Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:50 PM GMT

PDB ID	:	4G9I
Title	:	Crystal structure of T.kodakarensis HypF
Authors	:	Tominaga, T.; Watanabe, S.; Matsumi, R.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on	:	2012-07-24
Resolution	:	4.50 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
http://wwpdb.org/validation/2016/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:

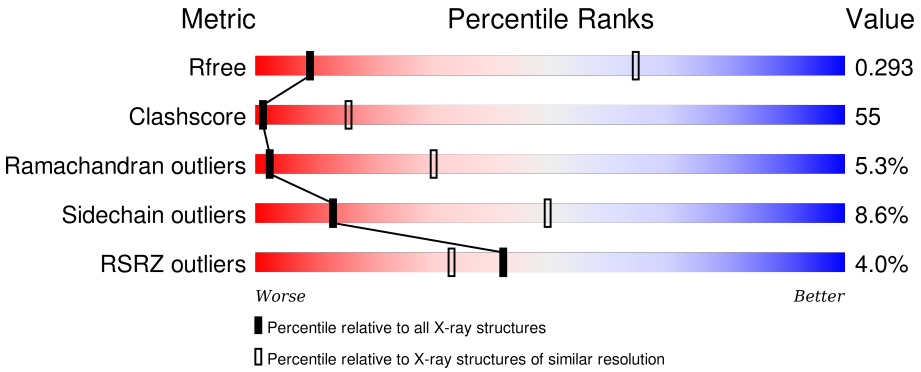
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 4.50 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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	772	2% 25% 64% 9%
1	B	772	5% 26% 63% 9%
1	C	772	2% 29% 60% 9%
1	D	772	4% 28% 63% 8%
1	E	772	5% 27% 63% 8%

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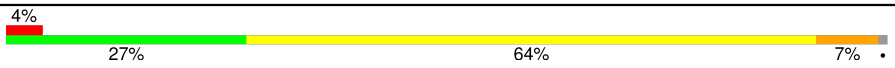
Mol	Chain	Length	Quality of chain
1	F	772	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 36065 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 Hydrogenase maturation protein HypF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	766	Total	C	N	O	S	Se	0	0	0
			6032	3862	1028	1113	11	18			
1	B	762	Total	C	N	O	S	Se	0	0	0
			6008	3847	1024	1108	11	18			
1	C	756	Total	C	N	O	S	Se	0	0	0
			5964	3819	1017	1100	11	17			
1	D	765	Total	C	N	O	S	Se	0	0	0
			6027	3859	1027	1112	11	18			
1	E	762	Total	C	N	O	S	Se	0	0	0
			6008	3847	1024	1108	11	18			
1	F	762	Total	C	N	O	S	Se	0	0	0
			6008	3847	1024	1108	11	18			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

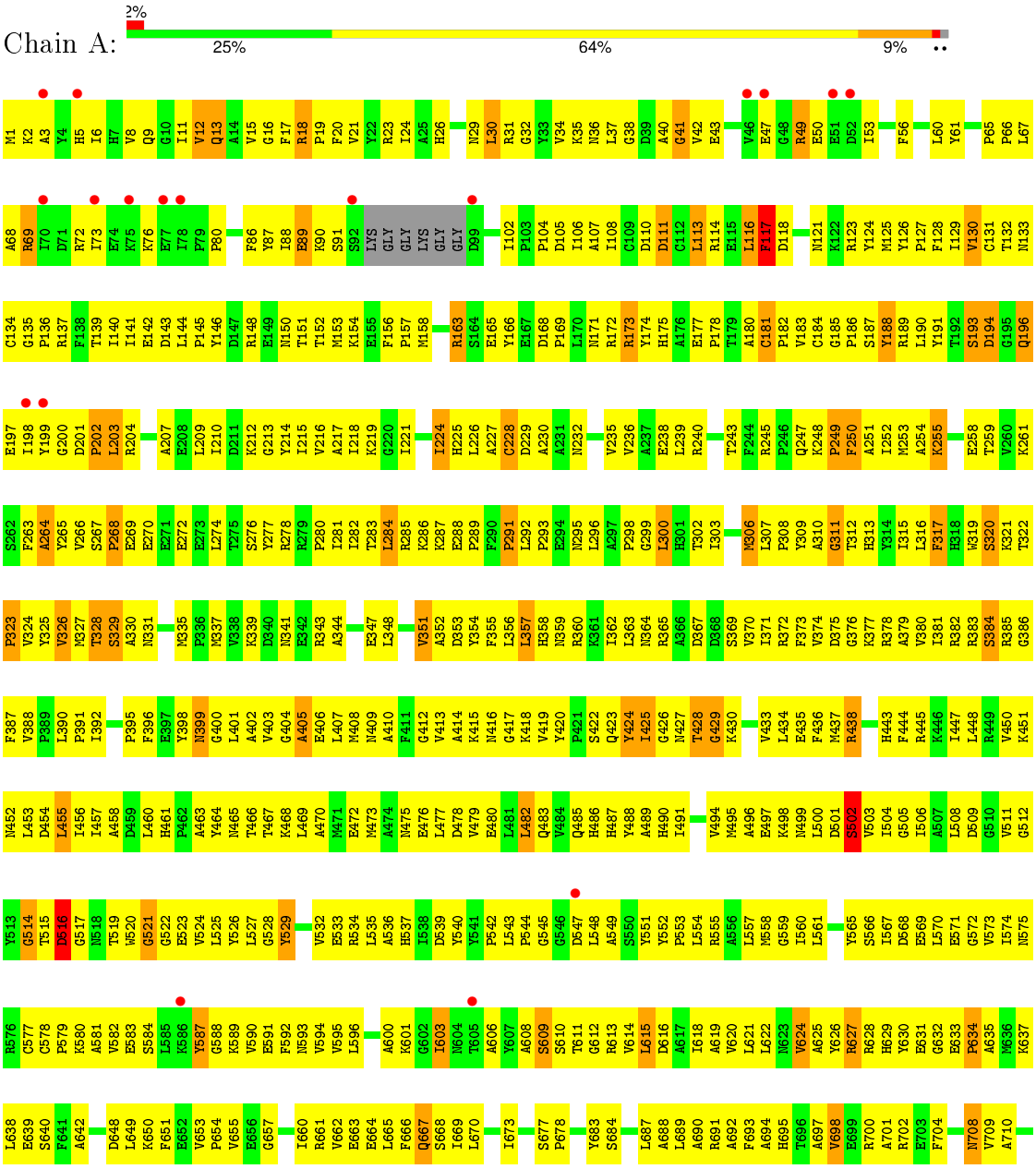
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total	Zn	0	0
			3	3		
2	E	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		
2	A	3	Total	Zn	0	0
			3	3		
2	F	3	Total	Zn	0	0
			3	3		

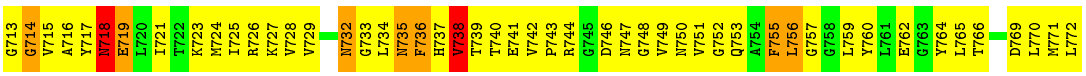
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Hydrogenase maturation protein HypF

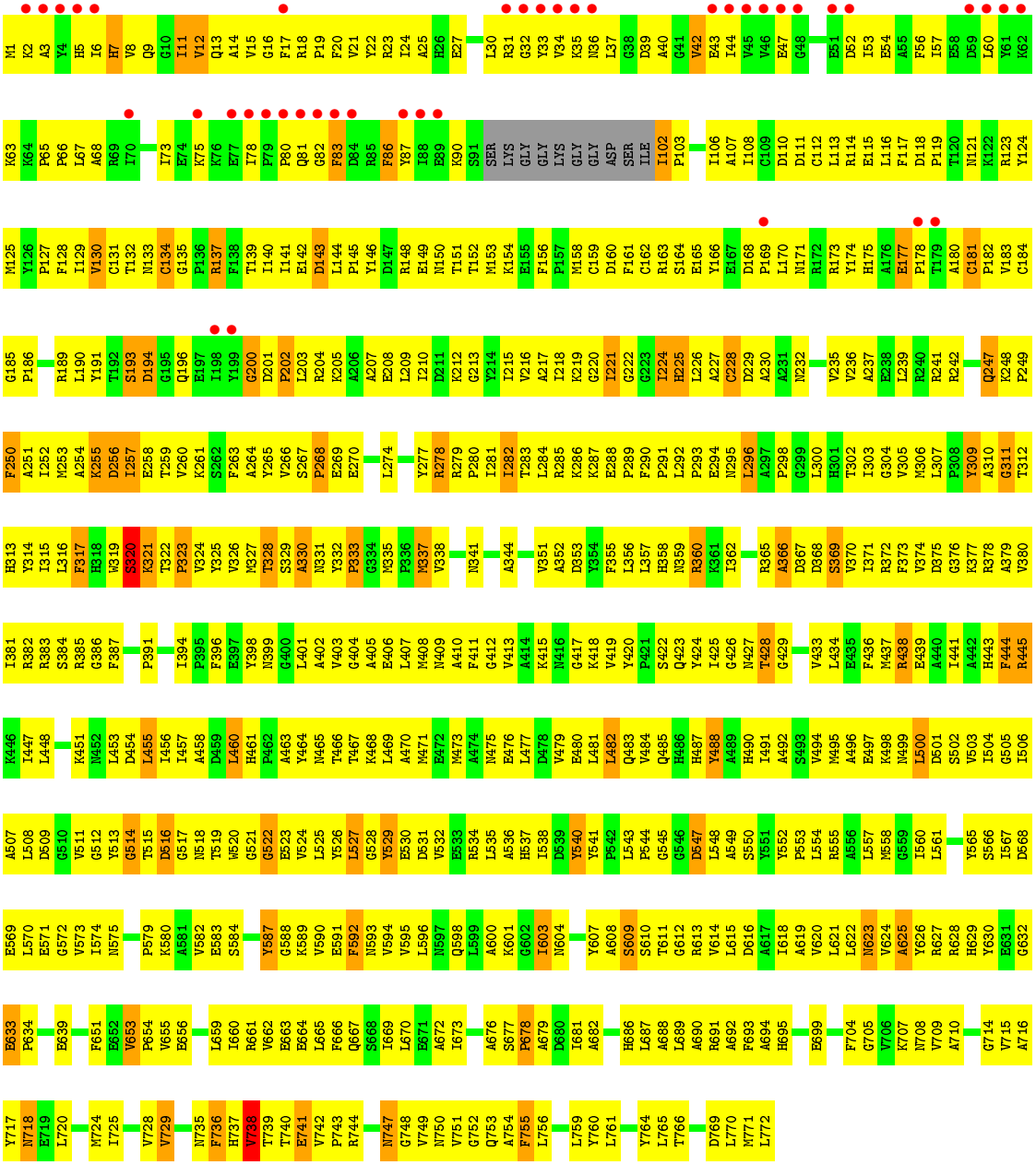
Chain A:





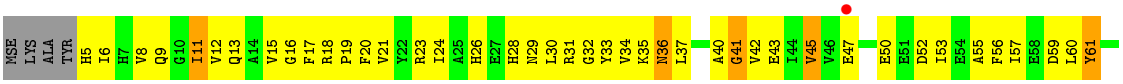
• Molecule 1: Hydrogenase maturation protein HypF

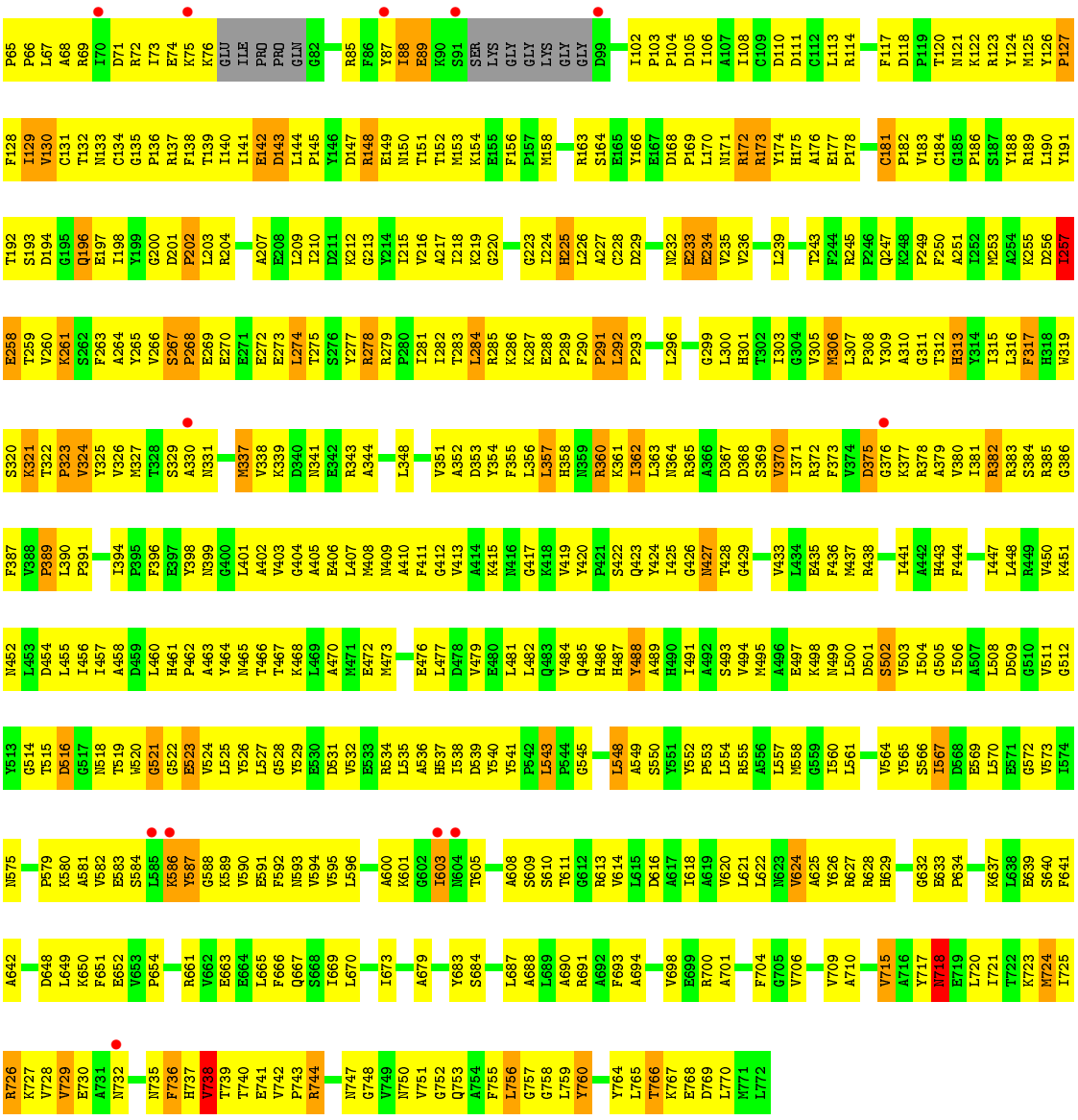
Chain B:



• Molecule 1: Hydrogenase maturation protein HypF

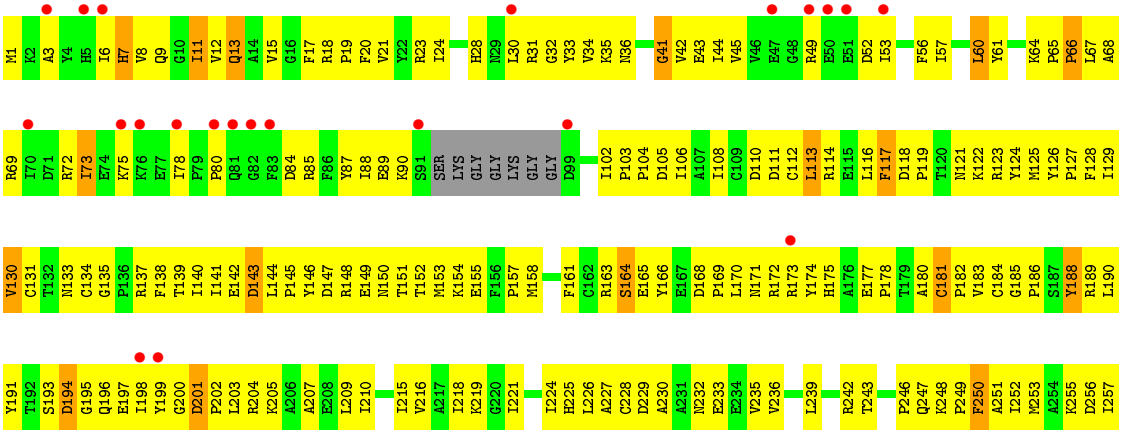
Chain C:

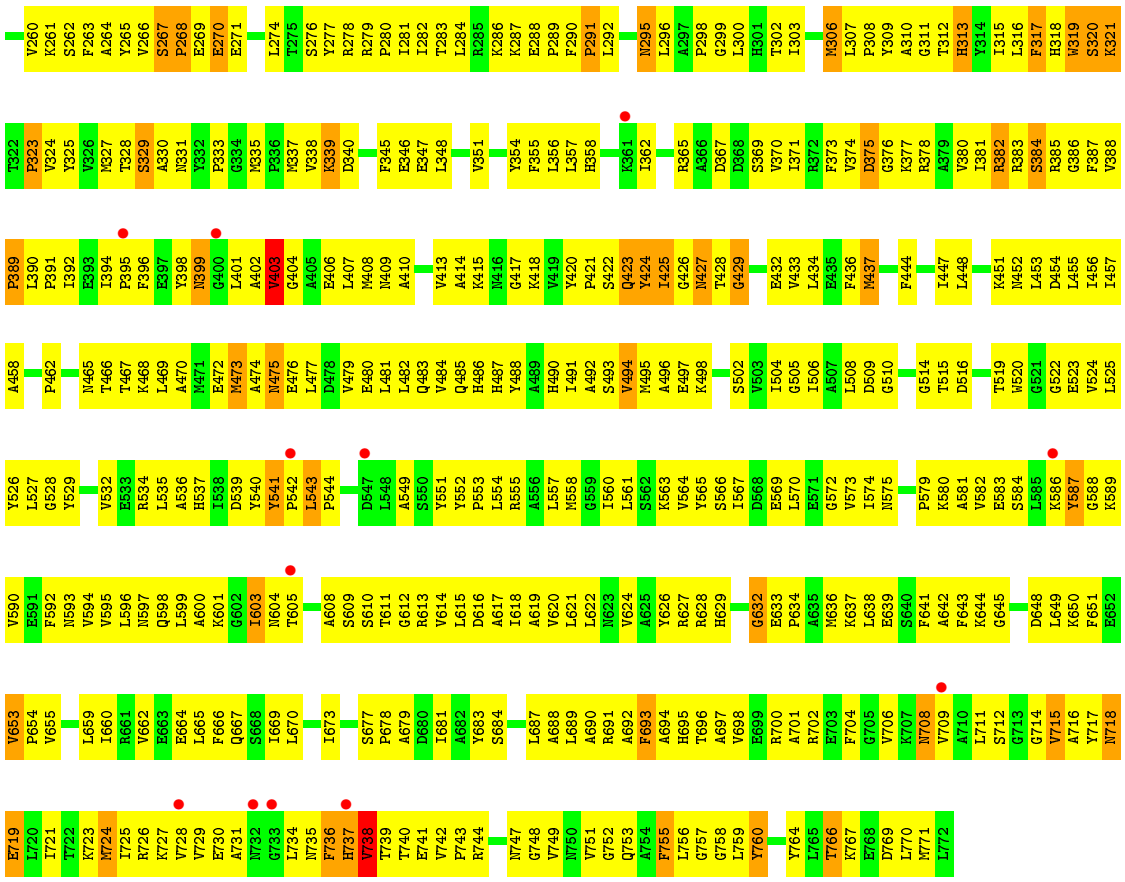




• Molecule 1: Hydrogenase maturation protein HypF

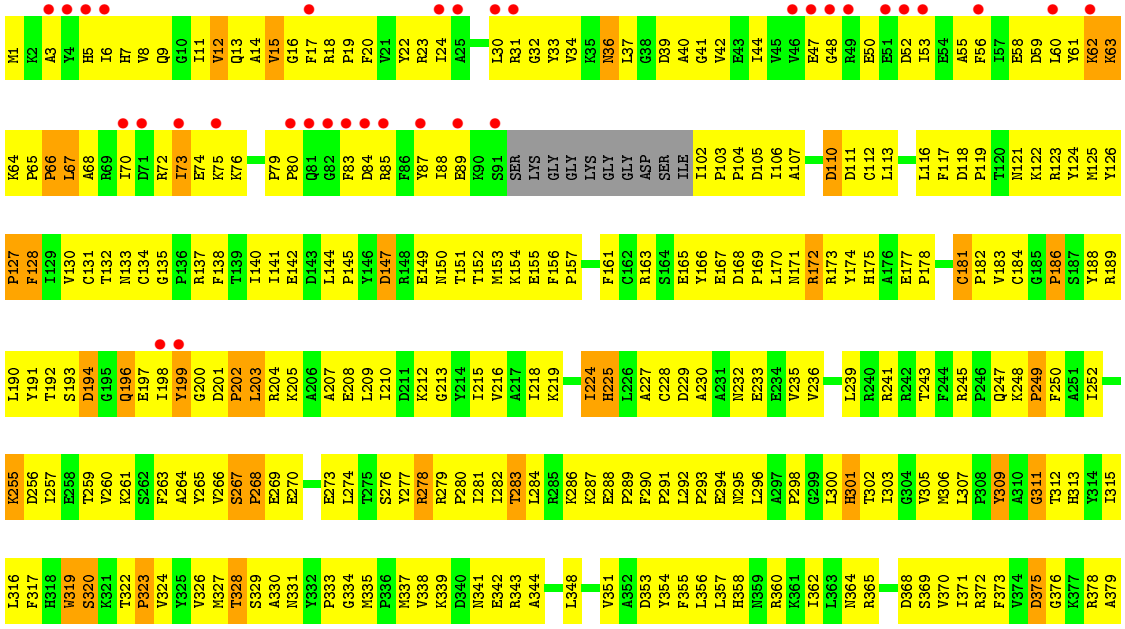
Chain D:

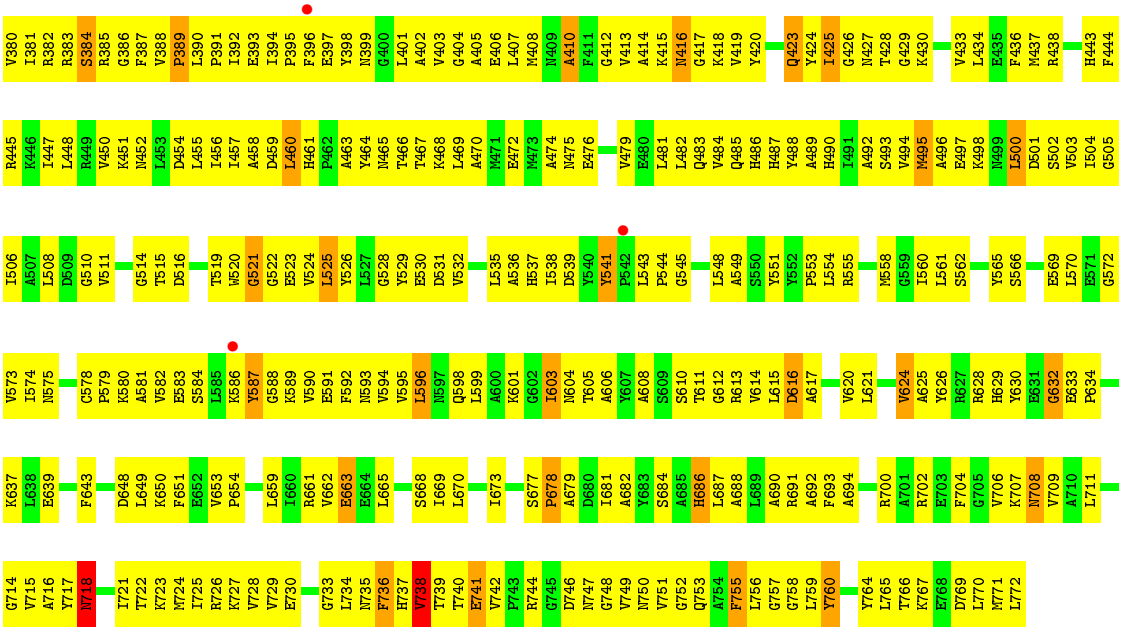




• Molecule 1: Hydrogenase maturation protein HypF

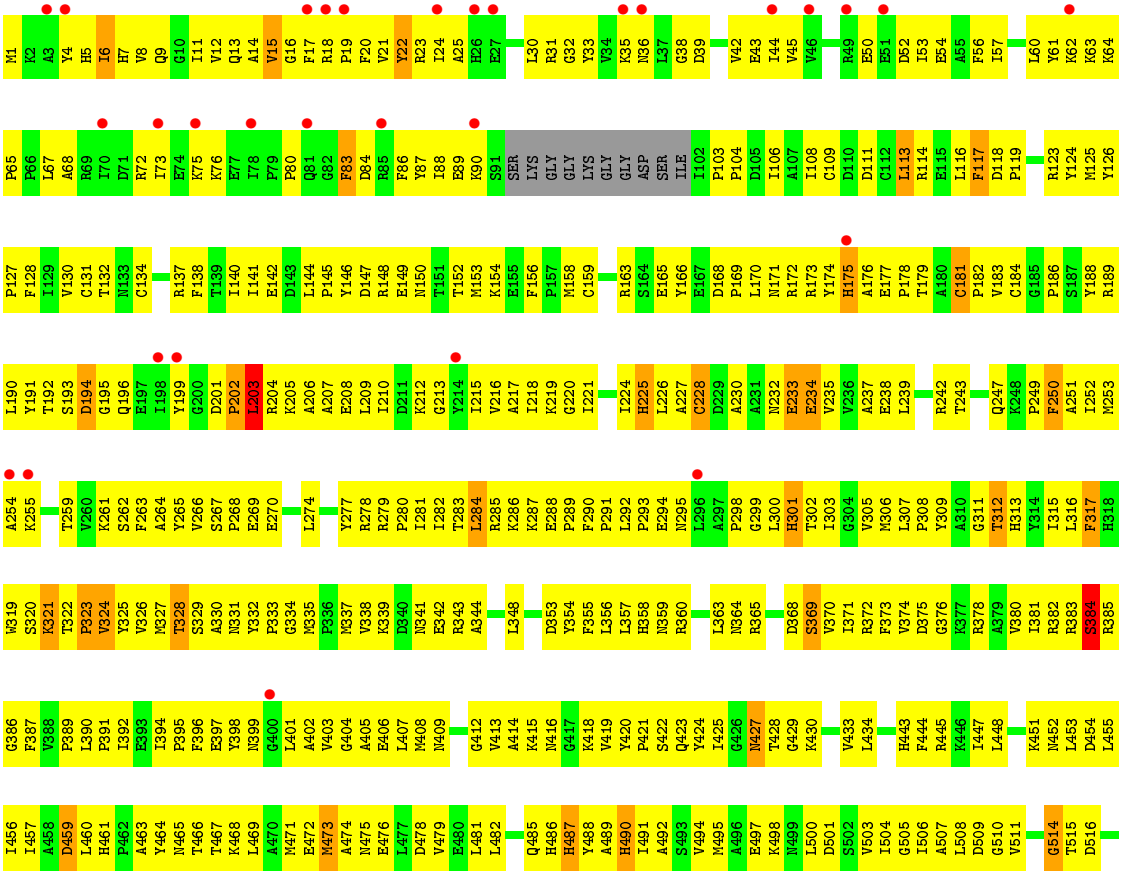
Chain E:

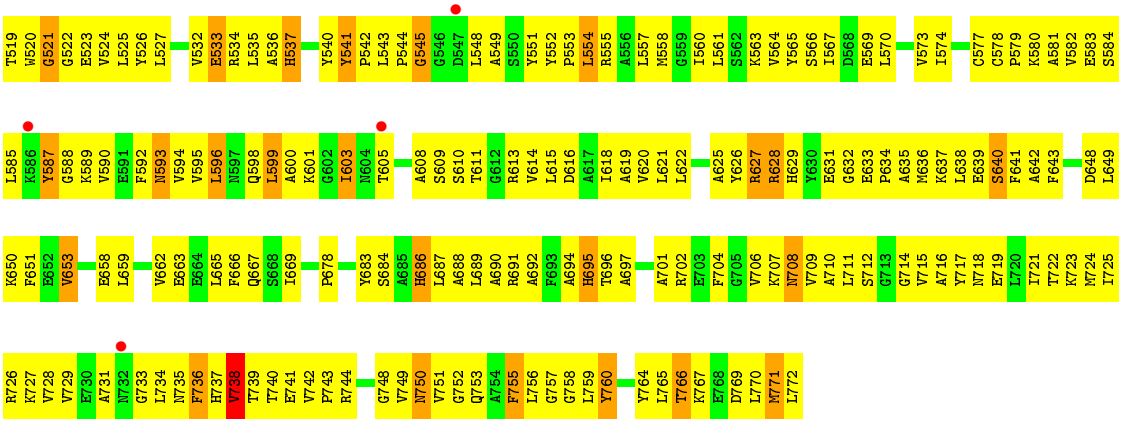




• Molecule 1: Hydrogenase maturation protein HypF

Chain F:




T519 W520 G521 G522 E523 V524 L525 Y526 L527 V532 E533 R534 L535 A536 H537 Y540 Y541 P542 L543 P544 G545 G546 D547 L548 A549 S550 Y551 Y552 P553 L554 R555 A556 L557 M558 G559 I560 L561 S562 K563 V564 Y565 S566 I567 D568 E569 L570 V573 I574 C577 C578 P579 K580 A581 V582 E583 S584
L585 K586 Y587 G588 K589 V590 E591 F592 N593 V594 V595 L596 N597 Q598 L599 A600 K601 G602 I603 N604 T605 A608 S609 S610 T611 G612 R613 V614 L615 D616 A617 I618 A619 V620 L621 L622 A625 Y626 R627 R628 H629 Y630 E631 G632 E633 P634 A635 M636 K637 L638 E639 S640 F641 A642 F643 D648 L649
K650 F651 E652 V653 E658 L659 V662 E663 E664 L665 F666 Q667 S668 I669 P678 Y683 S684 A685 H686 L687 A688 L689 A690 R691 A692 F693 A694 H695 T696 A697 A701 R702 E703 F704 G705 V706 K707 N708 V709 A710 L711 S712 G713 G714 V715 A716 Y717 N718 E719 L720 I721 T722 K723 M724 I725
R726 K727 V728 V729 E730 A731 N732 G733 L734 N735 F736 H737 V738 T739 T740 E741 V742 F743 R744 G748 V749 N750 V751 G752 Q753 A754 F755 L756 G757 G758 L759 Y760 Y764 L765 T766 K767 E768 D769 L770 N771 L772

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	265.81Å 265.81Å 693.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 4.50 49.77 – 4.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (15.00-4.50) 94.9 (49.77-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 4.45Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.279 , 0.300 0.298 , 0.293	Depositor DCC
R_{free} test set	3991 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	143.9	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 154.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 86313 reflections	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	36065	wwPDB-VP
Average B, all atoms (Å^2)	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.25	0/6151	0.49	0/8308
1	B	0.25	0/6127	0.49	1/8275 (0.0%)
1	C	0.25	0/6080	0.49	0/8208
1	D	0.25	0/6146	0.49	0/8301
1	E	0.25	0/6127	0.49	0/8275
1	F	0.25	0/6127	0.50	0/8275
All	All	0.25	0/36758	0.49	1/49642 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	200	GLY	N-CA-C	5.11	125.88	113.10

There are no chirality outliers.

There are no planarity outliers.

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	6032	0	5969	684	1
1	B	6008	0	5954	671	0
1	C	5964	0	5909	669	0
1	D	6027	0	5970	674	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	6008	0	5954	616	0
1	F	6008	0	5955	667	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
All	All	36065	0	35711	3925	1

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 55.

All (3925) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HG21	1:A:69:ARG:H	1.24	1.02
1:D:9:GLN:HE21	1:D:41:GLY:HA2	1.17	1.02
1:D:485:GLN:HE21	1:D:487:HIS:H	1.04	1.01
1:D:451:LYS:HA	1:D:477:LEU:HD21	1.41	0.99
1:F:394:ILE:HD11	1:F:419:VAL:HB	1.41	0.99
1:D:288:GLU:HB3	1:D:289:PRO:HD3	1.45	0.98
1:C:198:ILE:HG13	1:D:122:LYS:HD3	1.39	0.98
1:B:485:GLN:HE21	1:B:487:HIS:H	1.04	0.98
1:B:57:ILE:HG13	1:B:75:LYS:HZ3	1.28	0.98
1:B:456:ILE:HG22	1:B:457:ILE:H	1.26	0.98
1:A:485:GLN:HE21	1:A:487:HIS:H	1.10	0.97
1:A:268:PRO:HG2	1:A:378:ARG:HH22	1.28	0.97
1:B:225:HIS:HA	1:B:330:ALA:HB2	1.44	0.97
1:D:369:SER:H	1:D:385:ARG:HB2	1.28	0.97
1:E:39:ASP:HB3	1:E:144:LEU:HD13	1.45	0.97
1:F:485:GLN:HE21	1:F:487:HIS:H	1.01	0.97
1:F:288:GLU:HB3	1:F:289:PRO:HD3	1.46	0.96
1:E:127:PRO:HB3	1:E:312:THR:HG22	1.47	0.96
1:D:88:ILE:HG22	1:D:89:GLU:H	1.31	0.96
1:C:127:PRO:HB3	1:C:312:THR:HG22	1.46	0.96
1:B:288:GLU:HB3	1:B:289:PRO:HD3	1.47	0.95
1:A:587:TYR:HD1	1:A:588:GLY:H	1.14	0.95
1:A:557:LEU:HD21	1:A:621:LEU:HD13	1.49	0.95
1:C:191:TYR:HB2	1:C:355:PHE:HB2	1.47	0.95
1:A:475:ASN:HD22	1:B:591:GLU:HG2	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:485:GLN:HE21	1:E:487:HIS:H	0.96	0.94
1:A:181:CYS:SG	1:A:183:VAL:HG22	2.07	0.94
1:A:11:ILE:HG12	1:A:68:ALA:HA	1.49	0.94
1:E:369:SER:H	1:E:385:ARG:HB2	1.31	0.94
1:B:394:ILE:HD11	1:B:419:VAL:HB	1.47	0.94
1:F:216:VAL:HB	1:F:354:TYR:HB2	1.50	0.94
1:E:169:PRO:HG2	1:E:170:LEU:HD12	1.48	0.94
1:A:379:ALA:HB3	1:A:744:ARG:HH11	1.31	0.94
1:C:288:GLU:HB2	1:C:289:PRO:HD3	1.47	0.93
1:A:287:LYS:HG3	1:A:289:PRO:HD2	1.49	0.93
1:D:127:PRO:HB3	1:D:312:THR:HG22	1.48	0.93
1:B:268:PRO:HG2	1:B:378:ARG:HH22	1.31	0.93
1:E:394:ILE:HD11	1:E:419:VAL:HB	1.51	0.93
1:D:111:ASP:HB2	1:D:172:ARG:HH22	1.34	0.93
1:C:519:THR:HB	1:C:608:ALA:HA	1.51	0.93
1:B:612:GLY:HA2	1:B:615:LEU:HD12	1.51	0.93
1:C:504:ILE:HB	1:C:709:VAL:HG12	1.51	0.93
1:A:288:GLU:HB3	1:A:289:PRO:HD3	1.48	0.92
1:F:207:ALA:HB1	1:F:320:SER:HB2	1.49	0.92
1:A:553:PRO:HB2	1:A:620:VAL:HG21	1.50	0.92
1:F:190:LEU:HD21	1:F:206:ALA:HB2	1.50	0.92
1:D:11:ILE:HG12	1:D:68:ALA:HA	1.51	0.92
1:F:219:LYS:HD3	1:F:358:HIS:H	1.33	0.92
1:C:286:LYS:HD2	1:C:303:ILE:HD11	1.51	0.92
1:A:108:ILE:HG12	1:A:310:ALA:HA	1.52	0.92
1:E:738:VAL:HG23	1:E:744:ARG:HG2	1.51	0.92
1:A:380:VAL:HG12	1:A:381:ILE:H	1.34	0.91
1:E:149:GLU:HA	1:E:154:LYS:HG2	1.49	0.91
1:B:232:ASN:HB3	1:B:235:VAL:HG22	1.52	0.91
1:D:111:ASP:HB3	1:D:172:ARG:HH12	1.33	0.90
1:B:14:ALA:HB3	1:B:103:PRO:HG3	1.53	0.90
1:B:39:ASP:HB3	1:B:144:LEU:HD13	1.52	0.90
1:E:288:GLU:HB3	1:E:289:PRO:HD3	1.52	0.90
1:F:369:SER:H	1:F:385:ARG:HB2	1.35	0.90
1:F:508:LEU:HD22	1:F:611:THR:HG21	1.51	0.90
1:E:191:TYR:HB2	1:E:355:PHE:HB2	1.54	0.89
1:A:628:ARG:NH2	1:A:632:GLY:H	1.69	0.89
1:F:19:PRO:HG2	1:F:132:THR:HG21	1.53	0.89
1:E:287:LYS:HG3	1:E:289:PRO:HD2	1.51	0.89
1:E:494:VAL:HG22	1:E:738:VAL:HG22	1.54	0.89
1:B:149:GLU:HA	1:B:154:LYS:HG2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ILE:HG23	1:B:277:TYR:HB2	1.54	0.89
1:A:230:ALA:HB2	1:A:326:VAL:HG23	1.55	0.89
1:B:615:LEU:HA	1:B:618:ILE:HD12	1.55	0.89
1:D:331:ASN:HD22	1:D:337:MSE:HA	1.36	0.89
1:D:543:LEU:H	1:D:543:LEU:HD23	1.37	0.89
1:C:281:ILE:HB	1:C:370:VAL:HG12	1.52	0.89
1:A:219:LYS:HD3	1:A:358:HIS:H	1.37	0.88
1:D:281:ILE:HB	1:D:370:VAL:HG12	1.54	0.88
1:F:190:LEU:HG	1:F:202:PRO:HB3	1.55	0.88
1:D:458:ALA:HB1	1:D:467:THR:HG22	1.55	0.88
1:E:153:MSE:HE1	1:E:360:ARG:HD2	1.55	0.88
1:E:765:LEU:HD21	1:E:770:LEU:HD21	1.55	0.88
1:C:369:SER:H	1:C:385:ARG:HB2	1.38	0.88
1:F:282:ILE:HD12	1:F:371:ILE:HG23	1.53	0.87
1:F:261:LYS:NZ	1:F:266:VAL:HB	1.90	0.87
1:D:106:ILE:HG23	1:D:277:TYR:HB2	1.56	0.87
1:F:219:LYS:HA	1:F:224:ILE:HG12	1.56	0.87
1:F:281:ILE:HB	1:F:370:VAL:HG12	1.56	0.87
1:C:371:ILE:HD12	1:C:380:VAL:HG22	1.57	0.87
1:E:690:ALA:HB1	1:E:725:ILE:HG13	1.55	0.87
1:F:653:VAL:HG13	1:F:692:ALA:HB3	1.54	0.87
1:D:566:SER:H	1:D:569:GLU:HB2	1.39	0.86
1:E:485:GLN:NE2	1:E:487:HIS:H	1.73	0.86
1:F:380:VAL:HG23	1:F:740:THR:HA	1.57	0.86
1:C:207:ALA:HB1	1:C:320:SER:HB2	1.54	0.86
1:C:331:ASN:HD22	1:C:337:MSE:HA	1.41	0.86
1:A:456:ILE:HG22	1:A:457:ILE:H	1.40	0.86
1:D:9:GLN:HB2	1:D:72:ARG:HD2	1.56	0.86
1:D:370:VAL:HG22	1:D:382:ARG:HD2	1.57	0.86
1:E:485:GLN:HE21	1:E:487:HIS:N	1.73	0.86
1:B:128:PHE:HB3	1:B:360:ARG:HH22	1.38	0.86
1:A:371:ILE:HB	1:A:380:VAL:HG13	1.56	0.86
1:F:615:LEU:HD12	1:F:638:LEU:HD23	1.56	0.86
1:B:249:PRO:HG3	1:B:300:LEU:HD13	1.58	0.86
1:C:502:SER:HB3	1:C:528:GLY:HA2	1.58	0.86
1:C:485:GLN:HG3	1:C:488:TYR:H	1.41	0.85
1:D:102:ILE:HD11	1:D:144:LEU:HG	1.58	0.85
1:A:281:ILE:HG12	1:A:306:MSE:HG3	1.55	0.85
1:A:201:ASP:N	1:A:202:PRO:HD2	1.91	0.85
1:E:543:LEU:HD23	1:E:543:LEU:H	1.40	0.85
1:C:219:LYS:HA	1:C:224:ILE:HB	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ALA:HB1	1:A:467:THR:HG22	1.58	0.85
1:D:687:LEU:HB3	1:D:724:MSE:HE2	1.56	0.85
1:B:544:PRO:HB2	1:B:555:ARG:HH21	1.42	0.85
1:F:149:GLU:HA	1:F:154:LYS:HG2	1.57	0.85
1:C:153:MSE:HE1	1:C:360:ARG:HD3	1.57	0.85
1:B:765:LEU:HD21	1:B:770:LEU:HD21	1.59	0.85
1:C:543:LEU:HD23	1:C:543:LEU:H	1.41	0.85
1:B:369:SER:H	1:B:385:ARG:HB2	1.41	0.85
1:D:374:VAL:HG21	1:D:744:ARG:HH22	1.41	0.85
1:F:5:HIS:HB3	1:F:76:LYS:HB2	1.59	0.84
1:E:281:ILE:HB	1:E:370:VAL:HG12	1.58	0.84
1:F:589:LYS:HG3	1:F:590:VAL:H	1.42	0.84
1:C:485:GLN:HE22	1:C:514:GLY:HA2	1.42	0.84
1:D:181:CYS:SG	1:D:183:VAL:HG22	2.16	0.84
1:B:191:TYR:HB2	1:B:355:PHE:HB2	1.57	0.84
1:A:589:LYS:HG3	1:A:590:VAL:H	1.40	0.84
1:C:282:ILE:HD12	1:C:371:ILE:HG23	1.59	0.84
1:A:404:GLY:HA2	1:A:753:GLN:HE22	1.42	0.84
1:C:261:LYS:NZ	1:C:266:VAL:HB	1.93	0.84
1:D:247:GLN:HG3	1:D:298:PRO:HG2	1.59	0.84
1:A:425:ILE:HD12	1:A:437:MSE:HE2	1.59	0.84
1:E:270:GLU:HB2	1:E:373:PHE:HE2	1.42	0.84
1:A:524:VAL:HG22	1:A:536:ALA:HB3	1.60	0.84
1:D:233:GLU:HB2	1:D:295:ASN:HD21	1.40	0.83
1:C:258:GLU:HG3	1:C:259:THR:N	1.93	0.83
1:A:163:ARG:HH11	1:A:163:ARG:HB2	1.42	0.83
1:F:265:TYR:HE2	1:F:287:LYS:HD2	1.42	0.83
1:C:457:ILE:HG21	1:C:753:GLN:HB3	1.60	0.83
1:A:491:ILE:HG23	1:A:527:LEU:HD11	1.60	0.83
1:B:281:ILE:HB	1:B:370:VAL:HG12	1.60	0.83
1:C:409:ASN:HD22	1:C:425:ILE:HD11	1.43	0.83
1:A:267:SER:HB2	1:A:270:GLU:HB2	1.59	0.83
1:D:225:HIS:HA	1:D:330:ALA:HB2	1.60	0.83
1:E:425:ILE:HD12	1:E:437:MSE:HE2	1.60	0.83
1:F:57:ILE:HG13	1:F:75:LYS:NZ	1.94	0.83
1:E:18:ARG:HB2	1:E:19:PRO:HD3	1.61	0.83
1:D:506:ILE:HD11	1:D:694:ALA:HA	1.61	0.82
1:B:587:TYR:HD1	1:B:588:GLY:H	1.27	0.82
1:F:225:HIS:HA	1:F:330:ALA:HB2	1.59	0.82
1:A:404:GLY:HA2	1:A:753:GLN:NE2	1.94	0.82
1:E:210:ILE:HD11	1:E:228:CYS:HA	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MSE:HB3	1:D:80:PRO:HD2	1.61	0.82
1:B:494:VAL:HG22	1:B:738:VAL:HG22	1.59	0.82
1:D:519:THR:HB	1:D:608:ALA:HA	1.60	0.82
1:F:711:LEU:HD13	1:F:725:ILE:HG21	1.61	0.82
1:E:20:PHE:HD2	1:E:23:ARG:HH21	1.26	0.82
1:E:380:VAL:HG23	1:E:740:THR:HA	1.61	0.82
1:B:451:LYS:HA	1:B:477:LEU:HD21	1.61	0.82
1:C:470:ALA:HB1	1:C:481:LEU:HD11	1.61	0.82
1:E:181:CYS:SG	1:E:183:VAL:HG22	2.19	0.82
1:E:249:PRO:HG3	1:E:300:LEU:HD13	1.60	0.82
1:B:380:VAL:HG23	1:B:740:THR:HA	1.61	0.82
1:A:281:ILE:HB	1:A:370:VAL:HG12	1.60	0.82
1:E:201:ASP:N	1:E:202:PRO:HD2	1.94	0.82
1:A:495:MSE:SE	1:A:527:LEU:HD13	2.30	0.81
1:C:215:ILE:HD12	1:C:226:LEU:HD23	1.62	0.81
1:B:331:ASN:HD22	1:B:337:MSE:HA	1.45	0.81
1:E:331:ASN:HD22	1:E:337:MSE:HA	1.45	0.81
1:C:587:TYR:HD1	1:C:588:GLY:H	1.27	0.81
1:B:457:ILE:HG21	1:B:753:GLN:HB3	1.61	0.81
1:D:544:PRO:HG2	1:D:555:ARG:HB3	1.62	0.81
1:F:419:VAL:HG11	1:F:751:VAL:HG23	1.62	0.81
1:D:230:ALA:HB1	1:D:296:LEU:HD21	1.62	0.81
1:F:554:LEU:HD11	1:F:579:PRO:HB2	1.60	0.81
1:C:103:PRO:HG2	1:C:137:ARG:HD2	1.60	0.81
1:E:589:LYS:HG3	1:E:590:VAL:H	1.45	0.81
1:A:457:ILE:HG21	1:A:753:GLN:HB3	1.63	0.81
1:B:247:GLN:HE21	1:B:298:PRO:HG2	1.44	0.81
1:A:625:ALA:HB2	1:A:637:LYS:HD3	1.63	0.81
1:F:765:LEU:HD21	1:F:770:LEU:HD21	1.61	0.81
1:B:374:VAL:HG21	1:B:744:ARG:HH22	1.45	0.81
1:B:485:GLN:NE2	1:B:487:HIS:H	1.80	0.81
1:F:504:ILE:HB	1:F:709:VAL:HG12	1.63	0.81
1:C:6:ILE:HG22	1:C:8:VAL:HG23	1.63	0.81
1:F:247:GLN:HG3	1:F:298:PRO:HG2	1.62	0.81
1:B:485:GLN:HG3	1:B:488:TYR:H	1.46	0.80
1:E:484:VAL:HG12	1:E:770:LEU:HD13	1.63	0.80
1:C:225:HIS:HA	1:C:330:ALA:HB2	1.63	0.80
1:A:191:TYR:HB2	1:A:355:PHE:HB2	1.64	0.80
1:F:580:LYS:HG3	1:F:593:ASN:HD22	1.44	0.80
1:F:521:GLY:HA3	1:F:610:SER:HA	1.63	0.80
1:D:587:TYR:HD1	1:D:588:GLY:H	1.24	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:HD12	1:B:437:MSE:HE2	1.61	0.80
1:A:127:PRO:HB3	1:A:312:THR:HG22	1.62	0.80
1:B:519:THR:HB	1:B:608:ALA:HA	1.64	0.80
1:B:451:LYS:HG3	1:B:477:LEU:HD11	1.62	0.80
1:C:458:ALA:HB1	1:C:467:THR:HG22	1.63	0.80
1:C:181:CYS:SG	1:C:183:VAL:HG22	2.22	0.80
1:E:711:LEU:HD13	1:E:725:ILE:HG21	1.64	0.80
1:C:201:ASP:N	1:C:202:PRO:HD2	1.97	0.79
1:F:691:ARG:HD3	1:F:724:MSE:HE3	1.64	0.79
1:F:545:GLY:HA3	1:F:548:LEU:HB2	1.64	0.79
1:D:249:PRO:HG3	1:D:300:LEU:HD13	1.64	0.79
1:C:253:MSE:HG2	1:C:317:PHE:HE1	1.45	0.79
1:C:269:GLU:HB2	1:C:378:ARG:CZ	2.12	0.79
1:C:485:GLN:HB3	1:C:488:TYR:HB2	1.64	0.79
1:B:163:ARG:HB2	1:B:163:ARG:HH11	1.47	0.79
1:F:371:ILE:HD12	1:F:380:VAL:HG22	1.64	0.79
1:F:404:GLY:HA2	1:F:753:GLN:HE22	1.47	0.79
1:E:111:ASP:HB3	1:E:172:ARG:HH22	1.48	0.79
1:B:57:ILE:HG13	1:B:75:LYS:NZ	1.98	0.79
1:B:282:ILE:HD12	1:B:371:ILE:HG23	1.64	0.79
1:B:508:LEU:HD22	1:B:611:THR:HG21	1.65	0.79
1:B:653:VAL:HG13	1:B:692:ALA:HB3	1.64	0.79
1:A:335:MSE:HE1	1:A:430:LYS:HG3	1.63	0.78
1:C:219:LYS:HD3	1:C:358:HIS:H	1.48	0.78
1:C:66:PRO:HD2	1:C:133:ASN:HD22	1.48	0.78
1:E:24:ILE:HD11	1:E:56:PHE:HA	1.65	0.78
1:E:282:ILE:HD12	1:E:371:ILE:HG23	1.65	0.78
1:F:169:PRO:HG2	1:F:170:LEU:HD12	1.64	0.78
1:E:15:VAL:HG11	1:E:67:LEU:HB2	1.65	0.78
1:D:219:LYS:HD3	1:D:358:HIS:H	1.49	0.78
1:E:506:ILE:HB	1:E:711:LEU:HD12	1.65	0.78
1:F:249:PRO:HG3	1:F:300:LEU:HD13	1.65	0.78
1:A:435:GLU:HA	1:A:438:ARG:HD2	1.63	0.78
1:A:225:HIS:HA	1:A:330:ALA:HB2	1.66	0.78
1:A:331:ASN:HD22	1:A:337:MSE:HA	1.48	0.78
1:E:580:LYS:HG3	1:E:593:ASN:HD22	1.48	0.78
1:B:14:ALA:HB3	1:B:103:PRO:CG	2.12	0.78
1:F:269:GLU:HB2	1:F:378:ARG:CZ	2.14	0.78
1:E:268:PRO:HG2	1:E:378:ARG:HH22	1.49	0.78
1:C:690:ALA:HB1	1:C:725:ILE:HG13	1.66	0.78
1:E:412:GLY:HA3	1:E:750:ASN:HD22	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:VAL:HG22	1:C:738:VAL:HG22	1.66	0.78
1:B:337:MSE:HE3	1:B:367:ASP:HA	1.65	0.78
1:A:267:SER:HB2	1:A:270:GLU:CB	2.14	0.78
1:E:368:ASP:HA	1:E:385:ARG:HD3	1.66	0.78
1:B:526:TYR:O	1:B:532:VAL:HG13	1.83	0.78
1:C:329:SER:HB2	1:C:331:ASN:HD21	1.49	0.78
1:C:11:ILE:CG2	1:C:69:ARG:H	1.97	0.78
1:A:412:GLY:HA3	1:A:750:ASN:HD22	1.48	0.78
1:E:30:LEU:HD13	1:E:52:ASP:HB2	1.65	0.77
1:D:553:PRO:HB2	1:D:620:VAL:HG21	1.64	0.77
1:B:412:GLY:HA3	1:B:750:ASN:HD22	1.48	0.77
1:A:106:ILE:HG23	1:A:277:TYR:HB2	1.64	0.77
1:A:183:VAL:HG23	1:A:184:CYS:N	1.99	0.77
1:A:485:GLN:NE2	1:A:487:HIS:H	1.83	0.77
1:D:380:VAL:HG23	1:D:740:THR:HA	1.66	0.77
1:B:282:ILE:HG22	1:B:305:VAL:HB	1.65	0.77
1:D:88:ILE:HG22	1:D:89:GLU:N	1.99	0.77
1:C:687:LEU:HB3	1:C:724:MSE:HE2	1.65	0.77
1:B:371:ILE:HD12	1:B:380:VAL:HG22	1.66	0.77
1:C:207:ALA:O	1:C:210:ILE:HG22	1.85	0.77
1:E:210:ILE:HD13	1:E:216:VAL:HG12	1.65	0.77
1:F:6:ILE:HG23	1:F:73:ILE:HG23	1.67	0.77
1:F:633:GLU:H	1:F:634:PRO:HD2	1.50	0.76
1:F:373:PHE:CD1	1:F:378:ARG:HB3	2.21	0.76
1:C:456:ILE:HG22	1:C:457:ILE:H	1.50	0.76
1:E:729:VAL:HG11	1:E:735:ASN:HB3	1.66	0.76
1:A:11:ILE:HG21	1:A:69:ARG:N	2.00	0.76
1:B:165:GLU:HB3	1:B:171:ASN:ND2	2.01	0.76
1:B:201:ASP:N	1:B:202:PRO:HD2	2.01	0.76
1:C:690:ALA:HB2	1:C:721:ILE:HG23	1.68	0.76
1:F:35:LYS:HG3	1:F:90:LYS:HD2	1.65	0.76
1:B:267:SER:HB2	1:B:270:GLU:HB2	1.67	0.76
1:B:494:VAL:HG11	1:B:710:ALA:HB1	1.68	0.76
1:D:653:VAL:HG13	1:D:692:ALA:HB3	1.67	0.76
1:A:236:VAL:HG13	1:A:295:ASN:HD22	1.50	0.76
1:E:470:ALA:HB1	1:E:481:LEU:HD11	1.68	0.76
1:C:287:LYS:HG3	1:C:289:PRO:HD2	1.68	0.76
1:E:106:ILE:HG23	1:E:277:TYR:HB2	1.66	0.76
1:A:485:GLN:HG3	1:A:488:TYR:H	1.50	0.76
1:A:371:ILE:HD12	1:A:380:VAL:HG22	1.68	0.76
1:D:601:LYS:HD3	1:E:772:LEU:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PHE:HB3	1:B:360:ARG:NH2	2.01	0.75
1:C:11:ILE:HG21	1:C:69:ARG:H	1.49	0.75
1:C:110:ASP:O	1:C:113:LEU:HB3	1.86	0.75
1:B:225:HIS:NE2	1:B:327:MSE:HE3	2.01	0.75
1:F:404:GLY:HA2	1:F:753:GLN:NE2	2.00	0.75
1:E:371:ILE:HB	1:E:380:VAL:HG13	1.68	0.75
1:E:329:SER:HB2	1:E:331:ASN:HD21	1.51	0.75
1:C:198:ILE:HG13	1:D:122:LYS:CD	2.17	0.75
1:A:380:VAL:HG23	1:A:740:THR:HA	1.69	0.75
1:E:165:GLU:HB3	1:E:171:ASN:ND2	2.01	0.75
1:A:121:ASN:ND2	1:A:123:ARG:H	1.83	0.75
1:B:557:LEU:HD12	1:B:620:VAL:HB	1.69	0.75
1:F:111:ASP:HB2	1:F:172:ARG:HH22	1.51	0.75
1:D:589:LYS:HG3	1:D:590:VAL:H	1.51	0.75
1:F:255:LYS:HB2	1:F:323:PRO:HB3	1.69	0.75
1:E:215:ILE:HG22	1:E:228:CYS:HB2	1.67	0.75
1:A:628:ARG:HH21	1:A:632:GLY:H	1.33	0.75
1:A:190:LEU:O	1:A:196:GLN:HB2	1.87	0.75
1:A:456:ILE:HG22	1:A:457:ILE:N	2.01	0.75
1:E:633:GLU:H	1:E:634:PRO:HD2	1.52	0.75
1:A:502:SER:HB3	1:A:528:GLY:HA2	1.69	0.74
1:A:765:LEU:HD21	1:A:770:LEU:HD21	1.69	0.74
1:C:249:PRO:HG3	1:C:300:LEU:HD13	1.69	0.74
1:F:526:TYR:O	1:F:532:VAL:HG13	1.87	0.74
1:F:15:VAL:HG12	1:F:16:GLY:H	1.51	0.74
1:E:131:CYS:HB2	1:E:172:ARG:HG3	1.67	0.74
1:B:557:LEU:HD21	1:B:621:LEU:HD13	1.69	0.74
1:B:52:ASP:O	1:B:56:PHE:HB2	1.87	0.74
1:D:169:PRO:HG2	1:D:170:LEU:HD12	1.67	0.74
1:B:456:ILE:HG22	1:B:457:ILE:N	2.02	0.74
1:E:371:ILE:HD12	1:E:380:VAL:HG22	1.69	0.74
1:B:427:ASN:ND2	1:B:429:GLY:H	1.84	0.74
1:E:219:LYS:HG3	1:E:224:ILE:HG22	1.70	0.74
1:B:633:GLU:H	1:B:634:PRO:HD2	1.52	0.74
1:D:121:ASN:ND2	1:D:123:ARG:H	1.84	0.74
1:E:508:LEU:HD22	1:E:611:THR:HG21	1.67	0.74
1:B:287:LYS:HG3	1:B:289:PRO:HD2	1.68	0.74
1:D:371:ILE:HD12	1:D:380:VAL:HG22	1.70	0.74
1:B:108:ILE:HD11	1:B:314:TYR:CD2	2.22	0.74
1:A:521:GLY:HA3	1:A:610:SER:HA	1.69	0.74
1:E:270:GLU:OE1	1:E:284:LEU:HD21	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLU:O	1:B:212:LYS:HG2	1.87	0.74
1:C:190:LEU:HB2	1:C:202:PRO:HB3	1.68	0.74
1:B:502:SER:HB3	1:B:528:GLY:HA2	1.68	0.74
1:C:273:GLU:HG2	1:C:371:ILE:HD13	1.69	0.74
1:F:330:ALA:HB1	1:F:348:LEU:HD21	1.70	0.74
1:B:35:LYS:HG2	1:B:36:ASN:H	1.53	0.73
1:E:539:ASP:HA	1:E:659:LEU:HD11	1.69	0.73
1:C:415:LYS:HD3	1:C:448:LEU:HD22	1.70	0.73
1:A:461:HIS:CE1	1:A:463:ALA:HB3	2.23	0.73
1:B:236:VAL:HG13	1:B:295:ASN:HD22	1.51	0.73
1:C:373:PHE:CD1	1:C:378:ARG:HB3	2.24	0.73
1:C:650:LYS:HD2	1:C:691:ARG:HH22	1.53	0.73
1:E:144:LEU:HD12	1:E:447:ILE:HG23	1.69	0.73
1:D:35:LYS:HZ3	1:D:90:LYS:HD2	1.53	0.73
1:E:625:ALA:HB2	1:E:637:LYS:HD2	1.70	0.73
1:F:215:ILE:HG22	1:F:228:CYS:HB2	1.69	0.73
1:F:201:ASP:N	1:F:202:PRO:HD2	2.02	0.73
1:A:542:PRO:O	1:A:559:GLY:HA3	1.89	0.73
1:B:181:CYS:SG	1:B:183:VAL:HG22	2.28	0.73
1:B:485:GLN:HE21	1:B:487:HIS:N	1.84	0.73
1:F:690:ALA:HB2	1:F:721:ILE:HG23	1.69	0.73
1:A:584:SER:HB3	1:A:589:LYS:HB3	1.70	0.73
1:A:729:VAL:HG11	1:A:735:ASN:HB3	1.70	0.73
1:E:225:HIS:HA	1:E:330:ALA:HB2	1.71	0.73
1:D:406:GLU:HG3	1:D:407:LEU:HG	1.69	0.73
1:A:3:ALA:HB2	1:A:47:GLU:HA	1.70	0.73
1:B:550:SER:O	1:B:628:ARG:HG3	1.89	0.73
1:E:691:ARG:HE	1:E:724:MSE:HE2	1.52	0.73
1:B:225:HIS:HA	1:B:330:ALA:CB	2.18	0.73
1:D:219:LYS:HG3	1:D:224:ILE:HG22	1.69	0.73
1:E:654:PRO:HG2	1:E:661:ARG:HB3	1.69	0.73
1:C:339:LYS:HG3	1:C:365:ARG:NH1	2.04	0.73
1:A:268:PRO:HG2	1:A:378:ARG:NH2	2.02	0.72
1:C:284:LEU:HD21	1:C:305:VAL:HG21	1.70	0.72
1:C:292:LEU:HD13	1:C:293:PRO:HD2	1.71	0.72
1:A:111:ASP:HB3	1:A:172:ARG:HH12	1.52	0.72
1:C:11:ILE:O	1:C:11:ILE:HG13	1.88	0.72
1:F:181:CYS:SG	1:F:183:VAL:HG22	2.28	0.72
1:E:544:PRO:HG2	1:E:555:ARG:HB3	1.71	0.72
1:C:589:LYS:H	1:F:475:ASN:ND2	1.86	0.72
1:D:557:LEU:HD12	1:D:620:VAL:HB	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ALA:HB2	1:E:47:GLU:HA	1.70	0.72
1:E:587:TYR:HD1	1:E:588:GLY:H	1.37	0.72
1:C:30:LEU:HD13	1:C:52:ASP:HB2	1.70	0.72
1:C:485:GLN:NE2	1:C:514:GLY:HA2	2.05	0.72
1:F:281:ILE:HG12	1:F:306:MSE:HG2	1.69	0.72
1:D:193:SER:O	1:D:194:ASP:HB2	1.89	0.72
1:D:485:GLN:NE2	1:D:487:HIS:H	1.85	0.72
1:B:254:ALA:HB1	1:B:259:THR:HB	1.69	0.72
1:C:649:LEU:HB3	1:C:684:SER:HB3	1.70	0.72
1:B:169:PRO:HG2	1:B:170:LEU:HD12	1.71	0.72
1:F:587:TYR:HD1	1:F:588:GLY:H	1.38	0.72
1:E:22:TYR:CD2	1:E:169:PRO:HB3	2.25	0.72
1:A:379:ALA:HB3	1:A:744:ARG:NH1	2.03	0.72
1:D:225:HIS:NE2	1:D:327:MSE:HE3	2.04	0.72
1:A:15:VAL:HG12	1:A:16:GLY:H	1.55	0.72
1:F:18:ARG:HB2	1:F:19:PRO:HD3	1.70	0.72
1:E:404:GLY:HA2	1:E:753:GLN:HE22	1.53	0.72
1:F:191:TYR:HB2	1:F:355:PHE:HB2	1.71	0.72
1:E:239:LEU:O	1:E:243:THR:HG22	1.90	0.72
1:C:369:SER:H	1:C:385:ARG:CB	2.03	0.71
1:A:148:ARG:O	1:A:151:THR:HG22	1.89	0.71
1:A:274:LEU:HB3	1:A:307:LEU:HD11	1.70	0.71
1:F:108:ILE:HA	1:F:134:CYS:SG	2.31	0.71
1:F:331:ASN:HD22	1:F:337:MSE:HA	1.55	0.71
1:F:726:ARG:NH2	1:F:727:LYS:HG2	2.05	0.71
1:D:210:ILE:HD13	1:D:216:VAL:HG12	1.73	0.71
1:F:491:ILE:HG23	1:F:507:ALA:HB2	1.71	0.71
1:D:201:ASP:N	1:D:202:PRO:HD2	2.05	0.71
1:A:225:HIS:NE2	1:A:327:MSE:HE3	2.05	0.71
1:F:373:PHE:CE1	1:F:378:ARG:HB3	2.25	0.71
1:B:371:ILE:HB	1:B:380:VAL:HG13	1.72	0.71
1:B:380:VAL:HG12	1:B:381:ILE:H	1.56	0.71
1:B:373:PHE:CE1	1:B:378:ARG:HB3	2.26	0.71
1:E:153:MSE:CE	1:E:360:ARG:HD2	2.20	0.71
1:A:258:GLU:HA	1:A:261:LYS:HD3	1.73	0.71
1:D:11:ILE:HG21	1:D:69:ARG:H	1.56	0.71
1:B:20:PHE:CZ	1:B:63:LYS:HB2	2.25	0.71
1:E:724:MSE:O	1:E:728:VAL:HG23	1.91	0.71
1:D:330:ALA:HB1	1:D:348:LEU:HD21	1.71	0.71
1:D:170:LEU:H	1:D:170:LEU:HD12	1.54	0.71
1:D:539:ASP:HA	1:D:659:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LEU:HD22	1:D:307:LEU:HG	1.72	0.71
1:F:543:LEU:HD12	1:F:549:ALA:HB3	1.73	0.71
1:E:207:ALA:O	1:E:210:ILE:HG22	1.89	0.71
1:E:633:GLU:N	1:E:634:PRO:HD2	2.04	0.71
1:B:108:ILE:HA	1:B:134:CYS:SG	2.31	0.71
1:C:149:GLU:HA	1:C:154:LYS:HG2	1.72	0.71
1:F:554:LEU:O	1:F:558:MSE:HG3	1.89	0.71
1:C:404:GLY:HA2	1:C:753:GLN:NE2	2.06	0.71
1:D:225:HIS:HA	1:D:330:ALA:CB	2.20	0.71
1:B:279:ARG:HD3	1:B:307:LEU:HB2	1.72	0.71
1:D:485:GLN:HG3	1:D:488:TYR:H	1.55	0.70
1:E:445:ARG:HH21	1:E:452:ASN:HD22	1.39	0.70
1:B:495:MSE:HE2	1:B:755:PHE:HZ	1.55	0.70
1:C:136:PRO:HG3	1:C:360:ARG:NH1	2.06	0.70
1:E:553:PRO:HB2	1:E:620:VAL:HG21	1.73	0.70
1:F:687:LEU:HD22	1:F:724:MSE:HB2	1.72	0.70
1:E:583:GLU:H	1:E:583:GLU:CD	1.95	0.70
1:D:142:GLU:HB3	1:D:150:ASN:O	1.91	0.70
1:F:6:ILE:HG22	1:F:7:HIS:H	1.56	0.70
1:A:26:HIS:HE1	1:A:87:TYR:HB3	1.57	0.70
1:F:413:VAL:HG21	1:F:448:LEU:HD13	1.73	0.70
1:F:144:LEU:HD12	1:F:447:ILE:HG23	1.73	0.70
1:A:526:TYR:O	1:A:532:VAL:HG13	1.91	0.70
1:F:89:GLU:HG3	1:F:175:HIS:HE2	1.56	0.70
1:F:391:PRO:HB2	1:F:418:LYS:HB2	1.72	0.70
1:B:590:VAL:O	1:B:594:VAL:HG23	1.92	0.70
1:E:495:MSE:HE2	1:E:755:PHE:HZ	1.56	0.70
1:D:694:ALA:HB2	1:D:725:ILE:HG23	1.74	0.70
1:D:144:LEU:HD12	1:D:447:ILE:HG23	1.74	0.70
1:A:601:LYS:HD3	1:B:772:LEU:HD11	1.74	0.70
1:B:18:ARG:HB2	1:B:19:PRO:HD3	1.74	0.70
1:C:391:PRO:HB3	1:C:420:TYR:CE1	2.27	0.70
1:D:8:VAL:HA	1:D:72:ARG:HB2	1.74	0.70
1:D:190:LEU:HB2	1:D:202:PRO:HB2	1.72	0.70
1:A:207:ALA:HB1	1:A:320:SER:HB2	1.73	0.70
1:F:14:ALA:HB3	1:F:103:PRO:HD3	1.73	0.70
1:D:13:GLN:HE21	1:D:42:VAL:HG23	1.56	0.70
1:D:6:ILE:HB	1:D:44:ILE:HB	1.73	0.70
1:B:567:ILE:HG12	1:B:600:ALA:HB1	1.74	0.70
1:B:144:LEU:HD12	1:B:447:ILE:HG23	1.73	0.70
1:D:329:SER:HB2	1:D:331:ASN:HD21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:ALA:HB1	1:E:348:LEU:HD21	1.74	0.70
1:E:292:LEU:HD11	1:E:324:VAL:HG21	1.74	0.70
1:A:516:ASP:HA	1:B:603:ILE:HG23	1.73	0.70
1:E:14:ALA:O	1:E:103:PRO:HG3	1.92	0.70
1:F:434:LEU:HD13	1:F:465:ASN:HB3	1.72	0.70
1:C:18:ARG:HB2	1:C:19:PRO:HD3	1.74	0.70
1:F:225:HIS:NE2	1:F:327:MSE:HE3	2.07	0.70
1:D:263:PHE:HZ	1:D:303:ILE:HG21	1.56	0.70
1:E:208:GLU:O	1:E:212:LYS:HG2	1.91	0.69
1:F:409:ASN:HD22	1:F:425:ILE:HD11	1.56	0.69
1:C:506:ILE:HD11	1:C:694:ALA:HA	1.74	0.69
1:A:504:ILE:O	1:A:709:VAL:HA	1.91	0.69
1:D:374:VAL:HG21	1:D:744:ARG:NH2	2.07	0.69
1:D:207:ALA:O	1:D:210:ILE:HG22	1.91	0.69
1:A:649:LEU:HD12	1:A:650:LYS:H	1.56	0.69
1:F:127:PRO:O	1:F:311:GLY:HA3	1.92	0.69
1:F:495:MSE:HE2	1:F:755:PHE:HZ	1.57	0.69
1:A:379:ALA:CB	1:A:744:ARG:HH11	2.04	0.69
1:C:281:ILE:HG12	1:C:306:MSE:HG3	1.74	0.69
1:B:215:ILE:HD11	1:B:352:ALA:HA	1.72	0.69
1:D:287:LYS:HG3	1:D:289:PRO:HD2	1.74	0.69
1:F:210:ILE:HD11	1:F:227:ALA:C	2.12	0.69
1:A:207:ALA:O	1:A:210:ILE:HG22	1.92	0.69
1:A:380:VAL:HG12	1:A:381:ILE:N	2.06	0.69
1:E:190:LEU:HB2	1:E:202:PRO:HB3	1.74	0.69
1:D:582:VAL:HG11	1:D:626:TYR:O	1.92	0.69
1:B:20:PHE:HZ	1:B:63:LYS:HB2	1.57	0.69
1:D:205:LYS:O	1:D:209:LEU:HD13	1.92	0.69
1:B:589:LYS:HG3	1:B:590:VAL:H	1.58	0.69
1:C:317:PHE:HE2	1:C:323:PRO:HA	1.57	0.69
1:A:227:ALA:HA	1:A:326:VAL:O	1.92	0.69
1:A:32:GLY:O	1:A:87:TYR:HA	1.93	0.69
1:A:472:GLU:O	1:A:476:GLU:HG2	1.92	0.69
1:A:339:LYS:HA	1:A:362:ILE:HD11	1.74	0.69
1:B:729:VAL:HB	1:B:735:ASN:HD22	1.57	0.69
1:A:329:SER:HA	1:A:337:MSE:HE2	1.73	0.69
1:D:409:ASN:HD22	1:D:425:ILE:HD11	1.57	0.69
1:E:282:ILE:HG22	1:E:305:VAL:HB	1.75	0.69
1:C:329:SER:HB2	1:C:331:ASN:ND2	2.08	0.69
1:B:207:ALA:O	1:B:210:ILE:HG22	1.92	0.69
1:D:633:GLU:H	1:D:634:PRO:HD2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:SER:O	1:E:194:ASP:HB2	1.93	0.69
1:B:752:GLY:O	1:B:756:LEU:HB2	1.92	0.69
1:D:315:ILE:HG12	1:D:319:TRP:HZ3	1.56	0.69
1:F:19:PRO:HA	1:F:174:TYR:CD1	2.28	0.69
1:C:57:ILE:HG21	1:C:75:LYS:HE3	1.74	0.69
1:B:13:GLN:NE2	1:B:18:ARG:HH21	1.90	0.69
1:F:537:HIS:NE2	1:F:659:LEU:HD22	2.07	0.69
1:C:435:GLU:HA	1:C:438:ARG:HD2	1.74	0.69
1:A:662:VAL:O	1:A:665:LEU:HB3	1.93	0.69
1:A:383:ARG:HH21	1:A:392:ILE:HD11	1.57	0.68
1:E:267:SER:O	1:E:270:GLU:HB3	1.91	0.68
1:A:689:LEU:O	1:A:693:PHE:HB2	1.93	0.68
1:F:288:GLU:CB	1:F:289:PRO:HD3	2.22	0.68
1:A:590:VAL:H	1:B:475:ASN:HD21	1.41	0.68
1:C:385:ARG:HG3	1:C:386:GLY:H	1.58	0.68
1:F:760:TYR:HE2	1:F:767:LYS:HG2	1.59	0.68
1:E:572:GLY:HA2	1:E:575:ASN:HD22	1.57	0.68
1:F:267:SER:HB2	1:F:270:GLU:HB2	1.76	0.68
1:B:369:SER:HB2	1:B:385:ARG:CB	2.24	0.68
1:C:26:HIS:CE1	1:C:87:TYR:HB3	2.28	0.68
1:D:391:PRO:HB3	1:D:420:TYR:CE1	2.29	0.68
1:E:6:ILE:HA	1:E:74:GLU:O	1.93	0.68
1:B:514:GLY:HA3	1:B:520:TRP:CD1	2.29	0.68
1:D:369:SER:H	1:D:385:ARG:CB	2.06	0.68
1:A:215:ILE:HG22	1:A:228:CYS:HB2	1.74	0.68
1:E:639:GLU:HB2	1:E:718:ASN:HD21	1.58	0.68
1:F:230:ALA:HB3	1:F:324:VAL:HB	1.75	0.68
1:F:394:ILE:CD1	1:F:419:VAL:HB	2.21	0.68
1:C:355:PHE:HB3	1:C:357:LEU:HD21	1.75	0.68
1:B:534:ARG:HG2	1:B:535:LEU:N	2.08	0.68
1:E:229:ASP:OD1	1:E:322:THR:HG21	1.94	0.68
1:A:247:GLN:HE22	1:A:637:LYS:HE3	1.59	0.68
1:C:61:TYR:OH	1:C:73:ILE:HG21	1.92	0.68
1:C:88:ILE:HG22	1:C:89:GLU:H	1.57	0.68
1:D:373:PHE:CD1	1:D:378:ARG:HB3	2.28	0.68
1:E:8:VAL:HB	1:E:42:VAL:HB	1.75	0.68
1:F:208:GLU:O	1:F:212:LYS:HG2	1.94	0.68
1:F:653:VAL:HG11	1:F:689:LEU:HA	1.76	0.68
1:F:649:LEU:HB3	1:F:684:SER:HB3	1.76	0.68
1:A:553:PRO:CB	1:A:620:VAL:HG21	2.24	0.68
1:A:687:LEU:HD22	1:A:724:MSE:HE3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:341:ASN:HD22	1:F:357:LEU:HB3	1.59	0.68
1:C:460:LEU:O	1:C:462:PRO:HD3	1.94	0.68
1:B:286:LYS:HD2	1:B:303:ILE:HD11	1.75	0.67
1:B:524:VAL:HG22	1:B:536:ALA:HB3	1.76	0.67
1:C:589:LYS:HG3	1:C:590:VAL:H	1.57	0.67
1:B:460:LEU:HD12	1:B:483:GLN:HB3	1.76	0.67
1:F:165:GLU:HB3	1:F:171:ASN:ND2	2.09	0.67
1:B:469:LEU:HG	1:B:473:MSE:HG3	1.75	0.67
1:F:503:VAL:HB	1:F:708:ASN:O	1.94	0.67
1:E:282:ILE:HG13	1:E:283:THR:H	1.60	0.67
1:A:419:VAL:HG11	1:A:751:VAL:HG23	1.76	0.67
1:D:219:LYS:HE3	1:D:358:HIS:CE1	2.29	0.67
1:F:12:VAL:HG13	1:F:42:VAL:HG21	1.76	0.67
1:D:504:ILE:HG22	1:D:505:GLY:N	2.10	0.67
1:A:15:VAL:HG11	1:A:67:LEU:O	1.94	0.67
1:D:12:VAL:HG13	1:D:17:PHE:CG	2.29	0.67
1:A:373:PHE:CD1	1:A:378:ARG:HB3	2.29	0.67
1:C:267:SER:O	1:C:270:GLU:HB3	1.93	0.67
1:B:624:VAL:O	1:B:625:ALA:HB2	1.93	0.67
1:D:32:GLY:O	1:D:87:TYR:HA	1.94	0.67
1:A:249:PRO:HG3	1:A:300:LEU:HD13	1.76	0.67
1:E:408:MSE:HG3	1:E:424:TYR:CE1	2.29	0.67
1:F:544:PRO:HG2	1:F:555:ARG:HB3	1.76	0.67
1:E:428:THR:HA	1:E:433:VAL:HG11	1.76	0.67
1:C:30:LEU:HG	1:C:47:GLU:O	1.94	0.67
1:A:102:ILE:HD11	1:A:144:LEU:HG	1.77	0.67
1:E:121:ASN:ND2	1:E:123:ARG:H	1.92	0.67
1:C:131:CYS:HB2	1:C:172:ARG:HG3	1.76	0.67
1:C:369:SER:N	1:C:385:ARG:HB2	2.10	0.67
1:D:491:ILE:HD11	1:D:505:GLY:HA3	1.75	0.67
1:F:620:VAL:HG13	1:F:626:TYR:CD1	2.29	0.67
1:E:183:VAL:HG23	1:E:184:CYS:N	2.09	0.67
1:C:148:ARG:O	1:C:151:THR:HG22	1.94	0.67
1:A:6:ILE:HD12	1:A:73:ILE:HG23	1.76	0.67
1:A:391:PRO:HB3	1:A:420:TYR:CE1	2.29	0.67
1:D:369:SER:HB2	1:D:385:ARG:HB3	1.75	0.67
1:C:253:MSE:HE3	1:C:308:PRO:HB3	1.77	0.67
1:F:168:ASP:O	1:F:174:TYR:HB2	1.95	0.67
1:A:544:PRO:HD2	1:A:555:ARG:O	1.94	0.67
1:B:503:VAL:HB	1:B:708:ASN:O	1.94	0.67
1:B:394:ILE:HG23	1:B:755:PHE:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HA	1:A:224:ILE:HG22	1.76	0.67
1:C:521:GLY:HA3	1:C:610:SER:HA	1.76	0.67
1:C:13:GLN:HE21	1:C:42:VAL:HG23	1.58	0.67
1:C:170:LEU:H	1:C:170:LEU:HD12	1.60	0.67
1:E:415:LYS:HD3	1:E:448:LEU:HD22	1.77	0.67
1:A:225:HIS:HA	1:A:330:ALA:CB	2.24	0.67
1:C:102:ILE:HG23	1:C:141:ILE:HD13	1.76	0.67
1:D:526:TYR:O	1:D:532:VAL:HG13	1.95	0.67
1:B:288:GLU:CB	1:B:289:PRO:HD3	2.23	0.67
1:E:394:ILE:HG23	1:E:755:PHE:HB2	1.76	0.67
1:F:250:PHE:HE2	1:F:328:THR:HG1	1.43	0.67
1:A:148:ARG:NH2	1:A:158:MSE:HG3	2.08	0.67
1:F:396:PHE:CZ	1:F:759:LEU:HD13	2.30	0.66
1:B:268:PRO:HG2	1:B:378:ARG:NH2	2.07	0.66
1:E:738:VAL:HG12	1:E:742:VAL:HB	1.76	0.66
1:D:191:TYR:HB2	1:D:355:PHE:HB2	1.77	0.66
1:D:554:LEU:O	1:D:558:MSE:HG3	1.96	0.66
1:D:163:ARG:HB2	1:D:163:ARG:HH11	1.60	0.66
1:D:269:GLU:HB2	1:D:378:ARG:CZ	2.25	0.66
1:C:508:LEU:HD22	1:C:611:THR:HG21	1.77	0.66
1:C:649:LEU:HB3	1:C:684:SER:CB	2.25	0.66
1:C:34:VAL:HB	1:C:87:TYR:OH	1.95	0.66
1:A:261:LYS:HG3	1:A:266:VAL:HG21	1.75	0.66
1:D:279:ARG:HD2	1:D:308:PRO:O	1.96	0.66
1:C:738:VAL:HG12	1:C:742:VAL:O	1.95	0.66
1:F:580:LYS:HZ2	1:F:590:VAL:HG13	1.60	0.66
1:E:373:PHE:CD1	1:E:378:ARG:HB3	2.30	0.66
1:A:616:ASP:OD2	1:A:634:PRO:HG3	1.94	0.66
1:F:398:TYR:HB2	1:F:454:ASP:OD2	1.95	0.66
1:F:89:GLU:HG3	1:F:175:HIS:NE2	2.10	0.66
1:C:461:HIS:CE1	1:C:463:ALA:HB3	2.31	0.66
1:F:412:GLY:HA3	1:F:750:ASN:ND2	2.11	0.66
1:B:394:ILE:HG22	1:B:396:PHE:H	1.59	0.66
1:F:264:ALA:CB	1:F:286:LYS:HA	2.25	0.66
1:B:156:PHE:HZ	1:B:359:ASN:HB2	1.61	0.66
1:B:267:SER:HB2	1:B:270:GLU:CB	2.26	0.66
1:D:215:ILE:HG22	1:D:228:CYS:HB2	1.78	0.66
1:E:504:ILE:HB	1:E:709:VAL:HG12	1.77	0.66
1:D:508:LEU:HD22	1:D:611:THR:HG21	1.78	0.66
1:F:203:LEU:HD12	1:F:319:TRP:HZ3	1.61	0.66
1:B:227:ALA:HA	1:B:326:VAL:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:LYS:HZ1	1:F:266:VAL:HB	1.61	0.66
1:D:137:ARG:NH2	1:D:178:PRO:HG3	2.10	0.66
1:E:267:SER:HB2	1:E:270:GLU:HB2	1.77	0.66
1:B:142:GLU:HG3	1:B:143:ASP:OD1	1.95	0.66
1:C:756:LEU:O	1:C:759:LEU:HB3	1.96	0.66
1:D:580:LYS:HG3	1:D:593:ASN:HD22	1.61	0.66
1:B:22:TYR:CD2	1:B:169:PRO:HB3	2.31	0.66
1:E:286:LYS:HD2	1:E:303:ILE:HD11	1.78	0.66
1:E:312:THR:HA	1:E:315:ILE:HG22	1.78	0.66
1:A:589:LYS:HG3	1:A:590:VAL:N	2.11	0.66
1:C:506:ILE:HG12	1:C:524:VAL:HG12	1.78	0.66
1:C:484:VAL:HG12	1:C:770:LEU:HD22	1.77	0.66
1:D:384:SER:HA	1:D:388:VAL:HG23	1.78	0.66
1:D:502:SER:HB3	1:D:528:GLY:HA2	1.77	0.66
1:C:200:GLY:C	1:C:202:PRO:HD2	2.16	0.66
1:C:337:MSE:HG3	1:C:367:ASP:OD2	1.96	0.66
1:A:425:ILE:HA	1:A:436:PHE:HE1	1.59	0.66
1:E:649:LEU:HB3	1:E:684:SER:HB3	1.78	0.66
1:C:698:VAL:HG13	1:C:732:ASN:HD22	1.61	0.66
1:D:239:LEU:O	1:D:243:THR:HG22	1.96	0.66
1:D:491:ILE:HG23	1:D:527:LEU:HD21	1.76	0.65
1:C:103:PRO:CG	1:C:137:ARG:HD2	2.25	0.65
1:C:66:PRO:CD	1:C:133:ASN:HD22	2.08	0.65
1:F:301:HIS:HD2	1:F:302:THR:H	1.44	0.65
1:E:263:PHE:HZ	1:E:303:ILE:HG21	1.61	0.65
1:D:9:GLN:NE2	1:D:41:GLY:HA2	2.02	0.65
1:A:485:GLN:HE21	1:A:487:HIS:N	1.90	0.65
1:F:239:LEU:HD22	1:F:250:PHE:HZ	1.62	0.65
1:C:591:GLU:HG2	1:F:475:ASN:HD22	1.61	0.65
1:F:649:LEU:HD12	1:F:650:LYS:H	1.61	0.65
1:D:700:ARG:HH11	1:D:704:PHE:HE2	1.43	0.65
1:A:490:HIS:HE1	1:A:746:ASP:HA	1.61	0.65
1:C:412:GLY:HA3	1:C:750:ASN:HD22	1.61	0.65
1:F:570:LEU:O	1:F:573:VAL:HG12	1.97	0.65
1:F:619:ALA:HB1	1:F:625:ALA:HB3	1.76	0.65
1:F:615:LEU:CD1	1:F:638:LEU:HD23	2.25	0.65
1:D:570:LEU:O	1:D:573:VAL:HG12	1.97	0.65
1:E:12:VAL:HG23	1:E:68:ALA:HB1	1.79	0.65
1:D:181:CYS:SG	1:D:183:VAL:HG13	2.37	0.65
1:A:508:LEU:HD22	1:A:611:THR:HG21	1.79	0.65
1:A:166:TYR:CE1	1:A:175:HIS:HA	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:PRO:HG2	1:C:748:GLY:HA3	1.79	0.65
1:B:456:ILE:HD12	1:B:480:GLU:O	1.97	0.65
1:E:270:GLU:OE2	1:E:284:LEU:HD11	1.97	0.65
1:B:425:ILE:HG22	1:B:436:PHE:HE1	1.61	0.65
1:F:616:ASP:OD1	1:F:634:PRO:HG2	1.97	0.65
1:E:404:GLY:HA2	1:E:753:GLN:NE2	2.10	0.65
1:F:409:ASN:HB3	1:F:425:ILE:HD11	1.78	0.65
1:C:376:GLY:O	1:C:377:LYS:HG3	1.95	0.65
1:F:641:PHE:HZ	1:F:678:PRO:HB2	1.61	0.65
1:E:12:VAL:HA	1:E:68:ALA:HB1	1.77	0.65
1:C:620:VAL:HG22	1:C:626:TYR:HA	1.79	0.65
1:F:504:ILE:HG22	1:F:505:GLY:N	2.11	0.65
1:C:522:GLY:HA3	1:C:538:ILE:HD12	1.79	0.65
1:A:317:PHE:HE2	1:A:323:PRO:HA	1.62	0.65
1:D:20:PHE:HA	1:D:23:ARG:HH21	1.60	0.65
1:D:155:GLU:O	1:D:157:PRO:HD3	1.96	0.65
1:F:456:ILE:HG22	1:F:457:ILE:N	2.12	0.65
1:C:127:PRO:O	1:C:311:GLY:HA3	1.96	0.65
1:D:233:GLU:HB2	1:D:295:ASN:ND2	2.11	0.65
1:A:337:MSE:HG3	1:A:367:ASP:OD2	1.97	0.65
1:B:279:ARG:HB2	1:B:309:TYR:HB3	1.79	0.65
1:B:481:LEU:HD12	1:B:482:LEU:H	1.62	0.65
1:F:694:ALA:HB2	1:F:725:ILE:HG12	1.79	0.65
1:C:371:ILE:HB	1:C:380:VAL:HG13	1.78	0.65
1:E:590:VAL:O	1:E:594:VAL:HG23	1.96	0.65
1:A:165:GLU:HB3	1:A:171:ASN:ND2	2.11	0.65
1:D:456:ILE:HG22	1:D:457:ILE:H	1.60	0.65
1:F:408:MSE:HG3	1:F:424:TYR:CE1	2.32	0.65
1:F:743:PRO:HG2	1:F:748:GLY:HA3	1.79	0.65
1:B:498:LYS:HE3	1:B:736:PHE:HB2	1.79	0.65
1:B:690:ALA:HB1	1:B:725:ILE:HG13	1.79	0.65
1:E:30:LEU:CD1	1:E:52:ASP:HB2	2.27	0.65
1:C:700:ARG:HH11	1:C:704:PHE:HE2	1.43	0.65
1:E:232:ASN:HB3	1:E:235:VAL:HG22	1.79	0.65
1:A:589:LYS:H	1:B:475:ASN:ND2	1.95	0.64
1:C:281:ILE:HG12	1:C:306:MSE:CG	2.27	0.64
1:C:385:ARG:HG3	1:C:386:GLY:N	2.12	0.64
1:B:215:ILE:O	1:B:353:ASP:HB2	1.97	0.64
1:B:374:VAL:HG21	1:B:744:ARG:NH2	2.12	0.64
1:A:26:HIS:CE1	1:A:87:TYR:HB3	2.31	0.64
1:A:619:ALA:O	1:A:624:VAL:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:649:LEU:HD12	1:E:650:LYS:H	1.60	0.64
1:D:690:ALA:HB1	1:D:725:ILE:HG13	1.79	0.64
1:B:263:PHE:HZ	1:B:303:ILE:HG21	1.62	0.64
1:F:729:VAL:HG11	1:F:735:ASN:HB3	1.78	0.64
1:E:281:ILE:HG12	1:E:306:MSE:CG	2.27	0.64
1:E:329:SER:HA	1:E:337:MSE:HE2	1.80	0.64
1:E:651:PHE:HB2	1:E:688:ALA:CB	2.27	0.64
1:E:749:VAL:O	1:E:753:GLN:HG3	1.97	0.64
1:E:103:PRO:HG2	1:E:137:ARG:HD2	1.78	0.64
1:E:137:ARG:O	1:E:141:ILE:HG13	1.97	0.64
1:E:570:LEU:O	1:E:573:VAL:HG12	1.97	0.64
1:E:601:LYS:HB2	1:E:603:ILE:HG13	1.79	0.64
1:B:456:ILE:HD11	1:B:479:VAL:HB	1.79	0.64
1:B:219:LYS:HA	1:B:224:ILE:HB	1.77	0.64
1:C:292:LEU:HD12	1:C:296:LEU:HD21	1.79	0.64
1:A:200:GLY:C	1:A:202:PRO:HD2	2.18	0.64
1:C:405:ALA:O	1:C:466:THR:HG21	1.97	0.64
1:E:224:ILE:HG13	1:E:338:VAL:HG13	1.78	0.64
1:B:491:ILE:HD12	1:B:525:LEU:HD12	1.78	0.64
1:E:18:ARG:HH22	1:E:36:ASN:ND2	1.96	0.64
1:F:687:LEU:CD2	1:F:724:MSE:HB2	2.27	0.64
1:D:564:VAL:HG13	1:D:667:GLN:HE21	1.62	0.64
1:C:37:LEU:HD23	1:C:40:ALA:O	1.98	0.64
1:C:50:GLU:O	1:C:53:ILE:HG22	1.97	0.64
1:D:690:ALA:O	1:D:725:ILE:HG12	1.97	0.64
1:F:456:ILE:HG22	1:F:457:ILE:H	1.61	0.64
1:C:312:THR:O	1:C:315:ILE:HG22	1.98	0.64
1:A:475:ASN:ND2	1:B:591:GLU:HG2	2.10	0.64
1:D:491:ILE:HG23	1:D:527:LEU:HD11	1.80	0.64
1:A:653:VAL:HG13	1:A:692:ALA:HB3	1.80	0.64
1:A:292:LEU:HD11	1:A:324:VAL:HG21	1.80	0.64
1:C:409:ASN:ND2	1:C:425:ILE:HD11	2.12	0.64
1:A:232:ASN:HB3	1:A:235:VAL:HG22	1.79	0.64
1:A:451:LYS:HA	1:A:477:LEU:HD21	1.79	0.64
1:E:521:GLY:HA3	1:E:610:SER:HA	1.79	0.64
1:C:601:LYS:NZ	1:F:771:MSE:HE3	2.13	0.64
1:E:519:THR:HB	1:E:608:ALA:HA	1.79	0.64
1:C:188:TYR:CZ	1:C:312:THR:HG21	2.32	0.64
1:F:581:ALA:HA	1:F:584:SER:HB3	1.80	0.64
1:A:183:VAL:CG2	1:A:184:CYS:N	2.61	0.64
1:F:32:GLY:H	1:F:87:TYR:HD2	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:VAL:HG12	1:F:381:ILE:N	2.12	0.64
1:C:192:THR:C	1:C:194:ASP:H	1.99	0.64
1:C:437:MSE:O	1:C:441:ILE:HG13	1.98	0.64
1:B:549:ALA:HA	1:B:555:ARG:HB2	1.78	0.64
1:B:163:ARG:HB2	1:B:163:ARG:NH1	2.12	0.64
1:C:583:GLU:H	1:C:583:GLU:CD	2.01	0.64
1:F:142:GLU:HB3	1:F:150:ASN:O	1.98	0.64
1:B:6:ILE:HG23	1:B:73:ILE:HG23	1.80	0.64
1:A:282:ILE:HG13	1:A:283:THR:H	1.63	0.64
1:B:544:PRO:HB2	1:B:555:ARG:NH2	2.13	0.64
1:F:57:ILE:HG13	1:F:75:LYS:HZ3	1.61	0.64
1:D:216:VAL:HG23	1:D:354:TYR:C	2.18	0.64
1:C:394:ILE:HD11	1:C:419:VAL:HB	1.80	0.64
1:F:651:PHE:HB2	1:F:688:ALA:CB	2.28	0.64
1:A:759:LEU:HD22	1:A:765:LEU:HB2	1.79	0.63
1:D:524:VAL:HG23	1:D:536:ALA:H	1.62	0.63
1:A:633:GLU:N	1:A:634:PRO:HD2	2.14	0.63
1:A:49:ARG:CD	1:A:49:ARG:H	2.09	0.63
1:A:757:GLY:O	1:A:760:TYR:HB3	1.98	0.63
1:F:427:ASN:O	1:F:433:VAL:HG21	1.98	0.63
1:E:127:PRO:HB3	1:E:312:THR:CG2	2.27	0.63
1:C:338:VAL:HG23	1:C:343:ARG:HB2	1.79	0.63
1:C:12:VAL:HG13	1:C:13:GLN:H	1.61	0.63
1:A:615:LEU:HD11	1:A:635:ALA:HA	1.81	0.63
1:E:502:SER:HB3	1:E:528:GLY:HA2	1.80	0.63
1:D:232:ASN:HB3	1:D:235:VAL:HG22	1.80	0.63
1:D:529:TYR:HD1	1:D:764:TYR:HB3	1.63	0.63
1:A:752:GLY:O	1:A:756:LEU:HB2	1.97	0.63
1:F:373:PHE:CE2	1:F:378:ARG:HD3	2.34	0.63
1:F:549:ALA:HA	1:F:555:ARG:HB2	1.80	0.63
1:B:369:SER:HB2	1:B:385:ARG:HB2	1.81	0.63
1:D:161:PHE:O	1:D:164:SER:HB2	1.97	0.63
1:B:270:GLU:HB2	1:B:373:PHE:HE2	1.64	0.63
1:B:584:SER:HB3	1:B:589:LYS:HB3	1.80	0.63
1:E:380:VAL:HG12	1:E:381:ILE:H	1.63	0.63
1:A:485:GLN:OE1	1:A:514:GLY:HA2	1.99	0.63
1:F:589:LYS:HG3	1:F:590:VAL:N	2.12	0.63
1:D:653:VAL:HG11	1:D:689:LEU:HD12	1.79	0.63
1:F:263:PHE:HZ	1:F:303:ILE:HG21	1.62	0.63
1:A:17:PHE:O	1:A:21:VAL:HG23	1.97	0.63
1:F:221:ILE:HA	1:F:360:ARG:HH22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LYS:HG2	1:D:358:HIS:NE2	2.13	0.63
1:B:215:ILE:HG22	1:B:228:CYS:HB2	1.81	0.63
1:A:201:ASP:N	1:A:202:PRO:CD	2.61	0.63
1:B:580:LYS:HE2	1:B:593:ASN:ND2	2.13	0.63
1:F:126:TYR:CZ	1:F:128:PHE:HB2	2.34	0.63
1:B:566:SER:H	1:B:569:GLU:HB2	1.63	0.63
1:F:396:PHE:CE2	1:F:759:LEU:HB2	2.34	0.63
1:B:265:TYR:O	1:B:284:LEU:HD22	1.98	0.63
1:A:108:ILE:HG13	1:A:311:GLY:H	1.63	0.63
1:F:224:ILE:HD13	1:F:357:LEU:HD22	1.81	0.63
1:E:760:TYR:HE2	1:E:767:LYS:HG2	1.64	0.63
1:D:742:VAL:HG11	1:D:751:VAL:HG11	1.81	0.63
1:D:88:ILE:CG2	1:D:89:GLU:H	2.09	0.63
1:A:590:VAL:N	1:B:475:ASN:HD21	1.96	0.63
1:B:501:ASP:O	1:B:503:VAL:HG13	1.99	0.63
1:F:239:LEU:O	1:F:239:LEU:HD23	1.98	0.63
1:C:13:GLN:NE2	1:C:42:VAL:HG23	2.13	0.63
1:A:629:HIS:HB2	1:A:633:GLU:OE1	1.98	0.63
1:D:434:LEU:HD13	1:D:465:ASN:HB3	1.81	0.63
1:F:613:ARG:HE	1:F:613:ARG:HA	1.64	0.63
1:A:369:SER:H	1:A:385:ARG:HB2	1.64	0.63
1:A:114:ARG:O	1:A:118:ASP:HB2	1.98	0.63
1:C:253:MSE:O	1:C:324:VAL:HA	1.98	0.62
1:B:210:ILE:HD11	1:B:228:CYS:N	2.13	0.62
1:F:137:ARG:HH22	1:F:178:PRO:HG3	1.62	0.62
1:B:566:SER:N	1:B:569:GLU:HB2	2.14	0.62
1:A:5:HIS:HB3	1:A:76:LYS:HB2	1.80	0.62
1:F:697:ALA:HB1	1:F:709:VAL:HG11	1.80	0.62
1:C:261:LYS:HZ3	1:C:266:VAL:HB	1.63	0.62
1:A:148:ARG:CZ	1:A:158:MSE:HG3	2.28	0.62
1:B:374:VAL:HG11	1:B:744:ARG:HH22	1.64	0.62
1:F:430:LYS:HB2	1:F:433:VAL:HG23	1.80	0.62
1:B:651:PHE:HE2	1:B:669:ILE:HA	1.63	0.62
1:F:665:LEU:HD22	1:F:689:LEU:HD13	1.81	0.62
1:F:620:VAL:HG13	1:F:626:TYR:HD1	1.64	0.62
1:F:264:ALA:HB2	1:F:286:LYS:HA	1.80	0.62
1:C:239:LEU:O	1:C:243:THR:HG22	1.98	0.62
1:B:373:PHE:CD1	1:B:378:ARG:HB3	2.35	0.62
1:A:494:VAL:HG22	1:A:738:VAL:HG22	1.80	0.62
1:B:8:VAL:HG11	1:B:12:VAL:HG21	1.81	0.62
1:A:329:SER:HB2	1:A:331:ASN:HD21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PHE:O	1:A:24:ILE:HG22	1.99	0.62
1:D:385:ARG:HG3	1:D:386:GLY:N	2.14	0.62
1:C:281:ILE:HB	1:C:370:VAL:CG1	2.25	0.62
1:D:226:LEU:HD11	1:D:348:LEU:HD23	1.81	0.62
1:D:553:PRO:CD	1:D:627:ARG:HA	2.30	0.62
1:F:329:SER:HB2	1:F:331:ASN:HD21	1.65	0.62
1:D:649:LEU:HD12	1:D:650:LYS:H	1.64	0.62
1:A:708:ASN:HB3	1:A:734:LEU:O	1.99	0.62
1:E:5:HIS:HB3	1:E:76:LYS:HB2	1.80	0.62
1:E:66:PRO:HD2	1:E:133:ASN:ND2	2.15	0.62
1:D:408:MSE:HG3	1:D:424:TYR:CE1	2.34	0.62
1:A:497:GLU:OE2	1:A:741:GLU:HB3	2.00	0.62
1:C:104:PRO:HD3	1:C:390:LEU:HD21	1.82	0.62
1:B:281:ILE:HG12	1:B:306:MSE:HG2	1.80	0.62
1:F:729:VAL:HB	1:F:735:ASN:HD22	1.65	0.62
1:E:370:VAL:H	1:E:382:ARG:HB3	1.64	0.62
1:D:282:ILE:HD12	1:D:371:ILE:O	1.99	0.62
1:D:373:PHE:CE1	1:D:378:ARG:HB3	2.34	0.62
1:A:325:TYR:O	1:A:326:VAL:HG23	2.00	0.62
1:C:219:LYS:HE3	1:C:358:HIS:CE1	2.35	0.62
1:A:116:LEU:HB3	1:A:129:ILE:HD12	1.80	0.62
1:A:534:ARG:HG2	1:A:535:LEU:N	2.14	0.62
1:B:225:HIS:HB2	1:B:328:THR:O	2.00	0.62
1:C:534:ARG:HD3	1:C:537:HIS:HD2	1.65	0.62
1:C:258:GLU:HG3	1:C:259:THR:H	1.61	0.62
1:F:590:VAL:O	1:F:594:VAL:HG23	2.00	0.62
1:D:105:ASP:OD1	1:D:139:THR:HG23	1.99	0.62
1:F:464:TYR:HB2	1:F:467:THR:HG23	1.80	0.62
1:F:193:SER:O	1:F:194:ASP:HB2	2.00	0.62
1:A:475:ASN:ND2	1:B:589:LYS:H	1.98	0.62
1:E:168:ASP:O	1:E:174:TYR:HB2	2.00	0.62
1:E:111:ASP:HB3	1:E:172:ARG:NH2	2.15	0.62
1:C:649:LEU:HD12	1:C:650:LYS:H	1.64	0.62
1:D:408:MSE:HG3	1:D:424:TYR:HE1	1.64	0.62
1:C:570:LEU:O	1:C:573:VAL:HG12	2.00	0.62
1:E:142:GLU:HB3	1:E:150:ASN:O	1.99	0.62
1:A:65:PRO:HG2	1:A:68:ALA:HB3	1.80	0.62
1:E:380:VAL:HG12	1:E:381:ILE:N	2.15	0.62
1:C:495:MSE:SE	1:C:527:LEU:HD13	2.50	0.62
1:A:210:ILE:HD11	1:A:228:CYS:N	2.14	0.62
1:A:263:PHE:HZ	1:A:303:ILE:HG21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:VAL:O	1:A:753:GLN:HG3	2.00	0.62
1:E:210:ILE:HD11	1:E:228:CYS:CA	2.28	0.62
1:C:169:PRO:HG2	1:C:170:LEU:HD12	1.81	0.62
1:C:422:SER:HA	1:C:444:PHE:CZ	2.34	0.62
1:B:1:MSE:HG2	1:B:83:PHE:HD1	1.65	0.62
1:A:521:GLY:CA	1:A:610:SER:HA	2.30	0.62
1:F:190:LEU:HG	1:F:202:PRO:CB	2.29	0.62
1:C:253:MSE:HA	1:C:306:MSE:O	2.00	0.62
1:D:543:LEU:N	1:D:543:LEU:HD23	2.13	0.62
1:F:65:PRO:HG2	1:F:68:ALA:HB3	1.82	0.62
1:A:580:LYS:HG3	1:A:593:ASN:HD22	1.65	0.61
1:E:737:HIS:HB3	1:E:744:ARG:HD3	1.82	0.61
1:B:498:LYS:HB2	1:B:500:LEU:CD2	2.29	0.61
1:C:756:LEU:HD22	1:C:770:LEU:HD21	1.82	0.61
1:D:590:VAL:O	1:D:594:VAL:HG23	1.99	0.61
1:C:603:ILE:HG23	1:F:516:ASP:HA	1.81	0.61
1:D:61:TYR:OH	1:D:73:ILE:HD12	1.99	0.61
1:F:583:GLU:HG3	1:F:592:PHE:CD1	2.35	0.61
1:E:394:ILE:CD1	1:E:419:VAL:HB	2.28	0.61
1:E:445:ARG:HH21	1:E:452:ASN:ND2	1.97	0.61
1:B:525:LEU:HD23	1:B:534:ARG:HA	1.81	0.61
1:D:543:LEU:HD12	1:D:549:ALA:HB3	1.82	0.61
1:C:224:ILE:HG23	1:C:338:VAL:HG13	1.82	0.61
1:E:201:ASP:N	1:E:202:PRO:CD	2.63	0.61
1:A:236:VAL:HG13	1:A:295:ASN:ND2	2.15	0.61
1:E:61:TYR:CZ	1:E:73:ILE:HD12	2.34	0.61
1:E:204:ARG:HG2	1:E:319:TRP:CE2	2.35	0.61
1:D:8:VAL:O	1:D:9:GLN:HG3	2.00	0.61
1:F:498:LYS:HE3	1:F:736:PHE:HB2	1.83	0.61
1:C:226:LEU:HD21	1:C:351:VAL:HG12	1.81	0.61
1:F:385:ARG:HG3	1:F:386:GLY:H	1.64	0.61
1:C:138:PHE:HB2	1:C:389:PRO:HD3	1.82	0.61
1:E:111:ASP:CB	1:E:172:ARG:HH22	2.14	0.61
1:E:391:PRO:HB2	1:E:418:LYS:HB2	1.82	0.61
1:B:502:SER:CB	1:B:528:GLY:HA2	2.29	0.61
1:D:553:PRO:HD2	1:D:627:ARG:HA	1.82	0.61
1:F:255:LYS:HB2	1:F:323:PRO:CB	2.29	0.61
1:C:196:GLN:HG2	1:C:197:GLU:N	2.15	0.61
1:E:47:GLU:CB	1:E:80:PRO:HG2	2.30	0.61
1:B:743:PRO:HG3	1:B:747:ASN:HD21	1.66	0.61
1:E:485:GLN:OE1	1:E:514:GLY:HA2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLU:CG	1:C:259:THR:N	2.62	0.61
1:A:216:VAL:HB	1:A:354:TYR:HB2	1.82	0.61
1:D:601:LYS:HB2	1:D:603:ILE:HG13	1.82	0.61
1:F:292:LEU:HD11	1:F:324:VAL:HG21	1.82	0.61
1:D:427:ASN:ND2	1:D:429:GLY:H	1.98	0.61
1:B:485:GLN:CG	1:B:488:TYR:H	2.12	0.61
1:B:313:HIS:HE1	1:B:327:MSE:HE2	1.64	0.61
1:F:690:ALA:HB1	1:F:725:ILE:HG13	1.83	0.61
1:E:489:ALA:O	1:E:492:ALA:HB3	2.00	0.61
1:A:282:ILE:HG13	1:A:283:THR:N	2.16	0.61
1:B:125:MSE:O	1:B:127:PRO:HD3	2.01	0.61
1:C:232:ASN:OD1	1:C:234:GLU:HB3	2.00	0.61
1:D:257:ILE:HD12	1:D:260:VAL:HG21	1.83	0.61
1:B:380:VAL:HG12	1:B:381:ILE:N	2.16	0.61
1:F:106:ILE:CG2	1:F:277:TYR:HB2	2.30	0.61
1:F:61:TYR:OH	1:F:73:ILE:HD12	2.00	0.61
1:C:614:VAL:O	1:C:618:ILE:HG13	2.01	0.61
1:B:491:ILE:HG22	1:B:527:LEU:HD11	1.81	0.61
1:A:727:LYS:NZ	1:C:287:LYS:HE3	2.15	0.61
1:F:15:VAL:HG22	1:F:103:PRO:HB3	1.82	0.61
1:F:17:PHE:O	1:F:21:VAL:HG23	2.00	0.61
1:F:154:LYS:HD3	1:F:154:LYS:O	2.01	0.61
1:F:633:GLU:N	1:F:634:PRO:HD2	2.16	0.61
1:F:183:VAL:HG23	1:F:184:CYS:N	2.16	0.61
1:E:670:LEU:O	1:E:673:ILE:HG12	2.01	0.61
1:D:111:ASP:CB	1:D:172:ARG:HH22	2.10	0.61
1:F:614:VAL:O	1:F:618:ILE:HG13	2.01	0.61
1:C:584:SER:HB3	1:C:589:LYS:HB3	1.83	0.61
1:D:369:SER:N	1:D:385:ARG:HB2	2.10	0.60
1:A:590:VAL:O	1:A:594:VAL:HG23	2.01	0.60
1:C:759:LEU:CD1	1:C:764:TYR:HB2	2.30	0.60
1:F:370:VAL:H	1:F:382:ARG:HB3	1.65	0.60
1:B:200:GLY:C	1:B:202:PRO:HD2	2.21	0.60
1:C:450:VAL:HG22	1:C:451:LYS:H	1.66	0.60
1:A:123:ARG:NH2	1:A:173:ARG:HE	1.98	0.60
1:D:542:PRO:HD3	1:D:563:LYS:HE2	1.82	0.60
1:F:506:ILE:O	1:F:711:LEU:HD12	2.00	0.60
1:D:282:ILE:HG13	1:D:283:THR:N	2.16	0.60
1:A:142:GLU:HB3	1:A:150:ASN:O	2.00	0.60
1:C:456:ILE:HG22	1:C:457:ILE:N	2.16	0.60
1:F:35:LYS:HE2	1:F:90:LYS:NZ	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:ILE:HG22	1:D:457:ILE:N	2.16	0.60
1:A:49:ARG:O	1:A:53:ILE:HB	2.01	0.60
1:A:698:VAL:HG13	1:A:732:ASN:HD22	1.65	0.60
1:A:572:GLY:HA2	1:A:575:ASN:HD22	1.67	0.60
1:D:270:GLU:HB2	1:D:373:PHE:HE2	1.66	0.60
1:F:649:LEU:HB3	1:F:684:SER:CB	2.31	0.60
1:E:500:LEU:HD13	1:E:736:PHE:CZ	2.36	0.60
1:B:394:ILE:CD1	1:B:419:VAL:HB	2.25	0.60
1:C:504:ILE:O	1:C:709:VAL:HA	2.01	0.60
1:C:373:PHE:CE2	1:C:378:ARG:HD3	2.37	0.60
1:A:524:VAL:HG22	1:A:536:ALA:CB	2.31	0.60
1:B:729:VAL:CB	1:B:735:ASN:HD22	2.14	0.60
1:E:691:ARG:NE	1:E:724:MSE:HE2	2.14	0.60
1:F:469:LEU:O	1:F:473:MSE:HB2	2.01	0.60
1:F:287:LYS:HG3	1:F:289:PRO:HD2	1.83	0.60
1:D:253:MSE:O	1:D:324:VAL:HA	2.02	0.60
1:C:759:LEU:HD11	1:C:764:TYR:HB2	1.83	0.60
1:D:144:LEU:HD23	1:D:146:TYR:H	1.67	0.60
1:E:266:VAL:HG13	1:E:270:GLU:OE2	2.01	0.60
1:E:286:LYS:HE3	1:E:290:PHE:HB2	1.84	0.60
1:D:148:ARG:O	1:D:151:THR:HG22	2.01	0.60
1:A:616:ASP:CG	1:A:634:PRO:HG3	2.22	0.60
1:E:406:GLU:HG3	1:E:407:LEU:HG	1.82	0.60
1:B:373:PHE:CE2	1:B:378:ARG:HD3	2.36	0.60
1:E:759:LEU:HD11	1:E:764:TYR:HB2	1.83	0.60
1:D:504:ILE:O	1:D:709:VAL:HA	2.01	0.60
1:D:665:LEU:HD22	1:D:689:LEU:HD13	1.83	0.60
1:A:15:VAL:HG21	1:A:67:LEU:O	2.02	0.60
1:A:239:LEU:O	1:A:243:THR:HG22	2.02	0.60
1:B:408:MSE:HG3	1:B:424:TYR:CE1	2.37	0.60
1:D:572:GLY:HA2	1:D:575:ASN:HD22	1.66	0.60
1:E:257:ILE:HD12	1:E:260:VAL:HB	1.83	0.60
1:B:263:PHE:CZ	1:B:303:ILE:HG21	2.36	0.60
1:B:759:LEU:HD11	1:B:764:TYR:HB2	1.84	0.60
1:B:35:LYS:HG3	1:B:90:LYS:HD2	1.83	0.60
1:C:552:TYR:HE1	1:C:627:ARG:NE	1.99	0.60
1:B:401:LEU:HD12	1:B:402:ALA:H	1.67	0.60
1:C:485:GLN:CB	1:C:488:TYR:HB2	2.32	0.60
1:B:158:MSE:HE3	1:B:163:ARG:CZ	2.32	0.60
1:B:620:VAL:C	1:B:622:LEU:H	2.05	0.60
1:E:6:ILE:HD12	1:E:73:ILE:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:GLN:HB2	1:E:72:ARG:HD2	1.84	0.60
1:F:405:ALA:O	1:F:466:THR:HG21	2.01	0.60
1:D:371:ILE:CD1	1:D:380:VAL:HG22	2.31	0.60
1:A:282:ILE:HD12	1:A:371:ILE:O	2.02	0.60
1:B:653:VAL:HG13	1:B:692:ALA:CB	2.30	0.60
1:E:30:LEU:HG	1:E:48:GLY:HA3	1.84	0.60
1:A:634:PRO:HG2	1:A:635:ALA:H	1.67	0.60
1:C:204:ARG:HG2	1:C:319:TRP:CZ2	2.37	0.60
1:D:34:VAL:O	1:D:89:GLU:HA	2.02	0.60
1:A:587:TYR:HD1	1:A:588:GLY:N	1.93	0.60
1:E:281:ILE:HG12	1:E:306:MSE:HG2	1.83	0.60
1:E:726:ARG:HH21	1:E:727:LYS:HG2	1.67	0.60
1:B:274:LEU:HB3	1:B:307:LEU:HD11	1.84	0.60
1:B:540:TYR:HD1	1:B:540:TYR:H	1.48	0.60
1:D:409:ASN:ND2	1:D:425:ILE:HD11	2.17	0.60
1:A:299:GLY:O	1:A:300:LEU:HG	2.02	0.60
1:F:371:ILE:HD11	1:F:373:PHE:HE1	1.67	0.59
1:C:409:ASN:O	1:C:425:ILE:HG12	2.02	0.59
1:B:504:ILE:HG22	1:B:505:GLY:N	2.16	0.59
1:E:554:LEU:O	1:E:558:MSE:HG3	2.02	0.59
1:D:554:LEU:HD11	1:D:579:PRO:HB2	1.83	0.59
1:F:445:ARG:HH21	1:F:452:ASN:HD22	1.48	0.59
1:A:445:ARG:HH21	1:A:452:ASN:ND2	2.00	0.59
1:B:219:LYS:HD3	1:B:358:HIS:H	1.66	0.59
1:A:723:LYS:HE2	1:C:289:PRO:HG2	1.83	0.59
1:C:524:VAL:HG22	1:C:536:ALA:HB3	1.82	0.59
1:B:312:THR:O	1:B:315:ILE:HG22	2.02	0.59
1:D:566:SER:N	1:D:569:GLU:HB2	2.13	0.59
1:A:405:ALA:O	1:A:466:THR:HG21	2.02	0.59
1:E:261:LYS:HZ3	1:E:266:VAL:HB	1.67	0.59
1:E:329:SER:HB2	1:E:331:ASN:ND2	2.17	0.59
1:B:425:ILE:HG22	1:B:436:PHE:CE1	2.38	0.59
1:A:144:LEU:HD12	1:A:447:ILE:HG23	1.83	0.59
1:D:526:TYR:HB2	1:D:535:LEU:HD11	1.85	0.59
1:A:553:PRO:HG3	1:A:626:TYR:O	2.01	0.59
1:E:396:PHE:CE2	1:E:759:LEU:HB2	2.36	0.59
1:C:215:ILE:HG22	1:C:228:CYS:HB2	1.83	0.59
1:C:225:HIS:HA	1:C:330:ALA:CB	2.32	0.59
1:A:196:GLN:HG2	1:A:197:GLU:O	2.01	0.59
1:F:370:VAL:HG23	1:F:381:ILE:HD11	1.83	0.59
1:D:144:LEU:HD23	1:D:146:TYR:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:PRO:HB3	1:B:420:TYR:CE1	2.38	0.59
1:C:171:ASN:ND2	1:C:173:ARG:HB2	2.18	0.59
1:D:166:TYR:CE1	1:D:175:HIS:HA	2.38	0.59
1:E:156:PHE:CZ	1:E:186:PRO:HB3	2.38	0.59
1:D:614:VAL:O	1:D:618:ILE:HG13	2.02	0.59
1:A:554:LEU:O	1:A:558:MSE:HG3	2.02	0.59
1:E:419:VAL:HG11	1:E:751:VAL:HG23	1.83	0.59
1:A:253:MSE:HE2	1:A:317:PHE:CD1	2.37	0.59
1:C:724:MSE:O	1:C:728:VAL:HG23	2.03	0.59
1:B:107:ALA:O	1:B:134:CYS:HB2	2.02	0.59
1:C:554:LEU:O	1:C:558:MSE:HG3	2.03	0.59
1:D:468:LYS:HG3	1:E:587:TYR:OH	2.03	0.59
1:D:654:PRO:HG3	1:D:664:GLU:OE1	2.02	0.59
1:E:456:ILE:HG22	1:E:457:ILE:N	2.18	0.59
1:F:601:LYS:HB2	1:F:603:ILE:HG13	1.83	0.59
1:F:106:ILE:HG23	1:F:277:TYR:HB2	1.84	0.59
1:B:15:VAL:HG12	1:B:16:GLY:H	1.68	0.59
1:A:247:GLN:HG3	1:A:298:PRO:HG2	1.83	0.59
1:C:406:GLU:HG3	1:C:407:LEU:N	2.16	0.59
1:E:464:TYR:HB2	1:E:467:THR:HG23	1.84	0.59
1:B:239:LEU:O	1:B:239:LEU:HD23	2.03	0.59
1:D:171:ASN:ND2	1:D:173:ARG:H	2.00	0.59
1:A:267:SER:H	1:A:270:GLU:CD	2.06	0.59
1:B:282:ILE:HG23	1:B:283:THR:N	2.15	0.59
1:F:265:TYR:CE2	1:F:287:LYS:HD2	2.31	0.59
1:B:751:VAL:HG13	1:B:752:GLY:N	2.17	0.59
1:C:526:TYR:O	1:C:532:VAL:HG13	2.03	0.59
1:F:370:VAL:CG2	1:F:381:ILE:HD11	2.33	0.59
1:D:383:ARG:HB3	1:D:747:ASN:HD21	1.68	0.59
1:E:543:LEU:HD12	1:E:549:ALA:HB3	1.85	0.59
1:C:66:PRO:HG3	1:C:133:ASN:HB3	1.85	0.59
1:E:729:VAL:HB	1:E:735:ASN:HD22	1.66	0.59
1:E:572:GLY:HA2	1:E:575:ASN:ND2	2.17	0.59
1:F:254:ALA:HB1	1:F:259:THR:HB	1.85	0.59
1:D:398:TYR:HB2	1:D:454:ASP:OD2	2.03	0.59
1:B:281:ILE:HG12	1:B:306:MSE:CG	2.33	0.59
1:E:752:GLY:O	1:E:756:LEU:HB2	2.01	0.59
1:D:137:ARG:HH22	1:D:178:PRO:HG3	1.67	0.59
1:E:210:ILE:CD1	1:E:228:CYS:HA	2.32	0.59
1:B:374:VAL:CG2	1:B:744:ARG:HH22	2.14	0.59
1:E:677:SER:HB2	1:E:678:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:MSE:HE1	1:F:313:HIS:ND1	2.17	0.59
1:F:519:THR:HB	1:F:608:ALA:HA	1.83	0.59
1:B:402:ALA:HB2	1:B:457:ILE:HD12	1.84	0.59
1:A:485:GLN:CG	1:A:488:TYR:H	2.16	0.59
1:C:223:GLY:HA2	1:C:362:ILE:HD12	1.85	0.59
1:D:121:ASN:HD22	1:D:123:ARG:H	1.49	0.59
1:F:181:CYS:SG	1:F:183:VAL:HG13	2.43	0.59
1:F:213:GLY:CA	1:F:235:VAL:HG11	2.33	0.59
1:D:485:GLN:HE21	1:D:487:HIS:N	1.87	0.59
1:A:270:GLU:N	1:A:378:ARG:HH12	2.01	0.59
1:E:399:ASN:O	1:E:454:ASP:HB2	2.02	0.59
1:C:491:ILE:HG22	1:C:527:LEU:HD12	1.84	0.59
1:A:210:ILE:HG21	1:A:325:TYR:HE1	1.67	0.59
1:D:565:TYR:HB3	1:D:569:GLU:CB	2.33	0.59
1:A:408:MSE:HG3	1:A:424:TYR:HE1	1.68	0.59
1:B:237:ALA:HA	1:B:295:ASN:HD21	1.68	0.59
1:C:583:GLU:HG3	1:C:592:PHE:CD1	2.37	0.59
1:F:253:MSE:HE3	1:F:317:PHE:CE1	2.38	0.59
1:B:111:ASP:O	1:B:114:ARG:HG2	2.02	0.59
1:A:620:VAL:C	1:A:622:LEU:H	2.06	0.59
1:E:274:LEU:HB3	1:E:307:LEU:HD11	1.85	0.59
1:C:591:GLU:HG2	1:F:475:ASN:ND2	2.17	0.59
1:A:447:ILE:O	1:A:448:LEU:HD23	2.02	0.59
1:C:9:GLN:O	1:C:71:ASP:HB3	2.03	0.59
1:C:247:GLN:OE1	1:C:637:LYS:HE3	2.01	0.59
1:E:15:VAL:HG12	1:E:16:GLY:H	1.66	0.58
1:A:371:ILE:HG13	1:A:380:VAL:HA	1.85	0.58
1:A:405:ALA:H	1:A:749:VAL:HG11	1.68	0.58
1:F:498:LYS:HB2	1:F:500:LEU:HD23	1.85	0.58
1:F:506:ILE:HG12	1:F:524:VAL:HG12	1.85	0.58
1:D:18:ARG:HA	1:D:21:VAL:HG12	1.85	0.58
1:C:312:THR:HA	1:C:315:ILE:HG22	1.84	0.58
1:D:11:ILE:CG1	1:D:68:ALA:HA	2.29	0.58
1:B:232:ASN:HB3	1:B:235:VAL:CG2	2.31	0.58
1:D:724:MSE:O	1:D:728:VAL:HG23	2.03	0.58
1:E:589:LYS:HG3	1:E:590:VAL:N	2.17	0.58
1:B:433:VAL:O	1:B:436:PHE:HB3	2.04	0.58
1:C:642:ALA:O	1:C:683:TYR:HB2	2.03	0.58
1:B:108:ILE:HD11	1:B:314:TYR:CE2	2.38	0.58
1:A:140:ILE:HB	1:A:152:THR:CG2	2.33	0.58
1:B:220:GLY:H	1:B:224:ILE:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:VAL:HG22	1:D:382:ARG:HB2	1.85	0.58
1:D:65:PRO:HG2	1:D:68:ALA:CB	2.33	0.58
1:C:253:MSE:HG2	1:C:317:PHE:CE1	2.32	0.58
1:B:154:LYS:O	1:B:154:LYS:HD3	2.02	0.58
1:A:407:LEU:HD23	1:A:427:ASN:ND2	2.19	0.58
1:B:298:PRO:O	1:B:300:LEU:HD12	2.03	0.58
1:D:247:GLN:HE22	1:D:637:LYS:HE3	1.68	0.58
1:B:337:MSE:HG3	1:B:367:ASP:OD2	2.02	0.58
1:C:57:ILE:HG23	1:C:73:ILE:HD11	1.86	0.58
1:C:106:ILE:HG23	1:C:277:TYR:HB2	1.83	0.58
1:B:34:VAL:HG12	1:B:87:TYR:HE1	1.67	0.58
1:A:615:LEU:HD12	1:A:638:LEU:HD23	1.85	0.58
1:E:412:GLY:HA2	1:E:420:TYR:O	2.02	0.58
1:D:331:ASN:HD22	1:D:337:MSE:CA	2.13	0.58
1:A:183:VAL:HG23	1:A:184:CYS:H	1.68	0.58
1:F:15:VAL:HG11	1:F:67:LEU:O	2.03	0.58
1:E:376:GLY:HA2	1:E:726:ARG:HH11	1.68	0.58
1:D:216:VAL:HG23	1:D:354:TYR:O	2.03	0.58
1:B:278:ARG:CG	1:B:280:PRO:HD3	2.33	0.58
1:E:264:ALA:HB2	1:E:286:LYS:HA	1.86	0.58
1:A:140:ILE:HB	1:A:152:THR:HG22	1.84	0.58
1:C:500:LEU:HD13	1:C:736:PHE:CZ	2.38	0.58
1:F:524:VAL:HG22	1:F:536:ALA:O	2.04	0.58
1:E:398:TYR:HB2	1:E:454:ASP:OD2	2.04	0.58
1:C:225:HIS:ND1	1:C:337:MSE:HE1	2.18	0.58
1:B:329:SER:HB2	1:B:331:ASN:HD21	1.69	0.58
1:A:66:PRO:HG3	1:A:133:ASN:O	2.04	0.58
1:F:570:LEU:O	1:F:574:ILE:HG12	2.04	0.58
1:A:369:SER:N	1:A:385:ARG:HB2	2.19	0.58
1:A:543:LEU:H	1:A:543:LEU:HD23	1.67	0.58
1:A:374:VAL:HG11	1:A:744:ARG:HH22	1.69	0.58
1:A:759:LEU:HD21	1:A:764:TYR:HB2	1.85	0.58
1:A:190:LEU:HD12	1:A:355:PHE:O	2.04	0.58
1:F:580:LYS:HG3	1:F:593:ASN:ND2	2.17	0.58
1:B:729:VAL:HG11	1:B:735:ASN:HB3	1.85	0.58
1:C:11:ILE:HG12	1:C:68:ALA:HA	1.86	0.58
1:B:623:ASN:ND2	1:B:624:VAL:HG23	2.18	0.58
1:A:601:LYS:HB2	1:A:603:ILE:HG13	1.86	0.58
1:F:461:HIS:O	1:F:467:THR:HG21	2.02	0.58
1:F:583:GLU:HG3	1:F:592:PHE:CG	2.38	0.58
1:E:490:HIS:HE1	1:E:746:ASP:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLU:HB2	1:B:378:ARG:CZ	2.34	0.58
1:E:487:HIS:CD2	1:E:520:TRP:HB3	2.39	0.58
1:F:207:ALA:O	1:F:210:ILE:HG22	2.04	0.58
1:B:628:ARG:HD2	1:B:634:PRO:CD	2.34	0.58
1:C:620:VAL:C	1:C:622:LEU:H	2.04	0.58
1:E:472:GLU:O	1:E:476:GLU:HG2	2.03	0.58
1:A:434:LEU:HD13	1:A:465:ASN:HB3	1.85	0.58
1:C:216:VAL:HB	1:C:354:TYR:HB2	1.86	0.58
1:B:215:ILE:CD1	1:B:352:ALA:HA	2.33	0.58
1:B:554:LEU:O	1:B:558:MSE:HG3	2.03	0.58
1:B:189:ARG:HB3	1:B:191:TYR:CE2	2.39	0.58
1:D:225:HIS:HB2	1:D:328:THR:O	2.03	0.58
1:F:760:TYR:CE2	1:F:767:LYS:HG2	2.39	0.58
1:E:19:PRO:O	1:E:23:ARG:HG3	2.03	0.58
1:C:264:ALA:HB1	1:C:285:ARG:O	2.03	0.58
1:A:371:ILE:CB	1:A:380:VAL:HG13	2.33	0.58
1:F:281:ILE:HG12	1:F:306:MSE:CG	2.33	0.58
1:C:218:ILE:O	1:C:224:ILE:HG13	2.04	0.58
1:F:284:LEU:O	1:F:302:THR:HA	2.03	0.58
1:A:461:HIS:HE1	1:A:463:ALA:HB3	1.67	0.58
1:E:401:LEU:HD12	1:E:402:ALA:H	1.69	0.58
1:D:572:GLY:HA2	1:D:575:ASN:ND2	2.19	0.58
1:E:485:GLN:HG3	1:E:488:TYR:H	1.69	0.57
1:A:226:LEU:HD21	1:A:351:VAL:HG12	1.86	0.57
1:A:433:VAL:O	1:A:436:PHE:HB3	2.04	0.57
1:A:156:PHE:HZ	1:A:359:ASN:HB2	1.69	0.57
1:E:127:PRO:O	1:E:311:GLY:HA3	2.04	0.57
1:A:582:VAL:CG1	1:A:626:TYR:HB3	2.34	0.57
1:A:215:ILE:O	1:A:353:ASP:HB2	2.04	0.57
1:E:189:ARG:HD2	1:E:191:TYR:OH	2.04	0.57
1:F:620:VAL:C	1:F:622:LEU:H	2.06	0.57
1:E:265:TYR:O	1:E:284:LEU:HD13	2.04	0.57
1:B:23:ARG:O	1:B:27:GLU:HB2	2.04	0.57
1:A:443:HIS:O	1:A:447:ILE:HD12	2.04	0.57
1:B:283:THR:HA	1:B:303:ILE:O	2.04	0.57
1:F:729:VAL:O	1:F:729:VAL:HG12	2.05	0.57
1:E:700:ARG:HD2	1:E:704:PHE:HE2	1.68	0.57
1:F:239:LEU:O	1:F:243:THR:HG22	2.02	0.57
1:C:373:PHE:CE1	1:C:378:ARG:HB3	2.39	0.57
1:C:590:VAL:N	1:F:475:ASN:HD21	2.02	0.57
1:B:19:PRO:O	1:B:23:ARG:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LEU:HD21	1:C:760:TYR:HE1	1.69	0.57
1:F:375:ASP:OD1	1:F:723:LYS:HE2	2.03	0.57
1:F:708:ASN:N	1:F:708:ASN:ND2	2.51	0.57
1:B:270:GLU:OE1	1:B:284:LEU:HD21	2.04	0.57
1:E:394:ILE:HG22	1:E:396:PHE:H	1.69	0.57
1:A:263:PHE:CZ	1:A:303:ILE:HG21	2.38	0.57
1:F:278:ARG:HG3	1:F:280:PRO:HD3	1.86	0.57
1:B:579:PRO:HB3	1:B:626:TYR:CE1	2.39	0.57
1:B:504:ILE:HB	1:B:709:VAL:HG12	1.84	0.57
1:D:560:ILE:HD12	1:D:561:LEU:N	2.18	0.57
1:B:557:LEU:O	1:B:557:LEU:HD23	2.03	0.57
1:E:616:ASP:HB3	1:E:634:PRO:HG3	1.86	0.57
1:B:516:ASP:HB2	1:B:518:ASN:ND2	2.19	0.57
1:E:264:ALA:CB	1:E:286:LYS:HA	2.35	0.57
1:F:171:ASN:ND2	1:F:173:ARG:HB2	2.20	0.57
1:A:580:LYS:NZ	1:A:590:VAL:HG22	2.20	0.57
1:A:183:VAL:CG2	1:A:184:CYS:H	2.17	0.57
1:D:197:GLU:O	1:D:198:ILE:HD13	2.05	0.57
1:C:273:GLU:HG3	1:C:273:GLU:O	2.04	0.57
1:B:151:THR:HG23	1:B:153:MSE:H	1.69	0.57
1:C:183:VAL:HG23	1:C:184:CYS:N	2.19	0.57
1:B:572:GLY:HA2	1:B:575:ASN:HD22	1.69	0.57
1:E:653:VAL:HG13	1:E:692:ALA:HB3	1.86	0.57
1:B:541:TYR:CG	1:B:560:ILE:HG22	2.39	0.57
1:B:457:ILE:HG22	1:B:458:ALA:N	2.20	0.57
1:C:203:LEU:HD21	1:C:315:ILE:HD13	1.87	0.57
1:F:67:LEU:HD13	1:F:106:ILE:HD13	1.86	0.57
1:C:690:ALA:CB	1:C:721:ILE:HG23	2.33	0.57
1:A:603:ILE:HG23	1:B:516:ASP:HA	1.87	0.57
1:C:88:ILE:HG22	1:C:89:GLU:N	2.19	0.57
1:C:171:ASN:ND2	1:C:173:ARG:H	2.02	0.57
1:F:383:ARG:HD2	1:F:387:PHE:CD2	2.40	0.57
1:A:193:SER:O	1:A:194:ASP:HB2	2.05	0.57
1:B:37:LEU:O	1:B:37:LEU:HD13	2.04	0.57
1:B:282:ILE:HD12	1:B:371:ILE:CG2	2.35	0.57
1:D:21:VAL:HG11	1:D:34:VAL:HG21	1.87	0.57
1:A:217:ALA:O	1:A:218:ILE:HD13	2.03	0.57
1:A:30:LEU:HD11	1:A:53:ILE:HA	1.86	0.57
1:E:760:TYR:CE2	1:E:767:LYS:HG2	2.40	0.57
1:A:401:LEU:HD12	1:A:402:ALA:H	1.70	0.57
1:F:395:PRO:HG2	1:F:396:PHE:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:ILE:HG22	1:F:228:CYS:CB	2.35	0.57
1:A:219:LYS:HA	1:A:224:ILE:CG2	2.35	0.57
1:B:369:SER:HB2	1:B:385:ARG:HB3	1.86	0.57
1:E:52:ASP:O	1:E:56:PHE:HB2	2.04	0.57
1:C:21:VAL:HG11	1:C:34:VAL:HG21	1.87	0.57
1:D:633:GLU:N	1:D:634:PRO:HD2	2.19	0.57
1:D:700:ARG:HD2	1:D:704:PHE:HE2	1.70	0.57
1:D:670:LEU:HA	1:D:673:ILE:HG12	1.86	0.57
1:F:498:LYS:CB	1:F:500:LEU:HD23	2.35	0.57
1:C:201:ASP:N	1:C:202:PRO:CD	2.66	0.57
1:D:200:GLY:C	1:D:202:PRO:HD2	2.25	0.57
1:F:218:ILE:HD12	1:F:356:LEU:HD23	1.87	0.57
1:E:171:ASN:ND2	1:E:173:ARG:HB2	2.19	0.57
1:C:21:VAL:HA	1:C:24:ILE:HG22	1.87	0.57
1:C:169:PRO:HA	1:C:174:TYR:CD2	2.40	0.57
1:B:677:SER:HB2	1:B:678:PRO:HD2	1.86	0.57
1:B:268:PRO:C	1:B:270:GLU:H	2.09	0.57
1:E:494:VAL:C	1:E:496:ALA:H	2.08	0.57
1:B:759:LEU:CD1	1:B:764:TYR:HB2	2.35	0.57
1:C:504:ILE:HG22	1:C:505:GLY:N	2.19	0.57
1:E:288:GLU:CB	1:E:289:PRO:HD3	2.31	0.57
1:F:15:VAL:HG12	1:F:16:GLY:N	2.19	0.57
1:A:202:PRO:O	1:A:203:LEU:C	2.43	0.57
1:F:371:ILE:CD1	1:F:380:VAL:HG22	2.33	0.57
1:B:497:GLU:OE2	1:B:741:GLU:HB3	2.05	0.57
1:B:35:LYS:HE2	1:B:90:LYS:HD2	1.87	0.57
1:F:494:VAL:HG22	1:F:738:VAL:HG22	1.86	0.57
1:A:384:SER:HA	1:A:388:VAL:HG23	1.86	0.57
1:C:127:PRO:HB3	1:C:312:THR:CG2	2.28	0.56
1:A:502:SER:O	1:A:503:VAL:HG13	2.05	0.56
1:D:111:ASP:HB3	1:D:172:ARG:NH1	2.14	0.56
1:B:127:PRO:HB3	1:B:312:THR:HG22	1.87	0.56
1:E:189:ARG:HB3	1:E:191:TYR:CE2	2.40	0.56
1:C:105:ASP:CG	1:C:139:THR:HG23	2.25	0.56
1:B:19:PRO:HG3	1:B:174:TYR:HD1	1.69	0.56
1:A:24:ILE:HG23	1:A:56:PHE:CE1	2.40	0.56
1:E:457:ILE:HG22	1:E:458:ALA:H	1.70	0.56
1:D:760:TYR:HE2	1:D:767:LYS:HG2	1.70	0.56
1:A:269:GLU:HB2	1:A:378:ARG:CZ	2.35	0.56
1:A:759:LEU:O	1:A:762:GLU:HB2	2.04	0.56
1:D:380:VAL:HG21	1:D:740:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:MSE:HG3	1:C:424:TYR:CE1	2.40	0.56
1:F:582:VAL:HG13	1:F:627:ARG:HG2	1.88	0.56
1:D:495:MSE:HE2	1:D:755:PHE:HZ	1.68	0.56
1:E:331:ASN:ND2	1:E:337:MSE:HA	2.17	0.56
1:A:335:MSE:CE	1:A:430:LYS:HG3	2.32	0.56
1:A:171:ASN:HD21	1:A:173:ARG:HB2	1.70	0.56
1:F:301:HIS:CD2	1:F:302:THR:H	2.22	0.56
1:A:102:ILE:CD1	1:A:144:LEU:HG	2.34	0.56
1:A:144:LEU:HD23	1:A:146:TYR:H	1.69	0.56
1:F:140:ILE:HB	1:F:152:THR:HG22	1.87	0.56
1:F:192:THR:C	1:F:194:ASP:H	2.08	0.56
1:C:654:PRO:HG2	1:C:661:ARG:HB2	1.88	0.56
1:E:122:LYS:HE3	1:E:161:PHE:CZ	2.39	0.56
1:F:488:TYR:O	1:F:492:ALA:HB2	2.04	0.56
1:E:306:MSE:HE1	1:E:309:TYR:HE2	1.70	0.56
1:E:737:HIS:O	1:E:738:VAL:C	2.44	0.56
1:C:286:LYS:HE3	1:C:290:PHE:HA	1.88	0.56
1:F:381:ILE:HG22	1:F:717:TYR:CE1	2.40	0.56
1:D:665:LEU:O	1:D:669:ILE:HG13	2.05	0.56
1:E:408:MSE:HG3	1:E:424:TYR:HE1	1.69	0.56
1:A:612:GLY:O	1:A:616:ASP:HB2	2.06	0.56
1:A:5:HIS:CE1	1:A:43:GLU:HG2	2.40	0.56
1:B:689:LEU:O	1:B:693:PHE:HB2	2.04	0.56
1:D:567:ILE:HG12	1:D:600:ALA:HB1	1.85	0.56
1:A:398:TYR:HB2	1:A:454:ASP:OD2	2.05	0.56
1:D:756:LEU:O	1:D:759:LEU:HB3	2.05	0.56
1:B:296:LEU:HD12	1:B:296:LEU:H	1.70	0.56
1:E:756:LEU:O	1:E:759:LEU:HB3	2.05	0.56
1:C:126:TYR:CD1	1:C:182:PRO:HG3	2.40	0.56
1:C:683:TYR:CZ	1:C:687:LEU:HD11	2.40	0.56
1:E:341:ASN:O	1:E:344:ALA:HB3	2.05	0.56
1:C:18:ARG:HH21	1:C:36:ASN:HD22	1.53	0.56
1:A:136:PRO:HG3	1:A:360:ARG:NH1	2.21	0.56
1:B:398:TYR:HB2	1:B:454:ASP:CG	2.26	0.56
1:E:365:ARG:O	1:E:423:GLN:HG2	2.06	0.56
1:F:497:GLU:OE2	1:F:741:GLU:HB3	2.06	0.56
1:E:379:ALA:HB3	1:E:744:ARG:NH1	2.20	0.56
1:E:690:ALA:HB2	1:E:721:ILE:HG23	1.86	0.56
1:E:215:ILE:HG12	1:E:353:ASP:OD2	2.04	0.56
1:B:504:ILE:O	1:B:709:VAL:HA	2.06	0.56
1:C:137:ARG:O	1:C:141:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:ASP:O	1:D:620:VAL:HG23	2.05	0.56
1:E:633:GLU:N	1:E:634:PRO:CD	2.69	0.56
1:E:224:ILE:CG1	1:E:338:VAL:HG13	2.36	0.56
1:A:153:MSE:HE1	1:A:360:ARG:HD3	1.86	0.56
1:F:104:PRO:HD3	1:F:390:LEU:HD21	1.86	0.56
1:A:137:ARG:O	1:A:141:ILE:HG13	2.06	0.56
1:A:552:TYR:CZ	1:A:627:ARG:HD2	2.41	0.56
1:E:34:VAL:HB	1:E:87:TYR:OH	2.04	0.56
1:A:108:ILE:CG1	1:A:311:GLY:H	2.18	0.56
1:A:281:ILE:HG12	1:A:306:MSE:CG	2.32	0.56
1:B:215:ILE:HG12	1:B:353:ASP:OD2	2.05	0.56
1:F:653:VAL:HG13	1:F:692:ALA:CB	2.30	0.56
1:E:181:CYS:SG	1:E:182:PRO:N	2.79	0.56
1:B:148:ARG:CZ	1:B:158:MSE:HG3	2.35	0.56
1:D:561:LEU:HB2	1:D:570:LEU:HD11	1.88	0.56
1:A:522:GLY:HA3	1:A:611:THR:HG23	1.87	0.56
1:F:461:HIS:CE1	1:F:463:ALA:HB3	2.40	0.56
1:B:678:PRO:HG2	1:B:679:ALA:H	1.71	0.56
1:C:545:GLY:HA3	1:C:548:LEU:HD12	1.88	0.56
1:F:500:LEU:HD13	1:F:503:VAL:HG11	1.87	0.56
1:A:487:HIS:CE1	1:A:512:GLY:HA3	2.40	0.56
1:D:339:LYS:HG3	1:D:365:ARG:NH1	2.21	0.56
1:C:310:ALA:O	1:C:313:HIS:HB2	2.06	0.56
1:D:330:ALA:O	1:D:338:VAL:HG12	2.05	0.56
1:D:401:LEU:HD12	1:D:402:ALA:H	1.71	0.56
1:B:464:TYR:HB2	1:B:467:THR:HG23	1.86	0.56
1:C:629:HIS:HB2	1:C:633:GLU:OE1	2.06	0.56
1:B:498:LYS:HB2	1:B:500:LEU:HD23	1.88	0.56
1:F:344:ALA:HA	1:F:348:LEU:HD13	1.87	0.56
1:D:331:ASN:ND2	1:D:337:MSE:HA	2.13	0.56
1:C:457:ILE:CG2	1:C:753:GLN:HB3	2.34	0.56
1:E:558:MSE:HE1	1:E:593:ASN:OD1	2.06	0.56
1:A:236:VAL:CG1	1:A:295:ASN:HD22	2.18	0.56
1:F:409:ASN:O	1:F:425:ILE:HG12	2.06	0.56
1:D:228:CYS:SG	1:D:229:ASP:N	2.79	0.56
1:A:540:TYR:HD1	1:A:540:TYR:H	1.53	0.56
1:B:261:LYS:HE2	1:B:266:VAL:HG21	1.88	0.56
1:B:655:VAL:HG22	1:B:660:ILE:HG23	1.88	0.56
1:A:491:ILE:HG12	1:A:527:LEU:HD12	1.87	0.56
1:C:286:LYS:HZ2	1:C:291:PRO:HD2	1.71	0.56
1:A:226:LEU:HD11	1:A:348:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:ARG:HB2	1:B:629:HIS:CE1	2.41	0.56
1:F:756:LEU:HD21	1:F:770:LEU:CD2	2.36	0.56
1:B:171:ASN:HD21	1:B:173:ARG:HB2	1.71	0.56
1:F:123:ARG:HH22	1:F:173:ARG:HG2	1.71	0.56
1:E:678:PRO:HG2	1:E:679:ALA:H	1.71	0.56
1:E:708:ASN:HB3	1:E:734:LEU:O	2.05	0.56
1:B:485:GLN:OE1	1:B:514:GLY:HA2	2.06	0.56
1:B:503:VAL:O	1:B:527:LEU:HD12	2.06	0.56
1:C:524:VAL:HG23	1:C:535:LEU:HB2	1.88	0.56
1:C:282:ILE:HG22	1:C:305:VAL:HB	1.88	0.56
1:C:379:ALA:HB3	1:C:744:ARG:NH1	2.21	0.56
1:A:189:ARG:O	1:A:356:LEU:HD12	2.06	0.56
1:D:504:ILE:HD12	1:D:701:ALA:HA	1.88	0.56
1:B:413:VAL:HG21	1:B:448:LEU:HD13	1.86	0.56
1:C:650:LYS:HD2	1:C:691:ARG:NH2	2.21	0.56
1:A:37:LEU:HB3	1:A:41:GLY:HA3	1.88	0.56
1:B:434:LEU:HD13	1:B:465:ASN:HB3	1.87	0.55
1:E:700:ARG:HD2	1:E:704:PHE:CE2	2.41	0.55
1:B:524:VAL:HG23	1:B:535:LEU:HB2	1.88	0.55
1:D:312:THR:HA	1:D:315:ILE:HG22	1.89	0.55
1:C:516:ASP:HB2	1:C:518:ASN:ND2	2.21	0.55
1:C:269:GLU:O	1:C:272:GLU:HB3	2.06	0.55
1:C:219:LYS:NZ	1:C:362:ILE:HG12	2.20	0.55
1:C:102:ILE:HD11	1:C:144:LEU:HG	1.88	0.55
1:A:364:ASN:HD21	1:A:443:HIS:CD2	2.24	0.55
1:C:582:VAL:HG11	1:C:626:TYR:O	2.05	0.55
1:D:506:ILE:HB	1:D:711:LEU:HD12	1.87	0.55
1:E:380:VAL:HG12	1:E:382:ARG:H	1.71	0.55
1:D:370:VAL:HG23	1:D:381:ILE:CG1	2.37	0.55
1:C:525:LEU:HD23	1:C:534:ARG:HA	1.88	0.55
1:C:225:HIS:NE2	1:C:327:MSE:HE3	2.21	0.55
1:A:371:ILE:CD1	1:A:380:VAL:HG22	2.35	0.55
1:A:456:ILE:CG2	1:A:457:ILE:H	2.16	0.55
1:F:53:ILE:HG23	1:F:54:GLU:HG3	1.89	0.55
1:A:247:GLN:NE2	1:A:637:LYS:HE3	2.20	0.55
1:E:610:SER:O	1:E:614:VAL:HG23	2.07	0.55
1:C:561:LEU:HB2	1:C:570:LEU:HD11	1.88	0.55
1:C:665:LEU:O	1:C:669:ILE:HG13	2.07	0.55
1:E:401:LEU:O	1:E:456:ILE:HA	2.07	0.55
1:C:628:ARG:NH2	1:C:632:GLY:H	2.03	0.55
1:B:587:TYR:HD1	1:B:588:GLY:N	2.00	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ILE:HA	1:D:371:ILE:O	2.06	0.55
1:C:522:GLY:CA	1:C:611:THR:HG23	2.36	0.55
1:F:218:ILE:C	1:F:224:ILE:HG23	2.27	0.55
1:F:22:TYR:CE1	1:F:87:TYR:HB3	2.40	0.55
1:A:190:LEU:HD13	1:A:356:LEU:HD13	1.88	0.55
1:B:580:LYS:HG2	1:B:593:ASN:HD22	1.71	0.55
1:D:624:VAL:HG12	1:D:637:LYS:HD3	1.87	0.55
1:E:338:VAL:HG21	1:E:344:ALA:HA	1.88	0.55
1:C:339:LYS:HG3	1:C:365:ARG:HH12	1.70	0.55
1:C:554:LEU:HG	1:C:558:MSE:HE3	1.88	0.55
1:F:737:HIS:O	1:F:738:VAL:C	2.44	0.55
1:B:527:LEU:HD12	1:B:527:LEU:H	1.72	0.55
1:C:268:PRO:HG2	1:C:269:GLU:OE1	2.06	0.55
1:C:102:ILE:HG23	1:C:141:ILE:CD1	2.37	0.55
1:E:582:VAL:HG13	1:E:626:TYR:HB3	1.88	0.55
1:F:286:LYS:HB2	1:F:303:ILE:HD12	1.87	0.55
1:E:225:HIS:HA	1:E:330:ALA:CB	2.37	0.55
1:F:253:MSE:O	1:F:317:PHE:HZ	1.89	0.55
1:F:397:GLU:HB2	1:F:416:ASN:HA	1.88	0.55
1:F:8:VAL:HG12	1:F:12:VAL:HG11	1.88	0.55
1:C:219:LYS:HA	1:C:224:ILE:CB	2.35	0.55
1:F:580:LYS:HZ1	1:F:590:VAL:HG22	1.71	0.55
1:E:196:GLN:HG2	1:E:197:GLU:O	2.07	0.55
1:C:601:LYS:HD3	1:F:772:LEU:HD11	1.87	0.55
1:D:24:ILE:HG12	1:D:56:PHE:HD1	1.72	0.55
1:C:196:GLN:HG2	1:C:197:GLU:O	2.07	0.55
1:D:125:MSE:O	1:D:127:PRO:HD3	2.06	0.55
1:F:14:ALA:HB3	1:F:103:PRO:CD	2.36	0.55
1:B:123:ARG:HH22	1:B:173:ARG:HG2	1.72	0.55
1:D:457:ILE:HG21	1:D:753:GLN:HB3	1.89	0.55
1:D:522:GLY:HA2	1:D:611:THR:HG23	1.88	0.55
1:B:3:ALA:HB2	1:B:47:GLU:HA	1.89	0.55
1:F:406:GLU:HG3	1:F:407:LEU:HG	1.89	0.55
1:A:498:LYS:HE3	1:A:736:PHE:HB2	1.89	0.55
1:B:294:GLU:HG2	1:B:294:GLU:O	2.07	0.55
1:A:580:LYS:HZ2	1:A:590:VAL:HG13	1.71	0.55
1:B:491:ILE:CG2	1:B:527:LEU:HD11	2.36	0.55
1:A:216:VAL:HG23	1:A:354:TYR:C	2.27	0.55
1:F:665:LEU:HG	1:F:669:ILE:HD11	1.88	0.55
1:E:515:THR:O	1:E:516:ASP:HB2	2.05	0.55
1:E:330:ALA:O	1:E:338:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ARG:NH2	1:C:173:ARG:HE	2.05	0.55
1:F:399:ASN:HA	1:F:414:ALA:O	2.06	0.55
1:B:142:GLU:O	1:B:143:ASP:HB3	2.07	0.55
1:F:193:SER:O	1:F:194:ASP:CB	2.54	0.55
1:A:572:GLY:O	1:A:575:ASN:HB2	2.07	0.55
1:E:128:PHE:CD1	1:E:186:PRO:HG2	2.41	0.55
1:F:501:ASP:O	1:F:503:VAL:HG13	2.07	0.55
1:B:749:VAL:O	1:B:753:GLN:HG3	2.06	0.55
1:A:742:VAL:HG11	1:A:751:VAL:HG11	1.88	0.55
1:A:727:LYS:HZ1	1:C:287:LYS:HE3	1.71	0.55
1:A:408:MSE:HG3	1:A:424:TYR:CE1	2.41	0.55
1:B:738:VAL:HB	1:B:744:ARG:HG3	1.87	0.55
1:E:582:VAL:HG11	1:E:626:TYR:O	2.06	0.55
1:C:15:VAL:HG21	1:C:67:LEU:O	2.06	0.55
1:C:249:PRO:HG3	1:C:300:LEU:CD1	2.37	0.55
1:E:508:LEU:CD2	1:E:611:THR:HG21	2.37	0.55
1:E:649:LEU:HB3	1:E:684:SER:CB	2.36	0.55
1:A:522:GLY:CA	1:A:611:THR:HG23	2.37	0.55
1:A:193:SER:O	1:A:194:ASP:CB	2.54	0.55
1:F:494:VAL:HG11	1:F:710:ALA:HB1	1.88	0.55
1:C:670:LEU:HA	1:C:673:ILE:HG12	1.89	0.55
1:B:664:GLU:O	1:B:667:GLN:HB3	2.07	0.55
1:D:57:ILE:HG13	1:D:75:LYS:NZ	2.22	0.55
1:E:562:SER:HB3	1:E:599:LEU:HD11	1.88	0.55
1:B:11:ILE:O	1:B:11:ILE:HG23	2.07	0.55
1:B:252:ILE:HG23	1:B:325:TYR:O	2.07	0.55
1:B:707:LYS:HG3	1:B:708:ASN:ND2	2.22	0.55
1:D:401:LEU:HD12	1:D:402:ALA:N	2.22	0.55
1:C:500:LEU:HD13	1:C:736:PHE:CE2	2.42	0.55
1:E:147:ASP:HA	1:E:177:GLU:OE2	2.07	0.55
1:D:737:HIS:O	1:D:738:VAL:C	2.46	0.55
1:F:503:VAL:HG11	1:F:708:ASN:OD1	2.07	0.55
1:B:53:ILE:O	1:B:57:ILE:HG12	2.07	0.55
1:B:224:ILE:HG12	1:B:338:VAL:O	2.06	0.55
1:C:315:ILE:HG23	1:C:316:LEU:N	2.22	0.55
1:D:119:PRO:HA	1:D:124:TYR:CD2	2.42	0.55
1:B:525:LEU:HA	1:B:535:LEU:HD13	1.88	0.55
1:C:369:SER:HB2	1:C:385:ARG:HB3	1.88	0.55
1:F:545:GLY:HA3	1:F:548:LEU:HD12	1.89	0.55
1:C:67:LEU:HD11	1:C:106:ILE:HD11	1.89	0.55
1:E:538:ILE:HD11	1:E:611:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:TYR:HB2	1:B:454:ASP:OD2	2.07	0.55
1:F:20:PHE:HE1	1:F:60:LEU:HA	1.73	0.55
1:C:142:GLU:HB2	1:C:150:ASN:O	2.07	0.55
1:A:651:PHE:HB2	1:A:688:ALA:CB	2.36	0.55
1:F:239:LEU:HD22	1:F:250:PHE:CZ	2.42	0.54
1:A:724:MSE:O	1:A:728:VAL:HG23	2.07	0.54
1:A:282:ILE:HA	1:A:371:ILE:O	2.07	0.54
1:B:583:GLU:OE1	1:B:583:GLU:N	2.40	0.54
1:E:155:GLU:O	1:E:157:PRO:HD3	2.07	0.54
1:C:114:ARG:O	1:C:118:ASP:HB2	2.07	0.54
1:A:245:ARG:NE	1:A:248:LYS:HB3	2.22	0.54
1:F:237:ALA:HA	1:F:295:ASN:ND2	2.21	0.54
1:F:265:TYR:CD2	1:F:265:TYR:N	2.75	0.54
1:B:528:GLY:O	1:B:529:TYR:C	2.45	0.54
1:F:320:SER:O	1:F:321:LYS:C	2.46	0.54
1:B:124:TYR:CE2	1:B:125:MSE:HG2	2.42	0.54
1:B:213:GLY:CA	1:B:235:VAL:HG11	2.36	0.54
1:F:261:LYS:HZ3	1:F:266:VAL:HB	1.68	0.54
1:C:102:ILE:HD12	1:C:141:ILE:HG21	1.89	0.54
1:A:247:GLN:HE21	1:A:298:PRO:HG2	1.72	0.54
1:E:616:ASP:HA	1:E:634:PRO:HB2	1.90	0.54
1:B:35:LYS:HG2	1:B:36:ASN:N	2.22	0.54
1:D:140:ILE:HB	1:D:152:THR:CG2	2.38	0.54
1:F:506:ILE:HD11	1:F:697:ALA:HB2	1.88	0.54
1:A:494:VAL:HG11	1:A:710:ALA:HB1	1.89	0.54
1:D:315:ILE:HG12	1:D:319:TRP:CZ3	2.40	0.54
1:F:190:LEU:HD21	1:F:206:ALA:CB	2.32	0.54
1:D:601:LYS:CB	1:D:603:ILE:HG13	2.38	0.54
1:D:593:ASN:O	1:D:596:LEU:HB2	2.08	0.54
1:C:586:LYS:CB	1:C:627:ARG:HH12	2.20	0.54
1:E:565:TYR:HB3	1:E:569:GLU:HB2	1.90	0.54
1:A:558:MSE:HB3	1:A:570:LEU:HD21	1.89	0.54
1:C:227:ALA:HA	1:C:326:VAL:O	2.07	0.54
1:D:383:ARG:HG3	1:D:383:ARG:HH11	1.71	0.54
1:A:649:LEU:HB3	1:A:684:SER:CB	2.37	0.54
1:A:61:TYR:CZ	1:A:73:ILE:HD12	2.42	0.54
1:C:553:PRO:HB2	1:C:620:VAL:HG21	1.87	0.54
1:F:232:ASN:HB3	1:F:235:VAL:HG22	1.88	0.54
1:D:655:VAL:HG22	1:D:660:ILE:HG12	1.89	0.54
1:F:114:ARG:HG2	1:F:118:ASP:OD2	2.06	0.54
1:D:711:LEU:HD23	1:D:737:HIS:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:391:PRO:HB3	1:F:420:TYR:CE1	2.42	0.54
1:F:729:VAL:HB	1:F:735:ASN:ND2	2.23	0.54
1:E:273:GLU:HG2	1:E:371:ILE:HD13	1.88	0.54
1:B:484:VAL:HG12	1:B:770:LEU:HD13	1.89	0.54
1:F:215:ILE:HG21	1:F:239:LEU:HD12	1.90	0.54
1:F:341:ASN:ND2	1:F:357:LEU:HB3	2.22	0.54
1:C:370:VAL:HG23	1:C:381:ILE:HD11	1.88	0.54
1:A:317:PHE:CE2	1:A:323:PRO:HA	2.42	0.54
1:C:19:PRO:O	1:C:23:ARG:HG3	2.08	0.54
1:A:385:ARG:HG3	1:A:386:GLY:N	2.22	0.54
1:D:140:ILE:HB	1:D:152:THR:HG22	1.89	0.54
1:E:434:LEU:HD13	1:E:465:ASN:HB3	1.90	0.54
1:A:35:LYS:HG2	1:A:36:ASN:H	1.72	0.54
1:D:628:ARG:CZ	1:D:632:GLY:H	2.20	0.54
1:F:739:THR:HG23	1:F:741:GLU:H	1.71	0.54
1:C:738:VAL:CG2	1:C:744:ARG:HB3	2.37	0.54
1:F:369:SER:HB2	1:F:385:ARG:CB	2.37	0.54
1:B:374:VAL:HG11	1:B:744:ARG:NH2	2.22	0.54
1:B:406:GLU:O	1:B:428:THR:HG23	2.07	0.54
1:E:580:LYS:HG3	1:E:593:ASN:ND2	2.20	0.54
1:F:651:PHE:HB2	1:F:688:ALA:HB2	1.89	0.54
1:D:484:VAL:HG12	1:D:770:LEU:HD22	1.90	0.54
1:E:50:GLU:O	1:E:53:ILE:HG22	2.08	0.54
1:F:495:MSE:HE2	1:F:755:PHE:CZ	2.42	0.54
1:B:465:ASN:O	1:B:468:LYS:HB3	2.08	0.54
1:A:370:VAL:HG23	1:A:381:ILE:HD11	1.88	0.54
1:D:553:PRO:HB2	1:D:620:VAL:CG2	2.38	0.54
1:E:504:ILE:O	1:E:709:VAL:HA	2.06	0.54
1:E:339:LYS:HA	1:E:362:ILE:HD11	1.90	0.54
1:B:682:ALA:O	1:B:686:HIS:HB2	2.07	0.54
1:A:8:VAL:HA	1:A:72:ARG:O	2.08	0.54
1:C:215:ILE:HD11	1:C:352:ALA:HA	1.89	0.54
1:A:282:ILE:HD12	1:A:371:ILE:HG23	1.89	0.54
1:F:554:LEU:HD11	1:F:579:PRO:CB	2.36	0.54
1:B:183:VAL:HG23	1:B:184:CYS:N	2.23	0.54
1:E:312:THR:O	1:E:315:ILE:HG22	2.08	0.54
1:D:371:ILE:HB	1:D:380:VAL:HG13	1.90	0.54
1:F:103:PRO:HG2	1:F:137:ARG:HD2	1.89	0.54
1:F:21:VAL:HG12	1:F:87:TYR:OH	2.08	0.54
1:B:403:VAL:HG11	1:B:466:THR:HB	1.90	0.54
1:C:66:PRO:CD	1:C:133:ASN:HB3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:GLY:CA	1:D:611:THR:HG23	2.38	0.54
1:D:564:VAL:HG11	1:D:667:GLN:HG2	1.90	0.54
1:B:1:MSE:HE3	1:B:2:LYS:N	2.23	0.54
1:F:225:HIS:HA	1:F:330:ALA:CB	2.33	0.54
1:C:215:ILE:HG12	1:C:353:ASP:OD2	2.07	0.54
1:A:219:LYS:HG2	1:A:358:HIS:CE1	2.42	0.54
1:D:103:PRO:HG2	1:D:137:ARG:HD2	1.90	0.54
1:B:553:PRO:HB2	1:B:620:VAL:HG21	1.90	0.54
1:A:395:PRO:HG2	1:A:396:PHE:CE2	2.44	0.54
1:F:422:SER:HA	1:F:444:PHE:CZ	2.43	0.54
1:D:488:TYR:O	1:D:756:LEU:HD11	2.08	0.53
1:B:520:TRP:HA	1:B:609:SER:OG	2.08	0.53
1:D:252:ILE:N	1:D:252:ILE:HD12	2.23	0.53
1:F:12:VAL:HG23	1:F:17:PHE:CD2	2.44	0.53
1:A:197:GLU:HG2	1:A:201:ASP:OD2	2.08	0.53
1:B:729:VAL:HB	1:B:735:ASN:ND2	2.23	0.53
1:E:252:ILE:N	1:E:252:ILE:HD12	2.23	0.53
1:C:570:LEU:HD12	1:C:573:VAL:CG1	2.38	0.53
1:D:126:TYR:OH	1:D:185:GLY:HA3	2.08	0.53
1:B:596:LEU:HD23	1:B:596:LEU:O	2.08	0.53
1:B:267:SER:O	1:B:270:GLU:HB3	2.07	0.53
1:C:504:ILE:HG23	1:C:525:LEU:O	2.08	0.53
1:C:264:ALA:CB	1:C:286:LYS:HA	2.38	0.53
1:D:565:TYR:HB3	1:D:569:GLU:HB3	1.90	0.53
1:C:152:THR:HG21	1:C:360:ARG:HG3	1.90	0.53
1:E:267:SER:HB2	1:E:270:GLU:CB	2.39	0.53
1:C:404:GLY:HA2	1:C:753:GLN:HE22	1.70	0.53
1:C:18:ARG:NH2	1:C:36:ASN:HD22	2.06	0.53
1:F:497:GLU:OE2	1:F:739:THR:HG22	2.08	0.53
1:B:485:GLN:HB3	1:B:488:TYR:HB2	1.91	0.53
1:B:286:LYS:HE3	1:B:290:PHE:HB2	1.91	0.53
1:D:381:ILE:HG13	1:D:382:ARG:N	2.24	0.53
1:A:410:ALA:HB3	1:A:747:ASN:O	2.07	0.53
1:E:205:LYS:O	1:E:209:LEU:HD13	2.08	0.53
1:B:662:VAL:O	1:B:665:LEU:HB3	2.08	0.53
1:D:288:GLU:HB3	1:D:289:PRO:CD	2.30	0.53
1:B:330:ALA:O	1:B:338:VAL:HG12	2.08	0.53
1:A:374:VAL:CG2	1:A:744:ARG:HH12	2.22	0.53
1:D:196:GLN:HG2	1:D:197:GLU:N	2.23	0.53
1:C:380:VAL:HG12	1:C:381:ILE:H	1.74	0.53
1:C:587:TYR:CZ	1:F:468:LYS:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:581:ALA:HA	1:E:584:SER:HB3	1.90	0.53
1:F:760:TYR:HA	1:F:765:LEU:HB3	1.89	0.53
1:F:724:MSE:O	1:F:728:VAL:HG23	2.08	0.53
1:D:653:VAL:HG11	1:D:689:LEU:HA	1.90	0.53
1:B:620:VAL:HG22	1:B:625:ALA:O	2.09	0.53
1:E:613:ARG:HA	1:E:616:ASP:OD1	2.09	0.53
1:D:524:VAL:CG2	1:D:536:ALA:H	2.22	0.53
1:B:115:GLU:HG2	1:B:121:ASN:ND2	2.24	0.53
1:B:461:HIS:CE1	1:B:463:ALA:HB3	2.43	0.53
1:D:261:LYS:HZ3	1:D:266:VAL:HB	1.73	0.53
1:F:708:ASN:HB3	1:F:734:LEU:O	2.08	0.53
1:B:456:ILE:CG2	1:B:457:ILE:H	2.09	0.53
1:B:292:LEU:HD11	1:B:324:VAL:HG21	1.89	0.53
1:F:487:HIS:O	1:F:491:ILE:HG12	2.08	0.53
1:F:19:PRO:HG3	1:F:174:TYR:O	2.09	0.53
1:D:549:ALA:HA	1:D:555:ARG:HB2	1.89	0.53
1:F:560:ILE:HD12	1:F:561:LEU:N	2.24	0.53
1:F:580:LYS:NZ	1:F:590:VAL:HG22	2.23	0.53
1:B:331:ASN:ND2	1:B:337:MSE:HA	2.18	0.53
1:D:110:ASP:O	1:D:113:LEU:HB3	2.09	0.53
1:A:267:SER:HB3	1:A:268:PRO:HD2	1.90	0.53
1:E:387:PHE:O	1:E:390:LEU:HG	2.08	0.53
1:B:756:LEU:O	1:B:759:LEU:HB3	2.08	0.53
1:D:320:SER:O	1:D:321:LYS:C	2.47	0.53
1:D:190:LEU:HD13	1:D:356:LEU:HD13	1.90	0.53
1:F:219:LYS:HG3	1:F:224:ILE:HG12	1.89	0.53
1:C:258:GLU:O	1:C:261:LYS:HG2	2.09	0.53
1:D:104:PRO:HB3	1:D:387:PHE:O	2.09	0.53
1:D:247:GLN:NE2	1:D:637:LYS:HE3	2.23	0.53
1:E:126:TYR:CD1	1:E:182:PRO:HG3	2.43	0.53
1:F:33:TYR:OH	1:F:90:LYS:HE3	2.09	0.53
1:E:613:ARG:HA	1:E:613:ARG:NE	2.22	0.53
1:C:468:LYS:HG3	1:F:587:TYR:OH	2.08	0.53
1:D:274:LEU:HB3	1:D:307:LEU:HD11	1.90	0.53
1:D:339:LYS:HA	1:D:362:ILE:HD11	1.90	0.53
1:C:380:VAL:HG12	1:C:381:ILE:N	2.24	0.53
1:A:330:ALA:HB1	1:A:348:LEU:HD21	1.91	0.53
1:D:329:SER:HA	1:D:337:MSE:HE2	1.89	0.53
1:A:158:MSE:HE3	1:A:163:ARG:NH1	2.24	0.53
1:A:15:VAL:HG12	1:A:16:GLY:N	2.21	0.53
1:B:278:ARG:HG2	1:B:280:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:HG23	1:C:17:PHE:CG	2.42	0.53
1:B:487:HIS:CD2	1:B:520:TRP:HB3	2.44	0.53
1:B:264:ALA:HB1	1:B:285:ARG:O	2.09	0.53
1:A:468:LYS:HG3	1:B:587:TYR:OH	2.09	0.53
1:E:170:LEU:H	1:E:170:LEU:HD12	1.74	0.53
1:D:380:VAL:HG12	1:D:381:ILE:N	2.24	0.53
1:C:283:THR:HA	1:C:303:ILE:O	2.08	0.53
1:F:579:PRO:HB3	1:F:626:TYR:CE1	2.43	0.53
1:C:404:GLY:HA2	1:C:753:GLN:CD	2.29	0.53
1:E:216:VAL:HB	1:E:354:TYR:HB2	1.90	0.53
1:D:601:LYS:NZ	1:E:771:MSE:HE3	2.24	0.53
1:D:580:LYS:HG3	1:D:593:ASN:ND2	2.23	0.53
1:D:482:LEU:HD12	1:D:483:GLN:N	2.23	0.53
1:A:415:LYS:C	1:A:417:GLY:H	2.11	0.53
1:D:485:GLN:OE1	1:D:514:GLY:HA2	2.09	0.53
1:D:494:VAL:HG13	1:D:738:VAL:H	1.73	0.53
1:B:491:ILE:HD11	1:B:507:ALA:HB2	1.91	0.53
1:C:495:MSE:HE2	1:C:755:PHE:CZ	2.44	0.53
1:C:264:ALA:HB3	1:C:284:LEU:HD13	1.91	0.53
1:A:190:LEU:HB2	1:A:202:PRO:HB3	1.90	0.53
1:E:373:PHE:CE1	1:E:378:ARG:HB3	2.44	0.53
1:C:402:ALA:HB2	1:C:457:ILE:HB	1.89	0.53
1:A:438:ARG:HG2	1:A:438:ARG:HH11	1.74	0.53
1:E:661:ARG:HG3	1:E:663:GLU:OE2	2.08	0.53
1:A:633:GLU:H	1:A:634:PRO:HD2	1.73	0.53
1:A:543:LEU:HD12	1:A:549:ALA:CB	2.38	0.53
1:E:545:GLY:HA3	1:E:548:LEU:HB2	1.89	0.53
1:F:489:ALA:O	1:F:752:GLY:HA3	2.09	0.53
1:F:759:LEU:HD11	1:F:764:TYR:HB2	1.90	0.53
1:E:526:TYR:O	1:E:532:VAL:HG13	2.08	0.53
1:B:534:ARG:HG2	1:B:535:LEU:H	1.72	0.53
1:C:15:VAL:HG12	1:C:16:GLY:H	1.74	0.53
1:D:579:PRO:O	1:D:582:VAL:HG23	2.09	0.53
1:D:554:LEU:HD12	1:D:583:GLU:OE1	2.09	0.53
1:D:193:SER:O	1:D:194:ASP:CB	2.57	0.53
1:F:329:SER:HB2	1:F:331:ASN:ND2	2.24	0.53
1:F:39:ASP:H	1:F:144:LEU:HD13	1.74	0.53
1:E:572:GLY:O	1:E:575:ASN:HB2	2.09	0.53
1:C:239:LEU:HD22	1:C:250:PHE:HE1	1.74	0.53
1:A:156:PHE:CZ	1:A:186:PRO:HB3	2.44	0.53
1:A:687:LEU:HB3	1:A:724:MSE:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ALA:HB2	1:C:286:LYS:HA	1.90	0.52
1:E:191:TYR:HB2	1:E:355:PHE:CB	2.31	0.52
1:B:201:ASP:N	1:B:202:PRO:CD	2.71	0.52
1:E:200:GLY:C	1:E:202:PRO:HD2	2.28	0.52
1:A:312:THR:O	1:A:316:LEU:HB2	2.09	0.52
1:E:522:GLY:HA3	1:E:538:ILE:HD12	1.90	0.52
1:C:593:ASN:O	1:C:596:LEU:HB2	2.09	0.52
1:A:49:ARG:HD2	1:A:49:ARG:H	1.74	0.52
1:D:619:ALA:HB2	1:D:638:LEU:HB2	1.91	0.52
1:C:651:PHE:HB2	1:C:688:ALA:CB	2.39	0.52
1:D:509:ASP:CG	1:D:510:GLY:H	2.12	0.52
1:A:270:GLU:N	1:A:378:ARG:NH1	2.57	0.52
1:C:379:ALA:HB3	1:C:744:ARG:CZ	2.39	0.52
1:F:544:PRO:HG2	1:F:555:ARG:HE	1.75	0.52
1:F:57:ILE:HG13	1:F:75:LYS:HZ1	1.73	0.52
1:C:428:THR:HG21	1:C:466:THR:HG22	1.92	0.52
1:B:522:GLY:H	1:B:523:GLU:CD	2.12	0.52
1:D:603:ILE:HG23	1:E:516:ASP:HA	1.91	0.52
1:C:30:LEU:CD1	1:C:52:ASP:HB2	2.37	0.52
1:F:205:LYS:O	1:F:209:LEU:HD13	2.08	0.52
1:C:461:HIS:HE1	1:C:463:ALA:HB3	1.72	0.52
1:F:738:VAL:HB	1:F:744:ARG:HG2	1.91	0.52
1:E:617:ALA:O	1:E:621:LEU:HB2	2.09	0.52
1:F:503:VAL:HA	1:F:706:VAL:HG11	1.91	0.52
1:A:266:VAL:HA	1:A:270:GLU:OE2	2.09	0.52
1:A:267:SER:O	1:A:270:GLU:HB3	2.10	0.52
1:D:199:TYR:CG	1:D:200:GLY:N	2.77	0.52
1:D:183:VAL:HG23	1:D:184:CYS:N	2.24	0.52
1:C:402:ALA:CB	1:C:457:ILE:HB	2.39	0.52
1:F:447:ILE:O	1:F:447:ILE:HG22	2.08	0.52
1:B:565:TYR:HB3	1:B:569:GLU:HB3	1.92	0.52
1:F:192:THR:C	1:F:194:ASP:N	2.60	0.52
1:A:695:HIS:O	1:A:698:VAL:HB	2.09	0.52
1:F:148:ARG:CZ	1:F:158:MSE:HG3	2.39	0.52
1:B:381:ILE:HG13	1:B:382:ARG:N	2.23	0.52
1:F:459:ASP:OD2	1:F:486:HIS:HB2	2.09	0.52
1:E:391:PRO:HB3	1:E:420:TYR:CE1	2.45	0.52
1:B:524:VAL:CG2	1:B:536:ALA:H	2.23	0.52
1:D:201:ASP:N	1:D:202:PRO:CD	2.72	0.52
1:D:504:ILE:CG2	1:D:505:GLY:N	2.72	0.52
1:F:641:PHE:CZ	1:F:678:PRO:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ALA:HA	1:A:418:LYS:O	2.10	0.52
1:D:487:HIS:CD2	1:D:520:TRP:HB3	2.43	0.52
1:E:102:ILE:HG12	1:E:144:LEU:HD11	1.90	0.52
1:F:401:LEU:O	1:F:456:ILE:HA	2.08	0.52
1:D:21:VAL:HA	1:D:24:ILE:HG22	1.91	0.52
1:E:16:GLY:HA2	1:E:132:THR:OG1	2.08	0.52
1:D:218:ILE:O	1:D:224:ILE:HB	2.09	0.52
1:C:286:LYS:NZ	1:C:291:PRO:HD2	2.25	0.52
1:B:504:ILE:CG2	1:B:505:GLY:N	2.72	0.52
1:E:202:PRO:O	1:E:203:LEU:C	2.46	0.52
1:B:470:ALA:HB1	1:B:481:LEU:HD11	1.91	0.52
1:D:404:GLY:HA2	1:D:753:GLN:NE2	2.24	0.52
1:D:621:LEU:HD22	1:D:666:PHE:HD1	1.75	0.52
1:B:656:GLU:HG3	1:B:661:ARG:NH1	2.25	0.52
1:E:37:LEU:O	1:E:37:LEU:HD13	2.10	0.52
1:B:453:LEU:O	1:B:453:LEU:HG	2.09	0.52
1:B:371:ILE:HG13	1:B:380:VAL:HA	1.90	0.52
1:E:412:GLY:HA3	1:E:750:ASN:ND2	2.21	0.52
1:A:374:VAL:CG1	1:A:744:ARG:HH12	2.23	0.52
1:D:274:LEU:HB3	1:D:307:LEU:CD1	2.40	0.52
1:F:219:LYS:HE3	1:F:358:HIS:CE1	2.45	0.52
1:D:543:LEU:HD12	1:D:549:ALA:CB	2.39	0.52
1:B:385:ARG:HG3	1:B:386:GLY:H	1.75	0.52
1:D:541:TYR:CG	1:D:560:ILE:HG22	2.44	0.52
1:E:560:ILE:HD12	1:E:561:LEU:N	2.24	0.52
1:F:176:ALA:O	1:F:179:THR:HG22	2.10	0.52
1:D:385:ARG:HG3	1:D:386:GLY:H	1.75	0.52
1:E:364:ASN:HD21	1:E:443:HIS:CD2	2.27	0.52
1:F:485:GLN:NE2	1:F:487:HIS:H	1.86	0.52
1:D:78:ILE:O	1:D:80:PRO:HD3	2.09	0.52
1:F:300:LEU:HA	1:F:640:SER:OG	2.10	0.52
1:B:628:ARG:NH2	1:B:632:GLY:H	2.07	0.52
1:C:579:PRO:HB3	1:C:626:TYR:CE1	2.44	0.52
1:E:110:ASP:O	1:E:113:LEU:HB3	2.09	0.52
1:C:166:TYR:CE1	1:C:175:HIS:HA	2.44	0.52
1:F:402:ALA:HB2	1:F:457:ILE:HD12	1.92	0.52
1:B:594:VAL:HG12	1:B:594:VAL:O	2.10	0.52
1:E:279:ARG:HD3	1:E:307:LEU:HB2	1.91	0.52
1:C:207:ALA:HB1	1:C:320:SER:CB	2.34	0.52
1:C:269:GLU:HB2	1:C:378:ARG:NH1	2.24	0.52
1:F:369:SER:HB2	1:F:385:ARG:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:H	1:A:747:ASN:ND2	2.08	0.52
1:C:409:ASN:HD22	1:C:425:ILE:CD1	2.20	0.52
1:F:541:TYR:CE1	1:F:609:SER:HA	2.45	0.52
1:B:412:GLY:HA3	1:B:750:ASN:ND2	2.18	0.52
1:A:123:ARG:NE	1:A:173:ARG:NH2	2.58	0.52
1:F:429:GLY:HA2	1:F:465:ASN:HD22	1.75	0.52
1:A:105:ASP:CG	1:A:139:THR:HG23	2.30	0.52
1:A:690:ALA:HB2	1:A:721:ILE:HG23	1.91	0.52
1:D:451:LYS:HD3	1:D:477:LEU:HG	1.92	0.52
1:F:694:ALA:C	1:F:696:THR:H	2.13	0.52
1:C:489:ALA:HA	1:C:756:LEU:HD12	1.91	0.52
1:C:215:ILE:O	1:C:353:ASP:HB2	2.10	0.52
1:E:249:PRO:HG3	1:E:300:LEU:CD1	2.37	0.52
1:A:169:PRO:HA	1:A:174:TYR:CD2	2.45	0.52
1:B:32:GLY:H	1:B:87:TYR:HD2	1.57	0.52
1:A:447:ILE:HG22	1:A:447:ILE:O	2.10	0.52
1:C:666:PHE:HA	1:C:669:ILE:HD12	1.92	0.52
1:A:738:VAL:HG12	1:A:742:VAL:O	2.10	0.52
1:A:376:GLY:C	1:A:377:LYS:HG2	2.30	0.52
1:C:288:GLU:HB2	1:C:289:PRO:CD	2.32	0.52
1:A:199:TYR:CD1	1:A:200:GLY:N	2.76	0.52
1:D:691:ARG:HG2	1:D:695:HIS:CD2	2.45	0.52
1:E:269:GLU:HB2	1:E:378:ARG:CZ	2.40	0.52
1:D:226:LEU:HD21	1:D:351:VAL:HG12	1.91	0.52
1:E:183:VAL:CG2	1:E:184:CYS:N	2.73	0.52
1:B:729:VAL:HG12	1:B:729:VAL:O	2.10	0.52
1:E:247:GLN:HG3	1:E:298:PRO:CG	2.40	0.52
1:C:32:GLY:O	1:C:87:TYR:HA	2.09	0.52
1:D:403:VAL:HG11	1:D:466:THR:HB	1.92	0.52
1:A:254:ALA:HB1	1:A:259:THR:HB	1.92	0.52
1:F:332:TYR:HB3	1:F:333:PRO:HD2	1.91	0.52
1:D:18:ARG:HB2	1:D:19:PRO:HD3	1.91	0.51
1:E:306:MSE:HE1	1:E:368:ASP:OD2	2.10	0.51
1:C:396:PHE:CE2	1:C:759:LEU:HB2	2.44	0.51
1:C:370:VAL:CG2	1:C:381:ILE:HD11	2.41	0.51
1:C:751:VAL:HG13	1:C:752:GLY:N	2.25	0.51
1:A:284:LEU:HD12	1:A:284:LEU:O	2.10	0.51
1:A:348:LEU:N	1:A:348:LEU:HD12	2.24	0.51
1:C:105:ASP:OD1	1:C:139:THR:HG23	2.10	0.51
1:B:403:VAL:CG1	1:B:466:THR:HB	2.40	0.51
1:C:521:GLY:CA	1:C:610:SER:HA	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:SER:O	1:B:681:ILE:HG12	2.09	0.51
1:E:375:ASP:OD2	1:E:723:LYS:HA	2.10	0.51
1:B:229:ASP:OD1	1:B:322:THR:HG21	2.10	0.51
1:A:714:GLY:O	1:A:716:ALA:N	2.43	0.51
1:E:105:ASP:OD2	1:E:138:PHE:HB3	2.10	0.51
1:B:438:ARG:HG2	1:B:438:ARG:HH11	1.75	0.51
1:B:42:VAL:O	1:B:42:VAL:HG13	2.10	0.51
1:B:252:ILE:CG2	1:B:324:VAL:HB	2.41	0.51
1:C:408:MSE:HG3	1:C:424:TYR:HE1	1.75	0.51
1:B:15:VAL:CG1	1:B:67:LEU:HB2	2.41	0.51
1:A:383:ARG:NH2	1:A:392:ILE:HD11	2.24	0.51
1:B:505:GLY:HA2	1:B:710:ALA:H	1.76	0.51
1:D:558:MSE:HE2	1:D:574:ILE:HG13	1.93	0.51
1:E:247:GLN:OE1	1:E:637:LYS:HE3	2.10	0.51
1:C:584:SER:CB	1:C:589:LYS:HB3	2.39	0.51
1:F:127:PRO:HB2	1:F:188:TYR:HE2	1.75	0.51
1:C:111:ASP:CB	1:C:172:ARG:HH22	2.23	0.51
1:F:399:ASN:O	1:F:452:ASN:HB2	2.10	0.51
1:A:258:GLU:O	1:A:261:LYS:HB2	2.11	0.51
1:F:690:ALA:CB	1:F:721:ILE:HG23	2.39	0.51
1:E:168:ASP:OD1	1:E:169:PRO:HD2	2.10	0.51
1:E:88:ILE:HG22	1:E:89:GLU:N	2.26	0.51
1:D:381:ILE:HG22	1:D:717:TYR:CZ	2.45	0.51
1:F:8:VAL:C	1:F:9:GLN:HG3	2.30	0.51
1:D:603:ILE:HG22	1:D:604:ASN:N	2.25	0.51
1:B:620:VAL:C	1:B:622:LEU:N	2.63	0.51
1:D:169:PRO:HA	1:D:174:TYR:CD2	2.45	0.51
1:C:625:ALA:HB2	1:C:637:LYS:HD3	1.92	0.51
1:B:560:ILE:HD12	1:B:561:LEU:N	2.26	0.51
1:E:598:GLN:HG3	1:E:604:ASN:HD22	1.75	0.51
1:E:293:PRO:C	1:E:295:ASN:H	2.14	0.51
1:E:766:THR:OG1	1:E:769:ASP:HB2	2.10	0.51
1:E:497:GLU:OE2	1:E:741:GLU:HB3	2.10	0.51
1:E:31:ARG:HG2	1:E:85:ARG:O	2.10	0.51
1:F:707:LYS:O	1:F:733:GLY:HA3	2.11	0.51
1:B:296:LEU:CD1	1:B:296:LEU:H	2.23	0.51
1:F:488:TYR:CE1	1:F:525:LEU:HD13	2.46	0.51
1:A:215:ILE:HD12	1:A:226:LEU:HD23	1.91	0.51
1:A:286:LYS:HE3	1:A:291:PRO:HD2	1.92	0.51
1:E:199:TYR:CD1	1:E:200:GLY:N	2.79	0.51
1:E:593:ASN:O	1:E:596:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:VAL:HG13	1:D:692:ALA:CB	2.39	0.51
1:B:616:ASP:OD1	1:B:634:PRO:HG2	2.10	0.51
1:D:583:GLU:H	1:D:583:GLU:CD	2.13	0.51
1:D:209:LEU:HD23	1:D:354:TYR:CE2	2.45	0.51
1:F:523:GLU:OE2	1:F:537:HIS:HB2	2.09	0.51
1:F:221:ILE:HG22	1:F:360:ARG:NH2	2.26	0.51
1:F:613:ARG:HH22	1:F:628:ARG:NH2	2.09	0.51
1:C:497:GLU:OE2	1:C:741:GLU:HB3	2.10	0.51
1:F:495:MSE:SE	1:F:527:LEU:HD13	2.60	0.51
1:E:371:ILE:CD1	1:E:380:VAL:HG22	2.40	0.51
1:B:534:ARG:C	1:B:535:LEU:HD12	2.31	0.51
1:F:225:HIS:HB2	1:F:328:THR:O	2.10	0.51
1:D:253:MSE:HG2	1:D:317:PHE:HE1	1.75	0.51
1:D:697:ALA:HB1	1:D:709:VAL:HG11	1.93	0.51
1:C:181:CYS:SG	1:C:182:PRO:N	2.82	0.51
1:E:218:ILE:O	1:E:224:ILE:HB	2.11	0.51
1:F:124:TYR:CE2	1:F:125:MSE:HG2	2.45	0.51
1:D:434:LEU:HD11	1:D:465:ASN:O	2.10	0.51
1:C:383:ARG:HH11	1:C:383:ARG:HG3	1.76	0.51
1:F:253:MSE:HG2	1:F:317:PHE:CE1	2.45	0.51
1:F:374:VAL:HG21	1:F:744:ARG:NH2	2.26	0.51
1:A:519:THR:HB	1:A:608:ALA:HA	1.93	0.51
1:E:503:VAL:HB	1:E:708:ASN:O	2.09	0.51
1:F:138:PHE:HB2	1:F:389:PRO:HD3	1.92	0.51
1:B:404:GLY:HA2	1:B:753:GLN:NE2	2.26	0.51
1:F:485:GLN:OE1	1:F:514:GLY:HA2	2.10	0.51
1:F:491:ILE:CD1	1:F:525:LEU:HD12	2.41	0.51
1:E:12:VAL:HA	1:E:68:ALA:CB	2.40	0.51
1:C:487:HIS:CE1	1:C:512:GLY:HA3	2.45	0.51
1:F:106:ILE:HB	1:F:134:CYS:HA	1.93	0.51
1:F:267:SER:HB2	1:F:270:GLU:CB	2.39	0.51
1:E:690:ALA:CB	1:E:721:ILE:HG23	2.41	0.51
1:D:137:ARG:O	1:D:141:ILE:HG13	2.10	0.51
1:E:543:LEU:HD23	1:E:543:LEU:N	2.18	0.51
1:E:225:HIS:NE2	1:E:327:MSE:HE3	2.25	0.51
1:E:538:ILE:HG23	1:E:662:VAL:CG2	2.40	0.51
1:E:663:GLU:CD	1:E:663:GLU:H	2.13	0.51
1:A:66:PRO:HG2	1:A:67:LEU:H	1.76	0.51
1:A:649:LEU:HB3	1:A:684:SER:HB3	1.92	0.51
1:F:428:THR:HA	1:F:433:VAL:CG1	2.41	0.51
1:F:551:TYR:HA	1:F:628:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:739:THR:HG23	1:C:741:GLU:H	1.76	0.51
1:D:3:ALA:C	1:D:53:ILE:HD11	2.31	0.51
1:F:708:ASN:HD22	1:F:708:ASN:N	2.09	0.51
1:B:225:HIS:CA	1:B:330:ALA:HB2	2.28	0.51
1:B:526:TYR:HB3	1:B:535:LEU:HD11	1.93	0.51
1:C:729:VAL:HG11	1:C:735:ASN:HB3	1.91	0.51
1:C:738:VAL:HB	1:C:744:ARG:HG2	1.91	0.51
1:A:199:TYR:CG	1:A:200:GLY:N	2.79	0.51
1:E:153:MSE:SE	1:E:360:ARG:HD2	2.60	0.51
1:F:370:VAL:O	1:F:381:ILE:HG13	2.10	0.51
1:A:408:MSE:O	1:A:747:ASN:HA	2.11	0.51
1:C:144:LEU:HD23	1:C:145:PRO:HA	1.91	0.51
1:B:409:ASN:CG	1:B:425:ILE:HD11	2.30	0.51
1:D:598:GLN:HG3	1:D:604:ASN:HB2	1.93	0.51
1:D:210:ILE:HD11	1:D:227:ALA:C	2.31	0.51
1:E:9:GLN:NE2	1:E:40:ALA:HB1	2.25	0.51
1:D:424:TYR:C	1:D:426:GLY:H	2.13	0.51
1:D:655:VAL:HG11	1:D:696:THR:OG1	2.11	0.51
1:A:11:ILE:CG1	1:A:68:ALA:HA	2.32	0.51
1:A:554:LEU:HG	1:A:558:MSE:HE3	1.93	0.51
1:E:392:ILE:HB	1:E:419:VAL:HG12	1.93	0.51
1:D:204:ARG:HG2	1:D:319:TRP:CE2	2.46	0.51
1:B:614:VAL:HG13	1:B:666:PHE:CE2	2.46	0.51
1:B:127:PRO:O	1:B:311:GLY:HA3	2.11	0.51
1:F:543:LEU:HD12	1:F:549:ALA:CB	2.40	0.51
1:F:554:LEU:HG	1:F:620:VAL:HG11	1.92	0.51
1:B:544:PRO:HG2	1:B:555:ARG:HE	1.75	0.51
1:B:476:GLU:O	1:B:477:LEU:HB3	2.11	0.51
1:E:584:SER:CB	1:E:589:LYS:HB3	2.40	0.51
1:B:409:ASN:CB	1:B:425:ILE:HD11	2.41	0.51
1:E:633:GLU:H	1:E:634:PRO:CD	2.22	0.51
1:C:590:VAL:O	1:C:594:VAL:HG23	2.10	0.51
1:C:596:LEU:HD23	1:C:596:LEU:O	2.11	0.51
1:E:213:GLY:C	1:E:235:VAL:HG11	2.31	0.51
1:D:649:LEU:HB3	1:D:684:SER:HB3	1.92	0.51
1:D:57:ILE:HG21	1:D:75:LYS:HZ1	1.76	0.51
1:F:491:ILE:HD11	1:F:525:LEU:HD12	1.93	0.51
1:F:288:GLU:HB3	1:F:289:PRO:CD	2.32	0.51
1:D:33:TYR:HB2	1:D:88:ILE:O	2.11	0.51
1:A:580:LYS:HG3	1:A:593:ASN:ND2	2.26	0.51
1:E:274:LEU:C	1:E:276:SER:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ILE:HG12	1:D:306:MSE:HG2	1.91	0.51
1:C:286:LYS:HE3	1:C:290:PHE:HB3	1.93	0.51
1:A:196:GLN:HG2	1:A:197:GLU:N	2.26	0.51
1:A:424:TYR:C	1:A:426:GLY:H	2.14	0.51
1:A:406:GLU:O	1:A:428:THR:HG23	2.10	0.51
1:C:31:ARG:HG2	1:C:85:ARG:O	2.10	0.51
1:C:561:LEU:HB2	1:C:570:LEU:CD1	2.40	0.51
1:C:633:GLU:N	1:C:634:PRO:HD2	2.26	0.51
1:A:593:ASN:O	1:A:596:LEU:HB2	2.10	0.51
1:E:104:PRO:HD3	1:E:390:LEU:HD21	1.92	0.51
1:E:65:PRO:C	1:E:67:LEU:H	2.14	0.51
1:A:225:HIS:CA	1:A:330:ALA:HB2	2.39	0.51
1:A:410:ALA:HB2	1:A:747:ASN:OD1	2.11	0.51
1:D:492:ALA:O	1:D:495:MSE:HG2	2.11	0.51
1:E:190:LEU:HB2	1:E:202:PRO:CB	2.41	0.51
1:B:522:GLY:HA3	1:B:611:THR:HG23	1.93	0.51
1:A:476:GLU:C	1:A:478:ASP:H	2.13	0.51
1:D:523:GLU:HG3	1:D:537:HIS:CB	2.41	0.51
1:A:278:ARG:HG3	1:A:280:PRO:HD3	1.92	0.51
1:D:487:HIS:CE1	1:D:509:ASP:HB3	2.46	0.50
1:D:510:GLY:O	1:D:610:SER:HB2	2.11	0.50
1:F:504:ILE:HG22	1:F:505:GLY:H	1.75	0.50
1:A:589:LYS:HG3	1:A:590:VAL:HG23	1.92	0.50
1:A:491:ILE:HG12	1:A:527:LEU:CD1	2.40	0.50
1:C:534:ARG:HD3	1:C:537:HIS:CD2	2.46	0.50
1:A:455:LEU:HA	1:A:479:VAL:HG12	1.93	0.50
1:C:138:PHE:CG	1:C:389:PRO:HD3	2.45	0.50
1:B:624:VAL:O	1:B:625:ALA:CB	2.58	0.50
1:F:308:PRO:HA	1:F:313:HIS:HB3	1.93	0.50
1:D:612:GLY:HA2	1:D:615:LEU:HD12	1.93	0.50
1:D:751:VAL:HG13	1:D:752:GLY:N	2.26	0.50
1:B:264:ALA:HB2	1:B:286:LYS:HA	1.93	0.50
1:B:765:LEU:HD12	1:B:766:THR:H	1.76	0.50
1:D:252:ILE:HG23	1:D:325:TYR:O	2.11	0.50
1:C:488:TYR:CD1	1:C:525:LEU:HD13	2.46	0.50
1:C:522:GLY:HA3	1:C:611:THR:HG23	1.93	0.50
1:F:219:LYS:HB2	1:F:357:LEU:HA	1.93	0.50
1:A:209:LEU:HA	1:A:212:LYS:HB2	1.93	0.50
1:A:204:ARG:HG2	1:A:319:TRP:CE2	2.46	0.50
1:F:268:PRO:HG2	1:F:378:ARG:HH22	1.76	0.50
1:F:665:LEU:O	1:F:669:ILE:HG13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ILE:CG2	1:D:389:PRO:HG3	2.41	0.50
1:D:13:GLN:NE2	1:D:42:VAL:HG23	2.24	0.50
1:D:651:PHE:HB2	1:D:688:ALA:CB	2.42	0.50
1:A:543:LEU:N	1:A:543:LEU:HD23	2.26	0.50
1:A:373:PHE:CD2	1:A:378:ARG:HD3	2.46	0.50
1:B:381:ILE:HA	1:B:717:TYR:OH	2.10	0.50
1:E:385:ARG:HG3	1:E:386:GLY:N	2.26	0.50
1:B:419:VAL:HG11	1:B:751:VAL:HG23	1.92	0.50
1:A:376:GLY:HA2	1:A:726:ARG:HH11	1.74	0.50
1:C:261:LYS:HZ2	1:C:266:VAL:HB	1.75	0.50
1:A:252:ILE:HD12	1:A:252:ILE:N	2.25	0.50
1:A:281:ILE:HB	1:A:370:VAL:CG1	2.36	0.50
1:A:218:ILE:HD12	1:A:356:LEU:HD23	1.93	0.50
1:B:518:ASN:HB3	1:B:540:TYR:HE2	1.76	0.50
1:E:415:LYS:C	1:E:417:GLY:H	2.13	0.50
1:E:504:ILE:HG22	1:E:505:GLY:N	2.25	0.50
1:F:383:ARG:HG3	1:F:383:ARG:HH11	1.76	0.50
1:F:686:HIS:HE1	1:F:718:ASN:ND2	2.10	0.50
1:F:566:SER:H	1:F:569:GLU:HB3	1.77	0.50
1:C:504:ILE:HD12	1:C:701:ALA:HB2	1.93	0.50
1:D:65:PRO:HG2	1:D:68:ALA:HB3	1.92	0.50
1:C:251:ALA:O	1:C:326:VAL:HA	2.11	0.50
1:A:370:VAL:CG2	1:A:381:ILE:HD11	2.41	0.50
1:B:65:PRO:C	1:B:67:LEU:H	2.13	0.50
1:D:394:ILE:HG23	1:D:755:PHE:HB2	1.93	0.50
1:F:610:SER:O	1:F:614:VAL:HG23	2.12	0.50
1:D:587:TYR:OH	1:E:468:LYS:HG3	2.11	0.50
1:A:106:ILE:CG2	1:A:277:TYR:HB2	2.37	0.50
1:B:35:LYS:HG3	1:B:90:LYS:HB3	1.92	0.50
1:C:245:ARG:NE	1:C:250:PHE:HE2	2.09	0.50
1:F:406:GLU:HG3	1:F:407:LEU:N	2.27	0.50
1:C:142:GLU:HB2	1:C:150:ASN:C	2.32	0.50
1:B:537:HIS:HB3	1:B:659:LEU:HD23	1.92	0.50
1:D:748:GLY:O	1:D:751:VAL:HG12	2.11	0.50
1:F:456:ILE:O	1:F:482:LEU:HB3	2.12	0.50
1:F:504:ILE:HD11	1:F:701:ALA:HA	1.93	0.50
1:D:28:HIS:CD2	1:D:56:PHE:HB2	2.47	0.50
1:E:163:ARG:O	1:E:167:GLU:HG2	2.10	0.50
1:D:323:PRO:HG2	1:D:324:VAL:H	1.77	0.50
1:D:371:ILE:CG1	1:D:380:VAL:HG22	2.42	0.50
1:A:319:TRP:O	1:A:320:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:PRO:HG3	1:A:747:ASN:HD22	1.76	0.50
1:F:756:LEU:HD21	1:F:770:LEU:HD22	1.93	0.50
1:B:158:MSE:HE3	1:B:163:ARG:NH1	2.27	0.50
1:F:189:ARG:HD2	1:F:191:TYR:OH	2.11	0.50
1:D:508:LEU:HB3	1:D:715:VAL:HB	1.94	0.50
1:B:1:MSE:HE2	1:B:47:GLU:C	2.32	0.50
1:A:486:HIS:O	1:A:489:ALA:HB3	2.10	0.50
1:C:399:ASN:O	1:C:454:ASP:HB2	2.11	0.50
1:A:65:PRO:HG2	1:A:68:ALA:CB	2.42	0.50
1:E:523:GLU:OE2	1:E:537:HIS:HB2	2.11	0.50
1:E:32:GLY:O	1:E:87:TYR:HA	2.11	0.50
1:D:253:MSE:HE2	1:D:317:PHE:CE1	2.46	0.50
1:F:582:VAL:HG21	1:F:626:TYR:CD1	2.46	0.50
1:E:192:THR:HG23	1:E:353:ASP:O	2.12	0.50
1:C:138:PHE:HA	1:C:141:ILE:HD12	1.94	0.50
1:E:219:LYS:HG3	1:E:224:ILE:CG2	2.41	0.50
1:A:111:ASP:CB	1:A:172:ARG:HH22	2.25	0.50
1:F:140:ILE:HG21	1:F:360:ARG:NH1	2.26	0.50
1:F:232:ASN:OD1	1:F:234:GLU:HB3	2.11	0.50
1:C:247:GLN:HE22	1:C:637:LYS:NZ	2.09	0.50
1:C:498:LYS:HB2	1:C:500:LEU:HD12	1.94	0.50
1:B:399:ASN:O	1:B:454:ASP:HB2	2.11	0.50
1:E:535:LEU:HD23	1:E:700:ARG:HG3	1.93	0.50
1:B:396:PHE:CE2	1:B:759:LEU:HB2	2.47	0.50
1:D:267:SER:O	1:D:270:GLU:HB3	2.11	0.50
1:D:292:LEU:HB3	1:D:296:LEU:HD22	1.92	0.50
1:C:263:PHE:HE1	1:C:292:LEU:HB2	1.76	0.50
1:D:504:ILE:H	1:D:706:VAL:HG11	1.77	0.50
1:F:4:TYR:HA	1:F:76:LYS:O	2.11	0.50
1:E:284:LEU:O	1:E:302:THR:HA	2.11	0.50
1:E:714:GLY:C	1:E:716:ALA:H	2.14	0.50
1:D:497:GLU:OE1	1:D:738:VAL:HA	2.11	0.50
1:E:485:GLN:CG	1:E:488:TYR:H	2.23	0.50
1:E:36:ASN:HA	1:E:41:GLY:O	2.12	0.50
1:A:724:MSE:HE1	1:C:289:PRO:HB3	1.94	0.50
1:D:219:LYS:HA	1:D:224:ILE:HG22	1.94	0.50
1:D:279:ARG:HD3	1:D:307:LEU:HB2	1.93	0.50
1:E:582:VAL:CG1	1:E:626:TYR:HB3	2.40	0.50
1:C:181:CYS:SG	1:C:183:VAL:HG13	2.51	0.50
1:D:300:LEU:CD2	1:D:636:MSE:HE2	2.42	0.50
1:D:456:ILE:HD11	1:D:479:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:GLY:CA	1:E:235:VAL:HG11	2.42	0.50
1:F:140:ILE:HB	1:F:152:THR:CG2	2.42	0.50
1:E:456:ILE:HG22	1:E:457:ILE:H	1.77	0.50
1:F:233:GLU:HB2	1:F:293:PRO:HB3	1.93	0.50
1:D:641:PHE:HZ	1:D:678:PRO:HB2	1.76	0.50
1:F:476:GLU:C	1:F:478:ASP:H	2.14	0.50
1:D:613:ARG:HA	1:D:613:ARG:NE	2.27	0.50
1:A:582:VAL:C	1:A:584:SER:H	2.14	0.50
1:E:396:PHE:CZ	1:E:759:LEU:HD13	2.46	0.50
1:B:528:GLY:N	1:B:532:VAL:HG22	2.27	0.50
1:E:16:GLY:C	1:E:19:PRO:HD2	2.32	0.50
1:A:765:LEU:CD2	1:A:770:LEU:HD21	2.41	0.50
1:C:709:VAL:O	1:C:735:ASN:HB2	2.12	0.50
1:B:315:ILE:HG23	1:B:316:LEU:N	2.26	0.50
1:F:380:VAL:HG21	1:F:740:THR:HG23	1.94	0.50
1:D:383:ARG:HD2	1:D:387:PHE:CD2	2.46	0.50
1:C:477:LEU:HB3	1:C:479:VAL:HG23	1.94	0.50
1:C:15:VAL:HG11	1:C:67:LEU:HB2	1.94	0.50
1:F:35:LYS:HE2	1:F:90:LYS:HZ2	1.76	0.50
1:F:253:MSE:HG2	1:F:317:PHE:HE1	1.76	0.50
1:E:236:VAL:HG21	1:E:296:LEU:HD12	1.94	0.50
1:A:177:GLU:HB2	1:A:178:PRO:HD3	1.93	0.50
1:E:188:TYR:OH	1:E:312:THR:HG21	2.12	0.49
1:C:315:ILE:CG2	1:C:316:LEU:N	2.75	0.49
1:A:557:LEU:HD23	1:A:557:LEU:O	2.12	0.49
1:D:281:ILE:HG12	1:D:306:MSE:CG	2.42	0.49
1:A:381:ILE:HG22	1:A:717:TYR:CZ	2.47	0.49
1:A:189:ARG:HA	1:A:202:PRO:HG3	1.94	0.49
1:A:427:ASN:O	1:A:433:VAL:HG21	2.11	0.49
1:A:456:ILE:CG2	1:A:457:ILE:N	2.72	0.49
1:C:224:ILE:HG22	1:C:338:VAL:O	2.12	0.49
1:E:722:THR:O	1:E:726:ARG:HB2	2.11	0.49
1:D:589:LYS:H	1:E:475:ASN:ND2	2.10	0.49
1:E:230:ALA:HB3	1:E:324:VAL:HG23	1.94	0.49
1:C:123:ARG:HH22	1:C:173:ARG:HG2	1.76	0.49
1:E:457:ILE:HG22	1:E:458:ALA:N	2.27	0.49
1:E:233:GLU:O	1:E:236:VAL:HG12	2.12	0.49
1:C:427:ASN:O	1:C:433:VAL:HG11	2.12	0.49
1:B:543:LEU:H	1:B:543:LEU:HD23	1.77	0.49
1:C:266:VAL:HG22	1:C:284:LEU:HD22	1.93	0.49
1:C:306:MSE:HE1	1:C:368:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:HB2	1:A:326:VAL:CG2	2.36	0.49
1:A:286:LYS:HE3	1:A:291:PRO:CD	2.43	0.49
1:D:329:SER:HB3	1:D:337:MSE:HE2	1.94	0.49
1:D:475:ASN:ND2	1:E:589:LYS:H	2.09	0.49
1:C:415:LYS:C	1:C:417:GLY:H	2.15	0.49
1:B:515:THR:O	1:B:516:ASP:HB2	2.12	0.49
1:A:61:TYR:CE2	1:A:73:ILE:HD12	2.46	0.49
1:A:399:ASN:ND2	1:A:399:ASN:N	2.60	0.49
1:C:633:GLU:H	1:C:634:PRO:HD2	1.77	0.49
1:E:278:ARG:HG3	1:E:280:PRO:HD3	1.94	0.49
1:E:398:TYR:CZ	1:E:758:GLY:HA3	2.48	0.49
1:E:759:LEU:CD1	1:E:764:TYR:HB2	2.42	0.49
1:C:540:TYR:HA	1:C:608:ALA:O	2.12	0.49
1:A:409:ASN:ND2	1:A:425:ILE:HD11	2.27	0.49
1:D:394:ILE:HG22	1:D:396:PHE:H	1.76	0.49
1:C:220:GLY:H	1:C:224:ILE:HA	1.78	0.49
1:B:409:ASN:HB3	1:B:425:ILE:HD11	1.93	0.49
1:C:406:GLU:HA	1:C:466:THR:CG2	2.42	0.49
1:C:649:LEU:CD1	1:C:650:LYS:H	2.24	0.49
1:B:22:TYR:CE1	1:B:87:TYR:HB3	2.47	0.49
1:D:456:ILE:HD12	1:D:480:GLU:O	2.12	0.49
1:C:130:VAL:HG23	1:C:134:CYS:SG	2.53	0.49
1:C:586:LYS:CB	1:C:627:ARG:HH22	2.25	0.49
1:C:20:PHE:HE1	1:C:60:LEU:HD12	1.77	0.49
1:F:714:GLY:C	1:F:716:ALA:H	2.16	0.49
1:A:639:GLU:OE2	1:A:718:ASN:HA	2.13	0.49
1:B:379:ALA:HB2	1:B:737:HIS:HE1	1.77	0.49
1:C:287:LYS:CG	1:C:289:PRO:HD2	2.40	0.49
1:D:286:LYS:HD2	1:D:303:ILE:HD11	1.94	0.49
1:F:201:ASP:N	1:F:202:PRO:CD	2.75	0.49
1:F:16:GLY:C	1:F:19:PRO:HD2	2.32	0.49
1:B:593:ASN:C	1:B:595:VAL:H	2.16	0.49
1:A:148:ARG:NH1	1:A:158:MSE:HG3	2.27	0.49
1:B:633:GLU:N	1:B:634:PRO:HD2	2.23	0.49
1:A:111:ASP:HB3	1:A:172:ARG:NH1	2.25	0.49
1:F:204:ARG:O	1:F:208:GLU:HG3	2.13	0.49
1:D:149:GLU:O	1:D:154:LYS:HG3	2.12	0.49
1:E:458:ALA:HB1	1:E:467:THR:HG22	1.94	0.49
1:B:398:TYR:OH	1:B:754:ALA:HA	2.13	0.49
1:D:472:GLU:O	1:D:476:GLU:HG2	2.13	0.49
1:F:338:VAL:HG23	1:F:343:ARG:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:TYR:CE1	1:A:525:LEU:HD13	2.47	0.49
1:F:504:ILE:CG2	1:F:505:GLY:N	2.76	0.49
1:A:504:ILE:HD12	1:A:701:ALA:HA	1.94	0.49
1:C:320:SER:O	1:C:322:THR:N	2.44	0.49
1:F:280:PRO:HB2	1:F:371:ILE:HG22	1.95	0.49
1:E:428:THR:HA	1:E:433:VAL:CG1	2.41	0.49
1:C:12:VAL:HG13	1:C:13:GLN:CD	2.33	0.49
1:C:601:LYS:HZ2	1:F:771:MSE:HE3	1.76	0.49
1:D:257:ILE:CD1	1:D:271:GLU:HG3	2.43	0.49
1:C:760:TYR:HA	1:C:765:LEU:HB3	1.93	0.49
1:D:766:THR:OG1	1:D:769:ASP:HB2	2.11	0.49
1:C:565:TYR:HB3	1:C:569:GLU:HB3	1.93	0.49
1:D:506:ILE:HB	1:D:711:LEU:CD1	2.43	0.49
1:E:370:VAL:HG22	1:E:382:ARG:HD2	1.94	0.49
1:D:15:VAL:HG21	1:D:67:LEU:O	2.13	0.49
1:A:210:ILE:HD11	1:A:228:CYS:CA	2.43	0.49
1:F:137:ARG:O	1:F:141:ILE:HG13	2.13	0.49
1:D:415:LYS:HD2	1:D:448:LEU:HD22	1.95	0.49
1:B:549:ALA:HA	1:B:555:ARG:CB	2.42	0.49
1:B:191:TYR:CD1	1:B:196:GLN:HB3	2.48	0.49
1:F:111:ASP:HB3	1:F:172:ARG:HH12	1.76	0.49
1:E:613:ARG:HA	1:E:613:ARG:HE	1.78	0.49
1:B:205:LYS:O	1:B:209:LEU:HD13	2.12	0.49
1:B:279:ARG:CB	1:B:309:TYR:HB3	2.41	0.49
1:E:583:GLU:HG3	1:E:592:PHE:CD1	2.47	0.49
1:A:490:HIS:CG	1:A:713:GLY:HA2	2.48	0.49
1:A:445:ARG:HH21	1:A:452:ASN:HD22	1.58	0.49
1:E:541:TYR:OH	1:E:610:SER:O	2.30	0.49
1:A:369:SER:H	1:A:385:ARG:CB	2.26	0.49
1:C:216:VAL:HG23	1:C:354:TYR:O	2.12	0.49
1:D:399:ASN:O	1:D:452:ASN:HB2	2.12	0.49
1:D:743:PRO:HG2	1:D:748:GLY:HA3	1.95	0.49
1:F:413:VAL:HG13	1:F:420:TYR:HB2	1.95	0.49
1:A:475:ASN:ND2	1:B:589:LYS:N	2.60	0.49
1:E:282:ILE:HG23	1:E:283:THR:N	2.26	0.49
1:C:370:VAL:O	1:C:381:ILE:HG13	2.12	0.49
1:A:225:HIS:HB2	1:A:328:THR:O	2.12	0.49
1:A:217:ALA:HB1	1:A:224:ILE:CD1	2.41	0.49
1:E:210:ILE:HD13	1:E:216:VAL:CG1	2.37	0.49
1:E:227:ALA:HA	1:E:326:VAL:O	2.13	0.49
1:B:278:ARG:NH1	1:B:387:PHE:HE1	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:MSE:HG3	1:B:424:TYR:HE1	1.76	0.49
1:D:660:ILE:HG22	1:D:662:VAL:HG23	1.94	0.49
1:C:429:GLY:HA2	1:C:465:ASN:HD22	1.77	0.49
1:A:19:PRO:O	1:A:23:ARG:HG3	2.13	0.49
1:D:375:ASP:OD2	1:D:723:LYS:HA	2.13	0.49
1:B:545:GLY:HA3	1:B:548:LEU:HB2	1.95	0.49
1:D:708:ASN:HB3	1:D:734:LEU:O	2.13	0.49
1:F:334:GLY:HA3	1:F:335:MSE:HE2	1.93	0.49
1:F:457:ILE:HG21	1:F:753:GLN:HB3	1.95	0.49
1:E:757:GLY:C	1:E:759:LEU:H	2.16	0.49
1:B:495:MSE:SE	1:B:527:LEU:HD13	2.63	0.49
1:B:529:TYR:HD1	1:B:764:TYR:HB3	1.78	0.49
1:C:485:GLN:OE1	1:C:514:GLY:HA2	2.13	0.49
1:F:385:ARG:HG3	1:F:386:GLY:N	2.28	0.49
1:E:196:GLN:NE2	1:E:196:GLN:N	2.61	0.49
1:B:508:LEU:CD2	1:B:611:THR:HG21	2.41	0.49
1:E:24:ILE:HG23	1:E:56:PHE:CE1	2.47	0.49
1:A:331:ASN:ND2	1:A:337:MSE:HA	2.23	0.49
1:C:11:ILE:HG21	1:C:69:ARG:N	2.23	0.49
1:D:116:LEU:HD23	1:D:129:ILE:HG21	1.95	0.49
1:F:159:CYS:SG	1:F:183:VAL:HG21	2.53	0.49
1:C:170:LEU:HD12	1:C:170:LEU:N	2.27	0.49
1:C:232:ASN:OD1	1:C:235:VAL:HG22	2.13	0.49
1:F:237:ALA:HA	1:F:295:ASN:HD21	1.77	0.49
1:E:384:SER:HA	1:E:388:VAL:HG23	1.93	0.49
1:E:255:LYS:HG2	1:E:256:ASP:OD2	2.13	0.49
1:E:738:VAL:CG1	1:E:742:VAL:HB	2.41	0.49
1:B:495:MSE:HG3	1:B:755:PHE:CZ	2.47	0.49
1:A:404:GLY:HA2	1:A:753:GLN:CD	2.33	0.49
1:D:491:ILE:HD11	1:D:505:GLY:CA	2.41	0.49
1:A:107:ALA:O	1:A:134:CYS:HB2	2.11	0.49
1:C:28:HIS:HB3	1:C:52:ASP:HB3	1.95	0.49
1:E:9:GLN:HE21	1:E:40:ALA:HB1	1.77	0.49
1:C:163:ARG:HA	1:C:166:TYR:HB3	1.95	0.49
1:F:242:ARG:HH22	1:F:353:ASP:CG	2.17	0.49
1:B:193:SER:O	1:B:194:ASP:CB	2.60	0.49
1:F:725:ILE:O	1:F:729:VAL:HG23	2.13	0.49
1:C:190:LEU:HB2	1:C:202:PRO:CB	2.39	0.49
1:B:495:MSE:SE	1:B:527:LEU:HD22	2.63	0.49
1:A:751:VAL:HG13	1:A:752:GLY:N	2.27	0.49
1:C:309:TYR:CG	1:C:385:ARG:NH2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TYR:C	1:A:466:THR:N	2.67	0.49
1:D:104:PRO:O	1:D:137:ARG:HB2	2.12	0.49
1:F:181:CYS:SG	1:F:182:PRO:N	2.85	0.49
1:C:433:VAL:O	1:C:436:PHE:HB3	2.12	0.49
1:B:31:ARG:HB3	1:B:86:PHE:O	2.13	0.49
1:D:509:ASP:CG	1:D:510:GLY:N	2.66	0.48
1:A:557:LEU:HD12	1:A:620:VAL:HB	1.94	0.48
1:E:370:VAL:HG23	1:E:381:ILE:HG13	1.95	0.48
1:C:210:ILE:HG21	1:C:325:TYR:HE1	1.77	0.48
1:F:22:TYR:CD2	1:F:169:PRO:HB3	2.48	0.48
1:C:218:ILE:C	1:C:224:ILE:HG13	2.33	0.48
1:F:4:TYR:CB	1:F:53:ILE:HD11	2.43	0.48
1:D:519:THR:HB	1:D:608:ALA:CA	2.37	0.48
1:F:7:HIS:CD2	1:F:43:GLU:HB3	2.48	0.48
1:A:655:VAL:HG22	1:A:660:ILE:HG12	1.94	0.48
1:C:130:VAL:HG22	1:C:131:CYS:N	2.28	0.48
1:C:130:VAL:HG11	1:C:178:PRO:O	2.13	0.48
1:E:113:LEU:O	1:E:116:LEU:HG	2.13	0.48
1:C:566:SER:N	1:C:569:GLU:HB2	2.27	0.48
1:A:545:GLY:HA3	1:A:548:LEU:HD12	1.95	0.48
1:D:376:GLY:C	1:D:377:LYS:HD2	2.33	0.48
1:D:515:THR:O	1:D:516:ASP:HB2	2.12	0.48
1:A:502:SER:CB	1:A:528:GLY:HA2	2.43	0.48
1:D:219:LYS:HA	1:D:224:ILE:HB	1.95	0.48
1:D:274:LEU:C	1:D:276:SER:H	2.17	0.48
1:A:251:ALA:HB3	1:A:327:MSE:O	2.14	0.48
1:F:146:TYR:CE1	1:F:177:GLU:HG2	2.49	0.48
1:E:219:LYS:HD3	1:E:358:HIS:H	1.76	0.48
1:B:516:ASP:C	1:B:518:ASN:H	2.17	0.48
1:C:24:ILE:HG23	1:C:56:PHE:CE1	2.47	0.48
1:F:601:LYS:CB	1:F:603:ILE:HG13	2.43	0.48
1:D:398:TYR:HB2	1:D:454:ASP:CG	2.33	0.48
1:D:677:SER:O	1:D:681:ILE:HG12	2.13	0.48
1:C:256:ASP:O	1:C:257:ILE:C	2.52	0.48
1:F:216:VAL:O	1:F:227:ALA:HB3	2.13	0.48
1:C:225:HIS:N	1:C:225:HIS:CD2	2.81	0.48
1:C:270:GLU:N	1:C:378:ARG:NH1	2.62	0.48
1:B:16:GLY:HA2	1:B:132:THR:OG1	2.12	0.48
1:F:124:TYR:O	1:F:125:MSE:HB2	2.13	0.48
1:A:450:VAL:HG22	1:A:451:LYS:N	2.28	0.48
1:A:239:LEU:HD22	1:A:250:PHE:HZ	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:ARG:HB3	1:F:86:PHE:O	2.12	0.48
1:E:510:GLY:O	1:E:511:VAL:HG23	2.13	0.48
1:D:392:ILE:N	1:D:392:ILE:HD12	2.29	0.48
1:E:144:LEU:CD1	1:E:447:ILE:HG23	2.40	0.48
1:B:216:VAL:O	1:B:227:ALA:HB3	2.13	0.48
1:D:543:LEU:CD2	1:D:543:LEU:H	2.20	0.48
1:B:406:GLU:HA	1:B:466:THR:HG21	1.96	0.48
1:B:427:ASN:O	1:B:433:VAL:HG11	2.13	0.48
1:F:300:LEU:HD22	1:F:636:MSE:HE2	1.95	0.48
1:D:557:LEU:HD23	1:D:557:LEU:O	2.13	0.48
1:A:144:LEU:HD23	1:A:146:TYR:N	2.27	0.48
1:F:315:ILE:HG23	1:F:316:LEU:N	2.28	0.48
1:A:116:LEU:C	1:A:118:ASP:H	2.17	0.48
1:E:456:ILE:O	1:E:482:LEU:HB3	2.13	0.48
1:F:383:ARG:CZ	1:F:421:PRO:HG3	2.43	0.48
1:C:375:ASP:OD2	1:C:723:LYS:HA	2.13	0.48
1:D:714:GLY:C	1:D:716:ALA:H	2.16	0.48
1:F:490:HIS:C	1:F:492:ALA:H	2.17	0.48
1:C:253:MSE:HG3	1:C:306:MSE:O	2.14	0.48
1:C:317:PHE:CE2	1:C:323:PRO:HA	2.45	0.48
1:A:253:MSE:HA	1:A:306:MSE:O	2.13	0.48
1:A:309:TYR:CZ	1:A:313:HIS:NE2	2.81	0.48
1:F:11:ILE:HG23	1:F:11:ILE:O	2.12	0.48
1:F:15:VAL:C	1:F:17:PHE:H	2.17	0.48
1:E:265:TYR:O	1:E:284:LEU:HD22	2.13	0.48
1:D:170:LEU:N	1:D:170:LEU:HD12	2.25	0.48
1:E:539:ASP:CA	1:E:659:LEU:HD11	2.40	0.48
1:F:182:PRO:HB3	1:F:199:TYR:OH	2.14	0.48
1:B:170:LEU:H	1:B:170:LEU:HD12	1.79	0.48
1:C:21:VAL:HA	1:C:24:ILE:CG2	2.42	0.48
1:C:9:GLN:NE2	1:C:40:ALA:HB1	2.28	0.48
1:D:399:ASN:HA	1:D:414:ALA:O	2.13	0.48
1:D:690:ALA:CB	1:D:721:ILE:HG23	2.43	0.48
1:B:588:GLY:O	1:B:592:PHE:HD2	1.97	0.48
1:A:495:MSE:HG3	1:A:755:PHE:CE2	2.48	0.48
1:C:265:TYR:CE2	1:C:287:LYS:HD2	2.47	0.48
1:A:380:VAL:CG1	1:A:381:ILE:H	2.15	0.48
1:F:579:PRO:O	1:F:582:VAL:HG23	2.14	0.48
1:C:105:ASP:HA	1:C:137:ARG:HB2	1.94	0.48
1:B:725:ILE:O	1:B:729:VAL:HG23	2.13	0.48
1:C:415:LYS:HZ2	1:C:448:LEU:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:SER:HA	1:D:388:VAL:CG2	2.43	0.48
1:A:445:ARG:HH22	1:A:477:LEU:HD22	1.77	0.48
1:D:105:ASP:CG	1:D:139:THR:HG23	2.33	0.48
1:C:429:GLY:HA2	1:C:465:ASN:ND2	2.29	0.48
1:B:691:ARG:HD3	1:B:724:MSE:HE3	1.93	0.48
1:F:595:VAL:O	1:F:598:GLN:HB3	2.14	0.48
1:F:534:ARG:HG2	1:F:535:LEU:N	2.28	0.48
1:E:315:ILE:HG23	1:E:316:LEU:N	2.29	0.48
1:D:190:LEU:O	1:D:196:GLN:HB2	2.13	0.48
1:C:329:SER:HA	1:C:337:MSE:HE2	1.95	0.48
1:C:367:ASP:HB2	1:C:424:TYR:HB3	1.94	0.48
1:B:146:TYR:CE1	1:B:177:GLU:HG2	2.49	0.48
1:B:128:PHE:CD1	1:B:186:PRO:HG2	2.49	0.48
1:C:528:GLY:O	1:C:529:TYR:C	2.52	0.48
1:F:191:TYR:HA	1:F:195:GLY:O	2.14	0.48
1:C:111:ASP:HB3	1:C:172:ARG:HH22	1.79	0.48
1:A:613:ARG:NE	1:A:613:ARG:HA	2.28	0.48
1:F:312:THR:O	1:F:315:ILE:HG22	2.14	0.48
1:A:445:ARG:HH22	1:A:477:LEU:CD2	2.27	0.48
1:E:670:LEU:HA	1:E:673:ILE:HG12	1.94	0.48
1:F:495:MSE:HB3	1:F:500:LEU:HD11	1.96	0.48
1:A:610:SER:O	1:A:614:VAL:HG23	2.13	0.48
1:A:270:GLU:HB2	1:A:373:PHE:HE2	1.79	0.48
1:E:751:VAL:HG13	1:E:752:GLY:N	2.29	0.48
1:E:64:LYS:CB	1:E:65:PRO:HD2	2.43	0.48
1:D:339:LYS:HD2	1:D:362:ILE:O	2.14	0.48
1:D:373:PHE:CE2	1:D:378:ARG:HD3	2.48	0.48
1:D:381:ILE:HA	1:D:717:TYR:OH	2.13	0.48
1:C:215:ILE:HD11	1:C:351:VAL:O	2.14	0.48
1:A:255:LYS:HG3	1:A:317:PHE:CD2	2.49	0.48
1:F:108:ILE:HG22	1:F:109:CYS:O	2.14	0.48
1:D:648:ASP:OD1	1:D:687:LEU:HD12	2.14	0.48
1:B:595:VAL:HG12	1:B:595:VAL:O	2.13	0.48
1:E:591:GLU:O	1:E:594:VAL:HB	2.14	0.48
1:C:406:GLU:HB3	1:C:464:TYR:CG	2.48	0.48
1:C:728:VAL:C	1:C:730:GLU:H	2.17	0.48
1:C:31:ARG:HA	1:C:87:TYR:HB2	1.96	0.48
1:A:666:PHE:O	1:A:669:ILE:HB	2.14	0.48
1:D:151:THR:O	1:D:154:LYS:HB2	2.13	0.48
1:B:140:ILE:HB	1:B:152:THR:CG2	2.44	0.48
1:E:665:LEU:O	1:E:669:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:O	1:B:344:ALA:HB3	2.13	0.48
1:A:485:GLN:HB3	1:A:488:TYR:HB2	1.94	0.48
1:E:485:GLN:HG2	1:E:488:TYR:CD2	2.49	0.48
1:E:391:PRO:C	1:E:392:ILE:HD12	2.34	0.48
1:D:233:GLU:O	1:D:236:VAL:HG12	2.14	0.48
1:C:525:LEU:CD2	1:C:534:ARG:HA	2.44	0.48
1:D:496:ALA:HB2	1:D:755:PHE:CD2	2.49	0.48
1:B:409:ASN:O	1:B:425:ILE:HG12	2.14	0.48
1:E:130:VAL:HG22	1:E:131:CYS:O	2.14	0.48
1:B:171:ASN:HD21	1:B:173:ARG:CB	2.26	0.48
1:E:538:ILE:HG12	1:E:662:VAL:HG21	1.94	0.48
1:E:624:VAL:CG1	1:E:637:LYS:HB3	2.44	0.48
1:C:9:GLN:HE21	1:C:40:ALA:C	2.16	0.48
1:C:204:ARG:C	1:C:204:ARG:HD2	2.34	0.48
1:D:617:ALA:O	1:D:621:LEU:HB2	2.14	0.48
1:D:469:LEU:O	1:D:473:MSE:HB2	2.14	0.48
1:F:113:LEU:O	1:F:117:PHE:HB2	2.13	0.48
1:D:255:LYS:HG2	1:D:256:ASP:OD2	2.13	0.48
1:B:335:MSE:N	1:B:335:MSE:HE2	2.29	0.48
1:C:613:ARG:NE	1:C:613:ARG:HA	2.28	0.48
1:F:690:ALA:O	1:F:725:ILE:HG12	2.13	0.48
1:C:127:PRO:HG3	1:C:203:LEU:HD21	1.96	0.48
1:D:263:PHE:HD1	1:D:292:LEU:HD23	1.79	0.48
1:D:218:ILE:HD12	1:D:356:LEU:HD23	1.96	0.48
1:C:506:ILE:HG22	1:C:508:LEU:HG	1.95	0.48
1:F:16:GLY:HA2	1:F:132:THR:OG1	2.13	0.48
1:F:16:GLY:O	1:F:19:PRO:HD2	2.14	0.48
1:E:323:PRO:HG2	1:E:324:VAL:H	1.79	0.48
1:D:403:VAL:CG1	1:D:466:THR:HB	2.44	0.48
1:D:524:VAL:HG23	1:D:535:LEU:HB2	1.96	0.48
1:E:455:LEU:HA	1:E:479:VAL:HG12	1.95	0.48
1:D:470:ALA:HB1	1:D:481:LEU:HD11	1.96	0.48
1:E:17:PHE:HZ	1:E:60:LEU:HD21	1.77	0.48
1:F:460:LEU:HB2	1:F:485:GLN:HA	1.96	0.47
1:D:279:ARG:HG3	1:D:309:TYR:HB3	1.96	0.47
1:D:381:ILE:HG22	1:D:717:TYR:CE1	2.48	0.47
1:C:275:THR:HA	1:C:279:ARG:HE	1.79	0.47
1:F:380:VAL:CG1	1:F:381:ILE:N	2.77	0.47
1:F:50:GLU:O	1:F:53:ILE:HG22	2.15	0.47
1:E:228:CYS:SG	1:E:229:ASP:N	2.87	0.47
1:F:264:ALA:HB1	1:F:286:LYS:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:LYS:HG3	1:F:475:ASN:OD1	2.14	0.47
1:C:149:GLU:HB2	1:C:154:LYS:HZ3	1.78	0.47
1:E:177:GLU:HB2	1:E:178:PRO:HD3	1.96	0.47
1:E:118:ASP:HA	1:E:119:PRO:HD3	1.72	0.47
1:A:573:VAL:HG13	1:A:574:ILE:N	2.29	0.47
1:E:595:VAL:HG12	1:E:595:VAL:O	2.13	0.47
1:B:487:HIS:CE1	1:B:512:GLY:HA3	2.49	0.47
1:A:520:TRP:HA	1:A:609:SER:OG	2.14	0.47
1:A:534:ARG:HG2	1:A:535:LEU:H	1.76	0.47
1:F:485:GLN:HG3	1:F:486:HIS:N	2.29	0.47
1:F:487:HIS:CD2	1:F:520:TRP:HB3	2.49	0.47
1:C:357:LEU:HD23	1:C:357:LEU:N	2.29	0.47
1:D:270:GLU:CB	1:D:373:PHE:HE2	2.26	0.47
1:C:380:VAL:HG23	1:C:740:THR:HA	1.96	0.47
1:A:204:ARG:HG2	1:A:319:TRP:CZ2	2.48	0.47
1:B:204:ARG:HG3	1:B:319:TRP:CE2	2.49	0.47
1:D:709:VAL:O	1:D:735:ASN:HB2	2.14	0.47
1:F:662:VAL:O	1:F:662:VAL:HG12	2.13	0.47
1:F:301:HIS:CD2	1:F:302:THR:HG23	2.49	0.47
1:E:651:PHE:HB2	1:E:688:ALA:HB2	1.95	0.47
1:C:387:PHE:O	1:C:390:LEU:HG	2.14	0.47
1:B:424:TYR:CZ	1:B:426:GLY:HA2	2.50	0.47
1:F:407:LEU:HB3	1:F:631:GLU:OE1	2.14	0.47
1:A:18:ARG:HB2	1:A:19:PRO:HD3	1.96	0.47
1:C:567:ILE:HG23	1:C:600:ALA:HB2	1.95	0.47
1:F:453:LEU:O	1:F:453:LEU:HG	2.14	0.47
1:D:485:GLN:HB3	1:D:488:TYR:HB2	1.95	0.47
1:A:596:LEU:HD23	1:A:596:LEU:O	2.14	0.47
1:A:589:LYS:N	1:B:475:ASN:ND2	2.60	0.47
1:B:526:TYR:CB	1:B:535:LEU:HD11	2.44	0.47
1:B:496:ALA:HB2	1:B:755:PHE:CD2	2.49	0.47
1:B:756:LEU:HD21	1:B:770:LEU:HD22	1.96	0.47
1:A:505:GLY:HA2	1:A:710:ALA:H	1.77	0.47
1:C:487:HIS:HD2	1:C:520:TRP:HB3	1.79	0.47
1:C:370:VAL:HG23	1:C:382:ARG:HB2	1.96	0.47
1:D:394:ILE:HD12	1:D:755:PHE:HB2	1.96	0.47
1:D:495:MSE:SE	1:D:527:LEU:HD13	2.64	0.47
1:B:189:ARG:HA	1:B:202:PRO:HG3	1.97	0.47
1:E:210:ILE:CD1	1:E:216:VAL:HG12	2.38	0.47
1:E:183:VAL:HG23	1:E:184:CYS:H	1.76	0.47
1:A:247:GLN:HG3	1:A:298:PRO:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:PRO:HB2	1:B:620:VAL:CG2	2.45	0.47
1:D:554:LEU:HD21	1:D:579:PRO:CG	2.44	0.47
1:D:629:HIS:HB2	1:D:633:GLU:OE1	2.14	0.47
1:E:8:VAL:HA	1:E:72:ARG:O	2.14	0.47
1:B:261:LYS:NZ	1:B:266:VAL:HB	2.29	0.47
1:F:406:GLU:HG3	1:F:407:LEU:H	1.80	0.47
1:A:422:SER:HA	1:A:444:PHE:CZ	2.49	0.47
1:D:702:ARG:NH2	1:D:731:ALA:O	2.48	0.47
1:A:487:HIS:CE1	1:A:509:ASP:HB3	2.50	0.47
1:B:219:LYS:HA	1:B:224:ILE:CB	2.45	0.47
1:B:310:ALA:O	1:B:313:HIS:HB2	2.14	0.47
1:F:488:TYR:CD1	1:F:525:LEU:HD13	2.49	0.47
1:B:588:GLY:O	1:B:592:PHE:HB2	2.15	0.47
1:D:219:LYS:NZ	1:D:362:ILE:HG12	2.30	0.47
1:C:309:TYR:H	1:C:313:HIS:CD2	2.32	0.47
1:C:229:ASP:OD1	1:C:322:THR:HG21	2.14	0.47
1:E:270:GLU:N	1:E:378:ARG:NH1	2.62	0.47
1:A:154:LYS:O	1:A:154:LYS:HD3	2.14	0.47
1:E:181:CYS:SG	1:E:182:PRO:HD2	2.54	0.47
1:E:579:PRO:HB3	1:E:626:TYR:CE1	2.49	0.47
1:A:106:ILE:HG22	1:A:107:ALA:N	2.29	0.47
1:E:726:ARG:HG2	1:E:735:ASN:HD21	1.80	0.47
1:E:727:LYS:O	1:E:730:GLU:HG2	2.15	0.47
1:F:264:ALA:HB1	1:F:285:ARG:O	2.15	0.47
1:A:516:ASP:O	1:A:517:GLY:C	2.53	0.47
1:C:570:LEU:HD12	1:C:573:VAL:HG11	1.96	0.47
1:C:216:VAL:HG23	1:C:354:TYR:C	2.34	0.47
1:B:573:VAL:HG13	1:B:574:ILE:N	2.30	0.47
1:E:124:TYR:CD2	1:E:125:MSE:HG2	2.49	0.47
1:E:682:ALA:O	1:E:686:HIS:HB2	2.15	0.47
1:C:715:VAL:HG12	1:C:715:VAL:O	2.15	0.47
1:B:404:GLY:HA2	1:B:753:GLN:HE22	1.78	0.47
1:B:457:ILE:HG22	1:B:458:ALA:H	1.78	0.47
1:E:399:ASN:O	1:E:452:ASN:HB2	2.14	0.47
1:D:190:LEU:HB2	1:D:202:PRO:CB	2.41	0.47
1:A:218:ILE:O	1:A:224:ILE:HB	2.15	0.47
1:A:406:GLU:HA	1:A:466:THR:HG21	1.95	0.47
1:F:183:VAL:CG2	1:F:184:CYS:N	2.77	0.47
1:C:111:ASP:HB3	1:C:172:ARG:HH12	1.79	0.47
1:C:176:ALA:C	1:C:178:PRO:HD2	2.34	0.47
1:A:450:VAL:HG22	1:A:451:LYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:LYS:HE3	1:D:736:PHE:HB3	1.95	0.47
1:D:642:ALA:O	1:D:683:TYR:HB2	2.14	0.47
1:A:460:LEU:HD12	1:A:483:GLN:HB3	1.97	0.47
1:B:21:VAL:HG11	1:B:44:ILE:HD13	1.96	0.47
1:A:566:SER:N	1:A:569:GLU:HB3	2.28	0.47
1:A:267:SER:HB2	1:A:270:GLU:HB3	1.94	0.47
1:B:253:MSE:SE	1:B:313:HIS:ND1	2.97	0.47
1:C:356:LEU:C	1:C:357:LEU:HD23	2.35	0.47
1:E:398:TYR:HB2	1:E:454:ASP:CG	2.35	0.47
1:F:250:PHE:HE2	1:F:328:THR:OG1	1.96	0.47
1:A:302:THR:HG21	1:A:372:ARG:HE	1.78	0.47
1:D:183:VAL:CG2	1:D:184:CYS:N	2.78	0.47
1:E:373:PHE:CE2	1:E:378:ARG:HD3	2.49	0.47
1:E:553:PRO:HB2	1:E:620:VAL:CG2	2.41	0.47
1:C:8:VAL:HG13	1:C:72:ARG:O	2.15	0.47
1:D:246:PRO:CG	1:D:629:HIS:HB3	2.45	0.47
1:E:413:VAL:HG21	1:E:448:LEU:HD13	1.95	0.47
1:D:535:LEU:HD23	1:D:700:ARG:HG3	1.95	0.47
1:B:142:GLU:HB3	1:B:150:ASN:O	2.15	0.47
1:C:104:PRO:HG3	1:C:390:LEU:HD11	1.95	0.47
1:E:665:LEU:HG	1:E:669:ILE:HD11	1.97	0.47
1:D:451:LYS:HD3	1:D:477:LEU:CG	2.45	0.47
1:B:370:VAL:CG2	1:B:381:ILE:HD11	2.44	0.47
1:F:504:ILE:HG23	1:F:525:LEU:O	2.15	0.47
1:F:694:ALA:C	1:F:696:THR:N	2.68	0.47
1:A:582:VAL:HG13	1:A:626:TYR:HB3	1.95	0.47
1:E:166:TYR:CE1	1:E:175:HIS:HA	2.50	0.47
1:D:286:LYS:HB2	1:D:303:ILE:CD1	2.45	0.47
1:D:111:ASP:CB	1:D:172:ARG:HH12	2.17	0.47
1:C:729:VAL:HB	1:C:735:ASN:HD22	1.78	0.47
1:C:286:LYS:HE3	1:C:290:PHE:CA	2.43	0.47
1:A:264:ALA:HB1	1:A:285:ARG:O	2.15	0.47
1:F:283:THR:OG1	1:F:372:ARG:HB2	2.15	0.47
1:D:504:ILE:HG22	1:D:505:GLY:H	1.79	0.47
1:C:543:LEU:HD23	1:C:543:LEU:N	2.18	0.47
1:E:266:VAL:HG22	1:E:284:LEU:HD13	1.97	0.47
1:D:251:ALA:HB3	1:D:327:MSE:O	2.14	0.47
1:D:1:MSE:HE3	1:D:84:ASP:N	2.30	0.47
1:E:134:CYS:SG	1:E:135:GLY:N	2.87	0.47
1:F:300:LEU:CD2	1:F:636:MSE:HE2	2.45	0.47
1:D:13:GLN:HG3	1:D:42:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASP:O	1:B:174:TYR:HB2	2.15	0.47
1:E:252:ILE:HD13	1:E:303:ILE:CG2	2.45	0.47
1:D:403:VAL:HG23	1:D:457:ILE:O	2.15	0.47
1:A:660:ILE:O	1:A:662:VAL:HG23	2.14	0.47
1:F:408:MSE:HG3	1:F:424:TYR:HE1	1.78	0.47
1:C:760:TYR:HE2	1:C:767:LYS:HG2	1.80	0.47
1:F:374:VAL:HG21	1:F:744:ARG:CZ	2.45	0.47
1:A:677:SER:HB2	1:A:678:PRO:HD2	1.97	0.47
1:C:523:GLU:CD	1:C:523:GLU:N	2.68	0.47
1:D:130:VAL:HG21	1:D:135:GLY:HA3	1.96	0.47
1:E:370:VAL:HG23	1:E:381:ILE:CG1	2.45	0.47
1:A:253:MSE:HE2	1:A:317:PHE:HD1	1.79	0.47
1:F:306:MSE:O	1:F:307:LEU:HD23	2.15	0.47
1:C:451:LYS:HA	1:C:477:LEU:HD21	1.95	0.47
1:B:739:THR:O	1:B:742:VAL:O	2.33	0.47
1:E:190:LEU:O	1:E:196:GLN:HB2	2.15	0.47
1:F:509:ASP:CG	1:F:510:GLY:H	2.18	0.47
1:F:726:ARG:HH21	1:F:727:LYS:HG2	1.76	0.47
1:E:193:SER:O	1:E:194:ASP:CB	2.59	0.47
1:A:129:ILE:O	1:A:130:VAL:HB	2.15	0.47
1:D:257:ILE:HA	1:D:260:VAL:HG23	1.96	0.47
1:E:406:GLU:HB3	1:E:464:TYR:CG	2.50	0.47
1:A:128:PHE:CD1	1:A:186:PRO:HG2	2.50	0.47
1:D:126:TYR:CD1	1:D:182:PRO:HG3	2.50	0.47
1:F:595:VAL:HG12	1:F:595:VAL:O	2.15	0.47
1:F:766:THR:OG1	1:F:769:ASP:HB2	2.14	0.47
1:A:1:MSE:HB2	1:A:80:PRO:HD2	1.96	0.47
1:E:245:ARG:NE	1:E:248:LYS:HB3	2.30	0.47
1:E:144:LEU:HA	1:E:145:PRO:C	2.36	0.47
1:F:404:GLY:HA2	1:F:753:GLN:CD	2.35	0.47
1:F:404:GLY:O	1:F:459:ASP:HB2	2.15	0.47
1:B:284:LEU:O	1:B:302:THR:HA	2.14	0.47
1:D:320:SER:HG	1:D:325:TYR:HE1	1.61	0.47
1:C:210:ILE:HD11	1:C:228:CYS:N	2.30	0.47
1:A:252:ILE:HG22	1:A:253:MSE:N	2.30	0.47
1:A:283:THR:OG1	1:A:372:ARG:HB2	2.15	0.47
1:D:278:ARG:HG3	1:D:280:PRO:HD3	1.95	0.47
1:C:456:ILE:HD11	1:C:479:VAL:HB	1.96	0.47
1:A:315:ILE:HG23	1:A:316:LEU:N	2.30	0.47
1:F:286:LYS:CE	1:F:290:PHE:HB2	2.45	0.47
1:C:590:VAL:HG23	1:F:475:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:SG	1:A:133:ASN:HB2	2.54	0.47
1:A:515:THR:O	1:A:516:ASP:HB2	2.14	0.47
1:C:35:LYS:HG2	1:C:36:ASN:H	1.80	0.47
1:C:147:ASP:HA	1:C:177:GLU:OE2	2.15	0.47
1:E:204:ARG:HD2	1:E:204:ARG:C	2.36	0.47
1:E:566:SER:HB3	1:E:569:GLU:HG2	1.97	0.47
1:B:6:ILE:HG22	1:B:7:HIS:H	1.80	0.47
1:E:486:HIS:O	1:E:489:ALA:HB3	2.14	0.47
1:A:719:GLU:O	1:A:723:LYS:HB2	2.14	0.47
1:D:219:LYS:HA	1:D:224:ILE:CB	2.45	0.47
1:D:66:PRO:HG2	1:D:67:LEU:H	1.80	0.47
1:C:251:ALA:HB3	1:C:327:MSE:O	2.14	0.47
1:C:219:LYS:HZ2	1:C:362:ILE:HG12	1.80	0.47
1:C:66:PRO:CG	1:C:133:ASN:HB3	2.44	0.47
1:A:412:GLY:CA	1:A:750:ASN:HD22	2.22	0.47
1:D:17:PHE:CZ	1:D:60:LEU:HD11	2.50	0.47
1:B:566:SER:H	1:B:569:GLU:CB	2.28	0.47
1:B:665:LEU:O	1:B:669:ILE:HG13	2.15	0.47
1:D:540:TYR:O	1:D:563:LYS:HE3	2.15	0.47
1:C:625:ALA:HB2	1:C:637:LYS:CD	2.44	0.47
1:E:383:ARG:HG3	1:E:383:ARG:HH11	1.80	0.47
1:C:718:ASN:ND2	1:C:720:LEU:HB2	2.30	0.47
1:D:742:VAL:CG1	1:D:751:VAL:HG11	2.45	0.46
1:D:288:GLU:CB	1:D:289:PRO:HD3	2.30	0.46
1:E:485:GLN:NE2	1:E:486:HIS:H	2.13	0.46
1:D:371:ILE:HD11	1:D:373:PHE:HE1	1.80	0.46
1:C:274:LEU:O	1:C:307:LEU:HD12	2.15	0.46
1:A:323:PRO:HG2	1:A:324:VAL:H	1.79	0.46
1:E:287:LYS:O	1:E:288:GLU:C	2.53	0.46
1:E:216:VAL:O	1:E:227:ALA:HB3	2.15	0.46
1:D:299:GLY:O	1:D:300:LEU:HG	2.15	0.46
1:D:589:LYS:HG3	1:D:590:VAL:N	2.25	0.46
1:C:415:LYS:NZ	1:C:448:LEU:HA	2.30	0.46
1:C:558:MSE:HE1	1:C:593:ASN:OD1	2.15	0.46
1:D:409:ASN:HD22	1:D:437:MSE:HE2	1.80	0.46
1:C:172:ARG:HG2	1:C:173:ARG:N	2.30	0.46
1:F:445:ARG:HH21	1:F:452:ASN:ND2	2.13	0.46
1:B:651:PHE:HB2	1:B:688:ALA:HB2	1.97	0.46
1:F:472:GLU:HG3	1:F:473:MSE:N	2.30	0.46
1:F:213:GLY:C	1:F:235:VAL:HG11	2.35	0.46
1:C:427:ASN:ND2	1:C:429:GLY:H	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:LEU:O	1:F:30:LEU:HD23	2.14	0.46
1:F:1:MSE:CB	1:F:80:PRO:HD2	2.46	0.46
1:F:394:ILE:HG22	1:F:396:PHE:H	1.81	0.46
1:B:254:ALA:HB1	1:B:259:THR:CB	2.41	0.46
1:E:443:HIS:O	1:E:447:ILE:HD12	2.15	0.46
1:F:456:ILE:HD11	1:F:479:VAL:HB	1.98	0.46
1:F:507:ALA:HA	1:F:712:SER:O	2.16	0.46
1:E:694:ALA:HB2	1:E:725:ILE:HG23	1.96	0.46
1:A:403:VAL:CG1	1:A:466:THR:HB	2.45	0.46
1:F:584:SER:CB	1:F:589:LYS:HB3	2.46	0.46
1:A:400:GLY:O	1:A:413:VAL:HG23	2.15	0.46
1:B:1:MSE:HE3	1:B:2:LYS:H	1.79	0.46
1:D:398:TYR:CE1	1:D:758:GLY:HA3	2.50	0.46
1:D:678:PRO:HG2	1:D:679:ALA:H	1.80	0.46
1:C:572:GLY:HA2	1:C:575:ASN:HD22	1.80	0.46
1:B:137:ARG:O	1:B:141:ILE:HG13	2.15	0.46
1:B:217:ALA:O	1:B:218:ILE:HD13	2.16	0.46
1:B:491:ILE:CD1	1:B:525:LEU:HD12	2.45	0.46
1:C:323:PRO:HG2	1:C:324:VAL:H	1.80	0.46
1:B:154:LYS:HD3	1:B:154:LYS:C	2.36	0.46
1:F:282:ILE:HA	1:F:371:ILE:O	2.15	0.46
1:B:437:MSE:HG2	1:B:441:ILE:HD11	1.97	0.46
1:A:123:ARG:HE	1:A:173:ARG:HH21	1.62	0.46
1:D:455:LEU:HA	1:D:479:VAL:HG12	1.97	0.46
1:D:158:MSE:HE1	1:D:166:TYR:CD2	2.49	0.46
1:C:550:SER:O	1:C:628:ARG:HD2	2.14	0.46
1:D:472:GLU:HG3	1:D:473:MSE:N	2.30	0.46
1:B:365:ARG:O	1:B:423:GLN:HG2	2.16	0.46
1:E:343:ARG:HH11	1:E:343:ARG:HG2	1.81	0.46
1:A:88:ILE:HG22	1:A:89:GLU:N	2.30	0.46
1:F:495:MSE:HG3	1:F:755:PHE:CE2	2.50	0.46
1:D:18:ARG:O	1:D:21:VAL:HG12	2.16	0.46
1:B:584:SER:CB	1:B:589:LYS:HB3	2.44	0.46
1:B:707:LYS:HG3	1:B:708:ASN:CG	2.36	0.46
1:D:270:GLU:HB2	1:D:373:PHE:CE2	2.48	0.46
1:D:268:PRO:C	1:D:270:GLU:H	2.18	0.46
1:D:370:VAL:HG23	1:D:381:ILE:HG13	1.97	0.46
1:C:486:HIS:O	1:C:489:ALA:HB3	2.16	0.46
1:F:16:GLY:HA3	1:F:132:THR:O	2.15	0.46
1:B:582:VAL:CG1	1:B:626:TYR:HB3	2.46	0.46
1:C:409:ASN:HB3	1:C:425:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:VAL:HG22	1:C:72:ARG:O	2.16	0.46
1:B:428:THR:HG21	1:B:437:MSE:HE1	1.96	0.46
1:C:65:PRO:C	1:C:67:LEU:H	2.17	0.46
1:C:213:GLY:C	1:C:235:VAL:HG11	2.35	0.46
1:A:690:ALA:CB	1:A:721:ILE:HG23	2.46	0.46
1:F:335:MSE:HE2	1:F:335:MSE:N	2.30	0.46
1:E:124:TYR:CE2	1:E:125:MSE:HG2	2.50	0.46
1:F:279:ARG:HG3	1:F:309:TYR:HB3	1.96	0.46
1:B:376:GLY:O	1:B:377:LYS:HG3	2.15	0.46
1:E:312:THR:HA	1:E:315:ILE:CG2	2.45	0.46
1:B:269:GLU:HB2	1:B:378:ARG:NH2	2.31	0.46
1:E:88:ILE:N	1:E:88:ILE:HD12	2.30	0.46
1:C:330:ALA:HB1	1:C:348:LEU:HD21	1.96	0.46
1:F:380:VAL:HG12	1:F:381:ILE:H	1.78	0.46
1:F:380:VAL:HG23	1:F:740:THR:CA	2.39	0.46
1:B:555:ARG:NH2	1:B:595:VAL:HG11	2.31	0.46
1:D:225:HIS:HA	1:D:330:ALA:H	1.80	0.46
1:B:406:GLU:HG3	1:B:407:LEU:HG	1.97	0.46
1:B:522:GLY:CA	1:B:611:THR:HG23	2.46	0.46
1:D:123:ARG:HD3	1:D:129:ILE:HG13	1.98	0.46
1:F:203:LEU:HD12	1:F:319:TRP:CZ3	2.46	0.46
1:D:433:VAL:O	1:D:436:PHE:HB3	2.15	0.46
1:F:374:VAL:HG21	1:F:744:ARG:NH1	2.30	0.46
1:B:398:TYR:O	1:B:398:TYR:CG	2.69	0.46
1:A:18:ARG:HG3	1:A:18:ARG:NH1	2.30	0.46
1:B:371:ILE:CD1	1:B:380:VAL:HG22	2.42	0.46
1:A:582:VAL:HG11	1:A:626:TYR:HB3	1.97	0.46
1:E:742:VAL:HG11	1:E:751:VAL:HG11	1.98	0.46
1:C:522:GLY:HA2	1:C:611:THR:HG23	1.97	0.46
1:C:331:ASN:ND2	1:C:337:MSE:HA	2.20	0.46
1:C:273:GLU:CG	1:C:371:ILE:HD13	2.41	0.46
1:A:210:ILE:O	1:A:229:ASP:HB2	2.15	0.46
1:F:278:ARG:CG	1:F:280:PRO:HD3	2.46	0.46
1:D:383:ARG:H	1:D:747:ASN:ND2	2.13	0.46
1:D:447:ILE:O	1:D:447:ILE:HG22	2.16	0.46
1:E:707:LYS:O	1:E:733:GLY:HA3	2.15	0.46
1:B:165:GLU:HB3	1:B:171:ASN:CG	2.36	0.46
1:D:584:SER:HB3	1:D:589:LYS:HB3	1.98	0.46
1:B:24:ILE:HG23	1:B:56:PHE:CE1	2.50	0.46
1:A:542:PRO:O	1:A:559:GLY:CA	2.61	0.46
1:D:7:HIS:CD2	1:D:43:GLU:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:LYS:HD2	1:E:303:ILE:CD1	2.45	0.46
1:D:391:PRO:HB3	1:D:420:TYR:CD1	2.51	0.46
1:E:7:HIS:HB2	1:E:74:GLU:HB2	1.98	0.46
1:D:32:GLY:HA3	1:D:45:VAL:O	2.15	0.46
1:A:616:ASP:O	1:A:619:ALA:HB3	2.15	0.46
1:D:523:GLU:HG3	1:D:537:HIS:HB2	1.96	0.46
1:B:651:PHE:HB2	1:B:688:ALA:CB	2.46	0.46
1:D:618:ILE:O	1:D:622:LEU:HG	2.15	0.46
1:A:540:TYR:HA	1:A:608:ALA:O	2.15	0.46
1:A:592:PHE:O	1:A:595:VAL:HB	2.15	0.46
1:E:104:PRO:HB3	1:E:387:PHE:O	2.16	0.46
1:C:486:HIS:HD2	1:C:487:HIS:ND1	2.13	0.46
1:B:312:THR:HA	1:B:315:ILE:HG22	1.98	0.46
1:E:589:LYS:HG3	1:E:590:VAL:HG23	1.97	0.46
1:F:247:GLN:HG3	1:F:298:PRO:CG	2.41	0.46
1:A:171:ASN:ND2	1:A:173:ARG:HB2	2.30	0.46
1:D:749:VAL:O	1:D:753:GLN:HG3	2.16	0.46
1:C:620:VAL:C	1:C:622:LEU:N	2.68	0.46
1:E:570:LEU:O	1:E:574:ILE:HG12	2.16	0.46
1:A:239:LEU:O	1:A:239:LEU:HD23	2.16	0.46
1:A:239:LEU:HD13	1:A:250:PHE:CE1	2.50	0.46
1:B:255:LYS:HG2	1:B:256:ASP:OD2	2.16	0.46
1:D:57:ILE:HG13	1:D:75:LYS:HZ1	1.79	0.46
1:A:276:SER:OG	1:A:278:ARG:HG2	2.15	0.46
1:C:399:ASN:N	1:C:399:ASN:HD22	2.12	0.46
1:B:587:TYR:CD1	1:B:588:GLY:N	2.78	0.46
1:E:525:LEU:HA	1:E:535:LEU:HD13	1.98	0.46
1:E:16:GLY:O	1:E:19:PRO:HD2	2.16	0.46
1:D:127:PRO:O	1:D:311:GLY:HA3	2.16	0.46
1:D:190:LEU:HD12	1:D:355:PHE:O	2.16	0.46
1:D:286:LYS:HZ3	1:D:292:LEU:HB2	1.80	0.46
1:D:380:VAL:HG23	1:D:740:THR:CA	2.42	0.46
1:F:218:ILE:O	1:F:224:ILE:HG23	2.16	0.46
1:C:226:LEU:HD11	1:C:348:LEU:HD23	1.97	0.46
1:C:371:ILE:CD1	1:C:380:VAL:HG22	2.36	0.46
1:A:380:VAL:CG2	1:A:740:THR:HG23	2.45	0.46
1:D:475:ASN:HD21	1:E:590:VAL:N	2.14	0.46
1:B:181:CYS:SG	1:B:182:PRO:HD2	2.56	0.46
1:F:144:LEU:HA	1:F:145:PRO:C	2.36	0.46
1:A:664:GLU:O	1:A:667:GLN:HB3	2.16	0.46
1:F:413:VAL:CG1	1:F:420:TYR:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:460:LEU:CD2	1:F:515:THR:HG22	2.45	0.46
1:D:114:ARG:O	1:D:118:ASP:HB2	2.16	0.46
1:A:580:LYS:C	1:A:582:VAL:H	2.18	0.46
1:A:759:LEU:CD2	1:A:764:TYR:HB2	2.46	0.46
1:D:268:PRO:HG2	1:D:378:ARG:HH22	1.81	0.46
1:F:380:VAL:CG2	1:F:740:THR:HG23	2.46	0.46
1:A:464:TYR:C	1:A:466:THR:H	2.19	0.46
1:B:189:ARG:O	1:B:356:LEU:HA	2.15	0.46
1:A:121:ASN:HD22	1:A:123:ARG:H	1.63	0.46
1:F:205:LYS:HA	1:F:208:GLU:HG3	1.98	0.46
1:E:541:TYR:CG	1:E:560:ILE:HG22	2.51	0.46
1:B:410:ALA:HB3	1:B:747:ASN:O	2.16	0.46
1:E:545:GLY:HA3	1:E:548:LEU:HD12	1.98	0.46
1:F:542:PRO:HD2	1:F:563:LYS:HG3	1.98	0.46
1:E:335:MSE:CE	1:E:430:LYS:HG3	2.46	0.46
1:A:670:LEU:HA	1:A:673:ILE:HG12	1.98	0.46
1:E:369:SER:HB2	1:E:385:ARG:HB3	1.97	0.46
1:E:20:PHE:CZ	1:E:63:LYS:HB3	2.51	0.46
1:C:485:GLN:CG	1:C:488:TYR:H	2.20	0.46
1:C:738:VAL:HG21	1:C:744:ARG:HB3	1.98	0.46
1:A:225:HIS:CD2	1:A:327:MSE:HB3	2.51	0.46
1:B:228:CYS:SG	1:B:235:VAL:HG23	2.56	0.46
1:A:365:ARG:O	1:A:423:GLN:HG2	2.16	0.46
1:D:410:ALA:HB3	1:D:747:ASN:O	2.16	0.46
1:E:219:LYS:HA	1:E:224:ILE:HB	1.98	0.46
1:B:205:LYS:O	1:B:208:GLU:HB3	2.16	0.46
1:F:191:TYR:CD1	1:F:196:GLN:HB3	2.50	0.46
1:A:660:ILE:HG22	1:A:662:VAL:HG22	1.97	0.46
1:C:582:VAL:HG21	1:C:626:TYR:HB3	1.97	0.46
1:A:445:ARG:NH2	1:A:452:ASN:ND2	2.63	0.46
1:B:538:ILE:HG23	1:B:662:VAL:CG2	2.46	0.46
1:A:543:LEU:HD23	1:A:606:ALA:O	2.16	0.46
1:F:163:ARG:HA	1:F:166:TYR:HB3	1.97	0.46
1:A:126:TYR:OH	1:A:185:GLY:HA3	2.15	0.46
1:C:726:ARG:HH21	1:C:727:LYS:HA	1.81	0.46
1:E:301:HIS:CD2	1:E:301:HIS:N	2.83	0.46
1:D:432:GLU:H	1:D:432:GLU:CD	2.19	0.46
1:F:749:VAL:O	1:F:753:GLN:HG3	2.16	0.45
1:D:88:ILE:N	1:D:88:ILE:HD12	2.30	0.45
1:E:738:VAL:CG2	1:E:744:ARG:HG2	2.35	0.45
1:B:751:VAL:HG13	1:B:752:GLY:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:CB	1:A:289:PRO:HD3	2.34	0.45
1:D:233:GLU:HA	1:D:236:VAL:HG12	1.98	0.45
1:A:310:ALA:O	1:A:311:GLY:C	2.54	0.45
1:B:15:VAL:HG12	1:B:16:GLY:N	2.30	0.45
1:E:270:GLU:HB2	1:E:373:PHE:CE2	2.34	0.45
1:B:20:PHE:O	1:B:24:ILE:HG22	2.16	0.45
1:B:25:ALA:HA	1:B:56:PHE:HE1	1.80	0.45
1:C:649:LEU:HD12	1:C:650:LYS:N	2.31	0.45
1:D:406:GLU:HG3	1:D:407:LEU:N	2.31	0.45
1:C:595:VAL:HG12	1:C:595:VAL:O	2.16	0.45
1:C:151:THR:O	1:C:154:LYS:HB2	2.17	0.45
1:C:557:LEU:O	1:C:561:LEU:HG	2.15	0.45
1:A:651:PHE:HB2	1:A:688:ALA:HB2	1.97	0.45
1:E:62:LYS:O	1:E:63:LYS:HG3	2.16	0.45
1:C:485:GLN:CG	1:C:488:TYR:HB2	2.46	0.45
1:C:495:MSE:HE2	1:C:755:PHE:HZ	1.81	0.45
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.71	0.45
1:F:13:GLN:HB2	1:F:42:VAL:HG22	1.98	0.45
1:A:383:ARG:HD2	1:A:387:PHE:CD2	2.52	0.45
1:D:138:PHE:HB2	1:D:389:PRO:HD3	1.97	0.45
1:D:144:LEU:HA	1:D:145:PRO:C	2.37	0.45
1:D:181:CYS:HG	1:D:183:VAL:HG22	1.82	0.45
1:E:269:GLU:HB2	1:E:378:ARG:NH2	2.32	0.45
1:D:475:ASN:ND2	1:E:591:GLU:H	2.13	0.45
1:F:263:PHE:HD1	1:F:292:LEU:HD23	1.81	0.45
1:D:116:LEU:HG	1:D:117:PHE:N	2.32	0.45
1:A:451:LYS:HD3	1:A:477:LEU:HD11	1.97	0.45
1:D:261:LYS:HA	1:D:264:ALA:O	2.16	0.45
1:C:163:ARG:NH1	1:C:163:ARG:HB2	2.31	0.45
1:B:139:THR:HG21	1:B:222:GLY:HA3	1.97	0.45
1:A:9:GLN:NE2	1:A:40:ALA:HB1	2.31	0.45
1:D:752:GLY:O	1:D:756:LEU:HB2	2.16	0.45
1:F:506:ILE:CD1	1:F:694:ALA:HA	2.46	0.45
1:A:558:MSE:HE1	1:A:593:ASN:OD1	2.16	0.45
1:A:737:HIS:O	1:A:738:VAL:C	2.55	0.45
1:D:203:LEU:HD21	1:D:315:ILE:HG21	1.99	0.45
1:D:253:MSE:HE1	1:D:313:HIS:CG	2.51	0.45
1:D:370:VAL:CG2	1:D:381:ILE:HD11	2.47	0.45
1:A:216:VAL:O	1:A:227:ALA:HB3	2.16	0.45
1:F:619:ALA:HA	1:F:638:LEU:HD13	1.97	0.45
1:D:557:LEU:HD23	1:D:557:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:PRO:HG3	1:B:747:ASN:ND2	2.32	0.45
1:F:642:ALA:HB1	1:F:683:TYR:HA	1.98	0.45
1:F:217:ALA:HA	1:F:226:LEU:HA	1.97	0.45
1:E:485:GLN:NE2	1:E:486:HIS:N	2.64	0.45
1:E:15:VAL:HG12	1:E:16:GLY:N	2.31	0.45
1:A:739:THR:O	1:A:740:THR:C	2.55	0.45
1:C:140:ILE:HB	1:C:152:THR:CG2	2.46	0.45
1:F:589:LYS:HG3	1:F:590:VAL:HG23	1.98	0.45
1:A:158:MSE:HE3	1:A:163:ARG:HH12	1.81	0.45
1:B:738:VAL:HG12	1:B:742:VAL:O	2.17	0.45
1:C:67:LEU:HD21	1:C:106:ILE:HD11	1.98	0.45
1:A:134:CYS:SG	1:A:135:GLY:N	2.90	0.45
1:A:293:PRO:C	1:A:295:ASN:H	2.19	0.45
1:A:168:ASP:O	1:A:174:TYR:HD2	2.00	0.45
1:C:154:LYS:C	1:C:156:PHE:H	2.18	0.45
1:C:239:LEU:HD22	1:C:250:PHE:CE1	2.51	0.45
1:D:165:GLU:HB3	1:D:171:ASN:ND2	2.31	0.45
1:C:398:TYR:CE1	1:C:758:GLY:HA3	2.51	0.45
1:B:265:TYR:HE2	1:B:287:LYS:HD2	1.81	0.45
1:F:321:LYS:HB2	1:F:322:THR:H	1.61	0.45
1:A:288:GLU:HB3	1:A:289:PRO:CD	2.33	0.45
1:D:365:ARG:O	1:D:423:GLN:HG2	2.16	0.45
1:C:742:VAL:CG1	1:C:751:VAL:HG11	2.47	0.45
1:A:320:SER:O	1:A:322:THR:N	2.50	0.45
1:B:331:ASN:HD22	1:B:337:MSE:CA	2.23	0.45
1:D:142:GLU:O	1:D:143:ASP:HB2	2.16	0.45
1:D:391:PRO:HB2	1:D:418:LYS:HB2	1.98	0.45
1:C:411:PHE:CZ	1:C:441:ILE:HA	2.51	0.45
1:A:240:ARG:HB3	1:A:245:ARG:O	2.17	0.45
1:A:38:GLY:C	1:A:40:ALA:H	2.20	0.45
1:E:447:ILE:HG22	1:E:447:ILE:O	2.17	0.45
1:B:268:PRO:C	1:B:270:GLU:N	2.69	0.45
1:B:288:GLU:HB3	1:B:289:PRO:CD	2.33	0.45
1:A:553:PRO:HB2	1:A:620:VAL:CG2	2.33	0.45
1:A:591:GLU:O	1:A:594:VAL:HB	2.16	0.45
1:D:286:LYS:HE3	1:D:291:PRO:CD	2.46	0.45
1:C:331:ASN:HD22	1:C:337:MSE:CA	2.20	0.45
1:A:219:LYS:HG3	1:A:224:ILE:HG22	1.98	0.45
1:F:585:LEU:HB2	1:F:627:ARG:NH1	2.31	0.45
1:F:557:LEU:HD11	1:F:621:LEU:HA	1.99	0.45
1:B:374:VAL:CG1	1:B:744:ARG:HH22	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:579:PRO:O	1:E:582:VAL:HG23	2.17	0.45
1:D:249:PRO:HG3	1:D:300:LEU:CD1	2.40	0.45
1:A:235:VAL:HG23	1:A:236:VAL:N	2.32	0.45
1:B:134:CYS:SG	1:B:135:GLY:N	2.89	0.45
1:C:148:ARG:NH2	1:C:156:PHE:O	2.49	0.45
1:D:455:LEU:HD13	1:D:456:ILE:O	2.16	0.45
1:F:179:THR:HG23	1:F:179:THR:O	2.17	0.45
1:E:524:VAL:HG23	1:E:536:ALA:H	1.81	0.45
1:E:551:TYR:O	1:E:628:ARG:HB3	2.16	0.45
1:A:475:ASN:HD21	1:B:590:VAL:N	2.14	0.45
1:E:370:VAL:CG2	1:E:381:ILE:HD11	2.46	0.45
1:E:414:ALA:HB2	1:E:419:VAL:HA	1.99	0.45
1:E:450:VAL:HG22	1:E:451:LYS:N	2.31	0.45
1:B:524:VAL:HG22	1:B:536:ALA:H	1.81	0.45
1:B:765:LEU:HD21	1:B:770:LEU:CD2	2.40	0.45
1:D:202:PRO:O	1:D:203:LEU:C	2.54	0.45
1:C:306:MSE:CE	1:C:309:TYR:HE2	2.30	0.45
1:C:717:TYR:CE1	1:C:744:ARG:HG3	2.51	0.45
1:B:445:ARG:C	1:B:447:ILE:H	2.20	0.45
1:F:270:GLU:N	1:F:378:ARG:NH1	2.64	0.45
1:F:620:VAL:C	1:F:622:LEU:N	2.69	0.45
1:D:589:LYS:HG3	1:D:590:VAL:HG23	1.98	0.45
1:F:252:ILE:HG23	1:F:325:TYR:O	2.17	0.45
1:C:592:PHE:O	1:C:595:VAL:HB	2.17	0.45
1:E:415:LYS:HD3	1:E:448:LEU:CD2	2.44	0.45
1:A:633:GLU:N	1:A:634:PRO:CD	2.79	0.45
1:F:398:TYR:CG	1:F:398:TYR:O	2.70	0.45
1:D:239:LEU:C	1:D:239:LEU:HD23	2.37	0.45
1:F:428:THR:HA	1:F:433:VAL:HG11	1.99	0.45
1:F:613:ARG:HA	1:F:613:ARG:NE	2.29	0.45
1:E:335:MSE:HE1	1:E:430:LYS:HG3	1.99	0.45
1:B:130:VAL:HG11	1:B:178:PRO:O	2.17	0.45
1:D:31:ARG:HG2	1:D:85:ARG:HA	1.98	0.45
1:E:397:GLU:HB2	1:E:416:ASN:HA	1.99	0.45
1:A:589:LYS:HG2	1:B:475:ASN:OD1	2.17	0.45
1:B:766:THR:OG1	1:B:769:ASP:HB2	2.17	0.45
1:C:534:ARG:HG2	1:C:535:LEU:N	2.31	0.45
1:C:279:ARG:CB	1:C:309:TYR:HB3	2.47	0.45
1:E:151:THR:O	1:E:154:LYS:HB2	2.16	0.45
1:F:369:SER:OG	1:F:384:SER:N	2.49	0.45
1:F:282:ILE:HG23	1:F:283:THR:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:LEU:HB3	1:F:307:LEU:HD11	1.99	0.45
1:D:565:TYR:HB3	1:D:569:GLU:HB2	1.98	0.45
1:D:387:PHE:O	1:D:390:LEU:HG	2.17	0.45
1:C:61:TYR:CD2	1:C:61:TYR:N	2.85	0.45
1:B:616:ASP:HA	1:B:634:PRO:HB2	1.99	0.45
1:D:581:ALA:HA	1:D:584:SER:HB3	1.98	0.45
1:D:582:VAL:C	1:D:584:SER:H	2.19	0.45
1:E:629:HIS:HB2	1:E:633:GLU:OE1	2.17	0.45
1:A:532:VAL:HG12	1:A:533:GLU:N	2.32	0.45
1:F:429:GLY:HA2	1:F:465:ASN:ND2	2.32	0.45
1:E:393:GLU:HA	1:E:417:GLY:O	2.17	0.45
1:C:394:ILE:CD1	1:C:419:VAL:HB	2.47	0.45
1:E:460:LEU:HD12	1:E:483:GLN:HB3	1.98	0.45
1:A:124:TYR:CD2	1:A:125:MSE:HG2	2.51	0.45
1:B:530:GLU:O	1:B:531:ASP:HB2	2.16	0.45
1:D:345:PHE:C	1:D:347:GLU:H	2.20	0.45
1:B:250:PHE:CD2	1:B:328:THR:HG21	2.52	0.45
1:B:219:LYS:HE2	1:B:358:HIS:O	2.17	0.45
1:C:196:GLN:CG	1:C:197:GLU:N	2.77	0.45
1:B:270:GLU:CD	1:B:284:LEU:HD21	2.37	0.45
1:D:306:MSE:HE1	1:D:309:TYR:HE2	1.82	0.45
1:A:108:ILE:CG1	1:A:310:ALA:HA	2.34	0.45
1:A:292:LEU:HB3	1:A:296:LEU:HD22	1.99	0.45
1:B:443:HIS:O	1:B:447:ILE:HD12	2.16	0.45
1:F:373:PHE:CD2	1:F:378:ARG:HD3	2.52	0.45
1:E:474:ALA:HB2	1:E:481:LEU:HD13	1.98	0.45
1:A:3:ALA:HB2	1:A:47:GLU:CA	2.44	0.45
1:F:89:GLU:HG3	1:F:175:HIS:CE1	2.52	0.45
1:E:230:ALA:HB3	1:E:324:VAL:CG2	2.47	0.45
1:E:286:LYS:HE3	1:E:290:PHE:CB	2.46	0.45
1:A:653:VAL:CG1	1:A:692:ALA:HB3	2.46	0.45
1:C:553:PRO:HB2	1:C:620:VAL:CG2	2.46	0.45
1:E:521:GLY:CA	1:E:610:SER:HA	2.46	0.45
1:D:376:GLY:HA2	1:D:726:ARG:HH11	1.81	0.45
1:B:415:LYS:C	1:B:417:GLY:H	2.19	0.45
1:B:219:LYS:HB2	1:B:357:LEU:HA	1.99	0.45
1:B:371:ILE:CB	1:B:380:VAL:HG13	2.43	0.45
1:A:738:VAL:HB	1:A:744:ARG:HG2	1.98	0.45
1:D:292:LEU:HD12	1:D:296:LEU:HD21	1.99	0.45
1:D:739:THR:OG1	1:D:740:THR:N	2.49	0.45
1:B:614:VAL:HG13	1:B:666:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:GLU:O	1:C:274:LEU:HB2	2.16	0.45
1:A:207:ALA:HB1	1:A:320:SER:CB	2.42	0.45
1:A:225:HIS:HA	1:A:330:ALA:H	1.82	0.45
1:A:263:PHE:HE1	1:A:292:LEU:HG	1.81	0.45
1:F:384:SER:HB2	1:F:385:ARG:H	1.57	0.45
1:F:11:ILE:HG12	1:F:15:VAL:HG21	1.98	0.45
1:A:428:THR:HG21	1:A:466:THR:HG22	1.99	0.45
1:A:466:THR:OG1	1:A:467:THR:N	2.50	0.45
1:D:552:TYR:CD1	1:D:627:ARG:HG3	2.52	0.45
1:D:142:GLU:HB3	1:D:150:ASN:C	2.36	0.45
1:E:504:ILE:CG2	1:E:505:GLY:N	2.80	0.45
1:F:573:VAL:HG13	1:F:574:ILE:N	2.31	0.45
1:E:232:ASN:HB3	1:E:235:VAL:CG2	2.46	0.45
1:B:461:HIS:HB2	1:B:513:TYR:CB	2.47	0.45
1:C:641:PHE:CE2	1:C:679:ALA:HA	2.52	0.45
1:F:294:GLU:HG2	1:F:294:GLU:O	2.17	0.45
1:F:413:VAL:HG11	1:F:448:LEU:HD11	1.99	0.44
1:D:118:ASP:HA	1:D:119:PRO:HD3	1.74	0.44
1:B:270:GLU:OE2	1:B:284:LEU:HD21	2.17	0.44
1:E:523:GLU:HB2	1:E:525:LEU:HD21	1.99	0.44
1:A:157:PRO:O	1:A:184:CYS:HB2	2.16	0.44
1:E:372:ARG:NH2	1:E:717:TYR:HB3	2.31	0.44
1:A:709:VAL:O	1:A:735:ASN:HB2	2.17	0.44
1:D:191:TYR:HA	1:D:195:GLY:O	2.17	0.44
1:D:274:LEU:HD21	1:D:282:ILE:HG22	1.99	0.44
1:C:487:HIS:CD2	1:C:520:TRP:HB3	2.51	0.44
1:C:292:LEU:HD13	1:C:293:PRO:CD	2.43	0.44
1:A:409:ASN:CG	1:A:425:ILE:HD11	2.37	0.44
1:D:447:ILE:HD12	1:D:447:ILE:N	2.32	0.44
1:C:144:LEU:HA	1:C:145:PRO:C	2.37	0.44
1:D:300:LEU:HD21	1:D:636:MSE:HE2	1.99	0.44
1:B:506:ILE:HG22	1:B:508:LEU:HG	1.98	0.44
1:E:24:ILE:HG12	1:E:56:PHE:CD1	2.51	0.44
1:E:522:GLY:HA2	1:E:611:THR:HG23	1.98	0.44
1:B:159:CYS:SG	1:B:183:VAL:HG21	2.58	0.44
1:D:246:PRO:HG2	1:D:629:HIS:HB3	1.97	0.44
1:E:257:ILE:HA	1:E:260:VAL:CG2	2.46	0.44
1:F:44:ILE:HG22	1:F:45:VAL:H	1.82	0.44
1:B:568:ASP:O	1:B:571:GLU:HB3	2.17	0.44
1:F:497:GLU:CD	1:F:739:THR:HG22	2.37	0.44
1:B:487:HIS:CE1	1:B:509:ASP:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:HIS:CD2	1:B:43:GLU:HB3	2.52	0.44
1:F:524:VAL:CG2	1:F:536:ALA:H	2.30	0.44
1:D:253:MSE:HA	1:D:306:MSE:O	2.16	0.44
1:D:312:THR:O	1:D:315:ILE:HG22	2.18	0.44
1:C:233:GLU:HB2	1:C:293:PRO:HB3	1.99	0.44
1:A:251:ALA:O	1:A:326:VAL:HA	2.17	0.44
1:F:522:GLY:CA	1:F:611:THR:HG23	2.47	0.44
1:F:67:LEU:CD1	1:F:106:ILE:HD13	2.47	0.44
1:F:619:ALA:HB2	1:F:638:LEU:HD22	1.98	0.44
1:E:543:LEU:HD12	1:E:549:ALA:CB	2.46	0.44
1:E:425:ILE:HG22	1:E:436:PHE:CD1	2.52	0.44
1:C:66:PRO:HD3	1:C:133:ASN:HB3	1.99	0.44
1:D:552:TYR:HD1	1:D:627:ARG:HG3	1.82	0.44
1:F:35:LYS:CG	1:F:90:LYS:HD2	2.41	0.44
1:D:584:SER:CB	1:D:589:LYS:HB3	2.47	0.44
1:C:554:LEU:CG	1:C:558:MSE:HE3	2.47	0.44
1:C:34:VAL:HG23	1:C:43:GLU:O	2.18	0.44
1:A:116:LEU:HG	1:A:117:PHE:N	2.32	0.44
1:F:62:LYS:C	1:F:64:LYS:H	2.20	0.44
1:C:614:VAL:HG13	1:C:666:PHE:CE2	2.53	0.44
1:A:732:ASN:OD1	1:A:733:GLY:N	2.51	0.44
1:A:399:ASN:HA	1:A:414:ALA:O	2.17	0.44
1:F:639:GLU:OE2	1:F:718:ASN:HA	2.16	0.44
1:F:748:GLY:O	1:F:751:VAL:HG12	2.16	0.44
1:B:401:LEU:HD12	1:B:402:ALA:N	2.32	0.44
1:A:529:TYR:CE1	1:A:759:LEU:HD11	2.52	0.44
1:D:286:LYS:HE3	1:D:291:PRO:HD2	2.00	0.44
1:D:281:ILE:CB	1:D:370:VAL:HG12	2.36	0.44
1:A:263:PHE:O	1:A:264:ALA:HB2	2.18	0.44
1:B:15:VAL:HG21	1:B:67:LEU:O	2.18	0.44
1:D:504:ILE:HG13	1:D:706:VAL:HG21	1.99	0.44
1:D:601:LYS:HZ2	1:E:771:MSE:HE3	1.82	0.44
1:F:329:SER:HA	1:F:337:MSE:HE2	1.99	0.44
1:B:383:ARG:NH1	1:B:387:PHE:HB3	2.32	0.44
1:C:412:GLY:HA3	1:C:750:ASN:ND2	2.32	0.44
1:D:257:ILE:HD12	1:D:260:VAL:CG2	2.47	0.44
1:D:399:ASN:ND2	1:D:399:ASN:N	2.66	0.44
1:C:567:ILE:HG12	1:C:600:ALA:HB1	1.99	0.44
1:A:772:LEU:HD11	1:B:601:LYS:HD3	1.99	0.44
1:C:501:ASP:O	1:C:503:VAL:HG22	2.17	0.44
1:C:128:PHE:CD1	1:C:186:PRO:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:567:ILE:HG12	1:F:600:ALA:HB1	1.98	0.44
1:B:6:ILE:HG13	1:B:57:ILE:HD12	1.98	0.44
1:D:219:LYS:HG3	1:D:224:ILE:CG2	2.43	0.44
1:D:281:ILE:HG23	1:D:306:MSE:HG3	2.00	0.44
1:C:317:PHE:HE2	1:C:323:PRO:CA	2.27	0.44
1:A:252:ILE:CG2	1:A:324:VAL:HB	2.48	0.44
1:B:319:TRP:O	1:B:320:SER:O	2.36	0.44
1:B:337:MSE:CE	1:B:367:ASP:HA	2.41	0.44
1:A:312:THR:HA	1:A:315:ILE:HG22	2.00	0.44
1:B:25:ALA:HA	1:B:56:PHE:CE1	2.52	0.44
1:E:286:LYS:CE	1:E:290:PHE:HB2	2.46	0.44
1:E:498:LYS:HB2	1:E:500:LEU:CD1	2.48	0.44
1:D:261:LYS:HD3	1:D:266:VAL:CG2	2.47	0.44
1:F:736:PHE:N	1:F:736:PHE:CD2	2.84	0.44
1:B:313:HIS:CE1	1:B:327:MSE:HE2	2.49	0.44
1:A:582:VAL:HB	1:A:583:GLU:OE1	2.18	0.44
1:B:495:MSE:HA	1:B:500:LEU:HD21	2.00	0.44
1:F:215:ILE:CG2	1:F:239:LEU:HD12	2.47	0.44
1:A:748:GLY:O	1:A:751:VAL:HG12	2.18	0.44
1:D:219:LYS:HA	1:D:224:ILE:CG2	2.46	0.44
1:D:286:LYS:NZ	1:D:292:LEU:HB2	2.32	0.44
1:C:504:ILE:CG2	1:C:505:GLY:N	2.81	0.44
1:F:219:LYS:HG2	1:F:358:HIS:NE2	2.32	0.44
1:D:413:VAL:HG21	1:D:448:LEU:HD13	1.99	0.44
1:D:396:PHE:O	1:D:417:GLY:HA2	2.18	0.44
1:C:219:LYS:HE3	1:C:358:HIS:ND1	2.33	0.44
1:C:450:VAL:HG22	1:C:451:LYS:N	2.30	0.44
1:E:410:ALA:CA	1:E:425:ILE:HD11	2.47	0.44
1:B:738:VAL:HG23	1:B:744:ARG:HG2	1.99	0.44
1:B:422:SER:HA	1:B:444:PHE:CZ	2.53	0.44
1:F:230:ALA:HB2	1:F:325:TYR:O	2.17	0.44
1:C:30:LEU:O	1:C:30:LEU:HD23	2.18	0.44
1:F:443:HIS:O	1:F:447:ILE:HD12	2.18	0.44
1:C:87:TYR:C	1:C:88:ILE:HG13	2.37	0.44
1:C:278:ARG:CZ	1:C:387:PHE:HE1	2.29	0.44
1:B:572:GLY:O	1:B:575:ASN:HB2	2.17	0.44
1:B:541:TYR:CB	1:B:560:ILE:HG22	2.48	0.44
1:A:401:LEU:HD12	1:A:402:ALA:N	2.32	0.44
1:A:35:LYS:HG2	1:A:36:ASN:N	2.33	0.44
1:D:482:LEU:HD11	1:D:770:LEU:HD13	2.00	0.44
1:F:476:GLU:C	1:F:478:ASP:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:TYR:CE2	1:C:125:MSE:HG2	2.52	0.44
1:B:714:GLY:C	1:B:716:ALA:H	2.20	0.44
1:D:759:LEU:CD1	1:D:764:TYR:HB2	2.46	0.44
1:F:742:VAL:HG13	1:F:743:PRO:HD2	2.00	0.44
1:B:370:VAL:HG23	1:B:381:ILE:HD11	1.99	0.44
1:A:587:TYR:OH	1:B:468:LYS:HG3	2.18	0.44
1:E:278:ARG:CZ	1:E:387:PHE:HE1	2.30	0.44
1:D:312:THR:O	1:D:316:LEU:HB2	2.18	0.44
1:D:315:ILE:HG23	1:D:316:LEU:N	2.32	0.44
1:C:233:GLU:O	1:C:236:VAL:HG12	2.18	0.44
1:A:381:ILE:HG13	1:A:382:ARG:N	2.33	0.44
1:B:144:LEU:HA	1:B:145:PRO:C	2.37	0.44
1:A:188:TYR:CE1	1:A:358:HIS:HD2	2.36	0.44
1:D:491:ILE:CG2	1:D:527:LEU:HD21	2.44	0.44
1:C:451:LYS:O	1:C:452:ASN:C	2.55	0.44
1:D:225:HIS:CA	1:D:330:ALA:HB2	2.40	0.44
1:F:521:GLY:CA	1:F:610:SER:HA	2.41	0.44
1:B:653:VAL:CG1	1:B:692:ALA:HB3	2.43	0.44
1:C:132:THR:HG23	1:C:133:ASN:OD1	2.18	0.44
1:D:541:TYR:CZ	1:D:609:SER:HA	2.53	0.44
1:F:286:LYS:HE3	1:F:290:PHE:HB2	1.99	0.44
1:D:216:VAL:HB	1:D:354:TYR:HB2	1.99	0.44
1:A:144:LEU:HA	1:A:145:PRO:C	2.37	0.44
1:C:134:CYS:SG	1:C:135:GLY:N	2.90	0.44
1:C:192:THR:C	1:C:194:ASP:N	2.69	0.44
1:F:142:GLU:HB3	1:F:150:ASN:C	2.38	0.44
1:C:239:LEU:C	1:C:239:LEU:HD23	2.38	0.44
1:A:415:LYS:O	1:A:417:GLY:N	2.48	0.44
1:D:462:PRO:HG2	1:E:604:ASN:ND2	2.32	0.44
1:D:130:VAL:HG22	1:D:131:CYS:O	2.17	0.44
1:A:104:PRO:HG3	1:A:390:LEU:HD11	2.00	0.44
1:D:599:LEU:O	1:D:599:LEU:HD22	2.17	0.44
1:F:599:LEU:O	1:F:599:LEU:HD13	2.17	0.44
1:B:405:ALA:H	1:B:749:VAL:HG11	1.83	0.44
1:B:253:MSE:HE2	1:B:317:PHE:CD1	2.52	0.44
1:F:401:LEU:HD12	1:F:412:GLY:O	2.18	0.44
1:F:457:ILE:HA	1:F:482:LEU:O	2.17	0.44
1:D:269:GLU:HB2	1:D:378:ARG:NH2	2.33	0.44
1:C:485:GLN:CD	1:C:514:GLY:HA2	2.37	0.44
1:C:283:THR:OG1	1:C:372:ARG:HB2	2.17	0.44
1:B:210:ILE:HD11	1:B:228:CYS:CA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:ALA:HA	1:F:146:TYR:CD1	2.52	0.44
1:F:9:GLN:HB2	1:F:72:ARG:HH21	1.83	0.44
1:D:383:ARG:CZ	1:D:421:PRO:HG3	2.48	0.44
1:D:570:LEU:HD12	1:D:573:VAL:CG1	2.48	0.44
1:D:116:LEU:HG	1:D:117:PHE:H	1.83	0.44
1:D:428:THR:HG21	1:D:466:THR:HG22	2.00	0.44
1:A:612:GLY:HA2	1:A:615:LEU:HD23	1.99	0.44
1:A:615:LEU:HD21	1:A:635:ALA:CB	2.47	0.44
1:C:401:LEU:HD12	1:C:412:GLY:O	2.18	0.44
1:E:677:SER:O	1:E:681:ILE:HG12	2.17	0.44
1:F:565:TYR:HB3	1:F:569:GLU:HG2	2.00	0.44
1:D:727:LYS:O	1:D:730:GLU:HG2	2.17	0.44
1:F:1:MSE:HG2	1:F:83:PHE:HD1	1.83	0.44
1:F:707:LYS:HB3	1:F:708:ASN:HD22	1.83	0.44
1:B:288:GLU:CB	1:B:289:PRO:CD	2.94	0.44
1:A:584:SER:HA	1:A:587:TYR:O	2.17	0.44
1:E:756:LEU:HD21	1:E:770:LEU:HD22	2.00	0.44
1:F:251:ALA:O	1:F:326:VAL:HA	2.18	0.44
1:D:252:ILE:HD13	1:D:303:ILE:HG22	1.99	0.44
1:C:485:GLN:HE21	1:C:486:HIS:N	2.16	0.44
1:F:270:GLU:HA	1:F:373:PHE:HE2	1.83	0.44
1:F:543:LEU:HG	1:F:543:LEU:O	2.17	0.44
1:B:506:ILE:HD11	1:B:694:ALA:HA	1.99	0.44
1:A:213:GLY:O	1:A:235:VAL:HG11	2.17	0.44
1:D:579:PRO:HB3	1:D:626:TYR:CE1	2.52	0.44
1:B:54:GLU:C	1:B:56:PHE:H	2.20	0.44
1:E:341:ASN:HB3	1:E:357:LEU:HD13	2.00	0.44
1:B:181:CYS:SG	1:B:182:PRO:N	2.91	0.44
1:F:364:ASN:HD21	1:F:443:HIS:CD2	2.34	0.44
1:C:18:ARG:O	1:C:21:VAL:HG12	2.18	0.44
1:A:653:VAL:HG23	1:A:662:VAL:HA	1.99	0.44
1:F:125:MSE:O	1:F:315:ILE:HD12	2.18	0.44
1:F:315:ILE:HG12	1:F:319:TRP:CZ3	2.53	0.44
1:C:560:ILE:HD12	1:C:561:LEU:N	2.33	0.44
1:A:567:ILE:HG23	1:A:600:ALA:HB2	1.99	0.44
1:C:45:VAL:HG12	1:C:45:VAL:O	2.16	0.44
1:A:343:ARG:HG2	1:A:343:ARG:HH11	1.83	0.44
1:B:293:PRO:O	1:B:296:LEU:HD13	2.18	0.44
1:E:163:ARG:O	1:E:166:TYR:HB3	2.18	0.44
1:C:518:ASN:HB3	1:C:540:TYR:HE2	1.82	0.44
1:C:491:ILE:HD12	1:C:525:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LYS:HA	1:C:261:LYS:HD2	1.82	0.44
1:F:12:VAL:HG22	1:F:42:VAL:HG11	2.00	0.44
1:A:455:LEU:HB3	1:A:480:GLU:HB3	2.00	0.44
1:B:249:PRO:CG	1:B:300:LEU:HD13	2.37	0.44
1:B:413:VAL:CG1	1:B:420:TYR:HB2	2.47	0.44
1:B:412:GLY:HA2	1:B:420:TYR:O	2.17	0.44
1:C:447:ILE:C	1:C:448:LEU:HD23	2.38	0.44
1:C:581:ALA:HA	1:C:584:SER:HB3	1.98	0.44
1:C:603:ILE:HD11	1:F:772:LEU:HD21	1.99	0.44
1:B:1:MSE:HG2	1:B:83:PHE:CD1	2.50	0.44
1:B:687:LEU:HD22	1:B:724:MSE:SE	2.68	0.44
1:A:373:PHE:CE2	1:A:378:ARG:HD3	2.53	0.43
1:B:338:VAL:O	1:B:338:VAL:HG13	2.18	0.43
1:B:584:SER:HA	1:B:587:TYR:O	2.18	0.43
1:B:525:LEU:C	1:B:535:LEU:HD13	2.39	0.43
1:D:189:ARG:HD2	1:D:191:TYR:OH	2.18	0.43
1:C:370:VAL:CG2	1:C:382:ARG:HB2	2.48	0.43
1:B:8:VAL:O	1:B:9:GLN:HG3	2.18	0.43
1:E:718:ASN:HB3	1:E:721:ILE:HB	2.00	0.43
1:D:383:ARG:NH2	1:D:390:LEU:O	2.51	0.43
1:D:504:ILE:CG2	1:D:505:GLY:H	2.31	0.43
1:C:140:ILE:HB	1:C:152:THR:HG22	1.99	0.43
1:A:163:ARG:HB2	1:A:163:ARG:NH1	2.21	0.43
1:C:409:ASN:CG	1:C:410:ALA:H	2.22	0.43
1:A:312:THR:HA	1:A:315:ILE:CG2	2.48	0.43
1:F:629:HIS:HB2	1:F:633:GLU:OE1	2.17	0.43
1:C:299:GLY:C	1:C:300:LEU:HG	2.38	0.43
1:C:339:LYS:HB2	1:C:339:LYS:HE3	1.79	0.43
1:C:24:ILE:HD11	1:C:59:ASP:HB2	2.00	0.43
1:C:130:VAL:CG2	1:C:131:CYS:N	2.81	0.43
1:A:50:GLU:HA	1:A:53:ILE:HG22	2.01	0.43
1:F:613:ARG:HH22	1:F:628:ARG:HH22	1.66	0.43
1:B:651:PHE:CE2	1:B:669:ILE:HA	2.49	0.43
1:E:401:LEU:O	1:E:456:ILE:HG23	2.18	0.43
1:D:643:PHE:C	1:D:645:GLY:H	2.21	0.43
1:A:568:ASP:O	1:A:571:GLU:HB3	2.16	0.43
1:A:373:PHE:CE1	1:A:378:ARG:HB3	2.52	0.43
1:F:487:HIS:NE2	1:F:520:TRP:HB3	2.33	0.43
1:C:190:LEU:O	1:C:196:GLN:HA	2.19	0.43
1:B:492:ALA:CB	1:B:756:LEU:HD12	2.49	0.43
1:D:198:ILE:HG22	1:D:199:TYR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:LEU:HD12	1:C:330:ALA:HA	2.00	0.43
1:C:270:GLU:N	1:C:378:ARG:HH12	2.16	0.43
1:A:253:MSE:HE2	1:A:317:PHE:CE1	2.53	0.43
1:F:368:ASP:HA	1:F:385:ARG:HD3	2.00	0.43
1:B:65:PRO:HG2	1:B:68:ALA:HB3	1.99	0.43
1:F:282:ILE:HG22	1:F:305:VAL:HB	1.99	0.43
1:A:148:ARG:HH22	1:A:158:MSE:HG3	1.83	0.43
1:E:181:CYS:SG	1:E:182:PRO:CD	3.06	0.43
1:E:729:VAL:HG12	1:E:733:GLY:O	2.18	0.43
1:D:589:LYS:HG3	1:E:475:ASN:HD21	1.83	0.43
1:E:616:ASP:HB3	1:E:634:PRO:CG	2.47	0.43
1:D:12:VAL:HG22	1:D:17:PHE:CE1	2.53	0.43
1:F:383:ARG:NH1	1:F:387:PHE:HB3	2.32	0.43
1:B:691:ARG:HH11	1:B:695:HIS:HD2	1.65	0.43
1:E:334:GLY:HA3	1:E:335:MSE:HE2	2.00	0.43
1:E:578:CYS:O	1:E:578:CYS:SG	2.76	0.43
1:F:757:GLY:C	1:F:759:LEU:H	2.21	0.43
1:F:759:LEU:CD1	1:F:764:TYR:HB2	2.48	0.43
1:A:269:GLU:O	1:A:272:GLU:HB3	2.18	0.43
1:F:526:TYR:CB	1:F:535:LEU:HD11	2.47	0.43
1:E:18:ARG:HD2	1:E:175:HIS:ND1	2.33	0.43
1:D:204:ARG:C	1:D:204:ARG:HD2	2.38	0.43
1:D:102:ILE:HD12	1:D:141:ILE:HG21	2.00	0.43
1:D:491:ILE:HD11	1:D:505:GLY:C	2.38	0.43
1:C:543:LEU:HD12	1:C:549:ALA:HB3	2.00	0.43
1:D:338:VAL:HG11	1:D:348:LEU:HD11	1.99	0.43
1:E:620:VAL:HG13	1:E:626:TYR:HD1	1.82	0.43
1:B:409:ASN:ND2	1:B:425:ILE:HD11	2.33	0.43
1:A:329:SER:HB2	1:A:331:ASN:ND2	2.31	0.43
1:C:18:ARG:NH2	1:C:36:ASN:ND2	2.66	0.43
1:A:36:ASN:OD1	1:A:42:VAL:HG22	2.18	0.43
1:E:236:VAL:HG13	1:E:295:ASN:ND2	2.32	0.43
1:A:341:ASN:O	1:A:344:ALA:HB3	2.18	0.43
1:F:52:ASP:O	1:F:56:PHE:HB3	2.19	0.43
1:F:694:ALA:O	1:F:696:THR:N	2.51	0.43
1:F:729:VAL:CB	1:F:735:ASN:HD22	2.29	0.43
1:D:18:ARG:CB	1:D:19:PRO:HD3	2.48	0.43
1:A:560:ILE:HD12	1:A:561:LEU:N	2.33	0.43
1:E:395:PRO:HG2	1:E:396:PHE:CE2	2.52	0.43
1:B:396:PHE:CZ	1:B:759:LEU:HD13	2.54	0.43
1:C:348:LEU:HD12	1:C:348:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASP:CG	1:B:40:ALA:H	2.22	0.43
1:B:106:ILE:CG2	1:B:277:TYR:HB2	2.37	0.43
1:A:406:GLU:HA	1:A:466:THR:CG2	2.48	0.43
1:A:603:ILE:HD11	1:B:772:LEU:HD21	2.00	0.43
1:A:654:PRO:HG2	1:A:661:ARG:HB2	2.01	0.43
1:D:163:ARG:HB2	1:D:163:ARG:NH1	2.28	0.43
1:F:360:ARG:HG2	1:F:360:ARG:HH11	1.83	0.43
1:F:213:GLY:HA3	1:F:235:VAL:HG11	2.00	0.43
1:C:209:LEU:O	1:C:212:LYS:HB3	2.17	0.43
1:F:564:VAL:HG11	1:F:667:GLN:HB2	1.99	0.43
1:B:296:LEU:HD12	1:B:296:LEU:N	2.32	0.43
1:B:282:ILE:HA	1:B:371:ILE:O	2.18	0.43
1:C:197:GLU:OE2	1:D:124:TYR:CD1	2.71	0.43
1:A:595:VAL:HG12	1:A:595:VAL:O	2.18	0.43
1:E:494:VAL:O	1:E:496:ALA:N	2.51	0.43
1:F:227:ALA:HA	1:F:326:VAL:O	2.19	0.43
1:A:151:THR:O	1:A:154:LYS:HB2	2.18	0.43
1:E:207:ALA:HB1	1:E:320:SER:HB2	2.00	0.43
1:D:595:VAL:HG12	1:D:595:VAL:O	2.19	0.43
1:D:589:LYS:CG	1:E:475:ASN:HD21	2.31	0.43
1:F:302:THR:O	1:F:303:ILE:HG13	2.17	0.43
1:F:323:PRO:HG2	1:F:324:VAL:H	1.83	0.43
1:D:36:ASN:HA	1:D:42:VAL:HG22	2.01	0.43
1:C:28:HIS:CE1	1:C:55:ALA:HB1	2.54	0.43
1:D:539:ASP:CA	1:D:659:LEU:HD11	2.45	0.43
1:D:163:ARG:HA	1:D:166:TYR:HB3	1.99	0.43
1:D:20:PHE:CZ	1:D:64:LYS:HA	2.54	0.43
1:A:12:VAL:HG13	1:A:17:PHE:CD2	2.53	0.43
1:A:12:VAL:HG13	1:A:17:PHE:CG	2.53	0.43
1:F:221:ILE:HG22	1:F:360:ARG:HH21	1.82	0.43
1:C:364:ASN:HD21	1:C:443:HIS:CD2	2.35	0.43
1:C:472:GLU:HG3	1:C:473:MSE:N	2.32	0.43
1:F:498:LYS:HB2	1:F:500:LEU:CD2	2.47	0.43
1:B:230:ALA:HB2	1:B:325:TYR:O	2.18	0.43
1:B:323:PRO:HG2	1:B:324:VAL:H	1.83	0.43
1:B:219:LYS:CD	1:B:358:HIS:H	2.30	0.43
1:F:490:HIS:C	1:F:492:ALA:N	2.70	0.43
1:E:279:ARG:CB	1:E:309:TYR:HB3	2.48	0.43
1:E:370:VAL:HG22	1:E:382:ARG:HB2	2.00	0.43
1:A:501:ASP:O	1:A:502:SER:C	2.56	0.43
1:C:742:VAL:HG11	1:C:751:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ALA:HA	1:B:146:TYR:CD1	2.54	0.43
1:A:339:LYS:HG3	1:A:365:ARG:NH1	2.33	0.43
1:A:406:GLU:HG3	1:A:407:LEU:N	2.33	0.43
1:D:102:ILE:CD1	1:D:144:LEU:HG	2.40	0.43
1:E:425:ILE:HG22	1:E:436:PHE:CE1	2.53	0.43
1:E:584:SER:HB3	1:E:589:LYS:HB3	1.99	0.43
1:B:17:PHE:CZ	1:B:60:LEU:HG	2.54	0.43
1:E:502:SER:CB	1:E:528:GLY:HA2	2.48	0.43
1:D:614:VAL:HG13	1:D:666:PHE:CZ	2.53	0.43
1:F:383:ARG:CZ	1:F:421:PRO:CG	2.97	0.43
1:E:294:GLU:HG2	1:E:294:GLU:O	2.19	0.43
1:F:739:THR:O	1:F:742:VAL:O	2.37	0.43
1:B:485:GLN:HG3	1:B:487:HIS:N	2.34	0.43
1:B:253:MSE:HE1	1:B:313:HIS:ND1	2.34	0.43
1:F:485:GLN:HG2	1:F:488:TYR:CD2	2.54	0.43
1:E:392:ILE:HB	1:E:419:VAL:CG1	2.49	0.43
1:E:19:PRO:HG2	1:E:132:THR:HG21	2.01	0.43
1:A:742:VAL:CG1	1:A:751:VAL:HG11	2.48	0.43
1:C:261:LYS:CE	1:C:266:VAL:HB	2.49	0.43
1:F:577:CYS:SG	1:F:579:PRO:HD3	2.59	0.43
1:C:224:ILE:CG2	1:C:338:VAL:HG13	2.48	0.43
1:B:593:ASN:C	1:B:595:VAL:N	2.71	0.43
1:C:543:LEU:CD2	1:C:543:LEU:H	2.23	0.43
1:A:625:ALA:HB2	1:A:637:LYS:CD	2.42	0.43
1:B:547:ASP:O	1:B:550:SER:HB2	2.19	0.43
1:F:263:PHE:O	1:F:264:ALA:HB2	2.17	0.43
1:B:209:LEU:O	1:B:212:LYS:HB2	2.18	0.43
1:D:404:GLY:HA2	1:D:753:GLN:HE22	1.82	0.43
1:D:564:VAL:HG13	1:D:667:GLN:NE2	2.30	0.43
1:C:570:LEU:HA	1:C:573:VAL:HG12	2.01	0.43
1:F:118:ASP:HA	1:F:119:PRO:HD3	1.75	0.43
1:B:686:HIS:CD2	1:B:720:LEU:HD12	2.54	0.43
1:C:5:HIS:HB3	1:C:76:LYS:HD2	2.00	0.43
1:B:118:ASP:HA	1:B:119:PRO:HD3	1.74	0.43
1:D:738:VAL:HG11	1:D:742:VAL:HG12	2.01	0.43
1:B:286:LYS:CE	1:B:290:PHE:HB2	2.49	0.43
1:E:370:VAL:H	1:E:382:ARG:CB	2.32	0.43
1:A:766:THR:OG1	1:A:769:ASP:HB2	2.18	0.43
1:D:319:TRP:O	1:D:320:SER:C	2.55	0.43
1:D:380:VAL:CG2	1:D:740:THR:HG23	2.47	0.43
1:C:396:PHE:CZ	1:C:759:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD12	1:A:330:ALA:CB	2.49	0.43
1:A:348:LEU:HB3	1:A:351:VAL:HB	2.01	0.43
1:F:12:VAL:HG23	1:F:17:PHE:CG	2.53	0.43
1:A:457:ILE:CG2	1:A:753:GLN:HB3	2.41	0.43
1:D:415:LYS:C	1:D:417:GLY:H	2.22	0.43
1:B:494:VAL:HG22	1:B:738:VAL:CG2	2.40	0.43
1:B:406:GLU:HA	1:B:466:THR:CG2	2.49	0.43
1:B:506:ILE:HD12	1:B:725:ILE:HG23	2.00	0.43
1:E:171:ASN:HD21	1:E:173:ARG:HB2	1.82	0.43
1:B:159:CYS:O	1:B:160:ASP:C	2.57	0.43
1:B:34:VAL:HG12	1:B:87:TYR:CE1	2.49	0.43
1:E:286:LYS:HE3	1:E:290:PHE:CA	2.48	0.43
1:E:286:LYS:HE3	1:E:290:PHE:HA	2.01	0.43
1:A:665:LEU:O	1:A:669:ILE:HG13	2.18	0.43
1:F:123:ARG:NH2	1:F:173:ARG:HG2	2.33	0.43
1:C:621:LEU:O	1:C:622:LEU:HD23	2.18	0.43
1:C:560:ILE:H	1:C:560:ILE:HG13	1.61	0.43
1:A:434:LEU:HD11	1:A:465:ASN:O	2.18	0.43
1:C:564:VAL:HG11	1:C:667:GLN:HG3	2.01	0.43
1:F:25:ALA:HB1	1:F:30:LEU:O	2.19	0.43
1:A:110:ASP:O	1:A:113:LEU:HB3	2.19	0.43
1:F:456:ILE:CG2	1:F:457:ILE:N	2.81	0.43
1:E:315:ILE:CG2	1:E:316:LEU:N	2.82	0.43
1:A:584:SER:CB	1:A:589:LYS:HB3	2.43	0.43
1:A:468:LYS:HA	1:B:587:TYR:OH	2.18	0.43
1:E:170:LEU:N	1:E:170:LEU:HD12	2.34	0.43
1:D:252:ILE:CG2	1:D:324:VAL:HB	2.49	0.43
1:C:372:ARG:HD2	1:C:373:PHE:N	2.34	0.43
1:E:154:LYS:HD3	1:E:154:LYS:O	2.19	0.43
1:F:371:ILE:HD12	1:F:380:VAL:CG2	2.44	0.43
1:D:583:GLU:HG3	1:D:592:PHE:CD1	2.53	0.43
1:D:455:LEU:HD12	1:D:455:LEU:C	2.39	0.43
1:A:654:PRO:O	1:A:660:ILE:HG23	2.19	0.43
1:B:743:PRO:HG2	1:B:748:GLY:HA3	2.00	0.43
1:B:110:ASP:O	1:B:113:LEU:HB3	2.19	0.43
1:D:487:HIS:HE1	1:D:509:ASP:HB3	1.81	0.43
1:D:488:TYR:HE1	1:D:525:LEU:HB3	1.84	0.43
1:E:283:THR:OG1	1:E:372:ARG:HB2	2.19	0.43
1:E:757:GLY:C	1:E:759:LEU:N	2.73	0.43
1:B:614:VAL:HG12	1:B:618:ILE:HD11	2.01	0.43
1:C:768:GLU:C	1:C:770:LEU:H	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LYS:HE2	1:A:365:ARG:HH12	1.84	0.43
1:A:476:GLU:C	1:A:478:ASP:N	2.72	0.43
1:F:24:ILE:HD13	1:F:60:LEU:HD13	2.00	0.43
1:C:399:ASN:N	1:C:399:ASN:ND2	2.67	0.43
1:A:177:GLU:HB2	1:A:178:PRO:CD	2.49	0.43
1:B:545:GLY:HA3	1:B:548:LEU:HD12	2.01	0.43
1:A:29:ASN:O	1:A:31:ARG:HD2	2.19	0.43
1:D:108:ILE:HG13	1:D:310:ALA:HA	2.01	0.43
1:A:34:VAL:O	1:A:34:VAL:HG13	2.19	0.43
1:F:578:CYS:O	1:F:578:CYS:SG	2.77	0.43
1:D:520:TRP:HZ2	1:D:534:ARG:HH21	1.67	0.42
1:D:711:LEU:O	1:D:712:SER:HB2	2.19	0.42
1:F:524:VAL:O	1:F:525:LEU:HD23	2.19	0.42
1:F:265:TYR:HD2	1:F:265:TYR:N	2.14	0.42
1:E:450:VAL:HG22	1:E:451:LYS:H	1.84	0.42
1:E:755:PHE:CG	1:E:755:PHE:O	2.72	0.42
1:C:263:PHE:O	1:C:264:ALA:HB2	2.18	0.42
1:F:381:ILE:HG22	1:F:717:TYR:CZ	2.54	0.42
1:C:138:PHE:CB	1:C:389:PRO:HD3	2.47	0.42
1:C:183:VAL:CG2	1:C:184:CYS:N	2.81	0.42
1:E:225:HIS:HB2	1:E:328:THR:O	2.19	0.42
1:C:591:GLU:O	1:C:595:VAL:HG23	2.19	0.42
1:C:204:ARG:O	1:C:204:ARG:HD2	2.18	0.42
1:E:455:LEU:HA	1:E:479:VAL:CG1	2.49	0.42
1:B:116:LEU:HD23	1:B:129:ILE:HG21	2.01	0.42
1:B:131:CYS:SG	1:B:133:ASN:HB2	2.59	0.42
1:C:74:GLU:HG2	1:C:74:GLU:O	2.18	0.42
1:B:57:ILE:HG21	1:B:75:LYS:HE2	2.01	0.42
1:D:21:VAL:HA	1:D:24:ILE:CG2	2.49	0.42
1:E:371:ILE:CB	1:E:380:VAL:HG13	2.41	0.42
1:E:381:ILE:HG22	1:E:717:TYR:CE1	2.54	0.42
1:A:726:ARG:HH21	1:A:727:LYS:CG	2.32	0.42
1:A:265:TYR:O	1:A:284:LEU:HB2	2.18	0.42
1:F:371:ILE:CG1	1:F:380:VAL:HG22	2.49	0.42
1:E:210:ILE:HD11	1:E:228:CYS:N	2.34	0.42
1:D:475:ASN:HD22	1:E:591:GLU:HG2	1.83	0.42
1:F:541:TYR:OH	1:F:610:SER:N	2.52	0.42
1:B:427:ASN:HD21	1:B:429:GLY:H	1.65	0.42
1:B:171:ASN:ND2	1:B:173:ARG:H	2.17	0.42
1:E:225:HIS:HE2	1:E:327:MSE:HE3	1.84	0.42
1:B:540:TYR:CD1	1:B:540:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ILE:HG13	1:C:130:VAL:H	1.84	0.42
1:A:399:ASN:O	1:A:454:ASP:HB2	2.19	0.42
1:B:654:PRO:HG2	1:B:661:ARG:HB2	2.01	0.42
1:C:503:VAL:HA	1:C:706:VAL:CG1	2.50	0.42
1:D:335:MSE:HE2	1:D:335:MSE:N	2.33	0.42
1:D:719:GLU:O	1:D:719:GLU:HG3	2.19	0.42
1:B:670:LEU:O	1:B:673:ILE:HG12	2.19	0.42
1:A:485:GLN:HB3	1:A:488:TYR:HD2	1.83	0.42
1:B:381:ILE:HG22	1:B:717:TYR:CE1	2.54	0.42
1:C:188:TYR:CE1	1:C:312:THR:HG21	2.54	0.42
1:E:523:GLU:CD	1:E:537:HIS:HB2	2.40	0.42
1:A:181:CYS:SG	1:A:182:PRO:N	2.91	0.42
1:F:210:ILE:HD11	1:F:228:CYS:N	2.33	0.42
1:F:219:LYS:HA	1:F:224:ILE:HG23	2.00	0.42
1:C:372:ARG:O	1:C:379:ALA:O	2.37	0.42
1:A:370:VAL:CG2	1:A:382:ARG:HB2	2.50	0.42
1:B:9:GLN:HG2	1:B:40:ALA:HA	2.00	0.42
1:D:543:LEU:CD2	1:D:543:LEU:N	2.82	0.42
1:D:475:ASN:ND2	1:E:591:GLU:HG2	2.34	0.42
1:B:552:TYR:HA	1:B:553:PRO:HD2	1.92	0.42
1:F:38:GLY:CA	1:F:144:LEU:HB3	2.49	0.42
1:F:537:HIS:HE2	1:F:659:LEU:HD22	1.82	0.42
1:C:628:ARG:CZ	1:C:632:GLY:H	2.32	0.42
1:A:567:ILE:HG12	1:A:600:ALA:HB1	2.00	0.42
1:C:364:ASN:ND2	1:C:443:HIS:NE2	2.68	0.42
1:D:738:VAL:HG12	1:D:742:VAL:O	2.19	0.42
1:B:455:LEU:HD13	1:B:456:ILE:O	2.20	0.42
1:F:504:ILE:CG2	1:F:505:GLY:H	2.33	0.42
1:E:107:ALA:HB2	1:E:309:TYR:HB2	2.01	0.42
1:A:504:ILE:HG22	1:A:709:VAL:HG12	2.00	0.42
1:F:369:SER:HB2	1:F:385:ARG:HB2	2.00	0.42
1:E:261:LYS:NZ	1:E:266:VAL:HB	2.34	0.42
1:E:30:LEU:O	1:E:30:LEU:HD23	2.19	0.42
1:B:391:PRO:HB2	1:B:418:LYS:HB2	2.01	0.42
1:E:771:MSE:O	1:E:772:LEU:HD23	2.19	0.42
1:A:172:ARG:C	1:A:174:TYR:H	2.23	0.42
1:B:18:ARG:HB3	1:B:175:HIS:ND1	2.34	0.42
1:C:35:LYS:O	1:C:36:ASN:HB2	2.20	0.42
1:E:570:LEU:HA	1:E:573:VAL:HG12	2.01	0.42
1:E:528:GLY:O	1:E:529:TYR:C	2.56	0.42
1:C:204:ARG:HA	1:C:319:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ASN:HD22	1:D:173:ARG:H	1.67	0.42
1:B:256:ASP:O	1:B:258:GLU:N	2.52	0.42
1:E:138:PHE:HB2	1:E:389:PRO:HD3	2.01	0.42
1:C:639:GLU:OE2	1:C:718:ASN:HA	2.19	0.42
1:A:702:ARG:C	1:A:704:PHE:H	2.22	0.42
1:D:486:HIS:CD2	1:D:490:HIS:HE2	2.36	0.42
1:E:405:ALA:O	1:E:466:THR:HG21	2.19	0.42
1:D:30:LEU:HD22	1:D:52:ASP:O	2.19	0.42
1:D:610:SER:HB3	1:D:613:ARG:CG	2.50	0.42
1:B:251:ALA:HB3	1:B:327:MSE:O	2.20	0.42
1:A:587:TYR:OH	1:B:468:LYS:HA	2.19	0.42
1:E:451:LYS:O	1:E:452:ASN:C	2.57	0.42
1:B:528:GLY:H	1:B:532:VAL:HG22	1.85	0.42
1:A:687:LEU:HD22	1:A:724:MSE:CE	2.44	0.42
1:C:487:HIS:HE1	1:C:509:ASP:HB3	1.85	0.42
1:C:526:TYR:CB	1:C:535:LEU:HD11	2.49	0.42
1:C:260:VAL:HG12	1:C:266:VAL:CG2	2.49	0.42
1:A:215:ILE:HD11	1:A:352:ALA:HA	2.02	0.42
1:A:210:ILE:HD11	1:A:228:CYS:HA	2.02	0.42
1:A:253:MSE:SE	1:A:313:HIS:ND1	3.03	0.42
1:F:23:ARG:HD3	1:F:169:PRO:O	2.19	0.42
1:B:385:ARG:HG3	1:B:386:GLY:N	2.35	0.42
1:E:199:TYR:CG	1:E:200:GLY:N	2.87	0.42
1:E:137:ARG:C	1:E:141:ILE:HG13	2.39	0.42
1:C:18:ARG:HH21	1:C:36:ASN:ND2	2.15	0.42
1:D:401:LEU:O	1:D:456:ILE:HA	2.20	0.42
1:F:399:ASN:O	1:F:454:ASP:HB2	2.20	0.42
1:A:708:ASN:OD1	1:A:708:ASN:N	2.52	0.42
1:C:232:ASN:CG	1:C:235:VAL:HG22	2.40	0.42
1:C:204:ARG:HG2	1:C:319:TRP:CH2	2.55	0.42
1:E:599:LEU:O	1:E:599:LEU:HD22	2.19	0.42
1:F:20:PHE:CE1	1:F:60:LEU:HD12	2.54	0.42
1:F:500:LEU:HD22	1:F:736:PHE:CZ	2.54	0.42
1:F:520:TRP:HZ2	1:F:534:ARG:HH21	1.67	0.42
1:A:504:ILE:CG2	1:A:505:GLY:N	2.82	0.42
1:C:508:LEU:CD2	1:C:611:THR:HG21	2.48	0.42
1:C:270:GLU:HA	1:C:373:PHE:HE2	1.84	0.42
1:F:177:GLU:N	1:F:178:PRO:HD2	2.35	0.42
1:F:19:PRO:HA	1:F:174:TYR:HD1	1.81	0.42
1:A:427:ASN:C	1:A:429:GLY:H	2.22	0.42
1:B:406:GLU:HG3	1:B:407:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ARG:HG2	1:A:438:ARG:NH1	2.34	0.42
1:B:413:VAL:O	1:B:420:TYR:N	2.53	0.42
1:E:729:VAL:CB	1:E:735:ASN:HD22	2.30	0.42
1:F:301:HIS:CD2	1:F:302:THR:N	2.87	0.42
1:B:19:PRO:HA	1:B:174:TYR:CD1	2.54	0.42
1:C:88:ILE:CG2	1:C:89:GLU:H	2.23	0.42
1:E:58:GLU:HA	1:E:61:TYR:HD2	1.85	0.42
1:D:664:GLU:HA	1:D:667:GLN:HG3	2.01	0.42
1:C:9:GLN:HE21	1:C:41:GLY:N	2.16	0.42
1:C:383:ARG:CZ	1:C:387:PHE:HB3	2.50	0.42
1:E:503:VAL:HA	1:E:706:VAL:HG11	2.00	0.42
1:F:343:ARG:HD3	1:F:343:ARG:HA	1.81	0.42
1:B:570:LEU:HD12	1:B:573:VAL:CG1	2.50	0.42
1:E:438:ARG:NH2	1:E:469:LEU:HD21	2.34	0.42
1:B:639:GLU:HB2	1:B:718:ASN:HD21	1.83	0.42
1:D:520:TRP:HE1	1:D:534:ARG:NH2	2.17	0.42
1:F:216:VAL:HG23	1:F:354:TYR:C	2.40	0.42
1:A:495:MSE:HE2	1:A:755:PHE:HZ	1.84	0.42
1:A:765:LEU:HD12	1:A:766:THR:H	1.84	0.42
1:C:122:LYS:HD3	1:D:198:ILE:HD11	2.01	0.42
1:D:253:MSE:O	1:D:317:PHE:HZ	2.01	0.42
1:D:252:ILE:HG12	1:D:296:LEU:HD23	2.01	0.42
1:D:320:SER:HB3	1:D:325:TYR:OH	2.19	0.42
1:C:381:ILE:HG22	1:C:717:TYR:CZ	2.55	0.42
1:A:229:ASP:OD1	1:A:322:THR:HG21	2.20	0.42
1:B:102:ILE:CD1	1:B:103:PRO:HD2	2.50	0.42
1:A:365:ARG:HH21	1:A:436:PHE:HD2	1.67	0.42
1:D:383:ARG:HD2	1:D:387:PHE:HD2	1.84	0.42
1:D:597:ASN:HB3	1:D:601:LYS:HE3	2.01	0.42
1:C:649:LEU:CG	1:C:650:LYS:H	2.33	0.42
1:C:148:ARG:HH21	1:C:158:MSE:N	2.18	0.42
1:D:7:HIS:NE2	1:D:43:GLU:HG3	2.35	0.42
1:F:171:ASN:HD21	1:F:173:ARG:HB2	1.82	0.42
1:E:503:VAL:HG11	1:E:708:ASN:OD1	2.19	0.42
1:E:293:PRO:C	1:E:295:ASN:N	2.72	0.42
1:C:20:PHE:CE1	1:C:60:LEU:HD12	2.55	0.42
1:D:726:ARG:HH21	1:D:727:LYS:HG2	1.85	0.42
1:F:766:THR:HG21	1:F:769:ASP:OD2	2.19	0.42
1:C:718:ASN:HD22	1:C:720:LEU:HB2	1.83	0.42
1:A:88:ILE:HD12	1:A:88:ILE:N	2.34	0.42
1:C:482:LEU:HD21	1:C:757:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:HIS:NE2	1:A:521:GLY:HA2	2.35	0.42
1:B:264:ALA:CB	1:B:286:LYS:HA	2.50	0.42
1:B:226:LEU:CD1	1:B:330:ALA:HA	2.50	0.42
1:F:412:GLY:HA2	1:F:420:TYR:O	2.18	0.42
1:A:561:LEU:CB	1:A:570:LEU:HD13	2.50	0.42
1:B:751:VAL:CG1	1:B:752:GLY:N	2.82	0.42
1:E:34:VAL:HG23	1:E:44:ILE:HG12	2.02	0.42
1:C:487:HIS:CE1	1:C:509:ASP:HB3	2.55	0.42
1:D:65:PRO:HB2	1:D:66:PRO:HD2	2.00	0.42
1:C:253:MSE:HB3	1:C:325:TYR:HB2	2.02	0.42
1:F:621:LEU:HD22	1:F:666:PHE:HD1	1.84	0.42
1:E:543:LEU:HB2	1:E:549:ALA:CB	2.50	0.42
1:B:544:PRO:O	1:B:549:ALA:HB2	2.20	0.42
1:B:580:LYS:C	1:B:582:VAL:H	2.22	0.42
1:C:102:ILE:HG21	1:C:389:PRO:HG3	2.01	0.42
1:B:420:TYR:HB3	1:B:444:PHE:HE1	1.85	0.42
1:F:35:LYS:HE2	1:F:90:LYS:HZ3	1.82	0.42
1:E:247:GLN:HG3	1:E:298:PRO:HG2	2.02	0.42
1:E:79:PRO:HA	1:E:80:PRO:HD3	1.89	0.42
1:E:8:VAL:HG13	1:E:70:ILE:HG23	2.01	0.42
1:F:293:PRO:C	1:F:295:ASN:H	2.23	0.42
1:F:702:ARG:NH2	1:F:731:ALA:O	2.53	0.42
1:A:577:CYS:SG	1:A:579:PRO:HD3	2.59	0.42
1:E:530:GLU:HG3	1:E:531:ASP:OD2	2.20	0.42
1:D:287:LYS:HG3	1:D:288:GLU:N	2.35	0.42
1:C:202:PRO:O	1:C:203:LEU:C	2.57	0.42
1:E:702:ARG:C	1:E:704:PHE:H	2.23	0.42
1:F:215:ILE:HG13	1:F:215:ILE:O	2.20	0.42
1:E:11:ILE:HG23	1:E:12:VAL:N	2.34	0.42
1:E:19:PRO:HA	1:E:174:TYR:CD1	2.54	0.42
1:C:385:ARG:CG	1:C:386:GLY:N	2.74	0.42
1:C:424:TYR:C	1:C:426:GLY:H	2.23	0.42
1:F:385:ARG:HA	1:F:385:ARG:HD2	1.91	0.42
1:B:738:VAL:HG11	1:B:742:VAL:HG12	2.01	0.42
1:A:235:VAL:O	1:A:238:GLU:HB2	2.19	0.42
1:A:123:ARG:NH2	1:A:173:ARG:NE	2.68	0.42
1:F:38:GLY:HA2	1:F:145:PRO:HA	2.01	0.42
1:B:257:ILE:O	1:B:260:VAL:HB	2.20	0.42
1:F:279:ARG:HG3	1:F:309:TYR:CB	2.50	0.42
1:D:284:LEU:O	1:D:302:THR:HA	2.19	0.42
1:B:610:SER:HB3	1:B:613:ARG:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:ALA:O	1:B:676:ALA:HB3	2.20	0.42
1:D:690:ALA:HB2	1:D:721:ILE:HG23	2.02	0.42
1:B:225:HIS:CD2	1:B:225:HIS:N	2.86	0.42
1:B:281:ILE:HA	1:B:305:VAL:O	2.19	0.42
1:F:391:PRO:C	1:F:392:ILE:HD12	2.41	0.42
1:F:481:LEU:HD12	1:F:482:LEU:H	1.84	0.42
1:F:536:ALA:HA	1:F:658:GLU:O	2.20	0.42
1:E:748:GLY:O	1:E:751:VAL:HG12	2.19	0.42
1:B:524:VAL:O	1:B:535:LEU:HB2	2.20	0.42
1:F:210:ILE:HD11	1:F:227:ALA:O	2.20	0.42
1:E:12:VAL:O	1:E:12:VAL:HG22	2.20	0.42
1:C:515:THR:O	1:C:516:ASP:HB2	2.18	0.42
1:A:230:ALA:O	1:A:292:LEU:HD12	2.20	0.42
1:B:16:GLY:HA3	1:B:132:THR:HG23	2.02	0.42
1:D:329:SER:HB2	1:D:331:ASN:ND2	2.29	0.42
1:D:329:SER:CA	1:D:337:MSE:HE2	2.49	0.42
1:A:197:GLU:C	1:A:198:ILE:HG12	2.41	0.42
1:E:183:VAL:CG2	1:E:184:CYS:H	2.31	0.42
1:A:247:GLN:NE2	1:A:298:PRO:HG2	2.34	0.42
1:C:466:THR:OG1	1:C:467:THR:N	2.53	0.42
1:C:65:PRO:HG2	1:C:68:ALA:HB3	2.00	0.42
1:D:580:LYS:HD2	1:D:590:VAL:HA	2.01	0.42
1:F:376:GLY:HA2	1:F:726:ARG:HH11	1.84	0.42
1:D:239:LEU:HD22	1:D:250:PHE:CZ	2.55	0.42
1:A:670:LEU:O	1:A:673:ILE:HG12	2.20	0.42
1:C:766:THR:OG1	1:C:769:ASP:HB2	2.20	0.42
1:C:301:HIS:ND1	1:C:640:SER:HB3	2.35	0.42
1:F:339:LYS:HG3	1:F:365:ARG:NH1	2.34	0.42
1:A:589:LYS:CG	1:A:590:VAL:H	2.22	0.41
1:A:209:LEU:N	1:A:209:LEU:HD12	2.35	0.41
1:B:15:VAL:HG13	1:B:67:LEU:HB2	2.01	0.41
1:F:615:LEU:HD23	1:F:635:ALA:HB1	2.03	0.41
1:D:278:ARG:CG	1:D:280:PRO:HD3	2.49	0.41
1:E:543:LEU:HD23	1:E:606:ALA:O	2.20	0.41
1:D:561:LEU:HB2	1:D:570:LEU:CD1	2.50	0.41
1:A:123:ARG:HE	1:A:173:ARG:NH2	2.16	0.41
1:B:166:TYR:CZ	1:B:175:HIS:HA	2.55	0.41
1:A:359:ASN:O	1:A:360:ARG:C	2.58	0.41
1:F:383:ARG:CZ	1:F:387:PHE:HB3	2.50	0.41
1:C:209:LEU:HD12	1:C:209:LEU:N	2.35	0.41
1:D:639:GLU:HB2	1:D:718:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ILE:CB	1:B:370:VAL:HG12	2.42	0.41
1:B:283:THR:OG1	1:B:372:ARG:HB2	2.20	0.41
1:C:190:LEU:O	1:C:196:GLN:HB2	2.19	0.41
1:C:189:ARG:HA	1:C:202:PRO:HG3	2.02	0.41
1:E:526:TYR:CB	1:E:535:LEU:HD11	2.50	0.41
1:E:739:THR:O	1:E:742:VAL:O	2.37	0.41
1:E:18:ARG:HB2	1:E:19:PRO:CD	2.38	0.41
1:E:18:ARG:HH12	1:E:36:ASN:ND2	2.19	0.41
1:A:502:SER:HB3	1:A:527:LEU:O	2.20	0.41
1:B:67:LEU:HD22	1:B:106:ILE:HD13	2.01	0.41
1:D:168:ASP:O	1:D:174:TYR:HD2	2.03	0.41
1:E:522:GLY:HA3	1:E:538:ILE:CD1	2.50	0.41
1:B:481:LEU:HD12	1:B:482:LEU:N	2.33	0.41
1:B:166:TYR:CE1	1:B:175:HIS:HA	2.54	0.41
1:F:409:ASN:HD22	1:F:425:ILE:CD1	2.28	0.41
1:C:121:ASN:ND2	1:C:123:ARG:H	2.17	0.41
1:C:177:GLU:N	1:C:178:PRO:HD2	2.35	0.41
1:C:168:ASP:O	1:C:174:TYR:HD2	2.03	0.41
1:D:700:ARG:HD2	1:D:704:PHE:CE2	2.52	0.41
1:F:312:THR:HA	1:F:315:ILE:HG22	2.02	0.41
1:C:553:PRO:CG	1:C:620:VAL:HG21	2.50	0.41
1:C:580:LYS:C	1:C:582:VAL:H	2.23	0.41
1:D:257:ILE:HD11	1:D:271:GLU:HG3	2.01	0.41
1:F:387:PHE:O	1:F:390:LEU:HG	2.20	0.41
1:D:474:ALA:C	1:D:476:GLU:H	2.23	0.41
1:B:724:MSE:O	1:B:728:VAL:HG23	2.20	0.41
1:D:128:PHE:CG	1:D:186:PRO:HG2	2.56	0.41
1:E:312:THR:CA	1:E:315:ILE:HG22	2.47	0.41
1:E:106:ILE:HG22	1:E:107:ALA:N	2.35	0.41
1:D:312:THR:HA	1:D:315:ILE:CG2	2.50	0.41
1:C:217:ALA:HB1	1:C:224:ILE:HD11	2.02	0.41
1:F:584:SER:HB3	1:F:589:LYS:HB3	2.02	0.41
1:B:190:LEU:O	1:B:196:GLN:HB2	2.20	0.41
1:E:410:ALA:HA	1:E:425:ILE:HD11	2.02	0.41
1:F:247:GLN:OE1	1:F:637:LYS:HE3	2.21	0.41
1:F:299:GLY:O	1:F:300:LEU:HG	2.20	0.41
1:C:148:ARG:NH2	1:C:158:MSE:N	2.68	0.41
1:B:540:TYR:HD2	1:B:607:TYR:HB3	1.85	0.41
1:B:19:PRO:HG3	1:B:174:TYR:O	2.19	0.41
1:E:7:HIS:CB	1:E:74:GLU:HB2	2.51	0.41
1:B:140:ILE:HB	1:B:152:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:VAL:HG11	1:B:44:ILE:HG21	2.02	0.41
1:A:86:PHE:O	1:A:88:ILE:HD12	2.19	0.41
1:C:472:GLU:O	1:C:476:GLU:HG2	2.20	0.41
1:F:130:VAL:HG22	1:F:131:CYS:O	2.20	0.41
1:A:487:HIS:CD2	1:A:520:TRP:HB3	2.56	0.41
1:A:488:TYR:CD1	1:A:525:LEU:HD13	2.55	0.41
1:A:520:TRP:HZ2	1:A:534:ARG:HH21	1.68	0.41
1:E:493:SER:HB2	1:E:742:VAL:HG11	2.02	0.41
1:A:504:ILE:HD12	1:A:701:ALA:CA	2.51	0.41
1:D:219:LYS:HB2	1:D:357:LEU:HA	2.02	0.41
1:C:493:SER:HB2	1:C:751:VAL:HG13	2.01	0.41
1:A:370:VAL:HG23	1:A:382:ARG:HB2	2.02	0.41
1:B:125:MSE:HE3	1:B:319:TRP:CH2	2.56	0.41
1:B:65:PRO:O	1:B:67:LEU:N	2.54	0.41
1:B:582:VAL:HB	1:B:583:GLU:OE1	2.21	0.41
1:B:558:MSE:HE1	1:B:593:ASN:ND2	2.36	0.41
1:D:248:LYS:HA	1:D:249:PRO:HD3	1.97	0.41
1:F:39:ASP:HB3	1:F:144:LEU:HD13	2.02	0.41
1:F:38:GLY:HA2	1:F:144:LEU:HB3	2.02	0.41
1:F:209:LEU:HA	1:F:212:LYS:CG	2.50	0.41
1:B:258:GLU:O	1:B:261:LYS:N	2.52	0.41
1:F:415:LYS:O	1:F:416:ASN:HB2	2.20	0.41
1:A:1:MSE:HE3	1:A:2:LYS:H	1.85	0.41
1:A:1:MSE:N	1:A:80:PRO:HD2	2.36	0.41
1:E:55:ALA:O	1:E:59:ASP:HB2	2.19	0.41
1:B:161:PHE:O	1:B:164:SER:HB3	2.20	0.41
1:B:321:LYS:HA	1:B:321:LYS:HD3	1.93	0.41
1:D:752:GLY:O	1:D:756:LEU:HD12	2.19	0.41
1:E:488:TYR:CD1	1:E:525:LEU:HD13	2.55	0.41
1:E:700:ARG:HH11	1:E:704:PHE:HE2	1.67	0.41
1:A:738:VAL:HG11	1:A:742:VAL:HG12	2.02	0.41
1:D:188:TYR:CD2	1:D:203:LEU:HD13	2.55	0.41
1:D:236:VAL:HG21	1:D:296:LEU:HD12	2.03	0.41
1:D:306:MSE:HE1	1:D:309:TYR:CE2	2.54	0.41
1:C:292:LEU:HD12	1:C:296:LEU:CD2	2.47	0.41
1:F:11:ILE:O	1:F:11:ILE:HG12	2.20	0.41
1:A:456:ILE:HD12	1:A:456:ILE:N	2.36	0.41
1:F:557:LEU:HD23	1:F:561:LEU:HD12	2.02	0.41
1:F:620:VAL:HG22	1:F:625:ALA:O	2.20	0.41
1:D:278:ARG:NH1	1:D:387:PHE:HE1	2.18	0.41
1:B:368:ASP:HA	1:B:385:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:VAL:HG21	1:E:135:GLY:HA3	2.03	0.41
1:F:633:GLU:N	1:F:634:PRO:CD	2.81	0.41
1:D:595:VAL:O	1:D:598:GLN:HB3	2.20	0.41
1:B:383:ARG:CZ	1:B:387:PHE:HB3	2.50	0.41
1:B:18:ARG:N	1:B:19:PRO:CD	2.83	0.41
1:C:123:ARG:NH2	1:C:173:ARG:NE	2.67	0.41
1:F:398:TYR:CE1	1:F:758:GLY:HA3	2.56	0.41
1:B:1:MSE:HB2	1:B:80:PRO:HD2	2.02	0.41
1:A:180:ALA:HB1	1:A:185:GLY:HA3	2.02	0.41
1:C:503:VAL:HA	1:C:706:VAL:HG11	2.03	0.41
1:A:506:ILE:HD11	1:A:694:ALA:HA	2.02	0.41
1:F:186:PRO:HB3	1:F:359:ASN:HB2	2.03	0.41
1:D:493:SER:HB2	1:D:751:VAL:CG1	2.50	0.41
1:B:265:TYR:HE2	1:B:287:LYS:CD	2.33	0.41
1:E:12:VAL:CA	1:E:68:ALA:HB1	2.48	0.41
1:D:290:PHE:HA	1:D:291:PRO:HD3	1.90	0.41
1:C:371:ILE:CB	1:C:380:VAL:HG13	2.49	0.41
1:A:286:LYS:HB2	1:A:303:ILE:CD1	2.51	0.41
1:B:14:ALA:HA	1:B:146:TYR:CE1	2.56	0.41
1:F:522:GLY:HA3	1:F:611:THR:HG23	2.03	0.41
1:E:582:VAL:C	1:E:584:SER:H	2.23	0.41
1:F:510:GLY:HA2	1:F:610:SER:OG	2.19	0.41
1:C:181:CYS:SG	1:C:182:PRO:HD2	2.60	0.41
1:B:508:LEU:HD11	1:B:725:ILE:CD1	2.51	0.41
1:A:329:SER:CA	1:A:337:MSE:HE2	2.45	0.41
1:F:35:LYS:HG2	1:F:36:ASN:H	1.86	0.41
1:F:111:ASP:HB2	1:F:172:ARG:NH2	2.27	0.41
1:B:108:ILE:HG13	1:B:108:ILE:O	2.21	0.41
1:C:591:GLU:HG3	1:F:471:MSE:O	2.20	0.41
1:A:132:THR:HG23	1:A:133:ASN:OD1	2.21	0.41
1:C:37:LEU:HB2	1:C:41:GLY:HA3	2.03	0.41
1:E:498:LYS:CB	1:E:500:LEU:HD11	2.51	0.41
1:A:399:ASN:HD22	1:A:399:ASN:N	2.19	0.41
1:E:501:ASP:O	1:E:503:VAL:HG13	2.20	0.41
1:D:261:LYS:HD3	1:D:266:VAL:HG21	2.03	0.41
1:E:628:ARG:NH2	1:E:632:GLY:H	2.19	0.41
1:B:116:LEU:HB3	1:B:129:ILE:HD13	2.03	0.41
1:D:265:TYR:O	1:D:284:LEU:HD13	2.20	0.41
1:B:180:ALA:HB1	1:B:185:GLY:HA3	2.02	0.41
1:B:370:VAL:HG23	1:B:381:ILE:CG1	2.51	0.41
1:A:738:VAL:HB	1:A:744:ARG:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:582:VAL:HG22	1:D:626:TYR:HB3	2.03	0.41
1:E:687:LEU:HD22	1:E:724:MSE:SE	2.70	0.41
1:E:1:MSE:HB2	1:E:80:PRO:HD2	2.03	0.41
1:C:171:ASN:HD21	1:C:173:ARG:HB2	1.82	0.41
1:D:502:SER:CB	1:D:528:GLY:HA2	2.48	0.41
1:F:140:ILE:HG21	1:F:360:ARG:HH11	1.85	0.41
1:C:104:PRO:HB3	1:C:387:PHE:O	2.21	0.41
1:F:474:ALA:C	1:F:476:GLU:H	2.22	0.41
1:B:5:HIS:CD2	1:B:78:ILE:HD12	2.55	0.41
1:E:612:GLY:O	1:E:615:LEU:HB2	2.20	0.41
1:F:455:LEU:C	1:F:455:LEU:HD12	2.41	0.41
1:B:30:LEU:HD23	1:B:30:LEU:O	2.20	0.41
1:F:88:ILE:N	1:F:88:ILE:HD12	2.35	0.41
1:D:757:GLY:C	1:D:759:LEU:H	2.22	0.41
1:A:620:VAL:C	1:A:622:LEU:N	2.72	0.41
1:A:756:LEU:O	1:A:759:LEU:HB3	2.21	0.41
1:A:691:ARG:HG3	1:A:724:MSE:HG3	2.03	0.41
1:D:279:ARG:HH11	1:D:279:ARG:HG3	1.85	0.41
1:D:317:PHE:O	1:D:318:HIS:C	2.59	0.41
1:D:66:PRO:HD3	1:D:133:ASN:HD22	1.86	0.41
1:D:65:PRO:HG2	1:D:68:ALA:HB2	2.02	0.41
1:C:108:ILE:HG22	1:C:309:TYR:O	2.20	0.41
1:A:264:ALA:O	1:A:265:TYR:HD2	2.03	0.41
1:F:621:LEU:O	1:F:622:LEU:HD23	2.21	0.41
1:D:383:ARG:HB3	1:D:747:ASN:ND2	2.34	0.41
1:B:202:PRO:O	1:B:203:LEU:C	2.58	0.41
1:D:598:GLN:CG	1:D:604:ASN:HB2	2.50	0.41
1:E:219:LYS:HA	1:E:224:ILE:CB	2.51	0.41
1:C:413:VAL:CG2	1:C:448:LEU:HD12	2.51	0.41
1:A:472:GLU:HG3	1:A:473:MSE:N	2.36	0.41
1:E:142:GLU:HB3	1:E:150:ASN:C	2.41	0.41
1:C:564:VAL:HG12	1:C:565:TYR:CD1	2.56	0.41
1:E:461:HIS:CE1	1:E:463:ALA:HB3	2.56	0.41
1:A:469:LEU:O	1:A:470:ALA:C	2.59	0.41
1:A:578:CYS:SG	1:A:578:CYS:O	2.79	0.41
1:D:451:LYS:O	1:D:451:LYS:HG3	2.21	0.41
1:A:535:LEU:HD23	1:A:700:ARG:HG3	2.03	0.41
1:B:250:PHE:O	1:B:252:ILE:HD12	2.21	0.41
1:B:252:ILE:CD1	1:B:296:LEU:HD23	2.51	0.41
1:B:286:LYS:HB2	1:B:303:ILE:CD1	2.51	0.41
1:A:587:TYR:CD1	1:A:588:GLY:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:HIS:HD2	1:A:744:ARG:NE	2.19	0.41
1:E:22:TYR:CE1	1:E:87:TYR:HB3	2.56	0.41
1:A:504:ILE:HG22	1:A:505:GLY:N	2.35	0.41
1:A:528:GLY:O	1:A:529:TYR:C	2.59	0.41
1:A:376:GLY:HA2	1:A:726:ARG:NH1	2.35	0.41
1:D:233:GLU:HA	1:D:236:VAL:CG1	2.50	0.41
1:D:203:LEU:HD21	1:D:315:ILE:CG2	2.51	0.41
1:C:534:ARG:C	1:C:535:LEU:HD12	2.41	0.41
1:F:220:GLY:H	1:F:224:ILE:HA	1.85	0.41
1:C:253:MSE:HE1	1:C:313:HIS:CG	2.56	0.41
1:C:309:TYR:CZ	1:C:385:ARG:NH1	2.83	0.41
1:B:102:ILE:HA	1:B:102:ILE:HD13	1.91	0.41
1:E:288:GLU:HB3	1:E:289:PRO:CD	2.38	0.41
1:F:137:ARG:NH2	1:F:178:PRO:HG3	2.31	0.41
1:F:270:GLU:CA	1:F:373:PHE:HE2	2.34	0.41
1:E:690:ALA:HB2	1:E:721:ILE:HG12	2.03	0.41
1:A:339:LYS:HG3	1:A:365:ARG:HH12	1.84	0.41
1:A:456:ILE:HD12	1:A:480:GLU:O	2.20	0.41
1:A:409:ASN:CG	1:A:410:ALA:H	2.24	0.41
1:F:552:TYR:O	1:F:555:ARG:HG3	2.20	0.41
1:D:447:ILE:O	1:D:448:LEU:HD23	2.21	0.41
1:D:695:HIS:CE1	1:D:728:VAL:HG13	2.55	0.41
1:B:190:LEU:HB2	1:B:202:PRO:HB3	2.02	0.41
1:D:247:GLN:HG3	1:D:298:PRO:CG	2.38	0.41
1:D:348:LEU:N	1:D:348:LEU:HD12	2.36	0.41
1:C:102:ILE:CD1	1:C:144:LEU:HG	2.51	0.41
1:B:171:ASN:ND2	1:B:173:ARG:CB	2.84	0.41
1:B:619:ALA:HB1	1:B:625:ALA:CB	2.50	0.41
1:E:688:ALA:O	1:E:691:ARG:HB3	2.21	0.41
1:A:111:ASP:HB2	1:A:172:ARG:HH22	1.86	0.41
1:C:154:LYS:O	1:C:154:LYS:HD3	2.21	0.41
1:B:221:ILE:HD11	1:B:309:TYR:CE1	2.56	0.41
1:B:482:LEU:HD12	1:B:483:GLN:N	2.35	0.41
1:A:413:VAL:HG13	1:A:420:TYR:HB2	2.02	0.41
1:C:12:VAL:HG13	1:C:13:GLN:N	2.32	0.41
1:A:613:ARG:O	1:A:616:ASP:HB3	2.21	0.41
1:C:601:LYS:HB3	1:C:603:ILE:HG13	2.03	0.41
1:C:601:LYS:CB	1:C:603:ILE:HG13	2.51	0.41
1:F:64:LYS:CB	1:F:65:PRO:HD2	2.51	0.41
1:D:427:ASN:O	1:D:433:VAL:HG11	2.21	0.41
1:C:204:ARG:HG2	1:C:319:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:601:LYS:HD2	1:F:603:ILE:HD11	2.03	0.41
1:E:653:VAL:O	1:E:653:VAL:HG13	2.21	0.41
1:D:760:TYR:CE2	1:D:767:LYS:HG2	2.53	0.41
1:B:256:ASP:O	1:B:257:ILE:C	2.59	0.41
1:B:656:GLU:HG3	1:B:661:ARG:CZ	2.51	0.41
1:B:21:VAL:CG1	1:B:44:ILE:HD13	2.51	0.41
1:D:134:CYS:SG	1:D:135:GLY:N	2.93	0.41
1:F:596:LEU:O	1:F:600:ALA:N	2.54	0.41
1:B:639:GLU:OE2	1:B:718:ASN:HA	2.21	0.41
1:D:422:SER:HA	1:D:444:PHE:CZ	2.56	0.41
1:C:341:ASN:O	1:C:344:ALA:HB3	2.21	0.41
1:D:694:ALA:O	1:D:698:VAL:HG23	2.20	0.41
1:F:500:LEU:HD12	1:F:501:ASP:O	2.21	0.41
1:B:373:PHE:CZ	1:B:378:ARG:HD3	2.55	0.41
1:E:13:GLN:NE2	1:E:18:ARG:NH2	2.69	0.41
1:D:339:LYS:O	1:D:340:ASP:C	2.59	0.41
1:C:526:TYR:HB2	1:C:535:LEU:HD11	2.03	0.41
1:C:320:SER:O	1:C:321:LYS:C	2.58	0.41
1:C:494:VAL:HG11	1:C:710:ALA:HB1	2.02	0.41
1:A:286:LYS:HD2	1:A:303:ILE:HD11	2.02	0.41
1:B:15:VAL:HG21	1:B:68:ALA:HB2	2.03	0.41
1:D:147:ASP:HA	1:D:177:GLU:OE2	2.21	0.41
1:D:177:GLU:N	1:D:178:PRO:HD2	2.36	0.41
1:B:626:TYR:C	1:B:627:ARG:HG2	2.40	0.41
1:C:404:GLY:HA2	1:C:753:GLN:OE1	2.21	0.41
1:E:433:VAL:O	1:E:436:PHE:N	2.52	0.41
1:B:497:GLU:OE1	1:B:738:VAL:HA	2.21	0.41
1:E:198:ILE:O	1:E:199:TYR:HB3	2.21	0.41
1:D:557:LEU:O	1:D:561:LEU:HG	2.21	0.41
1:B:20:PHE:HE1	1:B:60:LEU:HA	1.86	0.41
1:C:554:LEU:HD23	1:C:583:GLU:OE2	2.21	0.41
1:B:309:TYR:C	1:B:309:TYR:CD1	2.94	0.41
1:E:8:VAL:O	1:E:42:VAL:HB	2.21	0.41
1:D:148:ARG:CZ	1:D:158:MSE:HG3	2.51	0.41
1:A:618:ILE:HG22	1:A:638:LEU:HD21	2.03	0.41
1:A:399:ASN:N	1:A:454:ASP:OD1	2.54	0.41
1:B:42:VAL:HG22	1:B:42:VAL:O	2.21	0.41
1:F:153:MSE:HA	1:F:156:PHE:HD2	1.86	0.41
1:B:598:GLN:HG3	1:B:604:ASN:HB2	2.03	0.41
1:B:761:LEU:O	1:B:761:LEU:HD12	2.20	0.41
1:E:739:THR:O	1:E:740:THR:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:VAL:CG2	1:B:536:ALA:HB3	2.47	0.40
1:A:496:ALA:HB2	1:A:755:PHE:CD2	2.56	0.40
1:A:252:ILE:HD13	1:A:303:ILE:CG2	2.51	0.40
1:F:552:TYR:HA	1:F:553:PRO:HD2	1.89	0.40
1:F:615:LEU:HD23	1:F:635:ALA:CB	2.52	0.40
1:C:543:LEU:HD12	1:C:549:ALA:CB	2.51	0.40
1:C:406:GLU:HA	1:C:466:THR:HG21	2.03	0.40
1:F:249:PRO:CG	1:F:300:LEU:HD13	2.45	0.40
1:D:170:LEU:H	1:D:170:LEU:CD1	2.29	0.40
1:E:218:ILE:HD12	1:E:356:LEU:CD2	2.51	0.40
1:D:205:LYS:HE3	1:D:205:LYS:HB2	1.84	0.40
1:B:460:LEU:CD2	1:B:515:THR:HG22	2.51	0.40
1:C:31:ARG:HG2	1:C:85:ARG:C	2.42	0.40
1:E:209:LEU:O	1:E:212:LYS:HB2	2.20	0.40
1:D:522:GLY:H	1:D:523:GLU:CD	2.23	0.40
1:A:50:GLU:O	1:A:53:ILE:HG22	2.21	0.40
1:E:66:PRO:HD2	1:E:133:ASN:HD21	1.85	0.40
1:D:171:ASN:HD21	1:D:173:ARG:HB2	1.86	0.40
1:A:630:TYR:HD1	1:A:631:GLU:N	2.19	0.40
1:F:743:PRO:HG2	1:F:748:GLY:CA	2.49	0.40
1:B:224:ILE:HG12	1:B:338:VAL:HG13	2.03	0.40
1:E:279:ARG:N	1:E:280:PRO:CD	2.84	0.40
1:B:525:LEU:CA	1:B:535:LEU:HD13	2.51	0.40
1:E:34:VAL:O	1:E:89:GLU:HA	2.21	0.40
1:A:683:TYR:O	1:A:687:LEU:HG	2.22	0.40
1:D:279:ARG:CG	1:D:279:ARG:HH11	2.34	0.40
1:C:282:ILE:HA	1:C:371:ILE:O	2.22	0.40
1:C:370:VAL:HG23	1:C:381:ILE:CD1	2.51	0.40
1:B:15:VAL:HG11	1:B:67:LEU:HB2	2.02	0.40
1:F:553:PRO:HG3	1:F:626:TYR:O	2.21	0.40
1:A:148:ARG:C	1:A:150:ASN:H	2.25	0.40
1:C:6:ILE:HG13	1:C:57:ILE:HD11	2.04	0.40
1:B:413:VAL:HG11	1:B:448:LEU:HD11	2.03	0.40
1:B:616:ASP:O	1:B:619:ALA:HB3	2.21	0.40
1:A:307:LEU:HB3	1:A:308:PRO:HD2	2.01	0.40
1:D:163:ARG:CB	1:D:163:ARG:HH11	2.32	0.40
1:D:649:LEU:HD23	1:D:651:PHE:HE1	1.86	0.40
1:A:398:TYR:CG	1:A:398:TYR:O	2.74	0.40
1:C:142:GLU:O	1:C:143:ASP:HB2	2.20	0.40
1:E:383:ARG:O	1:E:384:SER:HB3	2.21	0.40
1:B:365:ARG:O	1:B:366:ALA:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLY:C	1:A:40:ALA:N	2.74	0.40
1:A:694:ALA:O	1:A:697:ALA:N	2.54	0.40
1:B:332:TYR:HB3	1:B:333:PRO:HD2	2.03	0.40
1:B:242:ARG:HD3	1:B:351:VAL:O	2.21	0.40
1:D:453:LEU:HG	1:D:453:LEU:O	2.21	0.40
1:F:451:LYS:O	1:F:451:LYS:HG3	2.22	0.40
1:D:497:GLU:OE2	1:D:738:VAL:HG12	2.22	0.40
1:F:394:ILE:HG23	1:F:755:PHE:HB2	2.04	0.40
1:B:253:MSE:HE2	1:B:317:PHE:HD1	1.86	0.40
1:B:303:ILE:HG22	1:B:304:GLY:N	2.36	0.40
1:F:532:VAL:HG12	1:F:533:GLU:N	2.37	0.40
1:A:561:LEU:HB3	1:A:570:LEU:HD13	2.02	0.40
1:A:642:ALA:HB1	1:A:683:TYR:HA	2.03	0.40
1:D:292:LEU:HD11	1:D:324:VAL:HG21	2.02	0.40
1:A:108:ILE:HG13	1:A:311:GLY:N	2.32	0.40
1:F:270:GLU:CB	1:F:373:PHE:HE2	2.34	0.40
1:F:582:VAL:O	1:F:627:ARG:HD2	2.21	0.40
1:D:383:ARG:HG3	1:D:383:ARG:NH1	2.37	0.40
1:D:104:PRO:HD3	1:D:390:LEU:HD21	2.04	0.40
1:D:35:LYS:O	1:D:42:VAL:HG13	2.22	0.40
1:D:210:ILE:HD13	1:D:216:VAL:CG1	2.47	0.40
1:B:278:ARG:O	1:B:279:ARG:C	2.60	0.40
1:E:252:ILE:CG2	1:E:324:VAL:HB	2.51	0.40
1:D:437:MSE:HE1	1:D:466:THR:HG22	2.03	0.40
1:E:73:ILE:O	1:E:73:ILE:HG22	2.21	0.40
1:C:172:ARG:HG2	1:C:173:ARG:HD3	2.03	0.40
1:E:415:LYS:O	1:E:417:GLY:N	2.54	0.40
1:D:727:LYS:HA	1:D:730:GLU:HG2	2.03	0.40
1:E:140:ILE:HB	1:E:152:THR:CG2	2.51	0.40
1:F:722:THR:O	1:F:722:THR:HG22	2.22	0.40
1:B:217:ALA:HA	1:B:226:LEU:HA	2.02	0.40
1:B:253:MSE:HA	1:B:306:MSE:HB2	2.04	0.40
1:B:259:THR:O	1:B:263:PHE:HB2	2.22	0.40
1:F:413:VAL:CG2	1:F:448:LEU:HD13	2.48	0.40
1:C:312:THR:HA	1:C:315:ILE:CG2	2.49	0.40
1:A:561:LEU:HD22	1:A:565:TYR:CE2	2.57	0.40
1:A:588:GLY:O	1:A:592:PHE:CD2	2.75	0.40
1:E:11:ILE:O	1:E:13:GLN:N	2.55	0.40
1:D:125:MSE:HE3	1:D:319:TRP:CH2	2.56	0.40
1:D:219:LYS:HG2	1:D:358:HIS:CE1	2.55	0.40
1:C:424:TYR:HD1	1:C:747:ASN:HD22	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:HIS:O	1:C:738:VAL:C	2.58	0.40
1:A:207:ALA:C	1:A:209:LEU:N	2.75	0.40
1:A:228:CYS:O	1:A:326:VAL:HB	2.22	0.40
1:B:207:ALA:HB1	1:B:320:SER:CB	2.52	0.40
1:A:219:LYS:HB2	1:A:357:LEU:HA	2.03	0.40
1:A:457:ILE:HA	1:A:482:LEU:O	2.21	0.40
1:B:582:VAL:HG11	1:B:626:TYR:HB3	2.04	0.40
1:E:261:LYS:HD3	1:E:266:VAL:CG2	2.51	0.40
1:A:154:LYS:HD3	1:A:154:LYS:C	2.42	0.40
1:F:614:VAL:HG11	1:F:662:VAL:HG11	2.03	0.40
1:C:106:ILE:HG12	1:C:277:TYR:CD1	2.56	0.40
1:E:239:LEU:HD22	1:E:250:PHE:CZ	2.56	0.40
1:B:278:ARG:HG3	1:B:280:PRO:HD3	2.03	0.40
1:F:771:MSE:O	1:F:772:LEU:HD23	2.21	0.40
1:A:21:VAL:HA	1:A:24:ILE:CG2	2.52	0.40
1:A:116:LEU:HD12	1:A:116:LEU:C	2.42	0.40
1:E:406:GLU:HB3	1:E:464:TYR:CD2	2.56	0.40
1:D:152:THR:HG23	1:D:153:MSE:N	2.36	0.40
1:E:459:ASP:C	1:E:461:HIS:H	2.25	0.40
1:D:729:VAL:O	1:D:729:VAL:HG12	2.21	0.40
1:D:506:ILE:HG23	1:D:693:PHE:CE1	2.57	0.40
1:F:413:VAL:HG11	1:F:448:LEU:CD1	2.52	0.40
1:F:524:VAL:HG23	1:F:536:ALA:H	1.86	0.40
1:E:278:ARG:HG2	1:E:278:ARG:H	1.72	0.40
1:E:399:ASN:HA	1:E:414:ALA:O	2.22	0.40
1:C:516:ASP:HB2	1:C:518:ASN:HD22	1.84	0.40
1:B:228:CYS:O	1:B:326:VAL:HG23	2.21	0.40
1:F:8:VAL:O	1:F:9:GLN:HG3	2.22	0.40
1:D:543:LEU:HB2	1:D:549:ALA:CB	2.52	0.40
1:A:196:GLN:HE21	1:A:196:GLN:N	2.19	0.40
1:B:153:MSE:HE1	1:B:360:ARG:NE	2.36	0.40
1:F:557:LEU:HD11	1:F:621:LEU:CA	2.50	0.40
1:F:620:VAL:HG13	1:F:626:TYR:CE1	2.57	0.40
1:B:248:LYS:HA	1:B:249:PRO:HD3	1.97	0.40
1:D:394:ILE:HG23	1:D:395:PRO:HD2	2.02	0.40
1:D:395:PRO:HG2	1:D:396:PHE:CE2	2.55	0.40
1:C:555:ARG:NH1	1:C:592:PHE:CE1	2.90	0.40
1:D:6:ILE:O	1:D:43:GLU:HA	2.22	0.40
1:C:394:ILE:HD11	1:C:419:VAL:CG1	2.51	0.40
1:A:12:VAL:HG12	1:A:13:GLN:N	2.37	0.40
1:C:618:ILE:H	1:C:618:ILE:HG13	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:601:LYS:CD	1:F:603:ILE:HD11	2.51	0.40
1:A:105:ASP:OD1	1:A:139:THR:HG23	2.22	0.40
1:D:612:GLY:O	1:D:615:LEU:HB2	2.22	0.40
1:C:128:PHE:CE1	1:C:186:PRO:HG2	2.57	0.40
1:A:90:LYS:HB3	1:A:90:LYS:HE2	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:NH1	1:A:204:ARG:NH1[12_554]	1.95	0.25

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	762/772 (99%)	530 (70%)	179 (24%)	53 (7%)	1	23
1	B	758/772 (98%)	565 (74%)	145 (19%)	48 (6%)	2	26
1	C	750/772 (97%)	540 (72%)	170 (23%)	40 (5%)	2	30
1	D	761/772 (99%)	580 (76%)	148 (19%)	33 (4%)	3	35
1	E	758/772 (98%)	566 (75%)	149 (20%)	43 (6%)	2	28
1	F	758/772 (98%)	562 (74%)	171 (23%)	25 (3%)	5	42
All	All	4547/4632 (98%)	3343 (74%)	962 (21%)	242 (5%)	2	30

All (242) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ASP
1	A	203	LEU
1	A	264	ALA

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Mol	Chain	Res	Type
1	A	311	GLY
1	B	42	VAL
1	B	625	ALA
1	C	255	LYS
1	C	291	PRO
1	C	323	PRO
1	C	363	LEU
1	C	624	VAL
1	D	11	ILE
1	D	321	LYS
1	D	384	SER
1	D	603	ILE
1	D	738	VAL
1	E	255	LYS
1	E	384	SER
1	E	624	VAL
1	F	194	ASP
1	F	202	PRO
1	F	203	LEU
1	F	321	LYS
1	F	603	ILE
1	F	738	VAL
1	A	13	GLN
1	A	202	PRO
1	A	268	PRO
1	A	291	PRO
1	A	321	LYS
1	A	323	PRO
1	A	351	VAL
1	A	384	SER
1	A	428	THR
1	A	429	GLY
1	A	499	ASN
1	A	603	ILE
1	A	609	SER
1	A	624	VAL
1	A	725	ILE
1	B	291	PRO
1	B	320	SER
1	B	323	PRO
1	B	366	ALA
1	B	455	LEU

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Mol	Chain	Res	Type
1	B	529	TYR
1	B	741	GLU
1	C	41	GLY
1	C	321	LYS
1	C	362	ILE
1	C	384	SER
1	C	531	ASP
1	C	586	LYS
1	C	718	ASN
1	D	13	GLN
1	D	194	ASP
1	D	319	TRP
1	D	632	GLY
1	D	644	LYS
1	D	715	VAL
1	E	194	ASP
1	E	203	LEU
1	E	319	TRP
1	E	320	SER
1	E	429	GLY
1	E	495	MSE
1	E	603	ILE
1	E	632	GLY
1	E	715	VAL
1	E	738	VAL
1	F	291	PRO
1	F	363	LEU
1	F	384	SER
1	F	545	GLY
1	A	130	VAL
1	A	255	LYS
1	A	329	SER
1	A	363	LEU
1	A	424	TYR
1	A	657	GLY
1	A	714	GLY
1	A	715	VAL
1	A	732	ASN
1	B	81	GLN
1	B	83	PHE
1	B	194	ASP
1	B	268	PRO

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Mol	Chain	Res	Type
1	B	321	LYS
1	B	360	ARG
1	B	384	SER
1	B	715	VAL
1	B	738	VAL
1	C	29	ASN
1	C	234	GLU
1	C	360	ARG
1	C	423	GLN
1	C	539	ASP
1	C	609	SER
1	C	738	VAL
1	D	49	ARG
1	D	143	ASP
1	D	291	PRO
1	D	320	SER
1	D	323	PRO
1	E	12	VAL
1	E	83	PHE
1	E	199	TYR
1	E	202	PRO
1	E	268	PRO
1	E	291	PRO
1	E	586	LYS
1	E	648	ASP
1	E	718	ASN
1	F	715	VAL
1	A	113	LEU
1	A	502	SER
1	A	516	ASP
1	A	539	ASP
1	A	551	TYR
1	B	12	VAL
1	B	143	ASP
1	B	247	GLN
1	B	255	LYS
1	B	330	ALA
1	B	521	GLY
1	B	609	SER
1	C	143	ASP
1	C	361	LYS
1	C	521	GLY

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Mol	Chain	Res	Type
1	C	729	VAL
1	D	268	PRO
1	D	339	LYS
1	D	346	GLU
1	D	586	LYS
1	E	63	LYS
1	E	323	PRO
1	E	410	ALA
1	E	460	LEU
1	E	741	GLU
1	F	63	LYS
1	F	83	PHE
1	F	540	TYR
1	F	648	ASP
1	F	695	HIS
1	A	117	PHE
1	A	214	TYR
1	A	416	ASN
1	A	425	ILE
1	A	453	LEU
1	A	514	GLY
1	A	581	ALA
1	A	667	GLN
1	A	718	ASN
1	B	66	PRO
1	B	296	LEU
1	B	311	GLY
1	B	333	PRO
1	B	460	LEU
1	B	499	ASN
1	B	514	GLY
1	B	623	ASN
1	B	630	TYR
1	B	678	PRO
1	C	36	ASN
1	C	88	ILE
1	C	324	VAL
1	C	499	ASN
1	C	603	ILE
1	C	652	GLU
1	D	130	VAL
1	D	180	ALA

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Mol	Chain	Res	Type
1	D	424	TYR
1	E	15	VAL
1	E	36	ASN
1	E	66	PRO
1	E	127	PRO
1	E	416	ASN
1	E	678	PRO
1	F	6	ILE
1	F	234	GLU
1	F	514	GLY
1	F	521	GLY
1	A	12	VAL
1	A	143	ASP
1	A	405	ALA
1	A	521	GLY
1	B	137	ARG
1	B	633	GLU
1	C	268	PRO
1	C	567	ILE
1	D	329	SER
1	D	425	ILE
1	D	741	GLU
1	F	632	GLY
1	A	249	PRO
1	B	82	GLY
1	B	130	VAL
1	B	511	VAL
1	C	715	VAL
1	E	73	ILE
1	E	426	GLY
1	F	15	VAL
1	F	323	PRO
1	A	326	VAL
1	A	738	VAL
1	B	362	ILE
1	B	517	GLY
1	B	522	GLY
1	C	11	ILE
1	C	45	VAL
1	D	66	PRO
1	D	333	PRO
1	A	511	VAL

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Mol	Chain	Res	Type
1	A	634	PRO
1	B	202	PRO
1	B	603	ILE
1	B	705	GLY
1	D	429	GLY
1	E	521	GLY
1	F	324	VAL
1	A	41	GLY
1	C	127	PRO
1	C	202	PRO
1	C	257	ILE
1	D	41	GLY
1	D	73	ILE
1	D	403	VAL
1	E	333	PRO
1	E	351	VAL
1	E	425	ILE
1	F	511	VAL
1	A	698	VAL
1	B	257	ILE
1	B	729	VAL
1	C	130	VAL
1	C	511	VAL
1	E	186	PRO
1	E	249	PRO
1	E	311	GLY
1	E	389	PRO
1	D	389	PRO
1	C	389	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	632/627 (101%)	575 (91%)	57 (9%)	12 46
1	B	630/627 (100%)	574 (91%)	56 (9%)	12 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	626/627 (100%)	569 (91%)	57 (9%)	12 46
1	D	632/627 (101%)	584 (92%)	48 (8%)	16 55
1	E	630/627 (100%)	579 (92%)	51 (8%)	15 52
1	F	630/627 (100%)	573 (91%)	57 (9%)	12 46
All	All	3780/3762 (100%)	3454 (91%)	326 (9%)	13 49

All (326) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	30	LEU
1	A	49	ARG
1	A	60	LEU
1	A	69	ARG
1	A	89	GLU
1	A	91	SER
1	A	111	ASP
1	A	116	LEU
1	A	117	PHE
1	A	163	ARG
1	A	173	ARG
1	A	181	CYS
1	A	187	SER
1	A	188	TYR
1	A	193	SER
1	A	196	GLN
1	A	221	ILE
1	A	224	ILE
1	A	228	CYS
1	A	250	PHE
1	A	284	LEU
1	A	300	LEU
1	A	306	MSE
1	A	317	PHE
1	A	320	SER
1	A	328	THR
1	A	347	GLU
1	A	357	LEU
1	A	375	ASP
1	A	399	ASN
1	A	438	ARG

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Mol	Chain	Res	Type
1	A	455	LEU
1	A	482	LEU
1	A	500	LEU
1	A	502	SER
1	A	516	ASP
1	A	523	GLU
1	A	529	TYR
1	A	537	HIS
1	A	547	ASP
1	A	587	TYR
1	A	615	LEU
1	A	627	ARG
1	A	640	SER
1	A	648	ASP
1	A	663	GLU
1	A	668	SER
1	A	708	ASN
1	A	718	ASN
1	A	719	GLU
1	A	735	ASN
1	A	736	PHE
1	A	738	VAL
1	A	755	PHE
1	A	756	LEU
1	A	771	MSE
1	B	7	HIS
1	B	11	ILE
1	B	33	TYR
1	B	86	PHE
1	B	102	ILE
1	B	112	CYS
1	B	117	PHE
1	B	134	CYS
1	B	162	CYS
1	B	177	GLU
1	B	181	CYS
1	B	193	SER
1	B	221	ILE
1	B	224	ILE
1	B	225	HIS
1	B	228	CYS
1	B	241	ARG

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Mol	Chain	Res	Type
1	B	250	PHE
1	B	256	ASP
1	B	278	ARG
1	B	282	ILE
1	B	309	TYR
1	B	317	PHE
1	B	320	SER
1	B	328	THR
1	B	337	MSE
1	B	369	SER
1	B	375	ASP
1	B	411	PHE
1	B	428	THR
1	B	438	ARG
1	B	439	GLU
1	B	444	PHE
1	B	445	ARG
1	B	471	MSE
1	B	482	LEU
1	B	488	TYR
1	B	490	HIS
1	B	500	LEU
1	B	516	ASP
1	B	527	LEU
1	B	540	TYR
1	B	547	ASP
1	B	587	TYR
1	B	592	PHE
1	B	653	VAL
1	B	663	GLU
1	B	699	GLU
1	B	704	PHE
1	B	718	ASN
1	B	736	PHE
1	B	738	VAL
1	B	747	ASN
1	B	755	PHE
1	B	760	TYR
1	B	771	MSE
1	C	33	TYR
1	C	61	TYR
1	C	89	GLU

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Mol	Chain	Res	Type
1	C	117	PHE
1	C	120	THR
1	C	129	ILE
1	C	142	GLU
1	C	148	ARG
1	C	164	SER
1	C	172	ARG
1	C	173	ARG
1	C	181	CYS
1	C	193	SER
1	C	196	GLN
1	C	225	HIS
1	C	233	GLU
1	C	257	ILE
1	C	258	GLU
1	C	261	LYS
1	C	267	SER
1	C	274	LEU
1	C	278	ARG
1	C	284	LEU
1	C	292	LEU
1	C	306	MSE
1	C	313	HIS
1	C	317	PHE
1	C	337	MSE
1	C	357	LEU
1	C	370	VAL
1	C	375	ASP
1	C	382	ARG
1	C	403	VAL
1	C	427	ASN
1	C	488	TYR
1	C	502	SER
1	C	516	ASP
1	C	523	GLU
1	C	541	TYR
1	C	543	LEU
1	C	548	LEU
1	C	587	TYR
1	C	605	THR
1	C	616	ASP
1	C	624	VAL

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Mol	Chain	Res	Type
1	C	648	ASP
1	C	663	GLU
1	C	693	PHE
1	C	718	ASN
1	C	724	MSE
1	C	726	ARG
1	C	736	PHE
1	C	738	VAL
1	C	744	ARG
1	C	756	LEU
1	C	760	TYR
1	C	766	THR
1	D	7	HIS
1	D	60	LEU
1	D	112	CYS
1	D	113	LEU
1	D	117	PHE
1	D	164	SER
1	D	181	CYS
1	D	188	TYR
1	D	201	ASP
1	D	221	ILE
1	D	242	ARG
1	D	250	PHE
1	D	262	SER
1	D	267	SER
1	D	270	GLU
1	D	295	ASN
1	D	306	MSE
1	D	313	HIS
1	D	317	PHE
1	D	367	ASP
1	D	375	ASP
1	D	382	ARG
1	D	399	ASN
1	D	403	VAL
1	D	423	GLN
1	D	427	ASN
1	D	437	MSE
1	D	473	MSE
1	D	475	ASN
1	D	494	VAL

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Mol	Chain	Res	Type
1	D	541	TYR
1	D	543	LEU
1	D	551	TYR
1	D	587	TYR
1	D	605	THR
1	D	653	VAL
1	D	693	PHE
1	D	708	ASN
1	D	718	ASN
1	D	719	GLU
1	D	724	MSE
1	D	736	PHE
1	D	737	HIS
1	D	738	VAL
1	D	755	PHE
1	D	760	TYR
1	D	766	THR
1	D	771	MSE
1	E	33	TYR
1	E	62	LYS
1	E	67	LEU
1	E	75	LYS
1	E	84	ASP
1	E	110	ASP
1	E	112	CYS
1	E	117	PHE
1	E	128	PHE
1	E	147	ASP
1	E	172	ARG
1	E	181	CYS
1	E	196	GLN
1	E	224	ILE
1	E	225	HIS
1	E	241	ARG
1	E	259	THR
1	E	267	SER
1	E	278	ARG
1	E	283	THR
1	E	301	HIS
1	E	309	TYR
1	E	313	HIS
1	E	317	PHE

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Mol	Chain	Res	Type
1	E	328	THR
1	E	342	GLU
1	E	375	ASP
1	E	403	VAL
1	E	423	GLN
1	E	427	ASN
1	E	444	PHE
1	E	500	LEU
1	E	525	LEU
1	E	541	TYR
1	E	587	TYR
1	E	596	LEU
1	E	605	THR
1	E	616	ASP
1	E	630	TYR
1	E	643	PHE
1	E	663	GLU
1	E	668	SER
1	E	686	HIS
1	E	693	PHE
1	E	708	ASN
1	E	718	ASN
1	E	736	PHE
1	E	738	VAL
1	E	747	ASN
1	E	755	PHE
1	E	760	TYR
1	F	22	TYR
1	F	84	ASP
1	F	113	LEU
1	F	116	LEU
1	F	117	PHE
1	F	147	ASP
1	F	175	HIS
1	F	181	CYS
1	F	203	LEU
1	F	225	HIS
1	F	228	CYS
1	F	233	GLU
1	F	238	GLU
1	F	250	PHE
1	F	262	SER

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Mol	Chain	Res	Type
1	F	284	LEU
1	F	301	HIS
1	F	312	THR
1	F	317	PHE
1	F	328	THR
1	F	342	GLU
1	F	369	SER
1	F	384	SER
1	F	403	VAL
1	F	423	GLN
1	F	427	ASN
1	F	459	ASP
1	F	473	MSE
1	F	487	HIS
1	F	490	HIS
1	F	533	GLU
1	F	537	HIS
1	F	541	TYR
1	F	554	LEU
1	F	587	TYR
1	F	593	ASN
1	F	596	LEU
1	F	599	LEU
1	F	605	THR
1	F	627	ARG
1	F	628	ARG
1	F	640	SER
1	F	643	PHE
1	F	653	VAL
1	F	663	GLU
1	F	686	HIS
1	F	695	HIS
1	F	704	PHE
1	F	708	ASN
1	F	719	GLU
1	F	736	PHE
1	F	738	VAL
1	F	750	ASN
1	F	755	PHE
1	F	760	TYR
1	F	766	THR
1	F	771	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	121	ASN
1	A	171	ASN
1	A	196	GLN
1	A	247	GLN
1	A	295	ASN
1	A	331	ASN
1	A	427	ASN
1	A	452	ASN
1	A	475	ASN
1	A	485	GLN
1	A	575	ASN
1	A	593	ASN
1	A	718	ASN
1	A	737	HIS
1	A	747	ASN
1	A	750	ASN
1	B	5	HIS
1	B	13	GLN
1	B	36	ASN
1	B	121	ASN
1	B	171	ASN
1	B	247	GLN
1	B	295	ASN
1	B	318	HIS
1	B	331	ASN
1	B	399	ASN
1	B	427	ASN
1	B	475	ASN
1	B	483	GLN
1	B	485	GLN
1	B	490	HIS
1	B	575	ASN
1	B	593	ASN
1	B	623	ASN
1	B	667	GLN
1	B	695	HIS
1	B	735	ASN
1	B	747	ASN
1	B	750	ASN
1	C	9	GLN

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Mol	Chain	Res	Type
1	C	121	ASN
1	C	133	ASN
1	C	171	ASN
1	C	247	GLN
1	C	295	ASN
1	C	331	ASN
1	C	399	ASN
1	C	409	ASN
1	C	427	ASN
1	C	465	ASN
1	C	475	ASN
1	C	486	HIS
1	C	518	ASN
1	C	575	ASN
1	C	718	ASN
1	C	750	ASN
1	D	5	HIS
1	D	9	GLN
1	D	26	HIS
1	D	28	HIS
1	D	121	ASN
1	D	133	ASN
1	D	171	ASN
1	D	295	ASN
1	D	331	ASN
1	D	409	ASN
1	D	427	ASN
1	D	452	ASN
1	D	475	ASN
1	D	483	GLN
1	D	485	GLN
1	D	575	ASN
1	D	593	ASN
1	D	597	ASN
1	D	604	ASN
1	D	708	ASN
1	D	718	ASN
1	D	735	ASN
1	D	747	ASN
1	D	750	ASN
1	E	5	HIS
1	E	7	HIS

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Mol	Chain	Res	Type
1	E	13	GLN
1	E	36	ASN
1	E	121	ASN
1	E	133	ASN
1	E	171	ASN
1	E	196	GLN
1	E	295	ASN
1	E	301	HIS
1	E	331	ASN
1	E	364	ASN
1	E	427	ASN
1	E	452	ASN
1	E	475	ASN
1	E	485	GLN
1	E	575	ASN
1	E	593	ASN
1	E	604	ASN
1	E	686	HIS
1	E	718	ASN
1	E	747	ASN
1	E	750	ASN
1	E	753	GLN
1	F	7	HIS
1	F	171	ASN
1	F	295	ASN
1	F	301	HIS
1	F	331	ASN
1	F	341	ASN
1	F	427	ASN
1	F	452	ASN
1	F	465	ASN
1	F	475	ASN
1	F	593	ASN
1	F	604	ASN
1	F	686	HIS
1	F	708	ASN
1	F	750	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	748/772 (96%)	0.01	18 (2%)	62	52	97, 155, 228, 284	0
1	B	744/772 (96%)	0.26	42 (5%)	28	21	115, 179, 293, 361	0
1	C	739/772 (95%)	0.02	13 (1%)	71	62	118, 171, 229, 257	0
1	D	747/772 (96%)	0.17	34 (4%)	36	28	125, 189, 267, 339	0
1	E	744/772 (96%)	0.17	37 (4%)	32	25	110, 183, 285, 327	0
1	F	744/772 (96%)	0.24	34 (4%)	36	28	138, 191, 298, 348	0
All	All	4466/4632 (96%)	0.15	178 (3%)	42	33	97, 179, 272, 361	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	ILE	6.5
1	E	51	GLU	6.0
1	D	81	GLN	5.9
1	B	46	VAL	5.5
1	E	198	ILE	5.3
1	E	199	TYR	5.3
1	E	46	VAL	5.1
1	B	3	ALA	5.1
1	C	99	ASP	5.0
1	A	586	LYS	4.9
1	D	91	SER	4.6
1	A	99	ASP	4.5
1	F	70	ILE	4.5
1	B	31	ARG	4.5
1	F	35	LYS	4.4
1	F	18	ARG	4.3
1	E	49	ARG	4.2
1	B	89	GLU	4.1
1	D	82	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	47	GLU	4.1
1	B	51	GLU	4.1
1	F	175	HIS	4.0
1	B	87	TYR	3.9
1	B	80	PRO	3.9
1	F	400	GLY	3.8
1	F	17	PHE	3.8
1	B	88	ILE	3.7
1	B	2	LYS	3.6
1	F	199	TYR	3.6
1	B	4	TYR	3.5
1	B	81	GLN	3.5
1	B	62	LYS	3.5
1	E	3	ALA	3.5
1	B	45	VAL	3.4
1	B	32	GLY	3.4
1	F	19	PRO	3.4
1	F	78	ILE	3.3
1	E	80	PRO	3.3
1	A	78	ILE	3.3
1	D	49	ARG	3.3
1	B	60	LEU	3.3
1	E	47	GLU	3.3
1	E	75	LYS	3.2
1	E	85	ARG	3.2
1	D	198	ILE	3.2
1	F	255	LYS	3.2
1	F	62	LYS	3.2
1	B	6	ILE	3.2
1	B	199	TYR	3.2
1	D	586	LYS	3.1
1	B	79	PRO	3.1
1	E	81	GLN	3.1
1	C	91	SER	3.0
1	B	48	GLY	3.0
1	D	50	GLU	3.0
1	B	61	TYR	2.9
1	E	4	TYR	2.9
1	E	89	GLU	2.9
1	E	82	GLY	2.9
1	B	70	ILE	2.9
1	F	51	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	81	GLN	2.9
1	A	70	ILE	2.9
1	B	78	ILE	2.9
1	E	73	ILE	2.9
1	D	547	ASP	2.8
1	F	73	ILE	2.8
1	E	71	ASP	2.8
1	E	48	GLY	2.8
1	E	396	PHE	2.8
1	F	254	ALA	2.8
1	E	56	PHE	2.7
1	C	70	ILE	2.7
1	E	53	ILE	2.7
1	B	35	LYS	2.7
1	C	586	LYS	2.7
1	B	59	ASP	2.7
1	E	24	ILE	2.7
1	F	75	LYS	2.7
1	B	179	THR	2.7
1	F	296	LEU	2.7
1	B	44	ILE	2.7
1	D	75	LYS	2.6
1	B	17	PHE	2.6
1	D	80	PRO	2.6
1	B	75	LYS	2.6
1	F	90	LYS	2.6
1	D	53	ILE	2.6
1	D	400	GLY	2.6
1	F	605	THR	2.6
1	E	31	ARG	2.6
1	F	49	ARG	2.6
1	E	83	PHE	2.6
1	D	70	ILE	2.6
1	F	198	ILE	2.6
1	E	6	ILE	2.6
1	E	17	PHE	2.5
1	D	3	ALA	2.5
1	D	732	ASN	2.5
1	A	5	HIS	2.5
1	B	36	ASN	2.5
1	B	83	PHE	2.5
1	F	547	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	78	ILE	2.5
1	B	52	ASP	2.5
1	C	376	GLY	2.5
1	A	547	ASP	2.5
1	F	46	VAL	2.5
1	C	604	ASN	2.5
1	E	87	TYR	2.5
1	D	99	ASP	2.4
1	D	30	LEU	2.4
1	F	27	GLU	2.4
1	E	52	ASP	2.4
1	F	26	HIS	2.4
1	F	36	ASN	2.4
1	E	542	PRO	2.4
1	A	77	GLU	2.4
1	D	733	GLY	2.4
1	A	3	ALA	2.4
1	C	87	TYR	2.4
1	C	732	ASN	2.4
1	A	73	ILE	2.4
1	A	199	TYR	2.4
1	B	169	PRO	2.4
1	D	76	LYS	2.4
1	D	542	PRO	2.4
1	F	4	TYR	2.4
1	E	25	ALA	2.4
1	D	737	HIS	2.3
1	A	75	LYS	2.3
1	B	82	GLY	2.3
1	E	5	HIS	2.3
1	D	83	PHE	2.3
1	C	330	ALA	2.3
1	E	30	LEU	2.3
1	C	603	ILE	2.3
1	D	728	VAL	2.3
1	A	46	VAL	2.3
1	D	395	PRO	2.3
1	B	77	GLU	2.3
1	C	75	LYS	2.2
1	B	34	VAL	2.2
1	B	178	PRO	2.2
1	A	52	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	198	ILE	2.2
1	E	60	LEU	2.2
1	A	605	THR	2.2
1	F	85	ARG	2.2
1	F	24	ILE	2.1
1	F	732	ASN	2.1
1	D	51	GLU	2.1
1	C	47	GLU	2.1
1	E	91	SER	2.1
1	B	5	HIS	2.1
1	D	199	TYR	2.1
1	F	3	ALA	2.1
1	B	33	TYR	2.1
1	E	586	LYS	2.1
1	B	43	GLU	2.1
1	E	62	LYS	2.1
1	F	586	LYS	2.1
1	D	47	GLU	2.1
1	D	605	THR	2.1
1	E	84	ASP	2.1
1	D	361	LYS	2.1
1	C	585	LEU	2.1
1	B	84	ASP	2.1
1	D	709	VAL	2.1
1	D	5	HIS	2.1
1	A	51	GLU	2.0
1	F	44	ILE	2.0
1	D	173	ARG	2.0
1	A	47	GLU	2.0
1	A	92	SER	2.0
1	A	198	ILE	2.0
1	F	214	TYR	2.0
1	D	6	ILE	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	1001	1/1	0.98	0.28	1.02	144,144,144,144	0
2	ZN	F	1001	1/1	0.90	0.27	0.08	187,187,187,187	0
2	ZN	E	1001	1/1	0.98	0.26	-0.00	152,152,152,152	0
2	ZN	E	1003	1/1	0.97	0.21	-0.02	183,183,183,183	0
2	ZN	F	1003	1/1	0.98	0.25	-0.16	179,179,179,179	0
2	ZN	A	1003	1/1	0.94	0.24	-0.31	178,178,178,178	0
2	ZN	D	1001	1/1	0.99	0.24	-0.49	157,157,157,157	0
2	ZN	C	1001	1/1	0.95	0.19	-0.66	143,143,143,143	0
2	ZN	B	1001	1/1	0.98	0.22	-0.75	170,170,170,170	0
2	ZN	C	1003	1/1	0.96	0.23	-0.97	156,156,156,156	0
2	ZN	D	1003	1/1	0.88	0.21	-1.31	202,202,202,202	0
2	ZN	D	1002	1/1	0.94	0.08	-1.57	149,149,149,149	0
2	ZN	A	1002	1/1	0.99	0.12	-1.67	113,113,113,113	0
2	ZN	E	1002	1/1	0.91	0.08	-1.86	175,175,175,175	0
2	ZN	C	1002	1/1	0.95	0.13	-2.99	147,147,147,147	0
2	ZN	B	1002	1/1	0.98	0.03	-3.18	187,187,187,187	0
2	ZN	F	1002	1/1	0.89	0.11	-4.78	213,213,213,213	0
2	ZN	B	1003	1/1	0.80	0.32	-	180,180,180,180	0

6.5 Other polymers

There are no such residues in this entry.