Full wwPDB EM Validation Report (i)

Dec 13, 2022 – 12:14 AM EST

PDB ID	:	1SUV
Title	:	Structure of Human Transferrin Receptor-Transferrin Complex
Authors	:	Cheng, Y.; Zak, O.; Aisen, P.; Harrison, S.C.; Walz, T.
Deposited on	:	2004-03-26
Resolution	:	7.50 Å(reported)
Based on initial models	:	1CX8, 1JNF, 1A8E

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

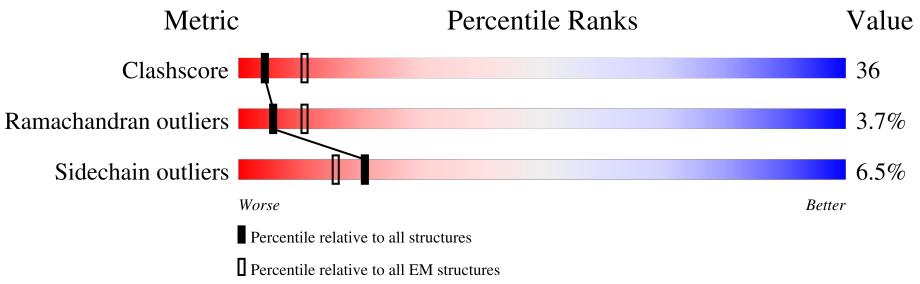
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.50 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	639	39% 50% 9% •
1	B	639	40% 49% 10% •
2	C	329	87% 12% •
2	D	329	86% 13% •
3	E	345	59% 34% 7%
3	F	345	60% 33% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	639	5056	3244	846	952	14	0	0
1	B	639	5056	3244	846	952	14	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	GLU	GLN	SEE REMARK 999	UNP P02786
A	613	GLU	ARG	SEE REMARK 999	UNP P02786
B	172	GLU	GLN	SEE REMARK 999	UNP P02786
B	613	GLU	ARG	SEE REMARK 999	UNP P02786

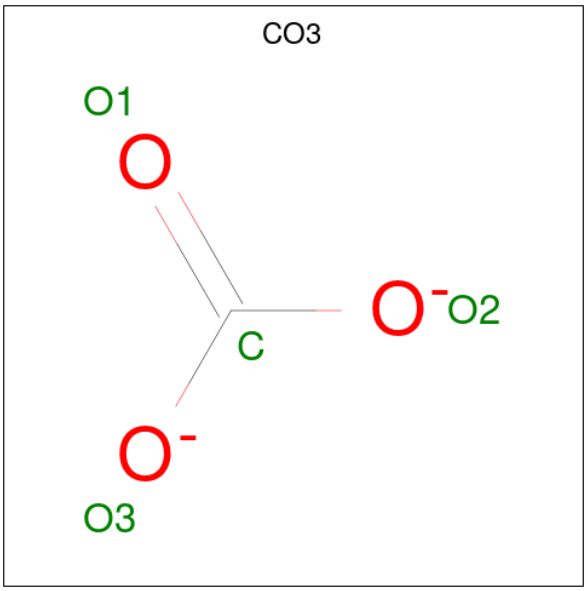
- Molecule 2 is a protein called Serotransferrin, N-lobe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	329	2567	1621	440	485	21	5	0
2	D	329	2567	1621	440	485	21	5	0

- Molecule 3 is a protein called Serotransferrin, C-lobe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	345	2669	1662	469	512	26	0	0
3	F	345	2669	1662	469	512	26	0	0

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	C	1	8	2	6	1
			Total	C	O	
4	D	1	8	2	6	1
			Total	C	O	
4	E	1	4	1	3	0
			Total	C	O	
4	F	1	4	1	3	0

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

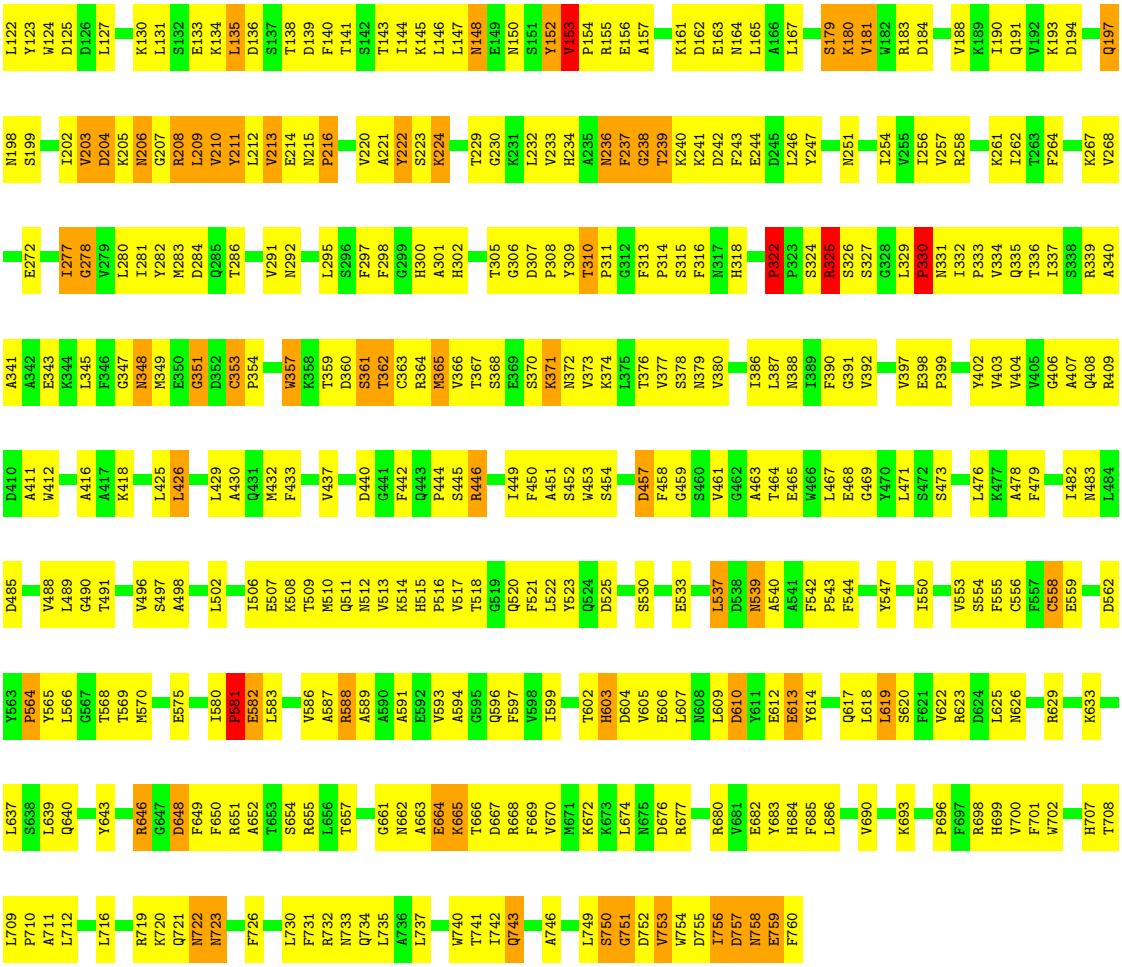
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
5	C	1	1	1	0
			Total	Fe	
5	D	1	1	1	0
			Total	Fe	
5	E	1	1	1	0
			Total	Fe	
5	F	1	1	1	0

3 Residue-property plots (i)

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

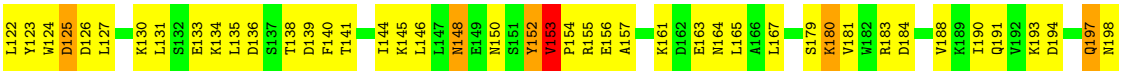
- Molecule 1: Transferrin receptor protein 1

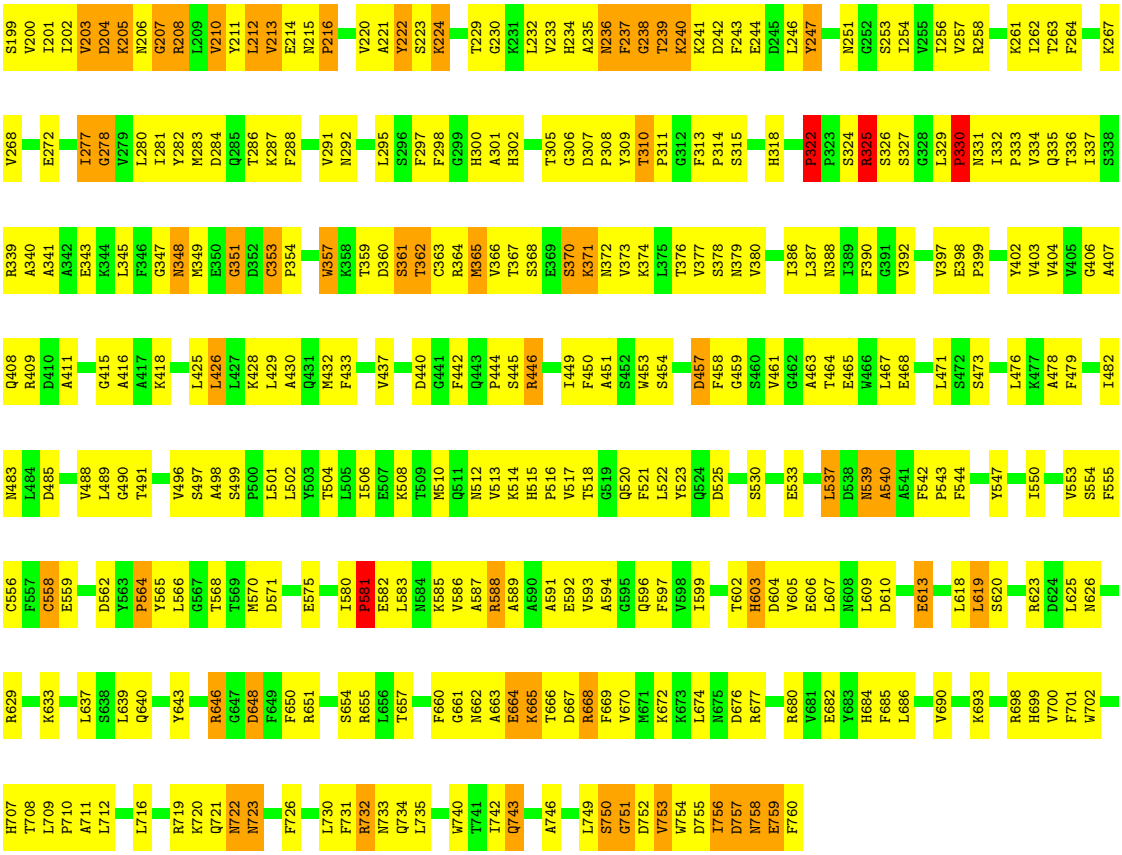
Chain A: 39% 50% 9%



- Molecule 1: Transferrin receptor protein 1

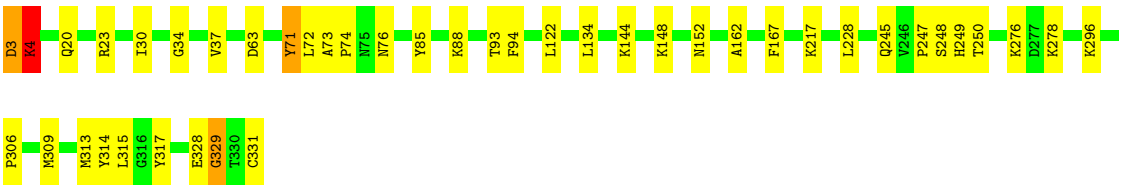
Chain B: 40% 49% 10%





- Molecule 2: Serotransferrin, N-lobe

Chain C:

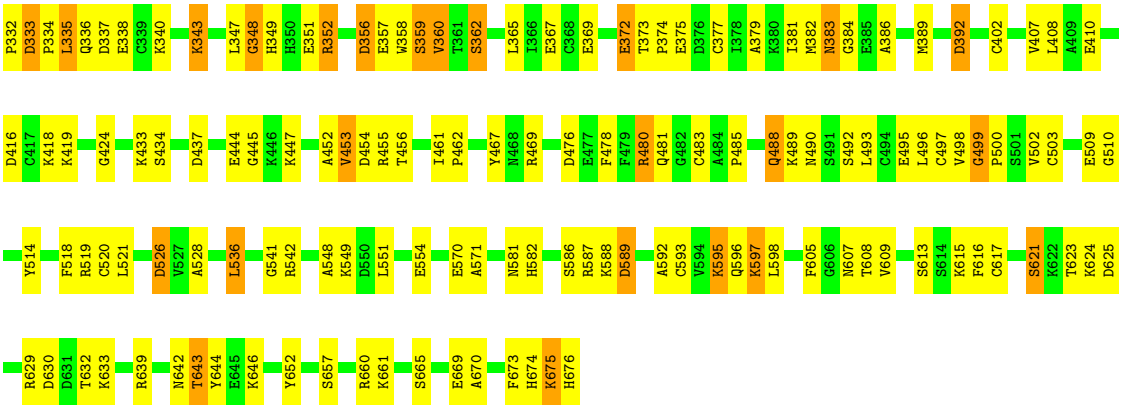


- Molecule 2: Serotransferrin, N-lobe

Chain D:

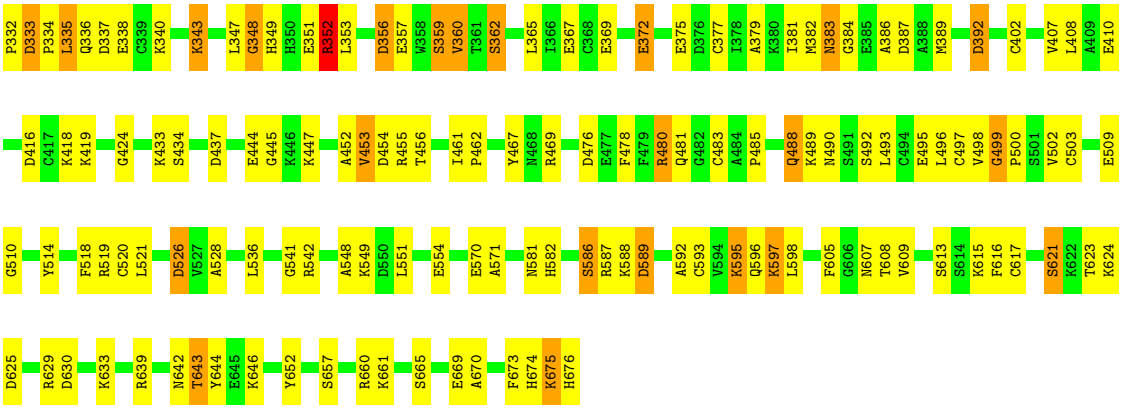
- Molecule 3: Serotransferrin, C-lobe

Chain E:



• Molecule 3: Serotransferrin, C-lobe

Chain F: 60% 33% 7%



GLOBAL-STATISTICS INFOmissingINFO

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, CO3

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	0.38	0/5177	0.61	1/7021 (0.0%)
1	B	0.38	0/5177	0.61	1/7021 (0.0%)
2	C	0.84	0/2648	0.88	5/3578 (0.1%)
2	D	0.84	0/2648	0.88	5/3578 (0.1%)
3	E	0.89	0/2723	1.03	9/3675 (0.2%)
3	F	0.89	0/2723	1.03	9/3675 (0.2%)
All	All	0.67	0/21096	0.81	30/28548 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	88	LYS	N-CA-CB	12.30	132.73	110.60
2	D	88	LYS	N-CA-CB	12.28	132.70	110.60
3	F	437	ASP	CB-CG-OD2	11.00	128.20	118.30
3	E	437	ASP	CB-CG-OD2	10.97	128.17	118.30
2	C	88	LYS	CA-CB-CG	-10.21	90.94	113.40
2	D	88	LYS	CA-CB-CG	-10.19	90.97	113.40
3	F	526	ASP	CB-CG-OD2	7.41	124.97	118.30
3	E	526	ASP	CB-CG-OD2	7.40	124.96	118.30
3	E	392	ASP	CB-CG-OD2	7.35	124.92	118.30
3	F	392	ASP	CB-CG-OD2	7.32	124.89	118.30
3	F	356	ASP	CB-CG-OD2	5.96	123.66	118.30
2	C	88	LYS	CB-CA-C	-5.96	98.49	110.40
2	D	88	LYS	CB-CA-C	-5.94	98.51	110.40
3	E	356	ASP	CB-CG-OD2	5.92	123.63	118.30
3	F	589	ASP	CB-CG-OD2	5.88	123.59	118.30
3	E	589	ASP	CB-CG-OD2	5.83	123.54	118.30
2	D	4	LYS	CA-CB-CG	-5.77	100.70	113.40
2	C	4	LYS	CA-CB-CG	-5.77	100.70	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	352	ARG	NE-CZ-NH2	-5.51	117.55	120.30
3	E	352	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	D	3	ASP	O-C-N	5.36	131.28	122.70
2	C	3	ASP	O-C-N	5.35	131.26	122.70
3	F	352	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	751	GLY	N-CA-C	-5.23	100.03	113.10
3	E	352	ARG	NE-CZ-NH1	5.22	122.91	120.30
3	F	542	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	751	GLY	N-CA-C	-5.13	100.28	113.10
3	E	542	ARG	NE-CZ-NH1	5.11	122.86	120.30
3	E	625	ASP	CB-CG-OD2	5.07	122.86	118.30
3	F	625	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5056	0	4980	582	0
1	B	5056	0	4982	575	0
2	C	2567	0	2482	94	0
2	D	2567	0	2482	95	0
3	E	2669	0	2574	197	0
3	F	2669	0	2575	205	0
4	C	8	0	0	0	0
4	D	8	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	20612	0	20075	1446	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 36.

All (1446) 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:D:317:TYR:CE1	3:F:383:ASN:HB2	1.19	1.66
2:C:317:TYR:CE1	3:E:383:ASN:HB2	1.19	1.65
1:B:623:ARG:HD2	3:F:360:VAL:CG2	1.16	1.62
1:A:623:ARG:CD	3:E:360:VAL:HG23	1.14	1.59
1:A:623:ARG:HB3	3:E:360:VAL:CG2	1.34	1.56
1:B:643:TYR:CD2	3:F:353:LEU:CD2	1.93	1.50
1:A:623:ARG:HD2	3:E:360:VAL:CG2	1.44	1.47
2:D:317:TYR:CE1	3:F:383:ASN:CB	2.02	1.43
1:B:646:ARG:NH2	3:F:352:ARG:HH21	1.09	1.42
1:B:623:ARG:CD	3:F:360:VAL:HG23	0.93	1.41
2:C:317:TYR:CE1	3:E:383:ASN:CB	2.02	1.40
2:C:94:PHE:CD1	3:E:675:LYS:HB2	1.55	1.40
1:A:623:ARG:CB	3:E:360:VAL:CG2	1.96	1.39
2:D:94:PHE:CD1	3:F:675:LYS:HB2	1.55	1.38
1:B:623:ARG:CB	3:F:360:VAL:HG22	1.53	1.37
1:B:623:ARG:HB3	3:F:360:VAL:CG2	1.53	1.36
1:B:646:ARG:NH2	3:F:352:ARG:NH2	1.75	1.34
1:B:643:TYR:CE2	3:F:353:LEU:HD22	1.59	1.34
1:B:623:ARG:CB	3:F:360:VAL:CG2	2.06	1.33
2:C:245:GLN:OE1	3:E:676:HIS:HA	1.25	1.33
2:D:245:GLN:OE1	3:F:676:HIS:HA	1.25	1.32
1:A:623:ARG:CB	3:E:360:VAL:HG22	1.52	1.30
2:C:317:TYR:CZ	3:E:383:ASN:HA	1.72	1.25
1:B:623:ARG:NH1	3:F:360:VAL:N	1.84	1.24
2:D:317:TYR:CZ	3:F:383:ASN:HA	1.72	1.23
1:A:623:ARG:NE	3:E:356:ASP:O	1.71	1.23
2:D:317:TYR:CZ	3:F:383:ASN:HB2	1.74	1.23
2:C:317:TYR:CZ	3:E:383:ASN:HB2	1.74	1.20
1:A:623:ARG:NH1	3:E:360:VAL:N	1.90	1.20
2:C:313:MET:CG	3:E:670:ALA:HB2	1.72	1.19
2:D:313:MET:CG	3:F:670:ALA:HB2	1.72	1.19
1:B:623:ARG:CD	3:F:360:VAL:CG2	1.85	1.17
1:B:623:ARG:CG	3:F:360:VAL:CG2	2.22	1.17
1:B:643:TYR:CD2	3:F:353:LEU:HD23	1.72	1.16
1:A:662:ASN:O	2:C:73:ALA:N	1.79	1.15
3:F:623:THR:HG22	3:F:624:LYS:H	1.05	1.15
1:A:662:ASN:O	2:C:72:LEU:HB3	1.50	1.12
1:A:153:VAL:HG13	1:A:154:PRO:HD3	1.20	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ARG:NE	3:F:356:ASP:O	1.82	1.11
1:B:643:TYR:CE2	3:F:353:LEU:CD2	2.23	1.11
3:E:623:THR:HG22	3:E:624:LYS:H	1.05	1.11
1:B:153:VAL:HG13	1:B:154:PRO:HD3	1.21	1.11
1:A:623:ARG:CG	3:E:360:VAL:HG23	1.81	1.10
2:C:315:LEU:O	3:E:674:HIS:NE2	1.85	1.10
2:D:315:LEU:O	3:F:674:HIS:NE2	1.85	1.10
1:B:759:GLU:OE2	3:F:500:PRO:HB3	1.52	1.09
2:C:313:MET:SD	3:E:670:ALA:HB2	1.93	1.09
1:A:623:ARG:CG	3:E:360:VAL:CG2	2.32	1.08
1:B:662:ASN:O	2:D:72:LEU:HB3	1.53	1.07
2:D:313:MET:SD	3:F:670:ALA:HB2	1.93	1.06
2:D:317:TYR:OH	3:F:383:ASN:HA	1.53	1.06
1:B:643:TYR:CD2	3:F:353:LEU:HD21	1.91	1.06
2:C:317:TYR:OH	3:E:383:ASN:HA	1.53	1.05
2:C:317:TYR:CZ	3:E:383:ASN:CA	2.40	1.05
2:C:313:MET:CG	3:E:670:ALA:CB	2.35	1.05
2:C:247:PRO:HG3	3:E:674:HIS:HE1	1.20	1.04
1:B:623:ARG:CG	3:F:360:VAL:HG23	1.83	1.04
2:D:317:TYR:CZ	3:F:383:ASN:CA	2.40	1.03
2:D:313:MET:HG2	3:F:670:ALA:CB	1.89	1.03
2:D:313:MET:CG	3:F:670:ALA:CB	2.35	1.02
1:B:359:THR:HG22	1:B:360:ASP:H	1.22	1.02
2:C:313:MET:HG2	3:E:670:ALA:CB	1.89	1.02
1:A:664:GLU:CD	2:C:74:PRO:HD3	1.81	1.01
1:B:210:VAL:HG13	1:B:211:TYR:H	1.22	1.01
1:B:662:ASN:O	2:D:73:ALA:N	1.92	1.01
1:A:629:ARG:NH1	3:E:357:GLU:OE1	1.94	1.01
2:C:317:TYR:CZ	3:E:383:ASN:CB	2.39	1.00
2:D:247:PRO:HG3	3:F:674:HIS:HE1	1.20	1.00
3:E:379:ALA:HA	3:E:382:MET:HE3	1.44	1.00
1:B:646:ARG:HH22	3:F:352:ARG:HH21	1.05	0.99
1:B:759:GLU:CD	3:F:500:PRO:HB3	1.83	0.99
2:C:94:PHE:CE1	3:E:675:LYS:HB2	1.97	0.99
1:A:359:THR:HG22	1:A:360:ASP:H	1.25	0.98
2:C:245:GLN:OE1	3:E:676:HIS:CA	2.12	0.98
2:D:94:PHE:CE1	3:F:675:LYS:HB2	1.97	0.97
2:D:94:PHE:CD1	3:F:675:LYS:CB	2.47	0.97
2:C:94:PHE:CD1	3:E:675:LYS:CB	2.47	0.97
3:F:379:ALA:HA	3:F:382:MET:HE3	1.46	0.97
2:D:245:GLN:OE1	3:F:676:HIS:CA	2.12	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASP:HB3	1:B:388:ASN:HB2	1.46	0.96
1:B:708:THR:HG22	1:B:711:ALA:H	1.31	0.95
1:B:646:ARG:HH21	3:F:352:ARG:HH21	0.96	0.95
1:B:664:GLU:OE1	2:D:74:PRO:HD3	1.68	0.94
1:B:306:GLY:HA2	1:B:461:VAL:HA	1.50	0.94
1:B:348:ASN:HB3	1:B:371:LYS:HE3	1.47	0.94
1:B:623:ARG:CG	3:F:360:VAL:HG22	1.93	0.94
1:A:759:GLU:CD	3:E:500:PRO:HB3	1.87	0.94
2:D:317:TYR:OH	3:F:383:ASN:CA	2.16	0.93
1:B:646:ARG:HH21	3:F:352:ARG:NH2	1.50	0.93
1:A:670:VAL:HG11	2:C:74:PRO:HB3	1.50	0.93
1:A:354:PRO:HD3	1:A:365:MET:SD	2.09	0.93
1:A:623:ARG:NH1	3:E:359:SER:C	2.20	0.93
2:C:317:TYR:OH	3:E:383:ASN:CA	2.16	0.93
3:F:623:THR:HG22	3:F:624:LYS:N	1.83	0.93
1:B:667:ASP:OD2	2:D:74:PRO:HG3	1.67	0.92
1:A:348:ASN:HB3	1:A:371:LYS:HE3	1.49	0.92
1:B:759:GLU:OE2	3:F:500:PRO:CB	2.17	0.92
1:B:664:GLU:CD	2:D:74:PRO:HD3	1.89	0.92
2:D:317:TYR:CZ	3:F:383:ASN:CB	2.39	0.92
1:A:203:VAL:HB	1:A:208:ARG:HA	1.49	0.91
1:A:664:GLU:OE2	2:C:74:PRO:CD	2.17	0.91
1:A:664:GLU:OE1	2:C:74:PRO:HD3	1.68	0.91
1:A:184:ASP:HB3	1:A:388:ASN:HB2	1.52	0.91
1:A:140:PHE:HE1	1:A:588:ARG:HA	1.36	0.90
1:A:209:LEU:HG	1:A:210:VAL:H	1.35	0.90
1:A:662:ASN:OD1	2:C:71:TYR:CE1	2.23	0.90
1:A:130:LYS:HE3	1:A:134:LYS:HD3	1.50	0.90
1:A:662:ASN:O	2:C:72:LEU:CB	2.18	0.90
1:B:623:ARG:CZ	3:F:360:VAL:H	1.84	0.90
1:B:623:ARG:HD2	3:F:360:VAL:CB	2.01	0.90
3:E:623:THR:HG22	3:E:624:LYS:N	1.83	0.89
2:C:313:MET:HG2	3:E:670:ALA:HB2	1.51	0.89
1:A:349:MET:HB2	1:A:364:ARG:HG3	1.54	0.89
1:A:623:ARG:HB3	3:E:360:VAL:HG21	1.54	0.89
1:B:130:LYS:HE3	1:B:134:LYS:HD3	1.54	0.89
1:B:349:MET:HB2	1:B:364:ARG:HG3	1.54	0.89
1:B:623:ARG:NH1	3:F:359:SER:C	2.24	0.88
1:A:623:ARG:CB	3:E:360:VAL:HG21	2.03	0.88
1:B:444:PRO:HB3	1:B:602:THR:HG21	1.56	0.88
1:A:153:VAL:CG1	1:A:154:PRO:HD3	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LYS:HA	1:B:164:ASN:HD22	1.39	0.88
1:A:161:LYS:HA	1:A:164:ASN:HD22	1.37	0.88
1:B:629:ARG:NH1	3:F:357:GLU:OE1	2.06	0.88
1:A:664:GLU:OE2	2:C:74:PRO:HD3	1.73	0.87
1:B:643:TYR:CG	3:F:353:LEU:HD21	2.08	0.87
1:B:670:VAL:HG11	2:D:74:PRO:HB3	1.54	0.87
1:B:300:HIS:HE1	1:B:302:HIS:HB3	1.39	0.87
1:B:140:PHE:HE1	1:B:588:ARG:HA	1.38	0.87
1:B:623:ARG:HD3	3:F:360:VAL:HG23	1.49	0.87
1:A:708:THR:HG22	1:A:711:ALA:H	1.39	0.87
1:B:623:ARG:CZ	3:F:360:VAL:N	2.27	0.87
1:B:201:ILE:HD11	1:B:208:ARG:HB2	1.57	0.86
1:A:239:THR:HB	1:A:244:GLU:HG2	1.55	0.86
1:A:353:CYS:HA	1:A:365:MET:SD	2.15	0.86
1:B:153:VAL:CG1	1:B:154:PRO:HD3	2.05	0.86
2:C:317:TYR:HE1	3:E:383:ASN:CB	1.64	0.86
1:B:354:PRO:HD3	1:B:365:MET:SD	2.14	0.86
1:B:667:ASP:HB3	1:B:670:VAL:HG22	1.57	0.86
1:A:662:ASN:HA	2:C:72:LEU:HD22	1.57	0.86
1:B:662:ASN:O	2:D:72:LEU:CB	2.22	0.86
1:A:623:ARG:CD	3:E:360:VAL:CG2	2.09	0.85
1:B:623:ARG:HB3	3:F:360:VAL:HG22	0.85	0.85
1:A:426:LEU:HD21	1:A:450:PHE:HB3	1.59	0.85
1:A:759:GLU:OE2	3:E:500:PRO:CA	2.25	0.85
1:A:153:VAL:HG13	1:A:154:PRO:CD	2.03	0.85
1:A:306:GLY:HA2	1:A:461:VAL:HA	1.59	0.85
1:A:662:ASN:HA	2:C:72:LEU:CD2	2.07	0.85
1:B:239:THR:HB	1:B:244:GLU:HG2	1.57	0.85
1:B:708:THR:HG23	1:B:710:PRO:HD2	1.59	0.85
1:A:300:HIS:HE1	1:A:302:HIS:HB3	1.42	0.84
1:B:353:CYS:HA	1:B:365:MET:SD	2.16	0.84
1:B:646:ARG:HG2	1:B:646:ARG:HH11	1.42	0.84
1:A:708:THR:HG23	1:A:710:PRO:HD2	1.59	0.84
1:B:623:ARG:CB	3:F:360:VAL:HG21	2.07	0.84
1:A:623:ARG:CA	3:E:360:VAL:HG21	2.08	0.84
1:A:662:ASN:O	2:C:72:LEU:CA	2.26	0.84
1:A:667:ASP:HB3	1:A:670:VAL:HG22	1.57	0.83
1:B:310:THR:OG1	1:B:468:GLU:OE1	1.96	0.83
1:A:662:ASN:OD1	2:C:71:TYR:CZ	2.31	0.83
1:A:759:GLU:OE2	3:E:500:PRO:HB3	1.79	0.83
3:E:623:THR:CG2	3:E:624:LYS:H	1.89	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:GLU:OE2	1:A:468:GLU:CD	2.17	0.83
1:A:442:PHE:CZ	1:A:444:PRO:HG3	2.13	0.83
1:B:153:VAL:HG13	1:B:154:PRO:CD	2.06	0.82
1:B:280:LEU:HD12	1:B:337:ILE:HD13	1.61	0.82
3:F:379:ALA:HA	3:F:382:MET:CE	2.09	0.82
1:A:667:ASP:OD2	2:C:74:PRO:HG3	1.79	0.82
1:B:426:LEU:HD21	1:B:450:PHE:HB3	1.58	0.82
1:A:664:GLU:CD	2:C:74:PRO:CD	2.47	0.82
1:B:643:TYR:HD2	3:F:353:LEU:HD23	1.39	0.82
1:B:640:GLN:HE22	3:F:349:HIS:CE1	1.98	0.82
1:B:662:ASN:OD1	2:D:71:TYR:OH	1.96	0.82
1:B:442:PHE:CZ	1:B:444:PRO:HG3	2.14	0.81
1:A:300:HIS:CE1	1:A:302:HIS:HB3	2.15	0.81
3:E:497:CYS:HB3	3:E:509:GLU:OE1	1.80	0.81
1:A:758:ASN:HB2	1:B:183:ARG:O	1.79	0.81
3:E:379:ALA:HA	3:E:382:MET:CE	2.09	0.81
1:B:662:ASN:OD1	2:D:71:TYR:CE1	2.32	0.81
2:D:247:PRO:HG3	3:F:674:HIS:CE1	2.13	0.81
1:A:310:THR:OG1	1:A:468:GLU:OE1	1.98	0.81
1:B:300:HIS:CE1	1:B:302:HIS:HB3	2.14	0.81
1:B:199:SER:HB2	1:B:212:LEU:HD11	1.63	0.81
3:F:623:THR:CG2	3:F:624:LYS:H	1.89	0.81
3:F:497:CYS:HB3	3:F:509:GLU:OE1	1.80	0.80
1:B:465:GLU:OE2	1:B:468:GLU:CD	2.19	0.80
1:A:623:ARG:HH11	3:E:360:VAL:N	1.79	0.80
1:B:662:ASN:OD1	2:D:71:TYR:CZ	2.34	0.80
1:A:444:PRO:HB3	1:A:602:THR:HG21	1.64	0.80
2:D:314:TYR:CE1	3:F:673:PHE:CZ	2.70	0.80
1:B:310:THR:HG21	1:B:315:SER:HB3	1.63	0.80
1:A:140:PHE:CE1	1:A:588:ARG:HA	2.17	0.80
1:B:309:TYR:HE2	1:B:325:ARG:HA	1.47	0.79
1:B:150:ASN:HA	1:B:153:VAL:HG12	1.64	0.79
2:C:247:PRO:HG3	3:E:674:HIS:CE1	2.13	0.79
2:C:314:TYR:CE1	3:E:673:PHE:CZ	2.70	0.79
1:B:759:GLU:OE2	3:F:500:PRO:CA	2.30	0.79
1:A:465:GLU:OE2	1:A:468:GLU:OE2	2.01	0.78
1:A:759:GLU:OE2	3:E:500:PRO:CB	2.31	0.78
1:B:496:VAL:HG11	1:B:506:ILE:HG21	1.65	0.78
1:A:280:LEU:HD12	1:A:337:ILE:HD13	1.66	0.78
1:B:140:PHE:CE1	1:B:588:ARG:HA	2.18	0.78
1:B:465:GLU:OE2	1:B:468:GLU:OE1	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ARG:HH11	1:A:646:ARG:HG2	1.46	0.78
1:B:623:ARG:CA	3:F:360:VAL:HG21	2.14	0.78
1:B:662:ASN:HA	2:D:72:LEU:CD2	2.14	0.78
1:B:662:ASN:HA	2:D:72:LEU:HD22	1.63	0.78
1:A:208:ARG:HD2	1:A:208:ARG:O	1.83	0.78
1:A:310:THR:HG21	1:A:315:SER:HB3	1.66	0.78
1:B:210:VAL:HG13	1:B:211:TYR:N	1.97	0.77
2:D:94:PHE:HD1	3:F:675:LYS:HB2	1.46	0.77
1:A:310:THR:OG1	1:A:310:THR:O	2.00	0.77
1:B:662:ASN:O	2:D:72:LEU:CA	2.32	0.77
1:B:664:GLU:CD	2:D:74:PRO:CD	2.53	0.77
1:B:664:GLU:OE2	2:D:74:PRO:CD	2.28	0.77
1:A:188:VAL:CG2	1:A:386:ILE:HD11	2.15	0.77
1:A:623:ARG:CA	3:E:360:VAL:CG2	2.62	0.77
1:B:518:THR:HG22	1:B:520:GLN:H	1.50	0.76
1:A:496:VAL:HG11	1:A:506:ILE:HG21	1.65	0.76
1:B:685:PHE:O	1:B:700:VAL:HG22	1.84	0.76
1:A:309:TYR:HE2	1:A:325:ARG:HA	1.50	0.76
1:A:623:ARG:HE	3:E:356:ASP:CA	1.98	0.76
1:B:232:LEU:HD22	1:B:373:VAL:HG11	1.68	0.76
1:A:310:THR:O	1:A:468:GLU:OE1	2.04	0.76
1:A:150:ASN:HA	1:A:153:VAL:HG12	1.69	0.75
1:B:664:GLU:OE2	2:D:74:PRO:HD3	1.86	0.75
1:A:465:GLU:CD	1:A:468:GLU:OE2	2.25	0.75
1:B:238:GLY:HA3	1:B:267:LYS:HG2	1.67	0.75
2:D:317:TYR:HE1	3:F:383:ASN:CB	1.64	0.75
1:A:640:GLN:HE22	3:E:349:HIS:CE1	2.04	0.74
2:C:317:TYR:CE1	3:E:383:ASN:HB3	2.21	0.74
2:C:94:PHE:HD1	3:E:675:LYS:HB2	1.46	0.74
1:A:220:VAL:HG21	1:A:334:VAL:HG12	1.69	0.74
1:B:318:HIS:O	1:B:322:PRO:HB3	1.88	0.74
1:B:646:ARG:HH22	3:F:352:ARG:NH2	1.70	0.74
1:A:191:GLN:HE22	1:A:223:SER:H	1.34	0.74
1:A:662:ASN:O	2:C:72:LEU:C	2.26	0.74
2:C:313:MET:HG2	3:E:670:ALA:HB1	1.69	0.74
1:A:278:GLY:H	1:A:332:ILE:HG23	1.53	0.74
1:A:662:ASN:OD1	2:C:71:TYR:OH	2.06	0.74
1:A:623:ARG:HE	3:E:356:ASP:C	1.91	0.74
1:B:295:LEU:HD21	1:B:568:THR:HG21	1.71	0.73
2:D:313:MET:HG2	3:F:670:ALA:HB1	1.69	0.73
3:F:407:VAL:HG13	3:F:408:LEU:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ARG:HD2	3:E:360:VAL:CB	2.18	0.73
1:B:191:GLN:HE22	1:B:223:SER:H	1.33	0.73
1:A:188:VAL:HG21	1:A:386:ILE:HD11	1.70	0.73
1:A:518:THR:HG22	1:A:520:GLN:H	1.54	0.73
2:C:94:PHE:CE1	3:E:675:LYS:CB	2.71	0.73
1:A:183:ARG:O	1:B:758:ASN:HB2	1.87	0.73
1:A:623:ARG:CZ	3:E:360:VAL:N	2.44	0.73
1:B:407:ALA:HB3	1:B:426:LEU:HD12	1.70	0.73
2:D:317:TYR:CE1	3:F:383:ASN:HB3	2.21	0.73
3:E:643:THR:HB	3:E:646:LYS:HD2	1.71	0.73
1:A:623:ARG:CZ	3:E:360:VAL:H	2.00	0.73
1:B:310:THR:OG1	1:B:310:THR:O	2.03	0.73
3:E:357:GLU:HG2	3:E:616:PHE:CE1	2.24	0.73
3:F:343:LYS:HD3	3:F:367:GLU:HB3	1.71	0.73
3:E:343:LYS:HD3	3:E:367:GLU:HB3	1.71	0.73
1:A:295:LEU:HD21	1:A:568:THR:HG21	1.70	0.72
3:E:407:VAL:HG13	3:E:408:LEU:N	2.03	0.72
1:A:232:LEU:HD22	1:A:373:VAL:HG11	1.70	0.72
1:B:183:ARG:NH1	1:B:387:LEU:HD21	2.04	0.72
1:B:229:THR:HB	1:B:374:LYS:HG3	1.70	0.72
3:F:357:GLU:HG2	3:F:616:PHE:CE1	2.23	0.72
1:A:212:LEU:HD21	1:A:215:ASN:HD21	1.55	0.72
3:F:643:THR:HB	3:F:646:LYS:HD2	1.71	0.72
1:A:318:HIS:O	1:A:322:PRO:HB3	1.90	0.72
3:F:418:LYS:O	3:F:639:ARG:NH2	2.23	0.72
1:A:685:PHE:O	1:A:700:VAL:HG22	1.90	0.71
1:A:515:HIS:HD2	1:A:517:VAL:H	1.37	0.71
1:A:643:TYR:HB2	3:E:349:HIS:NE2	2.04	0.71
1:B:278:GLY:H	1:B:332:ILE:HG23	1.53	0.71
1:A:663:ALA:HA	2:C:73:ALA:O	1.90	0.71
1:B:229:THR:HB	1:B:374:LYS:CG	2.21	0.71
1:A:397:VAL:C	1:A:399:PRO:HD3	2.10	0.71
1:B:732:ARG:HH11	1:B:732:ARG:HG3	1.55	0.71
1:A:740:TRP:CZ2	1:B:314:PRO:HB2	2.25	0.71
3:E:453:VAL:HG13	3:E:485:PRO:O	1.91	0.71
1:A:407:ALA:HB3	1:A:426:LEU:HD12	1.72	0.71
1:B:341:ALA:O	1:B:345:LEU:HD23	1.91	0.71
3:E:418:LYS:O	3:E:639:ARG:NH2	2.23	0.71
3:E:480:ARG:NH1	3:E:480:ARG:HA	2.05	0.71
3:F:480:ARG:HA	3:F:480:ARG:NH1	2.05	0.71
1:B:297:PHE:O	1:B:336:THR:HG21	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:PHE:CE1	3:F:675:LYS:CB	2.71	0.71
1:B:515:HIS:HD2	1:B:517:VAL:H	1.38	0.70
1:A:229:THR:HB	1:A:374:LYS:HG3	1.71	0.70
1:A:623:ARG:CZ	3:E:356:ASP:O	2.37	0.70
1:A:708:THR:CG2	1:A:710:PRO:HD2	2.21	0.70
1:B:305:THR:HG23	1:B:464:THR:HG21	1.71	0.70
1:B:397:VAL:C	1:B:399:PRO:HD3	2.12	0.70
1:B:465:GLU:CD	1:B:468:GLU:OE2	2.29	0.70
1:B:625:LEU:HD21	1:B:639:LEU:HD11	1.73	0.70
1:A:229:THR:HB	1:A:374:LYS:CG	2.21	0.70
1:A:623:ARG:NH1	3:E:360:VAL:H	1.89	0.70
1:A:623:ARG:CD	3:E:356:ASP:O	2.39	0.69
1:B:623:ARG:HB3	3:F:360:VAL:HG21	1.66	0.69
1:B:398:GLU:HB2	1:B:446:ARG:HG2	1.72	0.69
3:F:453:VAL:HG13	3:F:485:PRO:O	1.91	0.69
1:A:130:LYS:HE2	1:A:440:ASP:OD1	1.92	0.69
1:A:239:THR:HB	1:A:244:GLU:CG	2.22	0.69
1:A:623:ARG:NE	3:E:356:ASP:C	2.46	0.69
1:B:188:VAL:CG2	1:B:386:ILE:HD11	2.21	0.69
1:B:643:TYR:CZ	3:F:353:LEU:HD22	2.25	0.69
1:A:349:MET:HG2	1:A:367:THR:HA	1.73	0.69
1:B:351:GLY:O	1:B:364:ARG:HD3	1.93	0.69
1:B:542:PHE:HB3	1:B:543:PRO:HD3	1.75	0.69
1:A:183:ARG:NH1	1:A:387:LEU:HD21	2.08	0.69
1:A:732:ARG:HG3	1:A:732:ARG:HH11	1.58	0.69
1:A:623:ARG:HB3	3:E:360:VAL:HG22	0.70	0.69
1:B:150:ASN:HA	1:B:153:VAL:CG1	2.22	0.69
1:B:623:ARG:CZ	3:F:356:ASP:O	2.41	0.69
1:B:204:ASP:C	1:B:206:ASN:H	1.95	0.69
1:B:213:VAL:HG11	1:B:345:LEU:HD21	1.74	0.69
1:B:220:VAL:HG21	1:B:334:VAL:HG12	1.75	0.69
2:C:313:MET:CG	3:E:670:ALA:HB1	2.22	0.69
3:E:375:GLU:OE2	3:E:665:SER:OG	2.06	0.69
1:A:488:VAL:O	1:A:489:LEU:HD12	1.94	0.68
1:A:629:ARG:HH22	3:E:357:GLU:HB2	1.58	0.68
1:B:310:THR:O	1:B:468:GLU:OE1	2.11	0.68
1:A:214:GLU:O	1:A:216:PRO:HD3	1.94	0.68
1:B:313:PHE:O	1:B:468:GLU:OE1	2.12	0.68
1:A:623:ARG:HE	3:E:356:ASP:HA	1.58	0.68
1:A:640:GLN:NE2	3:E:349:HIS:CE1	2.62	0.68
1:B:167:LEU:HD22	1:B:183:ARG:HH22	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:GLY:HA3	1:B:267:LYS:CG	2.22	0.68
1:B:232:LEU:HB3	1:B:367:THR:HG23	1.76	0.68
1:A:398:GLU:HB2	1:A:446:ARG:HG2	1.75	0.68
1:A:626:ASN:HB3	1:A:629:ARG:HH21	1.58	0.68
1:B:506:ILE:O	1:B:510:MET:HG3	1.93	0.68
1:A:297:PHE:O	1:A:336:THR:HG21	1.94	0.67
1:B:183:ARG:HH12	1:B:387:LEU:HD21	1.58	0.67
1:A:330:PRO:O	1:A:331:ASN:HB3	1.93	0.67
1:A:759:GLU:OE2	3:E:500:PRO:HA	1.93	0.67
2:D:317:TYR:HH	3:F:383:ASN:HA	1.55	0.67
1:B:465:GLU:OE2	1:B:468:GLU:OE2	2.12	0.67
1:A:254:ILE:HA	1:A:277:ILE:O	1.95	0.67
3:E:347:LEU:O	3:E:348:GLY:O	2.13	0.67
1:B:330:PRO:O	1:B:331:ASN:HB3	1.94	0.67
1:B:254:ILE:HA	1:B:277:ILE:O	1.94	0.67
1:A:643:TYR:CB	3:E:349:HIS:NE2	2.58	0.67
1:B:239:THR:HB	1:B:244:GLU:CG	2.24	0.67
1:B:307:ASP:HB3	1:B:465:GLU:OE1	1.94	0.67
3:F:347:LEU:O	3:F:348:GLY:O	2.13	0.67
1:A:140:PHE:O	1:A:144:ILE:HG13	1.94	0.66
1:B:208:ARG:HG2	1:B:208:ARG:O	1.94	0.66
1:B:309:TYR:CE2	1:B:325:ARG:HA	2.28	0.66
1:B:646:ARG:NH2	3:F:352:ARG:CZ	2.57	0.66
2:D:313:MET:CG	3:F:670:ALA:HB1	2.22	0.66
1:A:629:ARG:CZ	3:E:357:GLU:OE1	2.43	0.66
1:A:686:LEU:HD23	1:A:699:HIS:CA	2.25	0.66
1:B:349:MET:HG2	1:B:367:THR:HA	1.76	0.66
1:B:353:CYS:HB2	1:B:363:CYS:O	1.95	0.66
2:D:317:TYR:OH	3:F:383:ASN:CB	2.43	0.66
1:A:155:ARG:HH21	1:A:165:LEU:HD22	1.60	0.66
1:A:351:GLY:O	1:A:364:ARG:HD3	1.95	0.66
1:B:188:VAL:HG21	1:B:386:ILE:HD11	1.76	0.66
2:D:313:MET:HG3	3:F:670:ALA:CB	2.26	0.66
1:A:337:ILE:HG23	1:A:341:ALA:HB3	1.76	0.66
1:A:490:GLY:HA3	1:A:559:GLU:HG2	1.76	0.66
1:A:311:PRO:O	1:A:693:LYS:HA	1.96	0.66
1:A:341:ALA:O	1:A:345:LEU:HD23	1.95	0.66
1:B:140:PHE:O	1:B:144:ILE:HG13	1.96	0.66
1:A:651:ARG:NH2	3:E:372:GLU:HG2	2.11	0.66
1:B:300:HIS:HE2	1:B:459:GLY:CA	2.07	0.66
1:A:232:LEU:HD21	1:A:256:ILE:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:GLU:CG	3:E:500:PRO:HB3	2.25	0.66
1:B:626:ASN:HB3	1:B:629:ARG:HH21	1.62	0.66
1:B:337:ILE:HG23	1:B:341:ALA:HB3	1.77	0.65
1:B:623:ARG:HH11	3:F:360:VAL:N	1.86	0.65
1:B:759:GLU:CG	3:F:500:PRO:HB3	2.26	0.65
3:E:499:GLY:HA3	3:E:509:GLU:HA	1.79	0.65
1:A:664:GLU:CD	1:A:664:GLU:H	2.00	0.65
1:B:623:ARG:NH1	3:F:360:VAL:CA	2.59	0.65
2:C:317:TYR:OH	3:E:383:ASN:CB	2.43	0.65
3:F:407:VAL:HG13	3:F:408:LEU:H	1.60	0.65
1:A:625:LEU:HD21	1:A:639:LEU:HD11	1.79	0.65
3:F:375:GLU:OE2	3:F:665:SER:OG	2.06	0.65
1:B:686:LEU:HD23	1:B:699:HIS:CA	2.26	0.65
1:A:150:ASN:HA	1:A:153:VAL:CG1	2.26	0.65
1:B:640:GLN:NE2	3:F:349:HIS:CE1	2.64	0.65
1:A:240:LYS:C	1:A:242:ASP:H	2.00	0.65
1:A:309:TYR:CE2	1:A:325:ARG:HA	2.30	0.65
1:B:359:THR:HG22	1:B:360:ASP:N	2.03	0.65
1:A:183:ARG:HH12	1:A:387:LEU:HD21	1.61	0.64
1:A:359:THR:HG22	1:A:360:ASP:N	2.06	0.64
1:A:353:CYS:HB2	1:A:363:CYS:O	1.97	0.64
1:B:130:LYS:HE2	1:B:440:ASP:OD1	1.97	0.64
1:B:229:THR:HB	1:B:374:LYS:CB	2.27	0.64
1:B:664:GLU:CD	1:B:664:GLU:H	2.01	0.64
1:A:246:LEU:HD12	1:A:247:TYR:N	2.12	0.64
3:F:499:GLY:HA3	3:F:509:GLU:HA	1.79	0.64
1:A:232:LEU:HD11	1:A:256:ILE:HG13	1.79	0.64
1:A:465:GLU:OE2	1:A:468:GLU:OE1	2.16	0.64
1:B:139:ASP:OD1	1:B:141:THR:HG22	1.97	0.64
1:B:201:ILE:HD13	1:B:212:LEU:HA	1.80	0.64
1:A:238:GLY:O	1:A:240:LYS:N	2.29	0.64
1:B:191:GLN:NE2	1:B:223:SER:H	1.95	0.64
1:A:661:GLY:O	2:C:72:LEU:HD22	1.96	0.64
3:E:407:VAL:HG13	3:E:408:LEU:H	1.60	0.64
1:A:232:LEU:HB3	1:A:367:THR:HG23	1.78	0.64
1:B:238:GLY:O	1:B:240:LYS:N	2.31	0.64
1:B:349:MET:HB3	1:B:366:VAL:O	1.98	0.64
2:C:313:MET:HG3	3:E:670:ALA:CB	2.26	0.64
1:A:758:ASN:N	1:A:758:ASN:HD22	1.96	0.63
1:A:238:GLY:HA3	1:A:267:LYS:HG2	1.79	0.63
1:A:488:VAL:C	1:A:489:LEU:HD12	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:HE2	1:A:440:ASP:CG	2.19	0.63
1:A:204:ASP:C	1:A:206:ASN:H	2.02	0.63
1:A:515:HIS:CD2	1:A:517:VAL:H	2.16	0.63
1:A:654:SER:O	1:A:657:THR:HG22	1.98	0.63
1:A:349:MET:HB3	1:A:366:VAL:O	1.99	0.63
1:A:623:ARG:CG	3:E:360:VAL:HG22	2.11	0.63
1:A:629:ARG:NH2	3:E:357:GLU:OE1	2.32	0.63
1:A:664:GLU:OE1	1:A:667:ASP:HB2	1.99	0.63
1:A:686:LEU:HD23	1:A:699:HIS:HA	1.79	0.63
1:B:167:LEU:CD2	1:B:183:ARG:HH22	2.11	0.63
1:A:238:GLY:HA3	1:A:267:LYS:CG	2.29	0.63
1:B:716:LEU:HD13	1:B:731:PHE:CE1	2.33	0.63
1:A:156:GLU:HG2	1:A:157:ALA:H	1.64	0.63
1:B:220:VAL:CG1	1:B:301:ALA:HB2	2.28	0.63
2:C:317:TYR:HE1	3:E:383:ASN:HB2	0.81	0.63
1:A:191:GLN:NE2	1:A:223:SER:H	1.97	0.63
1:A:210:VAL:HG22	1:A:211:TYR:H	1.63	0.63
1:B:708:THR:CG2	1:B:710:PRO:HD2	2.28	0.63
3:F:476:ASP:HB2	3:F:492:SER:OG	1.99	0.63
1:A:209:LEU:HG	1:A:210:VAL:N	2.11	0.63
1:B:324:SER:HB3	1:B:325:ARG:HE	1.64	0.63
1:A:555:PHE:CE2	1:A:593:VAL:HG23	2.34	0.63
2:D:313:MET:HG2	3:F:670:ALA:HB2	1.51	0.63
1:A:167:LEU:HD22	1:A:183:ARG:HH22	1.64	0.62
1:A:506:ILE:O	1:A:510:MET:HG3	2.00	0.62
1:B:152:TYR:HA	1:B:161:LYS:HE2	1.81	0.62
1:B:446:ARG:HD2	1:B:479:PHE:CE2	2.34	0.62
1:B:488:VAL:O	1:B:489:LEU:HD12	1.99	0.62
1:B:664:GLU:OE1	1:B:667:ASP:HB2	1.99	0.62
3:E:476:ASP:HB2	3:E:492:SER:OG	1.99	0.62
1:B:200:VAL:HG23	1:B:213:VAL:HB	1.79	0.62
1:B:348:ASN:N	1:B:348:ASN:HD22	1.97	0.62
1:B:758:ASN:N	1:B:758:ASN:HD22	1.97	0.62
1:A:539:ASN:HD22	1:A:540:ALA:N	1.97	0.62
1:A:542:PHE:HB3	1:A:543:PRO:HD3	1.80	0.62
1:A:662:ASN:C	2:C:73:ALA:H	2.02	0.62
1:B:349:MET:HB2	1:B:364:ARG:CG	2.27	0.62
1:B:155:ARG:HH21	1:B:165:LEU:HD22	1.64	0.62
1:B:686:LEU:HD23	1:B:699:HIS:HA	1.82	0.62
1:B:690:VAL:HG23	1:B:698:ARG:HG2	1.81	0.62
1:A:229:THR:HB	1:A:374:LYS:CB	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLU:HG2	1:B:157:ALA:H	1.64	0.62
1:B:238:GLY:C	1:B:240:LYS:H	2.03	0.62
1:B:625:LEU:CD2	1:B:639:LEU:HD11	2.28	0.62
1:B:623:ARG:CA	3:F:360:VAL:CG2	2.70	0.62
1:B:236:ASN:OD1	1:B:258:ARG:HD3	2.00	0.62
1:B:123:TYR:HB3	2:D:144:LYS:O	1.98	0.62
1:B:515:HIS:CD2	1:B:517:VAL:H	2.18	0.62
1:A:236:ASN:OD1	1:A:258:ARG:HD3	2.00	0.61
1:B:188:VAL:HG21	1:B:461:VAL:HG11	1.82	0.61
1:B:280:LEU:HD12	1:B:337:ILE:CD1	2.30	0.61
1:B:623:ARG:HH11	3:F:360:VAL:CA	2.12	0.61
1:A:446:ARG:H	1:A:602:THR:CG2	2.13	0.61
1:B:490:GLY:HA3	1:B:559:GLU:HG2	1.82	0.61
1:A:446:ARG:HD2	1:A:479:PHE:CE2	2.34	0.61
1:B:194:ASP:HB3	1:B:378:SER:O	2.00	0.61
1:B:246:LEU:HD12	1:B:247:TYR:N	2.16	0.61
1:A:139:ASP:OD1	1:A:141:THR:HG22	2.01	0.61
1:A:210:VAL:HG13	1:A:211:TYR:O	2.00	0.61
1:A:278:GLY:H	1:A:332:ILE:CG2	2.12	0.61
1:B:278:GLY:HA2	1:B:333:PRO:O	2.00	0.61
1:A:307:ASP:HB3	1:A:465:GLU:OE1	2.01	0.61
1:A:655:ARG:NH1	1:A:751:GLY:HA2	2.16	0.61
1:A:220:VAL:HG12	1:A:301:ALA:HB2	1.83	0.61
1:A:238:GLY:C	1:A:240:LYS:H	2.04	0.61
1:A:605:VAL:HG11	1:A:665:LYS:HB3	1.83	0.61
1:A:690:VAL:HG23	1:A:698:ARG:HG2	1.82	0.61
1:A:220:VAL:CG1	1:A:301:ALA:HB2	2.31	0.61
1:A:209:LEU:CG	1:A:210:VAL:H	2.07	0.61
1:B:623:ARG:HE	3:F:356:ASP:C	2.03	0.60
1:A:152:TYR:HA	1:A:161:LYS:HE2	1.84	0.60
1:A:167:LEU:CD2	1:A:183:ARG:HH22	2.14	0.60
1:A:191:GLN:HE22	1:A:223:SER:N	1.98	0.60
1:A:313:PHE:O	1:A:468:GLU:OE1	2.18	0.60
1:A:349:MET:HB2	1:A:364:ARG:CG	2.27	0.60
1:B:191:GLN:HE22	1:B:223:SER:N	1.98	0.60
1:B:654:SER:O	1:B:657:THR:HG22	2.01	0.60
1:A:336:THR:O	1:A:337:ILE:HD12	2.01	0.60
1:B:131:LEU:O	1:B:135:LEU:HD23	2.00	0.60
1:A:238:GLY:H	1:A:257:VAL:HB	1.65	0.60
1:B:368:SER:OG	1:B:371:LYS:HE2	2.01	0.60
1:A:348:ASN:HD22	1:A:348:ASN:N	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:MET:HA	1:A:367:THR:HA	1.83	0.60
1:B:256:ILE:HD11	1:B:349:MET:HE1	1.82	0.60
1:B:324:SER:CB	1:B:325:ARG:HE	2.15	0.60
2:D:317:TYR:HE1	3:F:383:ASN:HB2	0.81	0.60
1:B:403:VAL:HG22	1:B:479:PHE:CZ	2.37	0.60
2:D:249:HIS:CE1	2:D:296:LYS:HD2	2.37	0.60
1:B:623:ARG:HA	3:F:360:VAL:HG21	1.83	0.60
1:B:295:LEU:HD11	1:B:568:THR:OG1	2.01	0.60
1:B:759:GLU:OE2	3:F:500:PRO:HA	2.00	0.60
1:A:314:PRO:HB2	1:B:740:TRP:CZ2	2.37	0.60
1:B:588:ARG:HG3	1:B:588:ARG:HH11	1.67	0.60
1:A:131:LEU:O	1:A:135:LEU:HD23	2.01	0.60
1:B:130:LYS:O	1:B:134:LYS:HG2	2.02	0.60
3:E:643:THR:HG22	3:E:646:LYS:H	1.67	0.60
1:A:646:ARG:HG2	1:A:646:ARG:NH1	2.17	0.59
1:A:650:PHE:CE2	3:E:369:GLU:OE2	2.54	0.59
1:A:662:ASN:C	2:C:72:LEU:HB3	2.21	0.59
1:B:488:VAL:C	1:B:489:LEU:HD12	2.23	0.59
3:E:357:GLU:HG2	3:E:616:PHE:CD1	2.37	0.59
3:E:461:ILE:HB	3:E:462:PRO:HD3	1.84	0.59
3:F:357:GLU:HG2	3:F:616:PHE:CD1	2.37	0.59
3:F:643:THR:HG22	3:F:646:LYS:H	1.67	0.59
1:B:240:LYS:C	1:B:242:ASP:H	2.04	0.59
1:B:349:MET:HA	1:B:367:THR:HA	1.84	0.59
1:A:368:SER:OG	1:A:371:LYS:HE2	2.01	0.59
2:C:249:HIS:CE1	2:C:296:LYS:HD2	2.37	0.59
1:B:670:VAL:CG1	2:D:74:PRO:HB3	2.28	0.59
3:E:657:SER:HA	3:E:660:ARG:HG2	1.85	0.59
3:F:444:GLU:HG2	3:F:478:PHE:CE2	2.37	0.59
1:B:130:LYS:HE2	1:B:440:ASP:CG	2.23	0.59
1:A:345:LEU:O	1:A:349:MET:HG3	2.03	0.59
1:B:220:VAL:HG12	1:B:301:ALA:HB2	1.85	0.59
1:A:446:ARG:H	1:A:602:THR:HG23	1.68	0.59
1:B:167:LEU:HD22	1:B:183:ARG:NH2	2.17	0.59
1:B:278:GLY:H	1:B:332:ILE:CG2	2.16	0.59
1:B:646:ARG:HG2	1:B:646:ARG:NH1	2.11	0.59
2:C:315:LEU:O	3:E:674:HIS:CE1	2.55	0.59
3:F:461:ILE:HB	3:F:462:PRO:HD3	1.84	0.59
1:B:310:THR:OG1	1:B:465:GLU:OE2	2.20	0.59
1:B:662:ASN:O	2:D:72:LEU:C	2.40	0.59
1:A:515:HIS:CD2	1:A:516:PRO:HD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:PHE:CE2	1:B:444:PRO:HG3	2.38	0.58
2:D:314:TYR:O	3:F:673:PHE:CD2	2.56	0.58
1:A:298:PHE:HB2	1:A:412:TRP:CD2	2.38	0.58
3:E:444:GLU:HG2	3:E:478:PHE:CE2	2.37	0.58
1:A:237:PHE:CD2	1:A:258:ARG:HB2	2.38	0.58
1:A:670:VAL:CG1	2:C:74:PRO:HB3	2.29	0.58
1:B:664:GLU:C	1:B:666:THR:H	2.07	0.58
1:A:123:TYR:HB3	2:C:144:LYS:O	2.04	0.58
1:A:300:HIS:O	1:A:301:ALA:HB3	2.02	0.58
1:A:625:LEU:CD2	1:A:639:LEU:HD11	2.33	0.58
2:D:245:GLN:OE1	3:F:675:LYS:O	2.22	0.58
1:A:758:ASN:HD22	1:A:758:ASN:H	1.50	0.58
1:B:655:ARG:NH1	1:B:751:GLY:HA2	2.17	0.58
2:C:314:TYR:O	3:E:673:PHE:CD2	2.56	0.58
1:A:280:LEU:HD12	1:A:337:ILE:CD1	2.33	0.58
1:A:650:PHE:CZ	3:E:369:GLU:OE2	2.56	0.58
1:B:214:GLU:O	1:B:216:PRO:HD3	2.03	0.58
3:F:623:THR:CG2	3:F:624:LYS:N	2.55	0.58
1:B:496:VAL:HG11	1:B:506:ILE:CG2	2.34	0.58
2:C:245:GLN:OE1	3:E:675:LYS:O	2.22	0.58
1:A:237:PHE:HB2	1:A:243:PHE:HE1	1.69	0.57
1:A:307:ASP:H	1:A:461:VAL:HG13	1.68	0.57
1:B:345:LEU:O	1:B:349:MET:HG3	2.05	0.57
1:A:453:TRP:CD2	1:A:463:ALA:HB2	2.40	0.57
3:F:657:SER:HA	3:F:660:ARG:HG2	1.85	0.57
1:A:662:ASN:HA	2:C:72:LEU:HD23	1.86	0.57
1:A:672:LYS:HD3	1:A:676:ASP:OD2	2.05	0.57
1:B:237:PHE:HB2	1:B:243:PHE:HE1	1.67	0.57
1:A:699:HIS:HD2	1:A:702:TRP:H	1.51	0.57
1:B:268:VAL:HG21	1:B:334:VAL:HG21	1.86	0.57
1:B:555:PHE:CE2	1:B:593:VAL:HG23	2.39	0.57
1:B:643:TYR:CG	3:F:353:LEU:CD2	2.66	0.57
1:A:339:ARG:O	1:A:343:GLU:HG2	2.05	0.57
1:B:623:ARG:NE	3:F:360:VAL:H	2.02	0.57
3:E:333:ASP:O	3:E:335:LEU:N	2.38	0.57
3:E:424:GLY:HA2	3:E:581:ASN:OD1	2.05	0.57
3:F:333:ASP:O	3:F:335:LEU:N	2.38	0.57
3:F:424:GLY:HA2	3:F:581:ASN:OD1	2.05	0.57
1:A:324:SER:HB3	1:A:325:ARG:HE	1.68	0.57
1:A:719:ARG:HG3	1:A:719:ARG:HH11	1.68	0.57
1:B:238:GLY:O	1:B:262:ILE:HD11	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:OE2	1:B:330:PRO:O	2.23	0.57
1:B:446:ARG:H	1:B:602:THR:HG23	1.70	0.57
1:A:238:GLY:O	1:A:262:ILE:HD11	2.05	0.57
1:A:403:VAL:HG22	1:A:479:PHE:CZ	2.40	0.57
1:B:237:PHE:CD2	1:B:258:ARG:HB2	2.40	0.57
1:B:286:THR:CG2	1:B:360:ASP:HB2	2.35	0.57
1:B:618:LEU:HD11	1:B:742:ILE:HD13	1.87	0.57
1:A:202:ILE:HB	1:A:210:VAL:HG11	1.86	0.57
1:A:298:PHE:HE2	1:A:457:ASP:HB3	1.70	0.57
1:A:238:GLY:N	1:A:257:VAL:HB	2.20	0.56
1:A:264:PHE:CE2	1:A:281:ILE:HG21	2.39	0.56
1:B:426:LEU:CD2	1:B:450:PHE:HB3	2.31	0.56
1:B:661:GLY:O	2:D:72:LEU:HD22	2.05	0.56
1:B:719:ARG:HD3	1:B:726:PHE:CD2	2.40	0.56
1:A:433:PHE:O	1:A:437:VAL:HG23	2.04	0.56
1:B:239:THR:C	1:B:241:LYS:H	2.08	0.56
3:F:407:VAL:CG1	3:F:408:LEU:H	2.18	0.56
3:F:615:LYS:HG2	3:F:616:PHE:N	2.20	0.56
1:A:256:ILE:HD11	1:A:349:MET:HE1	1.86	0.56
1:A:670:VAL:O	1:A:674:LEU:HG	2.05	0.56
1:B:663:ALA:HA	2:D:73:ALA:O	2.05	0.56
1:B:756:ILE:HG22	1:B:756:ILE:O	2.04	0.56
3:F:607:ASN:OD1	3:F:608:THR:N	2.39	0.56
1:A:300:HIS:HE2	1:A:459:GLY:CA	2.18	0.56
3:E:615:LYS:HG2	3:E:616:PHE:N	2.20	0.56
1:A:167:LEU:HD22	1:A:183:ARG:NH2	2.20	0.56
1:A:268:VAL:HG21	1:A:334:VAL:HG21	1.87	0.56
1:A:324:SER:CB	1:A:325:ARG:HE	2.19	0.56
1:A:749:LEU:O	1:A:750:SER:CB	2.53	0.56
1:B:758:ASN:HD22	1:B:758:ASN:H	1.52	0.56
1:A:398:GLU:N	1:A:399:PRO:HD3	2.21	0.56
2:D:315:LEU:O	3:F:674:HIS:CE1	2.55	0.56
3:E:592:ALA:O	3:E:593:CYS:C	2.43	0.56
3:E:607:ASN:OD1	3:E:608:THR:N	2.39	0.56
1:B:646:ARG:HH22	3:F:352:ARG:HE	1.53	0.56
1:A:719:ARG:HD3	1:A:726:PHE:CD2	2.41	0.56
1:B:565:TYR:CE1	1:B:575:GLU:HB3	2.41	0.56
1:A:426:LEU:CD2	1:A:450:PHE:HB3	2.34	0.56
1:B:752:ASP:O	1:B:753:VAL:HB	2.06	0.56
1:A:272:GLU:OE2	1:A:330:PRO:O	2.23	0.55
1:A:756:ILE:HG22	1:A:756:ILE:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:HIS:O	1:B:301:ALA:HB3	2.06	0.55
3:E:407:VAL:CG1	3:E:408:LEU:H	2.18	0.55
3:E:407:VAL:CG1	3:E:408:LEU:N	2.68	0.55
1:A:232:LEU:HB3	1:A:367:THR:CG2	2.36	0.55
1:A:623:ARG:HD2	3:E:360:VAL:H	1.71	0.55
1:A:654:SER:HA	1:A:657:THR:HG22	1.89	0.55
1:A:664:GLU:C	1:A:666:THR:H	2.08	0.55
1:A:623:ARG:HD2	3:E:360:VAL:HG23	0.57	0.55
1:B:232:LEU:HB3	1:B:367:THR:CG2	2.35	0.55
1:B:676:ASP:O	1:B:680:ARG:HG3	2.06	0.55
1:B:749:LEU:O	1:B:750:SER:CB	2.55	0.55
1:B:756:ILE:H	1:B:756:ILE:HD12	1.71	0.55
1:A:194:ASP:HB3	1:A:378:SER:O	2.05	0.55
1:A:619:LEU:HD23	1:A:620:SER:N	2.22	0.55
1:B:336:THR:O	1:B:337:ILE:HD12	2.05	0.55
1:B:680:ARG:HB3	1:B:684:HIS:HD2	1.70	0.55
1:A:442:PHE:CE2	1:A:444:PRO:HG3	2.40	0.55
1:A:565:TYR:CE1	1:A:575:GLU:HB3	2.42	0.55
1:A:680:ARG:HB3	1:A:684:HIS:HD2	1.71	0.55
1:B:238:GLY:H	1:B:257:VAL:HB	1.72	0.55
1:A:286:THR:CG2	1:A:360:ASP:HB2	2.36	0.55
1:A:607:LEU:CD1	1:A:609:LEU:HG	2.36	0.55
1:B:446:ARG:H	1:B:602:THR:CG2	2.20	0.55
2:C:63:ASP:HA	2:C:249:HIS:CD2	2.42	0.55
1:A:453:TRP:CG	1:A:463:ALA:HB2	2.41	0.55
1:B:156:GLU:HG2	1:B:157:ALA:N	2.22	0.55
1:B:197:GLN:HE21	1:B:215:ASN:HB3	1.71	0.55
1:B:135:LEU:HD22	1:B:432:MET:SD	2.47	0.54
1:B:699:HIS:HD2	1:B:702:TRP:H	1.55	0.54
2:D:85:TYR:CE2	2:D:248[B]:SER:HB3	2.43	0.54
1:A:156:GLU:HG2	1:A:157:ALA:N	2.22	0.54
1:A:335:GLN:NE2	1:A:336:THR:HG22	2.23	0.54
1:A:425:LEU:HD22	1:A:591:ALA:HB2	1.88	0.54
1:B:222:TYR:HB3	1:B:329:LEU:HD23	1.89	0.54
1:B:398:GLU:N	1:B:399:PRO:HD3	2.22	0.54
1:B:646:ARG:HH22	3:F:352:ARG:CZ	2.18	0.54
3:F:407:VAL:CG1	3:F:408:LEU:N	2.68	0.54
1:A:237:PHE:CD1	1:A:261:LYS:HG3	2.42	0.54
2:C:85:TYR:CE2	2:C:248[B]:SER:HB3	2.42	0.54
2:C:317:TYR:OH	3:E:383:ASN:HB2	2.02	0.54
3:F:588:LYS:O	3:F:589:ASP:C	2.44	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD22	1:A:599:ILE:HD11	1.90	0.54
1:A:654:SER:C	1:A:657:THR:HG22	2.28	0.54
1:B:539:ASN:HD22	1:B:540:ALA:N	2.04	0.54
1:A:239:THR:C	1:A:241:LYS:H	2.10	0.54
1:A:278:GLY:HA2	1:A:333:PRO:O	2.08	0.54
1:B:654:SER:HA	1:B:657:THR:HG22	1.89	0.54
1:B:759:GLU:HG3	1:B:760:PHE:N	2.22	0.54
1:B:201:ILE:HB	1:B:212:LEU:HD12	1.90	0.54
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.88	0.54
3:E:362:SER:O	3:E:365:LEU:HD12	2.08	0.54
3:F:377:CYS:HB3	3:F:389:MET:SD	2.48	0.54
1:A:588:ARG:HG3	1:A:588:ARG:HH11	1.73	0.54
1:B:240:LYS:HA	1:B:262:ILE:HD13	1.90	0.54
1:B:580:ILE:HG23	1:B:580:ILE:O	2.08	0.54
1:A:306:GLY:HA2	1:A:461:VAL:CA	2.34	0.54
1:A:540:ALA:O	1:A:543:PRO:HD2	2.08	0.54
1:B:623:ARG:HH11	3:F:360:VAL:HA	1.72	0.54
3:E:377:CYS:HB3	3:E:389:MET:SD	2.47	0.54
1:A:471:LEU:HD13	1:A:547:TYR:OH	2.07	0.54
1:B:232:LEU:HD11	1:B:256:ILE:HG13	1.90	0.54
2:D:63:ASP:HA	2:D:249:HIS:CD2	2.42	0.54
3:F:362:SER:O	3:F:365:LEU:HD12	2.08	0.54
1:B:206:ASN:O	1:B:207:GLY:O	2.27	0.53
1:B:719:ARG:HG3	1:B:719:ARG:HH11	1.70	0.53
3:E:481:GLN:HE21	3:E:495:GLU:HB3	1.73	0.53
1:A:188:VAL:HG22	1:A:386:ILE:HD11	1.91	0.53
1:A:667:ASP:OD1	1:A:669:PHE:HB3	2.09	0.53
1:B:190:ILE:HG13	1:B:458:PHE:CD2	2.43	0.53
1:B:298:PHE:HE2	1:B:457:ASP:HB3	1.74	0.53
1:B:309:TYR:HE2	1:B:325:ARG:CA	2.21	0.53
1:B:347:GLY:C	1:B:348:ASN:HD22	2.11	0.53
1:B:618:LEU:HD13	1:B:701:PHE:HZ	1.72	0.53
1:B:623:ARG:HE	3:F:356:ASP:CA	2.21	0.53
1:A:743:GLN:O	1:A:746:ALA:HB3	2.09	0.53
3:E:588:LYS:O	3:E:589:ASP:C	2.44	0.53
1:A:232:LEU:CD2	1:A:256:ILE:HD11	2.38	0.53
1:A:513:VAL:HG21	1:A:593:VAL:HG12	1.89	0.53
1:B:502:LEU:O	1:B:506:ILE:HG13	2.08	0.53
1:B:756:ILE:HD12	1:B:756:ILE:N	2.24	0.53
3:E:452:ALA:HB3	3:E:455:ARG:HD3	1.91	0.53
3:F:481:GLN:HE21	3:F:495:GLU:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:GLY:C	1:A:348:ASN:HD22	2.11	0.53
3:E:623:THR:CG2	3:E:624:LYS:N	2.55	0.53
3:F:592:ALA:O	3:F:593:CYS:C	2.43	0.53
1:A:496:VAL:CG1	1:A:506:ILE:HD13	2.39	0.53
1:B:237:PHE:CD1	1:B:261:LYS:HG3	2.43	0.53
3:E:498:VAL:HG23	3:E:499:GLY:N	2.24	0.53
1:A:155:ARG:HA	1:A:161:LYS:HB2	1.90	0.53
1:A:197:GLN:HE21	1:A:215:ASN:HB3	1.74	0.53
1:A:295:LEU:HD11	1:A:568:THR:OG1	2.08	0.53
1:A:453:TRP:CE3	1:A:463:ALA:HA	2.44	0.53
1:A:623:ARG:HH12	3:E:359:SER:C	2.08	0.53
1:A:629:ARG:HH22	3:E:357:GLU:CD	2.10	0.53
1:A:752:ASP:O	1:A:753:VAL:HB	2.09	0.53
1:B:339:ARG:O	1:B:343:GLU:HG2	2.09	0.53
1:B:515:HIS:CD2	1:B:516:PRO:HD2	2.44	0.53
1:A:719:ARG:HH11	1:A:719:ARG:CG	2.22	0.53
1:B:210:VAL:CG1	1:B:211:TYR:H	2.02	0.53
1:B:498:ALA:HB2	1:B:553:VAL:HA	1.91	0.53
1:A:236:ASN:HB2	1:A:357:TRP:CD1	2.44	0.53
1:B:212:LEU:O	1:B:213:VAL:C	2.47	0.53
1:B:236:ASN:HB2	1:B:357:TRP:CD1	2.44	0.53
1:B:311:PRO:O	1:B:693:LYS:HA	2.08	0.53
1:B:523:TYR:HE1	1:B:530:SER:OG	1.91	0.53
1:B:719:ARG:HH11	1:B:719:ARG:CG	2.22	0.53
1:A:488:VAL:HG13	1:A:586:VAL:HG11	1.90	0.52
1:B:123:TYR:CB	2:D:144:LYS:O	2.57	0.52
1:B:619:LEU:HD23	1:B:620:SER:N	2.23	0.52
3:F:621:SER:HB3	3:F:630:ASP:OD1	2.10	0.52
1:A:212:LEU:CD2	1:A:215:ASN:HD21	2.21	0.52
1:A:515:HIS:CD2	1:A:516:PRO:CD	2.92	0.52
1:B:471:LEU:HD13	1:B:547:TYR:OH	2.08	0.52
1:B:539:ASN:O	1:B:542:PHE:N	2.39	0.52
2:C:317:TYR:CE2	3:E:383:ASN:HA	2.38	0.52
1:A:496:VAL:HG11	1:A:506:ILE:CG2	2.35	0.52
1:B:409:ARG:NH2	1:B:454:SER:HB2	2.24	0.52
1:B:513:VAL:HG21	1:B:593:VAL:HG12	1.90	0.52
1:A:473:SER:O	1:A:476:LEU:HB2	2.09	0.52
1:A:618:LEU:HD11	1:A:742:ILE:HD13	1.92	0.52
1:B:672:LYS:HD3	1:B:676:ASP:OD2	2.08	0.52
1:A:135:LEU:HD22	1:A:432:MET:SD	2.50	0.52
1:A:256:ILE:CD1	1:A:349:MET:HE1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ASN:CB	1:B:183:ARG:O	2.55	0.52
1:B:155:ARG:HA	1:B:161:LYS:HB2	1.91	0.52
1:B:540:ALA:O	1:B:543:PRO:HD2	2.10	0.52
3:E:382:MET:SD	3:E:402:CYS:HB3	2.50	0.52
1:A:130:LYS:O	1:A:134:LYS:HG2	2.10	0.52
1:A:502:LEU:O	1:A:506:ILE:HG13	2.10	0.52
1:B:564:PRO:HG2	1:B:565:TYR:H	1.74	0.52
1:B:565:TYR:HE1	1:B:575:GLU:HB3	1.75	0.52
3:F:452:ALA:HB3	3:F:455:ARG:HD3	1.91	0.52
1:B:201:ILE:HD12	1:B:202:ILE:N	2.25	0.52
1:B:306:GLY:HA2	1:B:461:VAL:CA	2.32	0.52
3:E:621:SER:HB3	3:E:630:ASP:OD1	2.10	0.52
3:F:498:VAL:HG23	3:F:499:GLY:N	2.24	0.52
1:A:145:LYS:O	1:A:148:ASN:HB2	2.09	0.52
1:A:163:GLU:O	1:A:167:LEU:HG	2.10	0.52
1:A:648:ASP:OD2	1:A:757:ASP:OD2	2.28	0.52
1:A:668:ARG:HD2	1:B:669:PHE:CD2	2.45	0.52
2:D:314:TYR:O	3:F:673:PHE:CE2	2.63	0.52
1:A:483:ASN:HD21	1:A:540:ALA:HB3	1.75	0.52
1:B:335:GLN:NE2	1:B:336:THR:HG22	2.25	0.52
1:A:232:LEU:HD11	1:A:256:ILE:CG1	2.40	0.51
1:A:623:ARG:HA	3:E:360:VAL:HG21	1.89	0.51
1:B:433:PHE:O	1:B:437:VAL:HG23	2.09	0.51
1:B:646:ARG:HH22	3:F:352:ARG:NE	2.08	0.51
1:B:667:ASP:HB3	1:B:670:VAL:CG2	2.37	0.51
2:D:314:TYR:CZ	3:F:673:PHE:CZ	2.98	0.51
1:A:188:VAL:HG21	1:A:461:VAL:HG11	1.92	0.51
1:B:361:SER:O	1:B:362:THR:CB	2.59	0.51
1:B:698:ARG:HA	1:B:707:HIS:NE2	2.24	0.51
1:A:305:THR:HG23	1:A:464:THR:HG21	1.93	0.51
1:A:669:PHE:CD2	1:B:668:ARG:HD2	2.46	0.51
1:B:232:LEU:HD21	1:B:256:ILE:HD11	1.91	0.51
1:B:651:ARG:NH2	3:F:372:GLU:OE1	2.44	0.51
1:B:553:VAL:HG22	1:B:554:SER:N	2.25	0.51
1:B:607:LEU:CD1	1:B:609:LEU:HG	2.40	0.51
1:B:651:ARG:NH2	3:F:372:GLU:HG2	2.25	0.51
1:B:749:LEU:O	1:B:750:SER:HB3	2.11	0.51
1:A:361:SER:O	1:A:362:THR:CB	2.58	0.51
1:A:676:ASP:O	1:A:680:ARG:HG3	2.10	0.51
1:B:198:ASN:OD1	1:B:378:SER:N	2.44	0.51
1:B:201:ILE:HD13	1:B:212:LEU:CA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ILE:CD1	1:B:349:MET:HE1	2.40	0.51
3:F:499:GLY:O	3:F:500:PRO:C	2.48	0.51
1:A:124:TRP:HH2	1:A:596:GLN:HG2	1.75	0.51
1:B:605:VAL:HG11	1:B:665:LYS:HB3	1.92	0.51
3:F:382:MET:SD	3:F:402:CYS:HB3	2.50	0.51
1:A:199:SER:O	1:A:376:THR:HG22	2.11	0.51
1:A:300:HIS:HE2	1:A:459:GLY:N	2.09	0.51
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.91	0.51
1:A:759:GLU:O	1:A:760:PHE:C	2.49	0.51
1:B:238:GLY:HA3	1:B:267:LYS:CD	2.41	0.51
2:C:314:TYR:O	3:E:673:PHE:CE2	2.63	0.51
1:A:651:ARG:HH21	3:E:372:GLU:HG2	1.75	0.51
1:B:145:LYS:O	1:B:148:ASN:HB2	2.11	0.51
1:B:286:THR:HG21	1:B:360:ASP:HB2	1.92	0.51
1:A:618:LEU:HD21	1:A:742:ILE:HG23	1.92	0.51
1:A:700:VAL:HG23	1:A:701:PHE:CD1	2.46	0.51
1:B:127:LEU:N	1:B:127:LEU:HD22	2.25	0.51
1:B:146:LEU:HD23	1:B:146:LEU:O	2.10	0.51
1:B:239:THR:C	1:B:241:LYS:N	2.64	0.51
1:B:750:SER:OG	1:B:751:GLY:N	2.42	0.51
1:A:498:ALA:HB2	1:A:553:VAL:HA	1.92	0.51
1:B:199:SER:CB	1:B:212:LEU:HD11	2.38	0.51
1:B:282:TYR:HE1	1:B:284:ASP:HB3	1.76	0.51
1:B:359:THR:CG2	1:B:360:ASP:H	2.02	0.51
1:B:453:TRP:CG	1:B:463:ALA:HB2	2.45	0.51
3:F:381:ILE:HA	3:F:386:ALA:O	2.10	0.51
1:A:238:GLY:HA3	1:A:267:LYS:CD	2.42	0.50
1:A:425:LEU:O	1:A:429:LEU:HB2	2.11	0.50
1:A:539:ASN:O	1:A:542:PHE:N	2.38	0.50
1:B:238:GLY:N	1:B:257:VAL:HB	2.26	0.50
2:C:314:TYR:CZ	3:E:673:PHE:CZ	2.98	0.50
3:E:381:ILE:HA	3:E:386:ALA:O	2.10	0.50
1:A:483:ASN:ND2	1:A:540:ALA:HB3	2.27	0.50
1:A:539:ASN:HD22	1:A:539:ASN:C	2.15	0.50
1:B:618:LEU:HD21	1:B:742:ILE:HG23	1.94	0.50
1:A:212:LEU:HD21	1:A:215:ASN:ND2	2.23	0.50
1:B:199:SER:O	1:B:376:THR:HG22	2.11	0.50
3:E:359:SER:O	3:E:360:VAL:C	2.50	0.50
3:F:499:GLY:HA3	3:F:510:GLY:H	1.76	0.50
1:A:349:MET:HA	1:A:368:SER:N	2.26	0.50
1:A:409:ARG:HB2	1:A:452:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:LEU:HD13	1:A:731:PHE:CE1	2.46	0.50
1:A:756:ILE:HD12	1:A:756:ILE:H	1.77	0.50
1:B:146:LEU:HD23	1:B:146:LEU:C	2.32	0.50
1:B:291:VAL:HG13	1:B:292:ASN:N	2.27	0.50
1:B:655:ARG:HH11	1:B:751:GLY:HA2	1.76	0.50
1:A:239:THR:C	1:A:241:LYS:N	2.65	0.50
1:A:623:ARG:HH11	3:E:360:VAL:CA	2.24	0.50
1:A:210:VAL:HG22	1:A:211:TYR:N	2.25	0.50
1:B:648:ASP:OD2	1:B:757:ASP:OD2	2.29	0.50
3:F:359:SER:O	3:F:360:VAL:C	2.50	0.50
1:A:222:TYR:HB3	1:A:329:LEU:HD23	1.94	0.50
1:A:361:SER:O	1:A:362:THR:HB	2.12	0.50
1:B:670:VAL:O	1:B:674:LEU:HG	2.12	0.50
1:B:682:GLU:OE2	1:B:699:HIS:CE1	2.64	0.50
1:A:224:LYS:HE3	1:A:224:LYS:HA	1.94	0.50
1:A:237:PHE:HB2	1:A:243:PHE:CE1	2.47	0.50
1:A:240:LYS:O	1:A:240:LYS:HG2	2.12	0.50
1:A:446:ARG:HH12	1:A:602:THR:HA	1.77	0.50
1:A:496:VAL:HG11	1:A:506:ILE:HD13	1.94	0.50
1:A:537:LEU:HD22	1:A:542:PHE:CE2	2.46	0.50
1:B:497:SER:OG	1:B:533:GLU:HB3	2.12	0.50
1:B:662:ASN:HA	2:D:72:LEU:HD23	1.91	0.50
3:E:548:ALA:HA	3:E:551:LEU:CD1	2.42	0.50
3:F:541:GLY:HA2	3:F:549:LYS:HD2	1.94	0.50
1:B:224:LYS:HE3	1:B:224:LYS:HA	1.93	0.50
1:B:264:PHE:CE2	1:B:281:ILE:HG21	2.47	0.50
1:B:307:ASP:H	1:B:461:VAL:HG13	1.76	0.50
1:B:349:MET:HA	1:B:368:SER:N	2.26	0.50
3:E:499:GLY:HA3	3:E:510:GLY:H	1.76	0.50
1:A:239:THR:HB	1:A:244:GLU:CD	2.33	0.49
1:A:307:ASP:N	1:A:461:VAL:HG13	2.26	0.49
1:A:677:ARG:NE	1:A:750:SER:HB2	2.26	0.49
1:B:453:TRP:CD2	1:B:463:ALA:HB2	2.47	0.49
1:B:654:SER:C	1:B:657:THR:HG22	2.32	0.49
3:F:548:ALA:HA	3:F:551:LEU:CD1	2.42	0.49
1:A:756:ILE:HD12	1:A:756:ILE:N	2.27	0.49
1:B:278:GLY:HA2	1:B:333:PRO:HG2	1.93	0.49
1:B:496:VAL:CG1	1:B:506:ILE:HD13	2.42	0.49
3:E:499:GLY:O	3:E:500:PRO:C	2.48	0.49
1:A:198:ASN:OD1	1:A:378:SER:N	2.44	0.49
1:A:553:VAL:HG22	1:A:554:SER:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:HIS:HE2	1:B:459:GLY:N	2.10	0.49
1:A:282:TYR:HE1	1:A:284:ASP:HB3	1.77	0.49
1:A:553:VAL:HG21	1:A:597:PHE:CE2	2.46	0.49
1:B:357:TRP:O	1:B:359:THR:N	2.44	0.49
1:B:425:LEU:O	1:B:429:LEU:HB2	2.13	0.49
1:B:667:ASP:OD1	1:B:669:PHE:HB3	2.12	0.49
1:A:209:LEU:O	1:A:210:VAL:HG12	2.13	0.49
1:A:523:TYR:HE1	1:A:530:SER:OG	1.95	0.49
1:A:682:GLU:OE2	1:A:699:HIS:CE1	2.65	0.49
1:A:759:GLU:HG3	1:A:760:PHE:N	2.27	0.49
1:B:197:GLN:NE2	1:B:215:ASN:HB3	2.27	0.49
1:B:623:ARG:HH12	3:F:359:SER:C	2.10	0.49
1:B:753:VAL:HG12	1:B:754:TRP:CG	2.48	0.49
3:F:595:LYS:O	3:F:598:LEU:N	2.46	0.49
1:A:153:VAL:HG22	1:A:154:PRO:CD	2.43	0.49
1:A:183:ARG:O	1:B:758:ASN:CB	2.58	0.49
1:A:240:LYS:O	1:A:241:LYS:HB3	2.13	0.49
1:B:237:PHE:HB2	1:B:243:PHE:CE1	2.46	0.49
1:A:286:THR:HG21	1:A:360:ASP:HB2	1.94	0.49
1:A:618:LEU:HD13	1:A:701:PHE:HZ	1.76	0.49
1:B:236:ASN:O	1:B:243:PHE:HD1	1.96	0.49
1:A:392:VAL:HG12	1:A:449:ILE:HB	1.94	0.49
1:A:655:ARG:HH11	1:A:751:GLY:HA2	1.76	0.49
1:B:568:THR:HG23	1:B:570:MET:H	1.76	0.49
1:B:650:PHE:CE2	3:F:369:GLU:OE2	2.65	0.49
3:E:541:GLY:HA2	3:E:549:LYS:HD2	1.94	0.49
1:A:580:ILE:HG23	1:A:580:ILE:O	2.13	0.49
1:A:238:GLY:HA3	1:A:267:LYS:HD3	1.94	0.49
1:A:408:GLN:HB3	1:A:485:ASP:OD1	2.12	0.49
1:B:163:GLU:O	1:B:167:LEU:HG	2.12	0.49
1:B:325:ARG:HG2	1:B:326:SER:N	2.28	0.49
2:D:134:LEU:HD13	2:D:228:LEU:HD21	1.94	0.48
2:D:317:TYR:OH	3:F:383:ASN:HB2	2.01	0.48
1:A:305:THR:HG23	1:A:305:THR:O	2.13	0.48
1:A:316:PHE:CZ	1:B:740:TRP:NE1	2.75	0.48
1:B:152:TYR:HA	1:B:161:LYS:HB3	1.95	0.48
1:B:230:GLY:O	1:B:372:ASN:HB2	2.14	0.48
1:B:537:LEU:HD22	1:B:542:PHE:CE2	2.48	0.48
1:B:677:ARG:NE	1:B:750:SER:HB2	2.27	0.48
1:A:324:SER:O	1:A:325:ARG:HB3	2.14	0.48
1:B:240:LYS:O	1:B:241:LYS:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ILE:CG2	1:B:454:SER:HB3	2.43	0.48
1:A:325:ARG:HG2	1:A:326:SER:N	2.29	0.48
1:A:357:TRP:O	1:A:359:THR:N	2.43	0.48
1:A:712:LEU:HD23	1:A:712:LEU:C	2.33	0.48
1:B:305:THR:HG23	1:B:305:THR:O	2.13	0.48
1:B:343:GLU:OE2	1:B:362:THR:HG21	2.14	0.48
1:B:712:LEU:C	1:B:712:LEU:HD23	2.34	0.48
1:A:152:TYR:HA	1:A:161:LYS:HB3	1.95	0.48
1:A:197:GLN:NE2	1:A:215:ASN:HB3	2.27	0.48
1:A:465:GLU:HA	1:A:468:GLU:HB2	1.95	0.48
1:A:497:SER:OG	1:A:533:GLU:HB3	2.14	0.48
1:A:680:ARG:HB3	1:A:684:HIS:CD2	2.48	0.48
1:A:700:VAL:HG23	1:A:701:PHE:HD1	1.79	0.48
1:B:229:THR:HB	1:B:374:LYS:HB2	1.96	0.48
1:B:361:SER:O	1:B:362:THR:HB	2.13	0.48
1:B:732:ARG:HH11	1:B:732:ARG:CG	2.25	0.48
1:A:278:GLY:HA2	1:A:333:PRO:HG2	1.94	0.48
1:B:680:ARG:HB3	1:B:684:HIS:CD2	2.47	0.48
3:F:392:ASP:HA	3:F:582:HIS:CD2	2.49	0.48
1:A:237:PHE:HD2	1:A:258:ARG:HB2	1.78	0.48
1:B:411:ALA:HA	1:B:457:ASP:OD2	2.13	0.48
3:E:392:ASP:HA	3:E:582:HIS:CD2	2.49	0.48
1:A:203:VAL:HG23	1:A:206:ASN:O	2.14	0.48
1:A:409:ARG:HG2	1:A:409:ARG:HH11	1.78	0.48
1:A:430:ALA:HA	1:A:450:PHE:CZ	2.49	0.48
1:A:677:ARG:HE	1:A:750:SER:HB2	1.78	0.48
1:B:239:THR:HB	1:B:244:GLU:CD	2.34	0.48
1:B:759:GLU:O	1:B:760:PHE:C	2.52	0.48
2:C:134:LEU:HD13	2:C:228:LEU:HD21	1.94	0.48
2:C:278:LYS:HE2	2:C:278:LYS:HB3	1.71	0.48
3:F:498:VAL:O	3:F:499:GLY:O	2.32	0.48
1:A:180:LYS:HD2	1:A:180:LYS:N	2.28	0.48
3:F:433:LYS:HD2	3:F:554:GLU:O	2.14	0.48
1:A:297:PHE:N	1:A:297:PHE:CD1	2.81	0.48
1:A:467:LEU:HD21	1:A:544:PHE:CZ	2.49	0.48
1:A:478:ALA:O	1:A:550:ILE:HD12	2.14	0.48
1:A:568:THR:HG23	1:A:570:MET:H	1.77	0.48
1:A:623:ARG:CD	3:E:360:VAL:H	2.26	0.48
3:E:498:VAL:O	3:E:499:GLY:O	2.32	0.48
1:A:213:VAL:HG11	1:A:345:LEU:CD2	2.44	0.47
1:A:232:LEU:HB2	1:A:373:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ASP:HB2	1:B:380:VAL:HG13	1.96	0.47
1:B:297:PHE:N	1:B:297:PHE:CD1	2.82	0.47
1:B:698:ARG:HA	1:B:707:HIS:HE2	1.78	0.47
1:A:134:LYS:O	1:A:138:THR:HG23	2.14	0.47
1:B:125:ASP:HB3	2:D:142:PRO:HB3	1.53	0.47
1:B:232:LEU:HD13	1:B:254:ILE:HG22	1.96	0.47
1:B:646:ARG:NH1	1:B:646:ARG:CG	2.77	0.47
2:C:23:ARG:HG3	2:C:37:VAL:O	2.14	0.47
2:D:23:ARG:HG3	2:D:37:VAL:O	2.14	0.47
1:A:131:LEU:HD22	1:A:599:ILE:CD1	2.43	0.47
1:A:213:VAL:O	1:A:214:GLU:HB2	2.13	0.47
1:A:240:LYS:HA	1:A:262:ILE:HD13	1.95	0.47
1:B:180:LYS:HD2	1:B:180:LYS:N	2.30	0.47
1:B:623:ARG:CD	3:F:356:ASP:O	2.62	0.47
2:C:314:TYR:CE1	3:E:673:PHE:CE1	3.03	0.47
3:F:548:ALA:HA	3:F:551:LEU:HG	1.97	0.47
1:A:238:GLY:HA2	1:A:257:VAL:HG11	1.95	0.47
1:A:662:ASN:OD1	2:C:71:TYR:HE1	1.93	0.47
1:A:753:VAL:HG11	1:B:402:TYR:CE1	2.50	0.47
1:B:222:TYR:CE2	1:B:308:PRO:HG3	2.50	0.47
1:B:453:TRP:CE3	1:B:463:ALA:HA	2.49	0.47
1:B:515:HIS:CD2	1:B:516:PRO:CD	2.97	0.47
3:E:548:ALA:HA	3:E:551:LEU:HG	1.97	0.47
3:F:392:ASP:HB2	3:F:582:HIS:CE1	2.49	0.47
1:A:180:LYS:HD2	1:A:180:LYS:H	1.80	0.47
1:A:643:TYR:HB3	3:E:349:HIS:NE2	2.29	0.47
1:B:425:LEU:HD22	1:B:591:ALA:HB2	1.96	0.47
1:B:473:SER:O	1:B:476:LEU:HB2	2.14	0.47
2:C:250[B]:THR:HG21	2:C:314:TYR:CE2	2.50	0.47
1:A:565:TYR:HE1	1:A:575:GLU:HB3	1.78	0.47
1:B:651:ARG:HH11	1:B:651:ARG:HG2	1.79	0.47
1:B:754:TRP:O	1:B:755:ASP:C	2.53	0.47
1:A:239:THR:O	1:A:243:PHE:HB2	2.15	0.47
1:A:330:PRO:O	1:A:331:ASN:CB	2.62	0.47
1:A:386:ILE:CG2	1:A:454:SER:HB3	2.44	0.47
1:A:582:GLU:CD	1:A:582:GLU:H	2.18	0.47
1:A:639:LEU:HD23	1:A:643:TYR:HE1	1.79	0.47
1:A:749:LEU:O	1:A:750:SER:HB3	2.14	0.47
1:B:161:LYS:O	1:B:164:ASN:HB2	2.14	0.47
1:B:204:ASP:OD1	1:B:205:LYS:N	2.43	0.47
1:B:211:TYR:CG	1:B:212:LEU:N	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ARG:HG2	1:B:409:ARG:HH11	1.79	0.47
2:C:30:ILE:CG2	2:C:34:GLY:HA3	2.45	0.47
2:D:94:PHE:HD1	3:F:675:LYS:CG	2.28	0.47
3:E:392:ASP:HB2	3:E:582:HIS:CE1	2.49	0.47
1:A:133:GLU:HA	1:A:136:ASP:HB2	1.95	0.47
1:A:161:LYS:O	1:A:164:ASN:HB2	2.14	0.47
1:A:236:ASN:O	1:A:243:PHE:HD1	1.97	0.47
1:B:743:GLN:O	1:B:746:ALA:HB3	2.15	0.47
2:C:94:PHE:HD1	3:E:675:LYS:CG	2.28	0.47
2:D:250[B]:THR:HG21	2:D:314:TYR:CE2	2.50	0.47
3:F:499:GLY:CA	3:F:510:GLY:H	2.28	0.47
1:A:154:PRO:HD2	1:A:161:LYS:HZ3	1.79	0.47
1:A:280:LEU:C	1:A:281:ILE:HD12	2.36	0.47
1:A:491:THR:HB	1:A:517:VAL:HG21	1.97	0.47
1:A:553:VAL:HG21	1:A:597:PHE:HE2	1.78	0.47
1:A:700:VAL:HG11	1:A:741:THR:HG21	1.97	0.47
1:B:153:VAL:HG22	1:B:154:PRO:CD	2.45	0.47
1:B:307:ASP:N	1:B:461:VAL:HG13	2.30	0.47
1:B:408:GLN:HB3	1:B:485:ASP:OD1	2.14	0.47
1:B:430:ALA:HA	1:B:450:PHE:CZ	2.50	0.47
3:E:433:LYS:HD2	3:E:554:GLU:O	2.14	0.47
1:A:683:TYR:CD1	1:A:686:LEU:HD12	2.50	0.47
1:B:203:VAL:HB	1:B:208:ARG:HA	1.97	0.47
2:D:30:ILE:CG2	2:D:34:GLY:HA3	2.45	0.47
2:D:314:TYR:CE1	3:F:673:PHE:CE1	3.03	0.47
3:E:499:GLY:CA	3:E:510:GLY:H	2.28	0.47
1:A:232:LEU:CD1	1:A:256:ILE:HG13	2.45	0.46
1:A:291:VAL:HG13	1:A:292:ASN:N	2.30	0.46
1:A:699:HIS:CD2	1:A:701:PHE:HB2	2.49	0.46
1:A:730:LEU:HG	1:A:734:GLN:OE1	2.15	0.46
1:B:240:LYS:O	1:B:240:LYS:HG2	2.15	0.46
2:D:93:THR:H	3:F:675:LYS:HD2	1.80	0.46
3:F:347:LEU:O	3:F:351:GLU:HB2	2.16	0.46
1:A:555:PHE:HZ	1:A:594:ALA:HB2	1.81	0.46
1:B:445:SER:N	1:B:602:THR:HG22	2.31	0.46
3:F:467:TYR:C	3:F:469:ARG:H	2.17	0.46
1:A:190:ILE:HG13	1:A:458:PHE:CD2	2.50	0.46
1:A:244:GLU:OE1	1:A:244:GLU:HA	2.15	0.46
1:A:359:THR:CG2	1:A:360:ASP:N	2.74	0.46
1:A:623:ARG:NE	3:E:360:VAL:H	2.13	0.46
1:A:699:HIS:CD2	1:A:702:TRP:H	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLN:OE1	1:B:197:GLN:HA	2.16	0.46
1:B:238:GLY:C	1:B:240:LYS:N	2.69	0.46
1:B:446:ARG:HH12	1:B:602:THR:HA	1.81	0.46
1:A:281:ILE:HD12	1:A:281:ILE:N	2.30	0.46
1:A:409:ARG:NH2	1:A:454:SER:HB2	2.31	0.46
1:A:667:ASP:HB3	1:A:670:VAL:CG2	2.36	0.46
1:B:198:ASN:OD1	1:B:377:VAL:HA	2.16	0.46
1:B:239:THR:O	1:B:241:LYS:N	2.48	0.46
2:D:314:TYR:CZ	3:F:673:PHE:HZ	2.33	0.46
3:E:595:LYS:O	3:E:598:LEU:N	2.46	0.46
1:A:547:TYR:HD1	1:A:696:PRO:O	1.99	0.46
1:A:654:SER:CA	1:A:657:THR:HG22	2.44	0.46
1:B:122:LEU:HD12	1:B:122:LEU:N	2.30	0.46
1:B:357:TRP:HE1	1:B:365:MET:CE	2.29	0.46
3:E:467:TYR:C	3:E:469:ARG:H	2.17	0.46
2:C:3:ASP:O	2:C:4:LYS:HB2	2.15	0.46
3:E:514:TYR:HE2	3:E:629:ARG:HD2	1.81	0.46
1:A:446:ARG:NH1	1:A:602:THR:HA	2.30	0.46
1:A:731:PHE:O	1:A:732:ARG:C	2.54	0.46
1:A:750:SER:OG	1:A:751:GLY:N	2.48	0.46
1:B:239:THR:O	1:B:243:PHE:HB2	2.15	0.46
2:C:314:TYR:CZ	3:E:673:PHE:HZ	2.33	0.46
3:F:483:CYS:HB2	3:F:496:LEU:HB2	1.97	0.46
1:A:146:LEU:C	1:A:146:LEU:HD23	2.36	0.46
1:A:390:PHE:CD2	1:A:449:ILE:HD11	2.51	0.46
1:A:580:ILE:N	1:A:581:PRO:HD3	2.31	0.46
1:A:753:VAL:HG12	1:A:754:TRP:CG	2.51	0.46
1:B:134:LYS:O	1:B:138:THR:HG23	2.16	0.46
1:B:504:THR:OG1	1:B:610:ASP:OD2	2.30	0.46
1:B:553:VAL:HG21	1:B:597:PHE:CE2	2.51	0.46
1:B:565:TYR:N	1:B:565:TYR:CD2	2.83	0.46
1:B:580:ILE:N	1:B:581:PRO:HD3	2.30	0.46
3:E:521:LEU:HB2	3:E:528:ALA:HB2	1.98	0.46
1:B:244:GLU:HA	1:B:244:GLU:OE1	2.14	0.46
1:B:639:LEU:HD23	1:B:643:TYR:HE1	1.80	0.46
3:E:347:LEU:O	3:E:351:GLU:HB2	2.16	0.46
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.17	0.46
1:A:623:ARG:C	3:E:360:VAL:HG21	2.36	0.46
1:B:204:ASP:C	1:B:206:ASN:N	2.63	0.46
1:B:759:GLU:HG3	1:B:760:PHE:H	1.80	0.46
1:A:190:ILE:CG2	1:A:191:GLN:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LYS:O	1:A:512:ASN:ND2	2.49	0.45
2:D:94:PHE:HD1	3:F:675:LYS:CB	2.15	0.45
3:E:483:CYS:HB2	3:E:496:LEU:HB2	1.97	0.45
1:A:564:PRO:HG2	1:A:565:TYR:H	1.80	0.45
1:A:209:LEU:CG	1:A:210:VAL:N	2.76	0.45
1:A:618:LEU:O	1:A:622:VAL:HG23	2.16	0.45
1:A:629:ARG:NH2	3:E:357:GLU:CD	2.70	0.45
1:A:262:ILE:HD11	1:A:267:LYS:HG2	1.98	0.45
1:A:553:VAL:HG11	1:A:597:PHE:CD2	2.52	0.45
1:A:698:ARG:HA	1:A:707:HIS:NE2	2.31	0.45
1:B:610:ASP:HB3	1:B:613:GLU:CG	2.47	0.45
2:D:3:ASP:O	2:D:4:LYS:HB2	2.15	0.45
2:D:309:MET:CE	3:F:669:GLU:OE2	2.65	0.45
1:A:664:GLU:OE1	2:C:74:PRO:CD	2.52	0.45
2:D:250[B]:THR:HG21	2:D:314:TYR:CZ	2.52	0.45
1:A:188:VAL:HG23	1:A:190:ILE:HD13	1.98	0.45
1:A:224:LYS:HB3	1:A:332:ILE:C	2.37	0.45
1:A:732:ARG:HG3	1:A:732:ARG:NH1	2.28	0.45
1:B:201:ILE:HD13	1:B:212:LEU:N	2.32	0.45
1:B:281:ILE:HD12	1:B:281:ILE:N	2.32	0.45
3:F:445:GLY:O	3:F:480:ARG:HB2	2.17	0.45
1:A:127:LEU:N	1:A:127:LEU:HD22	2.31	0.45
1:A:143:THR:O	1:A:147:LEU:HG	2.17	0.45
1:A:194:ASP:HB2	1:A:380:VAL:HG13	1.99	0.45
1:A:233:VAL:HG12	1:A:234:HIS:N	2.32	0.45
1:A:240:LYS:C	1:A:242:ASP:N	2.69	0.45
1:A:612:GLU:O	1:A:614:TYR:N	2.50	0.45
1:B:124:TRP:HH2	1:B:596:GLN:HG2	1.82	0.45
1:B:211:TYR:CE1	1:B:212:LEU:O	2.70	0.45
1:B:539:ASN:HD22	1:B:539:ASN:C	2.19	0.45
1:B:588:ARG:HG3	1:B:588:ARG:NH1	2.31	0.45
2:C:93:THR:H	3:E:675:LYS:HD2	1.81	0.45
2:D:309:MET:HE3	3:F:669:GLU:OE2	2.17	0.45
3:E:333:ASP:OD1	3:E:333:ASP:N	2.50	0.45
3:F:382:MET:HE3	3:F:382:MET:HB2	1.75	0.45
1:A:238:GLY:C	1:A:240:LYS:N	2.70	0.45
1:A:309:TYR:HE2	1:A:325:ARG:CA	2.24	0.45
1:A:340:ALA:O	1:A:343:GLU:HB2	2.16	0.45
1:A:607:LEU:HD11	1:A:609:LEU:HG	1.98	0.45
1:A:690:VAL:CG2	1:A:698:ARG:HG2	2.47	0.45
1:A:740:TRP:CD2	1:B:314:PRO:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:TYR:CE2	3:F:383:ASN:HA	2.38	0.45
1:A:651:ARG:NH2	3:E:372:GLU:CG	2.80	0.45
1:A:719:ARG:CG	1:A:719:ARG:NH1	2.80	0.45
1:B:232:LEU:HB2	1:B:373:VAL:CG1	2.47	0.45
1:B:237:PHE:HD2	1:B:258:ARG:HB2	1.82	0.45
1:B:496:VAL:HG11	1:B:506:ILE:HD13	1.99	0.45
1:B:556:CYS:C	1:B:558:CYS:H	2.19	0.45
1:B:699:HIS:CD2	1:B:702:TRP:CD1	3.05	0.45
3:F:333:ASP:OD1	3:F:333:ASP:N	2.50	0.45
1:A:123:TYR:CB	2:C:144:LYS:O	2.65	0.44
1:A:212:LEU:O	1:A:213:VAL:C	2.55	0.44
1:B:662:ASN:C	2:D:73:ALA:H	2.15	0.44
1:B:664:GLU:CD	1:B:664:GLU:N	2.70	0.44
1:B:700:VAL:HG23	1:B:701:PHE:CD1	2.51	0.44
3:E:488:GLN:O	3:E:490:ASN:N	2.50	0.44
3:F:488:GLN:O	3:F:490:ASN:N	2.50	0.44
1:A:190:ILE:HG23	1:A:191:GLN:N	2.32	0.44
1:A:754:TRP:O	1:A:755:ASP:C	2.55	0.44
1:B:392:VAL:HG12	1:B:449:ILE:HG13	1.99	0.44
3:F:521:LEU:HB2	3:F:528:ALA:HB2	1.98	0.44
1:A:721:GLN:O	1:A:723:ASN:N	2.50	0.44
1:B:340:ALA:O	1:B:343:GLU:HB2	2.17	0.44
1:B:499:SER:O	1:B:501:LEU:N	2.50	0.44
1:B:637:LEU:CD1	1:B:731:PHE:HE2	2.30	0.44
2:C:309:MET:CE	3:E:669:GLU:OE2	2.65	0.44
3:F:609:VAL:HG11	3:F:617:CYS:SG	2.58	0.44
1:A:343:GLU:OE2	1:A:362:THR:HG21	2.18	0.44
1:A:482:ILE:HG22	1:A:483:ASN:N	2.33	0.44
1:A:603:HIS:CD2	1:A:603:HIS:C	2.91	0.44
3:E:498:VAL:O	3:E:499:GLY:C	2.56	0.44
3:E:518:PHE:O	3:E:521:LEU:HB3	2.18	0.44
1:A:306:GLY:HA2	1:A:461:VAL:HG22	1.99	0.44
1:B:633:LYS:O	1:B:633:LYS:HD3	2.18	0.44
3:E:605:PHE:CE1	3:E:616:PHE:HB3	2.53	0.44
3:F:518:PHE:O	3:F:521:LEU:HB3	2.18	0.44
1:A:614:TYR:HA	1:A:617:GLN:HB2	1.99	0.44
1:A:733:ASN:O	1:A:734:GLN:C	2.55	0.44
1:B:224:LYS:HB3	1:B:332:ILE:C	2.37	0.44
1:B:664:GLU:O	1:B:666:THR:N	2.50	0.44
1:B:699:HIS:CD2	1:B:701:PHE:HB2	2.53	0.44
3:E:445:GLY:O	3:E:480:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ALA:O	1:A:223:SER:N	2.50	0.44
1:A:238:GLY:HA2	1:A:257:VAL:HB	2.00	0.44
1:A:349:MET:HG2	1:A:367:THR:HG22	2.00	0.44
1:A:221:ALA:O	1:A:301:ALA:HB3	2.18	0.44
1:A:239:THR:O	1:A:241:LYS:N	2.50	0.44
1:A:349:MET:CG	1:A:367:THR:HA	2.45	0.44
1:A:357:TRP:HE1	1:A:365:MET:CE	2.31	0.44
1:B:154:PRO:HD2	1:B:161:LYS:HZ3	1.82	0.44
1:B:465:GLU:HA	1:B:468:GLU:HB2	1.99	0.44
1:B:508:LYS:O	1:B:512:ASN:ND2	2.51	0.44
1:B:731:PHE:O	1:B:732:ARG:C	2.56	0.44
1:B:735:LEU:C	1:B:735:LEU:HD23	2.38	0.44
3:F:387:ASP:O	3:F:586:SER:OG	2.29	0.44
3:F:498:VAL:O	3:F:499:GLY:C	2.56	0.44
3:F:605:PHE:CE1	3:F:616:PHE:HB3	2.53	0.44
1:A:122:LEU:N	1:A:122:LEU:HD12	2.32	0.44
1:B:180:LYS:HD2	1:B:180:LYS:H	1.83	0.44
1:B:193:LYS:HA	1:B:379:ASN:OD1	2.17	0.44
1:B:204:ASP:OD2	1:B:370:SER:O	2.36	0.44
1:A:300:HIS:O	1:A:301:ALA:CB	2.66	0.43
1:A:633:LYS:O	1:A:633:LYS:HD3	2.18	0.43
1:B:188:VAL:HB	1:B:307:ASP:HB2	2.00	0.43
1:B:201:ILE:HD12	1:B:202:ILE:H	1.81	0.43
1:B:643:TYR:HB2	3:F:349:HIS:NE2	2.32	0.43
2:C:317:TYR:CE2	3:E:382:MET:O	2.71	0.43
2:D:317:TYR:CE2	3:F:382:MET:O	2.71	0.43
1:A:146:LEU:HD23	1:A:146:LEU:O	2.17	0.43
1:A:229:THR:HB	1:A:374:LYS:HB2	2.00	0.43
1:A:467:LEU:C	1:A:469:GLY:N	2.70	0.43
1:B:565:TYR:HB3	1:B:570:MET:HB3	1.99	0.43
1:B:654:SER:CA	1:B:657:THR:HG22	2.47	0.43
1:B:732:ARG:HG3	1:B:732:ARG:NH1	2.27	0.43
2:C:317:TYR:HH	3:E:383:ASN:HA	1.76	0.43
2:D:148:LYS:NZ	2:D:152:ASN:ND2	2.66	0.43
3:E:453:VAL:O	3:E:454:ASP:HB2	2.18	0.43
3:F:453:VAL:O	3:F:454:ASP:HB2	2.18	0.43
1:A:406:GLY:HA2	1:A:451:ALA:O	2.18	0.43
1:A:580:ILE:HG23	1:A:583:LEU:HB2	1.99	0.43
1:A:654:SER:HA	1:A:657:THR:CG2	2.48	0.43
1:A:732:ARG:HH11	1:A:732:ARG:CG	2.28	0.43
1:B:238:GLY:HA3	1:B:267:LYS:HD3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:LEU:HD22	2:C:162:ALA:HA	2.01	0.43
1:A:651:ARG:HG2	1:A:651:ARG:HH11	1.83	0.43
1:B:402:TYR:HB3	1:B:449:ILE:HG22	2.00	0.43
1:B:404:VAL:HA	1:B:449:ILE:HG23	2.00	0.43
3:E:593:CYS:O	3:E:597:LYS:HG2	2.19	0.43
3:E:609:VAL:HG11	3:E:617:CYS:SG	2.58	0.43
1:A:202:ILE:HG13	1:A:213:VAL:HG21	2.01	0.43
1:A:222:TYR:CE2	1:A:308:PRO:HG3	2.53	0.43
1:A:376:THR:HG23	1:A:376:THR:O	2.18	0.43
1:A:735:LEU:HD23	1:A:735:LEU:C	2.38	0.43
1:B:348:ASN:N	1:B:348:ASN:ND2	2.65	0.43
1:B:629:ARG:HH22	3:F:357:GLU:CD	2.21	0.43
2:C:148:LYS:NZ	2:C:152:ASN:ND2	2.66	0.43
2:C:250[B]:THR:HG21	2:C:314:TYR:CZ	2.52	0.43
3:E:335:LEU:O	3:E:336:GLN:HG3	2.19	0.43
3:F:381:ILE:O	3:F:587:ARG:HD3	2.19	0.43
1:A:214:GLU:OE1	1:A:341:ALA:HB2	2.19	0.43
1:A:556:CYS:C	1:A:558:CYS:H	2.21	0.43
1:A:639:LEU:O	1:A:643:TYR:CD1	2.72	0.43
1:B:467:LEU:HD21	1:B:544:PHE:CZ	2.54	0.43
1:B:582:GLU:CD	1:B:582:GLU:H	2.21	0.43
1:B:733:ASN:O	1:B:734:GLN:C	2.56	0.43
3:F:357:GLU:HG2	3:F:616:PHE:HE1	1.82	0.43
3:F:593:CYS:O	3:F:597:LYS:HG2	2.19	0.43
1:A:488:VAL:HG13	1:A:586:VAL:CG1	2.49	0.43
1:A:564:PRO:HG2	1:A:565:TYR:CD2	2.54	0.43
1:A:723:ASN:N	1:A:723:ASN:HD22	2.17	0.43
1:A:759:GLU:OE2	3:E:500:PRO:C	2.56	0.43
1:B:233:VAL:HG12	1:B:234:HIS:N	2.33	0.43
2:D:122:LEU:HD22	2:D:162:ALA:HA	2.01	0.43
3:E:382:MET:HE3	3:E:382:MET:HB2	1.75	0.43
1:A:145:LYS:O	1:A:148:ASN:N	2.52	0.43
1:A:146:LEU:C	1:A:148:ASN:H	2.22	0.43
1:A:603:HIS:ND1	1:A:604:ASP:OD1	2.52	0.43
1:A:637:LEU:CD1	1:A:731:PHE:HE2	2.31	0.43
1:B:754:TRP:HA	1:B:754:TRP:HE3	1.84	0.43
3:F:416:ASP:O	3:F:419:LYS:HG2	2.19	0.43
1:A:327:SER:N	1:A:329:LEU:HD12	2.34	0.43
1:A:749:LEU:O	1:A:749:LEU:HG	2.19	0.43
1:A:754:TRP:HE3	1:A:754:TRP:HA	1.84	0.43
1:B:133:GLU:HA	1:B:136:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:HG22	1:B:386:ILE:HD11	1.97	0.43
1:B:283:MET:HG3	1:B:297:PHE:CE1	2.54	0.43
1:B:603:HIS:ND1	1:B:604:ASP:OD1	2.52	0.43
3:E:502:VAL:O	3:E:503:CYS:CB	2.66	0.43
3:F:335:LEU:O	3:F:336:GLN:HG3	2.19	0.43
3:F:514:TYR:HE2	3:F:629:ARG:HD2	1.81	0.43
1:A:392:VAL:HG12	1:A:449:ILE:HG13	2.00	0.43
1:B:221:ALA:O	1:B:301:ALA:HB3	2.19	0.43
1:B:232:LEU:CD2	1:B:256:ILE:HD11	2.49	0.43
1:B:376:THR:HG23	1:B:376:THR:O	2.19	0.43
1:B:677:ARG:HE	1:B:750:SER:HB2	1.83	0.43
3:F:384:GLY:HA2	3:F:587:ARG:NH1	2.34	0.43
1:A:232:LEU:HD13	1:A:254:ILE:HG22	2.01	0.42
1:A:264:PHE:O	1:A:268:VAL:HG23	2.19	0.42
1:B:699:HIS:CD2	1:B:702:TRP:H	2.36	0.42
2:D:71:TYR:O	2:D:76:ASN:HA	2.19	0.42
3:E:384:GLY:HA2	3:E:587:ARG:NH1	2.34	0.42
1:A:326:SER:N	1:A:329:LEU:HD13	2.34	0.42
1:A:198:ASN:OD1	1:A:377:VAL:HA	2.19	0.42
1:A:402:TYR:HB3	1:A:449:ILE:HG22	2.01	0.42
1:A:513:VAL:HB	1:A:522:LEU:HD12	2.00	0.42
1:B:513:VAL:HB	1:B:522:LEU:HD12	2.00	0.42
1:B:730:LEU:HG	1:B:734:GLN:OE1	2.19	0.42
2:C:245:GLN:HE22	3:E:676:HIS:C	2.23	0.42
1:A:213:VAL:HG11	1:A:345:LEU:HD21	2.01	0.42
1:A:278:GLY:N	1:A:332:ILE:CG2	2.82	0.42
1:A:300:HIS:NE2	1:A:458:PHE:C	2.73	0.42
1:A:392:VAL:HG12	1:A:449:ILE:CB	2.48	0.42
1:A:411:ALA:HA	1:A:457:ASP:OD2	2.19	0.42
1:A:488:VAL:HG11	1:A:583:LEU:HD12	2.02	0.42
1:A:721:GLN:C	1:A:723:ASN:H	2.22	0.42
1:A:737:LEU:HD11	1:B:693:LYS:HE2	2.00	0.42
1:B:153:VAL:O	1:B:155:ARG:N	2.50	0.42
1:B:213:VAL:HG11	1:B:345:LEU:CD2	2.47	0.42
1:B:478:ALA:O	1:B:550:ILE:HD12	2.18	0.42
1:B:488:VAL:HG13	1:B:586:VAL:HG11	2.01	0.42
1:B:513:VAL:HG22	1:B:592:GLU:HG2	2.01	0.42
1:B:553:VAL:HG11	1:B:597:PHE:CD2	2.54	0.42
1:B:654:SER:HA	1:B:657:THR:CG2	2.50	0.42
3:F:502:VAL:O	3:F:503:CYS:CB	2.66	0.42
1:A:488:VAL:HG21	1:A:587:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HA	1:A:521:PHE:HA	2.00	0.42
1:B:148:ASN:HD21	1:B:416:ALA:HB2	1.85	0.42
1:B:330:PRO:O	1:B:331:ASN:CB	2.62	0.42
1:B:482:ILE:HG22	1:B:483:ASN:N	2.34	0.42
2:D:245:GLN:HE22	3:F:676:HIS:C	2.23	0.42
3:E:461:ILE:N	3:E:462:PRO:HD2	2.34	0.42
1:A:230:GLY:O	1:A:372:ASN:HB2	2.19	0.42
1:A:308:PRO:HB2	1:A:329:LEU:HD11	2.01	0.42
1:A:610:ASP:HB3	1:A:613:GLU:CG	2.49	0.42
1:B:146:LEU:C	1:B:148:ASN:H	2.22	0.42
1:B:210:VAL:CG1	1:B:211:TYR:N	2.69	0.42
1:B:514:LYS:HA	1:B:521:PHE:HA	2.02	0.42
2:C:71:TYR:O	2:C:76:ASN:HA	2.19	0.42
1:A:588:ARG:HD3	1:A:589:ALA:N	2.34	0.42
1:A:649:PHE:O	1:A:652:ALA:HB3	2.20	0.42
1:A:686:LEU:HD23	1:A:699:HIS:N	2.34	0.42
1:B:221:ALA:O	1:B:223:SER:N	2.52	0.42
1:B:428:LYS:HA	1:B:428:LYS:HD3	1.79	0.42
1:B:629:ARG:HH22	3:F:357:GLU:HB2	1.84	0.42
1:A:619:LEU:HD23	1:A:619:LEU:C	2.40	0.42
1:A:720:LYS:C	1:A:722:ASN:H	2.22	0.42
1:B:402:TYR:N	1:B:402:TYR:CD1	2.88	0.42
1:B:721:GLN:C	1:B:723:ASN:H	2.23	0.42
2:D:26:MET:HE2	2:D:26:MET:HB3	1.88	0.42
3:E:416:ASP:O	3:E:419:LYS:HG2	2.19	0.42
3:F:570:GLU:O	3:F:571:ALA:C	2.58	0.42
1:A:335:GLN:NE2	1:A:336:THR:H	2.18	0.42
1:A:516:PRO:HG3	1:A:586:VAL:HA	2.02	0.42
1:A:555:PHE:CZ	1:A:594:ALA:HB2	2.55	0.42
1:A:669:PHE:CE2	1:B:668:ARG:HD2	2.55	0.42
1:B:240:LYS:C	1:B:242:ASP:N	2.72	0.42
1:B:716:LEU:HD13	1:B:731:PHE:CZ	2.55	0.42
2:D:148:LYS:HD3	2:D:152:ASN:ND2	2.35	0.42
3:E:381:ILE:O	3:E:587:ARG:HD3	2.19	0.42
3:F:461:ILE:N	3:F:462:PRO:HD2	2.34	0.42
1:A:306:GLY:N	1:A:459:GLY:O	2.53	0.42
1:A:568:THR:C	1:A:570:MET:H	2.23	0.42
1:A:668:ARG:HD2	1:B:669:PHE:CG	2.55	0.42
1:A:753:VAL:HG12	1:A:754:TRP:N	2.35	0.42
1:B:238:GLY:HA2	1:B:257:VAL:HB	2.01	0.42
1:B:360:ASP:O	1:B:361:SER:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:SER:OG	1:B:371:LYS:HG3	2.20	0.42
3:E:456:THR:HG23	3:E:652:TYR:CE1	2.54	0.42
1:A:161:LYS:HA	1:A:164:ASN:ND2	2.19	0.41
1:A:349:MET:HA	1:A:367:THR:CA	2.50	0.41
1:A:402:TYR:CD1	1:A:402:TYR:N	2.87	0.41
1:A:402:TYR:CE1	1:B:753:VAL:HG11	2.55	0.41
1:B:588:ARG:HD3	1:B:589:ALA:N	2.34	0.41
2:C:331:CYS:OXT	3:E:332:PRO:HD3	2.20	0.41
3:F:598:LEU:HD23	3:F:598:LEU:HA	1.87	0.41
1:A:614:TYR:O	1:A:618:LEU:HB2	2.20	0.41
1:B:351:GLY:O	1:B:364:ARG:HB3	2.20	0.41
1:B:564:PRO:HG2	1:B:565:TYR:CD2	2.54	0.41
1:B:690:VAL:CG2	1:B:698:ARG:HG2	2.47	0.41
2:C:94:PHE:CD1	3:E:675:LYS:CG	3.04	0.41
2:C:328:GLU:HB2	2:C:329:GLY:H	1.73	0.41
3:E:343:LYS:HB2	3:E:343:LYS:HZ2	1.85	0.41
3:F:447:LYS:NZ	3:F:526:ASP:OD2	2.53	0.41
1:A:193:LYS:HA	1:A:379:ASN:OD1	2.20	0.41
1:A:283:MET:HG3	1:A:297:PHE:CE1	2.55	0.41
1:B:123:TYR:O	1:B:126:ASP:HB2	2.20	0.41
1:B:237:PHE:O	1:B:238:GLY:C	2.59	0.41
1:B:308:PRO:HB2	1:B:329:LEU:HD11	2.01	0.41
1:B:324:SER:O	1:B:325:ARG:HB3	2.19	0.41
1:B:623:ARG:CD	3:F:360:VAL:H	2.33	0.41
1:B:686:LEU:HD23	1:B:699:HIS:N	2.36	0.41
3:E:514:TYR:CE2	3:E:629:ARG:HD2	2.55	0.41
3:E:570:GLU:O	3:E:571:ALA:C	2.58	0.41
1:A:204:ASP:C	1:A:206:ASN:N	2.71	0.41
1:A:754:TRP:NE1	1:B:449:ILE:HD12	2.35	0.41
1:B:193:LYS:NZ	1:B:193:LYS:HB2	2.35	0.41
1:B:327:SER:N	1:B:329:LEU:HD12	2.35	0.41
1:B:415:GLY:HA2	1:B:571:ASP:CG	2.40	0.41
1:B:662:ASN:O	2:D:72:LEU:HA	2.16	0.41
3:E:332:PRO:C	3:E:333:ASP:O	2.59	0.41
3:E:447:LYS:NZ	3:E:526:ASP:OD2	2.53	0.41
3:F:519:ARG:O	3:F:520:CYS:C	2.57	0.41
1:A:181:VAL:HA	1:A:391:GLY:HA2	2.00	0.41
1:A:188:VAL:HB	1:A:307:ASP:HB2	2.03	0.41
1:A:445:SER:N	1:A:602:THR:HG22	2.36	0.41
1:A:664:GLU:C	1:A:666:THR:N	2.74	0.41
1:B:313:PHE:HA	1:B:314:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ALA:CB	1:B:553:VAL:HA	2.50	0.41
1:A:124:TRP:CH2	1:A:596:GLN:HG2	2.54	0.41
1:A:238:GLY:HA2	1:A:257:VAL:CB	2.50	0.41
1:A:307:ASP:HB3	1:A:310:THR:HG23	2.01	0.41
1:A:637:LEU:HD21	1:A:732:ARG:HE	1.85	0.41
1:B:139:ASP:OD1	1:B:141:THR:CG2	2.68	0.41
1:B:349:MET:HB2	1:B:364:ARG:CB	2.50	0.41
1:B:386:ILE:HG22	1:B:454:SER:HB3	2.02	0.41
1:B:488:VAL:HG21	1:B:587:ALA:HA	2.02	0.41
2:D:90:ASP:HA	2:D:91:PRO:HD2	1.89	0.41
3:E:519:ARG:O	3:E:520:CYS:C	2.58	0.41
1:A:280:LEU:N	1:A:280:LEU:HD22	2.36	0.41
1:B:201:ILE:HB	1:B:212:LEU:CD1	2.49	0.41
1:B:208:ARG:H	1:B:208:ARG:HD3	1.84	0.41
1:B:238:GLY:HA2	1:B:257:VAL:HG11	2.02	0.41
1:B:458:PHE:HB2	1:B:461:VAL:HG21	2.03	0.41
1:B:491:THR:HB	1:B:517:VAL:HG21	2.02	0.41
1:B:585:LYS:O	1:B:588:ARG:HB3	2.21	0.41
1:A:148:ASN:HD21	1:A:416:ALA:HB2	1.86	0.41
1:A:310:THR:OG1	1:A:465:GLU:OE2	2.38	0.41
1:A:565:TYR:HB3	1:A:570:MET:HB3	2.02	0.41
1:A:664:GLU:O	1:A:666:THR:N	2.54	0.41
1:A:730:LEU:O	1:A:734:GLN:HG3	2.21	0.41
1:B:190:ILE:HG23	1:B:191:GLN:N	2.36	0.41
1:B:222:TYR:CD2	1:B:308:PRO:HG3	2.56	0.41
1:B:232:LEU:HD11	1:B:256:ILE:CG1	2.51	0.41
1:B:280:LEU:N	1:B:280:LEU:HD22	2.36	0.41
1:B:390:PHE:CD2	1:B:449:ILE:HD11	2.56	0.41
1:B:623:ARG:HE	3:F:356:ASP:HA	1.85	0.41
1:B:662:ASN:OD1	2:D:71:TYR:HE1	1.99	0.41
1:B:720:LYS:C	1:B:722:ASN:H	2.24	0.41
3:F:410:GLU:OE1	3:F:582:HIS:HB2	2.21	0.41
3:F:456:THR:HG23	3:F:652:TYR:CE1	2.54	0.41
1:A:123:TYR:HH	2:C:167:PHE:HZ	1.65	0.41
1:A:179:SER:O	1:A:180:LYS:C	2.58	0.41
1:A:238:GLY:HA2	1:A:257:VAL:CG1	2.50	0.41
1:A:565:TYR:CD2	1:A:565:TYR:N	2.86	0.41
1:B:188:VAL:HG23	1:B:190:ILE:HD13	2.02	0.41
1:B:201:ILE:HD13	1:B:211:TYR:C	2.41	0.41
1:B:287:LYS:HB3	1:B:288:PHE:CD1	2.56	0.41
1:B:444:PRO:CB	1:B:602:THR:HG21	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:GLU:C	1:B:666:THR:N	2.73	0.41
1:B:667:ASP:O	1:B:669:PHE:N	2.54	0.41
1:B:754:TRP:HA	1:B:754:TRP:CE3	2.56	0.41
2:C:148:LYS:HD3	2:C:152:ASN:ND2	2.35	0.41
2:C:309:MET:CE	3:E:669:GLU:CD	2.90	0.41
2:C:313:MET:HG3	3:E:670:ALA:HB1	1.97	0.41
1:A:130:LYS:HA	1:A:130:LYS:HD2	1.88	0.41
1:A:180:LYS:H	1:A:180:LYS:CD	2.34	0.41
1:A:349:MET:HB2	1:A:364:ARG:CB	2.51	0.41
1:A:404:VAL:HA	1:A:449:ILE:HG23	2.03	0.41
1:A:509:THR:C	1:A:511:GLN:H	2.24	0.41
1:A:754:TRP:HA	1:A:754:TRP:CE3	2.56	0.41
1:B:131:LEU:HD22	1:B:599:ILE:HD11	2.01	0.41
1:B:235:ALA:O	1:B:236:ASN:C	2.60	0.41
1:B:262:ILE:HD11	1:B:267:LYS:HG2	2.02	0.41
1:B:263:THR:O	1:B:264:PHE:C	2.59	0.41
1:B:307:ASP:HB3	1:B:310:THR:HG23	2.02	0.41
1:B:406:GLY:HA2	1:B:451:ALA:O	2.20	0.41
1:B:488:VAL:HG11	1:B:583:LEU:HD12	2.01	0.41
1:B:721:GLN:O	1:B:723:ASN:N	2.53	0.41
2:C:306:PRO:CB	3:E:669:GLU:OE1	2.69	0.41
2:D:331:CYS:OXT	3:F:332:PRO:HD3	2.20	0.41
3:F:343:LYS:NZ	3:F:343:LYS:HB2	2.36	0.41
1:A:156:GLU:O	1:A:162:ASP:HB2	2.21	0.40
1:A:359:THR:CG2	1:A:360:ASP:H	2.04	0.40
1:B:326:SER:N	1:B:329:LEU:HD13	2.35	0.40
1:B:643:TYR:CB	3:F:349:HIS:NE2	2.84	0.40
3:E:343:LYS:HB2	3:E:343:LYS:NZ	2.36	0.40
3:E:410:GLU:OE1	3:E:582:HIS:HB2	2.21	0.40
3:E:498:VAL:CG2	3:E:499:GLY:N	2.84	0.40
3:F:498:VAL:CG2	3:F:499:GLY:N	2.84	0.40
1:A:759:GLU:HG3	1:A:760:PHE:H	1.85	0.40
1:B:398:GLU:N	1:B:399:PRO:CD	2.84	0.40
1:B:555:PHE:HZ	1:B:594:ALA:HB2	1.87	0.40
2:D:309:MET:CE	3:F:669:GLU:CD	2.90	0.40
3:E:358:TRP:O	3:E:362:SER:OG	2.31	0.40
3:F:514:TYR:CE2	3:F:629:ARG:HD2	2.55	0.40
1:A:237:PHE:O	1:A:238:GLY:C	2.59	0.40
1:A:280:LEU:HA	1:A:335:GLN:O	2.22	0.40
1:A:335:GLN:NE2	1:A:336:THR:N	2.68	0.40
1:B:349:MET:HA	1:B:367:THR:CA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:ASN:N	1:B:758:ASN:ND2	2.67	0.40
2:D:245:GLN:OE1	3:F:676:HIS:C	2.59	0.40
2:D:278:LYS:HB3	2:D:278:LYS:HE2	1.71	0.40
3:E:373:THR:HB	3:E:374:PRO:HD2	2.03	0.40
1:B:253:SER:C	1:B:277:ILE:HD12	2.41	0.40
1:B:308:PRO:HG2	1:B:309:TYR:CE1	2.56	0.40
1:B:651:ARG:HG2	1:B:651:ARG:NH1	2.37	0.40
1:B:709:LEU:CB	1:B:710:PRO:HD3	2.51	0.40
3:E:536:LEU:HD12	3:E:536:LEU:HA	1.97	0.40
1:B:204:ASP:OD1	1:B:205:LYS:HG3	2.22	0.40
1:B:309:TYR:CE2	1:B:324:SER:O	2.75	0.40
1:B:753:VAL:HG12	1:B:754:TRP:N	2.36	0.40
2:D:306:PRO:CB	3:F:669:GLU:OE1	2.70	0.40
3:E:629:ARG:O	3:E:632:THR:OG1	2.35	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	637/639 (100%)	499 (78%)	100 (16%)	38 (6%)	1 17
1	B	637/639 (100%)	497 (78%)	101 (16%)	39 (6%)	1 17
2	C	332/329 (101%)	315 (95%)	15 (4%)	2 (1%)	25 66
2	D	332/329 (101%)	315 (95%)	15 (4%)	2 (1%)	25 66
3	E	343/345 (99%)	309 (90%)	26 (8%)	8 (2%)	6 34
3	F	343/345 (99%)	309 (90%)	26 (8%)	8 (2%)	6 34
All	All	2624/2626 (100%)	2244 (86%)	283 (11%)	97 (4%)	6 24

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	210	VAL
1	A	251	ASN
1	A	330	PRO
1	A	361	SER
1	A	362	THR
1	A	722	ASN
1	A	750	SER
1	A	753	VAL
1	A	759	GLU
1	B	179	SER
1	B	207	GLY
1	B	210	VAL
1	B	251	ASN
1	B	361	SER
1	B	362	THR
1	B	722	ASN
1	B	750	SER
1	B	753	VAL
1	B	759	GLU
2	C	4	LYS
2	D	4	LYS
1	A	179	SER
1	A	207	GLY
1	A	209	LEU
1	A	236	ASN
1	A	613	GLU
1	B	213	VAL
1	B	222	TYR
1	B	238	GLY
1	B	278	GLY
1	B	330	PRO
1	B	665	LYS
2	C	329	GLY
2	D	329	GLY
3	E	334	PRO
3	E	348	GLY
3	E	489	LYS
3	E	499	GLY
3	E	595	LYS
3	F	334	PRO
3	F	348	GLY
3	F	489	LYS

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Mol	Chain	Res	Type
3	F	499	GLY
3	F	595	LYS
1	A	208	ARG
1	A	222	TYR
1	A	237	PHE
1	A	238	GLY
1	A	239	THR
1	A	278	GLY
1	A	322	PRO
1	A	325	ARG
1	A	370	SER
1	A	558	CYS
1	A	581	PRO
1	A	665	LYS
1	B	236	ASN
1	B	237	PHE
1	B	322	PRO
1	B	325	ARG
1	B	581	PRO
1	A	180	LYS
1	A	566	LEU
1	B	204	ASP
1	B	212	LEU
1	B	239	THR
1	B	566	LEU
1	B	613	GLU
1	A	213	VAL
1	A	507	GLU
1	B	180	LYS
1	B	205	LYS
1	B	240	LYS
1	B	370	SER
1	B	540	ALA
1	B	558	CYS
1	B	668	ARG
3	E	337	ASP
3	E	493	LEU
3	F	337	ASP
3	F	493	LEU
1	A	153	VAL
1	A	205	LYS
1	A	569	THR

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Mol	Chain	Res	Type
1	B	153	VAL
1	B	247	TYR
1	B	351	GLY
1	B	216	PRO
1	A	216	PRO
1	B	564	PRO
1	A	351	GLY
1	A	564	PRO
1	A	756	ILE
1	B	756	ILE
3	E	360	VAL
3	F	360	VAL

4.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	548/548 (100%)	505 (92%)	43 (8%)	12	36
1	B	548/548 (100%)	507 (92%)	41 (8%)	13	38
2	C	279/274 (102%)	275 (99%)	4 (1%)	67	80
2	D	279/274 (102%)	275 (99%)	4 (1%)	67	80
3	E	292/293 (100%)	266 (91%)	26 (9%)	9	30
3	F	292/293 (100%)	266 (91%)	26 (9%)	9	30
All	All	2238/2230 (100%)	2094 (94%)	144 (6%)	21	42

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ASP
1	A	135	LEU
1	A	148	ASN
1	A	152	TYR
1	A	153	VAL
1	A	181	VAL

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	203	VAL
1	A	204	ASP
1	A	211	TYR
1	A	224	LYS
1	A	277	ILE
1	A	310	THR
1	A	322	PRO
1	A	325	ARG
1	A	330	PRO
1	A	348	ASN
1	A	353	CYS
1	A	357	TRP
1	A	365	MET
1	A	371	LYS
1	A	418	LYS
1	A	426	LEU
1	A	446	ARG
1	A	457	ASP
1	A	525	ASP
1	A	537	LEU
1	A	539	ASN
1	A	562	ASP
1	A	581	PRO
1	A	582	GLU
1	A	588	ARG
1	A	603	HIS
1	A	606	GLU
1	A	610	ASP
1	A	619	LEU
1	A	646	ARG
1	A	648	ASP
1	A	664	GLU
1	A	723	ASN
1	A	743	GLN
1	A	757	ASP
1	A	758	ASN
1	B	125	ASP
1	B	148	ASN
1	B	152	TYR
1	B	153	VAL
1	B	181	VAL

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Mol	Chain	Res	Type
1	B	197	GLN
1	B	203	VAL
1	B	208	ARG
1	B	224	LYS
1	B	277	ILE
1	B	310	THR
1	B	322	PRO
1	B	325	ARG
1	B	330	PRO
1	B	348	ASN
1	B	353	CYS
1	B	357	TRP
1	B	365	MET
1	B	371	LYS
1	B	418	LYS
1	B	426	LEU
1	B	446	ARG
1	B	457	ASP
1	B	525	ASP
1	B	537	LEU
1	B	539	ASN
1	B	562	ASP
1	B	581	PRO
1	B	588	ARG
1	B	603	HIS
1	B	606	GLU
1	B	619	LEU
1	B	646	ARG
1	B	648	ASP
1	B	660	PHE
1	B	664	GLU
1	B	723	ASN
1	B	732	ARG
1	B	743	GLN
1	B	757	ASP
1	B	758	ASN
2	C	20	GLN
2	C	71	TYR
2	C	217	LYS
2	C	276	LYS
2	D	20	GLN
2	D	71	TYR

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Mol	Chain	Res	Type
2	D	217	LYS
2	D	276	LYS
3	E	333	ASP
3	E	335	LEU
3	E	338	GLU
3	E	340	LYS
3	E	343	LYS
3	E	352	ARG
3	E	359	SER
3	E	362	SER
3	E	372	GLU
3	E	383	ASN
3	E	434	SER
3	E	453	VAL
3	E	480	ARG
3	E	488	GLN
3	E	536	LEU
3	E	586	SER
3	E	596	GLN
3	E	597	LYS
3	E	613	SER
3	E	621	SER
3	E	633	LYS
3	E	642	ASN
3	E	643	THR
3	E	644	TYR
3	E	661	LYS
3	E	675	LYS
3	F	333	ASP
3	F	335	LEU
3	F	338	GLU
3	F	340	LYS
3	F	343	LYS
3	F	352	ARG
3	F	359	SER
3	F	362	SER
3	F	372	GLU
3	F	383	ASN
3	F	434	SER
3	F	453	VAL
3	F	480	ARG
3	F	488	GLN

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Mol	Chain	Res	Type
3	F	536	LEU
3	F	586	SER
3	F	596	GLN
3	F	597	LYS
3	F	613	SER
3	F	621	SER
3	F	633	LYS
3	F	642	ASN
3	F	643	THR
3	F	644	TYR
3	F	661	LYS
3	F	675	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	160	GLN
1	A	164	ASN
1	A	191	GLN
1	A	215	ASN
1	A	275	ASN
1	A	317	ASN
1	A	335	GLN
1	A	348	ASN
1	A	408	GLN
1	A	515	HIS
1	A	539	ASN
1	A	640	GLN
1	A	684	HIS
1	A	699	HIS
1	A	723	ASN
1	A	758	ASN
1	B	148	ASN
1	B	160	GLN
1	B	164	ASN
1	B	191	GLN
1	B	270	ASN
1	B	275	ASN
1	B	317	ASN
1	B	335	GLN
1	B	348	ASN

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Mol	Chain	Res	Type
1	B	408	GLN
1	B	515	HIS
1	B	539	ASN
1	B	640	GLN
1	B	684	HIS
1	B	699	HIS
1	B	723	ASN
1	B	758	ASN
2	C	25	HIS
2	C	108	GLN
2	C	152	ASN
2	C	325	ASN
2	D	25	HIS
2	D	108	GLN
2	D	152	ASN
2	D	325	ASN
3	E	481	GLN
3	F	481	GLN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CO3	F	701	5	2,3,3	0.35	0	2,3,3	1.59	1 (50%)
4	CO3	C	338[B]	5	2,3,3	0.70	0	2,3,3	0.55	0
4	CO3	C	338[A]	5	2,3,3	0.27	0	2,3,3	0.13	0
4	CO3	E	701	5	2,3,3	0.35	0	2,3,3	1.59	1 (50%)
4	CO3	D	338[B]	5	2,3,3	0.70	0	2,3,3	0.58	0
4	CO3	D	338[A]	5	2,3,3	0.26	0	2,3,3	0.10	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	701	CO3	O3-C-O1	2.12	125.04	119.55
4	F	701	CO3	O3-C-O1	2.12	125.04	119.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.