65
1:C:683:ARG:HD2	2:H:458:THR:OG1	1.95	0.65
1:B:475:CYS:O	1:B:479:PHE:HB2	1.96	0.65
1:B:570:PRO:O	1:B:573:THR:OG1	2.10	0.65
1:D:379:GLN:CG	1:D:380:ALA:H	1.86	0.65
1:D:381:SER:O	1:D:383:LYS:CA	2.45	0.65
2:H:318:SER:O	2:H:452:SER:OG	2.14	0.65
1:C:203:LYS:O	1:C:207:SER:N	2.30	0.65
1:B:691:LEU:O	2:E:427:LEU:N	2.28	0.65
2:F:352:LEU:HD23	2:F:372:GLN:OE1	1.96	0.65
1:B:382:GLU:C	1:B:384:GLN:H	1.99	0.65
1:B:555:ASN:O	1:B:559:PHE:N	2.30	0.65
1:C:151:LEU:HD12	1:C:198:LYS:HZ2	1.60	0.65
1:D:199:MET:HA	1:D:244:PHE:CE2	2.31	0.65
2:G:328:THR:O	2:G:332:GLN:NE2	2.25	0.65
1:A:397:GLU:HG2	1:A:400:LEU:HD12	1.78	0.65
1:B:500:GLN:O	1:B:503:SER:OG	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:VAL:HG12	1:B:567:TYR:CZ	2.30	0.65
1:D:151:LEU:HG	1:D:198:LYS:HD2	1.79	0.65
2:E:328:THR:O	2:E:332:GLN:NE2	2.22	0.65
2:E:411:GLN:O	2:E:415:LEU:N	2.28	0.65
1:C:189:MET:O	1:C:191:VAL:N	2.30	0.65
1:B:291:LYS:O	1:B:295:THR:HG23	1.96	0.65
1:D:556:VAL:HA	1:D:559:PHE:HD2	1.61	0.65
2:F:398:GLN:HB3	2:F:399:MET:HA	1.79	0.65
2:H:454:TYR:O	2:H:458:THR:OG1	2.14	0.65
1:B:97:LEU:HA	1:B:242:HIS:CD2	2.32	0.64
1:D:330:LEU:HD22	2:F:309:PHE:CE2	2.32	0.64
1:B:379:GLN:HE22	1:B:387:LEU:HD12	1.62	0.64
1:B:562:CYS:O	1:B:566:GLU:N	2.29	0.64
1:B:684:ALA:O	1:B:688:LEU:HD13	1.97	0.64
1:D:556:VAL:HA	1:D:559:PHE:CD2	2.33	0.64
1:A:476:PHE:O	1:A:480:LYS:HB2	1.97	0.64
1:C:325:ILE:O	1:C:328:LEU:N	2.29	0.64
1:D:296:THR:HG22	1:D:413:PHE:CD2	2.33	0.64
2:G:377:VAL:O	2:G:381:LYS:N	2.30	0.64
2:G:311:ILE:HG13	2:G:421:ILE:HG12	1.78	0.64
1:A:47:TYR:OH	1:A:329:GLN:OE1	2.13	0.64
1:C:555:ASN:O	1:C:559:PHE:N	2.31	0.64
2:H:304:GLN:OE1	2:H:446:TYR:OH	2.14	0.64
1:A:684:ALA:O	1:A:688:LEU:HD13	1.97	0.64
1:C:151:LEU:O	1:C:198:LYS:HE3	1.97	0.64
1:D:102:THR:OG1	1:D:273:ILE:HG12	1.98	0.64
1:A:102:THR:HG1	1:A:250:PHE:HE2	1.44	0.64
1:A:489:SER:HA	1:A:490:THR:HB	1.80	0.64
1:D:222:MET:HG3	1:D:250:PHE:CD1	2.33	0.64
1:A:397:GLU:O	1:A:401:LEU:HG	1.98	0.64
1:A:457:LEU:HG	1:A:559:PHE:CZ	2.32	0.64
1:A:448:TRP:CZ2	1:A:559:PHE:HB3	2.33	0.64
1:B:222:MET:HG3	1:B:250:PHE:CD1	2.33	0.64
1:A:690:LEU:O	2:G:426:HIS:HA	1.98	0.64
1:A:562:CYS:O	1:A:566:GLU:N	2.30	0.63
1:A:488:GLY:O	1:A:490:THR:OG1	2.16	0.63
1:A:694:ILE:HD13	1:A:704:VAL:HG13	1.81	0.63
2:H:373:LEU:HD22	2:H:412:LEU:HD21	1.81	0.63
1:B:50:ILE:O	1:B:54:MET:HG2	1.98	0.63
1:C:648:ASP:O	1:C:652:ALA:CB	2.46	0.63
1:D:379:GLN:CG	1:D:380:ALA:N	2.52	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:394:ASN:ND2	2:F:425:ASP:OD2	2.26	0.63
1:A:597:ARG:NH2	1:A:708:THR:OG1	2.31	0.63
1:B:216:VAL:HA	1:B:247:ILE:O	1.99	0.63
1:D:335:HIS:NE2	1:D:579:VAL:O	2.31	0.63
1:A:234:ILE:O	1:A:238:SER:CB	2.46	0.63
1:B:125:LEU:O	1:B:131:PRO:CD	2.46	0.63
1:B:202:LYS:HE2	1:B:213:PRO:HG2	1.81	0.63
1:C:147:PHE:CD2	1:C:233:PHE:CE2	2.86	0.63
1:C:112:THR:OG1	1:C:322:GLN:OE1	2.17	0.63
1:D:381:SER:O	1:D:382:GLU:C	2.34	0.63
1:C:152:ILE:HG23	1:C:198:LYS:N	2.14	0.63
2:G:298:PHE:HB3	2:G:330:MET:SD	2.39	0.63
1:B:488:GLY:O	1:B:490:THR:OG1	2.17	0.63
1:C:556:VAL:HA	1:C:559:PHE:HD2	1.64	0.63
1:B:147:PHE:HB2	1:B:233:PHE:CZ	2.34	0.63
1:B:52:GLN:O	1:B:56:SER:OG	2.10	0.63
1:B:335:HIS:NE2	1:B:579:VAL:O	2.32	0.63
1:C:563:LEU:N	1:C:567:TYR:HD2	1.95	0.63
1:D:209:GLN:N	1:D:210:TRP:HA	2.12	0.63
1:A:353:ARG:NH2	1:C:297:GLN:O	2.31	0.62
1:D:684:ALA:O	1:D:688:LEU:HD13	1.98	0.62
1:A:147:PHE:HB2	1:A:233:PHE:CZ	2.34	0.62
1:B:234:ILE:O	1:B:238:SER:CB	2.47	0.62
1:A:418:CYS:HA	1:A:479:PHE:CZ	2.34	0.62
1:C:216:VAL:HA	1:C:247:ILE:O	1.99	0.62
1:D:97:LEU:HA	1:D:242:HIS:CD2	2.34	0.62
1:B:202:LYS:HD2	1:B:244:PHE:HE1	1.62	0.62
1:B:397:GLU:HG2	1:B:400:LEU:HD12	1.82	0.62
1:C:688:LEU:HG	1:C:693:PHE:HB2	1.80	0.62
1:D:683:ARG:HH12	2:F:461:GLU:HB2	1.63	0.62
2:H:320:ARG:HH22	2:H:457:GLU:N	1.97	0.62
1:A:556:VAL:HA	1:A:559:PHE:CD2	2.34	0.62
1:B:330:LEU:HD13	1:B:592:LEU:HD21	1.81	0.62
1:C:155:LEU:HD11	1:C:215:VAL:HG21	1.80	0.62
1:C:475:CYS:O	1:C:479:PHE:HB3	1.98	0.62
1:D:147:PHE:CD2	1:D:233:PHE:CE2	2.88	0.62
2:G:298:PHE:HB3	2:G:330:MET:HG3	1.80	0.62
1:B:46:THR:O	1:B:50:ILE:HG13	1.99	0.62
1:C:563:LEU:CA	1:C:567:TYR:CD2	2.78	0.62
1:D:151:LEU:O	1:D:198:LYS:HE3	1.99	0.62
2:G:373:LEU:HD22	2:G:412:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ILE:O	1:D:54:MET:HG2	1.99	0.62
1:A:569:LEU:HB3	1:A:571:PRO:HD2	1.81	0.62
1:B:335:HIS:O	1:B:338:SER:N	2.26	0.62
1:B:209:GLN:N	1:B:210:TRP:HA	2.15	0.62
1:D:397:GLU:O	1:D:401:LEU:HG	1.99	0.62
1:A:392:ARG:HD3	1:C:484:GLU:HB3	1.82	0.62
1:A:548:LYS:O	1:A:552:LEU:N	2.29	0.62
1:B:99:GLU:N	1:B:241:LEU:HD12	2.15	0.62
1:C:452:GLU:N	1:C:452:GLU:OE1	2.28	0.62
1:C:152:ILE:HG21	1:C:197:PRO:CG	2.30	0.61
1:D:476:PHE:CE2	1:D:501:PHE:CD1	2.88	0.61
1:A:151:LEU:HD12	1:A:198:LYS:HZ2	1.63	0.61
1:C:563:LEU:HG	1:C:567:TYR:CE2	2.35	0.61
1:D:199:MET:CE	1:D:203:LYS:HE3	2.30	0.61
1:D:482:TYR:O	1:D:486:HIS:N	2.33	0.61
1:C:130:THR:OG1	1:C:131:PRO:HD3	2.01	0.61
1:C:132:TYR:O	1:C:215:VAL:HG22	2.00	0.61
1:C:684:ALA:O	1:C:688:LEU:HD13	1.99	0.61
1:D:324:PHE:O	1:D:328:LEU:HG	2.01	0.61
2:H:311:ILE:HG13	2:H:421:ILE:HG12	1.81	0.61
1:A:476:PHE:CE2	1:A:501:PHE:CD1	2.87	0.61
1:C:480:LYS:NZ	1:C:502:GLN:HG3	2.15	0.61
1:C:448:TRP:HZ2	1:C:559:PHE:HB3	1.65	0.61
1:D:314:PHE:HA	1:D:318:ASP:O	2.01	0.61
1:A:475:CYS:O	1:A:479:PHE:CD2	2.53	0.61
1:B:556:VAL:HA	1:B:559:PHE:CD2	2.36	0.61
1:D:429:TYR:HB3	1:D:433:ARG:HG2	1.82	0.61
1:A:272:CYS:SG	1:A:272:CYS:O	2.58	0.61
1:C:591:HIS:HA	2:H:445:TRP:O	1.99	0.61
1:D:152:ILE:HG21	1:D:197:PRO:CB	2.31	0.61
1:D:234:ILE:O	1:D:238:SER:CB	2.48	0.61
1:D:489:SER:HA	1:D:490:THR:HB	1.82	0.61
2:H:340:ASN:HB3	2:H:342:PHE:CE2	2.36	0.61
1:A:64:GLU:O	1:A:67:LYS:N	2.33	0.61
1:A:688:LEU:HG	1:A:693:PHE:HB2	1.82	0.61
1:B:453:TYR:OH	1:B:563:LEU:CD1	2.49	0.61
1:D:199:MET:HG2	1:D:244:PHE:HE2	1.65	0.61
1:A:420:HIS:CD2	1:A:435:ILE:HA	2.35	0.61
1:C:152:ILE:HG12	1:C:198:LYS:H	1.65	0.61
1:C:296:THR:HG22	1:C:413:PHE:CD2	2.35	0.61
1:D:489:SER:HA	1:D:490:THR:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:HIS:O	1:A:338:SER:N	2.27	0.61
1:B:155:LEU:CD1	1:B:198:LYS:HE2	2.30	0.61
1:B:453:TYR:OH	1:B:559:PHE:CE1	2.52	0.61
1:C:234:ILE:O	1:C:238:SER:CB	2.48	0.61
1:D:151:LEU:HD12	1:D:198:LYS:HZ2	1.66	0.61
1:B:353:ARG:NH2	1:D:297:GLN:O	2.34	0.61
2:E:428:ASN:O	2:E:431:LEU:HB3	1.99	0.61
2:E:318:SER:N	2:E:452:SER:O	2.28	0.61
2:F:311:ILE:HG13	2:F:421:ILE:HG12	1.83	0.61
2:H:287:LEU:HD22	2:H:451:TYR:HB2	1.82	0.61
1:A:104:ALA:HA	1:A:250:PHE:HD2	1.66	0.61
1:B:648:ASP:O	1:B:652:ALA:CB	2.48	0.61
1:C:46:THR:O	1:C:50:ILE:HG13	2.01	0.61
1:D:152:ILE:HG21	1:D:197:PRO:CG	2.31	0.61
1:D:590:GLU:O	2:F:445:TRP:HB2	2.00	0.61
1:A:147:PHE:CD2	1:A:233:PHE:CE2	2.89	0.60
1:B:409:HIS:HA	1:B:412:TYR:HD2	1.66	0.60
1:B:448:TRP:CZ2	1:B:559:PHE:HB3	2.36	0.60
1:C:330:LEU:O	1:C:334:GLU:CB	2.49	0.60
1:C:397:GLU:HG2	1:C:400:LEU:HD12	1.82	0.60
1:C:489:SER:HA	1:C:490:THR:CB	2.31	0.60
2:H:318:SER:N	2:H:452:SER:O	2.29	0.60
1:B:189:MET:O	1:B:191:VAL:N	2.34	0.60
1:B:429:TYR:HB3	1:B:433:ARG:HG2	1.83	0.60
1:A:155:LEU:CD1	1:A:215:VAL:HG21	2.31	0.60
1:A:297:GLN:HA	1:C:353:ARG:CZ	2.31	0.60
1:B:147:PHE:CD2	1:B:233:PHE:CE2	2.89	0.60
1:C:324:PHE:O	1:C:328:LEU:HG	2.02	0.60
1:A:297:GLN:O	1:C:353:ARG:NH1	2.34	0.60
1:B:397:GLU:O	1:B:401:LEU:HG	2.01	0.60
1:B:418:CYS:HA	1:B:479:PHE:CZ	2.36	0.60
1:D:330:LEU:HD22	2:F:309:PHE:HE2	1.66	0.60
1:B:47:TYR:OH	1:B:329:GLN:OE1	2.16	0.60
1:B:569:LEU:HB3	1:B:571:PRO:HD2	1.84	0.60
1:D:47:TYR:OH	1:D:329:GLN:OE1	2.13	0.60
2:F:340:ASN:HB3	2:F:342:PHE:CE2	2.37	0.60
1:A:420:HIS:NE2	1:A:438:LEU:HB2	2.16	0.60
1:B:43:ARG:NH2	1:B:342:SER:OG	2.35	0.60
1:C:226:ALA:O	1:C:230:LEU:N	2.34	0.60
1:D:695:LYS:HD2	1:D:707:LEU:CD1	2.29	0.60
1:D:453:TYR:OH	1:D:563:LEU:HD13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:THR:HA	1:A:133:VAL:CG2	2.32	0.60
1:B:64:GLU:O	1:B:67:LYS:N	2.35	0.60
1:D:202:LYS:HD2	1:D:244:PHE:CE1	2.36	0.60
1:D:310:LEU:O	1:D:313:ILE:HG22	2.01	0.60
1:D:480:LYS:NZ	1:D:502:GLN:HG3	2.17	0.60
2:E:320:ARG:HH22	2:E:457:GLU:N	1.99	0.60
1:A:155:LEU:CD1	1:A:198:LYS:HE2	2.31	0.60
1:C:152:ILE:HG21	1:C:197:PRO:CD	2.31	0.60
1:C:229:VAL:HG13	1:C:233:PHE:HE2	1.67	0.60
1:D:125:LEU:O	1:D:131:PRO:HD2	2.01	0.60
2:G:287:LEU:HD22	2:G:451:TYR:HB2	1.82	0.60
2:G:411:GLN:O	2:G:415:LEU:N	2.32	0.60
2:H:390:LEU:HD11	2:H:420:LEU:HD13	1.83	0.60
1:A:155:LEU:HD11	1:A:215:VAL:HG21	1.83	0.60
1:A:500:GLN:O	1:A:503:SER:OG	2.13	0.60
1:A:97:LEU:HA	1:A:242:HIS:CD2	2.36	0.60
1:D:693:PHE:CZ	2:F:427:LEU:HD21	2.37	0.60
1:C:219:LEU:HB2	1:C:222:MET:HG2	1.84	0.59
1:C:50:ILE:O	1:C:54:MET:HG2	2.01	0.59
2:G:337:VAL:HG22	2:G:359:VAL:HG21	1.83	0.59
1:A:189:MET:O	1:A:191:VAL:N	2.35	0.59
1:A:209:GLN:N	1:A:210:TRP:HA	2.17	0.59
1:D:99:GLU:N	1:D:241:LEU:HD12	2.17	0.59
1:D:695:LYS:HG3	1:D:696:PRO:HD2	1.84	0.59
1:B:683:ARG:HH12	2:E:461:GLU:HB2	1.66	0.59
1:B:480:LYS:O	1:B:484:GLU:CG	2.50	0.59
1:B:484:GLU:HG2	1:D:392:ARG:HD3	1.82	0.59
1:D:421:LYS:HB2	1:D:479:PHE:CE2	2.36	0.59
1:B:489:SER:HA	1:B:490:THR:HB	1.83	0.59
1:C:556:VAL:HA	1:C:559:PHE:CD2	2.37	0.59
1:D:155:LEU:CD1	1:D:198:LYS:HE2	2.33	0.59
1:D:44:PHE:HA	1:D:47:TYR:HB3	1.85	0.59
2:F:320:ARG:HH22	2:F:457:GLU:N	2.01	0.59
2:G:348:VAL:HA	2:G:351:VAL:HB	1.84	0.59
1:B:591:HIS:HA	2:E:445:TRP:O	2.01	0.59
1:B:651:GLU:O	1:B:655:THR:HG23	2.01	0.59
2:E:400:LEU:O	2:E:405:SER:OG	2.20	0.59
2:F:373:LEU:HD22	2:F:412:LEU:HD21	1.83	0.59
1:A:151:LEU:O	1:A:198:LYS:HE3	2.02	0.59
1:A:429:TYR:HB3	1:A:433:ARG:HG2	1.83	0.59
1:A:50:ILE:O	1:A:54:MET:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLN:HE22	1:B:387:LEU:HD11	1.66	0.59
1:D:405:LEU:N	1:D:574:GLN:OE1	2.36	0.59
2:G:305:LEU:O	2:G:419:TYR:CE1	2.56	0.59
1:B:230:LEU:HD21	1:B:263:LEU:HD23	1.84	0.59
1:C:446:ASN:OD1	1:C:569:LEU:HD11	2.02	0.59
1:D:152:ILE:HG21	1:D:197:PRO:CD	2.32	0.59
1:B:297:GLN:O	1:D:353:ARG:NH1	2.36	0.59
1:D:397:GLU:HG2	1:D:400:LEU:HD12	1.83	0.59
1:C:476:PHE:CE2	1:C:501:PHE:CD1	2.90	0.59
1:C:651:GLU:O	1:C:655:THR:HG23	2.02	0.59
2:H:331:LEU:HD11	2:H:391:LEU:HD11	1.84	0.59
1:A:131:PRO:HB3	1:A:214:PRO:O	2.02	0.59
1:A:99:GLU:N	1:A:241:LEU:HD12	2.18	0.59
1:C:397:GLU:O	1:C:401:LEU:HG	2.02	0.59
1:D:468:LEU:O	1:D:472:LEU:HG	2.03	0.59
1:A:648:ASP:O	1:A:652:ALA:CB	2.51	0.59
1:C:222:MET:HG3	1:C:250:PHE:CD1	2.37	0.59
1:C:202:LYS:CE	1:C:244:PHE:HE1	2.10	0.59
1:D:130:THR:OG1	1:D:131:PRO:HD3	2.02	0.59
2:E:311:ILE:HG13	2:E:421:ILE:HG12	1.85	0.59
2:H:323:LEU:HD22	2:H:391:LEU:HD13	1.84	0.59
1:A:199:MET:CE	1:A:203:LYS:HE3	2.33	0.58
1:B:147:PHE:O	1:B:151:LEU:HB2	2.02	0.58
1:B:151:LEU:HD12	1:B:198:LYS:HZ2	1.66	0.58
1:C:155:LEU:HG	1:C:198:LYS:HE2	1.85	0.58
1:C:152:ILE:HG12	1:C:198:LYS:CB	2.32	0.58
1:D:597:ARG:NH2	1:D:708:THR:OG1	2.35	0.58
1:D:645:ASN:HA	1:D:703:HIS:CE1	2.38	0.58
2:E:323:LEU:HD22	2:E:391:LEU:HD13	1.84	0.58
2:F:328:THR:O	2:F:332:GLN:NE2	2.28	0.58
2:F:412:LEU:HB3	2:F:418:ILE:HD11	1.84	0.58
1:B:476:PHE:CE2	1:B:501:PHE:CD1	2.90	0.58
1:B:489:SER:HA	1:B:490:THR:CB	2.33	0.58
1:C:694:ILE:HA	1:C:706:ARG:HA	1.86	0.58
2:E:340:ASN:HB3	2:E:342:PHE:CE2	2.39	0.58
2:G:366:PHE:N	2:G:372:GLN:HG2	2.18	0.58
1:A:296:THR:HB	1:A:410:MET:SD	2.42	0.58
1:A:489:SER:HA	1:A:490:THR:CB	2.33	0.58
1:B:155:LEU:CD1	1:B:215:VAL:HG21	2.33	0.58
1:C:335:HIS:O	1:C:338:SER:N	2.25	0.58
2:E:394:ASN:ND2	2:E:425:ASP:OD2	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:GLU:O	2:G:445:TRP:HB2	2.02	0.58
1:B:98:ARG:HA	1:B:238:SER:O	2.04	0.58
1:B:694:ILE:HD13	1:B:704:VAL:HG13	1.84	0.58
1:D:155:LEU:HD11	1:D:215:VAL:HG21	1.86	0.58
2:E:373:LEU:HD22	2:E:412:LEU:HD21	1.84	0.58
1:B:475:CYS:O	1:B:479:PHE:CD2	2.56	0.58
1:C:489:SER:HA	1:C:490:THR:HB	1.83	0.58
1:D:216:VAL:HA	1:D:247:ILE:O	2.04	0.58
1:D:271:LEU:HD13	1:D:273:ILE:HD11	1.86	0.58
1:D:629:ASP:OD2	1:D:680:ARG:NH1	2.37	0.58
2:E:352:LEU:O	2:E:356:THR:OG1	2.14	0.58
1:B:130:THR:OG1	1:B:131:PRO:HD3	2.03	0.58
1:B:152:ILE:HG21	1:B:197:PRO:CB	2.33	0.58
1:C:125:LEU:O	1:C:131:PRO:HD2	2.02	0.58
1:D:651:GLU:O	1:D:655:THR:HG23	2.03	0.58
1:D:683:ARG:HD2	2:F:458:THR:OG1	2.04	0.58
2:F:390:LEU:HD11	2:F:420:LEU:HD13	1.84	0.58
1:D:554:GLU:O	1:D:558:ASN:N	2.36	0.58
2:F:318:SER:N	2:F:452:SER:O	2.28	0.58
2:G:298:PHE:HB3	2:G:330:MET:CG	2.34	0.58
1:A:418:CYS:HA	1:A:479:PHE:CE2	2.39	0.58
1:C:152:ILE:HG12	1:C:198:LYS:HB2	1.86	0.58
1:C:314:PHE:HA	1:C:318:ASP:O	2.04	0.58
1:D:125:LEU:HD22	1:D:131:PRO:HG3	1.85	0.58
1:D:288:VAL:O	1:D:292:LEU:N	2.30	0.58
1:D:335:HIS:O	1:D:338:SER:N	2.28	0.58
1:D:420:HIS:CD2	1:D:438:LEU:HD22	2.39	0.58
1:D:648:ASP:O	1:D:652:ALA:CB	2.52	0.58
2:H:337:VAL:HG22	2:H:359:VAL:HG21	1.86	0.58
1:C:148:LEU:HG	1:C:233:PHE:HE1	1.69	0.58
1:C:488:GLY:O	1:C:490:THR:OG1	2.21	0.58
2:H:312:VAL:HB	2:H:445:TRP:HA	1.86	0.58
1:A:155:LEU:HG	1:A:198:LYS:HE2	1.86	0.58
1:B:147:PHE:CE1	1:B:225:PHE:CZ	2.92	0.58
1:B:151:LEU:O	1:B:198:LYS:HE3	2.03	0.58
1:C:147:PHE:CE2	1:C:229:VAL:HG11	2.39	0.58
1:D:125:LEU:O	1:D:131:PRO:CD	2.52	0.58
1:D:453:TYR:HH	1:D:559:PHE:HE1	1.44	0.58
2:E:287:LEU:HD22	2:E:451:TYR:HB2	1.84	0.58
2:F:352:LEU:HA	2:F:355:ILE:HG22	1.86	0.58
2:F:428:ASN:O	2:F:431:LEU:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:LEU:O	1:C:472:LEU:HG	2.03	0.57
1:D:267:VAL:HG12	1:D:271:LEU:HD11	1.86	0.57
1:B:591:HIS:CD2	2:E:445:TRP:O	2.57	0.57
1:A:302:ILE:HG23	1:A:306:VAL:HG22	1.84	0.57
1:B:152:ILE:HG21	1:B:197:PRO:CG	2.34	0.57
1:B:324:PHE:O	1:B:328:LEU:HG	2.04	0.57
1:C:379:GLN:CG	1:C:380:ALA:N	2.52	0.57
1:C:683:ARG:NH1	2:H:458:THR:HA	2.20	0.57
1:A:468:LEU:O	1:A:472:LEU:HG	2.05	0.57
1:C:480:LYS:O	1:C:484:GLU:CG	2.52	0.57
1:C:500:GLN:O	1:C:503:SER:OG	2.17	0.57
2:E:337:VAL:HG21	2:E:355:ILE:HG13	1.85	0.57
1:A:152:ILE:HG21	1:A:197:PRO:CG	2.34	0.57
1:D:302:ILE:HG23	1:D:306:VAL:HG22	1.87	0.57
2:E:331:LEU:HD11	2:E:391:LEU:HD11	1.85	0.57
2:H:317:GLY:O	2:H:319:LYS:NZ	2.38	0.57
1:B:310:LEU:O	1:B:313:ILE:HG22	2.04	0.57
1:B:326:LYS:O	1:B:330:LEU:HG	2.05	0.57
1:D:296:THR:HB	1:D:410:MET:SD	2.43	0.57
1:A:152:ILE:HG21	1:A:197:PRO:CB	2.34	0.57
1:B:480:LYS:HE2	1:B:498:LEU:HB3	1.86	0.57
1:B:685:VAL:CG1	1:B:704:VAL:HG21	2.34	0.57
1:C:310:LEU:O	1:C:313:ILE:HG22	2.05	0.57
1:D:226:ALA:O	1:D:230:LEU:N	2.38	0.57
1:D:384:GLN:O	1:D:388:LEU:HG	2.04	0.57
1:D:418:CYS:HA	1:D:479:PHE:CZ	2.39	0.57
2:H:352:LEU:HA	2:H:355:ILE:HG22	1.85	0.57
1:B:297:GLN:O	1:D:353:ARG:CZ	2.53	0.57
1:A:416:LEU:O	1:A:420:HIS:ND1	2.37	0.57
1:A:479:PHE:HA	1:A:482:TYR:HD2	1.70	0.57
1:B:376:VAL:HA	1:B:379:GLN:OE1	2.04	0.57
1:B:447:ILE:HG22	1:B:453:TYR:CG	2.40	0.57
1:B:482:TYR:O	1:B:487:LEU:N	2.33	0.57
1:C:302:ILE:HG23	1:C:306:VAL:HG22	1.85	0.57
1:D:147:PHE:O	1:D:151:LEU:HB2	2.04	0.57
1:D:230:LEU:HD21	1:D:263:LEU:HD23	1.86	0.57
1:D:98:ARG:HA	1:D:238:SER:O	2.05	0.57
2:F:337:VAL:HG22	2:F:359:VAL:HG21	1.86	0.57
2:F:323:LEU:HD22	2:F:391:LEU:HD13	1.86	0.57
2:G:331:LEU:HD11	2:G:391:LEU:HD11	1.87	0.57
1:A:310:LEU:O	1:A:313:ILE:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ARG:O	1:B:497:PHE:CD2	2.58	0.57
1:D:694:ILE:HB	1:D:704:VAL:HG13	1.86	0.57
1:C:101:PRO:O	1:C:247:ILE:HA	2.05	0.57
1:A:216:VAL:HA	1:A:247:ILE:O	2.05	0.56
1:A:271:LEU:HD13	1:A:273:ILE:HD11	1.87	0.56
2:G:323:LEU:HD22	2:G:391:LEU:HD13	1.87	0.56
1:C:155:LEU:CD1	1:C:215:VAL:HG21	2.35	0.56
1:C:563:LEU:N	1:C:567:TYR:CD2	2.73	0.56
1:A:134:VAL:HG22	1:A:154:GLN:HB3	1.87	0.56
1:A:43:ARG:NH2	1:A:342:SER:OG	2.38	0.56
1:A:560:ILE:HA	1:A:564:VAL:HB	1.88	0.56
1:C:52:GLN:O	1:C:56:SER:OG	2.12	0.56
2:F:416:HIS:O	2:F:419:TYR:CZ	2.59	0.56
2:G:352:LEU:HA	2:G:355:ILE:HG22	1.86	0.56
2:G:412:LEU:HB3	2:G:418:ILE:HD11	1.87	0.56
1:A:280:SER:O	1:A:284:HIS:ND1	2.38	0.56
1:B:494:ILE:HA	1:B:497:PHE:HD2	1.71	0.56
1:B:548:LYS:O	1:B:551:VAL:N	2.38	0.56
1:B:563:LEU:HA	1:B:567:TYR:HB2	1.86	0.56
1:D:234:ILE:O	1:D:238:SER:HB2	2.04	0.56
2:F:331:LEU:HD11	2:F:391:LEU:HD11	1.87	0.56
2:G:335:ILE:HG22	2:G:388:LEU:HA	1.87	0.56
2:G:400:LEU:O	2:G:405:SER:OG	2.23	0.56
1:A:421:LYS:HB2	1:A:479:PHE:CE2	2.40	0.56
1:A:648:ASP:HA	1:A:651:GLU:HB2	1.86	0.56
1:B:302:ILE:HG23	1:B:306:VAL:HG22	1.87	0.56
1:B:296:THR:HB	1:B:410:MET:SD	2.44	0.56
2:H:366:PHE:N	2:H:372:GLN:HG2	2.20	0.56
2:H:412:LEU:HB3	2:H:418:ILE:HD11	1.88	0.56
1:A:385:VAL:O	1:A:388:LEU:N	2.39	0.56
1:A:694:ILE:HD12	1:A:695:LYS:N	2.19	0.56
1:C:147:PHE:O	1:C:151:LEU:HB2	2.05	0.56
1:C:271:LEU:HD13	1:C:273:ILE:HD11	1.87	0.56
1:C:480:LYS:HE2	1:C:498:LEU:HB3	1.87	0.56
1:D:147:PHE:CE1	1:D:225:PHE:CZ	2.94	0.56
1:D:476:PHE:HB3	1:D:480:LYS:HE3	1.88	0.56
1:D:488:GLY:O	1:D:490:THR:OG1	2.23	0.56
1:D:64:GLU:O	1:D:67:LYS:N	2.38	0.56
2:E:412:LEU:HB3	2:E:418:ILE:HD11	1.88	0.56
2:E:304:GLN:OE1	2:E:446:TYR:OH	2.22	0.56
2:G:428:ASN:O	2:G:431:LEU:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:GLU:O	1:A:655:THR:HG23	2.05	0.56
1:C:429:TYR:CB	1:C:433:ARG:HG2	2.35	0.56
2:F:312:VAL:CG2	2:F:443:TRP:CE3	2.89	0.56
1:A:409:HIS:HA	1:A:412:TYR:HD2	1.69	0.56
1:C:296:THR:HB	1:C:410:MET:SD	2.46	0.56
1:C:447:ILE:HG22	1:C:453:TYR:CG	2.41	0.56
1:C:648:ASP:HA	1:C:651:GLU:HB2	1.88	0.56
1:D:104:ALA:HA	1:D:250:PHE:HD2	1.71	0.56
1:D:152:ILE:HG12	1:D:198:LYS:CB	2.35	0.56
1:D:412:TYR:O	1:D:415:VAL:N	2.38	0.56
1:D:446:ASN:HA	1:D:569:LEU:HD21	1.86	0.56
2:H:312:VAL:CG2	2:H:443:TRP:CE3	2.89	0.56
1:A:147:PHE:O	1:A:151:LEU:HB2	2.06	0.56
1:A:202:LYS:CE	1:A:215:VAL:HG23	2.36	0.56
1:A:230:LEU:HD21	1:A:263:LEU:HD23	1.86	0.56
1:D:147:PHE:HE1	1:D:225:PHE:CZ	2.24	0.56
1:B:330:LEU:HD21	2:E:309:PHE:CE2	2.40	0.56
1:A:482:TYR:O	1:A:486:HIS:N	2.39	0.56
1:A:46:THR:HA	1:A:49:LEU:HD12	1.88	0.56
1:B:648:ASP:HA	1:B:651:GLU:HB2	1.88	0.56
1:C:285:LEU:O	1:C:288:VAL:HG12	2.06	0.56
1:C:569:LEU:O	1:C:573:THR:CG2	2.54	0.56
1:C:64:GLU:O	1:C:67:LYS:N	2.38	0.56
2:H:305:LEU:O	2:H:419:TYR:CE1	2.59	0.56
1:A:234:ILE:O	1:A:238:SER:HB2	2.05	0.56
1:B:155:LEU:HD11	1:B:215:VAL:HG21	1.87	0.56
1:B:229:VAL:HG13	1:B:233:PHE:HE2	1.71	0.56
1:B:379:GLN:NE2	1:B:387:LEU:CD1	2.68	0.56
1:B:384:GLN:HG2	1:B:388:LEU:HD11	1.88	0.56
1:B:690:LEU:O	2:E:426:HIS:HA	2.06	0.56
1:C:458:GLN:O	1:C:462:MET:HG2	2.05	0.56
1:C:482:TYR:HA	1:C:486:HIS:ND1	2.21	0.56
1:D:148:LEU:HG	1:D:233:PHE:HE1	1.71	0.56
2:H:320:ARG:NH2	2:H:342:PHE:CZ	2.74	0.56
1:A:222:MET:HG3	1:A:250:PHE:CD1	2.41	0.55
1:A:324:PHE:O	1:A:328:LEU:HG	2.05	0.55
1:B:50:ILE:HG12	1:B:298:PHE:CD1	2.41	0.55
1:D:446:ASN:ND2	1:D:449:ASP:OD2	2.39	0.55
1:A:229:VAL:HG13	1:A:233:PHE:HE2	1.71	0.55
1:B:134:VAL:HG22	1:B:154:GLN:HB3	1.88	0.55
1:B:280:SER:O	1:B:284:HIS:ND1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLN:NE2	1:B:387:LEU:HD11	2.21	0.55
1:D:645:ASN:OD1	1:D:648:ASP:N	2.37	0.55
1:A:458:GLN:O	1:A:462:MET:HG2	2.05	0.55
1:C:155:LEU:HD12	1:C:198:LYS:CD	2.37	0.55
1:C:379:GLN:CG	1:C:380:ALA:H	1.86	0.55
1:C:464:ALA:HA	1:C:468:LEU:HD12	1.88	0.55
1:D:458:GLN:O	1:D:462:MET:HG2	2.07	0.55
2:E:352:LEU:HA	2:E:355:ILE:HG22	1.88	0.55
1:A:448:TRP:HZ2	1:A:559:PHE:HB3	1.71	0.55
1:A:695:LYS:HD2	1:A:707:LEU:HD11	1.87	0.55
1:B:464:ALA:HA	1:B:468:LEU:HD12	1.89	0.55
1:B:476:PHE:HB3	1:B:480:LYS:HE3	1.87	0.55
1:C:152:ILE:HA	1:C:198:LYS:HG3	1.87	0.55
1:D:81:HIS:CE1	1:D:214:PRO:HG3	2.41	0.55
1:D:369:LEU:HD11	1:D:576:LEU:HD23	1.87	0.55
1:D:479:PHE:HA	1:D:482:TYR:HD2	1.72	0.55
1:D:381:SER:O	1:D:383:LYS:C	2.44	0.55
1:D:43:ARG:NH2	1:D:342:SER:OG	2.39	0.55
1:D:480:LYS:HE2	1:D:498:LEU:HB3	1.88	0.55
2:E:366:PHE:O	2:E:372:GLN:CG	2.54	0.55
1:A:147:PHE:HE1	1:A:225:PHE:CZ	2.24	0.55
1:A:687:GLU:O	1:A:690:LEU:N	2.40	0.55
1:B:226:ALA:O	1:B:230:LEU:N	2.38	0.55
1:B:42:LEU:HD13	1:B:354:ARG:NH1	2.21	0.55
1:B:569:LEU:O	1:B:573:THR:CG2	2.55	0.55
1:B:645:ASN:HA	1:B:703:HIS:CE1	2.42	0.55
2:F:298:PHE:HB3	2:F:330:MET:SD	2.45	0.55
2:F:352:LEU:HD21	2:F:373:LEU:HD21	1.88	0.55
1:A:494:ILE:HA	1:A:497:PHE:HD2	1.72	0.55
1:B:152:ILE:HG21	1:B:197:PRO:CD	2.37	0.55
1:B:375:TYR:CZ	1:B:401:LEU:HD21	2.42	0.55
1:B:418:CYS:HA	1:B:479:PHE:CE2	2.42	0.55
1:B:560:ILE:HA	1:B:564:VAL:HB	1.88	0.55
1:C:429:TYR:CG	1:C:433:ARG:HG2	2.41	0.55
1:C:645:ASN:OD1	1:C:648:ASP:N	2.35	0.55
1:C:694:ILE:HD13	1:C:704:VAL:HG13	1.89	0.55
1:D:302:ILE:CG2	1:D:307:LEU:HG	2.37	0.55
2:G:295:GLU:O	2:G:298:PHE:HB2	2.07	0.55
2:G:390:LEU:HD11	2:G:420:LEU:HD13	1.89	0.55
2:H:298:PHE:HB3	2:H:330:MET:SD	2.47	0.55
2:H:325:ARG:O	2:H:329:THR:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ASN:CB	1:B:574:GLN:OE1	2.55	0.55
1:C:420:HIS:CD2	1:C:438:LEU:HD22	2.42	0.55
1:C:401:LEU:HD22	1:C:575:PRO:CG	2.37	0.55
1:C:683:ARG:NE	1:C:683:ARG:HA	2.20	0.55
1:D:464:ALA:HA	1:D:468:LEU:HD12	1.87	0.55
1:D:475:CYS:O	1:D:479:PHE:CD2	2.60	0.55
2:E:320:ARG:CZ	2:E:456:GLU:HB2	2.36	0.55
1:A:375:TYR:CZ	1:A:401:LEU:HD21	2.42	0.55
1:B:104:ALA:HA	1:B:250:PHE:HD2	1.72	0.55
1:B:202:LYS:HB2	1:B:244:PHE:CE1	2.42	0.55
1:C:234:ILE:O	1:C:238:SER:HB2	2.06	0.55
1:A:131:PRO:CB	1:A:214:PRO:O	2.55	0.54
1:B:369:LEU:HD11	1:B:576:LEU:HD23	1.89	0.54
1:C:152:ILE:HG21	1:C:197:PRO:CB	2.37	0.54
1:C:367:ARG:CZ	1:C:388:LEU:O	2.55	0.54
2:E:366:PHE:N	2:E:372:GLN:HG2	2.22	0.54
2:E:312:VAL:CG2	2:E:443:TRP:CE3	2.91	0.54
2:G:333:ASP:HB2	2:G:336:HIS:HE2	1.73	0.54
1:A:325:ILE:O	1:A:328:LEU:N	2.40	0.54
1:A:453:TYR:OH	1:A:563:LEU:CD1	2.55	0.54
1:C:367:ARG:HA	1:C:372:PHE:CE2	2.42	0.54
1:C:43:ARG:NH2	1:C:342:SER:H	2.05	0.54
1:D:229:VAL:HG13	1:D:233:PHE:HE2	1.71	0.54
2:F:305:LEU:O	2:F:419:TYR:CE1	2.61	0.54
2:G:397:SER:HB2	2:G:398:GLN:C	2.27	0.54
1:C:594:ALA:HB2	2:H:445:TRP:CE2	2.43	0.54
1:A:478:VAL:O	1:A:481:SER:HB3	2.07	0.54
1:B:285:LEU:O	1:B:288:VAL:HG12	2.07	0.54
1:B:479:PHE:HA	1:B:482:TYR:HD2	1.73	0.54
1:B:63:GLU:O	1:B:66:ASN:HB2	2.07	0.54
1:D:569:LEU:O	1:D:573:THR:CG2	2.56	0.54
2:H:337:VAL:HG21	2:H:355:ILE:HG13	1.88	0.54
1:A:128:ASN:HB2	1:A:130:THR:OG1	2.07	0.54
1:A:152:ILE:HG12	1:A:198:LYS:CB	2.37	0.54
1:A:369:LEU:HD11	1:A:576:LEU:HD23	1.90	0.54
1:A:352:LYS:NZ	1:A:403:GLU:OE2	2.30	0.54
1:A:476:PHE:HB3	1:A:480:LYS:HE3	1.90	0.54
1:B:45:GLU:O	1:B:49:LEU:HG	2.08	0.54
1:C:480:LYS:HE2	1:C:498:LEU:CB	2.38	0.54
1:D:63:GLU:O	1:D:66:ASN:HB2	2.07	0.54
2:E:325:ARG:O	2:E:329:THR:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:366:PHE:O	2:G:372:GLN:CG	2.55	0.54
2:H:320:ARG:CZ	2:H:456:GLU:HB2	2.37	0.54
1:B:330:LEU:O	1:B:334:GLU:CB	2.56	0.54
1:C:125:LEU:HD22	1:C:131:PRO:HG3	1.90	0.54
1:C:250:PHE:HB3	1:C:252:ILE:CD1	2.38	0.54
1:C:649:TRP:HZ3	1:C:704:VAL:HB	1.73	0.54
1:D:152:ILE:HG23	1:D:198:LYS:N	2.23	0.54
1:D:202:LYS:CD	1:D:244:PHE:CE1	2.91	0.54
2:E:298:PHE:HB3	2:E:330:MET:HG3	1.90	0.54
2:F:366:PHE:N	2:F:372:GLN:HG2	2.22	0.54
1:A:138:ALA:HB2	1:A:221:ASP:O	2.07	0.54
1:A:330:LEU:O	1:A:334:GLU:HB2	2.07	0.54
1:A:412:TYR:O	1:A:415:VAL:N	2.41	0.54
1:C:267:VAL:HG12	1:C:271:LEU:HD11	1.90	0.54
1:A:152:ILE:HG21	1:A:197:PRO:CD	2.38	0.54
1:A:267:VAL:HG12	1:A:271:LEU:HD11	1.89	0.54
1:A:330:LEU:O	1:A:334:GLU:CB	2.56	0.54
1:B:152:ILE:HG12	1:B:198:LYS:CB	2.38	0.54
1:B:421:LYS:HB2	1:B:479:PHE:CE2	2.43	0.54
1:B:420:HIS:CD2	1:B:438:LEU:HD22	2.43	0.54
1:C:479:PHE:HA	1:C:482:TYR:HD2	1.73	0.54
1:C:645:ASN:HA	1:C:703:HIS:CE1	2.42	0.54
1:D:420:HIS:NE2	1:D:438:LEU:HB2	2.21	0.54
1:D:417:ARG:O	1:D:479:PHE:CZ	2.60	0.54
1:D:152:ILE:HG12	1:D:198:LYS:H	1.71	0.54
1:A:480:LYS:HE2	1:A:498:LEU:HB3	1.90	0.54
1:B:202:LYS:CE	1:B:215:VAL:HG23	2.38	0.54
1:C:685:VAL:CG1	1:C:704:VAL:HG21	2.38	0.54
2:E:339:ILE:HD13	2:E:351:VAL:HG13	1.90	0.54
2:F:339:ILE:HD13	2:F:351:VAL:HG13	1.90	0.54
1:B:646:LEU:HA	1:B:649:TRP:HB3	1.90	0.54
1:D:199:MET:CE	1:D:244:PHE:CE2	2.91	0.54
2:E:352:LEU:HD21	2:E:373:LEU:HD21	1.90	0.54
2:F:287:LEU:HD22	2:F:451:TYR:HB2	1.90	0.54
1:A:230:LEU:HD11	1:A:263:LEU:HD22	1.89	0.53
1:A:342:SER:O	1:A:345:CYS:N	2.32	0.53
1:A:46:THR:O	1:A:50:ILE:HG13	2.09	0.53
1:D:141:CYS:HB3	1:D:147:PHE:CE2	2.43	0.53
1:D:683:ARG:CZ	1:D:686:SER:OG	2.56	0.53
2:H:335:ILE:HG22	2:H:388:LEU:HA	1.89	0.53
1:A:420:HIS:NE2	1:A:435:ILE:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:O	1:B:131:PRO:HD2	2.09	0.53
1:B:234:ILE:O	1:B:238:SER:HB3	2.08	0.53
1:C:401:LEU:HD22	1:C:575:PRO:HG3	1.89	0.53
2:E:320:ARG:NH2	2:E:342:PHE:CZ	2.75	0.53
2:F:320:ARG:NH2	2:F:342:PHE:CZ	2.76	0.53
2:G:352:LEU:HD21	2:G:373:LEU:HD21	1.89	0.53
2:H:302:MET:HA	2:H:305:LEU:HD12	1.89	0.53
1:A:99:GLU:C	1:A:241:LEU:CD1	2.77	0.53
1:D:409:HIS:HA	1:D:412:TYR:HD2	1.73	0.53
1:D:478:VAL:O	1:D:481:SER:HB3	2.08	0.53
2:E:305:LEU:O	2:E:419:TYR:CE1	2.60	0.53
1:B:142:PRO:HD2	1:B:146:HIS:ND1	2.24	0.53
1:B:145:LYS:HZ1	1:B:194:LYS:HE2	1.74	0.53
1:B:222:MET:HG3	1:B:250:PHE:CE1	2.43	0.53
1:B:271:LEU:HD13	1:B:273:ILE:HD11	1.90	0.53
1:C:548:LYS:O	1:C:552:LEU:N	2.39	0.53
1:D:401:LEU:HD22	1:D:575:PRO:CG	2.38	0.53
1:B:685:VAL:HG11	1:B:704:VAL:HG21	1.90	0.53
1:C:155:LEU:HD12	1:C:198:LYS:HD3	1.90	0.53
1:C:478:VAL:O	1:C:481:SER:HB3	2.07	0.53
1:C:562:CYS:CB	1:C:567:TYR:HE2	2.21	0.53
1:D:604:LEU:CD1	1:D:693:PHE:CZ	2.91	0.53
1:D:694:ILE:HD12	1:D:695:LYS:N	2.24	0.53
2:F:397:SER:HB2	2:F:398:GLN:C	2.29	0.53
1:A:591:HIS:CE1	2:G:446:TYR:CD1	2.96	0.53
2:H:446:TYR:CB	2:H:448:THR:HG23	2.38	0.53
1:A:226:ALA:O	1:A:230:LEU:N	2.40	0.53
1:A:453:TYR:OH	1:A:559:PHE:CE1	2.60	0.53
1:A:493:ARG:O	1:A:497:PHE:CD2	2.62	0.53
1:A:685:VAL:HG11	1:A:704:VAL:HG21	1.90	0.53
1:B:101:PRO:HA	1:B:272:CYS:HB3	1.89	0.53
1:B:694:ILE:HD12	1:B:695:LYS:N	2.23	0.53
1:C:494:ILE:O	1:C:498:LEU:HG	2.08	0.53
1:D:330:LEU:CD1	1:D:592:LEU:HD21	2.39	0.53
1:D:695:LYS:HG3	1:D:696:PRO:CD	2.38	0.53
2:E:298:PHE:HB3	2:E:330:MET:CG	2.38	0.53
2:G:320:ARG:HH22	2:G:457:GLU:N	2.06	0.53
2:G:340:ASN:HB3	2:G:342:PHE:CE2	2.44	0.53
1:A:209:GLN:HE22	1:A:213:PRO:HG3	1.72	0.53
1:A:330:LEU:HD13	1:A:592:LEU:HD21	1.91	0.53
1:B:234:ILE:O	1:B:238:SER:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:LEU:HG	1:D:198:LYS:HE2	1.91	0.53
1:D:429:TYR:CB	1:D:433:ARG:HG2	2.39	0.53
1:D:685:VAL:CG1	1:D:704:VAL:HG21	2.39	0.53
2:H:311:ILE:HB	2:H:446:TYR:CE2	2.44	0.53
1:B:148:LEU:O	1:B:151:LEU:HB3	2.09	0.53
1:B:155:LEU:HG	1:B:198:LYS:HE2	1.91	0.53
1:B:420:HIS:NE2	1:B:438:LEU:HB2	2.24	0.53
1:C:476:PHE:HB3	1:C:480:LYS:HE3	1.91	0.53
1:D:152:ILE:HG12	1:D:198:LYS:HB2	1.91	0.53
1:D:244:PHE:O	1:D:246:LEU:N	2.40	0.53
1:D:452:GLU:OE1	1:D:452:GLU:N	2.31	0.53
1:D:46:THR:O	1:D:50:ILE:HG13	2.08	0.53
1:D:687:GLU:O	1:D:690:LEU:N	2.42	0.53
2:H:416:HIS:O	2:H:419:TYR:CZ	2.61	0.53
1:A:464:ALA:HA	1:A:468:LEU:HD12	1.91	0.53
1:B:385:VAL:O	1:B:388:LEU:N	2.42	0.53
1:B:43:ARG:NH2	1:B:342:SER:H	2.07	0.53
1:B:687:GLU:O	1:B:690:LEU:N	2.42	0.53
1:B:99:GLU:C	1:B:241:LEU:CD1	2.77	0.53
1:C:335:HIS:CE1	1:C:579:VAL:HA	2.43	0.53
1:D:219:LEU:HB2	1:D:222:MET:HG2	1.91	0.53
1:D:418:CYS:SG	1:D:422:PHE:HE2	2.32	0.53
1:D:694:ILE:HD13	1:D:704:VAL:HG13	1.91	0.53
2:E:302:MET:HA	2:E:305:LEU:HD12	1.91	0.53
2:G:320:ARG:CZ	2:G:456:GLU:HB2	2.38	0.53
2:H:327:ARG:HA	2:H:331:LEU:HB2	1.91	0.53
1:A:147:PHE:CE2	1:A:229:VAL:HG11	2.43	0.53
1:A:483:CYS:HA	1:A:487:LEU:O	2.09	0.53
1:A:556:VAL:CA	1:A:559:PHE:HD2	2.21	0.53
1:B:268:SER:HA	1:B:271:LEU:HD12	1.91	0.53
1:B:412:TYR:O	1:B:415:VAL:N	2.40	0.53
1:C:330:LEU:O	1:C:334:GLU:HB2	2.09	0.53
1:C:369:LEU:HD11	1:C:576:LEU:HD23	1.90	0.53
1:D:563:LEU:HA	1:D:567:TYR:HB2	1.89	0.53
2:E:377:VAL:O	2:E:381:LYS:N	2.32	0.53
2:G:365:THR:HB	2:G:372:GLN:CD	2.29	0.53
1:A:387:LEU:HD22	1:A:394:LEU:HD13	1.90	0.52
1:A:403:GLU:O	1:A:407:VAL:HG23	2.08	0.52
1:A:301:LYS:N	1:A:580:VAL:O	2.39	0.52
1:B:152:ILE:HG23	1:B:198:LYS:N	2.24	0.52
1:B:429:TYR:CG	1:B:433:ARG:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD23	1:D:45:GLU:OE2	2.09	0.52
1:C:147:PHE:HE1	1:C:225:PHE:CZ	2.27	0.52
1:C:230:LEU:HD21	1:C:263:LEU:HD23	1.89	0.52
2:G:339:ILE:HD13	2:G:351:VAL:HG22	1.90	0.52
2:G:318:SER:N	2:G:452:SER:O	2.30	0.52
1:A:132:TYR:O	1:A:155:LEU:HD21	2.09	0.52
1:A:421:LYS:NZ	1:A:479:PHE:CD1	2.71	0.52
1:A:404:ASN:C	1:A:574:GLN:OE1	2.48	0.52
1:B:403:GLU:O	1:B:407:VAL:HG23	2.08	0.52
1:B:429:TYR:CB	1:B:433:ARG:HG2	2.39	0.52
1:B:478:VAL:O	1:B:481:SER:HB3	2.08	0.52
1:D:480:LYS:HE2	1:D:498:LEU:CB	2.39	0.52
2:E:348:VAL:HA	2:E:351:VAL:HB	1.90	0.52
1:C:155:LEU:CD1	1:C:198:LYS:HE2	2.39	0.52
1:C:238:SER:HA	1:C:241:LEU:HG	1.92	0.52
1:C:403:GLU:O	1:C:407:VAL:HG23	2.09	0.52
1:B:347:ASN:OD1	1:D:350:GLU:HG3	2.09	0.52
2:G:314:TYR:N	2:G:448:THR:OG1	2.43	0.52
1:A:101:PRO:O	1:A:247:ILE:HA	2.10	0.52
1:A:133:VAL:N	1:A:158:CYS:SG	2.83	0.52
1:A:368:ARG:O	1:A:373:ARG:HG3	2.09	0.52
1:C:144:MET:SD	1:C:233:PHE:CE2	3.02	0.52
1:C:461:ARG:HG2	1:C:552:LEU:CD2	2.39	0.52
2:E:295:GLU:O	2:E:298:PHE:HB2	2.10	0.52
2:E:373:LEU:O	2:E:377:VAL:HB	2.10	0.52
2:F:454:TYR:O	2:F:458:THR:OG1	2.23	0.52
2:H:365:THR:HB	2:H:372:GLN:CD	2.30	0.52
1:A:296:THR:HG22	1:A:413:PHE:CD2	2.45	0.52
1:A:371:SER:HA	1:A:374:ARG:HB2	1.91	0.52
1:B:97:LEU:HA	1:B:242:HIS:CG	2.45	0.52
1:B:448:TRP:HZ2	1:B:559:PHE:HB3	1.74	0.52
1:B:405:LEU:HD23	1:B:574:GLN:HB2	1.92	0.52
1:C:368:ARG:O	1:C:373:ARG:HG3	2.09	0.52
1:C:412:TYR:O	1:C:415:VAL:N	2.41	0.52
1:C:417:ARG:HD3	1:C:482:TYR:CE1	2.43	0.52
1:C:493:ARG:O	1:C:497:PHE:CD2	2.62	0.52
1:D:155:LEU:CD1	1:D:215:VAL:HG21	2.40	0.52
1:D:448:TRP:CZ2	1:D:559:PHE:HB3	2.44	0.52
2:E:347:SER:N	2:E:350:SER:OG	2.38	0.52
2:E:390:LEU:HD11	2:E:420:LEU:HD13	1.92	0.52
1:A:100:ILE:O	1:A:270:LEU:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:HIS:CD2	1:A:438:LEU:HD22	2.43	0.52
1:B:302:ILE:CG2	1:B:307:LEU:HG	2.40	0.52
1:B:468:LEU:O	1:B:472:LEU:HG	2.09	0.52
1:D:649:TRP:HZ3	1:D:704:VAL:HB	1.75	0.52
1:C:367:ARG:NE	1:C:388:LEU:O	2.43	0.52
1:D:369:LEU:HD13	1:D:370:PRO:O	2.10	0.52
2:F:304:GLN:OE1	2:F:446:TYR:OH	2.26	0.52
2:F:302:MET:HA	2:F:305:LEU:HD12	1.92	0.52
2:G:416:HIS:O	2:G:419:TYR:CZ	2.62	0.52
2:H:333:ASP:HB2	2:H:336:HIS:HE2	1.74	0.52
1:A:335:HIS:CE1	1:A:579:VAL:HA	2.45	0.52
1:B:202:LYS:HD2	1:B:244:PHE:CD1	2.45	0.52
1:B:342:SER:O	1:B:345:CYS:N	2.33	0.52
1:B:420:HIS:O	1:B:424:SER:N	2.28	0.52
1:C:144:MET:SD	1:C:232:ASP:HB2	2.49	0.52
1:C:420:HIS:NE2	1:C:438:LEU:HB2	2.25	0.52
1:C:446:ASN:HA	1:C:569:LEU:HD21	1.92	0.52
1:D:131:PRO:CB	1:D:214:PRO:O	2.57	0.52
1:D:330:LEU:O	1:D:334:GLU:HB2	2.10	0.52
1:D:368:ARG:O	1:D:373:ARG:HG3	2.10	0.52
1:D:453:TYR:OH	1:D:559:PHE:CD1	2.60	0.52
2:F:391:LEU:CD2	2:F:421:ILE:HB	2.40	0.52
2:G:337:VAL:HG21	2:G:355:ILE:HG13	1.92	0.52
1:A:429:TYR:CB	1:A:433:ARG:HG2	2.40	0.52
1:A:417:ARG:O	1:A:479:PHE:CZ	2.62	0.52
1:A:548:LYS:O	1:A:551:VAL:N	2.43	0.52
1:B:122:THR:HA	1:B:133:VAL:CG2	2.40	0.52
1:B:367:ARG:HA	1:B:372:PHE:CE2	2.45	0.52
1:B:66:ASN:HB3	1:B:70:PHE:CD2	2.44	0.52
1:C:384:GLN:O	1:C:387:LEU:HB2	2.10	0.52
1:D:147:PHE:CE2	1:D:229:VAL:HG11	2.45	0.52
1:D:288:VAL:CG2	1:D:292:LEU:HD12	2.40	0.52
2:E:347:SER:H	2:E:350:SER:HG	1.56	0.52
1:B:497:PHE:HB3	1:B:501:PHE:HE2	1.75	0.52
1:C:694:ILE:HD12	1:C:695:LYS:N	2.24	0.52
1:D:314:PHE:HD2	1:D:324:PHE:HB2	1.74	0.52
1:D:448:TRP:HZ2	1:D:559:PHE:HB3	1.74	0.52
2:E:397:SER:HB2	2:E:398:GLN:C	2.30	0.52
2:F:365:THR:HB	2:F:372:GLN:CD	2.30	0.52
2:H:352:LEU:HD21	2:H:373:LEU:HD21	1.91	0.52
1:A:554:GLU:O	1:A:558:ASN:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ARG:NH1	2:G:458:THR:HA	2.25	0.51
1:B:132:TYR:O	1:B:155:LEU:HD21	2.10	0.51
1:B:101:PRO:O	1:B:247:ILE:HA	2.10	0.51
1:B:337:TYR:OH	2:E:307:LEU:HD11	2.10	0.51
1:B:480:LYS:HE2	1:B:498:LEU:CB	2.41	0.51
1:C:133:VAL:N	1:C:158:CYS:SG	2.82	0.51
1:C:152:ILE:HD12	1:C:194:LYS:O	2.09	0.51
1:C:591:HIS:HA	2:H:445:TRP:H	1.75	0.51
1:D:202:LYS:CD	1:D:244:PHE:HE1	2.23	0.51
1:D:421:LYS:HZ3	1:D:478:VAL:HB	1.75	0.51
1:D:418:CYS:HA	1:D:479:PHE:CE2	2.45	0.51
1:D:691:LEU:O	2:F:427:LEU:N	2.39	0.51
1:D:99:GLU:C	1:D:241:LEU:CD1	2.79	0.51
2:F:325:ARG:O	2:F:329:THR:N	2.41	0.51
2:F:337:VAL:HG21	2:F:355:ILE:HG13	1.92	0.51
2:F:366:PHE:O	2:F:372:GLN:CG	2.58	0.51
1:A:63:GLU:O	1:A:66:ASN:HB2	2.11	0.51
1:A:685:VAL:CG1	1:A:704:VAL:HG21	2.40	0.51
1:B:152:ILE:HG12	1:B:198:LYS:HG3	1.92	0.51
1:B:330:LEU:O	1:B:334:GLU:HB2	2.10	0.51
1:B:404:ASN:C	1:B:574:GLN:OE1	2.49	0.51
1:C:226:ALA:HB3	1:C:229:VAL:HB	1.92	0.51
1:C:342:SER:O	1:C:345:CYS:N	2.35	0.51
1:C:409:HIS:HA	1:C:412:TYR:HD2	1.76	0.51
1:D:101:PRO:O	1:D:247:ILE:HA	2.10	0.51
1:D:325:ILE:O	1:D:328:LEU:N	2.41	0.51
1:D:556:VAL:CA	1:D:559:PHE:HD2	2.23	0.51
2:G:420:LEU:HD12	2:G:421:ILE:N	2.25	0.51
1:A:152:ILE:HG23	1:A:198:LYS:N	2.25	0.51
1:A:288:VAL:O	1:A:292:LEU:N	2.33	0.51
1:A:480:LYS:HE2	1:A:498:LEU:CB	2.40	0.51
1:A:569:LEU:O	1:A:573:THR:CG2	2.59	0.51
1:B:683:ARG:HG3	1:B:687:GLU:OE2	2.11	0.51
1:C:683:ARG:NE	2:H:458:THR:HG23	2.26	0.51
1:D:148:LEU:O	1:D:151:LEU:HB3	2.09	0.51
1:D:385:VAL:O	1:D:388:LEU:N	2.44	0.51
1:D:494:ILE:O	1:D:498:LEU:HG	2.10	0.51
1:D:645:ASN:OD1	1:D:648:ASP:HB2	2.10	0.51
1:A:152:ILE:HA	1:A:198:LYS:HG3	1.93	0.51
1:A:234:ILE:O	1:A:238:SER:HB3	2.10	0.51
1:B:401:LEU:HD22	1:B:575:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ALA:O	1:C:249:ILE:HA	2.11	0.51
1:C:405:LEU:HD23	1:C:574:GLN:HB2	1.93	0.51
1:D:461:ARG:HG2	1:D:552:LEU:CD2	2.40	0.51
1:D:482:TYR:O	1:D:487:LEU:N	2.36	0.51
1:A:333:LEU:HD13	2:G:307:LEU:HD13	1.92	0.51
1:A:110:ASN:HB3	1:A:281:CYS:SG	2.51	0.51
1:A:155:LEU:HD12	1:A:198:LYS:CD	2.41	0.51
1:B:421:LYS:HZ3	1:B:478:VAL:HB	1.75	0.51
1:B:645:ASN:OD1	1:B:648:ASP:HB2	2.10	0.51
1:C:244:PHE:CD2	1:C:246:LEU:HD11	2.15	0.51
1:C:453:TYR:OH	1:C:563:LEU:HD13	2.11	0.51
1:D:285:LEU:O	1:D:288:VAL:HG12	2.10	0.51
1:D:330:LEU:O	1:D:334:GLU:CB	2.58	0.51
1:D:429:TYR:CG	1:D:433:ARG:HG2	2.45	0.51
2:H:366:PHE:O	2:H:372:GLN:CG	2.58	0.51
2:H:397:SER:HB2	2:H:398:GLN:C	2.30	0.51
1:C:590:GLU:O	2:H:445:TRP:O	2.28	0.51
1:C:267:VAL:O	1:C:271:LEU:HG	2.11	0.51
1:C:387:LEU:HA	1:C:394:LEU:HB2	1.92	0.51
1:C:694:ILE:HB	1:C:704:VAL:HG13	1.92	0.51
1:D:306:VAL:HG12	1:D:585:ALA:HB2	1.91	0.51
1:D:330:LEU:HD13	1:D:592:LEU:HD21	1.93	0.51
1:D:405:LEU:HD23	1:D:574:GLN:HB2	1.93	0.51
2:E:416:HIS:O	2:E:419:TYR:CZ	2.64	0.51
2:H:339:ILE:HD13	2:H:351:VAL:HG13	1.93	0.51
1:A:401:LEU:HD22	1:A:575:PRO:CG	2.41	0.51
1:B:267:VAL:HG12	1:B:271:LEU:HD11	1.92	0.51
1:B:553:ARG:O	1:B:557:VAL:HG23	2.11	0.51
1:C:134:VAL:HG22	1:C:154:GLN:HB3	1.91	0.51
1:C:99:GLU:N	1:C:241:LEU:HD12	2.25	0.51
1:C:497:PHE:CE1	1:C:557:VAL:HG13	2.46	0.51
2:E:365:THR:HB	2:E:372:GLN:CD	2.31	0.51
1:A:202:LYS:CD	1:A:244:PHE:CE1	2.92	0.51
1:A:694:ILE:HA	1:A:706:ARG:HA	1.93	0.51
1:B:556:VAL:CA	1:B:559:PHE:HD2	2.22	0.51
1:C:268:SER:HA	1:C:271:LEU:HD12	1.92	0.51
1:C:371:SER:O	1:C:575:PRO:HB3	2.10	0.51
1:D:222:MET:SD	1:D:225:PHE:CE2	3.04	0.51
1:D:367:ARG:HA	1:D:372:PHE:CE2	2.46	0.51
1:D:563:LEU:HA	1:D:567:TYR:CD2	2.46	0.51
2:E:318:SER:HA	2:E:319:LYS:HZ1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:HG12	1:A:198:LYS:H	1.76	0.51
1:A:199:MET:CE	1:A:244:PHE:HE2	2.24	0.51
1:A:563:LEU:HA	1:A:567:TYR:HB2	1.92	0.51
1:B:417:ARG:O	1:B:479:PHE:CZ	2.63	0.51
1:B:683:ARG:HD2	2:E:458:THR:OG1	2.11	0.51
1:C:306:VAL:HG12	1:C:585:ALA:HB2	1.93	0.51
1:D:128:ASN:O	1:D:129:VAL:HB	2.11	0.51
1:D:293:LEU:HD21	1:D:328:LEU:HD13	1.92	0.51
1:D:563:LEU:HA	1:D:567:TYR:HD2	1.76	0.51
2:F:373:LEU:O	2:F:377:VAL:HB	2.11	0.51
1:C:326:LYS:HB3	2:H:442:ASN:HD21	1.76	0.51
1:A:98:ARG:HA	1:A:238:SER:O	2.10	0.51
1:A:553:ARG:O	1:A:557:VAL:HG23	2.10	0.51
1:A:689:GLU:CG	1:A:694:ILE:HD11	2.41	0.51
1:D:342:SER:O	1:D:345:CYS:N	2.31	0.51
1:C:693:PHE:CZ	2:H:427:LEU:HD21	2.46	0.51
2:H:446:TYR:HB3	2:H:448:THR:HG23	1.93	0.51
1:A:286:THR:HG22	1:A:436:ARG:HE	1.76	0.50
1:A:421:LYS:HZ3	1:A:478:VAL:HB	1.75	0.50
1:A:482:TYR:O	1:A:487:LEU:N	2.32	0.50
1:A:556:VAL:O	1:A:560:ILE:N	2.42	0.50
1:B:446:ASN:OD1	1:B:569:LEU:HD11	2.12	0.50
1:C:404:ASN:CB	1:C:574:GLN:OE1	2.59	0.50
1:C:66:ASN:HB3	1:C:70:PHE:CD2	2.46	0.50
1:D:252:ILE:HD13	1:D:259:ILE:HD11	1.92	0.50
1:D:281:CYS:HB3	1:D:319:PHE:O	2.10	0.50
1:D:691:LEU:O	2:F:426:HIS:HA	2.11	0.50
1:B:693:PHE:CZ	2:E:427:LEU:HD21	2.46	0.50
1:A:152:ILE:HG12	1:A:198:LYS:HB2	1.93	0.50
1:A:202:LYS:CD	1:A:244:PHE:HE1	2.23	0.50
1:A:367:ARG:HA	1:A:372:PHE:CE2	2.46	0.50
1:A:404:ASN:CB	1:A:574:GLN:OE1	2.59	0.50
1:B:132:TYR:O	1:B:155:LEU:CD2	2.59	0.50
1:B:288:VAL:CG2	1:B:292:LEU:HD12	2.42	0.50
1:B:415:VAL:O	1:B:418:CYS:HB3	2.11	0.50
1:C:44:PHE:HA	1:C:47:TYR:HB3	1.93	0.50
1:D:478:VAL:O	1:D:482:TYR:HD2	1.94	0.50
1:D:695:LYS:CG	1:D:696:PRO:HD2	2.41	0.50
1:D:66:ASN:HB3	1:D:70:PHE:CD2	2.45	0.50
1:D:71:ASP:O	1:D:75:GLU:CG	2.59	0.50
2:H:455:THR:CA	2:H:458:THR:HB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:CG	1:A:198:LYS:HE2	2.42	0.50
1:A:342:SER:OG	1:A:579:VAL:HG13	2.12	0.50
1:B:369:LEU:HD13	1:B:370:PRO:O	2.11	0.50
1:B:562:CYS:HB3	1:B:567:TYR:CE2	2.46	0.50
1:C:330:LEU:O	1:C:334:GLU:HB3	2.12	0.50
2:E:409:ILE:HG22	2:E:441:PHE:CE1	2.47	0.50
2:H:373:LEU:O	2:H:377:VAL:HB	2.11	0.50
1:A:683:ARG:CZ	2:G:458:THR:HG23	2.42	0.50
1:B:415:VAL:HG12	1:B:567:TYR:CE1	2.46	0.50
1:B:552:LEU:O	1:B:556:VAL:HG23	2.11	0.50
1:B:555:ASN:C	1:B:559:PHE:CD2	2.85	0.50
1:C:372:PHE:HA	1:C:375:TYR:HB3	1.92	0.50
1:C:591:HIS:HA	2:H:445:TRP:N	2.26	0.50
1:C:687:GLU:O	1:C:690:LEU:N	2.44	0.50
1:D:230:LEU:HD11	1:D:263:LEU:HD22	1.94	0.50
1:D:555:ASN:HA	1:D:558:ASN:HB2	1.94	0.50
2:F:373:LEU:CD2	2:F:412:LEU:HD21	2.42	0.50
2:H:400:LEU:O	2:H:405:SER:OG	2.29	0.50
2:H:412:LEU:HB3	2:H:418:ILE:CD1	2.42	0.50
1:A:429:TYR:CG	1:A:433:ARG:HG2	2.46	0.50
1:A:43:ARG:NH2	1:A:342:SER:H	2.10	0.50
1:A:707:LEU:N	1:A:707:LEU:HD12	2.26	0.50
1:A:66:ASN:HB3	1:A:70:PHE:CD2	2.46	0.50
1:B:148:LEU:HG	1:B:233:PHE:HE1	1.77	0.50
1:B:504:LEU:HD11	1:B:554:GLU:CD	2.32	0.50
1:C:355:ILE:HA	1:C:358:LEU:HG	1.94	0.50
1:D:366:ILE:O	1:D:372:PHE:CD2	2.64	0.50
1:D:43:ARG:NH2	1:D:342:SER:H	2.10	0.50
1:D:371:SER:OG	1:D:576:LEU:N	2.42	0.50
2:F:348:VAL:HA	2:F:351:VAL:HB	1.92	0.50
2:H:331:LEU:HB3	2:H:336:HIS:CG	2.47	0.50
2:H:410:GLY:O	2:H:414:SER:CB	2.59	0.50
1:A:202:LYS:HB2	1:A:244:PHE:CE1	2.47	0.50
1:B:155:LEU:HD12	1:B:198:LYS:CD	2.42	0.50
1:B:364:GLU:HA	1:B:367:ARG:HD2	1.93	0.50
1:B:597:ARG:NH2	1:B:708:THR:OG1	2.45	0.50
1:C:102:THR:HA	1:C:247:ILE:HG23	1.94	0.50
1:C:100:ILE:CG1	1:C:241:LEU:HD21	2.42	0.50
1:D:403:GLU:O	1:D:407:VAL:HG23	2.12	0.50
2:E:311:ILE:HD11	2:E:421:ILE:HG23	1.93	0.50
2:E:420:LEU:HD12	2:E:421:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:420:LEU:HD21	2:E:443:TRP:CH2	2.47	0.50
2:F:352:LEU:CD2	2:F:369:ILE:HG23	2.42	0.50
2:G:320:ARG:NH2	2:G:457:GLU:N	2.60	0.50
2:H:348:VAL:HA	2:H:351:VAL:HB	1.93	0.50
1:A:645:ASN:OD1	1:A:648:ASP:HB2	2.11	0.50
1:B:102:THR:OG1	1:B:273:ILE:HG12	2.11	0.50
1:B:152:ILE:HG12	1:B:198:LYS:H	1.76	0.50
1:B:306:VAL:O	1:B:310:LEU:HD13	2.11	0.50
1:C:81:HIS:CE1	1:C:214:PRO:HG3	2.46	0.50
1:C:219:LEU:HB2	1:C:222:MET:CG	2.41	0.50
1:C:478:VAL:O	1:C:482:TYR:HD2	1.95	0.50
1:C:482:TYR:O	1:C:487:LEU:N	2.34	0.50
1:C:548:LYS:O	1:C:551:VAL:N	2.45	0.50
1:D:148:LEU:HA	1:D:151:LEU:CD2	2.42	0.50
1:D:155:LEU:HD12	1:D:198:LYS:CD	2.42	0.50
1:D:386:ALA:O	1:D:390:ASN:O	2.29	0.50
1:D:553:ARG:O	1:D:557:VAL:HG23	2.11	0.50
1:A:148:LEU:O	1:A:151:LEU:HB3	2.12	0.50
1:A:219:LEU:HB2	1:A:222:MET:HG2	1.93	0.50
1:A:405:LEU:HD23	1:A:574:GLN:HB2	1.94	0.50
1:C:288:VAL:CG2	1:C:292:LEU:HD12	2.42	0.50
1:D:222:MET:HG3	1:D:250:PHE:HD1	1.75	0.50
1:D:329:GLN:O	1:D:332:LEU:N	2.44	0.50
2:E:355:ILE:O	2:E:360:LEU:HB2	2.12	0.50
2:F:339:ILE:HD13	2:F:351:VAL:HG22	1.93	0.50
1:A:369:LEU:HD13	1:A:370:PRO:O	2.12	0.50
1:A:379:GLN:CG	1:A:380:ALA:N	2.51	0.50
1:A:418:CYS:O	1:A:422:PHE:CD2	2.65	0.50
1:A:504:LEU:HD11	1:A:554:GLU:CD	2.32	0.50
1:A:446:ASN:HA	1:A:569:LEU:HD21	1.94	0.50
1:A:683:ARG:HD2	2:G:458:THR:OG1	2.12	0.50
1:B:306:VAL:HG12	1:B:585:ALA:HB2	1.93	0.50
1:B:404:ASN:O	1:B:407:VAL:HB	2.12	0.50
1:B:418:CYS:O	1:B:422:PHE:CD2	2.65	0.50
1:C:229:VAL:HG13	1:C:233:PHE:CE2	2.45	0.50
1:C:448:TRP:CZ2	1:C:559:PHE:HB3	2.45	0.50
1:C:604:LEU:CD1	1:C:693:PHE:CZ	2.95	0.50
1:D:493:ARG:O	1:D:497:PHE:CD2	2.64	0.50
2:E:298:PHE:CD2	2:E:330:MET:HG2	2.46	0.50
2:G:325:ARG:O	2:G:329:THR:N	2.39	0.50
2:G:369:ILE:HG12	2:G:372:GLN:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:320:ARG:NH2	2:H:457:GLU:N	2.60	0.50
1:A:244:PHE:O	1:A:246:LEU:N	2.41	0.49
1:A:330:LEU:CD1	1:A:592:LEU:HD21	2.42	0.49
1:A:645:ASN:OD1	1:A:648:ASP:N	2.37	0.49
1:B:297:GLN:O	1:D:353:ARG:NH2	2.44	0.49
1:B:418:CYS:SG	1:B:422:PHE:HE2	2.35	0.49
1:B:497:PHE:O	1:B:501:PHE:HD2	1.95	0.49
1:B:588:LEU:O	1:B:592:LEU:N	2.46	0.49
1:C:330:LEU:CD1	1:C:592:LEU:HD21	2.42	0.49
1:C:63:GLU:O	1:C:66:ASN:HB2	2.11	0.49
2:F:355:ILE:O	2:F:360:LEU:HB2	2.12	0.49
2:G:312:VAL:CG2	2:G:443:TRP:CE3	2.95	0.49
2:G:339:ILE:HD13	2:G:351:VAL:HG13	1.94	0.49
2:G:311:ILE:HD11	2:G:421:ILE:HG23	1.94	0.49
1:A:372:PHE:HA	1:A:375:TYR:HB3	1.94	0.49
1:A:461:ARG:HG2	1:A:552:LEU:CD2	2.42	0.49
1:A:494:ILE:O	1:A:498:LEU:HG	2.12	0.49
1:B:128:ASN:O	1:B:129:VAL:HB	2.12	0.49
1:B:255:SER:HB2	1:B:256:PRO:HD3	1.94	0.49
1:C:562:CYS:C	1:C:567:TYR:HD2	2.15	0.49
1:C:562:CYS:CB	1:C:567:TYR:CE2	2.90	0.49
2:E:317:GLY:O	2:E:319:LYS:NZ	2.44	0.49
2:G:302:MET:HA	2:G:305:LEU:HD12	1.94	0.49
1:B:125:LEU:HD22	1:B:131:PRO:HG3	1.94	0.49
1:B:148:LEU:HA	1:B:151:LEU:HD22	1.95	0.49
1:B:252:ILE:HD13	1:B:259:ILE:HD11	1.94	0.49
1:B:267:VAL:O	1:B:271:LEU:HG	2.13	0.49
1:B:314:PHE:HA	1:B:318:ASP:O	2.12	0.49
1:B:419:LEU:HB2	1:B:567:TYR:CE1	2.47	0.49
1:D:134:VAL:HG22	1:D:154:GLN:HB3	1.93	0.49
1:D:482:TYR:HA	1:D:486:HIS:ND1	2.28	0.49
1:D:560:ILE:HA	1:D:564:VAL:HB	1.93	0.49
2:F:311:ILE:HD11	2:F:421:ILE:HG23	1.93	0.49
1:A:417:ARG:HD3	1:A:482:TYR:CE1	2.47	0.49
1:A:71:ASP:O	1:A:75:GLU:CG	2.61	0.49
1:B:152:ILE:HG12	1:B:198:LYS:HB2	1.94	0.49
1:B:302:ILE:HG21	1:B:306:VAL:HG22	1.93	0.49
1:B:347:ASN:O	1:B:351:ALA:N	2.35	0.49
1:C:325:ILE:HG22	1:C:326:LYS:N	2.27	0.49
1:C:553:ARG:O	1:C:557:VAL:HG23	2.12	0.49
1:C:591:HIS:O	2:H:444:LEU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:THR:O	1:D:121:LEU:N	2.45	0.49
2:E:333:ASP:HB2	2:E:336:HIS:HE2	1.78	0.49
2:G:410:GLY:HA2	2:G:441:PHE:CE1	2.48	0.49
1:A:457:LEU:CG	1:A:559:PHE:CZ	2.96	0.49
1:C:122:THR:HA	1:C:133:VAL:CG2	2.43	0.49
1:C:132:TYR:O	1:C:155:LEU:HD21	2.12	0.49
1:C:281:CYS:HB3	1:C:319:PHE:O	2.12	0.49
1:D:202:LYS:HB2	1:D:244:PHE:CE1	2.42	0.49
1:D:229:VAL:HG13	1:D:233:PHE:CE2	2.47	0.49
1:D:419:LEU:HB2	1:D:567:TYR:CE1	2.47	0.49
1:D:480:LYS:O	1:D:484:GLU:CG	2.61	0.49
2:E:412:LEU:O	2:E:415:LEU:N	2.46	0.49
1:B:682:ILE:HD11	2:E:465:LEU:HD12	1.93	0.49
2:F:411:GLN:O	2:F:415:LEU:N	2.36	0.49
2:F:455:THR:O	2:F:459:SER:N	2.45	0.49
2:H:311:ILE:HD11	2:H:421:ILE:HG23	1.94	0.49
1:A:152:ILE:HG12	1:A:198:LYS:HG3	1.95	0.49
1:A:252:ILE:HD13	1:A:259:ILE:HD11	1.95	0.49
1:B:100:ILE:O	1:B:270:LEU:O	2.30	0.49
1:C:430:PRO:HB2	1:C:452:GLU:HB3	1.95	0.49
1:D:476:PHE:CZ	1:D:501:PHE:CG	3.00	0.49
2:F:397:SER:HB2	2:F:400:LEU:H	1.78	0.49
2:G:355:ILE:O	2:G:360:LEU:HB2	2.12	0.49
1:A:555:ASN:C	1:A:559:PHE:CD2	2.86	0.49
1:B:401:LEU:HD22	1:B:575:PRO:CG	2.42	0.49
1:C:349:PRO:O	1:C:353:ARG:HG3	2.12	0.49
1:C:372:PHE:CE2	1:C:376:VAL:HG21	2.47	0.49
1:C:418:CYS:SG	1:C:422:PHE:HE2	2.36	0.49
1:C:453:TYR:OH	1:C:559:PHE:HD1	1.94	0.49
1:C:453:TYR:OH	1:C:559:PHE:CD1	2.65	0.49
1:C:695:LYS:HD2	1:C:707:LEU:HD11	1.95	0.49
1:D:132:TYR:O	1:D:155:LEU:HD21	2.12	0.49
1:D:152:ILE:HD12	1:D:194:LYS:O	2.13	0.49
2:F:335:ILE:HG22	2:F:388:LEU:HA	1.93	0.49
1:A:199:MET:HE2	1:A:244:PHE:HE2	1.77	0.49
1:A:222:MET:SD	1:A:225:PHE:CE2	3.06	0.49
1:A:478:VAL:O	1:A:482:TYR:HD2	1.96	0.49
1:B:683:ARG:NE	1:B:683:ARG:HA	2.28	0.49
1:C:560:ILE:HA	1:C:564:VAL:HB	1.95	0.49
1:C:301:LYS:N	1:C:580:VAL:O	2.41	0.49
1:D:138:ALA:HB2	1:D:221:ASP:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:TYR:OH	2:F:307:LEU:HD11	2.13	0.49
1:D:347:ASN:HB3	1:D:349:PRO:HD2	1.94	0.49
1:D:415:VAL:HG12	1:D:567:TYR:CE2	2.48	0.49
1:D:504:LEU:HD21	1:D:550:GLU:HB3	1.94	0.49
1:A:148:LEU:HD23	1:A:151:LEU:HD22	1.93	0.49
1:A:501:PHE:CE1	1:A:554:GLU:CD	2.86	0.49
1:B:272:CYS:O	1:B:272:CYS:SG	2.71	0.49
1:B:554:GLU:O	1:B:558:ASN:N	2.41	0.49
1:C:222:MET:SD	1:C:225:PHE:CE2	3.06	0.49
1:A:347:ASN:ND2	1:C:350:GLU:OE2	2.45	0.49
1:C:447:ILE:HG22	1:C:453:TYR:CD1	2.47	0.49
1:B:349:PRO:HG2	1:D:347:ASN:CB	2.43	0.49
1:D:500:GLN:O	1:D:503:SER:OG	2.24	0.49
1:D:497:PHE:CE1	1:D:557:VAL:CG1	2.96	0.49
1:D:683:ARG:NE	1:D:683:ARG:HA	2.27	0.49
2:F:390:LEU:HD23	2:F:418:ILE:HD12	1.93	0.49
2:G:398:GLN:HG3	2:G:401:ARG:HG3	1.95	0.49
1:A:306:VAL:HG12	1:A:585:ALA:HB2	1.94	0.49
1:A:293:LEU:HD21	1:A:328:LEU:HD13	1.95	0.49
1:A:49:LEU:HD11	1:C:49:LEU:HD21	1.95	0.49
1:A:480:LYS:NZ	1:A:502:GLN:HG3	2.28	0.49
1:B:312:ASN:O	1:B:316:TYR:HB2	2.13	0.49
1:C:152:ILE:CG2	1:C:198:LYS:N	2.75	0.49
1:C:198:LYS:O	1:C:201:SER:N	2.46	0.49
1:C:50:ILE:HG12	1:C:298:PHE:CD1	2.47	0.49
1:D:144:MET:SD	1:D:232:ASP:HB2	2.53	0.49
1:D:569:LEU:CB	1:D:571:PRO:HD2	2.43	0.49
2:H:441:PHE:HB3	2:H:443:TRP:CE2	2.48	0.49
1:A:132:TYR:O	1:A:155:LEU:CD2	2.61	0.48
1:A:199:MET:HE2	1:A:244:PHE:CE2	2.48	0.48
1:A:303:ASN:ND2	1:A:581:TYR:HB3	2.28	0.48
1:B:453:TYR:HH	1:B:559:PHE:HE1	1.52	0.48
1:B:480:LYS:NZ	1:B:502:GLN:HG3	2.28	0.48
1:C:420:HIS:CG	1:C:435:ILE:HG12	2.47	0.48
1:A:49:LEU:HD22	1:C:45:GLU:HG2	1.94	0.48
1:D:202:LYS:HE3	1:D:215:VAL:HG21	1.95	0.48
1:D:355:ILE:HA	1:D:358:LEU:HG	1.95	0.48
1:A:683:ARG:HH12	2:G:461:GLU:HB2	1.78	0.48
1:A:387:LEU:HA	1:A:394:LEU:HB2	1.95	0.48
1:A:386:ALA:O	1:A:390:ASN:O	2.31	0.48
1:A:393:TYR:O	1:A:397:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASN:OD1	1:A:569:LEU:HD11	2.13	0.48
1:B:368:ARG:O	1:B:373:ARG:HG3	2.12	0.48
1:B:387:LEU:HD22	1:B:394:LEU:HD13	1.96	0.48
1:B:417:ARG:C	1:B:479:PHE:CE1	2.86	0.48
1:B:497:PHE:O	1:B:501:PHE:CD2	2.66	0.48
1:C:98:ARG:HA	1:C:238:SER:O	2.12	0.48
1:D:404:ASN:CB	1:D:574:GLN:OE1	2.61	0.48
2:E:320:ARG:NH2	2:E:457:GLU:N	2.61	0.48
1:A:100:ILE:HG12	1:A:241:LEU:HD21	1.95	0.48
1:A:341:LEU:HD21	1:A:365:ASN:CB	2.43	0.48
1:A:415:VAL:O	1:A:418:CYS:HB3	2.13	0.48
1:A:478:VAL:O	1:A:482:TYR:CD2	2.66	0.48
1:D:420:HIS:CG	1:D:435:ILE:HG12	2.47	0.48
1:D:447:ILE:HG22	1:D:453:TYR:CG	2.48	0.48
1:D:494:ILE:HA	1:D:497:PHE:HD2	1.77	0.48
2:G:410:GLY:O	2:G:414:SER:CB	2.61	0.48
2:G:446:TYR:CB	2:G:448:THR:HG23	2.43	0.48
2:H:455:THR:HA	2:H:458:THR:HB	1.96	0.48
1:A:263:LEU:HD13	1:A:271:LEU:HD11	1.96	0.48
1:A:355:ILE:HA	1:A:358:LEU:HG	1.94	0.48
1:A:382:GLU:C	1:A:384:GLN:N	2.67	0.48
1:B:105:LEU:O	1:B:250:PHE:O	2.32	0.48
1:B:494:ILE:O	1:B:498:LEU:HG	2.14	0.48
1:C:234:ILE:O	1:C:238:SER:HB3	2.14	0.48
1:D:152:ILE:HA	1:D:198:LYS:HG3	1.95	0.48
1:D:209:GLN:HE22	1:D:213:PRO:HG3	1.78	0.48
1:D:199:MET:HG2	1:D:244:PHE:CE2	2.48	0.48
2:E:347:SER:N	2:E:350:SER:HG	2.10	0.48
2:E:410:GLY:HA2	2:E:441:PHE:CE1	2.48	0.48
2:E:446:TYR:CB	2:E:448:THR:HG23	2.42	0.48
1:B:683:ARG:NH1	2:E:461:GLU:HB2	2.28	0.48
2:H:355:ILE:O	2:H:360:LEU:HB2	2.13	0.48
1:A:229:VAL:HG13	1:A:233:PHE:CE2	2.49	0.48
1:A:387:LEU:HD21	1:A:397:GLU:CD	2.32	0.48
1:A:552:LEU:O	1:A:556:VAL:HG23	2.13	0.48
1:C:293:LEU:HD21	1:C:328:LEU:HD13	1.94	0.48
1:C:404:ASN:C	1:C:574:GLN:OE1	2.51	0.48
1:C:334:GLU:HG3	1:C:582:PHE:CZ	2.48	0.48
1:D:683:ARG:CZ	2:F:458:THR:HG23	2.44	0.48
2:G:332:GLN:O	2:G:336:HIS:CD2	2.66	0.48
1:A:325:ILE:HG22	1:A:326:LYS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASN:O	1:A:351:ALA:N	2.34	0.48
1:A:475:CYS:O	1:A:479:PHE:CB	2.61	0.48
1:B:559:PHE:O	1:B:564:VAL:N	2.32	0.48
1:C:107:LEU:HD23	1:C:278:SER:HB2	1.96	0.48
1:C:244:PHE:CD2	1:C:246:LEU:HD12	2.39	0.48
1:C:252:ILE:HD13	1:C:259:ILE:HD11	1.96	0.48
1:D:126:GLN:HB3	1:D:162:ILE:HD11	1.94	0.48
1:D:478:VAL:O	1:D:482:TYR:CD2	2.66	0.48
1:D:552:LEU:O	1:D:556:VAL:HG23	2.13	0.48
2:E:397:SER:HB2	2:E:400:LEU:H	1.79	0.48
1:A:285:LEU:O	1:A:288:VAL:HG12	2.13	0.48
1:A:402:LEU:HA	1:A:405:LEU:HD12	1.96	0.48
1:A:417:ARG:C	1:A:479:PHE:CE1	2.87	0.48
1:A:480:LYS:O	1:A:484:GLU:CG	2.61	0.48
1:B:152:ILE:HA	1:B:198:LYS:HG3	1.96	0.48
1:B:226:ALA:HB3	1:B:229:VAL:HB	1.96	0.48
1:B:372:PHE:HA	1:B:375:TYR:HB3	1.95	0.48
1:B:482:TYR:HA	1:B:486:HIS:ND1	2.28	0.48
1:C:42:LEU:HD13	1:C:354:ARG:NH1	2.28	0.48
1:C:369:LEU:HD13	1:C:370:PRO:O	2.13	0.48
1:C:497:PHE:HE1	1:C:557:VAL:HG13	1.79	0.48
2:E:295:GLU:HG2	2:E:298:PHE:CE2	2.49	0.48
2:F:320:ARG:NH2	2:F:457:GLU:N	2.61	0.48
2:F:400:LEU:HD22	2:F:409:ILE:CD1	2.44	0.48
2:H:291:ASN:O	2:H:295:GLU:HG3	2.13	0.48
1:A:255:SER:HB2	1:A:256:PRO:HD3	1.95	0.48
1:A:302:ILE:CG2	1:A:307:LEU:HG	2.44	0.48
1:A:418:CYS:SG	1:A:422:PHE:HE2	2.37	0.48
1:A:590:GLU:O	2:G:445:TRP:O	2.32	0.48
1:B:100:ILE:HG12	1:B:241:LEU:HD21	1.95	0.48
1:B:461:ARG:HG2	1:B:552:LEU:CD2	2.44	0.48
1:B:483:CYS:HA	1:B:487:LEU:O	2.14	0.48
1:C:117:THR:O	1:C:121:LEU:N	2.47	0.48
1:C:79:LYS:O	1:C:83:GLY:N	2.36	0.48
2:G:373:LEU:O	2:G:377:VAL:HB	2.14	0.48
2:H:339:ILE:HD13	2:H:351:VAL:HG22	1.95	0.48
2:G:382:GLU:O	2:H:383:ASP:OD1	2.32	0.48
1:A:126:GLN:HB3	1:A:162:ILE:HD11	1.95	0.48
1:B:230:LEU:HD11	1:B:263:LEU:HD22	1.94	0.48
1:B:297:GLN:HA	1:D:353:ARG:CZ	2.43	0.48
1:C:128:ASN:O	1:C:129:VAL:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:THR:HB	1:C:209:GLN:HG2	1.96	0.48
1:C:138:ALA:HB2	1:C:221:ASP:O	2.14	0.48
1:C:386:ALA:O	1:C:390:ASN:O	2.31	0.48
1:C:414:LEU:HD13	1:C:494:ILE:HD11	1.94	0.48
1:C:50:ILE:HG12	1:C:298:PHE:CE1	2.49	0.48
1:D:151:LEU:CD1	1:D:198:LYS:HD2	2.43	0.48
1:D:341:LEU:HD21	1:D:365:ASN:CB	2.44	0.48
1:D:342:SER:OG	1:D:579:VAL:HG13	2.14	0.48
2:F:353:ASN:OD1	2:F:365:THR:N	2.45	0.48
2:F:369:ILE:HG21	2:F:408:ILE:CD1	2.43	0.48
2:F:420:LEU:HD21	2:F:443:TRP:CH2	2.49	0.48
2:H:297:LEU:HB3	2:H:301:TRP:NE1	2.28	0.48
2:H:339:ILE:CD1	2:H:351:VAL:HG13	2.44	0.48
2:H:352:LEU:CD2	2:H:369:ILE:HG23	2.44	0.48
1:A:151:LEU:CD1	1:A:198:LYS:HD2	2.44	0.48
1:A:226:ALA:HB3	1:A:229:VAL:HB	1.96	0.48
1:B:286:THR:HG22	1:B:436:ARG:HE	1.79	0.48
1:B:555:ASN:O	1:B:559:PHE:CD2	2.67	0.48
1:C:420:HIS:NE2	1:C:435:ILE:HA	2.28	0.48
1:C:552:LEU:O	1:C:556:VAL:HG23	2.14	0.48
1:C:683:ARG:CZ	1:C:686:SER:OG	2.62	0.48
1:D:417:ARG:C	1:D:479:PHE:CE1	2.87	0.48
1:D:476:PHE:O	1:D:480:LYS:CB	2.61	0.48
2:E:369:ILE:HG12	2:E:372:GLN:OE1	2.13	0.48
2:F:412:LEU:HB3	2:F:418:ILE:CD1	2.43	0.48
2:G:352:LEU:CD2	2:G:369:ILE:HG23	2.43	0.48
1:A:497:PHE:O	1:A:501:PHE:HD2	1.97	0.47
1:B:229:VAL:HG13	1:B:233:PHE:CE2	2.49	0.47
1:B:326:LYS:HA	1:B:329:GLN:HE21	1.78	0.47
1:B:349:PRO:O	1:B:353:ARG:HG3	2.14	0.47
1:B:371:SER:O	1:B:575:PRO:HB3	2.14	0.47
1:B:384:GLN:O	1:B:387:LEU:HB2	2.13	0.47
1:C:255:SER:HB2	1:C:256:PRO:HD3	1.96	0.47
1:C:420:HIS:CE1	1:C:435:ILE:HG23	2.49	0.47
1:C:632:ILE:O	1:C:636:LEU:HG	2.14	0.47
1:D:476:PHE:HB3	1:D:480:LYS:CE	2.44	0.47
2:F:317:GLY:O	2:F:319:LYS:NZ	2.47	0.47
2:H:298:PHE:HB3	2:H:330:MET:HG3	1.96	0.47
2:H:410:GLY:HA2	2:H:441:PHE:CE1	2.49	0.47
1:A:326:LYS:HA	1:A:329:GLN:HE21	1.79	0.47
1:A:588:LEU:O	1:A:592:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:LEU:O	2:G:426:HIS:CA	2.62	0.47
1:B:341:LEU:HD21	1:B:365:ASN:CB	2.44	0.47
1:B:352:LYS:HG2	1:B:355:ILE:HD12	1.95	0.47
1:B:355:ILE:HA	1:B:358:LEU:HG	1.95	0.47
1:B:478:VAL:O	1:B:482:TYR:HD2	1.96	0.47
1:A:347:ASN:CG	1:C:350:GLU:HG3	2.34	0.47
1:C:440:CYS:O	1:C:444:GLU:HG3	2.15	0.47
1:C:478:VAL:O	1:C:482:TYR:CD2	2.67	0.47
1:D:371:SER:O	1:D:575:PRO:HA	2.14	0.47
2:F:420:LEU:HD12	2:F:421:ILE:N	2.29	0.47
1:A:404:ASN:O	1:A:407:VAL:HB	2.14	0.47
1:A:646:LEU:HA	1:A:649:TRP:HB3	1.94	0.47
1:A:691:LEU:O	2:G:427:LEU:HG	2.14	0.47
1:A:695:LYS:HG3	1:A:696:PRO:HD2	1.95	0.47
1:B:349:PRO:HG2	1:D:347:ASN:HB3	1.95	0.47
1:B:694:ILE:HD13	1:B:704:VAL:HG22	1.96	0.47
2:G:320:ARG:HH22	2:G:457:GLU:CA	2.27	0.47
2:G:298:PHE:CD2	2:G:330:MET:HG2	2.49	0.47
2:H:353:ASN:OD1	2:H:365:THR:N	2.47	0.47
1:A:288:VAL:CG2	1:A:292:LEU:HD12	2.43	0.47
1:B:340:PRO:HB2	1:B:362:GLN:HE21	1.79	0.47
1:B:386:ALA:O	1:B:390:ASN:O	2.33	0.47
1:B:478:VAL:O	1:B:482:TYR:CD2	2.68	0.47
1:C:337:TYR:OH	2:H:307:LEU:HD11	2.14	0.47
1:C:422:PHE:HE1	1:C:472:LEU:HD22	1.78	0.47
2:F:327:ARG:HA	2:F:331:LEU:HB2	1.95	0.47
2:F:395:LEU:HD12	2:F:400:LEU:HD13	1.95	0.47
2:G:362:HIS:O	2:G:363:MET:HG2	2.15	0.47
2:G:409:ILE:HG22	2:G:441:PHE:CE1	2.49	0.47
2:G:425:ASP:OD1	2:G:454:TYR:OH	2.32	0.47
2:H:428:ASN:O	2:H:431:LEU:CB	2.61	0.47
1:A:102:THR:HA	1:A:247:ILE:HG23	1.97	0.47
1:A:199:MET:HG2	1:A:244:PHE:CE2	2.50	0.47
1:B:329:GLN:O	1:B:332:LEU:N	2.47	0.47
1:B:387:LEU:HA	1:B:394:LEU:HB2	1.95	0.47
1:B:649:TRP:HZ3	1:B:704:VAL:HB	1.79	0.47
1:B:81:HIS:NE2	1:B:214:PRO:HB3	2.30	0.47
1:C:152:ILE:CG1	1:C:198:LYS:H	2.26	0.47
1:C:41:LYS:HD2	1:C:44:PHE:HE2	1.80	0.47
1:C:70:PHE:HA	1:C:73:LEU:HB2	1.96	0.47
1:D:267:VAL:O	1:D:271:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:PHE:HE1	1:D:472:LEU:HD22	1.79	0.47
1:D:71:ASP:O	1:D:75:GLU:HB2	2.14	0.47
2:F:410:GLY:HA2	2:F:441:PHE:CE1	2.49	0.47
1:A:100:ILE:O	1:A:271:LEU:HA	2.14	0.47
1:B:148:LEU:HD23	1:B:151:LEU:HD22	1.94	0.47
1:C:219:LEU:CB	1:C:222:MET:HG2	2.44	0.47
1:C:306:VAL:O	1:C:310:LEU:HB2	2.14	0.47
1:C:554:GLU:O	1:C:558:ASN:N	2.42	0.47
1:D:423:THR:CG2	1:D:438:LEU:HD21	2.45	0.47
1:D:472:LEU:O	1:D:476:PHE:CD2	2.67	0.47
1:D:497:PHE:O	1:D:501:PHE:HD2	1.97	0.47
2:H:409:ILE:HG22	2:H:441:PHE:CE1	2.49	0.47
1:A:252:ILE:CD1	1:A:259:ILE:HD11	2.44	0.47
1:A:419:LEU:HD23	1:A:438:LEU:HD23	1.97	0.47
1:A:457:LEU:HG	1:A:559:PHE:HZ	1.77	0.47
1:B:148:LEU:HB2	1:B:195:THR:HG22	1.97	0.47
1:B:202:LYS:CD	1:B:244:PHE:CE1	2.96	0.47
1:B:386:ALA:HB1	1:B:393:TYR:CB	2.45	0.47
1:C:387:LEU:HD21	1:C:397:GLU:CD	2.34	0.47
1:C:497:PHE:O	1:C:501:PHE:HD2	1.98	0.47
1:D:152:ILE:HG12	1:D:198:LYS:HG3	1.96	0.47
1:D:472:LEU:O	1:D:475:CYS:N	2.46	0.47
1:D:461:ARG:HG2	1:D:552:LEU:HD21	1.96	0.47
2:G:327:ARG:HA	2:G:331:LEU:HB2	1.97	0.47
2:H:340:ASN:HB3	2:H:342:PHE:CZ	2.49	0.47
1:A:49:LEU:CD2	1:C:45:GLU:HG2	2.44	0.47
1:A:555:ASN:HA	1:A:558:ASN:HB2	1.97	0.47
1:B:144:MET:SD	1:B:232:ASP:HB2	2.55	0.47
1:B:310:LEU:O	1:B:313:ILE:N	2.47	0.47
1:B:688:LEU:HB3	1:B:694:ILE:HG13	1.97	0.47
1:C:341:LEU:HD21	1:C:365:ASN:CB	2.45	0.47
1:C:422:PHE:CE1	1:C:472:LEU:HD22	2.50	0.47
1:C:497:PHE:CD1	1:C:557:VAL:CG1	2.97	0.47
1:D:404:ASN:O	1:D:407:VAL:HB	2.13	0.47
1:D:51:TRP:CH2	1:D:55:LYS:HE3	2.50	0.47
2:H:369:ILE:HG21	2:H:408:ILE:CD1	2.45	0.47
1:A:405:LEU:HD21	1:A:575:PRO:O	2.15	0.47
1:B:381:SER:O	1:B:384:GLN:HB3	2.15	0.47
1:B:563:LEU:HA	1:B:567:TYR:HD2	1.80	0.47
1:B:563:LEU:HA	1:B:567:TYR:CD2	2.49	0.47
1:C:250:PHE:HB3	1:C:252:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ILE:O	1:C:372:PHE:CD2	2.68	0.47
1:C:355:ILE:O	1:C:395:LYS:HE3	2.15	0.47
1:C:404:ASN:O	1:C:407:VAL:HB	2.14	0.47
1:D:100:ILE:HG12	1:D:241:LEU:HD21	1.97	0.47
1:D:420:HIS:CE1	1:D:435:ILE:HG23	2.49	0.47
2:G:412:LEU:O	2:G:415:LEU:N	2.47	0.47
1:A:148:LEU:HA	1:A:151:LEU:CD2	2.45	0.47
1:A:645:ASN:HA	1:A:703:HIS:CE1	2.49	0.47
1:B:306:VAL:O	1:B:310:LEU:HB2	2.15	0.47
1:B:409:HIS:HA	1:B:412:TYR:CD2	2.50	0.47
1:C:148:LEU:HA	1:C:151:LEU:CD2	2.45	0.47
1:C:326:LYS:HA	1:C:329:GLN:HE21	1.80	0.47
1:D:226:ALA:HB3	1:D:229:VAL:HB	1.96	0.47
1:D:646:LEU:HA	1:D:649:TRP:HB3	1.97	0.47
2:H:342:PHE:CE1	2:H:343:PHE:CE1	3.02	0.47
1:A:422:PHE:CE1	1:A:472:LEU:HD22	2.50	0.47
1:A:44:PHE:HA	1:A:47:TYR:HB3	1.96	0.47
1:A:555:ASN:O	1:A:559:PHE:CD2	2.67	0.47
1:B:257:ILE:HG22	1:B:261:ARG:NE	2.30	0.47
1:B:282:LYS:O	1:B:286:THR:HG23	2.15	0.47
1:B:325:ILE:HG22	1:B:326:LYS:N	2.29	0.47
1:B:555:ASN:O	1:B:558:ASN:N	2.48	0.47
1:C:474:LYS:O	1:C:478:VAL:HG23	2.15	0.47
1:C:555:ASN:HA	1:C:558:ASN:HB2	1.97	0.47
1:D:152:ILE:CD1	1:D:195:THR:C	2.83	0.47
1:D:202:LYS:CE	1:D:215:VAL:HG23	2.45	0.47
1:D:417:ARG:HD3	1:D:482:TYR:CE1	2.49	0.47
1:D:646:LEU:HD12	1:D:702:ASP:HB3	1.97	0.47
2:F:327:ARG:HE	2:F:391:LEU:HD12	1.79	0.47
2:F:377:VAL:O	2:F:381:LYS:N	2.41	0.47
2:F:441:PHE:HB3	2:F:443:TRP:CE2	2.50	0.47
2:G:331:LEU:HD11	2:G:391:LEU:CD1	2.45	0.47
2:H:362:HIS:O	2:H:363:MET:HG2	2.15	0.47
1:A:234:ILE:HG21	1:A:267:VAL:HG13	1.96	0.46
1:A:267:VAL:O	1:A:271:LEU:HG	2.15	0.46
1:A:401:LEU:HD22	1:A:575:PRO:HG3	1.97	0.46
1:A:420:HIS:O	1:A:421:LYS:C	2.50	0.46
1:A:695:LYS:HD2	1:A:707:LEU:CD1	2.45	0.46
1:B:148:LEU:HA	1:B:151:LEU:CD2	2.44	0.46
1:B:254:THR:CB	1:B:258:ILE:HD12	2.44	0.46
1:C:148:LEU:HD23	1:C:151:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LYS:O	1:C:71:ASP:HB2	2.16	0.46
1:D:421:LYS:NZ	1:D:479:PHE:CE1	2.79	0.46
1:D:648:ASP:HA	1:D:651:GLU:HB2	1.97	0.46
2:E:332:GLN:O	2:E:336:HIS:CD2	2.68	0.46
2:F:332:GLN:O	2:F:336:HIS:CD2	2.68	0.46
2:H:373:LEU:CD2	2:H:412:LEU:HD21	2.43	0.46
2:H:443:TRP:HB2	2:H:445:TRP:NE1	2.30	0.46
1:A:297:GLN:O	1:C:353:ARG:CZ	2.63	0.46
1:A:306:VAL:O	1:A:310:LEU:HD13	2.15	0.46
1:B:694:ILE:HB	1:B:704:VAL:HG13	1.97	0.46
1:C:148:LEU:O	1:C:151:LEU:HB3	2.14	0.46
1:C:81:HIS:NE2	1:C:214:PRO:HB3	2.30	0.46
1:C:244:PHE:CG	1:C:246:LEU:HG	2.37	0.46
1:C:324:PHE:CE2	1:C:328:LEU:HD11	2.49	0.46
1:C:364:GLU:HA	1:C:367:ARG:HD2	1.97	0.46
1:C:476:PHE:O	1:C:480:LYS:CB	2.63	0.46
1:C:645:ASN:OD1	1:C:648:ASP:HB2	2.15	0.46
1:D:155:LEU:CG	1:D:198:LYS:HE2	2.45	0.46
1:D:222:MET:HG3	1:D:250:PHE:CE1	2.50	0.46
1:D:72:ASN:HA	1:D:75:GLU:HB2	1.97	0.46
1:D:77:LEU:CD2	1:D:247:ILE:HG21	2.46	0.46
2:F:333:ASP:HB2	2:F:336:HIS:HE2	1.79	0.46
2:F:340:ASN:O	2:F:343:PHE:HB2	2.15	0.46
2:F:339:ILE:CD1	2:F:351:VAL:HG13	2.45	0.46
2:G:325:ARG:HA	2:G:328:THR:OG1	2.15	0.46
2:H:331:LEU:HD11	2:H:391:LEU:CD1	2.44	0.46
1:A:125:LEU:HB3	1:A:133:VAL:HG11	1.97	0.46
1:A:222:MET:HG3	1:A:250:PHE:CE1	2.50	0.46
1:A:101:PRO:HB3	1:A:272:CYS:SG	2.55	0.46
1:A:50:ILE:HG12	1:A:298:PHE:CE1	2.50	0.46
1:B:151:LEU:CD1	1:B:198:LYS:HD2	2.45	0.46
1:B:131:PRO:CB	1:B:214:PRO:O	2.64	0.46
1:B:497:PHE:HE1	1:B:557:VAL:HG13	1.80	0.46
1:C:152:ILE:HG21	1:C:197:PRO:HD2	1.98	0.46
1:C:155:LEU:CG	1:C:198:LYS:HE2	2.44	0.46
1:C:342:SER:OG	1:C:579:VAL:HG13	2.15	0.46
1:D:335:HIS:CE1	1:D:579:VAL:HA	2.50	0.46
1:D:352:LYS:NZ	1:D:403:GLU:OE2	2.26	0.46
1:D:74:ILE:HD13	1:D:128:ASN:OD1	2.14	0.46
2:E:327:ARG:HA	2:E:331:LEU:HB2	1.97	0.46
2:E:331:LEU:HD11	2:E:391:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:311:ILE:HB	2:E:446:TYR:CE2	2.51	0.46
2:E:453:PRO:CA	2:E:454:TYR:HB2	2.45	0.46
2:G:441:PHE:HB3	2:G:443:TRP:CE2	2.50	0.46
1:A:366:ILE:O	1:A:372:PHE:CD2	2.68	0.46
1:A:420:HIS:CG	1:A:435:ILE:HG12	2.51	0.46
1:B:234:ILE:HG21	1:B:267:VAL:HG13	1.96	0.46
1:B:422:PHE:HE1	1:B:472:LEU:HD22	1.80	0.46
1:B:71:ASP:O	1:B:75:GLU:CG	2.63	0.46
1:D:306:VAL:O	1:D:310:LEU:HD13	2.16	0.46
1:D:420:HIS:NE2	1:D:435:ILE:HA	2.30	0.46
1:D:555:ASN:C	1:D:559:PHE:CD2	2.89	0.46
2:E:396:ASP:O	2:E:401:ARG:NE	2.48	0.46
2:G:336:HIS:ND1	2:G:389:PHE:HB2	2.30	0.46
1:A:202:LYS:HE3	1:A:215:VAL:CG2	2.46	0.46
1:A:422:PHE:HE1	1:A:472:LEU:HD22	1.80	0.46
1:B:151:LEU:HG	1:B:198:LYS:CD	2.45	0.46
1:B:70:PHE:HA	1:B:73:LEU:HB2	1.98	0.46
1:C:147:PHE:CE1	1:C:225:PHE:CE1	3.04	0.46
1:C:147:PHE:HB2	1:C:233:PHE:CE1	2.51	0.46
1:C:371:SER:O	1:C:375:TYR:HB2	2.16	0.46
1:D:100:ILE:CG1	1:D:241:LEU:HD21	2.46	0.46
1:D:50:ILE:HG12	1:D:298:PHE:CE1	2.50	0.46
1:D:401:LEU:HD22	1:D:575:PRO:HG3	1.96	0.46
1:D:371:SER:O	1:D:575:PRO:HB3	2.16	0.46
2:E:410:GLY:O	2:E:414:SER:CB	2.64	0.46
2:G:317:GLY:O	2:G:319:LYS:NZ	2.49	0.46
1:A:497:PHE:HE1	1:A:557:VAL:HG13	1.80	0.46
1:B:155:LEU:CG	1:B:198:LYS:HE2	2.45	0.46
1:B:81:HIS:CE1	1:B:214:PRO:HG3	2.50	0.46
1:B:254:THR:HB	1:B:258:ILE:HD12	1.96	0.46
1:B:420:HIS:CE1	1:B:435:ILE:HG23	2.50	0.46
1:B:422:PHE:CE1	1:B:472:LEU:HD22	2.49	0.46
1:B:42:LEU:O	1:B:46:THR:HG23	2.16	0.46
1:B:569:LEU:O	1:B:573:THR:HG23	2.14	0.46
1:C:141:CYS:HB3	1:C:147:PHE:CE2	2.49	0.46
1:C:152:ILE:HG12	1:C:198:LYS:N	2.31	0.46
1:C:572:GLU:O	1:C:573:THR:HG23	2.16	0.46
1:C:695:LYS:HG3	1:C:696:PRO:CD	2.46	0.46
1:D:548:LYS:O	1:D:551:VAL:N	2.48	0.46
1:D:569:LEU:O	1:D:573:THR:HG23	2.16	0.46
1:D:682:ILE:HD11	2:F:465:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:398:GLN:HG3	2:F:401:ARG:HG3	1.97	0.46
2:F:400:LEU:O	2:F:405:SER:OG	2.34	0.46
2:F:438:GLN:O	2:F:441:PHE:O	2.33	0.46
2:H:324:GLU:O	2:H:328:THR:HG23	2.16	0.46
2:H:390:LEU:HD23	2:H:418:ILE:HD12	1.98	0.46
1:A:130:THR:O	1:A:131:PRO:O	2.33	0.46
1:A:144:MET:SD	1:A:232:ASP:HB2	2.56	0.46
1:A:49:LEU:CD2	1:C:45:GLU:CG	2.94	0.46
1:B:325:ILE:O	1:B:328:LEU:N	2.49	0.46
1:B:371:SER:HA	1:B:374:ARG:HB2	1.97	0.46
1:B:44:PHE:HA	1:B:47:TYR:HB3	1.98	0.46
1:B:342:SER:OG	1:B:579:VAL:HG13	2.16	0.46
1:C:43:ARG:NH2	1:C:342:SER:OG	2.48	0.46
1:C:414:LEU:O	1:C:479:PHE:HE1	1.98	0.46
1:C:480:LYS:O	1:C:484:GLU:CB	2.64	0.46
1:C:497:PHE:CE1	1:C:557:VAL:CG1	2.99	0.46
1:C:646:LEU:HD12	1:C:702:ASP:HB3	1.97	0.46
1:C:71:ASP:O	1:C:75:GLU:CG	2.64	0.46
1:D:202:LYS:CE	1:D:215:VAL:CG2	2.94	0.46
1:D:384:GLN:HG2	1:D:388:LEU:HD11	1.97	0.46
1:D:296:THR:CB	1:D:410:MET:SD	3.03	0.46
2:F:369:ILE:HG12	2:F:372:GLN:OE1	2.16	0.46
2:G:324:GLU:O	2:G:328:THR:HG23	2.16	0.46
2:G:331:LEU:HB3	2:G:336:HIS:CG	2.50	0.46
1:A:416:LEU:HD12	1:A:567:TYR:HD1	1.80	0.46
1:A:569:LEU:O	1:A:573:THR:HG23	2.16	0.46
1:A:371:SER:O	1:A:575:PRO:HB3	2.15	0.46
1:B:104:ALA:HA	1:B:250:PHE:CD2	2.50	0.46
1:B:415:VAL:HG12	1:B:567:TYR:CE2	2.50	0.46
1:B:46:THR:HA	1:B:49:LEU:HD12	1.97	0.46
1:C:122:THR:HA	1:C:133:VAL:HG21	1.98	0.46
1:C:335:HIS:HB2	1:C:582:PHE:CG	2.51	0.46
1:C:480:LYS:O	1:C:484:GLU:HB2	2.16	0.46
1:D:216:VAL:HG11	1:D:249:ILE:CD1	2.46	0.46
1:D:450:SER:OG	1:D:452:GLU:OE1	2.31	0.46
1:D:414:LEU:HG	1:D:487:LEU:HD13	1.98	0.46
2:G:340:ASN:O	2:G:343:PHE:HB2	2.15	0.46
2:H:377:VAL:O	2:H:381:LYS:N	2.41	0.46
1:A:302:ILE:HG22	1:A:307:LEU:HG	1.98	0.46
1:A:497:PHE:CE1	1:A:557:VAL:CG1	2.98	0.46
1:B:106:VAL:O	1:B:278:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ILE:O	1:B:372:PHE:CD2	2.69	0.46
1:C:687:GLU:OE2	2:H:454:TYR:HB3	2.15	0.46
1:C:72:ASN:HA	1:C:75:GLU:HB2	1.98	0.46
1:D:199:MET:HE2	1:D:244:PHE:CE2	2.50	0.46
2:F:298:PHE:HB3	2:F:330:MET:HG3	1.98	0.46
2:F:446:TYR:CB	2:F:448:THR:HG23	2.46	0.46
2:H:311:ILE:CG1	2:H:421:ILE:HG12	2.46	0.46
2:H:438:GLN:O	2:H:441:PHE:O	2.34	0.46
1:A:572:GLU:O	1:A:573:THR:HG23	2.16	0.46
1:A:695:LYS:CD	1:A:707:LEU:HD11	2.46	0.46
1:B:152:ILE:CD1	1:B:195:THR:C	2.84	0.46
1:B:417:ARG:HD3	1:B:482:TYR:CE1	2.51	0.46
1:B:695:LYS:CG	1:B:696:PRO:HD2	2.46	0.46
1:A:347:ASN:HB2	1:C:347:ASN:OD1	2.15	0.46
1:C:504:LEU:HD11	1:C:554:GLU:CD	2.36	0.46
1:D:341:LEU:HD21	1:D:365:ASN:HB2	1.98	0.46
1:D:457:LEU:CG	1:D:559:PHE:CZ	2.98	0.46
2:E:337:VAL:CG2	2:E:359:VAL:HG21	2.46	0.46
2:E:395:LEU:HD12	2:E:400:LEU:HD13	1.98	0.46
2:E:444:LEU:O	2:E:446:TYR:CE2	2.69	0.46
2:F:340:ASN:HB2	2:F:343:PHE:CG	2.51	0.46
2:G:400:LEU:HD22	2:G:409:ILE:HD11	1.98	0.46
2:G:320:ARG:HH22	2:G:457:GLU:HG3	1.81	0.46
1:A:447:ILE:HG22	1:A:453:TYR:CG	2.50	0.45
1:B:476:PHE:HB3	1:B:480:LYS:CE	2.46	0.45
1:B:497:PHE:CE1	1:B:557:VAL:HG13	2.51	0.45
1:B:50:ILE:O	1:B:53:GLN:HB2	2.16	0.45
1:B:647:VAL:O	1:B:651:GLU:HB2	2.16	0.45
1:C:152:ILE:CD1	1:C:195:THR:C	2.84	0.45
1:C:504:LEU:HD21	1:C:550:GLU:HB3	1.98	0.45
1:D:421:LYS:NZ	1:D:479:PHE:CD1	2.72	0.45
1:D:683:ARG:NE	1:D:686:SER:OG	2.48	0.45
1:D:685:VAL:O	1:D:689:GLU:HG3	2.16	0.45
2:E:355:ILE:HG23	2:E:356:THR:N	2.31	0.45
2:F:295:GLU:O	2:F:298:PHE:HB2	2.16	0.45
2:F:331:LEU:HB3	2:F:336:HIS:CG	2.51	0.45
2:H:320:ARG:HH12	2:H:457:GLU:H	1.63	0.45
1:A:559:PHE:O	1:A:564:VAL:N	2.33	0.45
1:B:144:MET:SD	1:B:229:VAL:HA	2.56	0.45
1:B:222:MET:SD	1:B:225:PHE:CE2	3.09	0.45
1:B:402:LEU:HA	1:B:405:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LYS:O	1:B:484:GLU:CB	2.63	0.45
1:B:501:PHE:CE1	1:B:554:GLU:CD	2.90	0.45
1:C:695:LYS:CG	1:C:696:PRO:HD2	2.46	0.45
1:D:162:ILE:HG22	1:D:162:ILE:O	2.17	0.45
1:D:199:MET:CE	1:D:243:GLU:OE1	2.64	0.45
1:D:302:ILE:HG22	1:D:307:LEU:HG	1.99	0.45
1:D:313:ILE:HG12	1:D:318:ASP:OD1	2.16	0.45
1:D:414:LEU:HD13	1:D:494:ILE:HD11	1.97	0.45
1:D:70:PHE:HA	1:D:73:LEU:HB2	1.97	0.45
2:E:324:GLU:O	2:E:328:THR:HG23	2.16	0.45
2:G:295:GLU:HG2	2:G:298:PHE:CE2	2.51	0.45
1:A:419:LEU:HB2	1:A:567:TYR:CE1	2.50	0.45
1:A:695:LYS:CG	1:A:696:PRO:HD2	2.45	0.45
1:B:283:GLU:O	1:B:287:THR:HG23	2.16	0.45
1:B:332:LEU:HD23	1:B:336:PHE:CD2	2.51	0.45
1:B:414:LEU:HD13	1:B:494:ILE:HD11	1.97	0.45
1:C:691:LEU:O	2:H:426:HIS:HA	2.16	0.45
1:D:106:VAL:HG13	1:D:253:ALA:O	2.16	0.45
1:D:497:PHE:CE1	1:D:557:VAL:HG13	2.52	0.45
2:F:342:PHE:CE1	2:F:343:PHE:CE1	3.05	0.45
1:A:330:LEU:HD11	2:G:309:PHE:CE2	2.51	0.45
2:G:397:SER:HB2	2:G:400:LEU:H	1.80	0.45
1:B:475:CYS:O	1:B:479:PHE:HD2	1.98	0.45
1:B:548:LYS:O	1:B:552:LEU:HG	2.16	0.45
1:B:457:LEU:CG	1:B:559:PHE:CZ	2.97	0.45
1:C:370:PRO:C	1:C:372:PHE:H	2.20	0.45
1:D:302:ILE:HG21	1:D:306:VAL:HG22	1.98	0.45
1:D:306:VAL:O	1:D:310:LEU:HB2	2.16	0.45
1:D:325:ILE:HG22	1:D:326:LYS:N	2.31	0.45
2:E:335:ILE:O	2:E:335:ILE:HG22	2.17	0.45
2:E:339:ILE:HD13	2:E:351:VAL:HG22	1.99	0.45
2:F:455:THR:HA	2:F:458:THR:HB	1.99	0.45
2:H:340:ASN:O	2:H:343:PHE:HB2	2.16	0.45
2:H:336:HIS:ND1	2:H:389:PHE:HB2	2.32	0.45
2:H:301:TRP:NE1	2:H:446:TYR:CE1	2.84	0.45
1:A:128:ASN:O	1:A:129:VAL:HB	2.17	0.45
1:B:248:LEU:CD1	1:B:250:PHE:CZ	2.99	0.45
1:B:263:LEU:CD1	1:B:271:LEU:HD11	2.47	0.45
1:B:400:LEU:O	1:B:404:ASN:ND2	2.49	0.45
1:B:636:LEU:HD13	1:B:653:PHE:HD1	1.82	0.45
1:C:155:LEU:HB2	1:C:198:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ILE:HG22	1:C:307:LEU:HG	1.97	0.45
1:C:350:GLU:O	1:C:354:ARG:HG2	2.16	0.45
1:C:554:GLU:HA	1:C:557:VAL:HB	1.98	0.45
1:C:562:CYS:C	1:C:567:TYR:CD2	2.90	0.45
1:D:137:GLN:NE2	1:D:220:LYS:HD2	2.32	0.45
1:D:355:ILE:O	1:D:395:LYS:HE3	2.16	0.45
1:D:415:VAL:O	1:D:418:CYS:HB3	2.16	0.45
1:D:476:PHE:CZ	1:D:501:PHE:CD1	3.04	0.45
1:A:348:LEU:CD2	1:A:403:GLU:HA	2.46	0.45
1:A:421:LYS:NZ	1:A:479:PHE:CE1	2.79	0.45
1:A:636:LEU:O	1:A:639:GLU:N	2.49	0.45
1:B:244:PHE:O	1:B:246:LEU:N	2.45	0.45
1:C:689:GLU:CG	1:C:694:ILE:HD11	2.46	0.45
1:D:148:LEU:HB2	1:D:195:THR:HG22	1.98	0.45
1:D:387:LEU:HD22	1:D:394:LEU:HD13	1.99	0.45
1:D:404:ASN:C	1:D:574:GLN:OE1	2.55	0.45
2:G:348:VAL:HG22	2:G:400:LEU:HD23	1.99	0.45
2:G:311:ILE:CG1	2:G:421:ILE:HG12	2.45	0.45
2:H:412:LEU:O	2:H:415:LEU:N	2.49	0.45
1:A:341:LEU:HD21	1:A:365:ASN:HB3	1.99	0.45
1:B:302:ILE:HG22	1:B:307:LEU:HG	1.99	0.45
1:B:293:LEU:HD21	1:B:328:LEU:HD13	1.99	0.45
1:B:458:GLN:O	1:B:462:MET:HG2	2.16	0.45
1:B:51:TRP:CH2	1:B:55:LYS:HE3	2.52	0.45
1:C:209:GLN:HE22	1:C:213:PRO:HG3	1.82	0.45
1:C:332:LEU:HD23	1:C:336:PHE:CD2	2.52	0.45
1:C:694:ILE:HD13	1:C:704:VAL:HG22	1.99	0.45
1:C:69:LEU:HD22	1:C:277:GLN:O	2.16	0.45
1:D:100:ILE:O	1:D:271:LEU:HA	2.17	0.45
1:D:255:SER:HB2	1:D:256:PRO:HD3	1.97	0.45
2:F:425:ASP:OD1	2:F:454:TYR:OH	2.34	0.45
2:G:339:ILE:HG21	2:G:351:VAL:HG22	1.99	0.45
2:H:340:ASN:HB2	2:H:343:PHE:CG	2.52	0.45
2:H:397:SER:HB2	2:H:400:LEU:H	1.82	0.45
1:A:104:ALA:HA	1:A:250:PHE:CD2	2.50	0.45
1:A:44:PHE:HZ	1:A:337:TYR:CE1	2.35	0.45
1:A:597:ARG:CZ	1:A:708:THR:OG1	2.65	0.45
1:B:286:THR:HG22	1:B:436:ARG:NE	2.32	0.45
1:B:416:LEU:HD12	1:B:567:TYR:HD1	1.81	0.45
1:B:62:GLN:O	1:B:66:ASN:CG	2.56	0.45
1:C:288:VAL:O	1:C:292:LEU:N	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:PHE:HD2	1:C:324:PHE:HB2	1.81	0.45
1:C:405:LEU:HD11	1:C:576:LEU:HB2	1.98	0.45
1:C:646:LEU:HA	1:C:649:TRP:HB3	1.98	0.45
1:D:271:LEU:CB	1:D:273:ILE:HG13	2.46	0.45
1:D:421:LYS:HB2	1:D:479:PHE:CZ	2.52	0.45
1:D:74:ILE:O	1:D:78:GLN:HB2	2.17	0.45
2:E:441:PHE:HB3	2:E:443:TRP:CE2	2.52	0.45
2:G:412:LEU:HB3	2:G:418:ILE:CD1	2.46	0.45
2:H:369:ILE:HG12	2:H:372:GLN:OE1	2.17	0.45
1:C:708:THR:HB	2:H:427:LEU:HD12	1.98	0.45
2:H:455:THR:O	2:H:459:SER:N	2.50	0.45
1:A:148:LEU:HA	1:A:151:LEU:HD22	1.99	0.45
1:A:151:LEU:HG	1:A:198:LYS:CD	2.46	0.45
1:A:202:LYS:HD2	1:A:244:PHE:CD1	2.52	0.45
1:A:50:ILE:HG12	1:A:298:PHE:CD1	2.52	0.45
1:A:443:LEU:HA	1:A:570:PRO:HD3	1.99	0.45
1:A:683:ARG:HA	1:A:683:ARG:NE	2.32	0.45
1:A:70:PHE:HA	1:A:73:LEU:HB2	1.99	0.45
1:B:426:LEU:HD21	1:B:460:LEU:HG	1.99	0.45
1:B:472:LEU:O	1:B:475:CYS:N	2.49	0.45
1:C:563:LEU:HG	1:C:567:TYR:CD2	2.52	0.45
1:D:81:HIS:NE2	1:D:214:PRO:HB3	2.32	0.45
1:D:217:VAL:HG12	1:D:219:LEU:HD21	1.99	0.45
1:D:107:LEU:HD23	1:D:278:SER:HB2	1.99	0.45
1:D:695:LYS:CG	1:D:696:PRO:CD	2.94	0.45
2:E:339:ILE:CD1	2:E:351:VAL:HG13	2.47	0.45
2:E:352:LEU:CD2	2:E:369:ILE:HG23	2.46	0.45
2:F:325:ARG:HA	2:F:328:THR:OG1	2.17	0.45
2:G:355:ILE:HG23	2:G:356:THR:N	2.31	0.45
2:G:442:ASN:HD22	2:G:442:ASN:HA	1.68	0.45
2:H:325:ARG:HA	2:H:328:THR:OG1	2.17	0.45
1:A:148:LEU:HG	1:A:233:PHE:HE1	1.82	0.45
1:B:147:PHE:HE2	1:B:229:VAL:HG11	1.82	0.45
1:B:209:GLN:HE22	1:B:213:PRO:HG3	1.81	0.45
1:B:72:ASN:HA	1:B:75:GLU:HB2	1.99	0.45
1:B:74:ILE:O	1:B:78:GLN:HB2	2.16	0.45
1:C:151:LEU:CD1	1:C:198:LYS:HD2	2.47	0.45
1:C:371:SER:HA	1:C:374:ARG:HB2	1.99	0.45
1:C:414:LEU:HG	1:C:487:LEU:HD13	1.98	0.45
1:C:415:VAL:O	1:C:418:CYS:HB3	2.17	0.45
1:C:641:SER:OG	1:C:642:ARG:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:LEU:HD13	1:D:271:LEU:HD11	1.98	0.45
1:D:42:LEU:HD13	1:D:354:ARG:NH1	2.32	0.45
1:D:335:HIS:HB2	1:D:582:PHE:CG	2.52	0.45
1:D:686:SER:O	1:D:689:GLU:HB2	2.16	0.45
2:E:347:SER:HA	2:E:399:MET:HG3	1.99	0.45
1:D:591:HIS:CD2	2:F:445:TRP:O	2.70	0.45
1:A:122:THR:HA	1:A:133:VAL:HG23	1.98	0.44
1:A:384:GLN:O	1:A:387:LEU:HB2	2.16	0.44
1:B:152:ILE:CG2	1:B:198:LYS:N	2.80	0.44
1:B:420:HIS:NE2	1:B:435:ILE:HA	2.31	0.44
1:B:480:LYS:O	1:B:484:GLU:HB2	2.17	0.44
1:C:208:SER:HB2	1:C:210:TRP:CE2	2.52	0.44
1:C:209:GLN:OE1	1:C:211:GLN:O	2.35	0.44
1:C:238:SER:HA	1:C:241:LEU:CD1	2.47	0.44
1:C:252:ILE:CD1	1:C:259:ILE:HD11	2.47	0.44
1:D:139:LYS:C	1:D:141:CYS:H	2.21	0.44
1:D:148:LEU:HA	1:D:151:LEU:HD22	1.97	0.44
1:D:144:MET:SD	1:D:233:PHE:CE2	3.10	0.44
1:D:387:LEU:HD21	1:D:397:GLU:CD	2.36	0.44
1:D:548:LYS:O	1:D:552:LEU:N	2.42	0.44
1:D:501:PHE:CE1	1:D:554:GLU:CD	2.91	0.44
2:G:340:ASN:HB2	2:G:343:PHE:CG	2.52	0.44
2:G:369:ILE:HA	2:G:372:GLN:CG	2.47	0.44
2:H:326:PHE:O	2:H:331:LEU:N	2.46	0.44
1:A:138:ALA:O	1:A:141:CYS:HB2	2.17	0.44
1:A:104:ALA:CA	1:A:250:PHE:HD2	2.29	0.44
1:A:423:THR:HG21	1:A:438:LEU:HD21	2.00	0.44
1:C:305:LYS:O	1:C:309:VAL:HG23	2.17	0.44
1:C:472:LEU:O	1:C:475:CYS:N	2.50	0.44
1:D:446:ASN:OD1	1:D:569:LEU:HD11	2.17	0.44
2:F:298:PHE:CD2	2:F:330:MET:HG2	2.53	0.44
2:H:425:ASP:OD1	2:H:454:TYR:OH	2.35	0.44
1:C:683:ARG:HH11	2:H:458:THR:HA	1.81	0.44
1:A:425:SER:OG	1:A:471:ILE:HD13	2.18	0.44
1:A:497:PHE:HB3	1:A:501:PHE:HE2	1.83	0.44
1:A:415:VAL:HG12	1:A:567:TYR:CE1	2.52	0.44
1:B:296:THR:HG22	1:B:413:PHE:CD2	2.53	0.44
1:B:310:LEU:HB3	1:B:324:PHE:HE1	1.82	0.44
1:B:382:GLU:C	1:B:384:GLN:N	2.63	0.44
1:B:393:TYR:O	1:B:397:GLU:HG3	2.18	0.44
1:C:147:PHE:CE2	1:C:229:VAL:CG1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LEU:HB3	1:C:279:LEU:HD12	1.98	0.44
1:C:341:LEU:HD21	1:C:365:ASN:HB2	2.00	0.44
1:C:387:LEU:HD22	1:C:394:LEU:HD13	2.00	0.44
1:C:99:GLU:C	1:C:241:LEU:CD1	2.86	0.44
1:D:152:ILE:CG2	1:D:198:LYS:N	2.80	0.44
1:D:106:VAL:O	1:D:278:SER:HB2	2.17	0.44
1:D:284:HIS:HA	1:D:287:THR:OG1	2.18	0.44
1:D:476:PHE:CE2	1:D:501:PHE:CG	3.05	0.44
2:F:319:LYS:HE3	2:F:423:SER:HB2	2.00	0.44
1:A:268:SER:HA	1:A:271:LEU:HD12	1.99	0.44
1:A:373:ARG:O	1:A:377:GLU:HG3	2.18	0.44
1:A:497:PHE:CE1	1:A:557:VAL:HG13	2.53	0.44
1:B:191:VAL:HG12	1:B:191:VAL:O	2.18	0.44
1:B:348:LEU:O	1:B:352:LYS:HG3	2.17	0.44
1:B:419:LEU:HB2	1:B:567:TYR:CZ	2.53	0.44
1:B:58:ASN:O	1:B:62:GLN:HG3	2.17	0.44
1:B:649:TRP:O	1:B:653:PHE:HB3	2.17	0.44
1:C:683:ARG:HD3	1:C:686:SER:OG	2.17	0.44
1:D:421:LYS:HE3	1:D:479:PHE:CE1	2.53	0.44
1:D:475:CYS:O	1:D:479:PHE:CB	2.62	0.44
1:D:475:CYS:O	1:D:479:PHE:HD2	2.01	0.44
1:D:75:GLU:O	1:D:79:LYS:HG3	2.18	0.44
2:F:356:THR:HG22	2:F:363:MET:O	2.18	0.44
2:G:335:ILE:CG2	2:G:388:LEU:HB2	2.47	0.44
2:G:396:ASP:O	2:G:401:ARG:NE	2.51	0.44
1:A:152:ILE:CG2	1:A:198:LYS:N	2.81	0.44
1:A:216:VAL:HG11	1:A:249:ILE:CD1	2.47	0.44
1:A:415:VAL:HG12	1:A:567:TYR:CE2	2.53	0.44
1:A:414:LEU:HD13	1:A:494:ILE:HD11	1.99	0.44
1:A:81:HIS:CE1	1:A:214:PRO:HG3	2.53	0.44
1:B:79:LYS:O	1:B:83:GLY:N	2.39	0.44
1:C:144:MET:SD	1:C:232:ASP:CB	3.06	0.44
1:C:405:LEU:HD21	1:C:575:PRO:O	2.18	0.44
1:C:42:LEU:O	1:C:46:THR:HG23	2.17	0.44
1:D:384:GLN:O	1:D:387:LEU:HB2	2.17	0.44
1:D:480:LYS:HG2	1:D:498:LEU:HD22	2.00	0.44
1:D:582:PHE:CE1	1:D:583:SER:O	2.70	0.44
2:E:319:LYS:HE3	2:E:423:SER:HB2	2.00	0.44
2:F:312:VAL:HB	2:F:445:TRP:HA	2.00	0.44
2:H:332:GLN:O	2:H:336:HIS:CD2	2.71	0.44
1:C:691:LEU:HA	2:H:425:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:ARG:CZ	2:H:458:THR:HG23	2.47	0.44
1:A:134:VAL:HG13	1:A:154:GLN:CB	2.48	0.44
1:A:144:MET:SD	1:A:233:PHE:CE2	3.11	0.44
1:A:405:LEU:HD11	1:A:576:LEU:HB2	2.00	0.44
1:B:284:HIS:HA	1:B:287:THR:OG1	2.18	0.44
1:B:372:PHE:CE2	1:B:376:VAL:HG21	2.52	0.44
1:B:303:ASN:ND2	1:B:581:TYR:HB3	2.33	0.44
1:B:65:LEU:HB3	1:B:279:LEU:HD12	1.99	0.44
1:C:259:ILE:CG2	1:C:263:LEU:HD12	2.47	0.44
1:C:386:ALA:HB1	1:C:393:TYR:CB	2.48	0.44
1:C:683:ARG:HH12	2:H:461:GLU:HB2	1.82	0.44
1:D:222:MET:SD	1:D:225:PHE:CD2	3.11	0.44
1:D:69:LEU:HD13	1:D:278:SER:HA	2.00	0.44
1:D:42:LEU:O	1:D:46:THR:HG23	2.18	0.44
1:D:688:LEU:HB3	1:D:694:ILE:HG13	2.00	0.44
2:E:320:ARG:O	2:E:324:GLU:HB2	2.17	0.44
2:E:373:LEU:CD2	2:E:412:LEU:HD21	2.48	0.44
2:F:323:LEU:HD12	2:F:393:HIS:CE1	2.53	0.44
2:F:352:LEU:O	2:F:356:THR:OG1	2.15	0.44
2:F:398:GLN:CG	2:F:401:ARG:HG3	2.47	0.44
2:F:410:GLY:O	2:F:414:SER:CB	2.66	0.44
1:A:647:VAL:O	1:A:651:GLU:HB2	2.18	0.44
1:A:67:LYS:O	1:A:71:ASP:HB2	2.18	0.44
1:B:216:VAL:HG11	1:B:249:ILE:HG13	2.00	0.44
1:B:347:ASN:CG	1:D:350:GLU:HG3	2.37	0.44
1:B:384:GLN:O	1:B:388:LEU:HG	2.18	0.44
1:C:196:ASP:O	1:C:199:MET:HG2	2.18	0.44
1:C:100:ILE:HG12	1:C:241:LEU:HD21	2.00	0.44
1:C:202:LYS:HE3	1:C:244:PHE:HE1	1.82	0.44
1:C:333:LEU:HD13	2:H:307:LEU:HD13	1.99	0.44
1:C:557:VAL:O	1:C:561:ASP:HB2	2.18	0.44
1:C:636:LEU:HD13	1:C:653:PHE:HD1	1.83	0.44
1:C:685:VAL:O	1:C:689:GLU:HG3	2.18	0.44
1:D:234:ILE:O	1:D:238:SER:HB3	2.15	0.44
2:H:309:PHE:CD1	2:H:309:PHE:N	2.86	0.44
2:H:347:SER:CB	2:H:399:MET:HG3	2.48	0.44
1:A:100:ILE:HD11	1:A:237:SER:CB	2.48	0.44
1:A:416:LEU:HD12	1:A:567:TYR:CD1	2.53	0.44
1:A:43:ARG:O	1:A:46:THR:OG1	2.35	0.44
1:A:587:ALA:O	1:A:591:HIS:CD2	2.71	0.44
1:B:138:ALA:HB2	1:B:221:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HD11	1:B:237:SER:CB	2.48	0.44
1:B:105:LEU:HB2	1:B:250:PHE:O	2.18	0.44
1:B:367:ARG:NE	1:B:388:LEU:O	2.50	0.44
1:C:134:VAL:HG21	1:C:155:LEU:HG	2.00	0.44
1:C:302:ILE:CG2	1:C:307:LEU:HG	2.48	0.44
1:C:303:ASN:ND2	1:C:581:TYR:HB3	2.33	0.44
1:C:97:LEU:HA	1:C:242:HIS:CD2	2.53	0.44
1:D:148:LEU:HD23	1:D:151:LEU:HD22	1.98	0.44
1:D:250:PHE:HB3	1:D:252:ILE:HD11	2.00	0.44
1:D:286:THR:HG22	1:D:436:ARG:NE	2.33	0.44
1:D:402:LEU:HD21	1:D:576:LEU:HD13	1.99	0.44
1:D:504:LEU:HD11	1:D:554:GLU:CD	2.38	0.44
1:D:453:TYR:OH	1:D:563:LEU:CD1	2.64	0.44
2:E:311:ILE:CG1	2:E:421:ILE:HG12	2.47	0.44
2:G:369:ILE:HA	2:G:372:GLN:CD	2.38	0.44
2:H:287:LEU:CD2	2:H:451:TYR:HB2	2.47	0.44
1:A:563:LEU:HA	1:A:567:TYR:HD2	1.83	0.44
1:A:72:ASN:HA	1:A:75:GLU:HB2	1.99	0.44
1:B:387:LEU:HD21	1:B:397:GLU:CD	2.37	0.44
1:B:405:LEU:HD21	1:B:575:PRO:O	2.17	0.44
1:B:632:ILE:O	1:B:636:LEU:HG	2.17	0.44
1:C:104:ALA:HA	1:C:250:PHE:HB2	1.99	0.44
1:C:354:ARG:HA	1:C:357:PHE:HD2	1.82	0.44
1:C:286:THR:HG22	1:C:436:ARG:HE	1.83	0.44
1:C:482:TYR:CD1	1:C:486:HIS:CG	3.06	0.44
1:C:501:PHE:CE1	1:C:554:GLU:CD	2.92	0.44
1:C:556:VAL:CA	1:C:559:PHE:HD2	2.30	0.44
1:D:216:VAL:HG11	1:D:249:ILE:HG13	1.99	0.44
1:D:564:VAL:O	1:D:568:LEU:HD21	2.17	0.44
1:D:700:LYS:HD3	1:D:703:HIS:NE2	2.32	0.44
2:E:342:PHE:CE1	2:E:343:PHE:CE1	3.06	0.44
2:E:335:ILE:CG2	2:E:388:LEU:HB2	2.48	0.44
2:G:355:ILE:HD11	2:G:388:LEU:HD21	1.98	0.44
2:G:379:LYS:O	2:G:383:ASP:HB2	2.18	0.44
2:G:433:TRP:HB3	2:G:438:GLN:HG3	1.99	0.44
2:H:348:VAL:HG22	2:H:400:LEU:HD23	1.98	0.44
1:A:125:LEU:HB3	1:A:131:PRO:HG2	2.00	0.43
1:A:147:PHE:CE1	1:A:225:PHE:CE1	3.06	0.43
1:A:50:ILE:O	1:A:53:GLN:HB2	2.17	0.43
1:B:355:ILE:O	1:B:395:LYS:HE3	2.18	0.43
1:B:636:LEU:CD2	1:B:656:VAL:HG11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:VAL:O	1:C:388:LEU:N	2.51	0.43
1:C:44:PHE:HZ	1:C:337:TYR:CZ	2.36	0.43
1:D:387:LEU:HA	1:D:394:LEU:HB2	2.00	0.43
1:D:52:GLN:O	1:D:56:SER:OG	2.10	0.43
1:D:557:VAL:O	1:D:561:ASP:HB2	2.17	0.43
1:D:636:LEU:HD13	1:D:653:PHE:HD1	1.83	0.43
1:D:695:LYS:HB3	1:D:697:THR:CG2	2.48	0.43
2:G:323:LEU:HD12	2:G:393:HIS:CE1	2.53	0.43
2:G:320:ARG:NH2	2:G:342:PHE:CZ	2.85	0.43
2:H:325:ARG:O	2:H:329:THR:OG1	2.30	0.43
2:H:391:LEU:CD2	2:H:421:ILE:HB	2.44	0.43
2:H:420:LEU:HD21	2:H:443:TRP:CH2	2.53	0.43
1:A:199:MET:CE	1:A:244:PHE:CE2	3.01	0.43
1:A:279:LEU:HD22	1:A:283:GLU:OE1	2.18	0.43
1:A:557:VAL:HG22	1:A:561:ASP:OD2	2.17	0.43
1:A:697:THR:HG21	1:A:705:ALA:HB3	2.00	0.43
1:B:151:LEU:CG	1:B:198:LYS:HD2	2.48	0.43
1:B:51:TRP:CH2	1:B:329:GLN:NE2	2.86	0.43
1:B:367:ARG:NH2	1:B:391:GLU:HG2	2.33	0.43
1:B:636:LEU:O	1:B:639:GLU:N	2.50	0.43
1:C:106:VAL:O	1:C:278:SER:HB2	2.18	0.43
1:C:280:SER:O	1:C:284:HIS:ND1	2.51	0.43
1:C:688:LEU:HB3	1:C:694:ILE:HG13	2.00	0.43
1:C:685:VAL:HG13	1:C:704:VAL:HG21	2.00	0.43
1:D:221:ASP:N	1:D:221:ASP:OD1	2.47	0.43
1:D:332:LEU:HD23	1:D:336:PHE:CD2	2.53	0.43
1:D:422:PHE:CE1	1:D:472:LEU:HD22	2.53	0.43
1:D:69:LEU:HD22	1:D:277:GLN:O	2.18	0.43
2:E:295:GLU:HA	2:E:298:PHE:CD2	2.53	0.43
2:E:331:LEU:HD11	2:E:391:LEU:CG	2.49	0.43
2:E:398:GLN:HG3	2:E:401:ARG:HG3	2.00	0.43
2:E:425:ASP:OD1	2:E:454:TYR:OH	2.35	0.43
2:F:355:ILE:HG23	2:F:356:THR:N	2.32	0.43
1:A:418:CYS:O	1:A:422:PHE:HD2	2.01	0.43
1:A:42:LEU:HD13	1:A:354:ARG:NH1	2.32	0.43
1:B:371:SER:OG	1:B:576:LEU:N	2.49	0.43
1:B:572:GLU:O	1:B:573:THR:HG23	2.19	0.43
1:B:707:LEU:N	1:B:707:LEU:HD12	2.33	0.43
1:A:45:GLU:CD	1:C:49:LEU:HD23	2.39	0.43
1:D:334:GLU:HG3	1:D:582:PHE:CZ	2.54	0.43
2:E:411:GLN:O	2:E:415:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:420:LEU:HD21	2:E:443:TRP:HH2	1.82	0.43
2:G:304:GLN:OE1	2:G:446:TYR:OH	2.30	0.43
2:H:309:PHE:CE2	2:H:442:ASN:ND2	2.86	0.43
1:A:250:PHE:HB3	1:A:252:ILE:CD1	2.48	0.43
1:A:312:ASN:O	1:A:316:TYR:HB2	2.18	0.43
1:A:354:ARG:O	1:A:358:LEU:HG	2.19	0.43
1:A:632:ILE:O	1:A:636:LEU:HG	2.18	0.43
1:B:144:MET:SD	1:B:233:PHE:CE2	3.11	0.43
1:B:420:HIS:CG	1:B:435:ILE:HG12	2.53	0.43
1:B:474:LYS:O	1:B:478:VAL:HG23	2.19	0.43
1:B:475:CYS:O	1:B:479:PHE:CB	2.63	0.43
1:B:496:GLU:O	1:B:500:GLN:HG3	2.18	0.43
1:C:271:LEU:CB	1:C:273:ILE:HG13	2.49	0.43
1:D:250:PHE:HB3	1:D:252:ILE:CD1	2.47	0.43
1:D:401:LEU:HD12	1:D:576:LEU:HD11	1.99	0.43
1:D:497:PHE:CD1	1:D:557:VAL:CG1	3.01	0.43
1:D:644:ILE:HB	1:D:649:TRP:CE3	2.52	0.43
2:E:325:ARG:HA	2:E:328:THR:OG1	2.17	0.43
2:E:323:LEU:HD12	2:E:393:HIS:CE1	2.53	0.43
2:G:327:ARG:HA	2:G:331:LEU:HD12	2.01	0.43
2:H:411:GLN:O	2:H:415:LEU:HG	2.18	0.43
1:A:139:LYS:C	1:A:141:CYS:H	2.21	0.43
1:A:150:LYS:O	1:A:154:GLN:CG	2.66	0.43
1:A:254:THR:HB	1:A:258:ILE:HD12	2.00	0.43
1:A:335:HIS:HB2	1:A:582:PHE:CG	2.53	0.43
1:B:234:ILE:HD13	1:B:267:VAL:HG13	1.99	0.43
1:B:49:LEU:CD2	1:D:45:GLU:OE2	2.65	0.43
1:B:564:VAL:O	1:B:568:LEU:HD21	2.18	0.43
1:C:136:LEU:HB2	1:C:219:LEU:HD22	2.00	0.43
1:C:241:LEU:C	1:C:243:GLU:H	2.21	0.43
1:C:306:VAL:O	1:C:310:LEU:HD13	2.19	0.43
1:C:381:SER:C	1:C:383:LYS:H	2.21	0.43
1:C:427:PRO:C	1:C:429:TYR:H	2.22	0.43
1:C:461:ARG:HG2	1:C:552:LEU:HD22	1.99	0.43
1:C:71:ASP:O	1:C:75:GLU:HB2	2.19	0.43
1:D:259:ILE:CG2	1:D:263:LEU:HD12	2.47	0.43
1:D:412:TYR:HE1	1:D:568:LEU:O	2.02	0.43
1:D:636:LEU:O	1:D:639:GLU:N	2.50	0.43
2:E:412:LEU:HB3	2:E:418:ILE:CD1	2.49	0.43
1:A:191:VAL:O	1:A:191:VAL:HG12	2.19	0.43
1:A:310:LEU:O	1:A:313:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:PHE:CD1	1:A:480:LYS:HE3	2.53	0.43
1:A:557:VAL:O	1:A:561:ASP:HB2	2.18	0.43
1:A:694:ILE:HD13	1:A:704:VAL:HG22	2.00	0.43
1:B:476:PHE:CD1	1:B:480:LYS:HE3	2.53	0.43
1:B:556:VAL:O	1:B:560:ILE:N	2.42	0.43
1:B:564:VAL:O	1:B:568:LEU:HD11	2.18	0.43
1:C:69:LEU:HD13	1:C:278:SER:HA	2.00	0.43
1:C:371:SER:OG	1:C:576:LEU:N	2.50	0.43
1:C:423:THR:CG2	1:C:438:LEU:HD21	2.49	0.43
1:C:494:ILE:HA	1:C:497:PHE:HD2	1.82	0.43
1:C:457:LEU:CG	1:C:559:PHE:CZ	3.01	0.43
1:C:569:LEU:O	1:C:573:THR:HG23	2.18	0.43
1:C:685:VAL:HG11	1:C:704:VAL:HG21	2.00	0.43
1:D:152:ILE:CG1	1:D:198:LYS:H	2.31	0.43
1:D:419:LEU:HD22	1:D:567:TYR:CE1	2.54	0.43
1:D:476:PHE:CD1	1:D:480:LYS:HE3	2.54	0.43
1:C:682:ILE:HD11	2:H:465:LEU:HD12	2.00	0.43
1:A:134:VAL:O	1:A:218:ILE:HD12	2.18	0.43
1:A:478:VAL:HA	1:A:481:SER:HB3	2.01	0.43
1:A:461:ARG:HG2	1:A:552:LEU:HD21	2.01	0.43
1:A:564:VAL:O	1:A:568:LEU:HD21	2.18	0.43
1:B:370:PRO:C	1:B:372:PHE:H	2.21	0.43
1:B:408:TYR:HB3	1:B:412:TYR:HE2	1.83	0.43
1:D:152:ILE:HG21	1:D:197:PRO:CA	2.49	0.43
1:D:199:MET:HE3	1:D:244:PHE:CE2	2.53	0.43
1:D:370:PRO:C	1:D:372:PHE:H	2.22	0.43
1:D:430:PRO:HB2	1:D:452:GLU:HB3	1.99	0.43
1:D:564:VAL:O	1:D:568:LEU:HD11	2.18	0.43
1:D:335:HIS:HB2	1:D:582:PHE:CD1	2.53	0.43
1:D:58:ASN:ND2	1:D:325:ILE:HD11	2.34	0.43
2:G:295:GLU:HA	2:G:298:PHE:CD2	2.54	0.43
2:H:388:LEU:O	2:H:418:ILE:HA	2.19	0.43
1:A:427:PRO:C	1:A:429:TYR:H	2.22	0.43
1:A:453:TYR:OH	1:A:563:LEU:HD13	2.19	0.43
1:B:136:LEU:HD13	1:B:147:PHE:HD1	1.84	0.43
1:B:338:SER:O	1:B:339:GLN:HG3	2.19	0.43
1:B:560:ILE:O	1:B:565:ARG:HG3	2.19	0.43
1:B:59:GLU:O	1:B:63:GLU:HG3	2.18	0.43
1:B:645:ASN:OD1	1:B:648:ASP:N	2.41	0.43
1:C:110:ASN:HB3	1:C:281:CYS:SG	2.59	0.43
1:C:555:ASN:O	1:C:559:PHE:CD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:LYS:CG	1:C:696:PRO:CD	2.96	0.43
1:D:102:THR:HA	1:D:247:ILE:HG23	2.00	0.43
1:D:110:ASN:HB3	1:D:281:CYS:SG	2.58	0.43
1:D:326:LYS:HA	1:D:329:GLN:HE21	1.83	0.43
1:D:562:CYS:HB3	1:D:567:TYR:CE2	2.53	0.43
1:D:641:SER:OG	1:D:642:ARG:N	2.51	0.43
2:E:335:ILE:HG22	2:E:388:LEU:HA	2.01	0.43
2:E:400:LEU:HD22	2:E:409:ILE:HD11	2.00	0.43
2:E:294:TYR:CZ	2:E:448:THR:HA	2.54	0.43
2:F:291:ASN:O	2:F:295:GLU:HG3	2.19	0.43
2:F:327:ARG:HA	2:F:331:LEU:HD12	2.01	0.43
2:F:429:ALA:N	2:F:430:PRO:HD2	2.34	0.43
2:G:331:LEU:O	2:G:336:HIS:NE2	2.52	0.43
2:H:369:ILE:HA	2:H:372:GLN:CD	2.39	0.43
1:A:219:LEU:HD13	1:A:222:MET:SD	2.59	0.43
1:A:107:LEU:HD23	1:A:278:SER:HB2	2.00	0.43
1:A:355:ILE:O	1:A:395:LYS:HE3	2.19	0.43
1:A:286:THR:HG21	1:A:434:GLN:NE2	2.33	0.43
1:A:563:LEU:HA	1:A:567:TYR:CD2	2.54	0.43
1:B:125:LEU:O	1:B:131:PRO:CG	2.67	0.43
1:B:148:LEU:HD13	1:B:195:THR:HB	2.01	0.43
1:B:263:LEU:HD13	1:B:271:LEU:HD11	1.99	0.43
1:B:497:PHE:CE1	1:B:557:VAL:CG1	3.01	0.43
1:B:558:ASN:O	1:B:563:LEU:HD12	2.19	0.43
1:B:77:LEU:CD2	1:B:247:ILE:HG21	2.47	0.43
1:C:352:LYS:HG2	1:C:399:GLN:HG2	2.00	0.43
1:C:504:LEU:CD2	1:C:550:GLU:HB3	2.48	0.43
1:C:555:ASN:C	1:C:559:PHE:CD2	2.92	0.43
1:C:51:TRP:CH2	1:C:55:LYS:HE3	2.54	0.43
1:C:446:ASN:OD1	1:C:569:LEU:CD1	2.64	0.43
1:C:597:ARG:NH2	1:C:708:THR:OG1	2.51	0.43
1:D:371:SER:O	1:D:375:TYR:HB2	2.18	0.43
2:G:400:LEU:HD22	2:G:409:ILE:CD1	2.47	0.43
2:G:398:GLN:CG	2:G:401:ARG:HG3	2.49	0.43
1:A:693:PHE:CZ	2:G:427:LEU:HD21	2.53	0.43
2:H:400:LEU:HD22	2:H:409:ILE:HD11	2.00	0.43
1:A:372:PHE:CE2	1:A:376:VAL:HG21	2.54	0.43
1:A:476:PHE:HB3	1:A:480:LYS:CE	2.49	0.43
1:A:54:MET:HE3	1:A:292:LEU:HD13	2.01	0.43
1:A:448:TRP:CH2	1:A:559:PHE:HB3	2.54	0.43
1:A:71:ASP:O	1:A:75:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:MET:HE3	1:B:233:PHE:CE1	2.54	0.43
1:B:333:LEU:HB3	1:B:337:TYR:HE2	1.83	0.43
1:C:144:MET:O	1:C:233:PHE:HZ	2.02	0.43
1:C:150:LYS:O	1:C:154:GLN:CG	2.67	0.43
1:C:230:LEU:HD21	1:C:263:LEU:CD2	2.49	0.43
1:C:313:ILE:HG12	1:C:318:ASP:OD1	2.19	0.43
1:C:372:PHE:CE2	1:C:376:VAL:CG2	3.02	0.43
1:C:429:TYR:HB2	1:C:433:ARG:HE	1.83	0.43
1:C:549:PHE:HA	1:C:552:LEU:HB2	2.00	0.43
1:C:578:GLU:O	1:C:579:VAL:HB	2.19	0.43
1:D:286:THR:HG22	1:D:436:ARG:HE	1.84	0.43
1:D:419:LEU:HD23	1:D:438:LEU:HD23	2.01	0.43
1:D:501:PHE:CD1	1:D:554:GLU:OE2	2.71	0.43
1:D:689:GLU:CG	1:D:694:ILE:HD11	2.45	0.43
2:E:436:ALA:O	2:E:440:LEU:HG	2.19	0.43
2:F:340:ASN:HB3	2:F:342:PHE:CZ	2.54	0.43
2:G:377:VAL:HG13	2:G:381:LYS:HG3	2.01	0.43
2:H:320:ARG:NH1	2:H:457:GLU:CD	2.72	0.43
2:H:433:TRP:HB3	2:H:438:GLN:HG3	2.00	0.43
1:A:421:LYS:HE3	1:A:479:PHE:CE1	2.54	0.42
1:A:467:GLU:HG2	1:A:471:ILE:HD12	2.00	0.42
1:A:646:LEU:HD12	1:A:702:ASP:HB3	2.00	0.42
1:A:74:ILE:O	1:A:78:GLN:HB2	2.18	0.42
1:B:152:ILE:HD13	1:B:197:PRO:HD2	2.01	0.42
1:B:155:LEU:HD21	1:B:215:VAL:CG1	2.49	0.42
1:B:202:LYS:HE3	1:B:215:VAL:CG2	2.49	0.42
1:B:350:GLU:CD	1:D:350:GLU:OE2	2.57	0.42
1:B:457:LEU:HG	1:B:559:PHE:HZ	1.81	0.42
1:C:139:LYS:C	1:C:141:CYS:H	2.23	0.42
1:C:273:ILE:HG22	1:C:274:GLU:N	2.34	0.42
1:C:367:ARG:NH2	1:C:391:GLU:HG2	2.34	0.42
1:C:402:LEU:HA	1:C:405:LEU:HD12	2.01	0.42
1:C:552:LEU:O	1:C:556:VAL:CG2	2.67	0.42
1:C:657:VAL:HG12	1:C:677:ILE:HD11	2.01	0.42
1:D:333:LEU:HB3	1:D:337:TYR:HE2	1.83	0.42
2:E:320:ARG:NH1	2:E:457:GLU:CD	2.72	0.42
2:E:369:ILE:HA	2:E:372:GLN:CD	2.39	0.42
2:F:355:ILE:HD11	2:F:388:LEU:HD21	2.01	0.42
2:F:397:SER:CB	2:F:400:LEU:H	2.31	0.42
1:A:693:PHE:CE2	2:G:427:LEU:HD21	2.54	0.42
2:H:295:GLU:O	2:H:298:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HD13	1:A:267:VAL:HG13	2.00	0.42
1:A:371:SER:O	1:A:575:PRO:HA	2.18	0.42
1:A:370:PRO:C	1:A:372:PHE:H	2.22	0.42
1:A:419:LEU:HD22	1:A:567:TYR:CE1	2.53	0.42
1:B:494:ILE:HA	1:B:497:PHE:CD2	2.52	0.42
1:B:563:LEU:HG	1:B:567:TYR:CD2	2.55	0.42
1:A:49:LEU:HD22	1:C:45:GLU:CG	2.49	0.42
1:C:476:PHE:CE2	1:C:501:PHE:CG	3.07	0.42
1:C:335:HIS:HB2	1:C:582:PHE:CD1	2.53	0.42
1:C:636:LEU:CD2	1:C:656:VAL:HG11	2.50	0.42
1:D:107:LEU:HD22	1:D:114:HIS:NE2	2.34	0.42
1:D:352:LYS:O	1:D:355:ILE:HB	2.20	0.42
1:D:474:LYS:O	1:D:478:VAL:HG23	2.19	0.42
2:G:339:ILE:CD1	2:G:351:VAL:HG13	2.49	0.42
2:H:298:PHE:CD2	2:H:330:MET:HG2	2.54	0.42
2:H:355:ILE:HG23	2:H:356:THR:N	2.33	0.42
1:A:152:ILE:HD12	1:A:194:LYS:O	2.20	0.42
1:A:202:LYS:HE3	1:A:215:VAL:HG21	2.02	0.42
1:A:238:SER:HA	1:A:241:LEU:CD1	2.50	0.42
1:A:367:ARG:CZ	1:A:388:LEU:O	2.68	0.42
1:A:409:HIS:HA	1:A:412:TYR:CD2	2.53	0.42
1:A:44:PHE:HZ	1:A:337:TYR:CZ	2.37	0.42
1:A:649:TRP:O	1:A:653:PHE:HB3	2.18	0.42
1:B:476:PHE:CZ	1:B:501:PHE:CG	3.06	0.42
1:C:113:ASP:OD2	1:C:322:GLN:HG3	2.18	0.42
1:C:152:ILE:HD12	1:C:195:THR:HA	2.01	0.42
1:C:142:PRO:O	1:C:229:VAL:HG21	2.20	0.42
1:A:484:GLU:HG2	1:C:392:ARG:HD3	2.01	0.42
1:C:414:LEU:O	1:C:479:PHE:CE1	2.71	0.42
1:D:97:LEU:HA	1:D:242:HIS:CG	2.54	0.42
1:D:402:LEU:HA	1:D:405:LEU:HD12	2.00	0.42
1:D:54:MET:CE	1:D:292:LEU:HB3	2.49	0.42
1:D:552:LEU:O	1:D:556:VAL:CG2	2.67	0.42
1:D:71:ASP:O	1:D:75:GLU:CB	2.67	0.42
2:F:335:ILE:O	2:F:335:ILE:HG22	2.19	0.42
2:F:311:ILE:CG1	2:F:421:ILE:HG12	2.49	0.42
2:F:420:LEU:HD11	2:F:422:ALA:HB2	2.01	0.42
2:G:373:LEU:CD2	2:G:412:LEU:HD21	2.47	0.42
2:G:318:SER:HB2	2:G:457:GLU:OE1	2.19	0.42
1:A:100:ILE:HD11	1:A:237:SER:HB2	2.01	0.42
1:A:234:ILE:HD13	1:A:267:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:CYS:O	1:A:479:PHE:HD2	1.97	0.42
1:A:562:CYS:HB3	1:A:567:TYR:CE2	2.54	0.42
1:A:641:SER:OG	1:A:642:ARG:N	2.51	0.42
1:A:649:TRP:HZ3	1:A:704:VAL:HB	1.85	0.42
1:B:100:ILE:HD11	1:B:237:SER:HB2	2.02	0.42
1:B:71:ASP:O	1:B:75:GLU:HB2	2.19	0.42
1:C:76:PHE:CG	1:C:276:PHE:CZ	3.07	0.42
1:C:582:PHE:CE1	1:C:583:SER:O	2.72	0.42
1:D:227:THR:HA	1:D:230:LEU:HB3	2.02	0.42
1:D:556:VAL:O	1:D:560:ILE:N	2.50	0.42
1:D:649:TRP:CZ3	1:D:704:VAL:HB	2.53	0.42
2:F:318:SER:HA	2:F:319:LYS:HZ1	1.85	0.42
2:F:324:GLU:O	2:F:328:THR:HG23	2.19	0.42
2:G:362:HIS:HB3	2:G:379:LYS:NZ	2.34	0.42
2:G:319:LYS:HE3	2:G:423:SER:HB2	2.00	0.42
1:A:363:CYS:SG	1:A:391:GLU:CD	2.98	0.42
1:B:563:LEU:N	1:B:567:TYR:HD2	2.18	0.42
1:C:209:GLN:H	1:C:210:TRP:HA	1.82	0.42
1:C:252:ILE:HG22	1:C:253:ALA:N	2.34	0.42
1:C:563:LEU:HD23	1:C:567:TYR:CG	2.54	0.42
1:C:564:VAL:O	1:C:568:LEU:HD21	2.19	0.42
2:F:356:THR:OG1	2:F:365:THR:CG2	2.68	0.42
2:F:412:LEU:O	2:F:415:LEU:N	2.53	0.42
2:G:397:SER:CB	2:G:400:LEU:H	2.32	0.42
2:G:397:SER:HB3	2:G:400:LEU:HD12	2.02	0.42
2:H:331:LEU:O	2:H:336:HIS:NE2	2.52	0.42
2:H:410:GLY:O	2:H:414:SER:HB3	2.19	0.42
1:A:118:PHE:HB3	1:A:220:LYS:HE2	2.02	0.42
1:A:342:SER:O	1:A:345:CYS:CB	2.68	0.42
1:A:416:LEU:HA	1:A:567:TYR:HE1	1.84	0.42
1:B:341:LEU:HD21	1:B:365:ASN:HB2	2.00	0.42
1:B:446:ASN:HA	1:B:569:LEU:HD21	2.02	0.42
1:B:75:GLU:O	1:B:79:LYS:HG3	2.19	0.42
1:C:636:LEU:O	1:C:639:GLU:N	2.50	0.42
1:D:314:PHE:CD2	1:D:324:PHE:HB2	2.54	0.42
1:D:372:PHE:HA	1:D:375:TYR:HB3	2.01	0.42
1:D:398:THR:O	1:D:402:LEU:HG	2.19	0.42
1:D:480:LYS:HZ3	1:D:502:GLN:HG3	1.85	0.42
1:D:591:HIS:HA	2:F:445:TRP:H	1.85	0.42
1:D:632:ILE:O	1:D:636:LEU:HG	2.20	0.42
2:E:398:GLN:CG	2:E:401:ARG:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:347:SER:N	2:F:350:SER:OG	2.45	0.42
1:A:305:LYS:O	1:A:309:VAL:HG23	2.20	0.42
1:A:381:SER:HB3	1:A:382:GLU:H	1.52	0.42
1:A:387:LEU:HD23	1:A:394:LEU:HA	2.02	0.42
1:A:367:ARG:NE	1:A:388:LEU:O	2.52	0.42
1:A:408:TYR:HB3	1:A:412:TYR:HE2	1.84	0.42
1:A:694:ILE:CG1	1:A:704:VAL:HG13	2.49	0.42
1:B:152:ILE:HD12	1:B:194:LYS:O	2.20	0.42
1:B:152:ILE:CG1	1:B:198:LYS:HG3	2.50	0.42
1:C:162:ILE:O	1:C:162:ILE:HG22	2.19	0.42
1:C:402:LEU:HD21	1:C:576:LEU:HD13	2.02	0.42
1:C:286:THR:HG22	1:C:436:ARG:NE	2.34	0.42
1:D:104:ALA:CA	1:D:250:PHE:HD2	2.33	0.42
1:D:147:PHE:CE1	1:D:225:PHE:CE1	3.08	0.42
1:D:216:VAL:CG1	1:D:249:ILE:HG13	2.49	0.42
2:E:309:PHE:CD1	2:E:309:PHE:N	2.86	0.42
2:F:320:ARG:CZ	2:F:456:GLU:HB2	2.50	0.42
2:G:318:SER:HA	2:G:319:LYS:HZ1	1.85	0.42
2:H:298:PHE:HB3	2:H:330:MET:CG	2.49	0.42
1:A:217:VAL:HG12	1:A:219:LEU:HD21	2.00	0.42
1:A:106:VAL:O	1:A:278:SER:HB2	2.20	0.42
1:B:421:LYS:HB2	1:B:479:PHE:CZ	2.55	0.42
1:B:404:ASN:HB2	1:B:574:GLN:OE1	2.20	0.42
1:C:136:LEU:HB2	1:C:219:LEU:CD2	2.50	0.42
1:C:144:MET:HE3	1:C:233:PHE:CE1	2.54	0.42
1:C:263:LEU:CD1	1:C:271:LEU:HD11	2.50	0.42
1:C:302:ILE:HG21	1:C:306:VAL:HG22	1.98	0.42
1:C:330:LEU:HD21	2:H:309:PHE:CE2	2.54	0.42
1:C:552:LEU:O	1:C:556:VAL:HB	2.19	0.42
1:C:695:LYS:O	1:C:697:THR:HG23	2.20	0.42
1:D:113:ASP:OD2	1:D:322:GLN:HG3	2.20	0.42
1:D:426:LEU:HD21	1:D:460:LEU:HG	2.01	0.42
1:D:685:VAL:HG13	1:D:704:VAL:HG21	2.01	0.42
2:F:453:PRO:CA	2:F:454:TYR:HB2	2.46	0.42
2:H:394:ASN:ND2	2:H:425:ASP:OD2	2.32	0.42
1:A:152:ILE:HD13	1:A:197:PRO:HD2	2.02	0.42
1:A:147:PHE:CE1	1:A:225:PHE:CZ	3.07	0.42
1:A:386:ALA:HB1	1:A:393:TYR:CB	2.50	0.42
1:A:569:LEU:CB	1:A:571:PRO:HD2	2.48	0.42
1:A:79:LYS:O	1:A:83:GLY:N	2.38	0.42
1:B:216:VAL:HG11	1:B:249:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LYS:NZ	1:B:479:PHE:CD1	2.74	0.42
1:B:555:ASN:HB3	1:B:559:PHE:CE2	2.55	0.42
1:B:416:LEU:HA	1:B:567:TYR:HE1	1.84	0.42
1:C:132:TYR:O	1:C:155:LEU:CD2	2.68	0.42
1:C:131:PRO:CB	1:C:214:PRO:O	2.68	0.42
1:C:257:ILE:O	1:C:261:ARG:HG3	2.20	0.42
1:C:54:MET:HE3	1:C:292:LEU:HD13	2.01	0.42
1:C:330:LEU:HD13	1:C:592:LEU:HD21	2.00	0.42
1:C:330:LEU:HD21	2:H:309:PHE:CD2	2.55	0.42
1:C:400:LEU:O	1:C:404:ASN:ND2	2.53	0.42
1:C:686:SER:O	1:C:689:GLU:HB2	2.19	0.42
1:D:41:LYS:HD2	1:D:44:PHE:HE2	1.84	0.42
1:D:563:LEU:CA	1:D:567:TYR:HD2	2.33	0.42
1:D:67:LYS:O	1:D:71:ASP:HB2	2.19	0.42
2:F:309:PHE:N	2:F:309:PHE:CD1	2.87	0.42
2:H:320:ARG:HH22	2:H:457:GLU:CA	2.33	0.42
1:A:332:LEU:HD23	1:A:336:PHE:CD2	2.54	0.42
1:A:41:LYS:HD2	1:A:44:PHE:HE2	1.85	0.42
1:B:126:GLN:HB3	1:B:162:ILE:HD11	2.01	0.42
1:B:234:ILE:HD13	1:B:267:VAL:CG1	2.50	0.42
1:B:480:LYS:O	1:B:484:GLU:HG3	2.19	0.42
1:B:552:LEU:O	1:B:556:VAL:CG2	2.68	0.42
1:C:202:LYS:HE3	1:C:215:VAL:HG21	2.02	0.42
1:C:222:MET:SD	1:C:225:PHE:CD2	3.13	0.42
1:C:202:LYS:HZ2	1:C:244:PHE:CE1	1.78	0.42
1:C:310:LEU:HB3	1:C:324:PHE:HE1	1.84	0.42
1:C:352:LYS:O	1:C:355:ILE:HB	2.20	0.42
1:C:687:GLU:OE2	2:H:454:TYR:CB	2.68	0.42
1:C:75:GLU:O	1:C:79:LYS:HG3	2.20	0.42
2:G:332:GLN:O	2:G:336:HIS:HD2	2.03	0.42
1:A:594:ALA:HB2	2:G:445:TRP:CE2	2.55	0.42
1:C:591:HIS:CD2	2:H:445:TRP:O	2.73	0.42
1:A:81:HIS:NE2	1:A:214:PRO:HB3	2.35	0.41
1:A:474:LYS:O	1:A:478:VAL:HG23	2.20	0.41
1:A:569:LEU:HB3	1:A:570:PRO:HD2	2.01	0.41
1:A:570:PRO:O	1:A:573:THR:OG1	2.26	0.41
1:A:694:ILE:CD1	1:A:704:VAL:HG13	2.48	0.41
1:B:41:LYS:HD2	1:B:44:PHE:HE2	1.84	0.41
1:B:426:LEU:CD2	1:B:456:VAL:HG13	2.50	0.41
1:B:476:PHE:O	1:B:480:LYS:CB	2.63	0.41
1:C:376:VAL:HG13	1:C:384:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:LEU:HD21	1:C:460:LEU:HG	2.02	0.41
1:C:461:ARG:HG2	1:C:552:LEU:HD21	2.02	0.41
1:C:637:HIS:CD2	1:C:694:ILE:CG2	3.03	0.41
1:C:636:LEU:HD11	1:C:657:VAL:HG21	2.02	0.41
1:C:649:TRP:CZ3	1:C:704:VAL:HB	2.52	0.41
1:D:101:PRO:HA	1:D:271:LEU:O	2.20	0.41
1:D:199:MET:CE	1:D:243:GLU:HB3	2.50	0.41
1:D:419:LEU:HB2	1:D:567:TYR:CZ	2.55	0.41
1:D:552:LEU:O	1:D:556:VAL:HB	2.20	0.41
2:E:348:VAL:HG23	2:E:399:MET:HB2	2.03	0.41
2:F:332:GLN:O	2:F:333:ASP:C	2.59	0.41
2:F:362:HIS:O	2:F:363:MET:HG2	2.19	0.41
2:H:400:LEU:HD22	2:H:409:ILE:CD1	2.50	0.41
1:A:152:ILE:CD1	1:A:195:THR:C	2.88	0.41
1:A:75:GLU:O	1:A:79:LYS:HG3	2.21	0.41
1:B:338:SER:O	1:B:339:GLN:CG	2.69	0.41
1:B:476:PHE:CE2	1:B:501:PHE:CG	3.08	0.41
1:B:653:PHE:O	1:B:657:VAL:HB	2.20	0.41
1:C:152:ILE:HA	1:C:198:LYS:CG	2.50	0.41
1:C:255:SER:CB	1:C:256:PRO:CD	2.98	0.41
1:C:263:LEU:HD13	1:C:271:LEU:HD11	2.02	0.41
1:C:373:ARG:O	1:C:377:GLU:HG3	2.20	0.41
1:C:446:ASN:HB2	1:C:449:ASP:HB2	2.03	0.41
1:D:104:ALA:HA	1:D:250:PHE:CD2	2.52	0.41
1:D:255:SER:CB	1:D:256:PRO:CD	2.98	0.41
1:D:324:PHE:CE2	1:D:328:LEU:HD11	2.54	0.41
1:D:694:ILE:HD13	1:D:704:VAL:HG22	2.02	0.41
2:E:369:ILE:HG21	2:E:408:ILE:CD1	2.50	0.41
2:E:348:VAL:HG22	2:E:400:LEU:HD23	2.02	0.41
2:E:320:ARG:HH12	2:E:457:GLU:H	1.68	0.41
2:G:395:LEU:HD12	2:G:400:LEU:HD13	2.02	0.41
2:G:390:LEU:CD2	2:G:418:ILE:HD12	2.50	0.41
2:G:388:LEU:HB3	2:G:418:ILE:HG22	2.02	0.41
2:G:318:SER:HB2	2:G:454:TYR:H	1.86	0.41
2:G:320:ARG:NH2	2:G:457:GLU:HG3	2.35	0.41
2:H:321:ASP:O	2:H:325:ARG:HG3	2.20	0.41
2:H:453:PRO:CA	2:H:454:TYR:HB2	2.45	0.41
1:A:122:THR:HA	1:A:133:VAL:HG21	2.02	0.41
1:A:202:LYS:CE	1:A:215:VAL:CG2	2.98	0.41
1:A:255:SER:CB	1:A:256:PRO:CD	2.99	0.41
1:A:420:HIS:CE1	1:A:435:ILE:HG23	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLN:O	1:A:66:ASN:CG	2.58	0.41
1:A:604:LEU:CD1	1:A:693:PHE:CZ	3.03	0.41
1:A:695:LYS:O	1:A:697:THR:HG23	2.21	0.41
1:B:141:CYS:CB	1:B:147:PHE:CZ	3.01	0.41
1:B:58:ASN:ND2	1:B:325:ILE:HD11	2.35	0.41
1:B:333:LEU:O	1:B:336:PHE:N	2.52	0.41
1:B:371:SER:O	1:B:575:PRO:HA	2.20	0.41
1:B:421:LYS:NZ	1:B:479:PHE:CE1	2.81	0.41
1:B:482:TYR:HA	1:B:486:HIS:HB2	2.01	0.41
1:C:150:LYS:O	1:C:151:LEU:C	2.59	0.41
1:C:370:PRO:HA	1:C:373:ARG:HB2	2.02	0.41
1:C:413:PHE:O	1:C:414:LEU:C	2.59	0.41
1:C:439:TYR:O	1:C:443:LEU:HD13	2.20	0.41
1:C:595:ALA:HB1	1:C:598:ILE:HD12	2.03	0.41
1:C:700:LYS:HB3	1:C:703:HIS:CE1	2.55	0.41
1:D:482:TYR:CD1	1:D:486:HIS:CG	3.08	0.41
1:D:570:PRO:CD	1:D:571:PRO:HD3	2.50	0.41
2:E:298:PHE:CD2	2:E:330:MET:CG	3.03	0.41
2:E:356:THR:OG1	2:E:365:THR:CG2	2.68	0.41
2:F:342:PHE:O	2:F:344:PRO:HD3	2.20	0.41
2:F:396:ASP:O	2:F:401:ARG:NE	2.53	0.41
2:F:409:ILE:HG22	2:F:441:PHE:CE1	2.56	0.41
2:F:416:HIS:O	2:F:417:ASN:C	2.58	0.41
1:A:199:MET:HG2	1:A:244:PHE:HE2	1.85	0.41
1:A:238:SER:HA	1:A:241:LEU:HG	2.02	0.41
1:A:263:LEU:CD1	1:A:271:LEU:HD11	2.50	0.41
1:A:283:GLU:O	1:A:287:THR:HG23	2.20	0.41
1:A:352:LYS:HG2	1:A:355:ILE:HD12	2.02	0.41
1:A:401:LEU:HD12	1:A:576:LEU:HD11	2.03	0.41
1:A:426:LEU:HD21	1:A:460:LEU:HG	2.02	0.41
1:A:548:LYS:O	1:A:552:LEU:HG	2.20	0.41
1:B:147:PHE:HE1	1:B:225:PHE:CZ	2.37	0.41
1:B:350:GLU:HG3	1:D:347:ASN:OD1	2.20	0.41
1:C:43:ARG:O	1:C:46:THR:OG1	2.36	0.41
1:C:476:PHE:CZ	1:C:501:PHE:CG	3.08	0.41
1:D:199:MET:HE1	1:D:203:LYS:HE3	2.01	0.41
1:D:467:GLU:HG2	1:D:471:ILE:HD12	2.02	0.41
1:D:504:LEU:CD2	1:D:550:GLU:HB3	2.51	0.41
1:D:453:TYR:OH	1:D:559:PHE:HD1	2.02	0.41
1:D:405:LEU:HD21	1:D:575:PRO:O	2.21	0.41
1:D:694:ILE:CB	1:D:704:VAL:HG13	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:362:HIS:O	2:E:363:MET:HG2	2.19	0.41
2:E:393:HIS:HA	2:E:423:SER:OG	2.21	0.41
2:E:454:TYR:O	2:E:458:THR:OG1	2.29	0.41
2:F:298:PHE:HB3	2:F:330:MET:CG	2.51	0.41
2:F:320:ARG:HH22	2:F:457:GLU:CA	2.34	0.41
2:F:335:ILE:CG2	2:F:388:LEU:HB2	2.51	0.41
2:F:352:LEU:O	2:F:355:ILE:HG22	2.20	0.41
2:G:326:PHE:CE2	2:G:421:ILE:CD1	3.04	0.41
1:A:97:LEU:HA	1:A:242:HIS:CG	2.55	0.41
1:B:150:LYS:O	1:B:151:LEU:C	2.58	0.41
1:B:162:ILE:O	1:B:162:ILE:HG22	2.20	0.41
1:B:248:LEU:CD1	1:B:250:PHE:CE1	3.03	0.41
1:B:255:SER:CB	1:B:256:PRO:CD	2.98	0.41
1:B:107:LEU:HD23	1:B:278:SER:HB2	2.03	0.41
1:B:314:PHE:O	1:B:319:PHE:HD1	2.03	0.41
1:C:70:PHE:CZ	1:C:117:THR:HB	2.55	0.41
1:C:304:GLU:O	1:C:308:GLN:HG3	2.21	0.41
1:C:467:GLU:HG2	1:C:471:ILE:HD12	2.01	0.41
1:C:637:HIS:CD2	1:C:694:ILE:HG22	2.55	0.41
1:D:144:MET:SD	1:D:232:ASP:CB	3.09	0.41
1:D:423:THR:HG21	1:D:438:LEU:HD21	2.02	0.41
1:D:555:ASN:HB3	1:D:559:PHE:CE2	2.55	0.41
1:D:597:ARG:CZ	1:D:708:THR:OG1	2.69	0.41
1:D:685:VAL:HG11	1:D:704:VAL:HG21	2.01	0.41
2:E:295:GLU:HA	2:E:298:PHE:CG	2.56	0.41
2:E:335:ILE:HG22	2:E:388:LEU:HD13	2.03	0.41
2:E:369:ILE:HA	2:E:372:GLN:CG	2.51	0.41
2:E:409:ILE:O	2:E:413:SER:OG	2.36	0.41
2:E:433:TRP:HB3	2:E:438:GLN:HG3	2.02	0.41
2:F:304:GLN:HA	2:F:307:LEU:HD12	2.03	0.41
2:F:320:ARG:O	2:F:324:GLU:HB2	2.21	0.41
2:F:352:LEU:CA	2:F:355:ILE:HG22	2.50	0.41
1:A:337:TYR:CD1	2:G:300:LYS:HE3	2.56	0.41
1:A:153:SER:O	1:A:157:ASP:CG	2.59	0.41
1:A:202:LYS:C	1:A:206:THR:O	2.58	0.41
1:A:43:ARG:HH11	1:A:336:PHE:C	2.23	0.41
1:A:370:PRO:HA	1:A:373:ARG:HB2	2.02	0.41
1:A:419:LEU:HB2	1:A:567:TYR:OH	2.21	0.41
1:A:342:SER:CB	1:A:579:VAL:CG1	2.98	0.41
1:A:686:SER:O	1:A:690:LEU:HG	2.20	0.41
1:A:69:LEU:HD22	1:A:277:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLN:OE1	1:B:211:GLN:O	2.38	0.41
1:B:250:PHE:HB3	1:B:252:ILE:HD11	2.01	0.41
1:B:288:VAL:O	1:B:292:LEU:N	2.43	0.41
1:B:497:PHE:O	1:B:500:GLN:HB2	2.21	0.41
1:B:554:GLU:HA	1:B:557:VAL:HB	2.02	0.41
1:B:67:LYS:O	1:B:71:ASP:HB2	2.21	0.41
1:C:74:ILE:O	1:C:78:GLN:HB2	2.20	0.41
1:D:305:LYS:O	1:D:309:VAL:HG23	2.21	0.41
1:D:44:PHE:HZ	1:D:337:TYR:CZ	2.39	0.41
1:D:342:SER:CB	1:D:579:VAL:CG1	2.98	0.41
1:B:484:GLU:HB3	1:D:392:ARG:NE	2.35	0.41
1:D:707:LEU:HD12	1:D:707:LEU:N	2.35	0.41
2:G:295:GLU:HA	2:G:298:PHE:CG	2.55	0.41
2:H:380:PHE:O	2:H:383:ASP:O	2.39	0.41
1:A:147:PHE:CE2	1:A:229:VAL:CG1	3.03	0.41
1:A:209:GLN:OE1	1:A:211:GLN:O	2.39	0.41
1:A:266:ALA:O	1:A:270:LEU:HG	2.21	0.41
1:A:314:PHE:HD2	1:A:324:PHE:HB2	1.85	0.41
1:A:402:LEU:HD21	1:A:576:LEU:HD13	2.02	0.41
1:A:59:GLU:O	1:A:63:GLU:HG3	2.20	0.41
1:A:695:LYS:HG3	1:A:696:PRO:CD	2.50	0.41
1:B:121:LEU:HD21	1:B:125:LEU:HD12	2.03	0.41
1:B:416:LEU:HD12	1:B:567:TYR:CD1	2.56	0.41
1:B:427:PRO:C	1:B:429:TYR:H	2.23	0.41
1:C:125:LEU:O	1:C:131:PRO:CG	2.67	0.41
1:C:196:ASP:HB2	1:C:197:PRO:HD3	2.03	0.41
1:C:408:TYR:CE2	1:C:574:GLN:HG3	2.56	0.41
1:C:476:PHE:HB3	1:C:480:LYS:CE	2.51	0.41
1:C:497:PHE:O	1:C:500:GLN:N	2.54	0.41
1:C:501:PHE:CD1	1:C:554:GLU:CD	2.94	0.41
1:C:588:LEU:O	1:C:591:HIS:N	2.52	0.41
1:C:586:HIS:O	1:C:590:GLU:HG3	2.20	0.41
1:D:147:PHE:HB2	1:D:233:PHE:CE1	2.56	0.41
1:D:152:ILE:CG2	1:D:197:PRO:HB2	2.50	0.41
1:D:350:GLU:O	1:D:354:ARG:HG2	2.20	0.41
1:D:393:TYR:O	1:D:397:GLU:HG3	2.21	0.41
1:D:476:PHE:CZ	1:D:501:PHE:CD2	3.09	0.41
1:D:453:TYR:CZ	1:D:563:LEU:HD13	2.56	0.41
1:D:563:LEU:HD23	1:D:567:TYR:CG	2.56	0.41
2:F:355:ILE:O	2:F:359:VAL:HG23	2.21	0.41
2:H:335:ILE:CG2	2:H:388:LEU:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:NH2	1:A:391:GLU:HG2	2.36	0.41
1:A:421:LYS:HB2	1:A:479:PHE:CZ	2.56	0.41
1:A:497:PHE:O	1:A:500:GLN:HB2	2.21	0.41
1:A:501:PHE:CD1	1:A:554:GLU:OE2	2.73	0.41
1:A:578:GLU:O	1:A:579:VAL:HB	2.21	0.41
1:B:482:TYR:CD1	1:B:486:HIS:CG	3.09	0.41
1:B:709:TRP:N	1:B:709:TRP:CD1	2.87	0.41
1:C:282:LYS:O	1:C:286:THR:HG23	2.21	0.41
1:C:419:LEU:HD23	1:C:438:LEU:HD23	2.02	0.41
1:C:418:CYS:O	1:C:422:PHE:CD2	2.74	0.41
1:C:600:LEU:HB3	1:C:693:PHE:HZ	1.86	0.41
1:D:694:ILE:HA	1:D:706:ARG:HA	2.03	0.41
2:F:342:PHE:CE1	2:F:343:PHE:CD1	3.09	0.41
2:G:355:ILE:O	2:G:359:VAL:HG23	2.20	0.41
2:H:445:TRP:N	2:H:445:TRP:CD1	2.88	0.41
1:A:150:LYS:O	1:A:151:LEU:C	2.59	0.41
1:A:314:PHE:HA	1:A:318:ASP:O	2.21	0.41
1:A:423:THR:CG2	1:A:438:LEU:HD21	2.51	0.41
1:A:456:VAL:HA	1:A:459:LEU:HD12	2.02	0.41
1:A:476:PHE:CE2	1:A:501:PHE:CG	3.09	0.41
1:A:700:LYS:HB3	1:A:703:HIS:CE1	2.56	0.41
1:B:202:LYS:C	1:B:206:THR:O	2.59	0.41
1:B:221:ASP:N	1:B:221:ASP:OD1	2.52	0.41
1:B:282:LYS:HE3	1:B:319:PHE:CE2	2.56	0.41
1:B:373:ARG:O	1:B:377:GLU:HG3	2.21	0.41
1:B:425:SER:OG	1:B:471:ILE:HD13	2.20	0.41
1:B:50:ILE:HG12	1:B:298:PHE:CE1	2.55	0.41
1:C:217:VAL:N	1:C:247:ILE:O	2.46	0.41
1:C:375:TYR:CZ	1:C:401:LEU:HD21	2.54	0.41
1:C:404:ASN:O	1:C:408:TYR:HD2	2.04	0.41
1:C:482:TYR:HA	1:C:486:HIS:HB2	2.03	0.41
1:D:122:THR:HA	1:D:133:VAL:HG23	2.03	0.41
1:D:238:SER:HA	1:D:241:LEU:CD1	2.51	0.41
1:D:252:ILE:HG22	1:D:253:ALA:N	2.35	0.41
1:D:554:GLU:HA	1:D:557:VAL:HB	2.03	0.41
1:D:572:GLU:O	1:D:573:THR:HG23	2.20	0.41
2:E:327:ARG:HA	2:E:331:LEU:HD12	2.03	0.41
2:E:355:ILE:HD11	2:E:388:LEU:HD21	2.03	0.41
2:E:446:TYR:HB2	2:E:448:THR:HG23	2.03	0.41
2:G:318:SER:HA	2:G:319:LYS:NZ	2.36	0.41
1:A:144:MET:HE3	1:A:233:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HG22	1:A:162:ILE:O	2.21	0.41
1:A:282:LYS:O	1:A:285:LEU:HB3	2.21	0.41
1:A:335:HIS:HB2	1:A:582:PHE:CD1	2.56	0.41
1:A:482:TYR:CD1	1:A:486:HIS:CG	3.09	0.41
1:B:131:PRO:HB3	1:B:214:PRO:O	2.21	0.41
1:B:299:PRO:HB2	1:B:345:CYS:SG	2.61	0.41
1:B:370:PRO:HA	1:B:373:ARG:HB2	2.02	0.41
1:B:570:PRO:CD	1:B:571:PRO:HD3	2.51	0.41
1:C:217:VAL:HG12	1:C:219:LEU:HD21	2.02	0.41
1:C:244:PHE:O	1:C:246:LEU:N	2.51	0.41
1:C:97:LEU:HD22	1:C:242:HIS:CB	2.51	0.41
1:D:152:ILE:HG12	1:D:198:LYS:N	2.34	0.41
1:D:248:LEU:CD1	1:D:250:PHE:CE1	3.04	0.41
1:D:688:LEU:HD12	1:D:691:LEU:HD12	2.03	0.41
2:F:331:LEU:HD11	2:F:391:LEU:CD1	2.49	0.41
2:G:309:PHE:HB2	2:G:444:LEU:HD11	2.03	0.41
2:G:320:ARG:NE	2:G:456:GLU:HB2	2.36	0.41
1:A:126:GLN:HB3	1:A:162:ILE:CD1	2.51	0.41
1:A:199:MET:HE1	1:A:243:GLU:OE1	2.20	0.41
1:A:282:LYS:O	1:A:286:THR:HG23	2.21	0.41
1:A:306:VAL:O	1:A:310:LEU:HB2	2.21	0.41
1:A:332:LEU:HD23	1:A:336:PHE:HD2	1.86	0.41
1:B:139:LYS:C	1:B:141:CYS:H	2.24	0.41
1:B:118:PHE:HB3	1:B:220:LYS:HE2	2.03	0.41
1:B:144:MET:HE3	1:B:233:PHE:CZ	2.56	0.41
1:B:238:SER:HA	1:B:241:LEU:CD1	2.51	0.41
1:B:252:ILE:CD1	1:B:259:ILE:HD11	2.51	0.41
1:B:563:LEU:CA	1:B:567:TYR:HD2	2.34	0.41
1:C:151:LEU:CG	1:C:198:LYS:HD2	2.47	0.41
1:C:103:ALA:O	1:C:250:PHE:HD2	2.04	0.41
1:D:273:ILE:HG22	1:D:274:GLU:N	2.35	0.41
1:D:50:ILE:HG12	1:D:298:PHE:CD1	2.56	0.41
1:D:476:PHE:CD2	1:D:476:PHE:N	2.89	0.41
2:G:356:THR:OG1	2:G:365:THR:CG2	2.68	0.41
2:H:377:VAL:HG22	2:H:415:LEU:HD13	2.03	0.41
1:A:209:GLN:NE2	1:A:213:PRO:HG3	2.36	0.40
1:A:219:LEU:CB	1:A:222:MET:HG2	2.51	0.40
1:A:222:MET:HG3	1:A:250:PHE:HD1	1.83	0.40
1:A:252:ILE:HG22	1:A:253:ALA:N	2.36	0.40
1:A:555:ASN:O	1:A:558:ASN:N	2.54	0.40
1:B:153:SER:O	1:B:157:ASP:CG	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ILE:HG22	1:B:253:ALA:N	2.35	0.40
1:B:264:PRO:HG2	1:B:267:VAL:HG23	2.03	0.40
1:B:387:LEU:HD23	1:B:394:LEU:HA	2.03	0.40
1:B:589:ARG:HG3	1:B:593:ASN:OD1	2.22	0.40
1:B:60:ARG:O	1:B:63:GLU:HB2	2.21	0.40
1:B:689:GLU:CG	1:B:694:ILE:HD11	2.47	0.40
1:C:107:LEU:HD22	1:C:114:HIS:NE2	2.35	0.40
1:C:219:LEU:CD1	1:C:222:MET:SD	3.09	0.40
1:A:350:GLU:HG3	1:C:347:ASN:OD1	2.21	0.40
1:C:448:TRP:CZ2	1:C:559:PHE:CD1	3.09	0.40
1:C:480:LYS:O	1:C:484:GLU:HG3	2.19	0.40
1:C:683:ARG:HG3	1:C:687:GLU:OE2	2.22	0.40
1:C:688:LEU:O	1:C:693:PHE:N	2.55	0.40
1:C:694:ILE:CB	1:C:704:VAL:HG13	2.51	0.40
1:D:76:PHE:CG	1:D:276:PHE:CZ	3.09	0.40
1:D:279:LEU:HD22	1:D:283:GLU:OE1	2.20	0.40
1:D:321:VAL:O	1:D:325:ILE:HB	2.21	0.40
1:D:394:LEU:O	1:D:395:LYS:C	2.60	0.40
1:D:440:CYS:O	1:D:444:GLU:HG3	2.21	0.40
1:D:491:ALA:O	1:D:492:LYS:HB2	2.21	0.40
1:D:555:ASN:O	1:D:558:ASN:N	2.54	0.40
2:E:309:PHE:CE2	2:E:442:ASN:ND2	2.89	0.40
2:F:287:LEU:CD2	2:F:451:TYR:HB2	2.51	0.40
2:G:336:HIS:HA	2:G:389:PHE:O	2.21	0.40
2:H:340:ASN:HB2	2:H:343:PHE:CD2	2.57	0.40
2:H:352:LEU:O	2:H:365:THR:CG2	2.69	0.40
2:H:390:LEU:HG	2:H:419:TYR:O	2.21	0.40
1:A:97:LEU:HD23	1:A:242:HIS:CG	2.56	0.40
1:A:341:LEU:HD21	1:A:365:ASN:HB2	2.03	0.40
1:A:394:LEU:O	1:A:395:LYS:C	2.60	0.40
1:A:296:THR:CB	1:A:410:MET:SD	3.09	0.40
1:A:564:VAL:O	1:A:568:LEU:HD11	2.21	0.40
1:B:257:ILE:O	1:B:261:ARG:HG3	2.21	0.40
1:B:497:PHE:CD1	1:B:557:VAL:CG1	3.03	0.40
1:B:578:GLU:O	1:B:579:VAL:HB	2.20	0.40
1:C:144:MET:SD	1:C:229:VAL:HA	2.61	0.40
1:C:238:SER:HA	1:C:241:LEU:CG	2.51	0.40
1:C:343:VAL:HG13	1:C:354:ARG:HH11	1.87	0.40
1:D:191:VAL:HG12	1:D:191:VAL:O	2.22	0.40
1:D:310:LEU:HB3	1:D:324:PHE:HE1	1.86	0.40
1:D:472:LEU:O	1:D:476:PHE:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:599:ALA:O	1:D:603:ALA:HB2	2.21	0.40
1:D:600:LEU:HB3	1:D:693:PHE:HZ	1.86	0.40
2:E:318:SER:HB2	2:E:454:TYR:H	1.86	0.40
2:E:331:LEU:HB3	2:E:336:HIS:CE1	2.57	0.40
2:E:340:ASN:O	2:E:343:PHE:HB2	2.21	0.40
2:E:347:SER:O	2:E:350:SER:N	2.55	0.40
2:F:352:LEU:HA	2:F:355:ILE:CG2	2.50	0.40
2:G:319:LYS:HE3	2:G:423:SER:CB	2.51	0.40
2:G:433:TRP:HB3	2:G:438:GLN:CG	2.51	0.40
2:H:341:GLY:N	2:H:393:HIS:O	2.45	0.40
2:H:396:ASP:O	2:H:401:ARG:NE	2.55	0.40
1:A:221:ASP:N	1:A:221:ASP:OD1	2.51	0.40
1:A:552:LEU:O	1:A:556:VAL:CG2	2.69	0.40
1:A:685:VAL:O	1:A:689:GLU:HG3	2.21	0.40
1:B:109:VAL:O	1:B:109:VAL:HG22	2.21	0.40
1:B:151:LEU:HA	1:B:198:LYS:HZ2	1.86	0.40
1:B:386:ALA:CB	1:B:393:TYR:HB3	2.51	0.40
1:B:419:LEU:HB2	1:B:567:TYR:OH	2.21	0.40
1:B:420:HIS:CD2	1:B:435:ILE:HG12	2.56	0.40
1:B:504:LEU:CD1	1:B:554:GLU:CD	2.89	0.40
1:C:126:GLN:HB3	1:C:162:ILE:HD11	2.03	0.40
1:C:504:LEU:CD1	1:C:554:GLU:OE1	2.69	0.40
1:C:645:ASN:HA	1:C:703:HIS:NE2	2.36	0.40
1:C:700:LYS:HD3	1:C:703:HIS:NE2	2.35	0.40
1:D:152:ILE:HG21	1:D:197:PRO:HD2	2.03	0.40
1:D:241:LEU:HB3	1:D:242:HIS:CD2	2.57	0.40
1:D:364:GLU:O	1:D:368:ARG:HG3	2.21	0.40
1:D:472:LEU:O	1:D:475:CYS:HB2	2.21	0.40
1:D:415:VAL:O	1:D:567:TYR:CE1	2.75	0.40
1:D:709:TRP:CD1	1:D:709:TRP:N	2.89	0.40
2:E:397:SER:CB	2:E:400:LEU:H	2.34	0.40
2:E:326:PHE:CE2	2:E:421:ILE:CD1	3.05	0.40
2:F:369:ILE:HG21	2:F:408:ILE:HG12	2.02	0.40
2:F:373:LEU:O	2:F:377:VAL:HG23	2.21	0.40
2:F:455:THR:CA	2:F:458:THR:HB	2.52	0.40
2:G:393:HIS:HA	2:G:423:SER:OG	2.21	0.40
2:G:445:TRP:N	2:G:445:TRP:CD1	2.89	0.40
2:H:356:THR:OG1	2:H:365:THR:CG2	2.70	0.40
1:A:208:SER:HB2	1:A:210:TRP:CE2	2.57	0.40
1:A:199:MET:CE	1:A:243:GLU:OE1	2.69	0.40
1:A:55:LYS:HA	1:A:58:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HD13	1:B:222:MET:SD	2.62	0.40
1:B:404:ASN:HB2	1:B:574:GLN:NE2	2.36	0.40
1:C:74:ILE:HD13	1:C:128:ASN:OD1	2.22	0.40
2:E:400:LEU:HD22	2:E:409:ILE:CD1	2.52	0.40
2:E:438:GLN:O	2:E:441:PHE:O	2.39	0.40
2:F:397:SER:CB	2:F:398:GLN:CA	2.99	0.40
2:F:446:TYR:HB2	2:F:448:THR:HG23	2.04	0.40
2:G:420:LEU:HD21	2:G:443:TRP:HH2	1.86	0.40
2:G:309:PHE:CE2	2:G:442:ASN:OD1	2.75	0.40
2:H:331:LEU:HD11	2:H:391:LEU:CG	2.51	0.40
1:A:106:VAL:HG13	1:A:253:ALA:O	2.20	0.40
1:A:135:SER:HB2	1:A:220:LYS:HE3	2.02	0.40
1:A:227:THR:HA	1:A:230:LEU:HB3	2.04	0.40
1:A:257:ILE:HG22	1:A:261:ARG:NE	2.36	0.40
1:A:284:HIS:HA	1:A:287:THR:OG1	2.22	0.40
1:A:480:LYS:HG2	1:A:498:LEU:HD22	2.03	0.40
1:A:306:VAL:HG12	1:A:585:ALA:CB	2.52	0.40
1:B:102:THR:HA	1:B:247:ILE:HG23	2.04	0.40
1:B:342:SER:O	1:B:345:CYS:CB	2.70	0.40
1:B:421:LYS:HE3	1:B:479:PHE:CE1	2.56	0.40
1:B:476:PHE:CZ	1:B:501:PHE:CD1	3.09	0.40
1:C:306:VAL:HG12	1:C:585:ALA:CB	2.52	0.40
1:A:349:PRO:HG2	1:C:347:ASN:CG	2.42	0.40
1:C:378:LYS:O	1:C:379:GLN:HB2	2.21	0.40
1:C:479:PHE:HA	1:C:482:TYR:CD2	2.56	0.40
1:C:501:PHE:CE1	1:C:554:GLU:HB3	2.57	0.40
1:D:248:LEU:CD1	1:D:250:PHE:CZ	3.05	0.40
1:D:263:LEU:CD1	1:D:271:LEU:HD11	2.52	0.40
1:B:347:ASN:HD21	1:D:353:ARG:NH2	2.19	0.40
1:D:657:VAL:HG12	1:D:677:ILE:HD11	2.02	0.40
1:D:636:LEU:HD11	1:D:657:VAL:HG21	2.04	0.40
2:E:332:GLN:O	2:E:333:ASP:C	2.60	0.40
1:B:591:HIS:O	2:E:445:TRP:HD1	2.05	0.40
2:G:310:ASN:HB3	2:G:420:LEU:O	2.22	0.40
2:G:331:LEU:HD11	2:G:391:LEU:CG	2.51	0.40
2:G:332:GLN:O	2:G:333:ASP:C	2.60	0.40
2:G:350:SER:HA	2:G:353:ASN:HB2	2.04	0.40
2:G:388:LEU:O	2:G:418:ILE:HA	2.21	0.40
2:H:332:GLN:O	2:H:333:ASP:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	541/712 (76%)	460 (85%)	72 (13%)	9 (2%)	9	42
1	B	541/712 (76%)	463 (86%)	72 (13%)	6 (1%)	14	52
1	C	541/712 (76%)	462 (85%)	72 (13%)	7 (1%)	12	48
1	D	541/712 (76%)	464 (86%)	70 (13%)	7 (1%)	12	48
2	E	181/347 (52%)	161 (89%)	20 (11%)	0	100	100
2	F	181/347 (52%)	161 (89%)	20 (11%)	0	100	100
2	G	181/347 (52%)	161 (89%)	20 (11%)	0	100	100
2	H	181/347 (52%)	163 (90%)	18 (10%)	0	100	100
All	All	2888/4236 (68%)	2495 (86%)	364 (13%)	29 (1%)	15	54

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	VAL
1	A	130	THR
1	A	383	LYS
1	B	129	VAL
1	B	383	LYS
1	C	129	VAL
1	C	382	GLU
1	D	129	VAL
1	D	382	GLU
1	D	579	VAL
1	A	190	THR
1	A	381	SER
1	A	579	VAL
1	A	640	CYS
1	B	190	THR
1	B	579	VAL
1	B	640	CYS

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Mol	Chain	Res	Type
1	C	190	THR
1	C	579	VAL
1	C	640	CYS
1	D	190	THR
1	A	131	PRO
1	C	379	GLN
1	D	640	CYS
1	D	379	GLN
1	C	570	PRO
1	D	570	PRO
1	A	570	PRO
1	B	570	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 X-ray entries followed by that with respect to entries of similar resolution.

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	517/659 (78%)	504 (98%)	13 (2%)	47	68
1	B	517/659 (78%)	505 (98%)	12 (2%)	50	71
1	C	517/659 (78%)	506 (98%)	11 (2%)	53	72
1	D	517/659 (78%)	505 (98%)	12 (2%)	50	71
2	E	171/323 (53%)	168 (98%)	3 (2%)	59	77
2	F	171/323 (53%)	168 (98%)	3 (2%)	59	77
2	G	171/323 (53%)	166 (97%)	5 (3%)	42	64
2	H	171/323 (53%)	168 (98%)	3 (2%)	59	77
All	All	2752/3928 (70%)	2690 (98%)	62 (2%)	50	71

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	MET
1	A	225	PHE
1	A	248	LEU

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Mol	Chain	Res	Type
1	A	272	CYS
1	A	325	ILE
1	A	342	SER
1	A	381	SER
1	A	394	LEU
1	A	457	LEU
1	A	570	PRO
1	A	683	ARG
1	A	704	VAL
1	A	706	ARG
1	B	199	MET
1	B	225	PHE
1	B	248	LEU
1	B	342	SER
1	B	347	ASN
1	B	381	SER
1	B	394	LEU
1	B	416	LEU
1	B	457	LEU
1	B	683	ARG
1	B	704	VAL
1	B	706	ARG
1	C	110	ASN
1	C	225	PHE
1	C	325	ILE
1	C	342	SER
1	C	346	CYS
1	C	381	SER
1	C	394	LEU
1	C	416	LEU
1	C	457	LEU
1	C	704	VAL
1	C	706	ARG
1	D	110	ASN
1	D	199	MET
1	D	225	PHE
1	D	248	LEU
1	D	318	ASP
1	D	342	SER
1	D	381	SER
1	D	394	LEU
1	D	416	LEU

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Mol	Chain	Res	Type
1	D	457	LEU
1	D	637	HIS
1	D	706	ARG
2	E	388	LEU
2	E	423	SER
2	E	457	GLU
2	F	418	ILE
2	F	423	SER
2	F	457	GLU
2	G	388	LEU
2	G	418	ILE
2	G	423	SER
2	G	442	ASN
2	G	457	GLU
2	H	418	ILE
2	H	423	SER
2	H	457	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	ASN
1	A	384	GLN
1	B	110	ASN
1	B	209	GLN
1	B	242	HIS
1	C	384	GLN
1	D	242	HIS
1	D	384	GLN
2	F	435	HIS
2	H	442	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	553/712 (77%)	0.03	20 (3%)	42	38	214, 295, 363, 401	0
1	B	553/712 (77%)	0.12	21 (3%)	40	36	208, 300, 363, 410	0
1	C	553/712 (77%)	0.27	33 (5%)	21	21	219, 302, 365, 407	0
1	D	553/712 (77%)	0.22	29 (5%)	27	27	227, 299, 363, 406	0
2	E	183/347 (52%)	-0.02	4 (2%)	62	54	256, 307, 348, 381	0
2	F	183/347 (52%)	0.11	7 (3%)	40	36	254, 310, 353, 374	0
2	G	183/347 (52%)	0.07	10 (5%)	25	25	250, 306, 352, 375	0
2	H	183/347 (52%)	0.06	3 (1%)	72	64	248, 310, 349, 376	0
All	All	2944/4236 (69%)	0.13	127 (4%)	35	32	208, 303, 360, 410	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	164	SER	7.9
1	C	164	SER	5.1
1	D	163	LYS	5.0
2	G	463	SER	4.9
1	C	81	HIS	4.4
2	E	463	SER	4.2
1	B	643	LEU	4.1
1	A	700	LYS	4.1
1	C	161	ASP	4.0
1	B	163	LYS	4.0
1	A	643	LEU	4.0
2	G	338	VAL	3.9
1	A	642	ARG	3.9
2	G	284	SER	3.9
1	B	642	ARG	3.8
1	C	163	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	465	LYS	3.7
2	G	337	VAL	3.7
1	B	700	LYS	3.6
1	C	162	ILE	3.6
1	B	140	ASP	3.6
1	A	699	GLN	3.6
1	B	698	LYS	3.5
1	A	110	ASN	3.4
1	C	77	LEU	3.4
1	D	204	ARG	3.4
1	D	109	VAL	3.3
2	G	367	ARG	3.3
1	C	205	THR	3.3
1	D	162	ILE	3.3
1	A	81	HIS	3.3
1	A	109	VAL	3.3
1	C	78	GLN	3.2
1	B	164	SER	3.2
1	D	700	LYS	3.1
1	D	193	GLN	3.1
1	C	157	ASP	3.1
1	B	159	CYS	3.1
1	C	699	GLN	3.0
2	E	464	LEU	3.0
1	D	161	ASP	3.0
1	B	699	GLN	2.9
2	G	344	PRO	2.9
1	B	110	ASN	2.9
1	A	209	GLN	2.9
1	C	255	SER	2.8
1	C	204	ARG	2.8
1	C	676	ILE	2.8
1	B	142	PRO	2.7
1	A	240	HIS	2.7
1	C	708	THR	2.7
2	E	362	HIS	2.7
1	A	80	SER	2.7
1	D	81	HIS	2.7
1	D	143	ASP	2.7
1	C	656	VAL	2.6
1	C	657	VAL	2.6
1	D	240	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	211	GLN	2.6
1	B	197	PRO	2.6
1	D	676	ILE	2.6
2	F	462	ASN	2.5
1	D	122	THR	2.5
1	A	254	THR	2.5
1	A	140	ASP	2.5
2	G	464	LEU	2.5
1	B	137	GLN	2.5
1	D	657	VAL	2.5
1	B	210	TRP	2.5
2	F	292	GLN	2.5
1	C	160	VAL	2.5
2	F	466	VAL	2.5
2	H	460	TYR	2.5
1	A	701	THR	2.4
1	C	700	LYS	2.4
1	A	196	ASP	2.4
1	C	253	ALA	2.4
1	D	656	VAL	2.4
1	B	162	ILE	2.4
1	C	200	LEU	2.3
1	B	209	GLN	2.3
2	F	344	PRO	2.3
1	D	641	SER	2.3
1	A	137	GLN	2.3
1	D	77	LEU	2.3
1	D	78	GLN	2.3
1	D	114	HIS	2.3
1	D	108	GLY	2.3
1	C	127	ASN	2.3
1	C	254	THR	2.3
1	D	270	LEU	2.2
1	C	109	VAL	2.2
1	C	698	LYS	2.2
1	D	191	VAL	2.2
1	D	642	ARG	2.2
1	B	656	VAL	2.2
1	C	244	PHE	2.2
1	A	465	LYS	2.2
2	G	462	ASN	2.2
1	C	193	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	337	TYR	2.2
1	C	504	LEU	2.2
1	B	240	HIS	2.2
2	F	465	LEU	2.1
1	C	140	ASP	2.1
1	A	693	PHE	2.1
1	B	254	THR	2.1
1	D	489	SER	2.1
2	G	345	GLY	2.1
1	D	110	ASN	2.1
2	G	451	TYR	2.1
1	B	196	ASP	2.1
2	F	359	VAL	2.1
1	C	240	HIS	2.1
1	C	108	GLY	2.1
2	E	367	ARG	2.1
1	C	192	THR	2.1
1	C	653	PHE	2.0
1	A	709	TRP	2.0
2	F	348	VAL	2.0
1	D	196	ASP	2.0
1	A	139	LYS	2.0
1	A	595	ALA	2.0
2	H	463	SER	2.0
1	D	680	ARG	2.0
2	H	432	MET	2.0
1	D	504	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.