



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:51 am BST

PDB ID : 1UKL
Title : Crystal structure of Importin-beta and SREBP-2 complex
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Deposited on : 2003-08-26
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

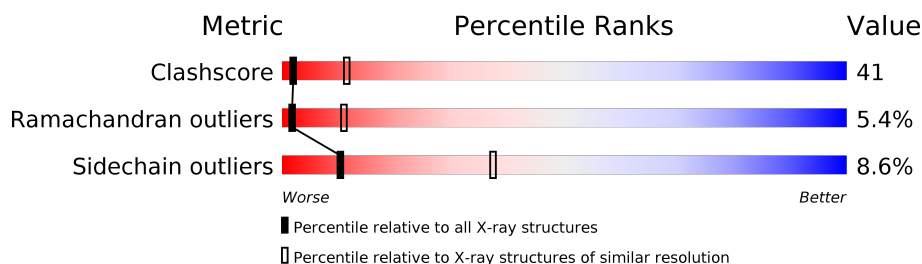
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	876	
1	B	876	
2	C	61	
2	D	61	
2	E	61	
2	F	61	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15606 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 Importin beta-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	876	Total	C	N	O	S	0	0	0
			6807	4286	1141	1334	46			
1	B	876	Total	C	N	O	S	0	0	0
			6807	4286	1141	1334	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	MET	VAL	SEE REMARK 999	UNP P70168
B	388	MET	VAL	SEE REMARK 999	UNP P70168

- Molecule 2 is a protein called Sterol regulatory element binding protein-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	61	Total	C	N	O	Se	0	0	0
			498	313	93	89	3			
2	D	61	Total	C	N	O	Se	0	0	0
			498	313	93	89	3			
2	E	61	Total	C	N	O	Se	0	0	0
			498	313	93	89	3			
2	F	61	Total	C	N	O	Se	0	0	0
			498	313	93	89	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	358	MSE	MET	MODIFIED RESIDUE	UNP Q12772
C	364	MSE	MET	MODIFIED RESIDUE	UNP Q12772
C	392	MSE	MET	MODIFIED RESIDUE	UNP Q12772
D	358	MSE	MET	MODIFIED RESIDUE	UNP Q12772
D	364	MSE	MET	MODIFIED RESIDUE	UNP Q12772
D	392	MSE	MET	MODIFIED RESIDUE	UNP Q12772

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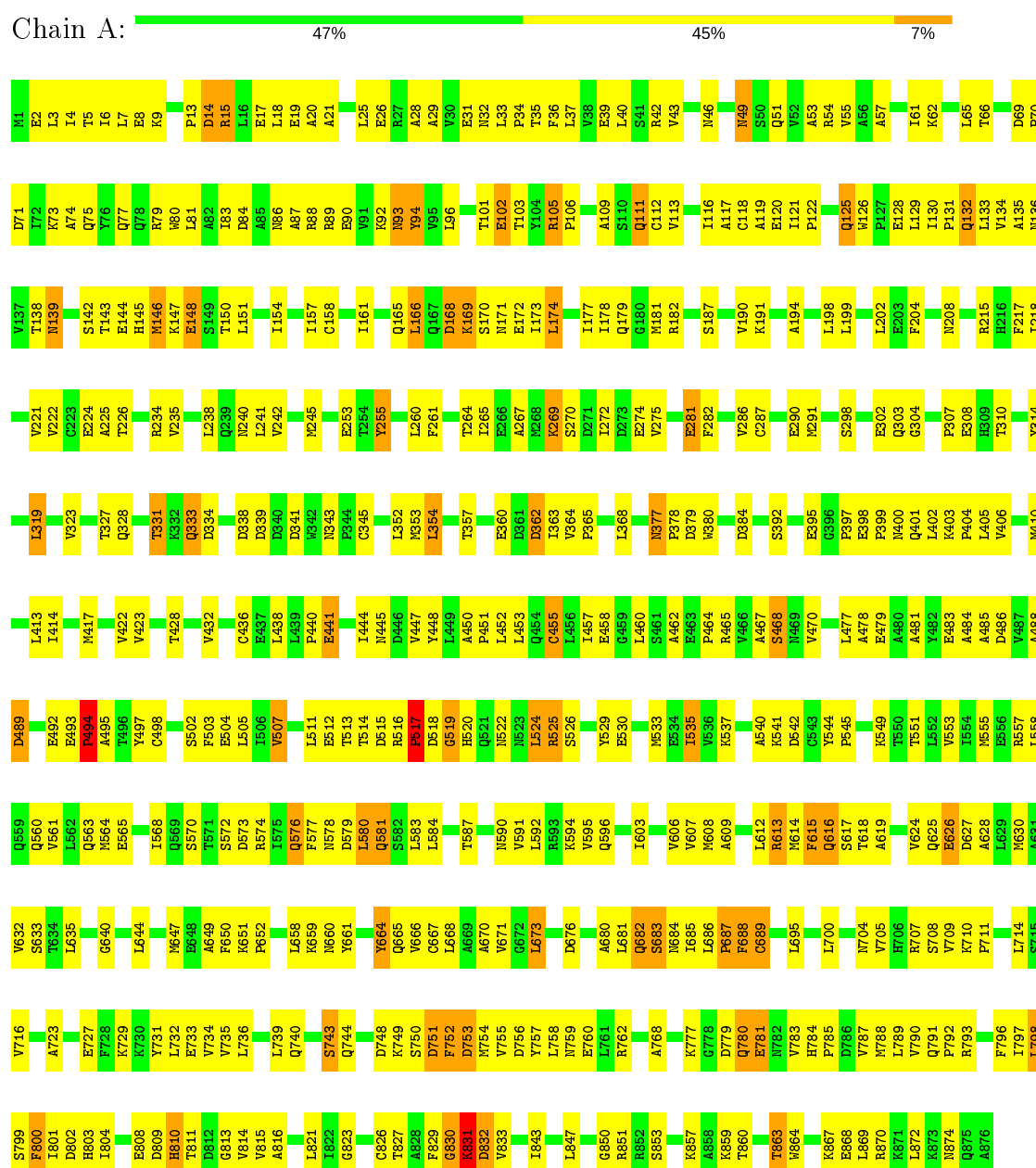
Chain	Residue	Modelled	Actual	Comment	Reference
E	358	MSE	MET	MODIFIED RESIDUE	UNP Q12772
E	364	MSE	MET	MODIFIED RESIDUE	UNP Q12772
E	392	MSE	MET	MODIFIED RESIDUE	UNP Q12772
F	358	MSE	MET	MODIFIED RESIDUE	UNP Q12772
F	364	MSE	MET	MODIFIED RESIDUE	UNP Q12772
F	392	MSE	MET	MODIFIED RESIDUE	UNP Q12772

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

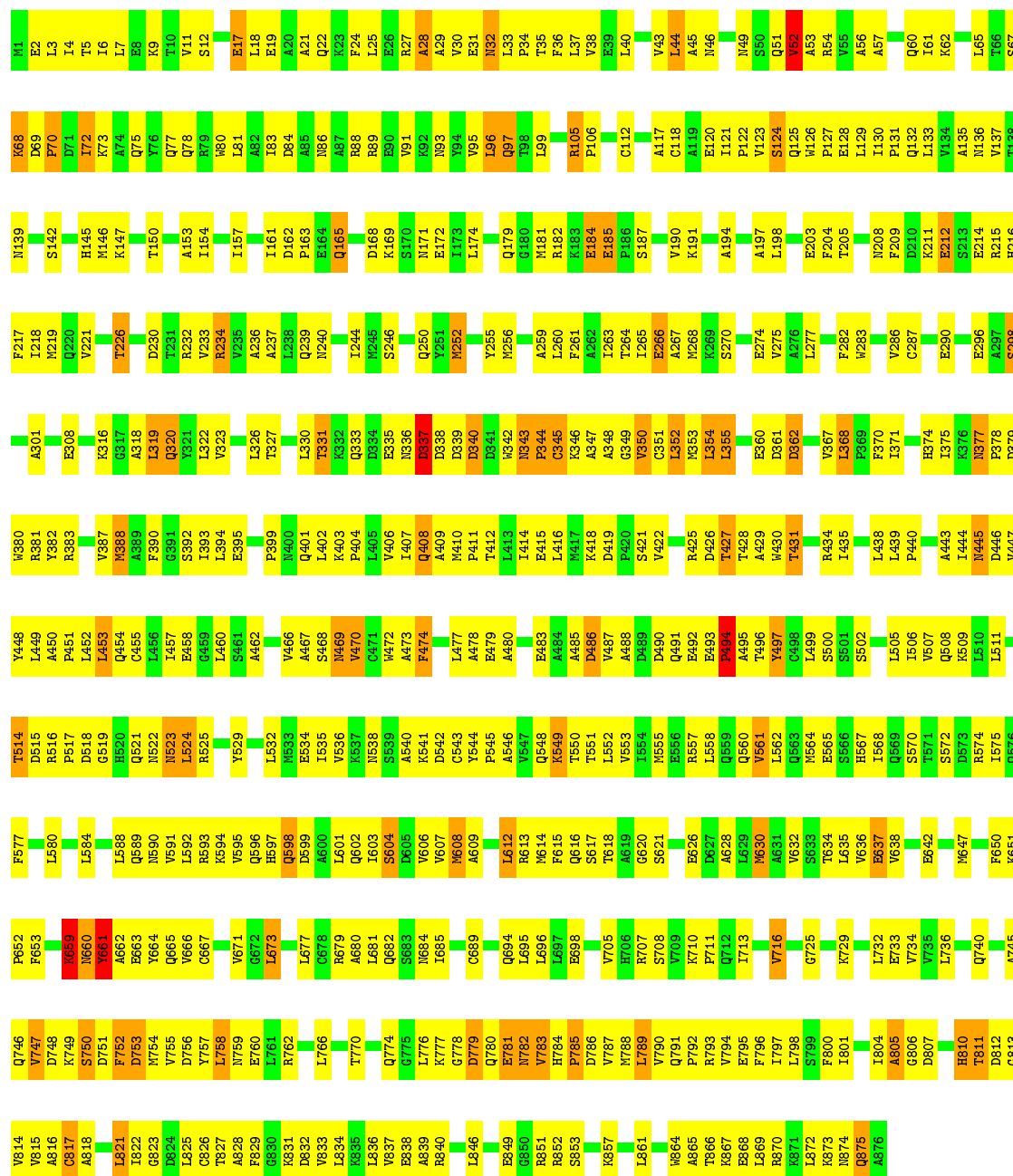
Note EDS was not executed.

- Molecule 1: Importin beta-1 subunit



- Molecule 1: Importin beta-1 subunit

Chain B: 



Chain D:  41% 52% 7%



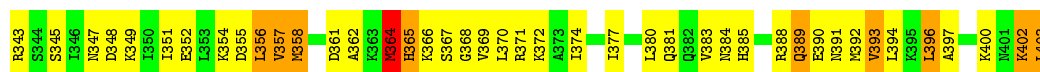
- Molecule 2: Sterol regulatory element binding protein-2

Chain E:  43% 44% 13%



- Molecule 2: Sterol regulatory element binding protein-2

Chain F:  31% 52% 15%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.09Å 113.28Å 240.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00	Depositor
% Data completeness (in resolution range)	99.1 (19.99-3.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15606	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.44	0/6918	0.69	6/9392 (0.1%)
1	B	0.44	0/6918	0.74	8/9392 (0.1%)
2	C	0.60	0/498	0.78	1/655 (0.2%)
2	D	0.50	0/498	0.68	0/655
2	E	0.67	0/498	0.94	3/655 (0.5%)
2	F	0.63	1/498 (0.2%)	0.80	0/655
All	All	0.46	1/15828 (0.0%)	0.73	18/21404 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	358	MSE	CG-SE	-5.93	1.75	1.95

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	PRO	CA-N-CD	-10.33	97.04	111.50
1	A	494	PRO	CA-N-CD	-10.19	97.23	111.50
2	E	368	GLY	N-CA-C	-9.03	90.53	113.10
1	A	810	HIS	CA-C-N	-7.43	100.85	117.20
1	B	494	PRO	CA-N-CD	-7.05	101.64	111.50
2	E	365	HIS	CA-C-N	-6.85	102.13	117.20
1	A	517	PRO	CA-N-CD	-6.62	102.24	111.50
2	E	367	SER	C-N-CA	6.42	135.78	122.30
1	B	337	ASP	CA-C-N	-6.36	103.20	117.20
2	C	362	ALA	C-N-CA	-6.09	106.47	121.70
1	B	785	PRO	CA-N-CD	-5.91	103.22	111.50
1	B	490	ASP	CA-C-N	-5.89	104.24	117.20
1	B	747	VAL	CA-C-N	-5.62	104.83	117.20
1	A	831	LYS	CA-C-N	-5.34	105.45	117.20
1	B	336	ASN	C-N-CA	-5.24	108.61	121.70
1	B	491	GLN	N-CA-C	-5.23	96.88	111.00
1	A	810	HIS	O-C-N	5.11	130.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	810	HIS	C-N-CA	5.11	134.46	121.70

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	6807	0	6802	506	1
1	B	6807	0	6802	621	0
2	C	498	0	539	53	0
2	D	498	0	539	39	0
2	E	498	0	539	78	0
2	F	498	0	539	53	1
All	All	15606	0	15760	1294	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 41.

All (1294) 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)
2:E:357:VAL:HG12	2:E:372:LYS:CE	1.52	1.39
1:A:870:ARG:NE	1:B:487:VAL:CG1	1.83	1.39
1:A:489:ASP:HB2	1:A:494:PRO:CD	1.63	1.26
1:A:870:ARG:NE	1:B:487:VAL:HG11	0.94	1.25
1:A:489:ASP:CB	1:A:494:PRO:HD3	1.68	1.23
2:E:357:VAL:CG1	2:E:372:LYS:HE3	1.69	1.22
2:F:347:ASN:OD1	2:F:348:ASP:N	1.69	1.22
2:E:357:VAL:HG11	2:E:372:LYS:CG	1.72	1.19
2:E:357:VAL:HG11	2:E:372:LYS:HG3	1.25	1.18
1:B:783:VAL:O	1:B:783:VAL:CG1	1.92	1.18
2:E:357:VAL:CG1	2:E:372:LYS:CE	2.21	1.17
2:C:358:MSE:SE	2:C:364:MSE:SE	2.62	1.16
2:F:364:MSE:SE	2:F:365:HIS:CE1	2.49	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:PHE:O	1:A:799:SER:HB2	1.46	1.12
2:E:357:VAL:HG12	2:E:372:LYS:HE2	1.18	1.11
2:E:358:MSE:HB3	2:E:372:LYS:HE2	1.30	1.09
1:A:784:HIS:HD2	1:A:785:PRO:HD2	1.14	1.08
1:A:870:ARG:CZ	1:B:487:VAL:CG1	2.31	1.07
1:A:762:ARG:HD3	1:A:800:PHE:HE1	1.17	1.06
1:A:762:ARG:HD3	1:A:800:PHE:CE1	1.90	1.06
2:F:365:HIS:HD2	2:F:367:SER:HB3	1.19	1.06
1:A:870:ARG:CZ	1:B:487:VAL:HG11	1.86	1.06
1:A:870:ARG:HE	1:B:487:VAL:CG1	1.56	1.06
1:B:659:LYS:HE3	1:B:659:LYS:HA	1.34	1.05
2:E:357:VAL:HG12	2:E:358:MSE:H	1.17	1.04
1:A:102:GLU:H	1:A:106:PRO:HG2	1.21	1.04
1:B:69:ASP:OD2	1:B:73:LYS:HE2	1.57	1.04
1:B:751:ASP:O	1:B:752:PHE:O	1.75	1.03
1:B:663:GLU:OE2	1:B:665:GLN:HB3	1.58	1.03
1:A:870:ARG:CD	1:B:487:VAL:HG11	1.90	1.01
1:B:663:GLU:OE2	1:B:665:GLN:CB	2.09	1.01
2:F:347:ASN:O	2:F:348:ASP:HB3	1.61	1.01
2:F:365:HIS:CD2	2:F:367:SER:HB3	1.96	1.01
1:A:514:THR:HG21	1:A:557:ARG:NH1	1.76	1.00
1:A:492:GLU:OE1	2:D:343:ARG:NH1	1.93	1.00
1:A:576:GLN:HA	1:A:576:GLN:HE21	1.27	1.00
1:B:777:LYS:HA	1:B:787:VAL:CG2	1.91	0.99
1:A:752:PHE:O	1:A:754:MET:N	1.95	0.99
2:F:347:ASN:CG	2:F:348:ASP:H	1.66	0.99
2:D:370:LEU:N	2:D:370:LEU:HD23	1.77	0.99
1:A:752:PHE:O	1:A:755:VAL:N	1.95	0.99
2:E:358:MSE:HB3	2:E:372:LYS:CE	1.94	0.98
1:A:752:PHE:O	1:A:753:ASP:C	1.99	0.98
1:A:514:THR:HG21	1:A:557:ARG:HH12	1.28	0.98
1:B:335:GLU:OE2	1:B:380:TRP:HZ2	1.47	0.97
1:B:38:VAL:HA	1:B:91:VAL:HG22	1.45	0.97
1:B:30:VAL:HG12	1:B:32:ASN:H	1.30	0.97
2:E:357:VAL:HG12	2:E:358:MSE:N	1.80	0.97
2:E:357:VAL:HG12	2:E:372:LYS:HE3	1.27	0.96
1:A:157:ILE:HG23	1:A:161:ILE:HD12	1.48	0.95
1:B:327:THR:HA	1:B:330:LEU:HD12	1.48	0.95
2:D:370:LEU:O	2:D:374:ILE:HD12	1.66	0.95
1:B:783:VAL:O	1:B:783:VAL:HG12	1.63	0.95
1:A:215:ARG:HD2	1:A:255:TYR:OH	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASP:HA	1:A:465:ARG:HH22	1.33	0.94
1:A:762:ARG:HD2	1:A:804:ILE:HD11	1.49	0.94
1:B:514:THR:HG21	1:B:557:ARG:HH12	1.33	0.94
1:B:749:LYS:HG3	1:B:750:SER:H	1.30	0.94
1:B:406:VAL:HG13	1:B:435:ILE:HD13	1.50	0.92
2:E:358:MSE:HE2	2:E:372:LYS:HG2	1.52	0.92
1:B:783:VAL:HG13	1:B:783:VAL:O	1.67	0.92
1:A:513:THR:O	1:A:516:ARG:HG3	1.70	0.92
1:B:337:ASP:O	1:B:338:ASP:OD1	1.88	0.92
1:B:606:VAL:O	1:B:609:ALA:HB3	1.70	0.91
2:D:370:LEU:HD23	2:D:370:LEU:H	1.32	0.91
1:B:130:ILE:HG22	1:B:169:LYS:HD2	1.53	0.91
1:A:102:GLU:HB3	1:A:106:PRO:HD3	1.50	0.91
1:A:489:ASP:HB2	1:A:494:PRO:HD3	0.92	0.90
1:A:515:ASP:O	1:A:516:ARG:HG2	1.69	0.90
1:A:762:ARG:CD	1:A:800:PHE:HE1	1.84	0.90
1:B:708:SER:O	1:B:711:PRO:HD2	1.71	0.90
1:A:135:ALA:HA	1:A:138:THR:HG22	1.53	0.90
2:E:358:MSE:CB	2:E:372:LYS:HE2	2.01	0.90
2:E:358:MSE:HG2	2:E:358:MSE:O	1.71	0.90
1:B:748:ASP:OD2	1:B:754:MET:HE1	1.72	0.89
1:A:515:ASP:O	1:A:516:ARG:CG	2.21	0.89
2:E:358:MSE:HE2	2:E:372:LYS:CG	2.02	0.89
1:B:749:LYS:HG3	1:B:750:SER:N	1.85	0.89
1:A:644:LEU:HD22	1:A:684:ASN:HD21	1.37	0.89
1:A:784:HIS:CD2	1:A:785:PRO:HD2	2.06	0.89
1:A:568:ILE:HD13	1:A:574:ARG:HD2	1.56	0.88
1:B:751:ASP:C	1:B:752:PHE:O	2.12	0.88
2:C:361:ASP:O	2:C:361:ASP:OD1	1.90	0.88
1:B:169:LYS:HB2	1:B:172:GLU:HB2	1.53	0.88
1:A:762:ARG:CD	1:A:800:PHE:CE1	2.55	0.87
2:E:346:ILE:HD12	2:E:349:LYS:HD2	1.57	0.86
1:B:494:PRO:O	1:B:541:LYS:HB2	1.76	0.86
1:B:335:GLU:OE2	1:B:380:TRP:CZ2	2.28	0.86
1:A:707:ARG:NH2	1:A:753:ASP:OD1	2.09	0.85
1:B:410:MET:O	1:B:414:ILE:HG13	1.77	0.85
1:A:84:ASP:HB3	1:A:87:ALA:HB2	1.57	0.85
1:A:489:ASP:HB2	1:A:494:PRO:CG	2.07	0.85
2:E:358:MSE:H	2:E:372:LYS:HE2	1.41	0.84
1:B:65:LEU:HB2	1:B:69:ASP:HB2	1.60	0.84
1:B:69:ASP:OD2	1:B:73:LYS:CE	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:LEU:HD22	1:A:684:ASN:ND2	1.93	0.84
1:B:33:LEU:HA	1:B:36:PHE:HB3	1.59	0.84
1:B:27:ARG:HG2	1:B:28:ALA:N	1.91	0.84
1:B:478:ALA:HB2	1:B:535:ILE:HD12	1.58	0.84
2:C:357:VAL:HG23	2:C:358:MSE:HG3	1.60	0.84
2:E:354:LYS:HE3	2:E:361:ASP:HA	1.57	0.83
1:B:468:SER:HB3	2:E:343:ARG:HH22	1.43	0.83
2:E:358:MSE:N	2:E:372:LYS:HE2	1.94	0.82
1:A:377:ASN:ND2	1:A:379:ASP:H	1.77	0.82
1:B:414:ILE:HG23	1:B:455:CYS:SG	2.19	0.82
1:B:430:TRP:HA	1:B:469:ASN:HD22	1.44	0.82
1:B:65:LEU:HD23	1:B:65:LEU:H	1.42	0.82
1:B:756:ASP:HA	1:B:759:ASN:HB2	1.62	0.82
1:A:684:ASN:O	1:A:687:PRO:HD2	1.78	0.82
1:A:799:SER:O	1:A:802:ASP:N	2.12	0.82
2:F:364:MSE:SE	2:F:365:HIS:HE1	2.14	0.81
2:E:358:MSE:O	2:E:358:MSE:CG	2.29	0.81
1:B:483:GLU:HA	1:B:486:ASP:OD1	1.81	0.81
1:B:89:ARG:O	1:B:93:ASN:HB2	1.79	0.81
1:A:544:TYR:HE1	1:A:595:VAL:HA	1.46	0.80
1:A:488:ALA:HA	1:B:870:ARG:HH12	1.46	0.80
1:A:751:ASP:O	1:A:754:MET:N	2.13	0.80
2:D:345:SER:HB2	2:D:349:LYS:HB2	1.63	0.80
2:E:357:VAL:CG1	2:E:358:MSE:H	1.78	0.80
1:A:32:ASN:HB3	1:A:35:THR:HB	1.63	0.80
1:B:485:ALA:O	1:B:487:VAL:N	2.12	0.80
1:A:377:ASN:HD22	1:A:378:PRO:N	1.79	0.80
1:B:105:ARG:HB3	1:B:106:PRO:CD	2.12	0.80
1:B:388:MET:HG2	1:B:427:THR:HG23	1.60	0.80
2:E:357:VAL:CG1	2:E:372:LYS:CG	2.59	0.80
1:A:808:GLU:O	1:A:810:HIS:N	2.15	0.80
1:B:483:GLU:HA	1:B:486:ASP:CG	2.01	0.80
1:A:516:ARG:HD3	1:A:524:LEU:CD1	2.13	0.79
1:A:51:GLN:HB2	1:A:105:ARG:HG3	1.63	0.79
1:B:483:GLU:HA	1:B:486:ASP:OD2	1.82	0.79
1:A:608:MET:HE1	1:A:632:VAL:HG22	1.64	0.79
1:B:736:LEU:HB3	1:B:793:ARG:HH12	1.48	0.79
1:B:811:THR:HG22	1:B:813:GLY:H	1.46	0.79
1:B:777:LYS:HA	1:B:787:VAL:HG21	1.63	0.79
1:A:353:MET:CG	1:A:392:SER:HB2	2.13	0.79
2:E:398:ASN:HD21	2:E:401:ASN:HA	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:MET:SD	1:A:603:ILE:HG23	2.23	0.78
1:B:777:LYS:CA	1:B:787:VAL:CG2	2.60	0.78
1:B:27:ARG:NH1	1:B:28:ALA:H	1.81	0.78
1:B:327:THR:O	1:B:330:LEU:HB2	1.82	0.78
1:B:153:ALA:O	1:B:157:ILE:HG13	1.82	0.78
1:B:748:ASP:OD2	1:B:754:MET:CE	2.32	0.78
1:A:736:LEU:HD13	1:A:793:ARG:HE	1.50	0.77
1:B:27:ARG:NH1	1:B:28:ALA:HA	1.98	0.77
1:B:402:LEU:O	1:B:406:VAL:HG23	1.84	0.77
1:A:353:MET:HG2	1:A:392:SER:HB2	1.66	0.77
1:A:516:ARG:HD3	1:A:524:LEU:HD11	1.67	0.77
1:A:640:GLY:O	1:A:680:ALA:HB1	1.85	0.76
1:B:483:GLU:O	1:B:486:ASP:OD2	2.03	0.76
1:B:777:LYS:HD2	1:B:780:GLN:HE21	1.50	0.76
1:B:402:LEU:HD23	1:B:439:LEU:HD11	1.67	0.76
1:B:751:ASP:O	1:B:752:PHE:C	2.23	0.76
1:B:834:LEU:HB2	1:B:872:LEU:HD13	1.67	0.76
1:A:533:MET:HG2	1:A:590:ASN:HD22	1.50	0.76
1:B:831:LYS:HA	1:B:872:LEU:HD22	1.66	0.76
2:C:361:ASP:O	2:C:361:ASP:CG	2.24	0.76
1:A:478:ALA:HB2	1:A:535:ILE:HD12	1.67	0.75
1:A:397:PRO:HB2	1:A:402:LEU:HD11	1.67	0.75
1:A:707:ARG:HG3	1:A:707:ARG:HH11	1.52	0.75
1:A:486:ASP:O	1:A:489:ASP:HB3	1.86	0.75
2:F:364:MSE:SE	2:F:365:HIS:ND1	2.68	0.75
1:A:102:GLU:N	1:A:106:PRO:HG2	1.98	0.75
1:B:256:MET:HA	1:B:260:LEU:HB2	1.67	0.75
1:B:261:PHE:CE1	1:B:265:ILE:HD11	2.22	0.74
1:B:753:ASP:OD1	2:E:372:LYS:NZ	2.19	0.74
1:A:34:PRO:HB3	1:A:83:ILE:HD11	1.68	0.74
1:B:707:ARG:NH2	1:B:753:ASP:O	2.21	0.74
1:A:80:TRP:HE1	1:A:120:GLU:CG	2.00	0.74
1:A:88:ARG:HD2	1:A:120:GLU:OE2	1.88	0.73
1:B:105:ARG:HB3	1:B:106:PRO:HD3	1.70	0.73
1:A:740:GLN:O	1:A:744:GLN:HG2	1.88	0.73
1:B:444:ILE:HA	1:B:449:LEU:HD13	1.68	0.73
2:F:365:HIS:HD2	2:F:367:SER:CB	1.98	0.73
1:A:558:LEU:HD11	1:A:614:MET:HE1	1.71	0.73
1:B:320:GLN:HE21	1:B:320:GLN:C	1.92	0.73
2:D:370:LEU:N	2:D:370:LEU:CD2	2.52	0.73
2:E:357:VAL:HG11	2:E:372:LYS:HG2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HD11	1:A:132:GLN:HG2	1.70	0.73
1:B:40:LEU:HD23	1:B:43:VAL:HB	1.71	0.73
1:A:682:GLN:O	1:A:684:ASN:N	2.22	0.72
1:B:37:LEU:HD13	1:B:61:ILE:HG12	1.70	0.72
1:A:667:CYS:O	1:A:671:VAL:HG23	1.88	0.72
1:B:27:ARG:O	1:B:29:ALA:N	2.19	0.72
1:B:353:MET:HG2	1:B:392:SER:HB2	1.72	0.72
1:A:495:ALA:O	1:A:542:ASP:HB3	1.90	0.72
1:B:558:LEU:O	1:B:562:LEU:HD13	1.88	0.72
1:A:492:GLU:O	1:A:493:GLU:HG3	1.88	0.72
1:B:410:MET:HE1	1:B:452:LEU:HD13	1.71	0.72
2:E:358:MSE:CE	2:E:372:LYS:HG2	2.19	0.72
1:B:679:ARG:CZ	2:F:343:ARG:N	2.53	0.72
1:A:417:MET:HG3	1:A:455:CYS:SG	2.29	0.72
1:A:544:TYR:CE1	1:A:595:VAL:HA	2.25	0.72
1:A:800:PHE:HA	1:A:803:HIS:HD2	1.53	0.71
1:A:790:VAL:HG23	1:A:829:PHE:HZ	1.54	0.71
1:B:667:CYS:O	1:B:671:VAL:HG23	1.89	0.71
1:B:174:LEU:HD13	1:B:205:THR:HG21	1.72	0.71
1:B:663:GLU:HG3	1:B:663:GLU:O	1.90	0.71
1:B:851:ARG:HH12	1:B:866:THR:HG21	1.56	0.71
1:A:682:GLN:O	1:A:685:ILE:N	2.16	0.71
1:B:126:TRP:N	1:B:127:PRO:HD3	2.06	0.71
1:A:551:THR:HG21	1:A:603:ILE:HD13	1.71	0.71
2:F:365:HIS:CD2	2:F:368:GLY:H	2.07	0.71
1:A:173:ILE:O	1:A:177:ILE:HG13	1.91	0.71
1:A:682:GLN:HA	1:A:723:ALA:HB1	1.73	0.71
1:B:162:ASP:O	1:B:165:GLN:HG3	1.90	0.71
1:B:430:TRP:CZ2	1:B:434:ARG:HD2	2.25	0.71
1:B:736:LEU:HB3	1:B:793:ARG:NH1	2.06	0.70
1:A:83:ILE:HG12	1:A:84:ASP:H	1.56	0.70
1:B:65:LEU:CB	1:B:69:ASP:HB2	2.21	0.70
1:A:51:GLN:HB2	1:A:105:ARG:CG	2.19	0.70
1:A:36:PHE:O	1:A:40:LEU:HG	1.91	0.70
1:B:705:VAL:HB	1:B:710:LYS:NZ	2.05	0.70
2:F:368:GLY:O	2:F:372:LYS:HB2	1.92	0.70
1:A:5:THR:O	1:A:9:LYS:HG2	1.90	0.70
1:A:80:TRP:O	1:A:83:ILE:HG22	1.92	0.70
1:B:169:LYS:C	1:B:171:ASN:H	1.95	0.70
1:B:234:ARG:NH2	1:B:275:VAL:HG11	2.06	0.70
1:B:374:HIS:HB3	1:B:382:TYR:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:347:ASN:O	2:F:348:ASP:CB	2.32	0.70
1:A:51:GLN:CB	1:A:105:ARG:HG3	2.20	0.70
1:A:700:LEU:CD2	1:A:710:LYS:HG3	2.21	0.70
1:B:418:LYS:NZ	1:B:458:GLU:HG2	2.05	0.70
1:A:568:ILE:HD12	1:A:574:ARG:NH1	2.06	0.70
1:B:696:LEU:HD22	1:B:713:ILE:HG23	1.74	0.70
1:B:758:LEU:CD2	1:B:762:ARG:HE	2.05	0.69
1:A:489:ASP:CG	1:A:494:PRO:HD3	2.12	0.69
2:C:346:ILE:O	2:C:350:ILE:HG12	1.92	0.69
1:A:516:ARG:C	1:A:518:ASP:H	1.95	0.69
1:B:467:ALA:O	1:B:470:VAL:HG12	1.92	0.69
1:A:174:LEU:O	1:A:178:ILE:HG13	1.92	0.69
1:A:444:ILE:HD12	1:A:481:ALA:HA	1.72	0.69
1:B:44:LEU:HD22	1:B:54:ARG:HB3	1.74	0.69
1:A:83:ILE:HG12	1:A:84:ASP:N	2.08	0.69
1:B:580:LEU:HD23	1:B:584:LEU:HG	1.75	0.69
1:B:410:MET:CE	1:B:452:LEU:HD13	2.23	0.69
2:D:370:LEU:O	2:D:374:ILE:CD1	2.39	0.68
1:A:84:ASP:HB3	1:A:87:ALA:CB	2.21	0.68
1:B:483:GLU:CA	1:B:486:ASP:OD2	2.41	0.68
1:A:514:THR:CG2	1:A:557:ARG:HH12	2.05	0.68
1:A:62:LYS:O	1:A:66:THR:HG22	1.94	0.68
1:B:575:ILE:O	1:B:575:ILE:HG22	1.92	0.68
1:B:588:LEU:HD21	1:B:607:VAL:HG23	1.75	0.68
1:B:49:ASN:HB2	1:B:54:ARG:HD2	1.74	0.68
2:F:403:LEU:H	2:F:403:LEU:HD23	1.59	0.68
1:B:758:LEU:HD21	1:B:762:ARG:HE	1.58	0.68
2:D:403:LEU:HD12	2:D:403:LEU:H	1.59	0.68
1:A:88:ARG:HH12	1:A:92:LYS:HD3	1.59	0.68
1:B:122:PRO:HG3	1:B:165:GLN:HE22	1.59	0.68
1:B:591:VAL:O	1:B:595:VAL:HG13	1.94	0.68
1:A:174:LEU:HD22	1:A:178:ILE:HD11	1.76	0.68
1:A:830:GLY:O	1:A:872:LEU:HD13	1.94	0.68
1:A:756:ASP:CG	2:C:371:ARG:HH22	1.96	0.67
1:A:142:SER:HB3	1:A:146:MET:HG2	1.76	0.67
2:E:358:MSE:CA	2:E:372:LYS:HE2	2.23	0.67
1:A:2:GLU:HB2	1:A:5:THR:OG1	1.94	0.67
1:B:219:MET:HG3	1:B:255:TYR:CE1	2.28	0.67
1:A:870:ARG:NH2	1:B:487:VAL:CG1	2.57	0.67
1:B:557:ARG:O	1:B:561:VAL:HG23	1.95	0.67
2:E:354:LYS:CE	2:E:361:ASP:HA	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:LEU:CD2	1:A:684:ASN:HD21	2.07	0.67
1:A:172:GLU:CD	1:A:172:GLU:H	1.99	0.67
2:E:358:MSE:HE2	2:E:372:LYS:CD	2.25	0.67
1:A:700:LEU:HD22	1:A:710:LYS:HE3	1.76	0.67
1:B:21:ALA:HA	1:B:24:PHE:HB3	1.78	0.66
1:B:130:ILE:CG2	1:B:169:LYS:HD2	2.24	0.66
1:B:445:ASN:O	1:B:447:VAL:N	2.28	0.66
1:B:27:ARG:NH1	1:B:28:ALA:N	2.42	0.66
1:A:170:SER:O	1:A:174:LEU:HB2	1.96	0.66
1:A:328:GLN:O	1:A:331:THR:HB	1.95	0.66
1:B:244:ILE:HG22	1:B:252:MET:CE	2.25	0.66
1:B:615:PHE:HB3	1:B:653:PHE:CD1	2.30	0.66
1:B:851:ARG:NH1	1:B:866:THR:HG21	2.10	0.66
2:E:357:VAL:CG1	2:E:372:LYS:HE2	2.04	0.66
1:A:14:ASP:HB3	1:A:17:GLU:HB3	1.78	0.65
1:A:665:GLN:NE2	2:C:363:LYS:O	2.29	0.65
1:B:752:PHE:HE2	2:E:372:LYS:HZ2	1.44	0.65
2:E:357:VAL:HG13	2:E:372:LYS:HE3	1.73	0.65
1:A:135:ALA:HA	1:A:138:THR:CG2	2.25	0.65
1:A:339:ASP:HB3	1:A:341:ASP:HB2	1.77	0.65
1:B:800:PHE:O	1:B:804:ILE:HG13	1.97	0.65
1:B:790:VAL:HG13	1:B:829:PHE:HZ	1.61	0.65
1:B:367:VAL:HG12	1:B:371:ILE:HD11	1.79	0.65
1:A:870:ARG:HE	1:B:487:VAL:HG11	0.83	0.65
1:A:15:ARG:NH1	1:A:18:LEU:HD12	2.11	0.65
1:A:494:PRO:O	1:A:541:LYS:HG2	1.97	0.65
1:A:377:ASN:HD22	1:A:377:ASN:C	1.98	0.65
1:A:511:LEU:O	1:A:514:THR:HB	1.96	0.65
1:B:287:CYS:HB2	1:B:354:LEU:CD1	2.27	0.65
1:B:511:LEU:HD22	1:B:553:VAL:HG11	1.78	0.65
1:B:580:LEU:HD23	1:B:580:LEU:O	1.97	0.65
2:C:388:ARG:HG3	2:D:387:LEU:HD11	1.78	0.65
1:B:462:ALA:H	1:B:516:ARG:HH12	1.45	0.64
2:F:396:LEU:HD13	2:F:397:ALA:N	2.12	0.64
1:B:532:LEU:O	1:B:535:ILE:HG22	1.96	0.64
1:B:758:LEU:O	1:B:762:ARG:HG3	1.96	0.64
1:A:867:LYS:HG3	1:A:870:ARG:HH22	1.61	0.64
1:B:568:ILE:CD1	1:B:574:ARG:HH11	2.09	0.64
1:A:544:TYR:N	1:A:545:PRO:HD2	2.13	0.64
1:A:756:ASP:O	1:A:760:GLU:HG3	1.98	0.64
1:A:808:GLU:C	1:A:810:HIS:H	1.99	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:GLU:OE2	1:B:665:GLN:HB2	1.94	0.64
1:B:40:LEU:HD23	1:B:40:LEU:O	1.98	0.63
1:B:780:GLN:HE22	1:B:827:THR:CG2	2.12	0.63
1:B:40:LEU:HD22	1:B:44:LEU:HG	1.79	0.63
1:B:427:THR:HG22	1:B:427:THR:O	1.98	0.63
1:A:81:LEU:HD13	1:A:88:ARG:HD3	1.81	0.63
1:B:174:LEU:CD1	1:B:205:THR:HG21	2.29	0.63
1:B:496:THR:HG23	1:B:500:SER:OG	1.99	0.63
1:A:338:ASP:CA	1:A:465:ARG:HH22	2.08	0.62
1:A:218:ILE:O	1:A:222:VAL:HG23	1.99	0.62
1:A:489:ASP:HB2	1:A:494:PRO:HG3	1.80	0.62
1:A:603:ILE:HG22	1:A:607:VAL:HG23	1.80	0.62
1:B:27:ARG:NH1	1:B:28:ALA:CA	2.62	0.62
1:B:660:ASN:ND2	1:B:663:GLU:H	1.97	0.62
2:C:357:VAL:HG23	2:C:358:MSE:N	2.14	0.62
1:A:752:PHE:C	1:A:754:MET:N	2.50	0.62
2:C:358:MSE:CE	2:C:364:MSE:SE	2.97	0.62
2:C:366:LYS:O	2:C:367:SER:OG	2.17	0.62
1:A:686:LEU:HD11	1:A:727:GLU:HG2	1.80	0.62
1:B:327:THR:HA	1:B:330:LEU:CD1	2.27	0.62
2:C:374:ILE:HG12	2:D:353:LEU:HD13	1.81	0.62
2:C:395:LYS:NZ	2:C:395:LYS:HB3	2.14	0.62
1:B:132:GLN:HE21	1:B:132:GLN:HA	1.64	0.62
1:B:286:VAL:O	1:B:290:GLU:HG3	1.99	0.62
1:B:857:LYS:O	1:B:861:LEU:HB3	1.97	0.62
2:C:363:LYS:O	2:C:363:LYS:HG3	2.00	0.62
1:A:80:TRP:HE1	1:A:120:GLU:CD	2.03	0.62
1:B:205:THR:HG1	1:B:209:PHE:HE1	1.46	0.62
1:B:326:LEU:O	1:B:330:LEU:HG	1.99	0.62
1:B:590:ASN:HD22	1:B:590:ASN:N	1.95	0.62
1:B:834:LEU:HD22	1:B:872:LEU:HB3	1.80	0.62
1:A:444:ILE:CD1	1:A:481:ALA:HA	2.29	0.62
1:B:479:GLU:HA	1:B:538:ASN:HD22	1.63	0.62
2:F:377:ILE:O	2:F:381:GLN:HG3	2.00	0.62
1:A:514:THR:HG21	1:A:529:TYR:OH	2.00	0.62
1:B:343:ASN:ND2	1:B:345:CYS:H	1.97	0.62
1:B:758:LEU:HD11	1:B:762:ARG:NH2	2.15	0.62
2:C:367:SER:HB3	2:D:347:ASN:HB2	1.82	0.62
1:B:449:LEU:HG	1:B:453:LEU:HD12	1.81	0.61
1:B:514:THR:HG21	1:B:557:ARG:NH1	2.10	0.61
2:E:346:ILE:O	2:E:350:ILE:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:391:ASN:O	2:E:395:LYS:HB2	2.00	0.61
1:A:129:LEU:HD11	1:A:133:LEU:HD11	1.83	0.61
1:B:406:VAL:HG21	1:B:439:LEU:HD13	1.82	0.61
1:B:777:LYS:CD	1:B:780:GLN:HE21	2.12	0.61
2:C:349:LYS:NZ	2:D:367:SER:HB2	2.15	0.61
1:B:319:LEU:O	1:B:323:VAL:HG23	2.01	0.61
1:A:102:GLU:HB3	1:A:106:PRO:CD	2.27	0.61
1:B:607:VAL:HG13	1:B:608:MET:H	1.65	0.61
1:A:368:LEU:HD11	1:A:405:LEU:HD21	1.83	0.61
1:A:42:ARG:HA	1:A:94:TYR:CE1	2.36	0.61
1:A:410:MET:HE1	1:A:452:LEU:HD13	1.82	0.61
1:B:603:ILE:HG22	1:B:607:VAL:HG12	1.82	0.61
1:A:242:VAL:HG11	1:A:281:GLU:HG2	1.83	0.61
1:A:488:ALA:CA	1:B:870:ARG:HH12	2.14	0.61
1:B:73:LYS:HG2	1:B:77:GLN:HE21	1.65	0.61
2:C:361:ASP:C	2:C:361:ASP:OD1	2.39	0.60
1:A:338:ASP:HA	1:A:465:ARG:NH2	2.11	0.60
1:B:544:TYR:N	1:B:545:PRO:HD2	2.16	0.60
1:B:194:ALA:O	1:B:197:ALA:HB3	2.01	0.60
1:B:31:GLU:C	1:B:34:PRO:HD2	2.21	0.60
1:B:35:THR:O	1:B:35:THR:HG22	2.01	0.60
2:C:354:LYS:HG2	2:C:369:VAL:HG21	1.83	0.60
1:A:402:LEU:O	1:A:406:VAL:HG23	2.00	0.60
1:B:497:TYR:HD1	1:B:500:SER:HG	1.49	0.60
1:B:261:PHE:O	1:B:265:ILE:HG12	2.00	0.60
1:A:516:ARG:C	1:A:518:ASP:N	2.54	0.60
1:A:796:PHE:O	1:A:799:SER:CB	2.35	0.60
1:A:870:ARG:CZ	1:B:487:VAL:HG12	2.30	0.60
1:A:576:GLN:NE2	1:A:576:GLN:HA	2.07	0.60
2:D:374:ILE:HG22	2:D:378:LYS:HE2	1.83	0.60
1:A:533:MET:CG	1:A:590:ASN:HD22	2.15	0.60
1:B:215:ARG:HG2	1:B:255:TYR:OH	2.02	0.60
1:B:399:PRO:O	1:B:403:LYS:HG3	2.02	0.60
1:B:616:GLN:HG2	1:B:653:PHE:CZ	2.37	0.60
1:B:754:MET:HA	1:B:757:TYR:HB3	1.82	0.60
1:A:377:ASN:HD22	1:A:379:ASP:H	1.49	0.60
1:B:169:LYS:C	1:B:171:ASN:N	2.54	0.60
1:B:163:PRO:HG3	1:B:204:PHE:CD1	2.37	0.60
1:B:663:GLU:HG3	1:B:666:VAL:HG23	1.84	0.59
1:B:133:LEU:O	1:B:150:THR:HG21	2.01	0.59
1:A:614:MET:O	1:A:618:THR:HB	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:LEU:HD21	1:A:709:VAL:HA	1.84	0.59
1:A:120:GLU:O	1:A:125:GLN:HB3	2.02	0.59
1:A:287:CYS:CB	1:A:354:LEU:HD13	2.32	0.59
1:A:560:GLN:HA	1:A:563:GLN:HE21	1.67	0.59
1:A:748:ASP:C	1:A:750:SER:H	2.05	0.59
1:B:450:ALA:HB3	1:B:451:PRO:HD3	1.84	0.59
1:B:30:VAL:HG12	1:B:31:GLU:N	2.17	0.59
1:B:496:THR:HG23	1:B:500:SER:CB	2.32	0.59
1:B:7:LEU:HD11	1:B:36:PHE:HZ	1.67	0.59
1:B:430:TRP:CA	1:B:469:ASN:HD22	2.13	0.59
2:E:366:LYS:O	2:E:367:SER:HB3	2.03	0.59
1:A:125:GLN:OE1	1:A:126:TRP:HB2	2.03	0.59
1:B:78:GLN:OE1	1:B:81:LEU:HD12	2.03	0.59
1:A:363:ILE:HG23	1:A:364:VAL:N	2.17	0.59
1:A:558:LEU:HD11	1:A:614:MET:CE	2.32	0.59
2:D:364:MSE:SE	2:D:368:GLY:O	2.71	0.59
1:A:222:VAL:O	1:A:226:THR:HG23	2.02	0.59
1:A:414:ILE:O	1:A:417:MET:HB2	2.03	0.59
1:B:244:ILE:HG22	1:B:252:MET:HE3	1.83	0.59
1:A:544:TYR:CZ	1:A:596:GLN:HG3	2.38	0.59
1:A:661:TYR:CE1	1:A:704:ASN:HB2	2.37	0.59
1:B:487:VAL:HG12	1:B:488:ALA:N	2.18	0.58
1:B:211:LYS:HD2	1:B:214:GLU:OE2	2.03	0.58
2:D:358:MSE:SE	2:D:372:LYS:HD2	2.53	0.58
1:A:15:ARG:HD3	1:A:15:ARG:C	2.23	0.58
1:A:29:ALA:HB1	1:A:33:LEU:HD13	1.85	0.58
1:B:588:LEU:O	1:B:591:VAL:HG22	2.03	0.58
2:E:357:VAL:CG1	2:E:372:LYS:HG3	2.18	0.58
1:A:120:GLU:HB3	1:A:125:GLN:OE1	2.04	0.58
1:A:43:VAL:HG13	1:A:49:ASN:ND2	2.18	0.58
1:B:444:ILE:N	1:B:444:ILE:HD12	2.19	0.58
1:A:265:ILE:O	1:A:269:LYS:HD2	2.04	0.58
1:A:870:ARG:NH2	1:B:487:VAL:HG13	2.18	0.58
1:A:851:ARG:C	1:A:853:SER:H	2.06	0.58
1:B:838:GLU:C	1:B:840:ARG:H	2.06	0.58
1:A:661:TYR:CB	1:A:705:VAL:HG12	2.33	0.58
1:B:125:GLN:C	1:B:127:PRO:HD3	2.24	0.58
1:B:834:LEU:HD21	1:B:873:LYS:HZ3	1.68	0.58
1:B:660:ASN:HD21	1:B:663:GLU:H	1.49	0.58
1:B:748:ASP:HB2	1:B:754:MET:HE2	1.85	0.58
1:B:811:THR:HB	1:B:814:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:VAL:HG13	1:B:608:MET:N	2.19	0.57
1:B:244:ILE:CG2	1:B:252:MET:HE1	2.35	0.57
1:B:411:PRO:HG3	1:B:448:TYR:CE1	2.39	0.57
1:B:73:LYS:C	1:B:75:GLN:H	2.06	0.57
2:C:395:LYS:O	2:C:399:GLN:HB2	2.04	0.57
2:C:346:ILE:CD1	2:D:367:SER:HB3	2.34	0.57
1:A:525:ARG:HG2	1:A:525:ARG:HH11	1.69	0.57
1:A:784:HIS:HD2	1:A:785:PRO:CD	2.02	0.57
1:B:128:GLU:O	1:B:131:PRO:HG2	2.04	0.57
1:B:394:LEU:HB3	1:B:438:LEU:HD12	1.86	0.57
1:B:694:GLN:HG3	1:B:698:GLU:OE2	2.05	0.57
1:A:800:PHE:HA	1:A:803:HIS:CD2	2.37	0.57
1:A:84:ASP:C	1:A:86:ASN:H	2.04	0.57
2:C:349:LYS:HZ1	2:D:367:SER:HB2	1.69	0.57
2:E:377:ILE:HG21	2:F:356:LEU:HD13	1.86	0.57
1:B:367:VAL:O	1:B:371:ILE:HG13	2.05	0.57
1:B:779:ASP:OD1	1:B:779:ASP:N	2.38	0.57
1:A:756:ASP:OD1	2:C:371:ARG:NH2	2.37	0.57
1:A:54:ARG:HH22	1:A:101:THR:CG2	2.17	0.57
1:B:27:ARG:HH12	1:B:28:ALA:HA	1.68	0.57
1:B:552:LEU:O	1:B:555:MET:HB3	2.05	0.57
1:A:464:PRO:O	1:A:468:SER:HB2	2.05	0.57
1:A:650:PHE:C	1:A:652:PRO:HD2	2.24	0.57
1:B:298:SER:O	1:B:301:ALA:HB3	2.04	0.57
1:B:377:ASN:HD22	1:B:378:PRO:N	2.03	0.57
1:B:756:ASP:HA	1:B:759:ASN:HD22	1.68	0.57
1:B:343:ASN:HB2	1:B:344:PRO:HD2	1.86	0.57
2:F:365:HIS:O	2:F:369:VAL:HG23	2.04	0.57
1:A:516:ARG:O	1:A:518:ASP:N	2.38	0.56
1:B:244:ILE:CG2	1:B:252:MET:CE	2.83	0.56
1:B:403:LYS:N	1:B:404:PRO:HD2	2.20	0.56
2:C:377:ILE:O	2:C:381:GLN:HG3	2.05	0.56
1:A:33:LEU:HB3	1:A:34:PRO:HD3	1.87	0.56
1:A:287:CYS:HB2	1:A:354:LEU:HD13	1.87	0.56
1:A:762:ARG:HD3	1:A:800:PHE:CZ	2.39	0.56
1:A:77:GLN:O	1:A:80:TRP:HB3	2.04	0.56
1:B:598:GLN:O	1:B:602:GLN:HG3	2.05	0.56
1:B:136:ASN:ND2	1:B:146:MET:HE2	2.21	0.56
1:B:681:LEU:O	1:B:684:ASN:HB2	2.06	0.56
1:B:805:ALA:HB2	1:B:846:LEU:HD22	1.87	0.56
1:A:618:THR:HG21	1:A:624:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:ILE:C	1:A:799:SER:N	2.58	0.56
1:A:797:ILE:O	1:A:799:SER:N	2.39	0.56
1:A:109:ALA:O	1:A:113:VAL:HG23	2.05	0.56
1:A:122:PRO:HB3	1:A:165:GLN:HE22	1.71	0.56
1:A:339:ASP:C	1:A:341:ASP:H	2.07	0.56
1:B:184:GLU:O	1:B:185:GLU:C	2.42	0.56
1:B:468:SER:C	1:B:470:VAL:H	2.09	0.56
1:B:616:GLN:HG2	1:B:653:PHE:HZ	1.71	0.56
1:B:659:LYS:CE	1:B:659:LYS:HA	2.17	0.56
1:A:681:LEU:O	1:A:682:GLN:CB	2.52	0.56
1:B:33:LEU:HA	1:B:36:PHE:CB	2.33	0.56
1:B:360:GLU:O	1:B:362:ASP:N	2.39	0.56
1:B:4:ILE:HD12	1:B:4:ILE:N	2.21	0.56
1:B:663:GLU:CG	1:B:666:VAL:HG23	2.35	0.56
1:A:353:MET:HG3	1:A:392:SER:HB2	1.87	0.56
1:A:492:GLU:O	1:A:493:GLU:CG	2.54	0.56
1:A:830:GLY:O	1:A:872:LEU:HD22	2.06	0.56
1:B:593:ARG:HH11	1:B:593:ARG:HA	1.70	0.56
2:E:353:LEU:O	2:E:357:VAL:HG23	2.06	0.56
1:B:525:ARG:HH12	1:B:580:LEU:HD12	1.69	0.56
1:B:681:LEU:N	1:B:681:LEU:HD23	2.20	0.56
1:B:38:VAL:HG22	1:B:91:VAL:CG2	2.36	0.56
2:E:357:VAL:CG1	2:E:358:MSE:N	2.45	0.56
1:A:464:PRO:HB2	1:A:522:ASN:HD22	1.69	0.55
1:A:801:ILE:HD11	1:A:843:ILE:CD1	2.36	0.55
1:A:762:ARG:NH1	1:A:804:ILE:HG12	2.21	0.55
1:A:15:ARG:O	1:A:15:ARG:HD3	2.05	0.55
1:A:740:GLN:HG3	1:A:796:PHE:CZ	2.41	0.55
2:C:346:ILE:HD13	2:D:367:SER:HB3	1.87	0.55
2:C:394:LEU:O	2:D:394:LEU:HD13	2.06	0.55
1:A:580:LEU:O	1:A:584:LEU:HG	2.06	0.55
1:A:743:SER:HG	1:A:796:PHE:HZ	1.53	0.55
1:A:762:ARG:HD2	1:A:800:PHE:CE1	2.41	0.55
1:B:740:GLN:HG3	1:B:796:PHE:CZ	2.42	0.55
1:A:790:VAL:HG23	1:A:829:PHE:CZ	2.40	0.55
1:A:810:HIS:CD2	1:A:815:VAL:CG2	2.89	0.55
1:B:756:ASP:CA	1:B:759:ASN:HB2	2.35	0.55
2:E:351:ILE:HD12	2:E:352:GLU:N	2.21	0.55
1:A:151:LEU:HD13	1:A:194:ALA:HB2	1.89	0.55
1:A:489:ASP:HA	1:A:494:PRO:HA	1.88	0.55
1:B:133:LEU:HD22	1:B:150:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ALA:O	1:B:25:LEU:HG	2.06	0.55
1:B:343:ASN:HD22	1:B:345:CYS:H	1.55	0.55
1:B:118:CYS:O	1:B:122:PRO:HG2	2.07	0.55
1:B:123:VAL:O	1:B:123:VAL:HG12	2.06	0.55
1:B:834:LEU:HD22	1:B:872:LEU:CB	2.36	0.55
1:A:801:ILE:HD11	1:A:843:ILE:HD13	1.89	0.55
1:B:377:ASN:ND2	1:B:379:ASP:H	2.04	0.55
1:B:335:GLU:CD	1:B:380:TRP:HZ2	2.09	0.55
1:B:468:SER:HB3	2:E:343:ARG:NH2	2.20	0.55
1:B:599:ASP:HA	1:B:602:GLN:HB2	1.88	0.55
1:B:83:ILE:HB	1:B:88:ARG:HD3	1.88	0.55
1:A:102:GLU:HG3	1:A:103:THR:H	1.70	0.55
1:B:161:ILE:HG23	1:B:165:GLN:OE1	2.07	0.55
1:B:647:MET:O	1:B:651:LYS:HG3	2.07	0.55
2:E:358:MSE:HE2	2:E:372:LYS:HD3	1.89	0.55
1:A:870:ARG:HH21	1:B:487:VAL:HG13	1.72	0.54
1:B:596:GLN:HE21	1:B:598:GLN:HG3	1.72	0.54
2:C:357:VAL:HG23	2:C:358:MSE:H	1.72	0.54
1:A:488:ALA:HA	1:B:870:ARG:NH1	2.21	0.54
1:A:516:ARG:O	1:A:519:GLY:N	2.27	0.54
1:B:129:LEU:HD11	1:B:133:LEU:HD11	1.89	0.54
1:B:429:ALA:HB2	1:B:466:VAL:HG13	1.89	0.54
1:B:394:LEU:HD12	1:B:434:ARG:HB3	1.88	0.54
1:A:286:VAL:O	1:A:290:GLU:HG3	2.08	0.54
1:B:182:ARG:NE	1:B:184:GLU:HB2	2.23	0.54
1:B:390:PHE:O	1:B:393:ILE:HG12	2.07	0.54
1:B:86:ASN:HA	1:B:89:ARG:HH12	1.72	0.54
2:C:358:MSE:HG2	2:C:372:LYS:HD2	1.90	0.54
2:F:348:ASP:OD2	2:F:351:ILE:HG13	2.07	0.54
1:B:24:PHE:HE1	1:B:27:ARG:HE	1.54	0.54
1:A:42:ARG:HA	1:A:94:TYR:CZ	2.42	0.54
1:A:616:GLN:O	1:A:619:ALA:HB2	2.07	0.54
1:B:182:ARG:HG3	1:B:184:GLU:HB2	1.88	0.54
2:E:367:SER:HA	2:E:370:LEU:HB2	1.90	0.54
1:A:603:ILE:HG22	1:A:607:VAL:CG2	2.38	0.54
1:A:831:LYS:C	1:A:833:VAL:H	2.09	0.54
2:F:392:MSE:C	2:F:394:LEU:H	2.10	0.54
1:A:302:GLU:O	1:A:303:GLN:HG3	2.08	0.54
1:A:714:LEU:HD12	1:A:714:LEU:H	1.73	0.54
1:B:150:THR:O	1:B:154:ILE:HG13	2.08	0.54
1:B:28:ALA:C	1:B:30:VAL:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:TRP:CZ2	1:B:381:ARG:NH1	2.75	0.54
1:B:753:ASP:OD1	2:E:358:MSE:HA	2.07	0.54
1:A:245:MET:HG3	1:A:282:PHE:CE1	2.42	0.54
1:A:797:ILE:C	1:A:799:SER:H	2.11	0.54
1:B:154:ILE:HA	1:B:157:ILE:HD12	1.89	0.54
1:B:264:THR:HG21	1:B:282:PHE:CD2	2.42	0.54
1:B:375:ILE:O	1:B:383:ARG:HG2	2.08	0.54
1:B:708:SER:C	1:B:711:PRO:HD2	2.27	0.54
1:A:592:LEU:O	1:A:595:VAL:HG22	2.08	0.54
1:B:483:GLU:O	1:B:486:ASP:CG	2.46	0.54
1:A:303:GLN:O	1:A:304:GLY:C	2.44	0.54
1:B:430:TRP:CE2	1:B:434:ARG:HD2	2.43	0.54
1:B:507:VAL:HG11	1:B:550:THR:OG1	2.08	0.54
1:B:777:LYS:CA	1:B:787:VAL:HG21	2.34	0.54
1:A:117:ALA:O	1:A:121:ILE:HG13	2.08	0.53
1:A:253:GLU:HA	1:A:314:TYR:OH	2.07	0.53
1:A:4:ILE:HG22	1:A:4:ILE:O	2.07	0.53
1:A:729:LYS:HD3	1:A:789:LEU:HD13	1.90	0.53
1:B:174:LEU:HD13	1:B:205:THR:CG2	2.37	0.53
1:B:548:GLN:O	1:B:551:THR:HB	2.08	0.53
1:B:827:THR:O	1:B:827:THR:HG22	2.08	0.53
1:A:478:ALA:HB2	1:A:535:ILE:CD1	2.36	0.53
1:A:626:GLU:HB2	1:A:666:VAL:HG22	1.90	0.53
1:B:450:ALA:HB3	1:B:451:PRO:CD	2.38	0.53
1:B:418:LYS:HZ2	1:B:458:GLU:HG2	1.72	0.53
1:B:821:LEU:O	1:B:825:LEU:HG	2.08	0.53
1:A:150:THR:O	1:A:154:ILE:HG13	2.09	0.53
1:A:756:ASP:OD2	2:C:371:ARG:NH2	2.41	0.53
1:B:776:LEU:HD22	1:B:786:ASP:HB3	1.90	0.53
2:C:396:LEU:C	2:C:398:ASN:H	2.09	0.53
1:A:823:GLY:HA3	1:A:864:TRP:CZ3	2.43	0.53
1:B:130:ILE:N	1:B:131:PRO:HD2	2.23	0.53
1:B:266:GLU:HG2	1:B:267:ALA:N	2.23	0.53
1:B:27:ARG:C	1:B:29:ALA:H	2.07	0.53
1:B:426:ASP:C	1:B:428:THR:H	2.10	0.53
1:B:444:ILE:H	1:B:444:ILE:HD12	1.74	0.53
1:A:682:GLN:O	1:A:683:SER:C	2.46	0.53
1:B:777:LYS:CA	1:B:787:VAL:HG22	2.38	0.53
1:A:515:ASP:O	1:A:516:ARG:HG3	2.03	0.53
1:B:745:ALA:O	1:B:747:VAL:HG23	2.09	0.53
2:C:350:ILE:O	2:C:354:LYS:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:C	1:A:119:ALA:H	2.12	0.53
1:B:473:ALA:O	1:B:477:LEU:HB2	2.09	0.53
1:B:77:GLN:O	1:B:81:LEU:HG	2.08	0.53
1:A:681:LEU:O	1:A:682:GLN:HB2	2.09	0.53
1:A:867:LYS:NZ	1:A:867:LYS:HB2	2.24	0.53
1:B:604:SER:HA	1:B:607:VAL:CG1	2.39	0.53
1:B:618:THR:C	1:B:620:GLY:H	2.10	0.53
1:B:404:PRO:O	1:B:408:GLN:HG2	2.10	0.53
1:B:561:VAL:HG21	1:B:580:LEU:HD22	1.91	0.53
1:B:707:ARG:HH12	1:B:754:MET:HG2	1.74	0.53
2:F:365:HIS:CD2	2:F:368:GLY:N	2.76	0.53
1:A:13:PRO:O	1:A:14:ASP:HB2	2.09	0.52
1:A:777:LYS:NZ	1:A:827:THR:HG21	2.24	0.52
1:B:236:ALA:HA	1:B:239:GLN:OE1	2.08	0.52
1:B:265:ILE:O	1:B:268:MET:HB2	2.09	0.52
1:B:377:ASN:HD22	1:B:379:ASP:H	1.57	0.52
2:E:363:LYS:HG3	2:E:363:LYS:O	2.09	0.52
2:E:395:LYS:NZ	2:E:395:LYS:HB3	2.24	0.52
1:A:121:ILE:N	1:A:122:PRO:CD	2.72	0.52
1:B:462:ALA:O	1:B:516:ARG:NH1	2.41	0.52
1:B:592:LEU:HA	1:B:595:VAL:HG22	1.91	0.52
1:B:589:GLN:HE22	1:B:630:MET:HB3	1.74	0.52
1:B:660:ASN:C	1:B:662:ALA:H	2.12	0.52
2:E:367:SER:OG	2:F:349:LYS:NZ	2.40	0.52
2:F:389:GLN:HE21	2:F:389:GLN:C	2.13	0.52
1:A:484:ALA:C	1:A:486:ASP:H	2.13	0.52
1:B:651:LYS:HB2	1:B:651:LYS:NZ	2.24	0.52
1:A:6:ILE:HG22	1:A:21:ALA:HB2	1.91	0.52
1:A:808:GLU:C	1:A:810:HIS:N	2.61	0.52
1:B:388:MET:HG2	1:B:427:THR:CG2	2.35	0.52
1:B:460:LEU:HD23	1:B:470:VAL:CG1	2.40	0.52
1:A:628:ALA:O	1:A:632:VAL:HG23	2.09	0.52
1:B:797:ILE:O	1:B:800:PHE:HB3	2.09	0.52
1:A:695:LEU:HD23	1:A:695:LEU:O	2.10	0.52
1:B:613:ARG:HD2	1:B:616:GLN:NE2	2.24	0.52
1:B:105:ARG:CB	1:B:106:PRO:CD	2.87	0.52
1:B:462:ALA:O	1:B:516:ARG:NH2	2.42	0.52
1:B:777:LYS:HA	1:B:787:VAL:HG23	1.84	0.52
1:B:777:LYS:N	1:B:787:VAL:HG22	2.25	0.52
1:A:492:GLU:CD	2:D:343:ARG:NH1	2.60	0.52
1:A:707:ARG:O	1:A:711:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:ASP:O	1:A:803:HIS:C	2.47	0.52
1:B:462:ALA:H	1:B:516:ARG:NH1	2.08	0.52
1:B:485:ALA:C	1:B:487:VAL:N	2.62	0.52
1:A:445:ASN:OD1	1:A:447:VAL:HG23	2.10	0.52
1:A:485:ALA:O	1:A:488:ALA:HB3	2.10	0.52
1:A:516:ARG:HD3	1:A:524:LEU:HD12	1.91	0.52
1:B:434:ARG:HG3	1:B:472:TRP:HH2	1.74	0.52
1:A:122:PRO:HB3	1:A:165:GLN:NE2	2.24	0.51
1:B:91:VAL:O	1:B:95:VAL:HG23	2.10	0.51
2:D:403:LEU:HD12	2:D:403:LEU:N	2.23	0.51
2:E:398:ASN:HD21	2:E:401:ASN:CA	2.17	0.51
2:E:398:ASN:ND2	2:E:401:ASN:H	2.08	0.51
1:A:26:GLU:C	1:A:28:ALA:H	2.14	0.51
1:A:787:VAL:HG23	1:A:788:MET:CE	2.40	0.51
2:E:346:ILE:CD1	2:F:367:SER:HA	2.40	0.51
1:A:380:TRP:HZ3	1:A:423:VAL:HG11	1.75	0.51
1:B:18:LEU:HD23	1:B:18:LEU:C	2.30	0.51
1:B:515:ASP:O	1:B:516:ARG:C	2.48	0.51
1:B:495:ALA:HA	1:B:541:LYS:HB3	1.92	0.51
2:D:350:ILE:HG22	2:D:369:VAL:HG11	1.92	0.51
2:E:346:ILE:CD1	2:E:349:LYS:HD2	2.37	0.51
1:A:103:THR:HA	1:A:145:HIS:CE1	2.45	0.51
1:A:651:LYS:N	1:A:652:PRO:HD2	2.25	0.51
1:B:333:GLN:O	1:B:381:ARG:NH2	2.43	0.51
1:B:331:THR:C	1:B:333:GLN:OE1	2.49	0.51
1:A:444:ILE:HD11	1:A:498:CYS:SG	2.50	0.51
1:A:801:ILE:HG13	1:A:802:ASP:N	2.25	0.51
2:C:389:GLN:O	2:C:392:MSE:N	2.38	0.51
2:F:389:GLN:HE21	2:F:390:GLU:N	2.08	0.51
1:A:398:GLU:OE1	1:A:400:ASN:HB2	2.10	0.51
1:A:514:THR:CG2	1:A:557:ARG:NH1	2.64	0.51
1:B:430:TRP:HA	1:B:469:ASN:ND2	2.21	0.51
1:B:801:ILE:O	1:B:804:ILE:HB	2.10	0.51
2:D:345:SER:HB2	2:D:349:LYS:CB	2.37	0.51
1:B:117:ALA:HB1	1:B:121:ILE:HD12	1.92	0.51
1:B:784:HIS:HE2	1:B:786:ASP:CG	2.14	0.51
1:A:489:ASP:OD1	1:A:493:GLU:N	2.44	0.51
1:B:179:GLN:O	1:B:182:ARG:HG2	2.10	0.51
1:B:323:VAL:CG1	1:B:367:VAL:HG22	2.40	0.51
1:B:608:MET:CE	1:B:632:VAL:HG22	2.40	0.51
1:B:377:ASN:C	1:B:377:ASN:HD22	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:GLU:CG	1:B:663:GLU:O	2.58	0.51
1:A:665:GLN:HE21	2:C:363:LYS:HG3	1.76	0.51
1:A:245:MET:HE1	1:A:286:VAL:HA	1.93	0.51
1:B:836:LEU:O	1:B:840:ARG:HD2	2.11	0.51
1:A:537:LYS:O	1:A:594:LYS:HE3	2.11	0.50
1:B:37:LEU:HD13	1:B:61:ILE:CG1	2.38	0.50
1:A:756:ASP:OD1	2:C:372:LYS:HE2	2.10	0.50
1:B:343:ASN:HD21	1:B:345:CYS:HB2	1.76	0.50
1:B:777:LYS:HD2	1:B:780:GLN:NE2	2.20	0.50
2:D:350:ILE:HG22	2:D:350:ILE:O	2.10	0.50
1:A:199:LEU:HD12	1:A:202:LEU:HD12	1.92	0.50
1:B:371:ILE:O	1:B:375:ILE:HB	2.11	0.50
1:B:483:GLU:C	1:B:486:ASP:OD2	2.50	0.50
2:D:345:SER:CB	2:D:349:LYS:HB2	2.38	0.50
2:E:398:ASN:HD22	2:E:398:ASN:C	2.13	0.50
1:A:102:GLU:CG	1:A:103:THR:H	2.25	0.50
1:A:811:THR:HG22	1:A:814:VAL:H	1.76	0.50
1:B:187:SER:OG	1:B:190:VAL:HG23	2.11	0.50
1:B:453:LEU:HD21	1:B:499:LEU:HD22	1.94	0.50
1:B:543:CYS:C	1:B:545:PRO:HD2	2.32	0.50
1:B:632:VAL:O	1:B:636:VAL:HG23	2.11	0.50
1:B:65:LEU:H	1:B:65:LEU:CD2	2.19	0.50
2:E:358:MSE:CB	2:E:372:LYS:CE	2.72	0.50
2:E:376:TYR:O	2:E:379:TYR:HB3	2.12	0.50
2:F:371:ARG:HG3	2:F:371:ARG:HH11	1.77	0.50
1:A:467:ALA:O	1:A:470:VAL:HB	2.11	0.50
1:A:576:GLN:CA	1:A:576:GLN:HE21	2.06	0.50
1:B:575:ILE:O	1:B:575:ILE:CG2	2.60	0.50
1:A:264:THR:O	1:A:267:ALA:HB3	2.11	0.50
1:A:811:THR:HG22	1:A:813:GLY:N	2.26	0.50
1:B:339:ASP:O	1:B:340:ASP:HB2	2.11	0.50
1:B:511:LEU:CD2	1:B:553:VAL:HG11	2.42	0.50
1:B:804:ILE:C	1:B:806:GLY:H	2.13	0.50
2:E:346:ILE:HD11	2:F:367:SER:HA	1.93	0.50
1:A:105:ARG:H	1:A:106:PRO:HD3	1.77	0.50
1:A:395:GLU:HB2	1:A:438:LEU:HD13	1.94	0.50
1:B:226:THR:O	1:B:234:ARG:HD3	2.12	0.50
1:B:756:ASP:O	1:B:760:GLU:N	2.42	0.50
1:A:3:LEU:HD12	1:A:3:LEU:N	2.27	0.50
1:A:591:VAL:HG23	1:A:592:LEU:N	2.27	0.50
1:A:73:LYS:C	1:A:75:GLN:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ARG:CD	1:A:800:PHE:CZ	2.95	0.50
1:A:88:ARG:NH1	1:A:92:LYS:HD3	2.25	0.50
1:B:35:THR:HA	1:B:38:VAL:CG2	2.41	0.50
1:B:460:LEU:HD11	1:B:474:PHE:HE2	1.76	0.50
1:B:522:ASN:O	1:B:524:LEU:N	2.45	0.50
1:B:478:ALA:O	1:B:538:ASN:HB3	2.12	0.50
1:B:758:LEU:O	1:B:758:LEU:HD22	2.12	0.50
1:A:549:LYS:O	1:A:553:VAL:HG23	2.12	0.49
1:B:135:ALA:O	1:B:139:ASN:HB2	2.12	0.49
2:F:366:LYS:O	2:F:370:LEU:HG	2.12	0.49
2:E:383:VAL:HG23	2:F:384:ASN:ND2	2.27	0.49
1:A:478:ALA:CB	1:A:535:ILE:HD12	2.41	0.49
1:B:35:THR:O	1:B:38:VAL:HB	2.12	0.49
1:B:426:ASP:O	1:B:428:THR:N	2.45	0.49
1:B:455:CYS:O	1:B:458:GLU:HB3	2.12	0.49
2:C:377:ILE:CG2	2:D:356:LEU:HD13	2.42	0.49
2:E:358:MSE:HE1	2:E:364:MSE:SE	2.62	0.49
1:A:708:SER:O	1:A:711:PRO:HD2	2.12	0.49
1:A:84:ASP:C	1:A:86:ASN:N	2.65	0.49
1:B:590:ASN:ND2	1:B:590:ASN:N	2.61	0.49
1:A:518:ASP:O	1:A:520:HIS:N	2.45	0.49
1:A:710:LYS:HB3	1:A:711:PRO:HD3	1.94	0.49
1:B:30:VAL:HG12	1:B:31:GLU:H	1.78	0.49
1:B:525:ARG:NH1	1:B:580:LEU:HD12	2.27	0.49
1:B:826:CYS:C	1:B:828:ALA:H	2.16	0.49
1:A:117:ALA:HB1	1:A:121:ILE:HD11	1.94	0.49
1:A:485:ALA:O	1:A:488:ALA:N	2.43	0.49
1:A:681:LEU:O	1:A:682:GLN:HG3	2.12	0.49
1:A:867:LYS:HA	1:A:870:ARG:NH2	2.27	0.49
1:B:136:ASN:HD22	1:B:146:MET:CG	2.26	0.49
1:B:335:GLU:HG3	1:B:381:ARG:HH12	1.76	0.49
1:B:426:ASP:C	1:B:428:THR:N	2.66	0.49
1:B:770:THR:HG22	1:B:774:GLN:HE21	1.77	0.49
1:A:353:MET:O	1:A:357:THR:HG23	2.12	0.49
1:A:557:ARG:O	1:A:561:VAL:HG23	2.13	0.49
1:B:139:ASN:HB3	1:B:142:SER:OG	2.12	0.49
1:B:46:ASN:O	1:B:49:ASN:ND2	2.45	0.49
1:B:777:LYS:CE	1:B:780:GLN:NE2	2.76	0.49
2:C:377:ILE:HG21	2:D:356:LEU:HD13	1.93	0.49
1:B:182:ARG:CD	1:B:184:GLU:HB2	2.43	0.49
2:F:370:LEU:C	2:F:372:LYS:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:THR:O	1:A:432:VAL:HG23	2.13	0.49
1:A:338:ASP:OD2	1:A:465:ARG:NH2	2.44	0.49
1:B:544:TYR:O	1:B:545:PRO:C	2.50	0.49
1:B:44:LEU:HD11	1:B:57:ALA:HB3	1.95	0.49
2:C:366:LYS:C	2:C:368:GLY:H	2.14	0.49
1:A:799:SER:O	1:A:801:ILE:N	2.46	0.49
1:B:33:LEU:HB3	1:B:34:PRO:HD3	1.94	0.49
1:B:603:ILE:HG22	1:B:607:VAL:CG1	2.41	0.49
1:B:776:LEU:O	1:B:784:HIS:CD2	2.66	0.49
1:B:791:GLN:O	1:B:794:VAL:HG23	2.13	0.49
2:F:396:LEU:O	2:F:396:LEU:HD22	2.12	0.49
1:B:663:GLU:O	1:B:665:GLN:N	2.46	0.48
1:B:495:ALA:HA	1:B:541:LYS:CB	2.43	0.48
1:B:791:GLN:C	1:B:793:ARG:H	2.17	0.48
1:A:488:ALA:CB	1:B:870:ARG:HH12	2.26	0.48
2:C:366:LYS:C	2:C:367:SER:OG	2.52	0.48
1:A:7:LEU:HD23	1:A:25:LEU:HD11	1.95	0.48
1:A:560:GLN:O	1:A:564:MET:HB2	2.13	0.48
1:B:38:VAL:HG22	1:B:91:VAL:HG21	1.95	0.48
1:B:451:PRO:O	1:B:454:GLN:N	2.47	0.48
1:B:65:LEU:HD23	1:B:65:LEU:N	2.21	0.48
1:A:444:ILE:HG12	1:A:444:ILE:O	2.13	0.48
1:A:707:ARG:NH1	1:A:707:ARG:HG3	2.24	0.48
1:B:126:TRP:N	1:B:127:PRO:CD	2.76	0.48
1:B:268:MET:HE1	1:B:283:TRP:CD1	2.48	0.48
2:E:370:LEU:O	2:E:374:ILE:HG13	2.14	0.48
1:A:689:CYS:HB3	1:A:731:TYR:OH	2.12	0.48
1:A:86:ASN:O	1:A:89:ARG:HB3	2.13	0.48
1:B:43:VAL:C	1:B:45:ALA:H	2.17	0.48
1:B:788:MET:O	1:B:790:VAL:N	2.46	0.48
1:A:399:PRO:O	1:A:403:LYS:HG3	2.13	0.48
1:A:661:TYR:HE1	1:A:704:ASN:HB2	1.76	0.48
1:A:69:ASP:O	1:A:71:ASP:N	2.47	0.48
1:B:99:LEU:HB2	1:B:146:MET:CE	2.44	0.48
1:B:19:GLU:HA	1:B:22:GLN:HE21	1.79	0.48
1:B:680:ALA:C	1:B:681:LEU:HD23	2.33	0.48
1:B:778:GLY:O	1:B:779:ASP:C	2.50	0.48
2:D:364:MSE:HE2	2:D:365:HIS:CE1	2.48	0.48
1:A:307:PRO:HG2	1:A:310:THR:HG22	1.96	0.48
1:A:62:LYS:HG3	1:A:112:CYS:SG	2.54	0.48
1:B:237:ALA:O	1:B:240:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ILE:O	1:B:445:ASN:HB2	2.13	0.48
1:B:682:GLN:O	1:B:685:ILE:HG22	2.14	0.48
1:B:752:PHE:HA	1:B:755:VAL:HG23	1.96	0.48
1:A:801:ILE:O	1:A:804:ILE:HB	2.14	0.48
1:A:831:LYS:C	1:A:833:VAL:N	2.67	0.48
1:A:80:TRP:O	1:A:83:ILE:CG2	2.61	0.48
2:E:358:MSE:HB3	2:E:372:LYS:CD	2.43	0.48
1:A:168:ASP:O	1:A:170:SER:N	2.47	0.48
1:A:681:LEU:C	1:A:682:GLN:HG3	2.34	0.48
1:A:751:ASP:O	1:A:752:PHE:C	2.52	0.48
1:B:350:VAL:HG12	1:B:351:CYS:N	2.29	0.48
1:B:495:ALA:O	1:B:496:THR:OG1	2.28	0.48
1:B:99:LEU:HB2	1:B:146:MET:HE1	1.94	0.48
1:A:51:GLN:HB2	1:A:105:ARG:CD	2.44	0.48
1:A:661:TYR:CG	1:A:705:VAL:HG12	2.48	0.48
1:A:700:LEU:HD23	1:A:710:LYS:HG3	1.94	0.48
1:A:789:LEU:O	1:A:792:PRO:HD2	2.14	0.48
1:B:705:VAL:HB	1:B:710:LYS:HZ1	1.77	0.48
2:D:364:MSE:HG3	2:D:365:HIS:H	1.78	0.48
2:F:393:VAL:HG22	2:F:393:VAL:O	2.13	0.48
1:A:591:VAL:HG23	1:A:592:LEU:H	1.79	0.47
1:A:784:HIS:O	1:A:787:VAL:HG22	2.13	0.47
1:A:798:LEU:O	1:A:801:ILE:HG12	2.14	0.47
1:B:318:ALA:O	1:B:322:LEU:HG	2.14	0.47
1:B:462:ALA:N	1:B:516:ARG:HH12	2.11	0.47
1:B:596:GLN:O	1:B:597:HIS:C	2.52	0.47
2:D:349:LYS:HG3	2:D:351:ILE:CG2	2.43	0.47
2:F:403:LEU:N	2:F:403:LEU:HD23	2.28	0.47
1:A:158:CYS:SG	1:A:204:PHE:HZ	2.37	0.47
1:A:736:LEU:HD13	1:A:793:ARG:NE	2.23	0.47
1:A:736:LEU:HD11	1:A:790:VAL:HG12	1.96	0.47
1:A:826:CYS:HA	1:A:830:GLY:HA2	1.96	0.47
1:B:169:LYS:HD3	1:B:172:GLU:HB2	1.96	0.47
1:B:343:ASN:HB2	1:B:344:PRO:CD	2.45	0.47
1:B:394:LEU:CB	1:B:438:LEU:HD12	2.43	0.47
1:A:787:VAL:HG23	1:A:788:MET:HE2	1.95	0.47
1:A:810:HIS:HD2	1:A:815:VAL:CG2	2.27	0.47
1:B:440:PRO:CB	1:B:480:ALA:HB2	2.44	0.47
1:B:483:GLU:CA	1:B:486:ASP:CG	2.77	0.47
2:F:351:ILE:O	2:F:354:LYS:HB3	2.14	0.47
1:A:126:TRP:CE2	1:A:129:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:O	1:A:242:VAL:HG23	2.14	0.47
1:A:323:VAL:O	1:A:327:THR:HG23	2.15	0.47
1:A:777:LYS:HZ1	1:A:827:THR:HG21	1.79	0.47
1:A:868:GLU:OE1	1:A:868:GLU:HA	2.14	0.47
1:B:752:PHE:C	1:B:754:MET:N	2.68	0.47
1:B:823:GLY:HA3	1:B:864:TRP:CZ3	2.50	0.47
1:B:96:LEU:HD22	1:B:126:TRP:CZ2	2.48	0.47
1:B:96:LEU:O	1:B:96:LEU:HG	2.15	0.47
1:A:37:LEU:HA	1:A:40:LEU:HD12	1.96	0.47
1:A:791:GLN:N	1:A:792:PRO:CD	2.78	0.47
1:A:867:LYS:HB2	1:A:867:LYS:HZ2	1.80	0.47
1:B:374:HIS:HA	1:B:377:ASN:HB2	1.96	0.47
1:B:412:THR:O	1:B:415:GLU:HB2	2.14	0.47
1:B:51:GLN:C	1:B:53:ALA:H	2.18	0.47
2:D:400:LYS:O	2:D:401:ASN:HB3	2.15	0.47
1:A:755:VAL:O	1:A:759:ASN:ND2	2.47	0.47
1:B:449:LEU:HG	1:B:453:LEU:CD1	2.44	0.47
1:B:822:ILE:HA	1:B:825:LEU:HD12	1.97	0.47
2:E:354:LYS:NZ	2:E:361:ASP:HA	2.29	0.47
1:A:681:LEU:C	1:A:682:GLN:CG	2.78	0.47
1:A:686:LEU:N	1:A:687:PRO:CD	2.77	0.47
1:A:90:GLU:O	1:A:94:TYR:HB2	2.15	0.47
1:B:316:LYS:O	1:B:319:LEU:HB2	2.15	0.47
1:B:780:GLN:HE22	1:B:827:THR:HG22	1.78	0.47
1:B:861:LEU:O	1:B:865:ALA:HB2	2.14	0.47
1:A:143:THR:O	1:A:146:MET:HB3	2.15	0.47
1:A:235:VAL:HG21	1:A:274:GLU:CG	2.45	0.47
1:A:777:LYS:HA	1:A:787:VAL:CG1	2.45	0.47
1:A:791:GLN:HB3	1:A:792:PRO:HD3	1.97	0.47
1:B:776:LEU:O	1:B:784:HIS:HD2	1.97	0.47
1:A:31:GLU:HG3	1:A:32:ASN:ND2	2.30	0.47
1:A:664:TYR:HB2	1:A:709:VAL:CG2	2.45	0.47
1:A:788:MET:O	1:A:791:GLN:HB2	2.14	0.47
1:B:570:SER:OG	1:B:572:SER:HB3	2.14	0.47
2:D:379:TYR:O	2:D:383:VAL:HG23	2.15	0.47
1:A:15:ARG:HH11	1:A:18:LEU:HD12	1.78	0.47
1:A:403:LYS:N	1:A:404:PRO:HD2	2.31	0.47
1:A:479:GLU:O	1:A:483:GLU:HG3	2.15	0.47
1:A:816:ALA:HB1	1:A:857:LYS:HG2	1.97	0.47
1:B:408:GLN:O	1:B:408:GLN:HG3	2.15	0.47
1:B:427:THR:O	1:B:427:THR:CG2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:GLN:HG3	1:B:634:THR:OG1	2.15	0.47
1:B:96:LEU:HD22	1:B:126:TRP:HZ2	1.79	0.47
1:A:484:ALA:C	1:A:486:ASP:N	2.69	0.46
1:A:513:THR:O	1:A:514:THR:C	2.53	0.46
1:A:33:LEU:HD22	1:A:79:ARG:HH21	1.80	0.46
1:A:851:ARG:C	1:A:853:SER:N	2.68	0.46
1:B:401:GLN:O	1:B:401:GLN:HG3	2.15	0.46
1:B:419:ASP:O	1:B:425:ARG:NH1	2.48	0.46
1:B:5:THR:O	1:B:9:LYS:HE2	2.14	0.46
2:F:380:LEU:HA	2:F:380:LEU:HD23	1.78	0.46
1:A:525:ARG:NH1	1:A:525:ARG:HG2	2.30	0.46
1:B:549:LYS:HA	1:B:552:LEU:HD12	1.97	0.46
1:B:695:LEU:O	1:B:696:LEU:C	2.54	0.46
1:B:812:ASP:O	1:B:815:VAL:HB	2.15	0.46
1:A:174:LEU:HD22	1:A:178:ILE:CD1	2.45	0.46
1:A:21:ALA:HB1	1:A:25:LEU:CD1	2.45	0.46
1:A:617:SER:O	1:A:619:ALA:N	2.43	0.46
1:B:2:GLU:OE1	1:B:4:ILE:HD13	2.15	0.46
1:B:867:LYS:O	1:B:870:ARG:HG2	2.16	0.46
2:C:387:LEU:N	2:C:387:LEU:HD23	2.30	0.46
1:A:54:ARG:HH22	1:A:101:THR:HG21	1.80	0.46
1:A:688:PHE:O	1:A:689:CYS:C	2.53	0.46
1:A:77:GLN:HG2	1:A:119:ALA:HB2	1.96	0.46
1:B:431:THR:O	1:B:435:ILE:HG13	2.14	0.46
2:C:395:LYS:HZ2	2:C:395:LYS:HB3	1.81	0.46
2:C:387:LEU:HD11	2:D:388:ARG:HE	1.79	0.46
2:E:377:ILE:O	2:E:381:GLN:HG3	2.16	0.46
1:A:118:CYS:HA	1:A:161:ILE:HG12	1.97	0.46
1:A:130:ILE:O	1:A:134:VAL:HG23	2.15	0.46
1:A:603:ILE:CG2	1:A:607:VAL:HG23	2.45	0.46
1:A:661:TYR:HB2	1:A:705:VAL:HG12	1.97	0.46
1:B:146:MET:HE2	1:B:150:THR:OG1	2.15	0.46
1:B:230:ASP:OD1	1:B:232:ARG:N	2.49	0.46
1:B:752:PHE:HE2	2:E:372:LYS:NZ	2.10	0.46
2:C:374:ILE:CG1	2:D:353:LEU:HD13	2.45	0.46
2:F:397:ALA:HA	2:F:400:LYS:HD3	1.97	0.46
1:B:502:SER:O	1:B:506:ILE:HG13	2.16	0.46
2:E:391:ASN:OD1	2:F:391:ASN:HB2	2.15	0.46
1:A:242:VAL:HG11	1:A:281:GLU:CG	2.46	0.46
1:A:35:THR:HG22	1:A:35:THR:O	2.15	0.46
1:B:28:ALA:HB1	1:B:33:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ILE:HG23	1:B:449:LEU:HD22	1.97	0.46
1:B:40:LEU:CD2	1:B:44:LEU:HG	2.46	0.46
1:B:497:TYR:HD1	1:B:497:TYR:H	1.63	0.46
1:B:561:VAL:O	1:B:561:VAL:HG12	2.16	0.46
1:B:580:LEU:CD2	1:B:584:LEU:HG	2.45	0.46
1:B:56:ALA:O	1:B:60:GLN:HG2	2.16	0.46
1:A:514:THR:HG23	1:A:529:TYR:CE2	2.50	0.46
1:A:647:MET:HG2	1:A:688:PHE:CZ	2.50	0.46
1:A:658:LEU:HG	1:A:670:ALA:HB1	1.98	0.46
1:B:169:LYS:HD3	1:B:172:GLU:CB	2.45	0.46
1:B:695:LEU:O	1:B:698:GLU:N	2.49	0.46
1:B:732:LEU:HD22	1:B:736:LEU:HD11	1.98	0.46
2:C:358:MSE:HE1	2:C:364:MSE:SE	2.65	0.46
2:E:358:MSE:CE	2:E:372:LYS:CG	2.83	0.46
1:A:126:TRP:C	1:A:128:GLU:H	2.17	0.46
1:A:608:MET:O	1:A:612:LEU:HB2	2.16	0.46
1:A:19:GLU:C	1:A:21:ALA:N	2.67	0.46
1:A:241:LEU:HD13	1:A:260:LEU:HD22	1.97	0.46
1:B:28:ALA:C	1:B:30:VAL:N	2.70	0.46
1:B:27:ARG:HH11	1:B:28:ALA:HA	1.77	0.46
1:B:493:GLU:C	1:B:494:PRO:O	2.51	0.46
1:B:875:GLN:OE1	1:B:875:GLN:HA	2.16	0.46
2:E:371:ARG:HA	2:E:374:ILE:HD12	1.98	0.46
1:A:144:GLU:CD	1:A:187:SER:HB2	2.37	0.45
1:B:73:LYS:C	1:B:75:GLN:N	2.68	0.45
2:E:349:LYS:NZ	2:F:367:SER:OG	2.42	0.45
1:B:3:LEU:H	1:B:4:ILE:HD12	1.80	0.45
1:A:53:ALA:O	1:A:57:ALA:HB2	2.16	0.45
1:A:93:ASN:HA	1:A:96:LEU:HB3	1.96	0.45
1:B:756:ASP:HA	1:B:759:ASN:ND2	2.31	0.45
1:B:780:GLN:HE22	1:B:827:THR:HG21	1.80	0.45
2:C:402:LYS:HG3	2:C:403:LEU:N	2.31	0.45
1:A:181:MET:CE	1:A:198:LEU:HD22	2.47	0.45
1:A:19:GLU:C	1:A:21:ALA:H	2.19	0.45
1:A:436:CYS:SG	1:A:477:LEU:HD13	2.57	0.45
1:A:533:MET:HG2	1:A:590:ASN:ND2	2.26	0.45
1:A:659:LYS:O	1:A:661:TYR:CD2	2.70	0.45
1:B:137:VAL:HA	1:B:147:LYS:HG2	1.97	0.45
1:B:208:ASN:ND2	1:B:214:GLU:OE1	2.44	0.45
1:B:419:ASP:C	1:B:421:SER:H	2.20	0.45
1:B:430:TRP:CZ2	1:B:434:ARG:CD	2.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:VAL:C	1:B:97:GLN:H	2.18	0.45
1:A:154:ILE:O	1:A:157:ILE:HB	2.16	0.45
1:A:37:LEU:O	1:A:40:LEU:HB2	2.17	0.45
1:A:609:ALA:O	1:A:613:ARG:HB3	2.16	0.45
1:A:673:LEU:HA	1:A:676:ASP:HB2	1.98	0.45
1:B:487:VAL:CG1	1:B:488:ALA:N	2.79	0.45
1:B:493:GLU:O	1:B:494:PRO:O	2.35	0.45
1:A:130:ILE:N	1:A:131:PRO:CD	2.79	0.45
1:A:19:GLU:O	1:A:21:ALA:N	2.50	0.45
1:A:287:CYS:O	1:A:291:MET:HG3	2.16	0.45
1:A:363:ILE:CG2	1:A:364:VAL:N	2.78	0.45
1:A:565:GLU:OE2	1:A:574:ARG:NH2	2.50	0.45
1:A:787:VAL:O	1:A:790:VAL:HG22	2.17	0.45
1:B:732:LEU:HD22	1:B:736:LEU:CD1	2.46	0.45
1:B:758:LEU:HD22	1:B:762:ARG:NE	2.31	0.45
1:B:139:ASN:HB3	1:B:142:SER:HG	1.81	0.45
1:B:407:ILE:HA	1:B:407:ILE:HD13	1.82	0.45
1:B:694:GLN:HE21	1:B:698:GLU:HG3	1.82	0.45
1:B:707:ARG:HH12	1:B:754:MET:CG	2.29	0.45
2:C:350:ILE:HD12	2:C:370:LEU:HD21	1.98	0.45
2:E:358:MSE:SE	2:E:364:MSE:CE	3.15	0.45
1:B:752:PHE:HE2	2:E:372:LYS:CE	2.29	0.45
1:A:29:ALA:O	1:A:33:LEU:N	2.49	0.45
1:A:401:GLN:O	1:A:405:LEU:HD13	2.17	0.45
1:A:608:MET:HE3	1:A:635:LEU:HD23	1.99	0.45
1:B:122:PRO:HA	1:B:165:GLN:NE2	2.32	0.45
1:B:661:TYR:CD1	1:B:661:TYR:C	2.90	0.45
1:B:673:LEU:HD22	1:B:677:LEU:HG	1.99	0.45
1:B:758:LEU:HD22	1:B:762:ARG:HE	1.80	0.45
2:D:357:VAL:HG11	2:D:372:LYS:HB3	1.97	0.45
1:A:235:VAL:HG21	1:A:274:GLU:HG2	1.99	0.45
1:A:319:LEU:HA	1:A:319:LEU:HD12	1.81	0.45
1:A:707:ARG:HH22	1:A:753:ASP:CG	2.20	0.45
1:B:194:ALA:O	1:B:197:ALA:N	2.50	0.45
1:B:351:CYS:O	1:B:355:LEU:HB2	2.17	0.45
1:A:33:LEU:N	1:A:34:PRO:CD	2.80	0.45
1:A:503:PHE:CE2	1:A:507:VAL:HG11	2.50	0.45
1:A:626:GLU:O	1:A:630:MET:HG2	2.17	0.45
1:A:683:SER:N	1:A:723:ALA:O	2.50	0.45
1:B:529:TYR:OH	1:B:557:ARG:NH1	2.49	0.45
1:B:787:VAL:O	1:B:790:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ARG:HB2	1:A:757:TYR:CZ	2.52	0.44
1:A:748:ASP:O	1:A:750:SER:N	2.44	0.44
1:B:326:LEU:CD2	1:B:348:ALA:HA	2.47	0.44
1:B:335:GLU:HG2	1:B:380:TRP:CZ2	2.53	0.44
1:B:864:TRP:O	1:B:868:GLU:HG2	2.17	0.44
1:B:679:ARG:NE	2:F:343:ARG:N	2.65	0.44
1:B:565:GLU:HB2	1:B:577:PHE:CE1	2.52	0.44
1:B:72:ILE:O	1:B:75:GLN:HB3	2.17	0.44
1:B:770:THR:CG2	1:B:774:GLN:HE21	2.31	0.44
2:C:354:LYS:HG2	2:C:369:VAL:CG2	2.48	0.44
1:A:616:GLN:CD	1:A:617:SER:N	2.70	0.44
1:A:618:THR:HG22	1:A:618:THR:O	2.18	0.44
1:B:154:ILE:O	1:B:157:ILE:HB	2.18	0.44
1:B:589:GLN:NE2	1:B:630:MET:HB3	2.32	0.44
1:B:637:GLU:OE1	1:B:638:VAL:HA	2.17	0.44
1:B:659:LYS:O	1:B:660:ASN:C	2.55	0.44
1:B:749:LYS:CG	1:B:750:SER:N	2.69	0.44
1:A:798:LEU:HA	1:A:798:LEU:HD23	1.88	0.44
1:A:81:LEU:CD1	1:A:88:ARG:HD3	2.45	0.44
1:B:40:LEU:O	1:B:43:VAL:N	2.44	0.44
1:B:410:MET:N	1:B:411:PRO:CD	2.80	0.44
1:B:457:ILE:HD13	1:B:505:LEU:HD23	2.00	0.44
1:B:544:TYR:O	1:B:548:GLN:N	2.47	0.44
1:B:651:LYS:N	1:B:652:PRO:CD	2.80	0.44
2:F:356:LEU:HA	2:F:356:LEU:HD23	1.84	0.44
1:A:15:ARG:HA	1:A:18:LEU:HG	2.00	0.44
1:B:597:HIS:O	1:B:598:GLN:C	2.55	0.44
2:E:348:ASP:O	2:E:351:ILE:HG13	2.17	0.44
1:A:25:LEU:HB3	1:A:36:PHE:HZ	1.83	0.44
1:B:136:ASN:ND2	1:B:146:MET:CE	2.81	0.44
1:B:468:SER:O	1:B:470:VAL:N	2.51	0.44
1:B:758:LEU:HD11	1:B:762:ARG:HH21	1.81	0.44
1:B:83:ILE:HG22	1:B:84:ASP:N	2.33	0.44
1:A:105:ARG:H	1:A:106:PRO:CD	2.30	0.44
1:A:39:GLU:HA	1:A:42:ARG:HD3	1.99	0.44
1:A:54:ARG:O	1:A:57:ALA:HB3	2.18	0.44
1:B:185:GLU:O	1:B:191:LYS:HE3	2.18	0.44
1:B:449:LEU:HD12	1:B:452:LEU:HD23	2.00	0.44
1:A:190:VAL:O	1:A:191:LYS:C	2.56	0.44
1:A:410:MET:HE1	1:A:452:LEU:HD22	1.98	0.44
1:A:756:ASP:CG	2:C:372:LYS:HE2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ILE:HD12	1:B:112:CYS:SG	2.58	0.44
1:B:342:TRP:CZ2	1:B:347:ALA:HB2	2.53	0.44
1:B:407:ILE:C	1:B:409:ALA:H	2.20	0.44
1:B:51:GLN:O	1:B:52:VAL:HG12	2.17	0.44
1:B:612:LEU:C	1:B:614:MET:H	2.22	0.44
1:B:838:GLU:C	1:B:840:ARG:N	2.71	0.44
2:F:361:ASP:O	2:F:362:ALA:HB2	2.17	0.44
1:A:158:CYS:HG	1:A:204:PHE:HZ	1.66	0.43
1:A:57:ALA:O	1:A:61:ILE:HG13	2.18	0.43
1:A:615:PHE:CE1	1:A:625:GLN:HG2	2.53	0.43
1:B:187:SER:HB3	1:B:190:VAL:CG2	2.48	0.43
1:B:450:ALA:N	1:B:451:PRO:HD2	2.33	0.43
1:B:508:GLN:HA	1:B:508:GLN:OE1	2.18	0.43
1:B:748:ASP:CB	1:B:754:MET:HE2	2.48	0.43
1:A:55:VAL:HG21	1:A:105:ARG:HD2	1.99	0.43
1:B:168:ASP:OD1	1:B:169:LYS:HG2	2.18	0.43
1:B:572:SER:O	1:B:575:ILE:N	2.51	0.43
1:B:660:ASN:O	1:B:662:ALA:N	2.51	0.43
1:B:766:LEU:HD13	1:B:818:ALA:N	2.32	0.43
1:A:133:LEU:O	1:A:136:ASN:HB2	2.18	0.43
1:A:368:LEU:HD21	1:A:405:LEU:HD23	2.00	0.43
1:B:606:VAL:O	1:B:609:ALA:CB	2.54	0.43
1:B:608:MET:HG2	1:B:635:LEU:CD2	2.48	0.43
1:B:69:ASP:CG	1:B:69:ASP:O	2.56	0.43
1:B:833:VAL:O	1:B:837:VAL:HG23	2.18	0.43
2:C:350:ILE:CD1	2:C:370:LEU:HD21	2.48	0.43
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.83	0.43
1:A:34:PRO:HG3	1:A:83:ILE:HG13	2.00	0.43
1:B:651:LYS:HB2	1:B:652:PRO:HD3	1.99	0.43
1:B:807:ASP:O	1:B:810:HIS:CD2	2.71	0.43
2:D:382:GLN:O	2:D:383:VAL:C	2.55	0.43
2:E:398:ASN:O	2:E:399:GLN:CG	2.66	0.43
2:F:396:LEU:C	2:F:396:LEU:HD13	2.37	0.43
1:A:121:ILE:HD12	1:A:161:ILE:HD13	2.00	0.43
1:A:51:GLN:HB2	1:A:105:ARG:HD2	1.99	0.43
1:A:659:LYS:O	1:A:661:TYR:HD2	2.01	0.43
1:A:714:LEU:O	1:A:768:ALA:HB2	2.18	0.43
1:A:827:THR:HG22	1:A:827:THR:O	2.18	0.43
1:B:323:VAL:HG13	1:B:367:VAL:HG22	2.00	0.43
1:B:449:LEU:O	1:B:453:LEU:HD12	2.18	0.43
2:E:380:LEU:HA	2:E:383:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD12	1:A:208:ASN:ND2	2.33	0.43
1:A:269:LYS:O	1:A:270:SER:C	2.56	0.43
1:A:440:PRO:HG2	1:A:441:GLU:H	1.84	0.43
1:A:465:ARG:HA	1:A:465:ARG:HD3	1.68	0.43
1:A:606:VAL:O	1:A:609:ALA:HB3	2.18	0.43
1:A:870:ARG:CZ	1:A:870:ARG:HB3	2.48	0.43
1:B:105:ARG:HH11	1:B:105:ARG:HG3	1.84	0.43
1:B:522:ASN:O	1:B:523:ASN:OD1	2.36	0.43
1:B:551:THR:HG22	1:B:552:LEU:N	2.34	0.43
1:B:804:ILE:C	1:B:806:GLY:N	2.71	0.43
2:F:371:ARG:HG3	2:F:371:ARG:NH1	2.34	0.43
1:B:483:GLU:C	1:B:486:ASP:CG	2.77	0.43
1:B:565:GLU:C	1:B:567:HIS:H	2.22	0.43
1:B:798:LEU:HD11	1:B:833:VAL:HG13	2.00	0.43
2:C:366:LYS:HG2	2:C:366:LYS:H	1.55	0.43
1:A:739:LEU:O	1:A:743:SER:HB3	2.19	0.43
1:A:779:ASP:O	1:A:780:GLN:HG3	2.18	0.43
1:A:780:GLN:O	1:A:781:GLU:C	2.57	0.43
1:B:233:VAL:O	1:B:234:ARG:C	2.57	0.43
1:B:331:THR:HG23	1:B:331:THR:O	2.18	0.43
1:B:615:PHE:CE2	1:B:628:ALA:HB3	2.54	0.43
2:D:370:LEU:HA	2:D:373:ALA:HB3	1.99	0.43
1:B:748:ASP:OD2	1:B:754:MET:HE2	2.16	0.43
1:B:846:LEU:HD12	1:B:849:GLU:OE1	2.18	0.43
2:C:365:HIS:O	2:C:369:VAL:HG23	2.19	0.43
2:F:402:LYS:O	2:F:403:LEU:O	2.37	0.43
1:A:135:ALA:CA	1:A:138:THR:HG22	2.38	0.43
1:A:46:ASN:HB3	1:A:49:ASN:ND2	2.33	0.43
1:A:505:LEU:HD12	1:A:505:LEU:O	2.19	0.43
1:A:533:MET:SD	1:A:590:ASN:ND2	2.92	0.43
1:B:132:GLN:HA	1:B:132:GLN:NE2	2.31	0.43
1:B:33:LEU:C	1:B:35:THR:H	2.22	0.43
1:B:522:ASN:C	1:B:524:LEU:N	2.72	0.43
1:B:592:LEU:HA	1:B:595:VAL:CG2	2.49	0.43
1:B:716:VAL:HG13	1:B:716:VAL:O	2.18	0.43
2:C:370:LEU:O	2:C:374:ILE:HG13	2.19	0.43
1:A:458:GLU:O	1:A:460:LEU:N	2.52	0.42
1:A:608:MET:CE	1:A:635:LEU:HD23	2.49	0.42
1:B:126:TRP:CD1	1:B:126:TRP:O	2.71	0.42
1:B:182:ARG:HD2	1:B:184:GLU:OE1	2.19	0.42
1:B:263:ILE:HG22	1:B:264:THR:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:CYS:CB	1:B:354:LEU:CD1	2.96	0.42
1:B:608:MET:HE3	1:B:632:VAL:HG22	2.00	0.42
2:E:358:MSE:SE	2:E:364:MSE:SE	3.37	0.42
2:F:403:LEU:H	2:F:403:LEU:CD2	2.30	0.42
1:A:272:ILE:O	1:A:275:VAL:HB	2.19	0.42
1:A:39:GLU:HA	1:A:42:ARG:CD	2.50	0.42
1:A:682:GLN:C	1:A:684:ASN:N	2.72	0.42
1:A:751:ASP:O	1:A:754:MET:HB2	2.18	0.42
1:A:34:PRO:CB	1:A:83:ILE:HD11	2.45	0.42
1:B:468:SER:C	1:B:470:VAL:N	2.71	0.42
1:B:663:GLU:HG3	1:B:666:VAL:H	1.83	0.42
2:F:348:ASP:OD1	2:F:351:ILE:HD11	2.18	0.42
1:A:217:PHE:O	1:A:221:VAL:HG23	2.19	0.42
1:A:587:THR:O	1:A:591:VAL:HG22	2.20	0.42
1:B:129:LEU:C	1:B:131:PRO:HD2	2.38	0.42
1:B:367:VAL:HG12	1:B:367:VAL:O	2.20	0.42
1:B:440:PRO:HB3	1:B:480:ALA:HB2	2.01	0.42
1:B:65:LEU:HB3	1:B:69:ASP:OD2	2.19	0.42
1:B:834:LEU:HD13	1:B:872:LEU:HD12	2.00	0.42
1:A:338:ASP:CB	1:A:465:ARG:HH22	2.32	0.42
1:A:570:SER:C	1:A:572:SER:N	2.72	0.42
1:A:748:ASP:C	1:A:750:SER:N	2.72	0.42
1:B:234:ARG:CZ	1:B:275:VAL:HG11	2.49	0.42
1:B:349:GLY:O	1:B:352:LEU:N	2.53	0.42
1:B:517:PRO:C	1:B:519:GLY:H	2.22	0.42
1:B:560:GLN:C	1:B:562:LEU:H	2.23	0.42
1:B:603:ILE:O	1:B:604:SER:C	2.58	0.42
1:B:205:THR:OG1	1:B:209:PHE:HE1	2.03	0.42
1:B:335:GLU:CG	1:B:380:TRP:HZ2	2.32	0.42
1:B:546:ALA:O	1:B:549:LYS:HG3	2.20	0.42
1:B:777:LYS:CB	1:B:787:VAL:HG21	2.49	0.42
1:B:831:LYS:O	1:B:834:LEU:N	2.51	0.42
1:A:139:ASN:C	1:A:139:ASN:ND2	2.71	0.42
1:A:34:PRO:HB3	1:A:83:ILE:CD1	2.44	0.42
1:B:457:ILE:HG22	1:B:509:LYS:HG2	2.01	0.42
1:B:546:ALA:C	1:B:548:GLN:N	2.72	0.42
1:B:589:GLN:C	1:B:590:ASN:HD22	2.23	0.42
1:B:816:ALA:O	1:B:817:CYS:C	2.57	0.42
1:B:834:LEU:HD21	1:B:873:LYS:NZ	2.34	0.42
1:A:6:ILE:HG22	1:A:21:ALA:CB	2.50	0.42
1:A:450:ALA:N	1:A:451:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:TYR:OH	1:A:596:GLN:N	2.35	0.42
1:A:847:LEU:O	1:A:851:ARG:HG3	2.20	0.42
1:B:353:MET:CG	1:B:392:SER:HB2	2.46	0.42
1:B:594:LYS:HG3	1:B:594:LYS:O	2.19	0.42
2:D:345:SER:OG	2:D:349:LYS:HD2	2.19	0.42
1:A:65:LEU:HD13	1:A:116:ILE:HG12	2.01	0.42
1:B:444:ILE:H	1:B:444:ILE:CD1	2.31	0.42
1:B:615:PHE:CZ	1:B:628:ALA:HB3	2.55	0.42
1:B:777:LYS:HE3	1:B:780:GLN:NE2	2.35	0.42
1:A:514:THR:O	1:A:525:ARG:HD3	2.19	0.42
1:A:668:LEU:CD2	1:A:709:VAL:HA	2.50	0.42
1:B:319:LEU:HD12	1:B:319:LEU:HA	1.84	0.42
1:B:368:LEU:HD23	1:B:368:LEU:HA	1.89	0.42
1:B:729:LYS:HG2	1:B:789:LEU:CD1	2.49	0.42
2:C:357:VAL:CG2	2:C:358:MSE:N	2.82	0.42
1:A:8:GLU:OE1	1:A:53:ALA:HB2	2.20	0.42
1:A:544:TYR:N	1:A:545:PRO:CD	2.82	0.42
1:A:578:ASN:O	1:A:581:GLN:HB3	2.20	0.42
1:B:607:VAL:O	1:B:608:MET:C	2.57	0.42
1:B:790:VAL:O	1:B:793:ARG:HB2	2.19	0.42
1:B:831:LYS:HE2	1:B:872:LEU:O	2.20	0.42
1:A:169:LYS:HB2	1:A:172:GLU:OE1	2.20	0.41
1:B:123:VAL:O	1:B:124:SER:C	2.58	0.41
1:B:613:ARG:O	1:B:617:SER:HB2	2.20	0.41
1:B:608:MET:HE1	1:B:632:VAL:HG22	2.01	0.41
1:B:781:GLU:O	1:B:782:ASN:HB2	2.20	0.41
1:B:791:GLN:N	1:B:792:PRO:HD2	2.35	0.41
1:A:151:LEU:HA	1:A:154:ILE:HD12	2.02	0.41
1:A:826:CYS:SG	1:A:869:LEU:HD23	2.60	0.41
1:A:34:PRO:CG	1:A:83:ILE:HG13	2.50	0.41
1:A:870:ARG:HH11	1:A:870:ARG:HG2	1.85	0.41
1:B:169:LYS:HG3	1:B:169:LYS:O	2.20	0.41
1:B:217:PHE:O	1:B:221:VAL:HG23	2.19	0.41
1:B:326:LEU:HD22	1:B:348:ALA:O	2.20	0.41
1:B:440:PRO:O	1:B:443:ALA:HB3	2.20	0.41
1:B:562:LEU:C	1:B:564:MET:H	2.22	0.41
1:B:6:ILE:O	1:B:6:ILE:HG22	2.20	0.41
1:A:338:ASP:OD2	1:A:338:ASP:O	2.39	0.41
1:A:617:SER:C	1:A:619:ALA:H	2.22	0.41
1:A:762:ARG:HD2	1:A:804:ILE:CD1	2.36	0.41
1:B:27:ARG:HH11	1:B:28:ALA:N	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:PHE:C	1:B:38:VAL:N	2.73	0.41
1:A:665:GLN:NE2	2:C:363:LYS:HG3	2.35	0.41
1:B:182:ARG:CG	1:B:184:GLU:HB2	2.51	0.41
1:B:535:ILE:CG2	1:B:536:VAL:N	2.83	0.41
1:B:758:LEU:HD22	1:B:762:ARG:HG3	2.02	0.41
1:B:857:LYS:O	1:B:861:LEU:CB	2.68	0.41
1:A:126:TRP:HA	1:A:128:GLU:OE1	2.21	0.41
1:B:33:LEU:N	1:B:34:PRO:CD	2.84	0.41
1:B:618:THR:C	1:B:620:GLY:N	2.71	0.41
1:B:804:ILE:O	1:B:806:GLY:N	2.53	0.41
1:B:861:LEU:O	1:B:865:ALA:CB	2.69	0.41
1:B:86:ASN:HA	1:B:89:ARG:NH1	2.35	0.41
2:E:366:LYS:O	2:E:367:SER:CB	2.67	0.41
1:A:362:ASP:O	1:A:365:PRO:HG2	2.20	0.41
1:A:333:GLN:OE1	1:A:384:ASP:OD2	2.38	0.41
1:A:707:ARG:NH2	1:A:753:ASP:CG	2.72	0.41
1:B:126:TRP:O	1:B:128:GLU:N	2.46	0.41
1:B:174:LEU:HD21	1:B:218:ILE:HD11	2.03	0.41
1:B:497:TYR:CD1	1:B:540:ALA:HB2	2.56	0.41
1:B:496:THR:OG1	1:B:542:ASP:OD1	2.36	0.41
2:F:347:ASN:CG	2:F:348:ASP:N	2.32	0.41
1:A:125:GLN:HG2	1:A:126:TRP:H	1.86	0.41
1:A:734:VAL:HG23	1:A:735:VAL:N	2.36	0.41
1:A:80:TRP:HE1	1:A:120:GLU:HG3	1.79	0.41
2:E:358:MSE:N	2:E:372:LYS:CE	2.76	0.41
1:A:365:PRO:HG3	2:E:392:MSE:CE	2.51	0.41
1:A:21:ALA:HB1	1:A:25:LEU:HD12	2.03	0.41
1:B:387:VAL:HG11	1:B:428:THR:OG1	2.21	0.41
1:B:434:ARG:HG2	1:B:434:ARG:HH11	1.86	0.41
1:B:509:LYS:HD3	1:B:509:LYS:HA	1.92	0.41
2:D:382:GLN:O	2:D:385:HIS:N	2.54	0.41
1:A:179:GLN:O	1:A:182:ARG:HG2	2.21	0.41
1:A:540:ALA:HB3	1:A:542:ASP:OD1	2.21	0.41
1:B:395:GLU:HB2	1:B:438:LEU:HD13	2.01	0.41
1:B:451:PRO:O	1:B:455:CYS:N	2.49	0.41
2:F:352:GLU:HA	2:F:355:ASP:OD2	2.21	0.41
1:A:512:GLU:O	1:A:515:ASP:HB2	2.20	0.41
1:A:565:GLU:HB2	1:A:577:PHE:CZ	2.56	0.41
1:A:867:LYS:CG	1:A:870:ARG:HH22	2.31	0.41
1:B:758:LEU:CD2	1:B:762:ARG:NE	2.76	0.41
1:B:740:GLN:HA	1:B:796:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD11	1:B:36:PHE:CZ	2.50	0.41
1:B:80:TRP:HE1	1:B:120:GLU:CD	2.23	0.41
2:E:398:ASN:ND2	2:E:398:ASN:C	2.74	0.41
1:A:360:GLU:O	1:A:363:ILE:HG22	2.21	0.41
1:A:686:LEU:CD1	1:A:727:GLU:HG2	2.50	0.41
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.83	0.41
1:B:27:ARG:CG	1:B:28:ALA:N	2.73	0.41
1:A:488:ALA:HB2	1:B:870:ARG:HH22	1.86	0.41
1:A:224:GLU:O	1:A:226:THR:N	2.54	0.40
1:A:626:GLU:HB2	1:A:666:VAL:CG2	2.50	0.40
1:A:850:GLY:O	1:A:859:LYS:HA	2.20	0.40
1:B:28:ALA:O	1:B:33:LEU:HD23	2.21	0.40
1:B:401:GLN:O	1:B:401:GLN:CG	2.69	0.40
1:B:479:GLU:HA	1:B:538:ASN:ND2	2.33	0.40
1:B:740:GLN:HG3	1:B:796:PHE:CE2	2.56	0.40
1:A:287:CYS:HB3	1:A:354:LEU:HD13	2.03	0.40
1:B:36:PHE:C	1:B:38:VAL:H	2.24	0.40
1:B:444:ILE:N	1:B:444:ILE:CD1	2.84	0.40
1:B:612:LEU:O	1:B:616:GLN:HG3	2.22	0.40
2:C:360:THR:O	2:C:361:ASP:HB3	2.21	0.40
2:E:380:LEU:HB2	2:F:380:LEU:HD13	2.03	0.40
1:A:51:GLN:NE2	1:A:105:ARG:NE	2.69	0.40
1:A:62:LYS:HG2	1:A:111:GLN:HB3	2.02	0.40
1:A:202:LEU:HD11	1:A:240:ASN:HD22	1.85	0.40
1:A:260:LEU:O	1:A:261:PHE:C	2.59	0.40
1:A:343:ASN:HD21	1:A:345:CYS:HB3	1.86	0.40
1:A:448:TYR:C	1:A:451:PRO:HD2	2.41	0.40
1:A:453:LEU:O	1:A:457:ILE:HG13	2.22	0.40
1:A:89:ARG:HH11	1:A:89:ARG:HG3	1.86	0.40
1:B:181:MET:HE1	1:B:198:LEU:HB2	2.04	0.40
1:B:460:LEU:HD11	1:B:474:PHE:CE2	2.56	0.40
1:B:867:LYS:C	1:B:869:LEU:H	2.25	0.40
1:A:147:LYS:O	1:A:148:GLU:C	2.60	0.40
1:A:515:ASP:C	1:A:516:ARG:CG	2.84	0.40
1:A:859:LYS:HE3	1:A:859:LYS:HB2	1.89	0.40
1:B:27:ARG:HH11	1:B:27:ARG:HG2	1.86	0.40
1:B:335:GLU:CG	1:B:380:TRP:CZ2	3.04	0.40
1:B:370:PHE:CD1	1:B:370:PHE:C	2.94	0.40
1:B:522:ASN:C	1:B:524:LEU:H	2.24	0.40
1:B:831:LYS:O	1:B:833:VAL:N	2.54	0.40
2:F:357:VAL:HG12	2:F:358:MSE:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:392:MSE:C	2:F:394:LEU:N	2.74	0.40
1:A:172:GLU:CD	1:A:172:GLU:N	2.72	0.40
1:A:514:THR:CG2	1:A:529:TYR:CZ	3.05	0.40
1:A:579:ASP:O	1:A:583:LEU:HG	2.21	0.40
1:A:859:LYS:O	1:A:863:THR:OG1	2.39	0.40
1:B:212:GLU:C	1:B:216:HIS:HD2	2.25	0.40
1:B:599:ASP:O	1:B:603:ILE:N	2.55	0.40
1:B:811:THR:C	1:B:813:GLY:N	2.74	0.40
2:F:370:LEU:O	2:F:374:ILE:HG13	2.22	0.40
2:F:385:HIS:O	2:F:388:ARG:HG2	2.21	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:171:ASN:CB	2:F:402:LYS:NZ[4_556]	1.72	0.48

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	874/876 (100%)	695 (80%)	146 (17%)	33 (4%)	3	18
1	B	874/876 (100%)	671 (77%)	143 (16%)	60 (7%)	1	6
2	C	59/61 (97%)	47 (80%)	12 (20%)	0	100	100
2	D	59/61 (97%)	45 (76%)	8 (14%)	6 (10%)	0	2
2	E	59/61 (97%)	48 (81%)	8 (14%)	3 (5%)	2	12
2	F	59/61 (97%)	45 (76%)	8 (14%)	6 (10%)	0	2
All	All	1984/1996 (99%)	1551 (78%)	325 (16%)	108 (5%)	2	11

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	A	168	ASP
1	A	169	LYS
1	A	462	ALA
1	A	683	SER
1	A	752	PHE
1	A	753	ASP
1	A	809	ASP
1	B	28	ALA
1	B	52	VAL
1	B	212	GLU
1	B	340	ASP
1	B	446	ASP
1	B	486	ASP
1	B	523	ASN
1	B	604	SER
1	B	621	SER
1	B	660	ASN
1	B	752	PHE
1	B	874	ASN
2	D	366	LYS
2	E	357	VAL
2	E	361	ASP
2	E	365	HIS
2	F	345	SER
2	F	357	VAL
2	F	365	HIS
2	F	402	LYS
1	A	49	ASN
1	A	225	ALA
1	A	519	GLY
1	A	800	PHE
1	A	830	GLY
1	B	12	SER
1	B	68	LYS
1	B	252	MET
1	B	259	ALA
1	B	270	SER
1	B	361	ASP
1	B	445	ASN
1	B	469	ASN
1	B	664	TYR
1	B	689	CYS

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Mol	Chain	Res	Type
1	B	725	GLY
1	B	733	GLU
1	B	746	GLN
1	B	750	SER
1	B	789	LEU
1	B	811	THR
1	B	852	ARG
1	B	853	SER
2	D	397	ALA
2	D	398	ASN
2	D	401	ASN
2	F	364	MSE
2	F	393	VAL
1	A	14	ASP
1	A	70	PRO
1	A	74	ALA
1	A	132	GLN
1	A	616	GLN
1	A	660	ASN
1	A	682	GLN
1	A	749	LYS
1	A	780	GLN
1	B	17	GLU
1	B	44	LEU
1	B	96	LEU
1	B	105	ARG
1	B	344	PRO
1	B	427	THR
1	B	659	LYS
1	B	805	ALA
1	B	832	ASP
1	B	875	GLN
2	D	367	SER
1	A	93	ASN
1	A	733	GLU
1	A	781	GLU
1	A	832	ASP
1	B	72	ILE
1	B	184	GLU
1	B	518	ASP
1	B	598	GLN
1	B	650	PHE

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Mol	Chain	Res	Type
1	B	661	TYR
1	B	782	ASN
1	B	795	GLU
1	A	20	ALA
1	A	517	PRO
1	A	649	ALA
1	A	798	LEU
1	B	62	LYS
1	B	124	SER
1	B	185	GLU
1	B	408	GLN
1	B	416	LEU
1	B	524	LEU
1	B	839	ALA
2	D	361	ASP
1	A	664	TYR
1	A	783	VAL
1	B	11	VAL
1	B	431	THR
1	B	561	VAL
1	B	734	VAL
1	B	494	PRO
1	A	105	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	753/753 (100%)	688 (91%)	65 (9%)	10	37
1	B	753/753 (100%)	688 (91%)	65 (9%)	10	37
2	C	56/53 (106%)	52 (93%)	4 (7%)	14	46
2	D	56/53 (106%)	52 (93%)	4 (7%)	14	46
2	E	56/53 (106%)	51 (91%)	5 (9%)	9	35
2	F	56/53 (106%)	50 (89%)	6 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1730/1718 (101%)	1581 (91%)	149 (9%)	10	37

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

Mol	Chain	Res	Type
1	A	15	ARG
1	A	94	TYR
1	A	102	GLU
1	A	111	GLN
1	A	125	GLN
1	A	139	ASN
1	A	146	MET
1	A	148	GLU
1	A	166	LEU
1	A	174	LEU
1	A	234	ARG
1	A	255	TYR
1	A	269	LYS
1	A	281	GLU
1	A	298	SER
1	A	308	GLU
1	A	319	LEU
1	A	331	THR
1	A	333	GLN
1	A	334	ASP
1	A	352	LEU
1	A	354	LEU
1	A	362	ASP
1	A	377	ASN
1	A	413	LEU
1	A	422	VAL
1	A	441	GLU
1	A	455	CYS
1	A	468	SER
1	A	489	ASP
1	A	494	PRO
1	A	497	TYR
1	A	502	SER
1	A	504	GLU
1	A	507	VAL
1	A	517	PRO
1	A	524	LEU

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Mol	Chain	Res	Type
1	A	525	ARG
1	A	526	SER
1	A	530	GLU
1	A	535	ILE
1	A	573	ASP
1	A	576	GLN
1	A	580	LEU
1	A	581	GLN
1	A	613	ARG
1	A	615	PHE
1	A	626	GLU
1	A	627	ASP
1	A	633	SER
1	A	673	LEU
1	A	687	PRO
1	A	688	PHE
1	A	689	CYS
1	A	716	VAL
1	A	732	LEU
1	A	743	SER
1	A	751	ASP
1	A	758	LEU
1	A	821	LEU
1	A	831	LYS
1	A	832	ASP
1	A	860	THR
1	A	863	THR
1	A	874	ASN
1	B	17	GLU
1	B	32	ASN
1	B	52	VAL
1	B	67	SER
1	B	68	LYS
1	B	70	PRO
1	B	97	GLN
1	B	145	HIS
1	B	165	GLN
1	B	203	GLU
1	B	226	THR
1	B	234	ARG
1	B	246	SER
1	B	250	GLN

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Mol	Chain	Res	Type
1	B	266	GLU
1	B	274	GLU
1	B	296	GLU
1	B	298	SER
1	B	308	GLU
1	B	319	LEU
1	B	320	GLN
1	B	331	THR
1	B	337	ASP
1	B	343	ASN
1	B	345	CYS
1	B	346	LYS
1	B	350	VAL
1	B	352	LEU
1	B	354	LEU
1	B	355	LEU
1	B	362	ASP
1	B	368	LEU
1	B	377	ASN
1	B	388	MET
1	B	422	VAL
1	B	453	LEU
1	B	470	VAL
1	B	474	PHE
1	B	492	GLU
1	B	494	PRO
1	B	497	TYR
1	B	514	THR
1	B	521	GLN
1	B	534	GLU
1	B	549	LYS
1	B	601	LEU
1	B	608	MET
1	B	612	LEU
1	B	626	GLU
1	B	630	MET
1	B	637	GLU
1	B	642	GLU
1	B	659	LYS
1	B	661	TYR
1	B	673	LEU
1	B	716	VAL

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Mol	Chain	Res	Type
1	B	753	ASP
1	B	758	LEU
1	B	779	ASP
1	B	781	GLU
1	B	783	VAL
1	B	785	PRO
1	B	810	HIS
1	B	817	CYS
1	B	821	LEU
2	C	356	LEU
2	C	361	ASP
2	C	364	MSE
2	C	367	SER
2	D	364	MSE
2	D	370	LEU
2	D	386	LYS
2	D	399	GLN
2	E	348	ASP
2	E	355	ASP
2	E	364	MSE
2	E	395	LYS
2	E	398	ASN
2	F	356	LEU
2	F	364	MSE
2	F	383	VAL
2	F	389	GLN
2	F	396	LEU
2	F	403	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	32	ASN
1	A	49	ASN
1	A	111	GLN
1	A	139	ASN
1	A	141	ASN
1	A	165	GLN
1	A	196	ASN
1	A	208	ASN
1	A	220	GLN

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Mol	Chain	Res	Type
1	A	240	ASN
1	A	278	GLN
1	A	328	GLN
1	A	336	ASN
1	A	377	ASN
1	A	401	GLN
1	A	520	HIS
1	A	523	ASN
1	A	563	GLN
1	A	576	GLN
1	A	590	ASN
1	A	596	GLN
1	A	625	GLN
1	A	660	ASN
1	A	684	ASN
1	A	702	ASN
1	A	741	GLN
1	A	784	HIS
1	A	803	HIS
1	A	874	ASN
1	B	22	GLN
1	B	32	ASN
1	B	49	ASN
1	B	97	GLN
1	B	132	GLN
1	B	141	ASN
1	B	159	GLN
1	B	165	GLN
1	B	167	GLN
1	B	179	GLN
1	B	220	GLN
1	B	240	ASN
1	B	320	GLN
1	B	343	ASN
1	B	377	ASN
1	B	454	GLN
1	B	469	ASN
1	B	522	ASN
1	B	548	GLN
1	B	578	ASN
1	B	589	GLN
1	B	590	ASN

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Mol	Chain	Res	Type
1	B	596	GLN
1	B	616	GLN
1	B	625	GLN
1	B	660	ASN
1	B	694	GLN
1	B	774	GLN
1	B	780	GLN
1	B	791	GLN
2	D	381	GLN
2	D	385	HIS
2	D	391	ASN
2	D	398	ASN
2	E	398	ASN
2	F	365	HIS
2	F	389	GLN
2	F	398	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.