



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:18 PM GMT

PDB ID : 4E3C
Title : X-ray crystal structure of human IKK2 in an active conformation
Authors : Polley, S.; Huang, D.B.; Hauenstein, A.V.; Ghosh, G.; Huxford, T.
Deposited on : 2012-03-09
Resolution : 3.98 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

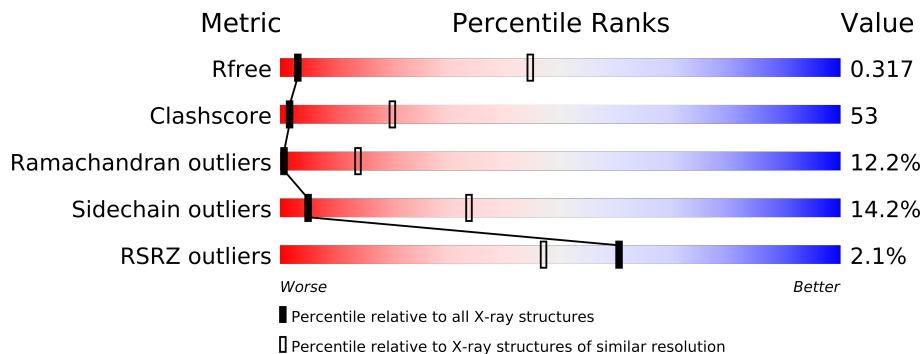
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1031 (4.50-3.46)
Clashscore	79885	1202 (4.46-3.50)
Ramachandran outliers	78287	1143 (4.46-3.50)
Sidechain outliers	78261	1130 (4.46-3.50)
RSRZ outliers	66119	1031 (4.50-3.46)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	669	
1	B	669	
1	C	669	
1	D	669	
1	E	669	
1	F	669	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30416 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Inhibitor of nuclear factor kappa-B kinase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	B	632	Total	C	N	O	S	0	0	0
			5116	3219	904	959	34			
1	C	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	D	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	E	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	F	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASN	-	EXPRESSION TAG	UNP O14920
A	2	LEU	-	EXPRESSION TAG	UNP O14920
A	3	TYR	-	EXPRESSION TAG	UNP O14920
A	4	PHE	-	EXPRESSION TAG	UNP O14920
A	5	GLN	-	EXPRESSION TAG	UNP O14920
A	6	GLY	-	EXPRESSION TAG	UNP O14920
A	7	ALA	-	EXPRESSION TAG	UNP O14920
A	8	MET	-	EXPRESSION TAG	UNP O14920
A	9	GLY	-	EXPRESSION TAG	UNP O14920
A	10	SER	-	EXPRESSION TAG	UNP O14920
A	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
A	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
B	1	ASN	-	EXPRESSION TAG	UNP O14920
B	2	LEU	-	EXPRESSION TAG	UNP O14920
B	3	TYR	-	EXPRESSION TAG	UNP O14920
B	4	PHE	-	EXPRESSION TAG	UNP O14920
B	5	GLN	-	EXPRESSION TAG	UNP O14920

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	GLY	-	EXPRESSION TAG	UNP O14920
B	7	ALA	-	EXPRESSION TAG	UNP O14920
B	8	MET	-	EXPRESSION TAG	UNP O14920
B	9	GLY	-	EXPRESSION TAG	UNP O14920
B	10	SER	-	EXPRESSION TAG	UNP O14920
B	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
B	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
C	1	ASN	-	EXPRESSION TAG	UNP O14920
C	2	LEU	-	EXPRESSION TAG	UNP O14920
C	3	TYR	-	EXPRESSION TAG	UNP O14920
C	4	PHE	-	EXPRESSION TAG	UNP O14920
C	5	GLN	-	EXPRESSION TAG	UNP O14920
C	6	GLY	-	EXPRESSION TAG	UNP O14920
C	7	ALA	-	EXPRESSION TAG	UNP O14920
C	8	MET	-	EXPRESSION TAG	UNP O14920
C	9	GLY	-	EXPRESSION TAG	UNP O14920
C	10	SER	-	EXPRESSION TAG	UNP O14920
C	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
C	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
D	1	ASN	-	EXPRESSION TAG	UNP O14920
D	2	LEU	-	EXPRESSION TAG	UNP O14920
D	3	TYR	-	EXPRESSION TAG	UNP O14920
D	4	PHE	-	EXPRESSION TAG	UNP O14920
D	5	GLN	-	EXPRESSION TAG	UNP O14920
D	6	GLY	-	EXPRESSION TAG	UNP O14920
D	7	ALA	-	EXPRESSION TAG	UNP O14920
D	8	MET	-	EXPRESSION TAG	UNP O14920
D	9	GLY	-	EXPRESSION TAG	UNP O14920
D	10	SER	-	EXPRESSION TAG	UNP O14920
D	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
D	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
E	1	ASN	-	EXPRESSION TAG	UNP O14920
E	2	LEU	-	EXPRESSION TAG	UNP O14920
E	3	TYR	-	EXPRESSION TAG	UNP O14920
E	4	PHE	-	EXPRESSION TAG	UNP O14920
E	5	GLN	-	EXPRESSION TAG	UNP O14920
E	6	GLY	-	EXPRESSION TAG	UNP O14920
E	7	ALA	-	EXPRESSION TAG	UNP O14920
E	8	MET	-	EXPRESSION TAG	UNP O14920
E	9	GLY	-	EXPRESSION TAG	UNP O14920
E	10	SER	-	EXPRESSION TAG	UNP O14920
E	177	GLU	SER	ENGINEERED MUTATION	UNP O14920

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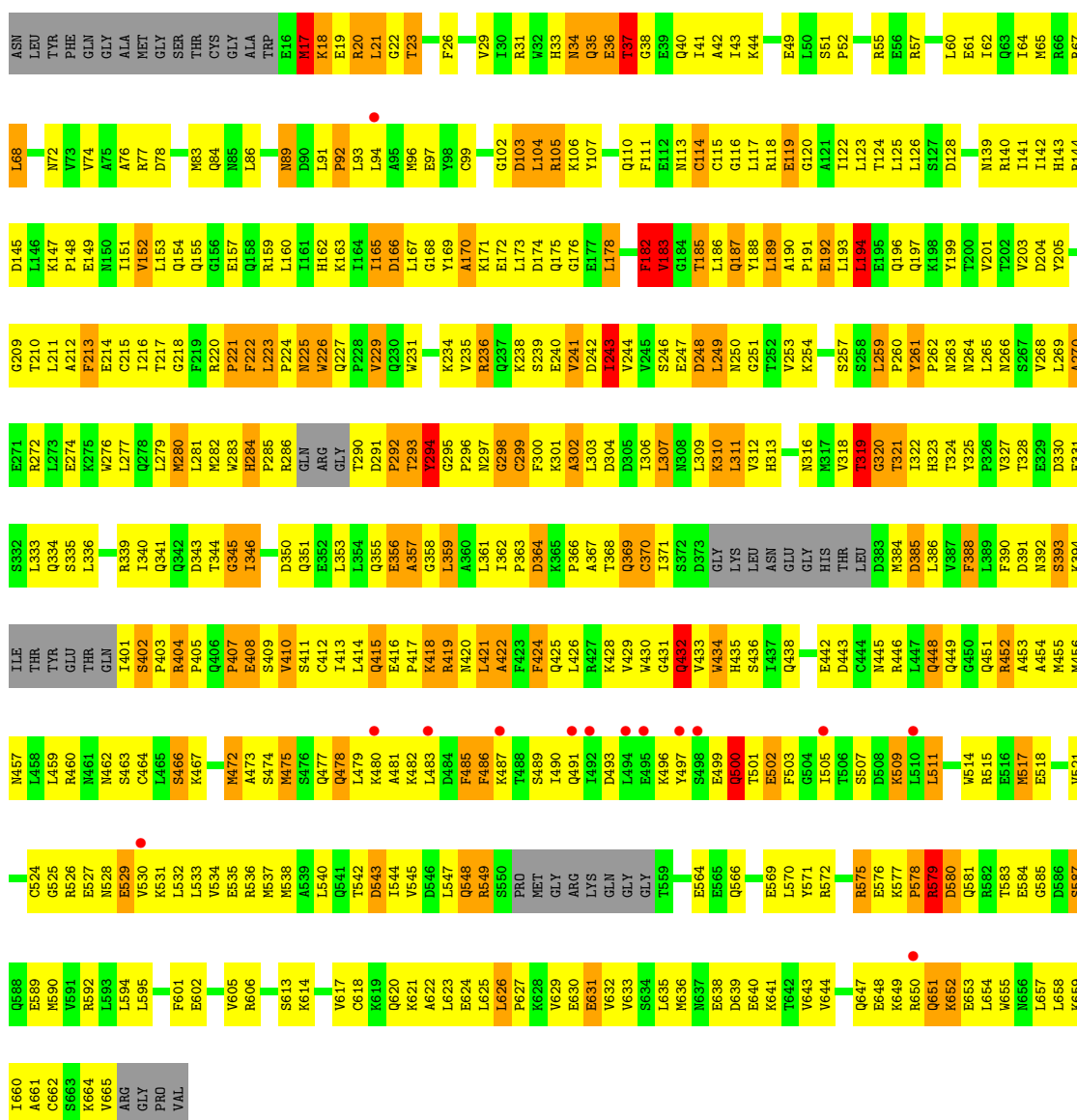
Chain	Residue	Modelled	Actual	Comment	Reference
E	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
F	1	ASN	-	EXPRESSION TAG	UNP O14920
F	2	LEU	-	EXPRESSION TAG	UNP O14920
F	3	TYR	-	EXPRESSION TAG	UNP O14920
F	4	PHE	-	EXPRESSION TAG	UNP O14920
F	5	GLN	-	EXPRESSION TAG	UNP O14920
F	6	GLY	-	EXPRESSION TAG	UNP O14920
F	7	ALA	-	EXPRESSION TAG	UNP O14920
F	8	MET	-	EXPRESSION TAG	UNP O14920
F	9	GLY	-	EXPRESSION TAG	UNP O14920
F	10	SER	-	EXPRESSION TAG	UNP O14920
F	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
F	181	GLU	SER	ENGINEERED MUTATION	UNP O14920

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

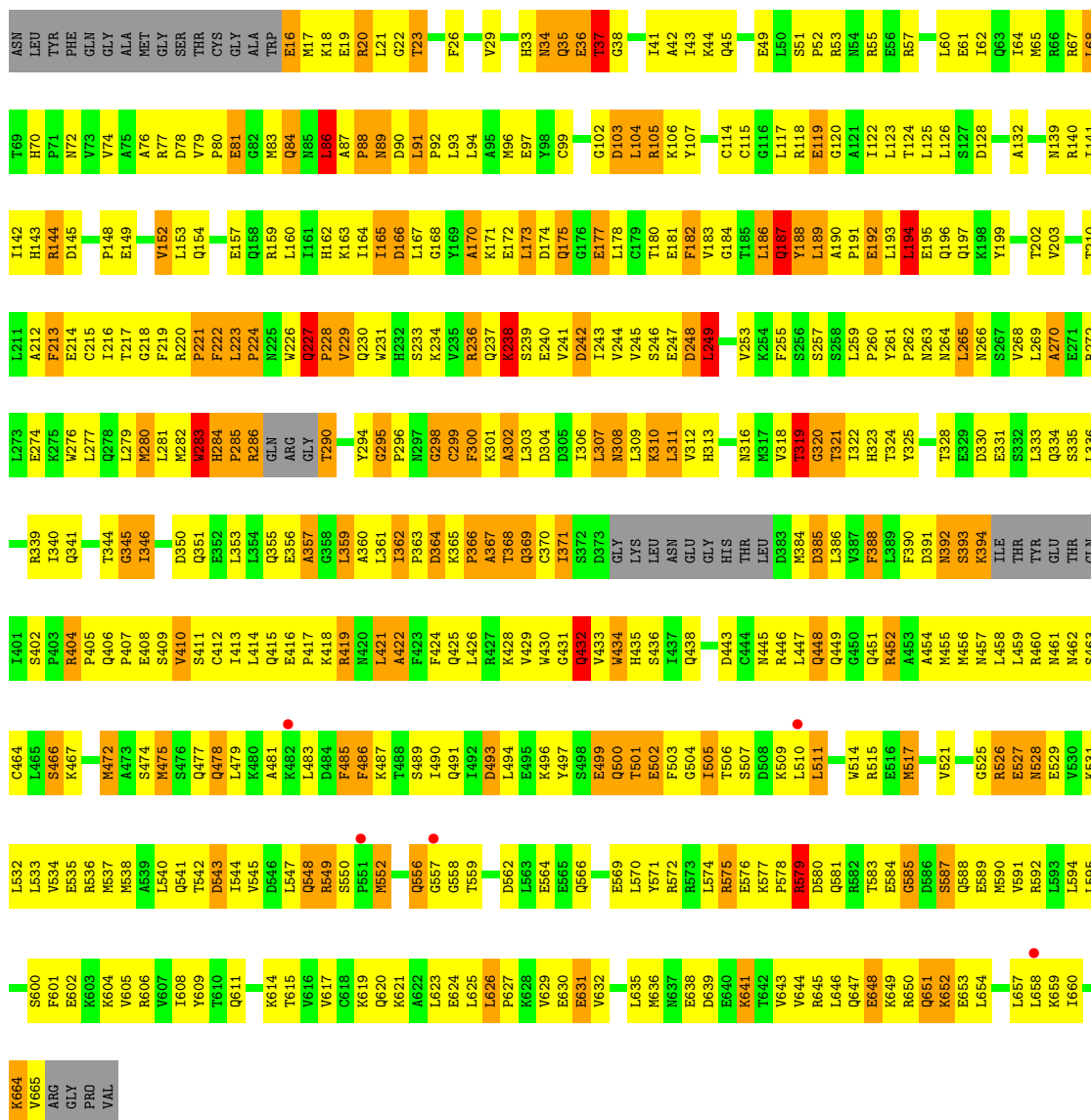
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain A: 



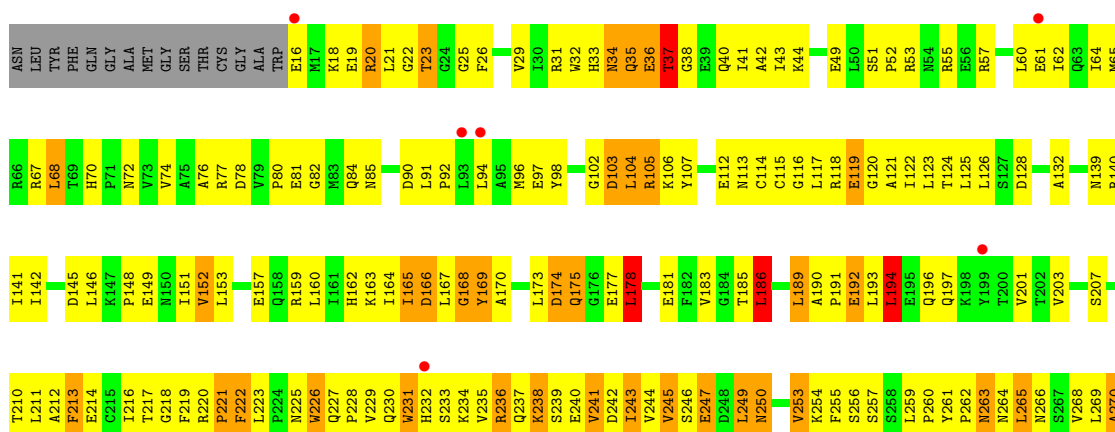
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

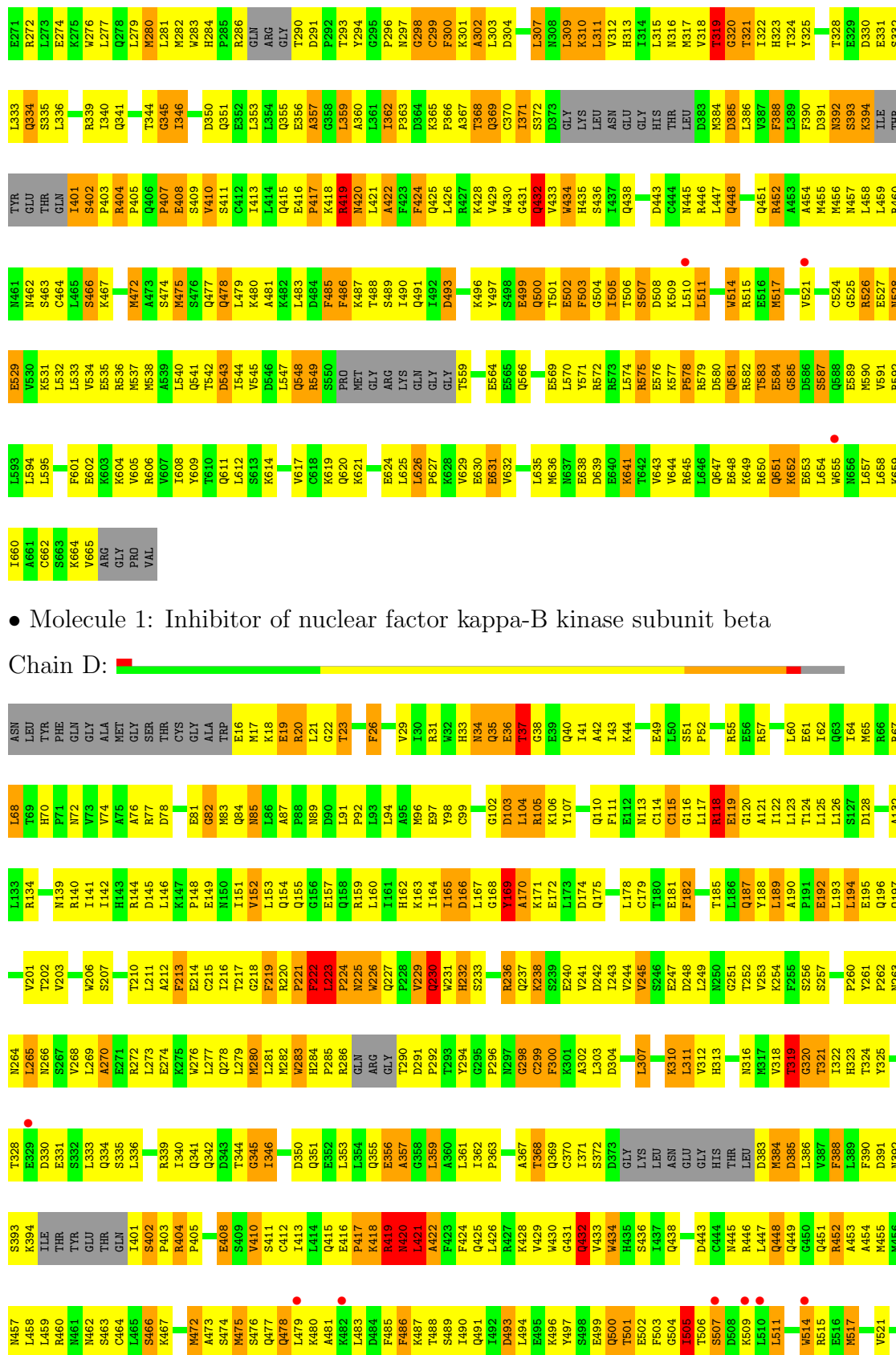
Chain B:

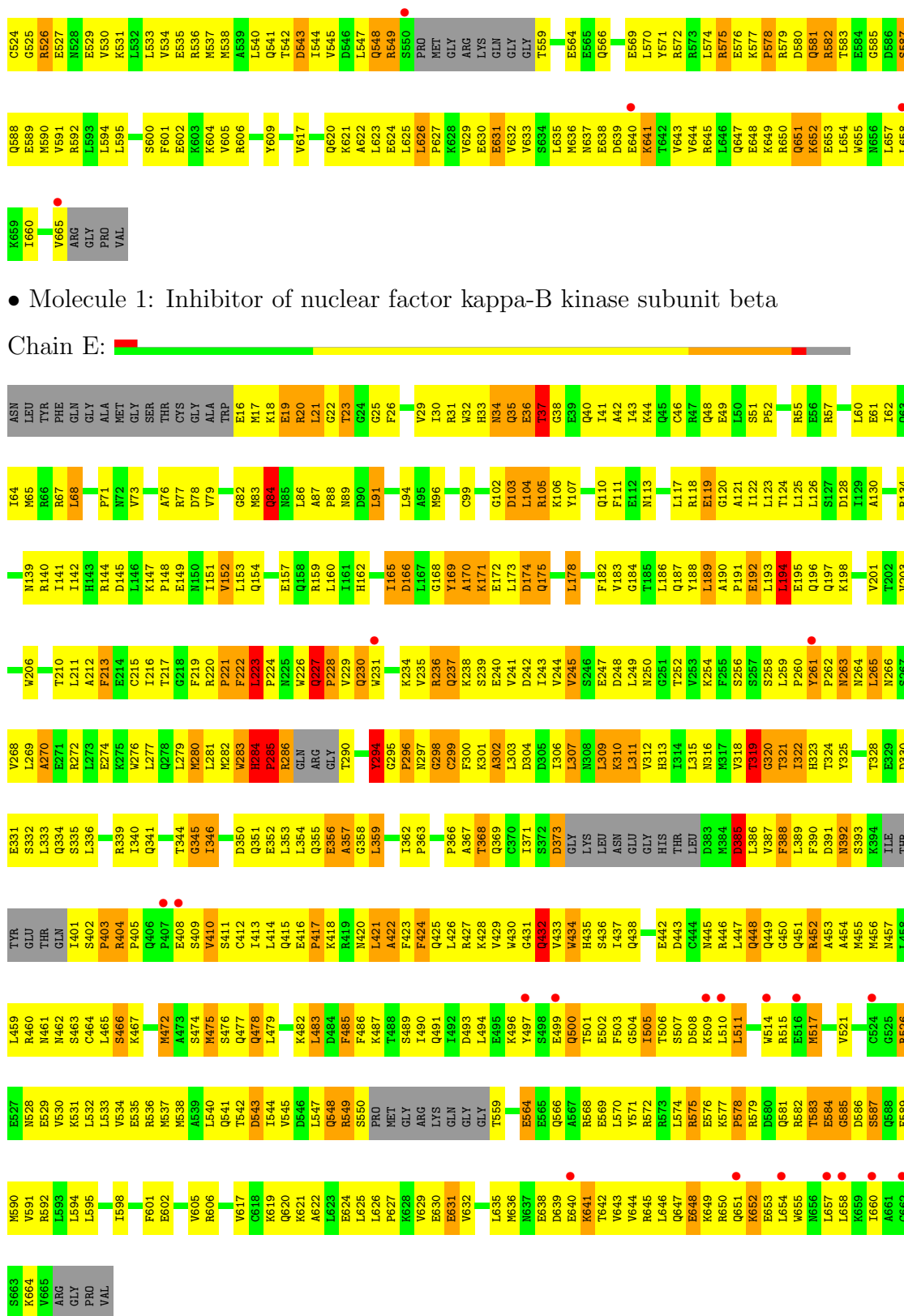


- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain C:







L646	Q647	E648	K649	R650	R651	K652	E653	L654	W655	R656	R657	R658	R659	R660	R661	R662	R663	K664	V665	ARG	GLY	PRO	VAL																																										
R582	T583	W514	R515	E516	M517	V521	G525	R526	E527	L528	N528	GLU	E529	V530	K531	V534	E535	R536	M537	K538	V605	R606	V607	L608																																									
Q448	Q449	W514	R515	E516	M517	V521	G525	R526	E527	L528	N528	GLU	E529	V530	K531	V534	E535	R536	M537	K538	V605	R606	V607	L608																																									
L386	V387	F388	L389	F390	D391	N392	S393	K394	I395	T396	T397	G398	T399	T400	T401	S402	P403	R404	Q405	Q406	S409	V410	S411	C412	L413	L414	Q415	L416	P417	K418	R419	M420	A421	A422	F423	F424	Q425	L426	R427	K428	V429	H430	G431	Q432	W433	H434	H435	S436	I437	Q438	T439	D442	D443	C444	M445	R446	L447								
Q448	Q449	C450	Q451	R452	R453	A454	A455	M456	N457	L458	L459	R460	N461	N462	S463	C464	L465	S466	K467	M472	A473	S474	M475	S476	Q477	Q478	L479	K480	E481	K482	L483	D484	F485	F486	K487	T488	S489	L490	Q491	L492	L493	D493	K496	Y497	S498	E499	Q500	T501	E502	F503	Q504	L505	T506	S507	B508	R509	L510	L511							
L386	V387	F388	L389	F390	D391	N392	S393	K394	I395	T396	T397	G398	T399	T400	T401	S402	P403	R404	Q405	Q406	S409	V410	S411	C412	L413	L414	Q415	L416	P417	K418	R419	M420	A421	A422	F423	F424	Q425	L426	R427	K428	V429	H430	G431	Q432	W433	H434	H435	S436	I437	Q438	T439	D442	D443	C444	M445	R446	L447								
P260	Y261	P262	N263	L264	L265	N266	S267	V268	L269	A270	E271	R272	L273	E274	K275	W276	L277	Q278	L279	M280	L281	M282	W283	H284	P285	R286	GLN	ARG	GLY	T290	D291	P292	T293	Y294	G295	P296	V297	G298	C299	F300	K301	A302	L303	D304	P305	L306	L307	N308	L309	K310	L311	V312	GLY	H313	R316	K317	V318	T319	G320						
T321	I322	H323	T324	Y325	T328	E329	D330	E331	S332	L333	Q334	Q335	L336	R339	I340	L341	Q341	T344	G345	L346	D350	Q351	E352	L353	L354	Q355	E356	A357	G358	L359	L361	I362	P363	D364	K365	P366	A367	T368	Q369	C370	I371	S372	L373	GLY	L375	L376	L377	L378	L379	F382	V383	G384	T385	L386	Q387	W388	L389	A390	L391	L392	L393	L394	L395	L396	L397
K198	Y199	T200	V201	T202	V203	D204	S207	F208	G209	T210	L211	A212	F213	E214	C215	L216	T217	G218	F219	R220	P221	F222	L223	P224	N225	W226	Q227	ARG	P228	V229	W230	W231	K234	V235	R236	Q237	R238	S239	E240	V241	D242	T243	V244	V245	S246	E247	D248	L249	W250	G251	L252	V253	K254	F255	S256	S257	G258	L259							
A132	L133	R134	N139	R140	I141	L142	H143	R144	D145	A146	R147	P148	E149	N150	I151	V152	L153	E157	Q158	R159	L160	I161	H162	K163	I164	I165	L166	L167	H168	Y169	A170	K171	E172	L173	D174	Q175	G176	E177	L178	C179	F182	V183	G184	L185	T186	Q187	G188	A189	L190	L191	L192	E193	L194	L195	L196	Q197									
M65	R66	R67	L68	T69	H70	R71	W72	W73	A74	A75	A76	R77	D78	V79	P80	E81	Q82	N83	Q84	H85	L86	A87	P88	N89	D90	L91	P92	L93	L94	A95	H96	E97	Y98	C99	G102	D103	L104	R105	K106	Y107	N113	C114	C115	G116	L117	R118	P119	E120	A121	L122	L123	T124	L125	L126	S127	D128									
ASN	LEU	TRP	PHE	GLN	GLY	ALA	MET	GLY	THR	SER	CYS	GLY	ALA	TRP	E16	M17	K18	E19	R20	L21	G22	T23	F26	V29	I30	R31	W32	H33	N34	Q35	E36	T37	G38	E39	Q40	I41	A42	I43	K44	Q45	C46	E49	L50	S51	P52	R53	H54	R55	L56	R57	L60	E61	I62	Q63	I64										

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.81 Å 170.81 Å 509.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.98 49.73 – 3.97	Depositor EDS
% Data completeness (in resolution range)	81.0 (29.84-3.98) 88.5 (49.73-3.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 4.00 Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.267 , 0.299 0.285 , 0.317	Depositor DCC
R_{free} test set	2221 reflections (3.82%)	DCC
Wilson B-factor (Å ²)	113.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 110.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 63509 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	30416	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.47	0/5142	0.61	3/6937 (0.0%)
1	B	0.47	0/5200	0.69	3/7014 (0.0%)
1	C	0.44	0/5142	0.58	0/6937
1	D	0.45	0/5142	0.69	3/6937 (0.0%)
1	E	0.44	0/5142	0.57	0/6937
1	F	0.42	0/5142	0.57	0/6937
All	All	0.45	0/30910	0.62	9/41699 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH1	-21.84	109.38	120.30
1	D	118	ARG	NE-CZ-NH2	21.77	131.18	120.30
1	B	144	ARG	NE-CZ-NH1	-20.91	109.84	120.30
1	B	144	ARG	NE-CZ-NH2	19.92	130.26	120.30
1	D	118	ARG	CD-NE-CZ	9.85	137.39	123.60
1	B	144	ARG	CD-NE-CZ	8.65	135.72	123.60
1	A	500	GLN	CA-C-N	-7.28	101.18	117.20
1	A	422	ALA	N-CA-C	-6.32	93.93	111.00
1	A	500	GLN	CA-C-O	5.59	131.84	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5060	0	5109	581	0
1	B	5116	0	5169	569	0
1	C	5060	0	5109	522	0
1	D	5060	0	5109	557	0
1	E	5060	0	5107	554	0
1	F	5060	0	5107	584	0
All	All	30416	0	30710	3237	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 53.

All (3237) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:419:ARG:HB2	1:B:419:ARG:NH1	1.55	1.18
1:B:366:PRO:HB2	1:B:368:THR:HG23	1.29	1.14
1:C:496:LYS:HE2	1:C:654:LEU:HD21	1.20	1.14
1:F:626:LEU:H	1:F:627:PRO:HD2	1.13	1.13
1:D:479:LEU:HD11	1:D:641:LYS:HG2	1.28	1.11
1:C:479:LEU:HD11	1:C:641:LYS:HG2	1.30	1.08
1:A:417:PRO:HA	1:B:320:GLY:HA3	1.35	1.08
1:F:401:ILE:HG12	1:F:403:PRO:HD3	1.31	1.08
1:E:284:HIS:HB3	1:E:285:PRO:HD2	1.42	1.02
1:E:265:LEU:HG	1:E:266:ASN:H	1.23	1.02
1:B:479:LEU:HD11	1:B:641:LYS:HG2	1.41	1.02
1:C:418:LYS:HZ2	1:C:421:LEU:HD12	1.25	1.01
1:A:533:LEU:HD22	1:A:629:VAL:HG12	1.41	1.01
1:B:571:TYR:HB3	1:B:575:ARG:HH21	1.24	1.01
1:B:419:ARG:HB2	1:B:419:ARG:HH11	1.24	1.00
1:A:279:LEU:HA	1:A:286:ARG:HH12	1.24	1.00
1:F:279:LEU:HD22	1:F:292:PRO:HD3	1.43	1.00
1:F:387:VAL:HG11	1:F:450:GLY:HA2	1.43	0.99
1:A:419:ARG:NE	1:A:419:ARG:H	1.59	0.99
1:C:402:SER:H	1:C:403:PRO:HD2	1.27	0.99
1:C:417:PRO:HA	1:D:320:GLY:HA3	1.44	0.98
1:C:259:LEU:HD22	1:C:260:PRO:HD2	1.41	0.98
1:C:571:TYR:HB3	1:C:575:ARG:HH21	1.29	0.98
1:F:389:LEU:HD21	1:F:454:ALA:HB2	1.45	0.98
1:E:387:VAL:HG11	1:E:450:GLY:HA2	1.46	0.98
1:A:571:TYR:HB3	1:A:575:ARG:HH21	1.28	0.98
1:A:417:PRO:HA	1:B:320:GLY:CA	1.94	0.97

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:419:ARG:HH22	1:D:345:GLY:HA3	1.30	0.97
1:A:402:SER:H	1:A:403:PRO:HD3	1.30	0.97
1:E:571:TYR:HB3	1:E:575:ARG:HH21	1.27	0.97
1:F:266:ASN:HB3	1:F:269:LEU:HB2	1.47	0.96
1:F:389:LEU:HD21	1:F:454:ALA:CB	1.94	0.96
1:F:142:ILE:HG13	1:F:173:LEU:HD11	1.44	0.96
1:F:571:TYR:HB3	1:F:575:ARG:HH21	1.31	0.96
1:D:571:TYR:HB3	1:D:575:ARG:HH21	1.29	0.96
1:B:165:ILE:HG22	1:B:166:ASP:H	1.30	0.96
1:D:229:VAL:HG23	1:D:230:GLN:H	1.30	0.96
1:F:357:ALA:HA	1:F:452:ARG:HH12	1.32	0.95
1:D:582:ARG:H	1:D:582:ARG:HE	1.00	0.95
1:F:427:ARG:HE	1:F:575:ARG:HG3	1.28	0.95
1:A:266:ASN:HB3	1:A:269:LEU:HB2	1.48	0.95
1:D:165:ILE:HG22	1:D:166:ASP:H	1.32	0.94
1:A:223:LEU:HD22	1:A:235:VAL:HG23	1.47	0.94
1:D:213:PHE:CE1	1:D:221:PRO:HB2	2.02	0.94
1:A:579:ARG:H	1:A:579:ARG:HD3	1.29	0.94
1:D:402:SER:H	1:D:403:PRO:HD2	1.32	0.93
1:D:266:ASN:HB3	1:D:269:LEU:HB2	1.49	0.93
1:B:654:LEU:HD23	1:C:654:LEU:HD23	1.48	0.93
1:F:80:PRO:HB2	1:F:83:MET:HB2	1.51	0.93
1:A:265:LEU:HD23	1:A:266:ASN:H	1.34	0.93
1:F:229:VAL:HG22	1:F:230:GLN:H	1.34	0.93
1:B:87:ALA:HB2	1:B:93:LEU:HD11	1.49	0.93
1:C:55:ARG:NH1	1:C:91:LEU:HD11	1.83	0.93
1:D:404:ARG:NH2	1:D:404:ARG:H	1.67	0.93
1:C:266:ASN:HB3	1:C:269:LEU:HB2	1.51	0.92
1:B:266:ASN:HB3	1:B:269:LEU:HB2	1.50	0.92
1:E:266:ASN:HB3	1:E:269:LEU:HB2	1.49	0.92
1:A:118:ARG:HB2	1:A:264:ASN:HB3	1.47	0.92
1:B:226:TRP:O	1:B:227:GLN:HG3	1.70	0.92
1:A:417:PRO:CA	1:B:320:GLY:HA3	1.98	0.91
1:C:511:LEU:HG	1:C:515:ARG:HH12	1.35	0.91
1:C:165:ILE:HG22	1:C:166:ASP:H	1.35	0.91
1:B:496:LYS:HE2	1:B:654:LEU:HD21	1.51	0.91
1:A:421:LEU:HD13	1:A:585:GLY:HA3	1.51	0.90
1:E:505:ILE:HD12	1:E:506:THR:H	1.36	0.90
1:A:292:PRO:HG3	1:A:297:ASN:HD22	1.37	0.90
1:E:165:ILE:HG22	1:E:166:ASP:H	1.35	0.90
1:C:500:GLN:HE22	1:C:504:GLY:HA3	1.34	0.90
1:E:17:MET:HG2	1:E:33:HIS:H	1.37	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:165:ILE:HG22	1:F:166:ASP:H	1.37	0.90
1:B:511:LEU:HG	1:B:515:ARG:HH12	1.36	0.90
1:E:410:VAL:HG12	1:E:411:SER:H	1.37	0.89
1:E:244:VAL:HB	1:E:256:SER:HB3	1.51	0.89
1:E:259:LEU:HD22	1:E:274:GLU:HG3	1.55	0.89
1:D:505:ILE:HD12	1:D:506:THR:H	1.38	0.89
1:C:447:LEU:HD23	1:C:609:TYR:HE1	1.37	0.89
1:E:295:GLY:H	1:E:296:PRO:HD2	1.37	0.88
1:B:80:PRO:HB2	1:B:83:MET:HB2	1.56	0.88
1:C:486:PHE:CE1	1:C:647:GLN:HB3	2.07	0.88
1:F:410:VAL:HG12	1:F:411:SER:H	1.39	0.88
1:A:473:ALA:HB1	1:A:530:VAL:HG11	1.56	0.88
1:A:213:PHE:HA	1:A:277:LEU:HD21	1.57	0.87
1:A:511:LEU:HG	1:A:515:ARG:HH12	1.40	0.87
1:E:265:LEU:HD11	1:E:270:ALA:HA	1.56	0.87
1:D:481:ALA:HB1	1:E:482:LYS:HD2	1.56	0.87
1:A:165:ILE:HG22	1:A:166:ASP:H	1.38	0.87
1:F:352:GLU:OE2	1:F:619:LYS:HE2	1.72	0.87
1:C:221:PRO:O	1:C:222:PHE:HB2	1.70	0.87
1:D:170:ALA:HB3	1:D:178:LEU:HD23	1.56	0.87
1:E:144:ARG:HD2	1:E:171:LYS:HB2	1.57	0.87
1:F:279:LEU:HD12	1:F:286:ARG:HG2	1.54	0.87
1:A:434:TRP:HB3	1:A:571:TYR:CZ	2.09	0.86
1:E:511:LEU:HG	1:E:515:ARG:HH12	1.40	0.86
1:F:626:LEU:N	1:F:627:PRO:HD2	1.85	0.86
1:D:192:GLU:HG2	1:D:283:TRP:HB3	1.57	0.86
1:C:410:VAL:HG12	1:C:411:SER:H	1.39	0.86
1:C:458:LEU:HD11	1:C:544:ILE:HG21	1.56	0.86
1:B:500:GLN:HE22	1:B:504:GLY:HA3	1.39	0.86
1:D:533:LEU:HD22	1:D:629:VAL:HG12	1.57	0.86
1:A:118:ARG:HH22	1:A:438:GLN:HG2	1.41	0.86
1:F:49:GLU:HG2	1:F:91:LEU:HD11	1.58	0.86
1:D:511:LEU:HG	1:D:515:ARG:HH12	1.39	0.86
1:F:511:LEU:HG	1:F:515:ARG:HH12	1.40	0.86
1:B:410:VAL:HG12	1:B:411:SER:H	1.40	0.85
1:D:227:GLN:HB2	1:D:229:VAL:HG22	1.58	0.85
1:F:220:ARG:H	1:F:223:LEU:HD12	1.40	0.85
1:A:500:GLN:C	1:A:500:GLN:HE21	1.79	0.85
1:D:410:VAL:HG12	1:D:411:SER:H	1.41	0.85
1:F:458:LEU:HD21	1:F:619:LYS:HA	1.57	0.85
1:E:193:LEU:HD22	1:E:203:VAL:HG21	1.58	0.85
1:D:240:GLU:HG3	1:D:241:VAL:HG23	1.58	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:319:THR:HG23	1:A:320:GLY:H	1.40	0.85
1:B:419:ARG:HB2	1:B:419:ARG:CZ	2.05	0.85
1:B:171:LYS:HG2	1:B:177:GLU:HA	1.58	0.85
1:D:582:ARG:N	1:D:582:ARG:HE	1.73	0.85
1:F:318:VAL:HG21	1:F:346:ILE:HD11	1.59	0.85
1:B:319:THR:HG23	1:B:320:GLY:H	1.42	0.85
1:C:18:LYS:HB2	1:C:31:ARG:HB3	1.59	0.85
1:A:318:VAL:HG21	1:A:346:ILE:HD11	1.58	0.85
1:F:387:VAL:CG1	1:F:450:GLY:HA2	2.07	0.84
1:E:321:THR:HG21	1:E:447:LEU:HD11	1.60	0.84
1:A:358:GLY:CA	1:A:457:ASN:HB2	2.08	0.84
1:D:144:ARG:HD2	1:D:171:LYS:HB3	1.59	0.84
1:F:67:ARG:HH21	1:F:68:LEU:HD12	1.43	0.84
1:E:530:VAL:HG22	1:E:632:VAL:HG12	1.59	0.84
1:A:481:ALA:HB1	1:F:482:LYS:NZ	1.92	0.84
1:B:172:GLU:HG3	1:B:175:GLN:H	1.42	0.84
1:D:193:LEU:HD22	1:D:203:VAL:HG21	1.60	0.84
1:E:111:PHE:CD1	1:E:575:ARG:HD2	2.13	0.83
1:C:418:LYS:NZ	1:C:421:LEU:HD12	1.92	0.83
1:A:193:LEU:HD22	1:A:203:VAL:HG21	1.60	0.83
1:F:126:LEU:HB3	1:F:303:LEU:HD21	1.60	0.83
1:C:496:LYS:HE2	1:C:654:LEU:CD2	2.06	0.83
1:D:657:LEU:HD23	1:E:658:LEU:HD21	1.59	0.83
1:A:655:TRP:CD1	1:F:500:GLN:HG2	2.14	0.83
1:E:430:TRP:HE1	1:E:587:SER:HA	1.40	0.83
1:F:427:ARG:HH21	1:F:575:ARG:HG2	1.43	0.83
1:A:652:LYS:HA	1:F:496:LYS:HE2	1.59	0.83
1:E:279:LEU:HD11	1:E:290:THR:HB	1.61	0.83
1:A:659:LYS:HD3	1:F:500:GLN:HE22	1.41	0.82
1:A:67:ARG:HH21	1:A:68:LEU:HD12	1.44	0.82
1:B:353:LEU:HB3	1:B:386:LEU:HD11	1.59	0.82
1:A:419:ARG:CZ	1:A:419:ARG:H	1.93	0.82
1:D:318:VAL:HG21	1:D:346:ILE:HD11	1.60	0.82
1:F:32:TRP:HZ3	1:F:83:MET:HB3	1.44	0.82
1:A:410:VAL:HG12	1:A:411:SER:H	1.44	0.82
1:C:193:LEU:HD22	1:C:203:VAL:HG21	1.60	0.82
1:B:318:VAL:HG21	1:B:346:ILE:HD11	1.62	0.82
1:E:427:ARG:HE	1:E:575:ARG:HG3	1.43	0.82
1:B:193:LEU:HD22	1:B:203:VAL:HG21	1.60	0.82
1:A:481:ALA:HB1	1:F:482:LYS:HZ2	1.45	0.82
1:A:657:LEU:O	1:F:658:LEU:HD11	1.79	0.82
1:E:265:LEU:HG	1:E:266:ASN:N	1.94	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:213:PHE:CE1	1:A:221:PRO:HB2	2.15	0.81
1:C:67:ARG:HH21	1:C:68:LEU:HD12	1.44	0.81
1:F:249:LEU:HD21	1:F:418:LYS:HE2	1.61	0.81
1:D:115:CYS:O	1:D:218:GLY:HA3	1.80	0.81
1:F:213:PHE:HA	1:F:277:LEU:HD21	1.61	0.81
1:C:421:LEU:HG	1:D:342:GLN:O	1.80	0.81
1:C:402:SER:N	1:C:403:PRO:HD2	1.94	0.81
1:B:67:ARG:HH21	1:B:68:LEU:HD12	1.45	0.81
1:F:282:MET:HG2	1:F:286:ARG:CZ	2.11	0.81
1:E:126:LEU:HB3	1:E:303:LEU:HD21	1.63	0.81
1:E:309:LEU:HD22	1:E:310:LYS:N	1.95	0.81
1:F:321:THR:HG21	1:F:447:LEU:HD11	1.62	0.80
1:D:319:THR:HG23	1:D:320:GLY:H	1.45	0.80
1:F:421:LEU:HB3	1:F:586:ASP:HA	1.61	0.80
1:E:431:GLY:HA2	1:E:571:TYR:CE2	2.15	0.80
1:A:61:GLU:HB2	1:A:178:LEU:HD21	1.60	0.80
1:F:319:THR:HG23	1:F:320:GLY:H	1.46	0.80
1:F:353:LEU:HB3	1:F:386:LEU:HD11	1.62	0.80
1:A:292:PRO:HG3	1:A:296:PRO:O	1.81	0.80
1:C:401:ILE:O	1:C:401:ILE:HD13	1.82	0.80
1:F:236:ARG:HH22	1:F:283:TRP:HE1	1.29	0.80
1:F:193:LEU:HD22	1:F:203:VAL:HG21	1.61	0.79
1:D:654:LEU:HD23	1:E:654:LEU:HD23	1.63	0.79
1:C:318:VAL:HG21	1:C:346:ILE:HD11	1.62	0.79
1:C:279:LEU:O	1:C:286:ARG:HD2	1.82	0.79
1:A:547:LEU:HD22	1:A:614:LYS:HE2	1.65	0.79
1:F:467:LYS:HD3	1:F:541:GLN:CG	2.13	0.79
1:B:360:ALA:HB3	1:E:36:GLU:HG3	1.62	0.79
1:C:418:LYS:O	1:C:419:ARG:HB3	1.81	0.79
1:E:319:THR:HG23	1:E:320:GLY:H	1.47	0.79
1:D:536:ARG:NH1	1:D:625:LEU:HD13	1.96	0.79
1:F:116:GLY:HA3	1:F:217:THR:O	1.82	0.79
1:A:627:PRO:HA	1:A:630:GLU:HB3	1.65	0.79
1:E:282:MET:HB3	1:E:286:ARG:HG3	1.63	0.79
1:A:320:GLY:HA3	1:B:417:PRO:HA	1.65	0.79
1:B:490:ILE:HD11	1:B:651:GLN:HG2	1.64	0.79
1:F:354:LEU:HD22	1:F:457:ASN:HB2	1.65	0.79
1:A:479:LEU:HB3	1:A:640:GLU:HG2	1.65	0.79
1:A:490:ILE:HG21	1:A:518:GLU:HB2	1.65	0.78
1:C:320:GLY:HA3	1:D:417:PRO:HA	1.64	0.78
1:B:481:ALA:CB	1:C:478:GLN:HG3	2.13	0.78
1:A:657:LEU:HB3	1:F:658:LEU:HD21	1.63	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:517:MET:HG2	1:D:650:ARG:CZ	2.14	0.78
1:A:480:LYS:HG2	1:A:527:GLU:HB2	1.64	0.78
1:D:279:LEU:O	1:D:286:ARG:HD2	1.82	0.78
1:F:430:TRP:HE1	1:F:587:SER:HA	1.48	0.78
1:E:427:ARG:HH21	1:E:575:ARG:HG2	1.46	0.78
1:F:426:LEU:HA	1:F:429:VAL:HB	1.66	0.78
1:C:649:LYS:HA	1:C:652:LYS:HB3	1.66	0.78
1:E:424:PHE:HD1	1:E:582:ARG:CZ	1.97	0.78
1:F:17:MET:O	1:F:18:LYS:HD2	1.83	0.78
1:F:486:PHE:HZ	1:F:651:GLN:OE1	1.67	0.78
1:E:318:VAL:HG21	1:E:346:ILE:HD11	1.66	0.78
1:A:479:LEU:HD12	1:A:640:GLU:CG	2.14	0.78
1:E:578:PRO:HB2	1:E:581:GLN:OE1	1.83	0.77
1:D:479:LEU:CD1	1:D:641:LYS:HG2	2.14	0.77
1:C:458:LEU:HD11	1:C:544:ILE:CG2	2.14	0.77
1:C:419:ARG:NH2	1:D:345:GLY:HA3	1.99	0.77
1:A:192:GLU:HG2	1:A:283:TRP:HB2	1.67	0.77
1:A:353:LEU:HB3	1:A:386:LEU:HD11	1.67	0.77
1:C:259:LEU:HB2	1:C:274:GLU:HG3	1.65	0.77
1:F:89:ASN:HB2	1:F:91:LEU:HG	1.66	0.77
1:D:290:THR:HG23	1:D:296:PRO:HA	1.67	0.77
1:D:67:ARG:HH21	1:D:68:LEU:HD12	1.47	0.77
1:D:478:GLN:HA	1:E:478:GLN:HG3	1.66	0.77
1:E:356:GLU:HA	1:E:453:ALA:HB2	1.65	0.77
1:D:261:TYR:N	1:D:262:PRO:HD2	2.00	0.77
1:D:404:ARG:H	1:D:404:ARG:HH21	1.29	0.76
1:C:21:LEU:HG	1:C:165:ILE:HD13	1.67	0.76
1:B:213:PHE:CE2	1:B:221:PRO:HG2	2.20	0.76
1:D:467:LYS:HD3	1:D:541:GLN:NE2	2.00	0.76
1:C:185:THR:O	1:C:186:LEU:HD23	1.85	0.76
1:E:531:LYS:HB3	1:E:531:LYS:HZ3	1.50	0.76
1:F:626:LEU:H	1:F:627:PRO:CD	1.94	0.76
1:F:263:ASN:ND2	1:F:265:LEU:HD22	2.00	0.76
1:E:223:LEU:H	1:E:224:PRO:HD2	1.48	0.76
1:E:353:LEU:HB3	1:E:386:LEU:HD11	1.68	0.76
1:F:104:LEU:HD23	1:F:148:PRO:HB3	1.67	0.76
1:B:286:ARG:HA	1:B:290:THR:HG21	1.67	0.76
1:F:627:PRO:HA	1:F:630:GLU:HB3	1.67	0.76
1:F:263:ASN:HD21	1:F:265:LEU:HD22	1.50	0.76
1:B:260:PRO:C	1:B:262:PRO:HD2	2.05	0.76
1:B:589:GLU:HG3	1:B:592:ARG:HH12	1.50	0.76
1:E:420:ASN:O	1:E:421:LEU:HB2	1.84	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:387:VAL:CG1	1:E:450:GLY:HA2	2.15	0.76
1:E:574:LEU:HD21	1:E:582:ARG:HH22	1.50	0.76
1:B:649:LYS:HA	1:B:652:LYS:HB3	1.66	0.76
1:A:402:SER:N	1:A:403:PRO:HD3	2.01	0.76
1:D:21:LEU:HG	1:D:165:ILE:HD13	1.68	0.76
1:A:21:LEU:HG	1:A:165:ILE:HD13	1.66	0.76
1:E:362:ILE:H	1:E:362:ILE:HD12	1.50	0.76
1:C:362:ILE:H	1:C:362:ILE:HD12	1.51	0.76
1:C:486:PHE:CZ	1:C:647:GLN:HB3	2.21	0.75
1:C:319:THR:HG23	1:C:320:GLY:H	1.50	0.75
1:E:105:ARG:HD2	1:E:148:PRO:HB2	1.67	0.75
1:A:140:ARG:HE	1:A:173:LEU:HD23	1.51	0.75
1:F:192:GLU:HG2	1:F:283:TRP:HB3	1.68	0.75
1:E:67:ARG:HH21	1:E:68:LEU:HD12	1.50	0.75
1:A:61:GLU:OE1	1:A:168:GLY:HA2	1.87	0.75
1:E:282:MET:HG2	1:E:286:ARG:HE	1.49	0.75
1:C:570:LEU:HD22	1:C:590:MET:HE2	1.67	0.75
1:F:362:ILE:H	1:F:362:ILE:HD12	1.51	0.75
1:D:214:GLU:HG3	1:D:220:ARG:H	1.51	0.75
1:E:309:LEU:HD22	1:E:310:LYS:H	1.50	0.75
1:D:496:LYS:HA	1:E:655:TRP:NE1	2.02	0.75
1:F:430:TRP:CZ3	1:F:570:LEU:HB3	2.22	0.75
1:E:540:LEU:HA	1:E:543:ASP:HB2	1.69	0.75
1:A:282:MET:HG3	1:A:283:TRP:CE3	2.21	0.74
1:C:506:THR:HG22	1:C:507:SER:H	1.52	0.74
1:F:214:GLU:HG3	1:F:219:PHE:HA	1.69	0.74
1:A:657:LEU:C	1:F:658:LEU:HD11	2.08	0.74
1:C:540:LEU:HA	1:C:543:ASP:HB2	1.69	0.74
1:D:223:LEU:HD12	1:D:226:TRP:HB2	1.69	0.74
1:B:457:ASN:HD21	1:B:619:LYS:NZ	1.84	0.74
1:D:223:LEU:HB3	1:D:231:TRP:CZ3	2.22	0.74
1:D:232:HIS:O	1:D:236:ARG:HB2	1.88	0.74
1:B:447:LEU:HD23	1:B:609:TYR:HE1	1.51	0.74
1:E:505:ILE:HD12	1:E:506:THR:N	2.02	0.74
1:B:367:ALA:C	1:B:369:GLN:H	1.90	0.74
1:A:417:PRO:C	1:B:320:GLY:HA3	2.08	0.74
1:A:434:TRP:HB3	1:A:571:TYR:OH	1.88	0.74
1:B:362:ILE:H	1:B:362:ILE:HD12	1.53	0.74
1:E:366:PRO:HG2	1:E:368:THR:HG22	1.70	0.74
1:D:117:LEU:HB2	1:D:215:CYS:O	1.88	0.74
1:A:362:ILE:HD12	1:A:362:ILE:H	1.53	0.74
1:C:496:LYS:NZ	1:C:654:LEU:HD11	2.03	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:265:LEU:CG	1:E:266:ASN:H	2.00	0.74
1:A:490:ILE:HG12	1:A:517:MET:CE	2.17	0.74
1:B:451:GLN:NE2	1:B:611:GLN:HB3	2.03	0.74
1:A:579:ARG:N	1:A:579:ARG:HH11	1.85	0.73
1:E:21:LEU:HB3	1:E:165:ILE:HG21	1.69	0.73
1:E:627:PRO:HA	1:E:630:GLU:HB3	1.68	0.73
1:F:570:LEU:HD22	1:F:590:MET:HE2	1.70	0.73
1:D:283:TRP:CE3	1:D:285:PRO:HD2	2.23	0.73
1:B:261:TYR:N	1:B:262:PRO:HD2	2.03	0.73
1:D:410:VAL:HA	1:D:413:ILE:HG22	1.68	0.73
1:A:358:GLY:HA3	1:A:457:ASN:HB2	1.70	0.73
1:A:309:LEU:HD11	1:A:311:LEU:HD23	1.70	0.73
1:D:242:ASP:OD1	1:D:257:SER:HB3	1.88	0.73
1:C:589:GLU:HG3	1:C:592:ARG:HH12	1.53	0.73
1:E:284:HIS:HB3	1:E:285:PRO:CD	2.17	0.73
1:A:533:LEU:HD13	1:A:629:VAL:HA	1.69	0.73
1:D:265:LEU:HG	1:D:266:ASN:H	1.53	0.73
1:F:29:VAL:HG12	1:F:44:LYS:HB2	1.70	0.73
1:B:226:TRP:C	1:B:227:GLN:HG3	2.07	0.73
1:E:61:GLU:HB2	1:E:178:LEU:HD11	1.70	0.73
1:E:626:LEU:H	1:E:627:PRO:HD2	1.54	0.73
1:F:540:LEU:HA	1:F:543:ASP:HB2	1.70	0.73
1:D:649:LYS:HA	1:D:652:LYS:HB3	1.70	0.73
1:B:410:VAL:HA	1:B:413:ILE:HG22	1.71	0.73
1:C:410:VAL:HA	1:C:413:ILE:HG22	1.71	0.73
1:E:368:THR:HG23	1:E:369:GLN:H	1.54	0.73
1:B:486:PHE:CZ	1:B:647:GLN:HB3	2.23	0.73
1:A:589:GLU:HG3	1:A:592:ARG:HH12	1.53	0.73
1:C:426:LEU:HA	1:C:429:VAL:HB	1.71	0.73
1:F:430:TRP:HZ3	1:F:570:LEU:HB3	1.52	0.73
1:D:55:ARG:HH11	1:D:91:LEU:HD21	1.52	0.73
1:A:417:PRO:O	1:B:320:GLY:HA3	1.89	0.73
1:E:192:GLU:HG2	1:E:283:TRP:HB3	1.70	0.73
1:A:205:TYR:HD1	1:A:290:THR:HG23	1.53	0.72
1:A:410:VAL:HA	1:A:413:ILE:HG22	1.69	0.72
1:A:117:LEU:HD12	1:A:215:CYS:O	1.90	0.72
1:D:353:LEU:HB3	1:D:386:LEU:HD11	1.71	0.72
1:A:294:TYR:O	1:A:301:LYS:HD3	1.88	0.72
1:F:265:LEU:O	1:F:266:ASN:HB2	1.88	0.72
1:F:223:LEU:N	1:F:224:PRO:HD2	2.04	0.72
1:A:290:THR:N	1:A:298:GLY:H	1.87	0.72
1:B:126:LEU:HB3	1:B:303:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:140:ARG:HH21	1:C:173:LEU:HD22	1.54	0.72
1:C:223:LEU:HG	1:C:245:VAL:HG12	1.70	0.72
1:F:649:LYS:HA	1:F:652:LYS:HB3	1.72	0.72
1:A:570:LEU:HD22	1:A:590:MET:HE2	1.72	0.72
1:B:422:ALA:O	1:B:585:GLY:HA2	1.90	0.72
1:F:245:VAL:HG13	1:F:255:PHE:HB3	1.70	0.72
1:E:19:GLU:O	1:E:20:ARG:HD3	1.89	0.72
1:A:659:LYS:HD3	1:F:500:GLN:NE2	2.03	0.72
1:B:506:THR:HG22	1:B:507:SER:H	1.55	0.72
1:A:340:ILE:HD11	1:A:351:GLN:OE1	1.90	0.72
1:C:249:LEU:HD23	1:C:418:LYS:NZ	2.05	0.72
1:D:223:LEU:HD13	1:D:224:PRO:HD2	1.71	0.72
1:C:500:GLN:NE2	1:C:504:GLY:HA3	2.05	0.72
1:E:410:VAL:HA	1:E:413:ILE:HG22	1.70	0.72
1:C:186:LEU:HG	1:C:228:PRO:HG2	1.71	0.72
1:E:649:LYS:HA	1:E:652:LYS:HB3	1.71	0.72
1:C:457:ASN:HD21	1:C:619:LYS:NZ	1.86	0.72
1:A:540:LEU:HA	1:A:543:ASP:HB2	1.70	0.72
1:A:477:GLN:OE1	1:F:478:GLN:NE2	2.23	0.72
1:A:661:ALA:HB1	1:F:662:CYS:SG	2.30	0.72
1:E:118:ARG:HB2	1:E:264:ASN:HB3	1.70	0.72
1:A:231:TRP:NE1	1:A:235:VAL:HG21	2.04	0.71
1:B:528:ASN:H	1:B:528:ASN:HD22	1.36	0.71
1:B:19:GLU:O	1:B:20:ARG:HD3	1.90	0.71
1:D:290:THR:HG22	1:D:291:ASP:H	1.54	0.71
1:A:480:LYS:CG	1:A:527:GLU:HB2	2.20	0.71
1:D:118:ARG:HH12	1:D:438:GLN:HG2	1.54	0.71
1:A:626:LEU:H	1:A:627:PRO:HD2	1.53	0.71
1:F:279:LEU:HD21	1:F:291:ASP:HA	1.71	0.71
1:B:142:ILE:HG22	1:B:144:ARG:HG2	1.73	0.71
1:B:394:LYS:HD3	1:B:402:SER:H	1.54	0.71
1:A:486:PHE:HE2	1:A:518:GLU:HA	1.56	0.71
1:B:140:ARG:HB3	1:B:173:LEU:HD11	1.72	0.71
1:C:340:ILE:HD11	1:C:351:GLN:OE1	1.90	0.71
1:B:627:PRO:HA	1:B:630:GLU:HB3	1.70	0.71
1:E:354:LEU:CD1	1:E:454:ALA:HA	2.20	0.71
1:D:419:ARG:NH2	1:D:420:ASN:HB2	2.06	0.71
1:F:467:LYS:HD3	1:F:541:GLN:HG2	1.73	0.71
1:B:120:GLY:O	1:B:123:LEU:HD23	1.91	0.71
1:A:312:VAL:HG22	1:A:313:HIS:H	1.56	0.71
1:F:589:GLU:HG3	1:F:592:ARG:HH12	1.55	0.71
1:B:478:GLN:HG3	1:C:481:ALA:CB	2.20	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:426:LEU:HA	1:D:429:VAL:HB	1.72	0.71
1:E:500:GLN:CD	1:E:505:ILE:HG12	2.10	0.71
1:C:118:ARG:HH22	1:C:438:GLN:HG2	1.56	0.71
1:E:46:CYS:SG	1:E:91:LEU:HD11	2.31	0.71
1:A:533:LEU:CD2	1:A:629:VAL:HG12	2.17	0.71
1:F:357:ALA:C	1:F:456:MET:HG2	2.10	0.71
1:E:426:LEU:HA	1:E:429:VAL:HB	1.72	0.71
1:F:430:TRP:C	1:F:571:TYR:HE2	1.94	0.71
1:B:243:ILE:HG22	1:B:281:LEU:HD23	1.72	0.71
1:B:408:GLU:HG3	1:B:409:SER:H	1.55	0.71
1:F:384:MET:HG2	1:F:385:ASP:N	2.04	0.70
1:D:187:GLN:HE21	1:D:220:ARG:HH11	1.38	0.70
1:C:447:LEU:HD23	1:C:609:TYR:CE1	2.25	0.70
1:D:627:PRO:HA	1:D:630:GLU:HB3	1.73	0.70
1:B:242:ASP:HA	1:B:257:SER:OG	1.91	0.70
1:A:19:GLU:O	1:A:20:ARG:HD3	1.91	0.70
1:B:426:LEU:HA	1:B:429:VAL:HB	1.71	0.70
1:F:410:VAL:HA	1:F:413:ILE:HG22	1.74	0.70
1:D:540:LEU:HD21	1:D:622:ALA:HB2	1.71	0.70
1:A:355:GLN:HE22	1:A:370:CYS:HA	1.54	0.70
1:F:16:GLU:HB3	1:F:33:HIS:H	1.55	0.70
1:E:240:GLU:HG3	1:E:241:VAL:HG23	1.74	0.70
1:D:479:LEU:HD11	1:D:641:LYS:CG	2.17	0.70
1:E:213:PHE:HA	1:E:277:LEU:HD21	1.72	0.70
1:F:220:ARG:NE	1:F:221:PRO:HD2	2.05	0.70
1:B:221:PRO:O	1:B:222:PHE:HB2	1.91	0.70
1:D:55:ARG:HD2	1:D:91:LEU:HD21	1.74	0.70
1:E:357:ALA:C	1:E:456:MET:HG2	2.11	0.70
1:D:505:ILE:CD1	1:D:506:THR:H	2.04	0.70
1:D:540:LEU:HA	1:D:543:ASP:HB2	1.73	0.70
1:E:105:ARG:CD	1:E:148:PRO:HB2	2.22	0.70
1:D:372:SER:H	1:D:384:MET:HE2	1.53	0.70
1:E:392:ASN:CG	1:E:393:SER:H	1.94	0.70
1:C:407:PRO:HG2	1:C:408:GLU:H	1.56	0.70
1:D:61:GLU:HB2	1:D:178:LEU:HD11	1.73	0.70
1:E:333:LEU:HD23	1:E:363:PRO:HA	1.72	0.70
1:F:240:GLU:HG3	1:F:241:VAL:HG23	1.72	0.70
1:D:589:GLU:HG3	1:D:592:ARG:HH12	1.56	0.70
1:A:283:TRP:CD1	1:A:285:PRO:HD2	2.26	0.70
1:B:366:PRO:HB2	1:B:368:THR:CG2	2.14	0.70
1:F:17:MET:HG2	1:F:32:TRP:HE1	1.57	0.70
1:F:431:GLY:HA2	1:F:571:TYR:CE2	2.27	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:ARG:N	1:A:221:PRO:HD3	2.07	0.69
1:C:55:ARG:HH12	1:C:91:LEU:HD11	1.57	0.69
1:A:182:PHE:O	1:A:183:VAL:HG22	1.92	0.69
1:B:117:LEU:HB3	1:B:119:GLU:OE1	1.92	0.69
1:F:279:LEU:O	1:F:286:ARG:HB3	1.91	0.69
1:A:649:LYS:HA	1:A:652:LYS:HB3	1.73	0.69
1:E:589:GLU:HG3	1:E:592:ARG:HH12	1.56	0.69
1:E:284:HIS:CB	1:E:285:PRO:HD2	2.20	0.69
1:D:227:GLN:H	1:D:227:GLN:CD	1.96	0.69
1:D:500:GLN:HB3	1:D:505:ILE:HG12	1.72	0.69
1:B:558:GLY:HA2	1:B:562:ASP:HB2	1.74	0.69
1:F:70:HIS:HE1	1:F:132:ALA:HA	1.56	0.69
1:B:419:ARG:HH22	1:B:588:GLN:HG3	1.57	0.69
1:B:500:GLN:NE2	1:B:504:GLY:HA3	2.07	0.69
1:B:29:VAL:HG12	1:B:44:LYS:HB2	1.74	0.69
1:D:549:ARG:HB2	1:D:549:ARG:NH1	2.07	0.69
1:A:292:PRO:HG3	1:A:297:ASN:ND2	2.05	0.69
1:F:265:LEU:H	1:F:265:LEU:HD23	1.57	0.69
1:F:19:GLU:O	1:F:20:ARG:HD3	1.91	0.69
1:E:29:VAL:HG12	1:E:44:LYS:HB2	1.74	0.69
1:D:626:LEU:O	1:D:629:VAL:HG22	1.92	0.69
1:D:118:ARG:HB2	1:D:264:ASN:OD1	1.91	0.69
1:C:627:PRO:HA	1:C:630:GLU:HB3	1.75	0.69
1:F:17:MET:HG2	1:F:32:TRP:NE1	2.08	0.69
1:A:285:PRO:O	1:A:290:THR:HB	1.93	0.69
1:C:290:THR:HG22	1:C:296:PRO:O	1.93	0.69
1:C:500:GLN:HB3	1:C:505:ILE:HG23	1.74	0.69
1:B:457:ASN:HD21	1:B:619:LYS:HZ1	1.40	0.69
1:B:570:LEU:HD22	1:B:590:MET:HE2	1.74	0.69
1:D:77:ARG:H	1:D:96:MET:HA	1.58	0.69
1:E:117:LEU:HB2	1:E:215:CYS:O	1.93	0.69
1:B:540:LEU:HA	1:B:543:ASP:HB2	1.75	0.69
1:B:496:LYS:CE	1:B:654:LEU:HD21	2.22	0.69
1:C:434:TRP:HB3	1:C:571:TYR:CZ	2.26	0.69
1:D:580:ASP:HA	1:D:582:ARG:CZ	2.22	0.69
1:B:312:VAL:HG22	1:B:313:HIS:H	1.57	0.69
1:D:17:MET:O	1:D:18:LYS:HD2	1.92	0.69
1:F:430:TRP:CZ3	1:F:570:LEU:HD23	2.29	0.69
1:D:187:GLN:HE21	1:D:220:ARG:NH1	1.90	0.69
1:B:279:LEU:HA	1:B:286:ARG:HH12	1.58	0.69
1:B:290:THR:HA	1:B:296:PRO:HA	1.75	0.69
1:C:526:ARG:NE	1:C:526:ARG:HA	2.07	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:17:MET:HG2	1:E:33:HIS:N	2.08	0.68
1:D:170:ALA:HB3	1:D:178:LEU:CD2	2.23	0.68
1:E:248:ASP:OD1	1:E:254:LYS:HE2	1.93	0.68
1:D:477:GLN:HG3	1:E:478:GLN:HB2	1.75	0.68
1:F:333:LEU:HD23	1:F:363:PRO:HA	1.74	0.68
1:A:394:LYS:CG	1:A:401:ILE:HG13	2.23	0.68
1:A:480:LYS:HG2	1:A:527:GLU:CD	2.14	0.68
1:A:333:LEU:HD23	1:A:363:PRO:HA	1.73	0.68
1:D:403:PRO:HA	1:D:404:ARG:HH21	1.57	0.68
1:D:115:CYS:SG	1:D:116:GLY:N	2.65	0.68
1:E:226:TRP:CH2	1:E:228:PRO:HB2	2.28	0.68
1:F:394:LYS:HE3	1:F:401:ILE:N	2.08	0.68
1:D:536:ARG:CZ	1:D:625:LEU:HD13	2.23	0.68
1:D:333:LEU:HD23	1:D:363:PRO:HA	1.75	0.68
1:C:353:LEU:HB3	1:C:386:LEU:HD11	1.75	0.68
1:E:362:ILE:N	1:E:362:ILE:HD12	2.09	0.68
1:B:213:PHE:HA	1:B:277:LEU:HD21	1.76	0.68
1:D:486:PHE:CZ	1:D:647:GLN:HB3	2.28	0.68
1:A:259:LEU:HD13	1:A:259:LEU:O	1.94	0.68
1:F:362:ILE:N	1:F:362:ILE:HD12	2.09	0.68
1:A:361:LEU:HD23	1:A:369:GLN:HE21	1.59	0.68
1:C:19:GLU:O	1:C:20:ARG:HD3	1.93	0.68
1:B:467:LYS:HD3	1:B:541:GLN:NE2	2.08	0.68
1:F:430:TRP:CH2	1:F:570:LEU:HD23	2.29	0.68
1:E:366:PRO:HG2	1:E:368:THR:CG2	2.23	0.68
1:A:356:GLU:HA	1:A:453:ALA:CB	2.24	0.68
1:D:16:GLU:N	1:D:33:HIS:H	1.91	0.68
1:C:420:ASN:ND2	1:C:421:LEU:H	1.92	0.67
1:D:490:ILE:HG21	1:D:517:MET:HE2	1.76	0.67
1:D:221:PRO:O	1:D:222:PHE:HB2	1.93	0.67
1:D:480:LYS:HG2	1:D:527:GLU:CD	2.15	0.67
1:D:362:ILE:H	1:D:362:ILE:HD12	1.59	0.67
1:C:249:LEU:HD23	1:C:418:LYS:HZ3	1.55	0.67
1:E:570:LEU:HD22	1:E:590:MET:HE2	1.75	0.67
1:C:362:ILE:HD12	1:C:362:ILE:N	2.09	0.67
1:A:362:ILE:HD12	1:A:362:ILE:N	2.09	0.67
1:A:29:VAL:HG12	1:A:44:LYS:HB2	1.76	0.67
1:B:325:TYR:CE2	1:B:340:ILE:HG22	2.29	0.67
1:D:120:GLY:O	1:D:123:LEU:HD23	1.94	0.67
1:F:602:GLU:O	1:F:606:ARG:HG2	1.95	0.67
1:F:421:LEU:CB	1:F:586:ASP:HA	2.24	0.67
1:B:229:VAL:HG23	1:B:230:GLN:H	1.59	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:57:ARG:O	1:C:60:LEU:HB3	1.95	0.67
1:F:501:THR:O	1:F:502:GLU:HB2	1.93	0.67
1:A:49:GLU:OE2	1:A:89:ASN:HA	1.94	0.67
1:F:394:LYS:HD2	1:F:401:ILE:O	1.95	0.67
1:A:279:LEU:HA	1:A:286:ARG:NH1	2.05	0.67
1:E:602:GLU:O	1:E:606:ARG:HG2	1.95	0.67
1:D:229:VAL:C	1:D:231:TRP:H	1.98	0.67
1:D:29:VAL:HG12	1:D:44:LYS:HB2	1.75	0.67
1:F:458:LEU:CD2	1:F:619:LYS:HA	2.23	0.67
1:C:407:PRO:O	1:C:408:GLU:HB2	1.92	0.67
1:F:187:GLN:CD	1:F:223:LEU:HG	2.15	0.67
1:B:171:LYS:HG3	1:B:199:TYR:OH	1.95	0.67
1:B:236:ARG:HD3	1:B:283:TRP:CZ3	2.30	0.67
1:E:102:GLY:HA2	1:E:153:LEU:H	1.60	0.67
1:A:325:TYR:CE2	1:A:340:ILE:HG22	2.29	0.67
1:B:102:GLY:HA2	1:B:153:LEU:H	1.58	0.67
1:B:479:LEU:CD1	1:B:641:LYS:HG2	2.21	0.67
1:C:419:ARG:N	1:C:419:ARG:HD3	2.08	0.67
1:F:236:ARG:NH2	1:F:283:TRP:HE1	1.93	0.67
1:D:416:GLU:C	1:D:418:LYS:H	1.98	0.67
1:A:118:ARG:CB	1:A:264:ASN:HB3	2.24	0.66
1:D:486:PHE:CE1	1:D:647:GLN:HB3	2.28	0.66
1:C:240:GLU:HG3	1:C:241:VAL:HG23	1.75	0.66
1:B:458:LEU:HD11	1:B:544:ILE:HG21	1.77	0.66
1:A:420:ASN:HD22	1:B:345:GLY:HA3	1.60	0.66
1:C:462:ASN:O	1:C:466:SER:HB3	1.95	0.66
1:F:480:LYS:HG2	1:F:527:GLU:HB3	1.77	0.66
1:E:295:GLY:N	1:E:296:PRO:HD2	2.08	0.66
1:F:422:ALA:O	1:F:585:GLY:HA3	1.95	0.66
1:C:490:ILE:HG21	1:C:517:MET:HE2	1.75	0.66
1:C:213:PHE:HA	1:C:277:LEU:HD21	1.76	0.66
1:D:496:LYS:HD2	1:E:655:TRP:CD1	2.30	0.66
1:D:328:THR:HG23	1:D:331:GLU:HG3	1.77	0.66
1:F:227:GLN:HA	1:F:231:TRP:CE3	2.31	0.66
1:D:626:LEU:HB3	1:D:627:PRO:CD	2.26	0.66
1:A:172:GLU:HG3	1:A:174:ASP:H	1.61	0.66
1:A:420:ASN:ND2	1:B:345:GLY:HA3	2.10	0.66
1:A:490:ILE:HG12	1:A:517:MET:HE1	1.77	0.66
1:D:310:LYS:HB2	1:D:310:LYS:HZ3	1.61	0.66
1:F:354:LEU:CD1	1:F:454:ALA:HA	2.26	0.66
1:F:421:LEU:CG	1:F:586:ASP:HA	2.24	0.66
1:B:340:ILE:HD11	1:B:351:GLN:OE1	1.96	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:118:ARG:HB2	1:F:264:ASN:OD1	1.96	0.66
1:B:415:GLN:O	1:B:419:ARG:HG3	1.95	0.66
1:D:404:ARG:N	1:D:404:ARG:HH21	1.93	0.66
1:D:496:LYS:HA	1:E:655:TRP:HE1	1.61	0.66
1:A:117:LEU:HB3	1:A:119:GLU:OE1	1.95	0.66
1:E:434:TRP:CZ3	1:E:568:ARG:HB2	2.31	0.66
1:C:77:ARG:H	1:C:96:MET:HA	1.60	0.66
1:B:77:ARG:H	1:B:96:MET:HA	1.60	0.66
1:F:312:VAL:HG22	1:F:313:HIS:H	1.61	0.66
1:B:282:MET:HG3	1:B:283:TRP:CD1	2.30	0.66
1:E:236:ARG:HH22	1:E:283:TRP:HE1	1.42	0.66
1:A:533:LEU:HD13	1:A:629:VAL:CB	2.26	0.66
1:D:182:PHE:HZ	1:D:194:LEU:HD23	1.61	0.65
1:B:362:ILE:N	1:B:362:ILE:HD12	2.11	0.65
1:A:246:SER:O	1:A:253:VAL:HA	1.96	0.65
1:A:528:ASN:O	1:A:532:LEU:HD23	1.96	0.65
1:C:517:MET:HG2	1:C:650:ARG:CZ	2.26	0.65
1:B:220:ARG:N	1:B:221:PRO:HD3	2.11	0.65
1:D:418:LYS:HE3	1:D:421:LEU:HD12	1.79	0.65
1:A:213:PHE:CE2	1:A:221:PRO:HG2	2.30	0.65
1:C:479:LEU:CD1	1:C:641:LYS:HG2	2.17	0.65
1:F:357:ALA:CA	1:F:452:ARG:HH12	2.07	0.65
1:E:57:ARG:O	1:E:60:LEU:HB3	1.96	0.65
1:C:20:ARG:CB	1:C:23:THR:HB	2.27	0.65
1:A:426:LEU:HA	1:A:429:VAL:HB	1.78	0.65
1:F:427:ARG:HH21	1:F:575:ARG:CG	2.09	0.65
1:D:418:LYS:NZ	1:D:421:LEU:HD12	2.11	0.65
1:D:19:GLU:O	1:D:20:ARG:HD3	1.96	0.65
1:E:249:LEU:HD13	1:E:414:LEU:HG	1.78	0.65
1:F:371:ILE:HA	1:F:384:MET:HE1	1.79	0.65
1:A:529:GLU:OE2	1:A:632:VAL:HG21	1.97	0.65
1:A:102:GLY:HA2	1:A:153:LEU:H	1.62	0.65
1:D:422:ALA:O	1:D:585:GLY:HA3	1.97	0.65
1:E:577:LYS:HG3	1:E:578:PRO:HD2	1.79	0.65
1:B:451:GLN:HA	1:B:454:ALA:HB3	1.79	0.65
1:B:102:GLY:CA	1:B:153:LEU:H	2.09	0.65
1:F:423:PHE:HD1	1:F:583:THR:HA	1.61	0.65
1:B:245:VAL:O	1:B:245:VAL:HG12	1.96	0.65
1:F:285:PRO:HG2	1:F:286:ARG:HE	1.62	0.65
1:F:428:LYS:HG3	1:F:429:VAL:N	2.10	0.65
1:A:243:ILE:HG22	1:A:281:LEU:HD23	1.78	0.65
1:F:212:ALA:O	1:F:216:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:ARG:H	1:A:96:MET:HA	1.61	0.65
1:B:602:GLU:O	1:B:606:ARG:HG2	1.97	0.65
1:F:310:LYS:HB2	1:F:310:LYS:HZ3	1.62	0.65
1:B:36:GLU:OE2	1:E:359:LEU:HA	1.97	0.65
1:A:102:GLY:CA	1:A:153:LEU:H	2.10	0.65
1:C:217:THR:HA	1:C:263:ASN:CG	2.17	0.64
1:F:389:LEU:HD21	1:F:454:ALA:HB1	1.74	0.64
1:A:231:TRP:CE2	1:A:235:VAL:HG21	2.32	0.64
1:F:102:GLY:HA2	1:F:153:LEU:H	1.61	0.64
1:A:89:ASN:HD22	1:A:89:ASN:H	1.43	0.64
1:F:57:ARG:O	1:F:60:LEU:HB3	1.97	0.64
1:C:365:LYS:HE2	1:C:365:LYS:HA	1.79	0.64
1:F:394:LYS:HG2	1:F:401:ILE:N	2.12	0.64
1:B:626:LEU:HB3	1:B:627:PRO:CD	2.27	0.64
1:A:451:GLN:HA	1:A:454:ALA:HB3	1.79	0.64
1:D:451:GLN:HA	1:D:454:ALA:HB3	1.78	0.64
1:E:77:ARG:H	1:E:96:MET:HA	1.61	0.64
1:F:626:LEU:N	1:F:627:PRO:CD	2.50	0.64
1:D:213:PHE:CE2	1:D:221:PRO:HG2	2.33	0.64
1:F:21:LEU:HG	1:F:165:ILE:HD13	1.80	0.64
1:D:481:ALA:CB	1:E:482:LYS:HD2	2.25	0.64
1:A:20:ARG:CB	1:A:23:THR:HB	2.28	0.64
1:D:545:VAL:HA	1:D:548:GLN:HE22	1.62	0.64
1:C:29:VAL:HG12	1:C:44:LYS:HB2	1.79	0.64
1:B:392:ASN:CG	1:B:393:SER:H	2.01	0.64
1:C:114:CYS:SG	1:C:115:CYS:N	2.71	0.64
1:E:577:LYS:HE3	1:E:584:GLU:OE1	1.96	0.64
1:C:282:MET:HG3	1:C:283:TRP:CE3	2.33	0.64
1:F:426:LEU:O	1:F:430:TRP:HB2	1.98	0.64
1:F:80:PRO:CB	1:F:83:MET:HB2	2.27	0.64
1:B:20:ARG:CB	1:B:23:THR:HB	2.28	0.64
1:C:517:MET:HG2	1:C:650:ARG:NE	2.12	0.64
1:B:104:LEU:HD23	1:B:148:PRO:HB3	1.78	0.64
1:F:577:LYS:HG3	1:F:578:PRO:HD2	1.80	0.64
1:D:602:GLU:O	1:D:606:ARG:HG2	1.97	0.64
1:F:465:LEU:O	1:F:626:LEU:HD11	1.98	0.64
1:A:417:PRO:HA	1:B:320:GLY:HA2	1.79	0.64
1:E:286:ARG:HB3	1:E:286:ARG:HH11	1.62	0.64
1:C:570:LEU:HD22	1:C:590:MET:CE	2.28	0.64
1:B:428:LYS:HG3	1:B:429:VAL:N	2.12	0.64
1:A:394:LYS:HG2	1:A:401:ILE:HG13	1.80	0.64
1:C:402:SER:H	1:C:403:PRO:CD	2.06	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:426:LEU:O	1:E:430:TRP:HB2	1.98	0.64
1:E:60:LEU:HD13	1:E:175:GLN:HG2	1.80	0.64
1:A:655:TRP:O	1:F:500:GLN:OE1	2.16	0.64
1:E:368:THR:O	1:E:371:ILE:HG22	1.98	0.64
1:E:328:THR:HG23	1:E:331:GLU:HG3	1.80	0.64
1:A:263:ASN:OD1	1:A:265:LEU:HD22	1.96	0.63
1:A:265:LEU:HD23	1:A:266:ASN:N	2.10	0.63
1:C:312:VAL:HG22	1:C:313:HIS:H	1.61	0.63
1:E:631:GLU:O	1:E:635:LEU:HG	1.98	0.63
1:C:320:GLY:HA2	1:C:405:PRO:HG3	1.79	0.63
1:C:126:LEU:HB3	1:C:303:LEU:HD21	1.80	0.63
1:D:655:TRP:CD1	1:E:496:LYS:HD2	2.33	0.63
1:C:496:LYS:HZ3	1:C:654:LEU:HD11	1.62	0.63
1:C:402:SER:N	1:C:403:PRO:CD	2.62	0.63
1:E:21:LEU:HD23	1:E:165:ILE:HG23	1.81	0.63
1:E:120:GLY:O	1:E:123:LEU:HD23	1.98	0.63
1:E:310:LYS:HZ3	1:E:310:LYS:HB2	1.63	0.63
1:E:102:GLY:CA	1:E:153:LEU:H	2.12	0.63
1:D:655:TRP:CE2	1:E:496:LYS:HD2	2.34	0.63
1:B:193:LEU:HD22	1:B:203:VAL:CG2	2.29	0.63
1:E:16:GLU:HG3	1:E:32:TRP:NE1	2.14	0.63
1:D:193:LEU:HD22	1:D:203:VAL:CG2	2.27	0.63
1:B:528:ASN:N	1:B:528:ASN:HD22	1.95	0.63
1:C:104:LEU:HD23	1:C:148:PRO:HB3	1.81	0.63
1:E:340:ILE:HD11	1:E:351:GLN:OE1	1.99	0.63
1:D:223:LEU:CD1	1:D:226:TRP:HB2	2.29	0.63
1:B:333:LEU:HD23	1:B:363:PRO:HA	1.79	0.63
1:D:428:LYS:HG3	1:D:429:VAL:N	2.13	0.63
1:A:651:GLN:HB2	1:F:493:ASP:OD2	1.99	0.63
1:A:117:LEU:HB2	1:A:215:CYS:O	1.99	0.63
1:A:57:ARG:O	1:A:60:LEU:HB3	1.98	0.63
1:C:602:GLU:O	1:C:606:ARG:HG2	1.99	0.63
1:A:193:LEU:HD22	1:A:203:VAL:CG2	2.29	0.63
1:F:77:ARG:H	1:F:96:MET:HA	1.64	0.63
1:C:451:GLN:HA	1:C:454:ALA:HB3	1.79	0.63
1:E:462:ASN:O	1:E:466:SER:HB3	1.99	0.63
1:C:418:LYS:HA	1:D:344:THR:HG23	1.80	0.62
1:C:511:LEU:CG	1:C:515:ARG:HH12	2.11	0.62
1:C:533:LEU:HD22	1:C:629:VAL:HG12	1.80	0.62
1:C:114:CYS:SG	1:C:575:ARG:NH1	2.70	0.62
1:F:570:LEU:HD22	1:F:590:MET:CE	2.29	0.62
1:E:20:ARG:CB	1:E:23:THR:HB	2.28	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:517:MET:HG2	1:D:650:ARG:NE	2.14	0.62
1:A:480:LYS:HG2	1:A:527:GLU:CG	2.30	0.62
1:B:434:TRP:HB3	1:B:571:TYR:CZ	2.34	0.62
1:F:296:PRO:HG2	1:F:297:ASN:H	1.63	0.62
1:F:455:MET:O	1:F:459:LEU:HD13	1.99	0.62
1:F:544:ILE:O	1:F:547:LEU:HG	1.99	0.62
1:D:21:LEU:HB3	1:D:165:ILE:HG21	1.80	0.62
1:B:213:PHE:CD2	1:B:221:PRO:HG2	2.33	0.62
1:B:310:LYS:HB2	1:B:310:LYS:HZ3	1.65	0.62
1:F:401:ILE:HG12	1:F:403:PRO:CD	2.20	0.62
1:A:286:ARG:HA	1:A:290:THR:OG1	1.99	0.62
1:D:182:PHE:CZ	1:D:195:GLU:HG2	2.35	0.62
1:F:210:THR:HG22	1:F:220:ARG:HB2	1.80	0.62
1:C:545:VAL:HA	1:C:548:GLN:HE22	1.64	0.62
1:D:408:GLU:CG	1:D:413:ILE:HD13	2.29	0.62
1:A:169:TYR:OH	1:A:183:VAL:HG21	1.99	0.62
1:C:120:GLY:O	1:C:123:LEU:HD23	1.99	0.62
1:C:90:ASP:O	1:C:91:LEU:HD22	2.00	0.62
1:F:340:ILE:HD11	1:F:351:GLN:OE1	1.99	0.62
1:A:434:TRP:HB3	1:A:571:TYR:CE1	2.34	0.62
1:F:185:THR:HG22	1:F:187:GLN:H	1.65	0.62
1:B:355:GLN:O	1:B:359:LEU:HD11	1.99	0.62
1:D:213:PHE:CD1	1:D:221:PRO:HB2	2.35	0.62
1:F:631:GLU:O	1:F:635:LEU:HG	1.99	0.62
1:D:84:GLN:HE22	1:D:85:ASN:HB2	1.63	0.62
1:F:309:LEU:HD11	1:F:311:LEU:HD23	1.82	0.62
1:D:325:TYR:CE2	1:D:340:ILE:HG22	2.35	0.62
1:C:417:PRO:CA	1:D:320:GLY:HA3	2.26	0.62
1:F:542:THR:HA	1:F:545:VAL:HG22	1.81	0.62
1:D:418:LYS:CE	1:D:421:LEU:HD12	2.30	0.62
1:C:325:TYR:CE2	1:C:340:ILE:HG22	2.34	0.62
1:D:244:VAL:HB	1:D:256:SER:HB2	1.81	0.62
1:D:213:PHE:HA	1:D:277:LEU:HD21	1.81	0.62
1:A:480:LYS:HG2	1:A:527:GLU:CB	2.29	0.62
1:F:486:PHE:CZ	1:F:651:GLN:OE1	2.52	0.62
1:E:237:GLN:HG2	1:E:238:LYS:HD2	1.81	0.62
1:A:540:LEU:HD21	1:A:622:ALA:HB2	1.80	0.62
1:A:361:LEU:HD22	1:A:369:GLN:HG3	1.82	0.62
1:B:328:THR:HG23	1:B:331:GLU:HG3	1.79	0.62
1:A:583:THR:HG23	1:A:584:GLU:H	1.64	0.62
1:C:426:LEU:O	1:C:430:TRP:HB2	2.00	0.62
1:A:212:ALA:O	1:A:216:ILE:HG13	2.00	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:223:LEU:HD21	1:C:253:VAL:HG12	1.81	0.62
1:F:354:LEU:HD13	1:F:453:ALA:O	2.00	0.62
1:B:227:GLN:NE2	1:B:229:VAL:HG13	2.15	0.62
1:B:545:VAL:HA	1:B:548:GLN:HE22	1.64	0.62
1:C:366:PRO:O	1:C:368:THR:HG23	2.00	0.62
1:C:123:LEU:HD12	1:C:307:LEU:HD13	1.81	0.62
1:D:245:VAL:HA	1:D:254:LYS:O	2.00	0.62
1:C:276:TRP:CE2	1:C:280:MET:HG3	2.35	0.62
1:E:186:LEU:HD12	1:E:189:LEU:HD23	1.82	0.61
1:F:282:MET:HG2	1:F:286:ARG:NH2	2.14	0.61
1:A:505:ILE:HG12	1:A:511:LEU:HD13	1.82	0.61
1:E:649:LYS:O	1:E:653:GLU:HG3	2.00	0.61
1:A:363:PRO:HG2	1:A:364:ASP:OD1	2.00	0.61
1:E:526:ARG:HD2	1:E:636:MET:HG2	1.82	0.61
1:A:533:LEU:HD13	1:A:629:VAL:HG12	1.82	0.61
1:F:451:GLN:HA	1:F:454:ALA:HB3	1.81	0.61
1:D:105:ARG:HD2	1:D:148:PRO:HB2	1.82	0.61
1:E:21:LEU:HG	1:E:165:ILE:HD13	1.81	0.61
1:B:17:MET:N	1:B:17:MET:SD	2.73	0.61
1:A:486:PHE:HZ	1:A:517:MET:SD	2.23	0.61
1:D:118:ARG:HH12	1:D:438:GLN:CG	2.14	0.61
1:E:467:LYS:HD3	1:E:541:GLN:NE2	2.15	0.61
1:E:312:VAL:HG22	1:E:313:HIS:H	1.66	0.61
1:E:357:ALA:HA	1:E:452:ARG:HH12	1.65	0.61
1:F:34:ASN:OD1	1:F:83:MET:SD	2.58	0.61
1:C:570:LEU:HD12	1:C:570:LEU:N	2.16	0.61
1:E:451:GLN:HA	1:E:454:ALA:HB3	1.82	0.61
1:E:49:GLU:HG3	1:E:89:ASN:HD22	1.65	0.61
1:F:325:TYR:CE2	1:F:340:ILE:HG22	2.35	0.61
1:A:602:GLU:O	1:A:606:ARG:HG2	2.00	0.61
1:D:126:LEU:HB3	1:D:303:LEU:HD21	1.81	0.61
1:A:244:VAL:HG21	1:A:260:PRO:HD3	1.82	0.61
1:A:658:LEU:HD21	1:F:497:TYR:HE1	1.66	0.61
1:D:84:GLN:NE2	1:D:85:ASN:HB2	2.15	0.61
1:E:401:ILE:HG22	1:E:402:SER:H	1.65	0.61
1:B:81:GLU:CD	1:B:81:GLU:H	2.04	0.61
1:E:427:ARG:HH21	1:E:575:ARG:CG	2.14	0.61
1:D:107:TYR:CE2	1:D:153:LEU:HD22	2.35	0.61
1:C:21:LEU:HB3	1:C:165:ILE:HG21	1.81	0.61
1:E:542:THR:HA	1:E:545:VAL:HG22	1.83	0.61
1:B:61:GLU:OE1	1:B:168:GLY:HA2	2.01	0.61
1:B:421:LEU:H	1:B:421:LEU:HD12	1.64	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:387:VAL:HG11	1:E:450:GLY:CA	2.25	0.61
1:F:57:ARG:HD2	1:F:177:GLU:O	2.01	0.61
1:A:126:LEU:HB3	1:A:303:LEU:HD21	1.82	0.61
1:F:626:LEU:O	1:F:629:VAL:HG22	2.00	0.61
1:B:57:ARG:O	1:B:60:LEU:HB3	2.00	0.61
1:F:61:GLU:OE1	1:F:168:GLY:HA2	2.01	0.61
1:F:82:GLY:C	1:F:84:GLN:H	2.04	0.61
1:C:490:ILE:CG1	1:C:650:ARG:HB3	2.31	0.61
1:B:165:ILE:HG22	1:B:166:ASP:N	2.11	0.61
1:D:244:VAL:CG2	1:D:260:PRO:HD3	2.31	0.61
1:B:84:GLN:O	1:B:86:LEU:HG	2.00	0.61
1:E:193:LEU:HD22	1:E:203:VAL:CG2	2.28	0.61
1:F:120:GLY:O	1:F:123:LEU:HD23	2.00	0.61
1:F:514:TRP:CH2	1:F:653:GLU:HB2	2.36	0.61
1:E:401:ILE:HB	1:E:403:PRO:HD3	1.82	0.61
1:C:80:PRO:HB2	1:C:84:GLN:NE2	2.16	0.61
1:F:328:THR:HG23	1:F:331:GLU:HG3	1.82	0.61
1:C:286:ARG:N	1:C:290:THR:HG23	2.15	0.61
1:F:32:TRP:CZ3	1:F:83:MET:HB3	2.33	0.61
1:B:213:PHE:CE1	1:B:221:PRO:HB2	2.35	0.61
1:C:542:THR:HA	1:C:545:VAL:HG22	1.83	0.61
1:A:545:VAL:HA	1:A:548:GLN:HE22	1.63	0.61
1:A:486:PHE:CE2	1:A:518:GLU:HA	2.36	0.61
1:A:107:TYR:CE2	1:A:153:LEU:HD22	2.36	0.61
1:B:187:GLN:HB3	1:B:220:ARG:CZ	2.31	0.61
1:E:22:GLY:N	1:E:165:ILE:HG21	2.15	0.61
1:F:21:LEU:HD23	1:F:165:ILE:HG23	1.82	0.61
1:D:408:GLU:HG2	1:D:413:ILE:HD13	1.82	0.61
1:D:57:ARG:O	1:D:60:LEU:HB3	2.01	0.61
1:E:325:TYR:CE2	1:E:340:ILE:HG22	2.36	0.60
1:F:123:LEU:HD12	1:F:307:LEU:HD13	1.81	0.60
1:C:526:ARG:HH11	1:C:529:GLU:HG2	1.66	0.60
1:F:276:TRP:CE2	1:F:280:MET:HG3	2.36	0.60
1:C:316:ASN:ND2	1:C:344:THR:HG21	2.16	0.60
1:A:528:ASN:HA	1:A:531:LYS:HZ2	1.65	0.60
1:A:533:LEU:HD13	1:A:629:VAL:CA	2.30	0.60
1:F:279:LEU:CD2	1:F:292:PRO:HD3	2.26	0.60
1:A:402:SER:H	1:A:403:PRO:CD	2.10	0.60
1:B:21:LEU:HG	1:B:165:ILE:HD13	1.82	0.60
1:B:283:TRP:HB2	1:B:284:HIS:ND1	2.16	0.60
1:C:118:ARG:HD3	1:C:435:HIS:NE2	2.16	0.60
1:F:117:LEU:O	1:F:118:ARG:HB3	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:477:GLN:HE21	1:C:477:GLN:NE2	1.99	0.60
1:B:415:GLN:NE2	1:B:419:ARG:HG2	2.16	0.60
1:A:419:ARG:NE	1:A:419:ARG:N	2.41	0.60
1:C:222:PHE:HA	1:C:245:VAL:HB	1.84	0.60
1:B:286:ARG:HA	1:B:290:THR:CG2	2.32	0.60
1:A:481:ALA:C	1:F:482:LYS:HZ1	2.05	0.60
1:F:526:ARG:HH22	1:F:635:LEU:HB3	1.67	0.60
1:A:192:GLU:HG2	1:A:283:TRP:CB	2.31	0.60
1:F:426:LEU:HD11	1:F:574:LEU:HD11	1.82	0.60
1:B:415:GLN:HE21	1:B:419:ARG:CG	2.14	0.60
1:C:417:PRO:HG3	1:D:405:PRO:HG3	1.82	0.60
1:D:402:SER:N	1:D:403:PRO:HD2	2.11	0.60
1:E:430:TRP:C	1:E:571:TYR:HE2	2.04	0.60
1:C:626:LEU:O	1:C:629:VAL:HG22	2.01	0.60
1:D:340:ILE:HD11	1:D:351:GLN:OE1	2.00	0.60
1:E:276:TRP:CE2	1:E:280:MET:HG3	2.37	0.60
1:A:316:ASN:ND2	1:A:344:THR:HG21	2.16	0.60
1:C:310:LYS:HZ3	1:C:310:LYS:HB2	1.66	0.60
1:A:292:PRO:C	1:A:294:TYR:H	2.04	0.60
1:A:658:LEU:HA	1:F:658:LEU:CD1	2.31	0.60
1:E:416:GLU:C	1:E:418:LYS:H	2.04	0.60
1:A:120:GLY:O	1:A:123:LEU:HD23	2.00	0.60
1:A:213:PHE:CE1	1:A:243:ILE:HB	2.37	0.60
1:C:244:VAL:HB	1:C:256:SER:HB3	1.84	0.60
1:B:626:LEU:O	1:B:629:VAL:HG22	2.02	0.60
1:C:333:LEU:HD23	1:C:363:PRO:HA	1.83	0.60
1:D:434:TRP:HB3	1:D:571:TYR:CZ	2.37	0.60
1:D:244:VAL:HG21	1:D:260:PRO:HD3	1.83	0.60
1:E:16:GLU:HG3	1:E:32:TRP:HE1	1.65	0.60
1:A:503:PHE:HB2	1:F:659:LYS:CD	2.31	0.60
1:D:517:MET:HB3	1:D:650:ARG:NH2	2.17	0.60
1:A:428:LYS:HG3	1:A:429:VAL:N	2.16	0.60
1:A:283:TRP:CD1	1:A:284:HIS:N	2.69	0.60
1:E:16:GLU:N	1:E:30:ILE:HG21	2.17	0.60
1:A:479:LEU:HD12	1:A:640:GLU:HG2	1.83	0.60
1:F:193:LEU:HD22	1:F:203:VAL:CG2	2.29	0.60
1:B:367:ALA:C	1:B:369:GLN:N	2.56	0.60
1:C:366:PRO:C	1:C:368:THR:H	2.06	0.60
1:D:665:VAL:HG13	1:E:664:LYS:O	2.02	0.60
1:B:455:MET:O	1:B:459:LEU:HD13	2.02	0.60
1:D:631:GLU:O	1:D:635:LEU:HG	2.02	0.60
1:F:421:LEU:HG	1:F:586:ASP:HA	1.82	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:224:PRO:HG2	1:D:225:ASN:H	1.67	0.59
1:D:236:ARG:HH22	1:D:283:TRP:HE1	1.47	0.59
1:D:496:LYS:HE2	1:D:654:LEU:HD21	1.84	0.59
1:A:170:ALA:O	1:A:178:LEU:HB2	2.02	0.59
1:F:526:ARG:NH2	1:F:635:LEU:HB3	2.16	0.59
1:E:545:VAL:HA	1:E:548:GLN:HE22	1.66	0.59
1:A:533:LEU:HD22	1:A:629:VAL:CG1	2.25	0.59
1:A:291:ASP:C	1:A:293:THR:H	2.04	0.59
1:D:21:LEU:HG	1:D:165:ILE:CD1	2.32	0.59
1:F:102:GLY:CA	1:F:153:LEU:H	2.15	0.59
1:B:35:GLN:HG2	1:E:465:LEU:HG	1.83	0.59
1:C:193:LEU:HD22	1:C:203:VAL:CG2	2.30	0.59
1:B:447:LEU:HD23	1:B:609:TYR:CE1	2.34	0.59
1:C:510:LEU:HB3	1:C:653:GLU:OE2	2.02	0.59
1:A:503:PHE:HB2	1:F:659:LYS:HD2	1.83	0.59
1:A:655:TRP:HD1	1:F:500:GLN:HG2	1.62	0.59
1:D:282:MET:HB2	1:D:286:ARG:CZ	2.31	0.59
1:E:229:VAL:HG22	1:E:230:GLN:OE1	2.03	0.59
1:C:486:PHE:CE2	1:C:521:VAL:HG21	2.37	0.59
1:F:284:HIS:CG	1:F:285:PRO:HD3	2.38	0.59
1:D:426:LEU:O	1:D:430:TRP:HB2	2.03	0.59
1:A:361:LEU:CD2	1:A:369:GLN:HE21	2.15	0.59
1:E:428:LYS:HG3	1:E:429:VAL:N	2.16	0.59
1:B:284:HIS:H	1:B:285:PRO:HD2	1.68	0.59
1:A:631:GLU:O	1:A:635:LEU:HG	2.02	0.59
1:B:365:LYS:C	1:B:367:ALA:H	2.06	0.59
1:E:626:LEU:O	1:E:629:VAL:HG22	2.03	0.59
1:F:427:ARG:HE	1:F:575:ARG:CG	2.10	0.59
1:F:20:ARG:CB	1:F:23:THR:HB	2.33	0.59
1:C:404:ARG:O	1:C:404:ARG:HD3	2.01	0.59
1:D:581:GLN:H	1:D:582:ARG:NE	2.01	0.59
1:A:579:ARG:N	1:A:579:ARG:HD3	2.10	0.59
1:D:500:GLN:HE22	1:D:504:GLY:HA3	1.66	0.59
1:D:171:LYS:HD2	1:D:172:GLU:H	1.68	0.59
1:D:416:GLU:O	1:D:418:LYS:N	2.36	0.59
1:A:367:ALA:O	1:A:369:GLN:N	2.35	0.59
1:D:362:ILE:N	1:D:362:ILE:HD12	2.17	0.59
1:F:223:LEU:H	1:F:224:PRO:HD2	1.67	0.59
1:B:202:THR:HG21	1:B:284:HIS:HA	1.84	0.59
1:C:366:PRO:O	1:C:368:THR:N	2.33	0.59
1:C:113:ASN:OD1	1:C:117:LEU:HD23	2.02	0.59
1:D:488:THR:HG22	1:E:648:GLU:HB3	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:186:LEU:HD11	1:E:189:LEU:HB2	1.85	0.59
1:F:458:LEU:HD23	1:F:619:LYS:CB	2.33	0.59
1:B:118:ARG:HD3	1:B:435:HIS:NE2	2.18	0.59
1:D:402:SER:H	1:D:403:PRO:CD	2.12	0.59
1:C:500:GLN:O	1:C:502:GLU:N	2.36	0.59
1:A:462:ASN:O	1:A:466:SER:HB3	2.03	0.59
1:D:140:ARG:O	1:D:172:GLU:HG3	2.03	0.59
1:D:172:GLU:HG2	1:D:174:ASP:H	1.66	0.59
1:E:316:ASN:ND2	1:E:344:THR:HG21	2.18	0.59
1:A:105:ARG:HD2	1:A:148:PRO:HB2	1.85	0.59
1:A:282:MET:CE	1:A:286:ARG:HH21	2.16	0.58
1:A:402:SER:N	1:A:403:PRO:CD	2.65	0.58
1:F:213:PHE:CZ	1:F:243:ILE:HB	2.38	0.58
1:F:21:LEU:HB3	1:F:165:ILE:HG21	1.85	0.58
1:D:649:LYS:O	1:D:653:GLU:HG3	2.03	0.58
1:E:352:GLU:OE2	1:E:619:LYS:HE2	2.03	0.58
1:C:239:SER:HA	1:C:242:ASP:OD1	2.03	0.58
1:A:419:ARG:CZ	1:A:419:ARG:N	2.64	0.58
1:D:223:LEU:HD11	1:D:226:TRP:CE3	2.38	0.58
1:B:268:VAL:HG13	1:B:269:LEU:N	2.17	0.58
1:B:279:LEU:HA	1:B:286:ARG:NH1	2.18	0.58
1:E:410:VAL:HG12	1:E:411:SER:N	2.14	0.58
1:B:577:LYS:HG2	1:B:581:GLN:HE21	1.67	0.58
1:C:531:LYS:HB3	1:C:531:LYS:HZ3	1.68	0.58
1:C:421:LEU:O	1:C:585:GLY:HA3	2.03	0.58
1:C:223:LEU:HB3	1:C:226:TRP:CD1	2.38	0.58
1:E:455:MET:O	1:E:459:LEU:HD13	2.04	0.58
1:F:229:VAL:HG22	1:F:230:GLN:N	2.11	0.58
1:A:21:LEU:HB3	1:A:165:ILE:HG21	1.85	0.58
1:E:118:ARG:HD3	1:E:435:HIS:NE2	2.18	0.58
1:B:542:THR:HA	1:B:545:VAL:HG22	1.85	0.58
1:B:458:LEU:HD11	1:B:544:ILE:CG2	2.34	0.58
1:D:41:ILE:HG22	1:D:42:ALA:H	1.68	0.58
1:B:321:THR:H	1:B:405:PRO:HG3	1.68	0.58
1:B:276:TRP:CE2	1:B:280:MET:HG3	2.39	0.58
1:B:511:LEU:CG	1:B:515:ARG:HH12	2.12	0.58
1:A:21:LEU:HD23	1:A:165:ILE:HG23	1.85	0.58
1:D:20:ARG:CB	1:D:23:THR:HB	2.34	0.58
1:A:426:LEU:O	1:A:430:TRP:HB2	2.03	0.58
1:D:655:TRP:CD2	1:E:496:LYS:HD2	2.38	0.58
1:E:276:TRP:NE1	1:E:280:MET:HG3	2.19	0.58
1:F:421:LEU:HB3	1:F:586:ASP:CA	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:102:GLY:CA	1:D:153:LEU:H	2.15	0.58
1:D:104:LEU:HD23	1:D:148:PRO:HB3	1.85	0.58
1:F:20:ARG:HB3	1:F:29:VAL:O	2.03	0.58
1:A:358:GLY:HA2	1:A:457:ASN:HB2	1.82	0.58
1:A:490:ILE:HG12	1:A:517:MET:HE2	1.85	0.58
1:A:328:THR:HG23	1:A:331:GLU:HG3	1.86	0.58
1:B:426:LEU:O	1:B:430:TRP:HB2	2.02	0.58
1:C:475:MET:O	1:C:478:GLN:HB3	2.04	0.58
1:C:37:THR:HG22	1:F:362:ILE:HG13	1.86	0.58
1:E:356:GLU:O	1:E:452:ARG:NH1	2.35	0.58
1:C:18:LYS:CB	1:C:31:ARG:HD3	2.33	0.58
1:D:276:TRP:CE2	1:D:280:MET:HG3	2.38	0.58
1:D:36:GLU:HG3	1:D:37:THR:H	1.68	0.58
1:F:279:LEU:CD2	1:F:291:ASP:HA	2.33	0.58
1:F:317:MET:SD	1:F:450:GLY:HA3	2.43	0.58
1:F:410:VAL:HG12	1:F:411:SER:N	2.15	0.58
1:A:60:LEU:HD13	1:A:175:GLN:NE2	2.19	0.58
1:B:312:VAL:HG22	1:B:313:HIS:N	2.18	0.58
1:D:462:ASN:O	1:D:466:SER:HB3	2.03	0.58
1:F:355:GLN:O	1:F:359:LEU:HD11	2.03	0.58
1:D:165:ILE:HG22	1:D:166:ASP:N	2.12	0.58
1:B:171:LYS:HG2	1:B:177:GLU:CA	2.32	0.58
1:A:481:ALA:CB	1:F:482:LYS:NZ	2.64	0.58
1:B:316:ASN:ND2	1:B:344:THR:HG21	2.18	0.58
1:B:570:LEU:HD22	1:B:590:MET:CE	2.34	0.58
1:A:455:MET:O	1:A:459:LEU:HD13	2.04	0.58
1:F:217:THR:HB	1:F:260:PRO:HG3	1.86	0.58
1:C:102:GLY:HA2	1:C:153:LEU:H	1.68	0.58
1:A:511:LEU:CG	1:A:515:ARG:HH12	2.16	0.58
1:F:458:LEU:HD23	1:F:619:LYS:HB2	1.86	0.58
1:D:282:MET:HG2	1:D:286:ARG:NH2	2.18	0.58
1:A:355:GLN:O	1:A:359:LEU:HD11	2.03	0.58
1:D:542:THR:HA	1:D:545:VAL:HG22	1.85	0.58
1:F:306:ILE:O	1:F:309:LEU:HD23	2.03	0.58
1:C:419:ARG:HH21	1:C:420:ASN:HB3	1.68	0.58
1:C:428:LYS:HG3	1:C:429:VAL:N	2.18	0.58
1:C:223:LEU:HD23	1:C:246:SER:HA	1.86	0.58
1:E:430:TRP:CZ3	1:E:570:LEU:HB3	2.39	0.58
1:D:213:PHE:CE1	1:D:243:ILE:HB	2.39	0.58
1:B:80:PRO:HB3	1:B:83:MET:SD	2.44	0.58
1:D:167:LEU:O	1:D:170:ALA:HB2	2.04	0.58
1:B:321:THR:N	1:B:405:PRO:HG3	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:214:GLU:OE1	1:C:220:ARG:HD3	2.04	0.57
1:A:312:VAL:HG22	1:A:313:HIS:N	2.19	0.57
1:A:194:LEU:HB3	1:A:196:GLN:HE22	1.68	0.57
1:D:265:LEU:HG	1:D:266:ASN:N	2.19	0.57
1:A:21:LEU:HG	1:A:165:ILE:CD1	2.34	0.57
1:E:420:ASN:O	1:E:421:LEU:CB	2.52	0.57
1:C:430:TRP:CZ3	1:C:574:LEU:HD12	2.40	0.57
1:F:545:VAL:HA	1:F:548:GLN:HE22	1.69	0.57
1:E:36:GLU:O	1:E:38:GLY:N	2.38	0.57
1:F:65:MET:HB3	1:F:76:ALA:HB2	1.86	0.57
1:C:636:MET:C	1:C:638:GLU:H	2.07	0.57
1:B:311:LEU:O	1:B:311:LEU:HD12	2.04	0.57
1:A:294:TYR:N	1:A:294:TYR:CD2	2.68	0.57
1:B:213:PHE:CE2	1:B:217:THR:HG21	2.40	0.57
1:F:316:ASN:ND2	1:F:344:THR:HG21	2.19	0.57
1:A:542:THR:HA	1:A:545:VAL:HG22	1.87	0.57
1:E:234:LYS:O	1:E:237:GLN:HB3	2.05	0.57
1:D:655:TRP:CG	1:E:496:LYS:HD2	2.39	0.57
1:B:501:THR:O	1:B:505:ILE:HG12	2.03	0.57
1:A:186:LEU:HD13	1:A:186:LEU:C	2.25	0.57
1:D:316:ASN:ND2	1:D:344:THR:HG21	2.19	0.57
1:C:270:ALA:O	1:C:274:GLU:HB2	2.05	0.57
1:E:570:LEU:HD22	1:E:590:MET:CE	2.33	0.57
1:B:194:LEU:HB3	1:B:196:GLN:HE22	1.69	0.57
1:F:89:ASN:HD22	1:F:91:LEU:HB2	1.68	0.57
1:E:220:ARG:HG2	1:E:220:ARG:NH1	2.19	0.57
1:A:394:LYS:NZ	1:A:613:SER:HB2	2.19	0.57
1:C:328:THR:HG23	1:C:331:GLU:HG3	1.85	0.57
1:C:169:TYR:HE1	1:C:183:VAL:HB	1.69	0.57
1:D:394:LYS:HG2	1:D:401:ILE:N	2.20	0.57
1:A:265:LEU:HD21	1:A:270:ALA:HB2	1.87	0.57
1:C:21:LEU:HG	1:C:165:ILE:CD1	2.34	0.57
1:D:144:ARG:HD3	1:D:169:TYR:O	2.05	0.57
1:A:649:LYS:O	1:A:653:GLU:HG3	2.05	0.57
1:F:502:GLU:HA	1:F:502:GLU:OE1	2.03	0.57
1:B:448:GLN:OE1	1:B:608:ILE:HD12	2.04	0.57
1:E:355:GLN:O	1:E:359:LEU:HD11	2.05	0.57
1:F:229:VAL:HG13	1:F:230:GLN:N	2.19	0.57
1:C:21:LEU:HD23	1:C:165:ILE:HG23	1.86	0.57
1:D:500:GLN:OE1	1:D:505:ILE:HG23	2.05	0.57
1:D:408:GLU:HA	1:D:408:GLU:OE1	2.04	0.57
1:C:36:GLU:HG3	1:C:37:THR:H	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:312:VAL:HG23	1:A:370:CYS:SG	2.45	0.57
1:E:117:LEU:HB3	1:E:119:GLU:OE1	2.05	0.57
1:A:531:LYS:HB3	1:A:531:LYS:HZ3	1.69	0.57
1:B:631:GLU:O	1:B:635:LEU:HG	2.05	0.57
1:A:292:PRO:O	1:A:294:TYR:N	2.38	0.57
1:A:500:GLN:CD	1:A:502:GLU:HG3	2.25	0.57
1:F:649:LYS:O	1:F:653:GLU:HG3	2.05	0.57
1:B:408:GLU:HG3	1:B:409:SER:N	2.19	0.57
1:D:17:MET:HG3	1:D:17:MET:O	2.05	0.57
1:F:276:TRP:NE1	1:F:280:MET:HG3	2.19	0.57
1:D:247:GLU:HA	1:D:252:THR:O	2.05	0.57
1:C:631:GLU:O	1:C:635:LEU:HG	2.04	0.57
1:B:489:SER:C	1:B:490:ILE:HD12	2.26	0.56
1:C:490:ILE:HG12	1:C:650:ARG:HB3	1.87	0.56
1:C:416:GLU:C	1:C:418:LYS:H	2.07	0.56
1:A:626:LEU:O	1:A:629:VAL:HG22	2.05	0.56
1:B:571:TYR:HB3	1:B:575:ARG:NH2	2.08	0.56
1:A:259:LEU:N	1:A:259:LEU:HD12	2.20	0.56
1:E:294:TYR:CG	1:E:296:PRO:HD2	2.39	0.56
1:B:62:ILE:HG13	1:B:94:LEU:HD13	1.87	0.56
1:D:636:MET:C	1:D:638:GLU:H	2.07	0.56
1:A:225:ASN:ND2	1:A:225:ASN:H	2.02	0.56
1:A:225:ASN:ND2	1:A:225:ASN:N	2.52	0.56
1:C:489:SER:C	1:C:490:ILE:HD12	2.26	0.56
1:E:270:ALA:O	1:E:274:GLU:HB2	2.05	0.56
1:C:428:LYS:O	1:C:432:GLN:HG2	2.05	0.56
1:B:36:GLU:HG3	1:B:37:THR:H	1.69	0.56
1:D:21:LEU:HD23	1:D:165:ILE:HG23	1.88	0.56
1:B:20:ARG:HB3	1:B:29:VAL:O	2.04	0.56
1:E:245:VAL:HA	1:E:254:LYS:O	2.04	0.56
1:B:419:ARG:CB	1:B:419:ARG:CZ	2.82	0.56
1:C:649:LYS:O	1:C:653:GLU:HG3	2.05	0.56
1:C:221:PRO:O	1:C:222:PHE:CB	2.48	0.56
1:F:389:LEU:CD2	1:F:454:ALA:HB1	2.35	0.56
1:E:430:TRP:HE1	1:E:587:SER:CA	2.15	0.56
1:E:570:LEU:N	1:E:570:LEU:HD12	2.21	0.56
1:A:268:VAL:O	1:A:272:ARG:HB2	2.05	0.56
1:E:21:LEU:C	1:E:165:ILE:HD13	2.26	0.56
1:D:511:LEU:CG	1:D:515:ARG:HH12	2.16	0.56
1:A:544:ILE:O	1:A:547:LEU:HG	2.05	0.56
1:B:462:ASN:O	1:B:466:SER:HB3	2.05	0.56
1:E:626:LEU:N	1:E:627:PRO:HD2	2.20	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:592:ARG:NH1	1:C:592:ARG:HB3	2.21	0.56
1:D:549:ARG:HB2	1:D:549:ARG:CZ	2.35	0.56
1:E:229:VAL:HG13	1:E:230:GLN:CD	2.25	0.56
1:D:41:ILE:HG22	1:D:42:ALA:N	2.19	0.56
1:D:570:LEU:HD12	1:D:570:LEU:N	2.20	0.56
1:D:65:MET:HB3	1:D:76:ALA:HB2	1.87	0.56
1:D:99:CYS:HB3	1:D:154:GLN:HB2	1.86	0.56
1:D:455:MET:O	1:D:459:LEU:HD13	2.06	0.56
1:C:41:ILE:HG22	1:C:42:ALA:H	1.70	0.56
1:E:220:ARG:HB2	1:E:221:PRO:HD2	1.87	0.56
1:E:284:HIS:CB	1:E:285:PRO:CD	2.82	0.56
1:C:245:VAL:HA	1:C:254:LYS:O	2.05	0.56
1:D:26:PHE:CE1	1:D:179:CYS:HB3	2.41	0.56
1:E:170:ALA:HB3	1:E:178:LEU:HG	1.88	0.56
1:E:223:LEU:HA	1:E:227:GLN:OE1	2.06	0.56
1:C:404:ARG:HE	1:C:601:PHE:HE2	1.53	0.56
1:C:392:ASN:CG	1:C:393:SER:H	2.08	0.56
1:F:335:SER:O	1:F:339:ARG:HG3	2.06	0.56
1:F:290:THR:HG23	1:F:296:PRO:O	2.04	0.56
1:D:182:PHE:CZ	1:D:194:LEU:HD23	2.40	0.56
1:B:16:GLU:C	1:B:17:MET:SD	2.84	0.56
1:D:55:ARG:HB3	1:D:91:LEU:HD21	1.88	0.56
1:D:383:ASP:O	1:D:384:MET:HB2	2.06	0.56
1:B:533:LEU:HD22	1:B:629:VAL:HG12	1.87	0.56
1:C:451:GLN:NE2	1:C:611:GLN:HB3	2.21	0.56
1:C:309:LEU:HD11	1:C:311:LEU:HD23	1.86	0.56
1:F:36:GLU:HG3	1:F:37:THR:H	1.70	0.56
1:C:213:PHE:CD1	1:C:221:PRO:HG2	2.41	0.56
1:F:265:LEU:HD11	1:F:270:ALA:HA	1.88	0.56
1:F:220:ARG:NH2	1:F:221:PRO:HB2	2.21	0.56
1:D:506:THR:HG22	1:D:507:SER:H	1.68	0.56
1:E:653:GLU:O	1:E:657:LEU:HD13	2.05	0.56
1:A:570:LEU:N	1:A:570:LEU:HD12	2.21	0.56
1:A:430:TRP:HE1	1:A:587:SER:HB3	1.69	0.56
1:B:88:PRO:HG2	1:B:89:ASN:H	1.71	0.56
1:B:559:THR:HG22	1:B:600:SER:OG	2.05	0.56
1:B:649:LYS:O	1:B:653:GLU:HG3	2.05	0.56
1:F:220:ARG:CZ	1:F:221:PRO:HB2	2.36	0.56
1:C:410:VAL:O	1:C:411:SER:HB3	2.06	0.56
1:C:276:TRP:NE1	1:C:280:MET:HG3	2.20	0.56
1:A:186:LEU:HD22	1:A:186:LEU:O	2.06	0.56
1:F:643:VAL:O	1:F:647:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:392:ASN:CG	1:F:393:SER:H	2.09	0.56
1:A:213:PHE:CA	1:A:277:LEU:HD21	2.33	0.56
1:F:428:LYS:O	1:F:432:GLN:HG2	2.06	0.56
1:B:187:GLN:HB3	1:B:220:ARG:NH1	2.20	0.56
1:B:118:ARG:HB2	1:B:264:ASN:OD1	2.05	0.56
1:B:636:MET:C	1:B:638:GLU:H	2.08	0.56
1:C:486:PHE:HE1	1:C:647:GLN:HB3	1.67	0.56
1:E:171:LYS:NZ	1:E:173:LEU:HD23	2.21	0.56
1:D:570:LEU:HD22	1:D:590:MET:HE2	1.87	0.56
1:A:171:LYS:HD2	1:A:199:TYR:OH	2.06	0.56
1:B:41:ILE:HG22	1:B:42:ALA:H	1.71	0.56
1:D:478:GLN:HB2	1:E:478:GLN:HA	1.87	0.56
1:C:265:LEU:HD11	1:C:270:ALA:HA	1.86	0.56
1:D:229:VAL:HG23	1:D:230:GLN:N	2.12	0.56
1:B:227:GLN:HE22	1:B:229:VAL:HG13	1.70	0.56
1:A:20:ARG:HB3	1:A:29:VAL:O	2.06	0.56
1:E:489:SER:C	1:E:490:ILE:HD12	2.26	0.56
1:B:648:GLU:HB3	1:C:488:THR:CG2	2.36	0.56
1:E:216:ILE:HG22	1:E:263:ASN:OD1	2.05	0.55
1:E:434:TRP:HB3	1:E:571:TYR:CE1	2.41	0.55
1:B:186:LEU:N	1:B:187:GLN:HE21	2.04	0.55
1:A:422:ALA:O	1:A:585:GLY:HA2	2.06	0.55
1:A:544:ILE:HG22	1:A:618:CYS:SG	2.46	0.55
1:C:118:ARG:HB2	1:C:264:ASN:HB3	1.87	0.55
1:B:55:ARG:HD2	1:B:91:LEU:HD11	1.87	0.55
1:C:350:ASP:HB2	1:C:391:ASP:H	1.70	0.55
1:C:122:ILE:HD13	1:C:216:ILE:HG12	1.87	0.55
1:C:65:MET:HB3	1:C:76:ALA:HB2	1.88	0.55
1:F:627:PRO:HA	1:F:630:GLU:CB	2.34	0.55
1:E:220:ARG:HH11	1:E:220:ARG:HG2	1.70	0.55
1:C:418:LYS:C	1:C:419:ARG:HD3	2.26	0.55
1:A:286:ARG:C	1:A:290:THR:HG21	2.25	0.55
1:C:286:ARG:HA	1:C:290:THR:N	2.21	0.55
1:B:272:ARG:HH11	1:B:272:ARG:HG3	1.72	0.55
1:B:285:PRO:O	1:B:286:ARG:HG3	2.06	0.55
1:B:394:LYS:C	1:B:394:LYS:HZ3	2.09	0.55
1:C:118:ARG:HA	1:C:264:ASN:O	2.05	0.55
1:D:570:LEU:HD22	1:D:590:MET:CE	2.36	0.55
1:A:335:SER:O	1:A:339:ARG:HG3	2.06	0.55
1:A:239:SER:HB2	1:A:242:ASP:HB2	1.88	0.55
1:D:335:SER:O	1:D:339:ARG:HG3	2.06	0.55
1:B:249:LEU:HD12	1:B:414:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:404:ARG:N	1:D:404:ARG:HD3	2.21	0.55
1:A:213:PHE:CZ	1:A:243:ILE:HB	2.42	0.55
1:A:292:PRO:C	1:A:294:TYR:N	2.60	0.55
1:C:290:THR:HB	1:C:296:PRO:HA	1.88	0.55
1:E:111:PHE:HD1	1:E:575:ARG:HD2	1.68	0.55
1:B:122:ILE:HD13	1:B:216:ILE:HG12	1.88	0.55
1:F:68:LEU:HD13	1:F:139:ASN:CG	2.27	0.55
1:A:486:PHE:CZ	1:A:517:MET:SD	2.99	0.55
1:A:489:SER:C	1:A:490:ILE:HD12	2.27	0.55
1:C:457:ASN:HD21	1:C:619:LYS:HZ1	1.53	0.55
1:B:426:LEU:HD11	1:B:574:LEU:HD11	1.88	0.55
1:E:483:LEU:HD13	1:E:640:GLU:OE1	2.05	0.55
1:A:276:TRP:CE2	1:A:280:MET:HG3	2.41	0.55
1:B:415:GLN:HE21	1:B:419:ARG:HG2	1.70	0.55
1:C:644:VAL:O	1:C:647:GLN:HB2	2.07	0.55
1:F:294:TYR:HE1	1:F:301:LYS:HZ2	1.55	0.55
1:D:236:ARG:O	1:D:237:GLN:C	2.45	0.55
1:D:261:TYR:N	1:D:262:PRO:CD	2.69	0.55
1:E:592:ARG:NH1	1:E:592:ARG:HB3	2.22	0.55
1:C:626:LEU:HB3	1:C:627:PRO:CD	2.37	0.55
1:D:62:ILE:HG13	1:D:94:LEU:HD13	1.88	0.55
1:B:536:ARG:CZ	1:B:625:LEU:HD13	2.36	0.55
1:E:87:ALA:HB1	1:E:88:PRO:HD2	1.89	0.55
1:C:490:ILE:HG21	1:C:517:MET:CE	2.36	0.55
1:E:187:GLN:HG2	1:E:220:ARG:HH21	1.72	0.55
1:F:583:THR:O	1:F:585:GLY:N	2.40	0.55
1:C:455:MET:O	1:C:459:LEU:HD13	2.06	0.55
1:E:213:PHE:CE2	1:E:217:THR:HG21	2.40	0.55
1:C:222:PHE:HB3	1:C:231:TRP:CZ2	2.41	0.55
1:E:294:TYR:CE1	1:E:301:LYS:HB3	2.42	0.55
1:E:549:ARG:CZ	1:E:549:ARG:HA	2.37	0.55
1:B:487:LYS:HA	1:B:491:GLN:HB2	1.89	0.55
1:F:431:GLY:N	1:F:571:TYR:HE2	2.05	0.55
1:D:168:GLY:C	1:D:170:ALA:H	2.10	0.55
1:E:627:PRO:HA	1:E:630:GLU:CB	2.36	0.55
1:D:592:ARG:NH1	1:D:592:ARG:HB3	2.22	0.55
1:C:105:ARG:HD3	1:C:149:GLU:CD	2.27	0.55
1:E:51:SER:HB2	1:E:52:PRO:HD2	1.89	0.55
1:D:316:ASN:HA	1:D:388:PHE:CE1	2.42	0.55
1:C:222:PHE:HE2	1:C:281:LEU:HD21	1.70	0.55
1:E:387:VAL:HG21	1:E:449:GLN:O	2.07	0.55
1:D:19:GLU:H	1:D:19:GLU:CD	2.10	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:118:ARG:HB2	1:B:264:ASN:ND2	2.21	0.55
1:D:276:TRP:NE1	1:D:280:MET:HG3	2.22	0.55
1:E:65:MET:HB3	1:E:76:ALA:HB2	1.89	0.55
1:A:626:LEU:HB3	1:A:627:PRO:CD	2.37	0.55
1:B:34:ASN:ND2	1:B:83:MET:SD	2.80	0.55
1:A:320:GLY:HA2	1:A:405:PRO:HG3	1.89	0.55
1:E:226:TRP:CE3	1:E:229:VAL:HG12	2.42	0.55
1:D:312:VAL:HG22	1:D:313:HIS:H	1.71	0.55
1:F:636:MET:C	1:F:638:GLU:H	2.09	0.55
1:B:265:LEU:HD21	1:B:270:ALA:HB2	1.88	0.55
1:F:295:GLY:N	1:F:296:PRO:CD	2.70	0.55
1:C:434:TRP:HB3	1:C:571:TYR:OH	2.05	0.55
1:F:462:ASN:O	1:F:466:SER:HB3	2.07	0.55
1:A:114:CYS:SG	1:A:575:ARG:NH1	2.79	0.55
1:B:213:PHE:CD1	1:B:221:PRO:HB2	2.41	0.55
1:E:60:LEU:O	1:E:64:ILE:HG12	2.07	0.55
1:C:548:GLN:O	1:C:549:ARG:HG3	2.07	0.55
1:E:48:GLN:HA	1:E:89:ASN:HD21	1.72	0.55
1:F:117:LEU:HG	1:F:119:GLU:OE2	2.07	0.55
1:A:310:LYS:HZ3	1:A:310:LYS:HB2	1.70	0.55
1:E:216:ILE:HD12	1:E:277:LEU:HD22	1.87	0.54
1:D:219:PHE:O	1:D:220:ARG:C	2.45	0.54
1:D:272:ARG:HG3	1:D:272:ARG:HH11	1.71	0.54
1:C:165:ILE:CG2	1:C:166:ASP:H	2.12	0.54
1:D:55:ARG:HH11	1:D:91:LEU:CD2	2.19	0.54
1:D:122:ILE:HD13	1:D:216:ILE:HG12	1.89	0.54
1:C:170:ALA:O	1:C:178:LEU:HB2	2.07	0.54
1:D:404:ARG:HD2	1:D:605:VAL:HG11	1.89	0.54
1:A:286:ARG:O	1:A:290:THR:OG1	2.25	0.54
1:F:259:LEU:HD11	1:F:270:ALA:HB1	1.89	0.54
1:B:213:PHE:CE1	1:B:243:ILE:HB	2.42	0.54
1:E:295:GLY:N	1:E:296:PRO:CD	2.70	0.54
1:A:592:ARG:NH1	1:A:592:ARG:HB3	2.21	0.54
1:D:111:PHE:O	1:D:114:CYS:HB2	2.07	0.54
1:D:559:THR:HB	1:D:604:LYS:NZ	2.22	0.54
1:B:366:PRO:O	1:B:368:THR:N	2.40	0.54
1:B:172:GLU:HG2	1:B:175:GLN:OE1	2.07	0.54
1:E:220:ARG:HB2	1:E:221:PRO:CD	2.38	0.54
1:F:213:PHE:CE2	1:F:217:THR:HG21	2.43	0.54
1:B:282:MET:HB2	1:B:286:ARG:HH21	1.73	0.54
1:A:410:VAL:O	1:A:411:SER:HB3	2.08	0.54
1:A:311:LEU:HD12	1:A:311:LEU:O	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:570:LEU:N	1:B:570:LEU:HD12	2.23	0.54
1:B:477:GLN:NE2	1:C:477:GLN:HE21	2.05	0.54
1:A:297:ASN:O	1:A:298:GLY:O	2.26	0.54
1:F:142:ILE:CG1	1:F:173:LEU:HD11	2.28	0.54
1:B:276:TRP:NE1	1:B:280:MET:HG3	2.23	0.54
1:E:494:LEU:HD21	1:E:515:ARG:HG2	1.90	0.54
1:A:530:VAL:CG1	1:A:633:VAL:HG12	2.38	0.54
1:A:659:LYS:CD	1:F:500:GLN:HE22	2.15	0.54
1:A:316:ASN:CG	1:A:344:THR:HG21	2.27	0.54
1:B:41:ILE:HG22	1:B:42:ALA:N	2.22	0.54
1:A:291:ASP:O	1:A:293:THR:N	2.41	0.54
1:B:279:LEU:HD12	1:B:286:ARG:HG2	1.90	0.54
1:E:511:LEU:CG	1:E:515:ARG:HH12	2.17	0.54
1:E:17:MET:HB3	1:E:31:ARG:O	2.08	0.54
1:E:18:LYS:CB	1:E:31:ARG:HD3	2.38	0.54
1:E:20:ARG:HB3	1:E:29:VAL:O	2.07	0.54
1:F:511:LEU:CG	1:F:515:ARG:HH12	2.16	0.54
1:E:530:VAL:HG22	1:E:632:VAL:CG1	2.36	0.54
1:C:457:ASN:HA	1:C:460:ARG:HG3	1.89	0.54
1:B:234:LYS:O	1:B:237:GLN:HB3	2.08	0.54
1:D:123:LEU:HD12	1:D:307:LEU:HD13	1.90	0.54
1:C:241:VAL:HG12	1:C:241:VAL:O	2.08	0.54
1:F:118:ARG:HH22	1:F:438:GLN:HG2	1.73	0.54
1:C:312:VAL:HG22	1:C:313:HIS:N	2.22	0.54
1:E:544:ILE:O	1:E:547:LEU:HG	2.08	0.54
1:B:118:ARG:HD2	1:B:264:ASN:HD21	1.72	0.54
1:B:118:ARG:HH22	1:B:438:GLN:HG2	1.73	0.54
1:B:581:GLN:H	1:B:581:GLN:CD	2.10	0.54
1:C:212:ALA:O	1:C:216:ILE:HG13	2.07	0.54
1:F:625:LEU:HD22	1:F:628:LYS:HD2	1.88	0.54
1:E:194:LEU:HB3	1:E:196:GLN:HE22	1.72	0.54
1:C:220:ARG:N	1:C:221:PRO:CD	2.71	0.54
1:E:434:TRP:HB3	1:E:571:TYR:CZ	2.42	0.54
1:B:294:TYR:CG	1:B:301:LYS:HD3	2.43	0.54
1:F:467:LYS:HA	1:F:541:GLN:NE2	2.23	0.54
1:B:18:LYS:HB3	1:B:19:GLU:OE2	2.08	0.54
1:A:279:LEU:C	1:A:281:LEU:H	2.10	0.54
1:F:259:LEU:H	1:F:274:GLU:HG3	1.73	0.54
1:D:213:PHE:CE2	1:D:217:THR:HG21	2.43	0.54
1:D:268:VAL:HG13	1:D:269:LEU:N	2.23	0.54
1:F:243:ILE:O	1:F:245:VAL:HG23	2.07	0.54
1:C:410:VAL:HG12	1:C:411:SER:N	2.17	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:394:LYS:HE2	1:C:612:LEU:CD1	2.38	0.54
1:B:114:CYS:O	1:B:115:CYS:HB3	2.08	0.54
1:B:428:LYS:O	1:B:432:GLN:HG2	2.08	0.54
1:A:239:SER:HA	1:A:242:ASP:OD2	2.06	0.54
1:B:335:SER:O	1:B:339:ARG:HG3	2.07	0.54
1:D:194:LEU:HB3	1:D:196:GLN:HE22	1.72	0.54
1:F:316:ASN:HA	1:F:388:PHE:CE1	2.43	0.54
1:D:282:MET:CB	1:D:286:ARG:CZ	2.85	0.54
1:B:118:ARG:HB2	1:B:264:ASN:CG	2.29	0.54
1:C:41:ILE:HG22	1:C:42:ALA:N	2.22	0.54
1:C:81:GLU:CD	1:F:364:ASP:HB2	2.28	0.54
1:C:261:TYR:N	1:C:262:PRO:HD2	2.23	0.54
1:B:434:TRP:HB3	1:B:571:TYR:OH	2.08	0.54
1:E:430:TRP:CZ3	1:E:570:LEU:HD23	2.43	0.54
1:B:21:LEU:HB3	1:B:165:ILE:HG21	1.90	0.54
1:D:514:TRP:HA	1:D:650:ARG:NH1	2.22	0.54
1:C:506:THR:O	1:C:508:ASP:N	2.41	0.54
1:A:394:LYS:HZ3	1:A:613:SER:HB2	1.71	0.54
1:B:548:GLN:O	1:B:549:ARG:HD2	2.08	0.54
1:B:51:SER:HB2	1:B:52:PRO:HD2	1.89	0.54
1:A:36:GLU:HG3	1:A:37:THR:H	1.72	0.54
1:A:118:ARG:NH2	1:A:438:GLN:HG2	2.16	0.53
1:E:431:GLY:CA	1:E:571:TYR:CE2	2.88	0.53
1:D:105:ARG:HD3	1:D:149:GLU:CD	2.28	0.53
1:A:570:LEU:HD22	1:A:590:MET:CE	2.36	0.53
1:F:501:THR:HG23	1:F:505:ILE:HG21	1.90	0.53
1:F:60:LEU:O	1:F:64:ILE:HG12	2.08	0.53
1:D:355:GLN:O	1:D:359:LEU:HD11	2.09	0.53
1:D:474:SER:O	1:D:477:GLN:HG2	2.09	0.53
1:C:231:TRP:C	1:C:233:SER:H	2.10	0.53
1:A:114:CYS:SG	1:A:115:CYS:N	2.81	0.53
1:E:504:GLY:O	1:E:505:ILE:HG23	2.09	0.53
1:F:105:ARG:HD3	1:F:149:GLU:CD	2.29	0.53
1:C:173:LEU:HD23	1:C:173:LEU:O	2.07	0.53
1:C:20:ARG:HB3	1:C:29:VAL:O	2.08	0.53
1:B:65:MET:HB3	1:B:76:ALA:HB2	1.89	0.53
1:E:160:LEU:N	1:E:160:LEU:HD12	2.23	0.53
1:A:43:ILE:HD12	1:A:43:ILE:N	2.24	0.53
1:F:62:ILE:HG13	1:F:94:LEU:HD13	1.90	0.53
1:A:65:MET:HB3	1:A:76:ALA:HB2	1.90	0.53
1:F:238:LYS:HE3	1:F:238:LYS:HA	1.89	0.53
1:B:286:ARG:HA	1:B:290:THR:OG1	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:35:GLN:HG2	1:E:465:LEU:CG	2.38	0.53
1:A:517:MET:HG2	1:A:650:ARG:CZ	2.38	0.53
1:D:487:LYS:HA	1:D:491:GLN:HB2	1.91	0.53
1:E:279:LEU:C	1:E:281:LEU:H	2.12	0.53
1:E:431:GLY:CA	1:E:571:TYR:HE2	2.20	0.53
1:A:547:LEU:HD22	1:A:614:LYS:CE	2.38	0.53
1:E:316:ASN:CG	1:E:344:THR:HG21	2.29	0.53
1:E:415:GLN:O	1:E:418:LYS:O	2.26	0.53
1:B:626:LEU:HB3	1:B:627:PRO:HD3	1.91	0.53
1:E:113:ASN:OD1	1:E:117:LEU:HG	2.09	0.53
1:F:312:VAL:HG22	1:F:313:HIS:N	2.24	0.53
1:E:517:MET:HG2	1:E:650:ARG:CZ	2.39	0.53
1:F:387:VAL:HG11	1:F:450:GLY:CA	2.28	0.53
1:F:316:ASN:CG	1:F:344:THR:HG21	2.29	0.53
1:A:276:TRP:NE1	1:A:280:MET:HG3	2.24	0.53
1:C:487:LYS:HA	1:C:491:GLN:HB2	1.90	0.53
1:C:37:THR:CG2	1:F:362:ILE:HG13	2.39	0.53
1:F:261:TYR:H	1:F:262:PRO:HD2	1.74	0.53
1:A:578:PRO:O	1:A:580:ASP:N	2.41	0.53
1:D:500:GLN:CA	1:D:500:GLN:HE21	2.21	0.53
1:D:500:GLN:C	1:D:500:GLN:HE21	2.12	0.53
1:D:410:VAL:HG12	1:D:411:SER:N	2.19	0.53
1:D:620:GLN:O	1:D:624:GLU:HG2	2.08	0.53
1:E:227:GLN:HA	1:E:231:TRP:HB2	1.91	0.53
1:E:620:GLN:O	1:E:624:GLU:HG2	2.07	0.53
1:B:419:ARG:NH2	1:B:588:GLN:HG3	2.24	0.53
1:C:213:PHE:CE2	1:C:221:PRO:HG3	2.44	0.53
1:B:294:TYR:OH	1:B:302:ALA:HB2	2.08	0.53
1:C:547:LEU:HD22	1:C:614:LYS:HE2	1.91	0.53
1:B:67:ARG:NH2	1:B:68:LEU:HD12	2.21	0.53
1:B:316:ASN:HA	1:B:388:PHE:CE1	2.44	0.53
1:A:430:TRP:HE1	1:A:587:SER:CB	2.21	0.53
1:E:636:MET:C	1:E:638:GLU:H	2.11	0.53
1:C:272:ARG:HH11	1:C:272:ARG:HG3	1.73	0.53
1:A:118:ARG:HD3	1:A:435:HIS:CE1	2.44	0.53
1:A:23:THR:HA	1:A:29:VAL:HG22	1.90	0.53
1:D:544:ILE:O	1:D:547:LEU:HG	2.09	0.53
1:E:226:TRP:HE3	1:E:229:VAL:HG12	1.73	0.53
1:D:644:VAL:O	1:D:647:GLN:HB2	2.09	0.53
1:B:355:GLN:HB3	1:B:359:LEU:CD1	2.38	0.53
1:B:355:GLN:HB3	1:B:359:LEU:HD13	1.91	0.53
1:B:270:ALA:O	1:B:274:GLU:HB2	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:335:SER:O	1:C:339:ARG:HG3	2.09	0.53
1:E:122:ILE:HD13	1:E:216:ILE:HG12	1.90	0.53
1:A:533:LEU:CD1	1:A:629:VAL:HA	2.38	0.53
1:C:192:GLU:HG2	1:C:283:TRP:HB2	1.91	0.53
1:A:118:ARG:HB2	1:A:264:ASN:CB	2.31	0.53
1:E:430:TRP:NE1	1:E:587:SER:HA	2.17	0.53
1:F:430:TRP:CE2	1:F:590:MET:HB2	2.44	0.53
1:C:49:GLU:OE2	1:C:90:ASP:HB2	2.09	0.53
1:D:410:VAL:O	1:D:411:SER:HB3	2.08	0.53
1:B:644:VAL:O	1:B:647:GLN:HB2	2.08	0.53
1:B:433:VAL:O	1:B:436:SER:HB3	2.09	0.53
1:D:480:LYS:HG2	1:D:527:GLU:OE2	2.09	0.53
1:C:474:SER:O	1:C:477:GLN:HG2	2.09	0.53
1:D:457:ASN:HA	1:D:460:ARG:HG3	1.91	0.53
1:B:536:ARG:HG2	1:B:536:ARG:HH11	1.73	0.53
1:A:549:ARG:HA	1:A:549:ARG:NE	2.23	0.53
1:B:70:HIS:HE1	1:B:132:ALA:HA	1.73	0.53
1:B:490:ILE:CD1	1:B:651:GLN:HG2	2.36	0.53
1:A:221:PRO:HB3	1:A:244:VAL:HA	1.89	0.53
1:C:227:GLN:O	1:C:231:TRP:HB2	2.09	0.53
1:D:102:GLY:HA2	1:D:153:LEU:H	1.72	0.53
1:B:298:GLY:O	1:B:299:CYS:C	2.47	0.53
1:B:57:ARG:HH21	1:B:177:GLU:HG2	1.74	0.53
1:A:658:LEU:HD21	1:F:497:TYR:CE1	2.43	0.53
1:E:36:GLU:HG3	1:E:37:THR:H	1.73	0.53
1:B:365:LYS:O	1:B:367:ALA:N	2.42	0.53
1:A:105:ARG:HD3	1:A:149:GLU:CD	2.28	0.53
1:C:239:SER:HB2	1:C:242:ASP:HB2	1.91	0.53
1:A:185:THR:O	1:A:186:LEU:HB3	2.08	0.53
1:C:577:LYS:HG3	1:C:578:PRO:HD2	1.91	0.53
1:F:145:ASP:HB3	1:F:169:TYR:HB3	1.91	0.53
1:C:643:VAL:O	1:C:647:GLN:HG2	2.09	0.52
1:B:496:LYS:HD2	1:C:655:TRP:HA	1.90	0.52
1:A:636:MET:C	1:A:638:GLU:H	2.10	0.52
1:D:540:LEU:CD2	1:D:622:ALA:HB2	2.39	0.52
1:A:261:TYR:N	1:A:262:PRO:HD2	2.24	0.52
1:B:653:GLU:O	1:B:657:LEU:HD13	2.09	0.52
1:C:213:PHE:CE2	1:C:217:THR:HG21	2.44	0.52
1:C:279:LEU:C	1:C:281:LEU:H	2.11	0.52
1:D:213:PHE:CG	1:D:221:PRO:HD2	2.44	0.52
1:F:214:GLU:HG3	1:F:219:PHE:CA	2.39	0.52
1:D:654:LEU:HB3	1:E:654:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:316:ASN:CG	1:B:344:THR:HG21	2.29	0.52
1:D:536:ARG:HG2	1:D:536:ARG:HH11	1.75	0.52
1:A:474:SER:O	1:A:477:GLN:HG2	2.10	0.52
1:C:61:GLU:HB2	1:C:178:LEU:HD21	1.90	0.52
1:A:620:GLN:O	1:A:624:GLU:HG2	2.08	0.52
1:F:487:LYS:HA	1:F:491:GLN:HB2	1.91	0.52
1:C:226:TRP:HD1	1:C:226:TRP:H	1.58	0.52
1:A:223:LEU:HB3	1:A:231:TRP:CZ3	2.44	0.52
1:B:286:ARG:HA	1:B:290:THR:CB	2.38	0.52
1:E:500:GLN:HE21	1:E:500:GLN:C	2.12	0.52
1:B:457:ASN:ND2	1:B:619:LYS:NZ	2.55	0.52
1:B:544:ILE:O	1:B:547:LEU:HG	2.09	0.52
1:C:367:ALA:C	1:C:369:GLN:H	2.11	0.52
1:B:91:LEU:HB3	1:B:92:PRO:CD	2.38	0.52
1:A:249:LEU:HD11	1:A:414:LEU:HG	1.92	0.52
1:E:298:GLY:O	1:E:299:CYS:C	2.48	0.52
1:C:536:ARG:HH11	1:C:536:ARG:HG2	1.74	0.52
1:B:493:ASP:HA	1:B:496:LYS:HG3	1.92	0.52
1:F:282:MET:HB3	1:F:286:ARG:HB2	1.90	0.52
1:E:431:GLY:HA2	1:E:571:TYR:CD2	2.43	0.52
1:F:270:ALA:O	1:F:274:GLU:HB2	2.09	0.52
1:D:152:VAL:HG13	1:D:165:ILE:HD11	1.91	0.52
1:E:371:ILE:C	1:E:373:ASP:H	2.11	0.52
1:A:661:ALA:CB	1:F:662:CYS:SG	2.97	0.52
1:C:368:THR:C	1:C:370:CYS:H	2.12	0.52
1:C:62:ILE:HG13	1:C:94:LEU:HD13	1.91	0.52
1:A:51:SER:HB2	1:A:52:PRO:HD2	1.91	0.52
1:B:579:ARG:O	1:B:579:ARG:HG2	2.10	0.52
1:B:475:MET:O	1:B:478:GLN:HB3	2.09	0.52
1:C:407:PRO:O	1:C:408:GLU:CB	2.58	0.52
1:F:268:VAL:O	1:F:272:ARG:HB2	2.09	0.52
1:D:283:TRP:HE3	1:D:285:PRO:HD2	1.72	0.52
1:C:18:LYS:HG3	1:C:31:ARG:HG2	1.91	0.52
1:C:316:ASN:CG	1:C:344:THR:HG21	2.30	0.52
1:E:369:GLN:C	1:E:371:ILE:H	2.12	0.52
1:E:354:LEU:HD22	1:E:457:ASN:HB2	1.90	0.52
1:F:528:ASN:O	1:F:531:LYS:HB3	2.10	0.52
1:A:643:VAL:O	1:A:647:GLN:HG2	2.10	0.52
1:F:489:SER:C	1:F:490:ILE:HD12	2.29	0.52
1:A:533:LEU:HD13	1:A:629:VAL:CG1	2.40	0.52
1:F:261:TYR:N	1:F:262:PRO:HD2	2.25	0.52
1:D:582:ARG:H	1:D:582:ARG:NE	1.85	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:626:LEU:HD23	1:D:627:PRO:N	2.25	0.52
1:F:592:ARG:NH1	1:F:592:ARG:HB3	2.24	0.52
1:A:62:ILE:HG13	1:A:94:LEU:HD13	1.90	0.52
1:C:72:ASN:HA	1:C:163:LYS:HA	1.91	0.52
1:F:72:ASN:HA	1:F:163:LYS:HA	1.91	0.52
1:B:659:LYS:HE2	1:C:499:GLU:OE1	2.09	0.52
1:A:214:GLU:OE1	1:A:220:ARG:HD3	2.09	0.52
1:A:282:MET:HE3	1:A:286:ARG:HH21	1.73	0.52
1:F:362:ILE:HD12	1:F:369:GLN:HE22	1.75	0.52
1:F:142:ILE:HG12	1:F:201:VAL:HG13	1.92	0.52
1:B:86:LEU:HD12	1:B:87:ALA:H	1.75	0.52
1:D:643:VAL:O	1:D:647:GLN:HG2	2.09	0.52
1:B:547:LEU:HD22	1:B:614:LYS:HE2	1.91	0.52
1:B:556:GLN:NE2	1:B:559:THR:OG1	2.42	0.52
1:C:74:VAL:HG23	1:C:164:ILE:O	2.09	0.52
1:A:665:VAL:HG23	1:F:665:VAL:HB	1.90	0.52
1:A:407:PRO:O	1:A:408:GLU:HB2	2.09	0.52
1:C:262:PRO:HB2	1:C:432:GLN:NE2	2.25	0.52
1:A:626:LEU:N	1:A:627:PRO:HD2	2.24	0.52
1:F:294:TYR:CZ	1:F:301:LYS:HD3	2.44	0.52
1:C:36:GLU:O	1:C:38:GLY:N	2.43	0.52
1:F:265:LEU:H	1:F:265:LEU:CD2	2.22	0.52
1:B:500:GLN:CA	1:B:500:GLN:HE21	2.23	0.52
1:D:171:LYS:HD2	1:D:172:GLU:N	2.25	0.52
1:D:493:ASP:HA	1:D:496:LYS:HG3	1.91	0.52
1:E:105:ARG:HD3	1:E:149:GLU:CD	2.31	0.52
1:C:366:PRO:O	1:C:367:ALA:HB3	2.10	0.52
1:C:355:GLN:O	1:C:359:LEU:HD11	2.09	0.52
1:A:343:ASP:O	1:B:418:LYS:HB3	2.10	0.52
1:E:187:GLN:CG	1:E:220:ARG:HH21	2.23	0.52
1:F:229:VAL:C	1:F:231:TRP:H	2.13	0.52
1:E:23:THR:HA	1:E:29:VAL:HG22	1.91	0.52
1:B:362:ILE:HG23	1:E:37:THR:HG21	1.91	0.52
1:B:107:TYR:CE2	1:B:153:LEU:HD22	2.45	0.52
1:F:434:TRP:HZ3	1:F:564:GLU:OE1	1.93	0.52
1:B:74:VAL:HG23	1:B:164:ILE:O	2.10	0.52
1:F:624:GLU:O	1:F:627:PRO:HG2	2.10	0.52
1:A:627:PRO:HA	1:A:630:GLU:CB	2.37	0.52
1:A:286:ARG:HA	1:A:290:THR:CB	2.40	0.52
1:E:355:GLN:HB3	1:E:359:LEU:CD1	2.40	0.52
1:E:424:PHE:CD1	1:E:582:ARG:CZ	2.86	0.52
1:B:213:PHE:CE1	1:B:221:PRO:CB	2.93	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:657:LEU:CB	1:F:658:LEU:HD21	2.37	0.52
1:A:104:LEU:HD23	1:A:148:PRO:HB3	1.92	0.52
1:D:36:GLU:O	1:D:38:GLY:N	2.43	0.52
1:E:335:SER:O	1:E:339:ARG:HG3	2.10	0.52
1:D:270:ALA:O	1:D:274:GLU:HB2	2.10	0.52
1:F:456:MET:HE3	1:F:459:LEU:HD22	1.92	0.51
1:F:430:TRP:HE1	1:F:587:SER:CA	2.21	0.51
1:A:270:ALA:O	1:A:274:GLU:HB2	2.10	0.51
1:B:89:ASN:HD22	1:B:90:ASP:N	2.08	0.51
1:A:241:VAL:HG12	1:A:241:VAL:O	2.10	0.51
1:F:350:ASP:HB2	1:F:391:ASP:H	1.75	0.51
1:B:160:LEU:HD12	1:B:160:LEU:N	2.25	0.51
1:D:404:ARG:HB3	1:D:405:PRO:HD2	1.93	0.51
1:C:279:LEU:HD11	1:C:290:THR:N	2.25	0.51
1:E:355:GLN:HB3	1:E:359:LEU:HD13	1.92	0.51
1:B:243:ILE:HG22	1:B:281:LEU:CD2	2.41	0.51
1:E:316:ASN:HA	1:E:388:PHE:CE1	2.45	0.51
1:B:460:ARG:C	1:B:462:ASN:H	2.13	0.51
1:B:627:PRO:HA	1:B:630:GLU:CB	2.39	0.51
1:A:428:LYS:O	1:A:432:GLN:HG2	2.10	0.51
1:B:559:THR:HB	1:B:604:LYS:HZ1	1.75	0.51
1:A:487:LYS:HA	1:A:491:GLN:HB2	1.91	0.51
1:E:272:ARG:HG3	1:E:272:ARG:HH11	1.75	0.51
1:F:295:GLY:N	1:F:296:PRO:HD2	2.26	0.51
1:C:226:TRP:CD1	1:C:226:TRP:N	2.77	0.51
1:C:231:TRP:CD1	1:C:235:VAL:HG21	2.45	0.51
1:F:223:LEU:N	1:F:224:PRO:CD	2.74	0.51
1:B:216:ILE:HD12	1:B:277:LEU:HD22	1.93	0.51
1:C:102:GLY:CA	1:C:153:LEU:H	2.22	0.51
1:E:500:GLN:HE21	1:E:500:GLN:CA	2.22	0.51
1:B:500:GLN:C	1:B:500:GLN:HE21	2.14	0.51
1:F:321:THR:HG21	1:F:447:LEU:CD1	2.35	0.51
1:D:489:SER:C	1:D:490:ILE:HD12	2.30	0.51
1:B:173:LEU:HD12	1:B:174:ASP:H	1.75	0.51
1:D:559:THR:HG22	1:D:600:SER:OG	2.11	0.51
1:B:214:GLU:O	1:B:218:GLY:HA2	2.10	0.51
1:C:371:ILE:HG12	1:C:384:MET:O	2.10	0.51
1:B:658:LEU:HD23	1:C:496:LYS:NZ	2.25	0.51
1:A:295:GLY:CA	1:A:301:LYS:HD3	2.41	0.51
1:A:295:GLY:HA3	1:A:301:LYS:HD3	1.93	0.51
1:F:16:GLU:CB	1:F:33:HIS:H	2.20	0.51
1:C:152:VAL:HG13	1:C:165:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:371:ILE:HG22	1:C:372:SER:H	1.74	0.51
1:D:125:LEU:C	1:D:125:LEU:HD13	2.31	0.51
1:E:528:ASN:O	1:E:532:LEU:HD23	2.10	0.51
1:E:125:LEU:HD13	1:E:125:LEU:C	2.31	0.51
1:D:43:ILE:N	1:D:43:ILE:HD12	2.25	0.51
1:C:514:TRP:HA	1:C:650:ARG:NH1	2.25	0.51
1:D:475:MET:O	1:D:478:GLN:HB3	2.11	0.51
1:A:284:HIS:HB3	1:A:285:PRO:CD	2.40	0.51
1:F:418:LYS:HB3	1:F:420:ASN:OD1	2.11	0.51
1:A:355:GLN:HB3	1:A:359:LEU:CD1	2.40	0.51
1:E:476:SER:HB2	1:E:636:MET:CE	2.40	0.51
1:B:89:ASN:OD1	1:B:91:LEU:HB2	2.10	0.51
1:F:483:LEU:HD12	1:F:644:VAL:HG21	1.92	0.51
1:E:41:ILE:HG22	1:E:42:ALA:H	1.76	0.51
1:B:308:ASN:HD22	1:B:308:ASN:N	2.09	0.51
1:F:620:GLN:O	1:F:624:GLU:HG2	2.11	0.51
1:E:219:PHE:CE2	1:E:260:PRO:HG3	2.46	0.51
1:E:428:LYS:O	1:E:432:GLN:HG2	2.10	0.51
1:B:213:PHE:CZ	1:B:221:PRO:HG2	2.45	0.51
1:C:500:GLN:HE21	1:C:500:GLN:CA	2.24	0.51
1:A:369:GLN:HA	1:A:369:GLN:OE1	2.10	0.51
1:A:225:ASN:N	1:A:225:ASN:HD22	2.09	0.51
1:C:81:GLU:CG	1:F:364:ASP:HB2	2.40	0.51
1:A:41:ILE:HG22	1:A:42:ALA:N	2.25	0.51
1:F:536:ARG:HH11	1:F:536:ARG:HG2	1.76	0.51
1:B:418:LYS:O	1:B:419:ARG:HD3	2.10	0.51
1:D:316:ASN:CG	1:D:344:THR:HG21	2.30	0.51
1:F:279:LEU:C	1:F:281:LEU:H	2.13	0.51
1:F:460:ARG:C	1:F:462:ASN:H	2.14	0.51
1:E:434:TRP:CE3	1:E:568:ARG:HB2	2.45	0.51
1:E:426:LEU:HD11	1:E:574:LEU:HD11	1.91	0.51
1:D:434:TRP:HB3	1:D:571:TYR:OH	2.09	0.51
1:B:68:LEU:HD13	1:B:139:ASN:CG	2.31	0.51
1:A:213:PHE:CE2	1:A:217:THR:HG21	2.45	0.51
1:E:434:TRP:CZ3	1:E:568:ARG:NE	2.79	0.51
1:A:223:LEU:HG	1:A:226:TRP:CD1	2.46	0.51
1:F:23:THR:HA	1:F:29:VAL:HG22	1.93	0.51
1:C:51:SER:HB2	1:C:52:PRO:HD2	1.92	0.51
1:E:497:TYR:CE2	1:E:511:LEU:HD21	2.46	0.51
1:D:627:PRO:HA	1:D:630:GLU:CB	2.41	0.51
1:D:144:ARG:HD2	1:D:171:LYS:CB	2.37	0.51
1:F:500:GLN:CA	1:F:500:GLN:HE21	2.23	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:570:LEU:H	1:C:570:LEU:HD12	1.73	0.51
1:E:438:GLN:HA	1:E:564:GLU:HG3	1.93	0.51
1:D:20:ARG:HB3	1:D:29:VAL:O	2.10	0.51
1:A:493:ASP:HA	1:A:496:LYS:HG3	1.92	0.51
1:A:384:MET:O	1:A:384:MET:HG3	2.11	0.51
1:A:292:PRO:CG	1:A:296:PRO:O	2.57	0.51
1:B:592:ARG:NH1	1:B:592:ARG:HB3	2.26	0.51
1:B:486:PHE:CE1	1:B:647:GLN:HB3	2.44	0.51
1:C:60:LEU:O	1:C:64:ILE:HG12	2.11	0.51
1:B:125:LEU:C	1:B:125:LEU:HD13	2.31	0.51
1:E:408:GLU:HG3	1:E:409:SER:N	2.25	0.51
1:B:510:LEU:HB3	1:B:653:GLU:OE2	2.11	0.51
1:C:517:MET:HB3	1:C:650:ARG:NH2	2.26	0.51
1:F:394:LYS:CG	1:F:401:ILE:HG22	2.41	0.51
1:E:268:VAL:HG13	1:E:269:LEU:N	2.26	0.51
1:C:431:GLY:C	1:C:433:VAL:H	2.14	0.51
1:C:213:PHE:CZ	1:C:243:ILE:HB	2.46	0.51
1:F:426:LEU:HD22	1:F:586:ASP:O	2.11	0.51
1:A:268:VAL:HG13	1:A:269:LEU:N	2.26	0.51
1:D:115:CYS:O	1:D:217:THR:O	2.28	0.51
1:F:230:GLN:O	1:F:234:LYS:N	2.39	0.51
1:E:165:ILE:HG22	1:E:166:ASP:N	2.15	0.51
1:E:282:MET:HG2	1:E:286:ARG:NE	2.23	0.51
1:F:113:ASN:HB3	1:F:117:LEU:HD12	1.93	0.51
1:E:493:ASP:HA	1:E:496:LYS:HG3	1.93	0.51
1:C:80:PRO:HB2	1:C:84:GLN:HE21	1.76	0.51
1:A:41:ILE:HG22	1:A:42:ALA:H	1.76	0.51
1:A:534:VAL:O	1:A:538:MET:HB2	2.11	0.51
1:B:410:VAL:HG12	1:B:411:SER:N	2.18	0.50
1:B:249:LEU:HD23	1:B:418:LYS:HZ1	1.76	0.50
1:F:420:ASN:C	1:F:421:LEU:HD22	2.32	0.50
1:D:578:PRO:C	1:D:580:ASP:H	2.14	0.50
1:D:219:PHE:CD1	1:D:221:PRO:HG3	2.47	0.50
1:F:227:GLN:O	1:F:231:TRP:HB3	2.11	0.50
1:E:117:LEU:HD23	1:E:119:GLU:OE1	2.11	0.50
1:E:245:VAL:HG12	1:E:245:VAL:O	2.10	0.50
1:A:430:TRP:HE1	1:A:587:SER:HA	1.76	0.50
1:A:583:THR:HG23	1:A:584:GLU:OE2	2.10	0.50
1:B:556:GLN:NE2	1:B:604:LYS:NZ	2.59	0.50
1:D:361:LEU:HD22	1:D:370:CYS:SG	2.51	0.50
1:E:265:LEU:HD11	1:E:270:ALA:CA	2.34	0.50
1:F:355:GLN:HB3	1:F:359:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:152:VAL:HG13	1:B:165:ILE:HD11	1.92	0.50
1:D:428:LYS:O	1:D:432:GLN:HG2	2.10	0.50
1:D:418:LYS:HZ1	1:D:421:LEU:HD12	1.76	0.50
1:E:223:LEU:HD13	1:E:224:PRO:N	2.26	0.50
1:E:77:ARG:HD2	1:E:78:ASP:H	1.76	0.50
1:E:41:ILE:HG22	1:E:42:ALA:N	2.26	0.50
1:B:366:PRO:C	1:B:368:THR:H	2.15	0.50
1:D:654:LEU:HD23	1:E:654:LEU:HB3	1.93	0.50
1:F:493:ASP:HA	1:F:496:LYS:HG3	1.94	0.50
1:A:410:VAL:HG12	1:A:411:SER:N	2.22	0.50
1:D:419:ARG:HE	1:D:419:ARG:N	2.09	0.50
1:E:371:ILE:HG23	1:E:371:ILE:O	2.11	0.50
1:B:457:ASN:HA	1:B:460:ARG:HG3	1.93	0.50
1:B:367:ALA:O	1:B:369:GLN:N	2.44	0.50
1:D:49:GLU:HG2	1:D:91:LEU:HD13	1.91	0.50
1:A:336:LEU:HD23	1:A:340:ILE:HG23	1.93	0.50
1:F:475:MET:O	1:F:478:GLN:HB3	2.11	0.50
1:A:477:GLN:CD	1:F:478:GLN:NE2	2.65	0.50
1:B:20:ARG:HB2	1:B:23:THR:HB	1.92	0.50
1:C:365:LYS:HD3	1:C:366:PRO:HD2	1.93	0.50
1:B:536:ARG:NH1	1:B:625:LEU:HD13	2.27	0.50
1:C:577:LYS:O	1:C:579:ARG:N	2.40	0.50
1:C:443:ASP:HA	1:C:446:ARG:HG3	1.94	0.50
1:C:653:GLU:O	1:C:657:LEU:HD13	2.11	0.50
1:D:582:ARG:N	1:D:582:ARG:NE	2.52	0.50
1:F:336:LEU:HD23	1:F:340:ILE:HG23	1.92	0.50
1:E:643:VAL:O	1:E:647:GLN:HG2	2.11	0.50
1:B:474:SER:O	1:B:477:GLN:HG2	2.12	0.50
1:B:455:MET:HB2	1:B:615:THR:HG21	1.93	0.50
1:B:536:ARG:NH2	1:B:625:LEU:HD13	2.27	0.50
1:F:41:ILE:HG22	1:F:42:ALA:H	1.76	0.50
1:C:493:ASP:HA	1:C:496:LYS:HG3	1.93	0.50
1:F:294:TYR:HD2	1:F:296:PRO:HD2	1.75	0.50
1:D:231:TRP:O	1:D:233:SER:N	2.44	0.50
1:F:423:PHE:CD1	1:F:583:THR:HA	2.46	0.50
1:A:36:GLU:O	1:A:38:GLY:N	2.44	0.50
1:B:99:CYS:HB3	1:B:154:GLN:HB2	1.93	0.50
1:B:350:ASP:HB2	1:B:391:ASP:H	1.77	0.50
1:A:350:ASP:HB2	1:A:391:ASP:H	1.76	0.50
1:C:641:LYS:HD2	1:C:645:ARG:NH1	2.26	0.50
1:A:220:ARG:N	1:A:221:PRO:CD	2.71	0.50
1:C:192:GLU:HG2	1:C:283:TRP:CB	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:433:VAL:O	1:E:436:SER:HB3	2.11	0.50
1:A:635:LEU:O	1:A:639:ASP:HB3	2.12	0.50
1:D:384:MET:SD	1:D:385:ASP:N	2.85	0.50
1:B:548:GLN:OE1	1:B:548:GLN:N	2.45	0.50
1:D:60:LEU:O	1:D:64:ILE:HG12	2.12	0.50
1:C:311:LEU:O	1:C:311:LEU:HD12	2.11	0.50
1:A:189:LEU:HD22	1:A:189:LEU:N	2.27	0.50
1:A:122:ILE:HD13	1:A:216:ILE:HG12	1.94	0.50
1:F:355:GLN:HB3	1:F:359:LEU:CD1	2.41	0.50
1:A:236:ARG:NH1	1:A:236:ARG:HG3	2.26	0.50
1:F:213:PHE:CA	1:F:277:LEU:HD21	2.38	0.50
1:B:284:HIS:N	1:B:285:PRO:HD2	2.26	0.50
1:D:167:LEU:O	1:D:170:ALA:CB	2.60	0.50
1:D:626:LEU:HD23	1:D:626:LEU:C	2.32	0.50
1:E:373:ASP:O	1:E:385:ASP:N	2.45	0.50
1:D:117:LEU:HB3	1:D:119:GLU:OE1	2.11	0.50
1:E:392:ASN:CG	1:E:393:SER:N	2.64	0.50
1:D:23:THR:HA	1:D:29:VAL:HG22	1.94	0.50
1:B:578:PRO:C	1:B:580:ASP:H	2.15	0.50
1:E:517:MET:HG2	1:E:650:ARG:NE	2.27	0.50
1:F:170:ALA:HB3	1:F:178:LEU:HD12	1.94	0.50
1:B:189:LEU:N	1:B:189:LEU:HD22	2.27	0.50
1:F:194:LEU:HB3	1:F:196:GLN:HE22	1.77	0.50
1:A:125:LEU:HA	1:A:162:HIS:CD2	2.46	0.50
1:D:139:ASN:O	1:D:141:ILE:HD12	2.11	0.50
1:A:536:ARG:HG2	1:A:536:ARG:HH11	1.76	0.50
1:B:479:LEU:HD11	1:B:641:LYS:CG	2.28	0.50
1:C:417:PRO:HA	1:D:320:GLY:CA	2.28	0.50
1:B:282:MET:HB2	1:B:286:ARG:NH2	2.27	0.50
1:C:544:ILE:O	1:C:547:LEU:HG	2.12	0.50
1:B:103:ASP:O	1:B:105:ARG:N	2.45	0.50
1:C:77:ARG:HD2	1:C:78:ASP:H	1.77	0.50
1:C:234:LYS:NZ	1:C:237:GLN:HE22	2.10	0.50
1:A:419:ARG:NH1	1:A:419:ARG:O	2.45	0.50
1:F:249:LEU:HG	1:F:414:LEU:HG	1.93	0.50
1:B:285:PRO:O	1:B:290:THR:HG21	2.12	0.50
1:E:19:GLU:CD	1:E:19:GLU:H	2.16	0.50
1:A:653:GLU:O	1:A:657:LEU:HD13	2.12	0.50
1:C:320:GLY:CA	1:D:417:PRO:HA	2.37	0.50
1:B:365:LYS:C	1:B:367:ALA:N	2.66	0.50
1:B:643:VAL:O	1:B:647:GLN:HG2	2.12	0.50
1:A:355:GLN:HB3	1:A:359:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:525:GLY:HA2	1:D:640:GLU:OE2	2.12	0.50
1:F:577:LYS:CG	1:F:578:PRO:HD2	2.42	0.50
1:F:77:ARG:HD2	1:F:78:ASP:H	1.76	0.50
1:F:635:LEU:O	1:F:639:ASP:HB3	2.12	0.50
1:C:631:GLU:HG3	1:C:632:VAL:N	2.27	0.50
1:A:665:VAL:HG21	1:F:664:LYS:HB3	1.94	0.50
1:F:41:ILE:HG22	1:F:42:ALA:N	2.26	0.50
1:D:350:ASP:HB2	1:D:391:ASP:H	1.77	0.50
1:C:620:GLN:O	1:C:624:GLU:HG2	2.11	0.50
1:B:410:VAL:O	1:B:411:SER:HB3	2.11	0.49
1:E:434:TRP:HB3	1:E:571:TYR:OH	2.12	0.49
1:B:268:VAL:O	1:B:272:ARG:HB2	2.11	0.49
1:D:533:LEU:HD13	1:D:629:VAL:HG12	1.94	0.49
1:A:144:ARG:HD3	1:A:169:TYR:O	2.12	0.49
1:B:117:LEU:HD12	1:B:215:CYS:O	2.12	0.49
1:D:77:ARG:N	1:D:96:MET:HA	2.26	0.49
1:C:20:ARG:HB2	1:C:23:THR:HB	1.92	0.49
1:F:480:LYS:HG2	1:F:527:GLU:CB	2.42	0.49
1:A:316:ASN:HA	1:A:388:PHE:CE1	2.47	0.49
1:A:644:VAL:O	1:A:647:GLN:HB2	2.11	0.49
1:D:534:VAL:O	1:D:538:MET:HB2	2.12	0.49
1:E:311:LEU:O	1:E:311:LEU:HD12	2.12	0.49
1:C:298:GLY:O	1:C:299:CYS:C	2.49	0.49
1:B:658:LEU:HD23	1:C:496:LYS:HZ2	1.78	0.49
1:A:282:MET:HG3	1:A:283:TRP:CZ3	2.47	0.49
1:F:116:GLY:O	1:F:216:ILE:O	2.30	0.49
1:B:272:ARG:NH1	1:B:272:ARG:HG3	2.27	0.49
1:F:467:LYS:CD	1:F:541:GLN:HG2	2.41	0.49
1:D:621:LYS:O	1:D:625:LEU:HD12	2.12	0.49
1:D:51:SER:HB2	1:D:52:PRO:HD2	1.94	0.49
1:F:118:ARG:HD2	1:F:264:ASN:OD1	2.13	0.49
1:E:239:SER:O	1:E:242:ASP:HB2	2.11	0.49
1:A:243:ILE:HG22	1:A:281:LEU:CD2	2.42	0.49
1:F:389:LEU:CD2	1:F:454:ALA:CB	2.79	0.49
1:E:358:GLY:HA2	1:E:453:ALA:O	2.12	0.49
1:E:111:PHE:CE1	1:E:575:ARG:HD2	2.47	0.49
1:D:103:ASP:O	1:D:106:LYS:N	2.44	0.49
1:E:306:ILE:O	1:E:309:LEU:HB3	2.11	0.49
1:A:367:ALA:C	1:A:369:GLN:N	2.66	0.49
1:A:20:ARG:HB2	1:A:23:THR:HB	1.93	0.49
1:C:23:THR:HA	1:C:29:VAL:HG22	1.93	0.49
1:D:16:GLU:HG3	1:D:33:HIS:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:103:ASP:O	1:C:105:ARG:N	2.45	0.49
1:E:463:SER:HA	1:E:467:LYS:HB3	1.94	0.49
1:D:128:ASP:HB3	1:D:162:HIS:HB2	1.93	0.49
1:E:487:LYS:HA	1:E:491:GLN:HB2	1.94	0.49
1:B:594:LEU:C	1:B:594:LEU:HD13	2.33	0.49
1:B:496:LYS:NZ	1:C:658:LEU:HD23	2.28	0.49
1:E:312:VAL:HG22	1:E:313:HIS:N	2.28	0.49
1:B:36:GLU:O	1:B:38:GLY:N	2.45	0.49
1:F:122:ILE:HD13	1:F:216:ILE:HG12	1.95	0.49
1:A:655:TRP:HZ2	1:F:499:GLU:CD	2.14	0.49
1:C:67:ARG:NH2	1:C:68:LEU:HD12	2.22	0.49
1:B:462:ASN:C	1:B:464:CYS:H	2.16	0.49
1:B:528:ASN:O	1:B:532:LEU:HD23	2.12	0.49
1:D:476:SER:HB2	1:D:636:MET:CE	2.43	0.49
1:F:36:GLU:O	1:F:38:GLY:N	2.45	0.49
1:B:620:GLN:O	1:B:624:GLU:HG2	2.12	0.49
1:F:621:LYS:O	1:F:625:LEU:HD12	2.12	0.49
1:F:51:SER:HB2	1:F:52:PRO:HD2	1.93	0.49
1:E:99:CYS:HB3	1:E:154:GLN:HB2	1.95	0.49
1:D:394:LYS:HZ3	1:D:401:ILE:N	2.11	0.49
1:F:294:TYR:HB2	1:F:296:PRO:HD2	1.93	0.49
1:F:457:ASN:HA	1:F:460:ARG:HG3	1.94	0.49
1:E:357:ALA:O	1:E:456:MET:HG2	2.10	0.49
1:E:434:TRP:HZ3	1:E:568:ARG:HE	1.59	0.49
1:F:570:LEU:N	1:F:570:LEU:HD12	2.27	0.49
1:D:105:ARG:CD	1:D:148:PRO:HB2	2.42	0.49
1:F:18:LYS:HB3	1:F:19:GLU:OE2	2.12	0.49
1:A:657:LEU:HA	1:A:660:ILE:HG22	1.94	0.49
1:E:241:VAL:HG12	1:E:241:VAL:O	2.13	0.49
1:D:55:ARG:HD2	1:D:91:LEU:HD11	1.94	0.49
1:D:371:ILE:HB	1:D:384:MET:HE2	1.94	0.49
1:E:118:ARG:HH22	1:E:438:GLN:HG2	1.78	0.49
1:C:627:PRO:HA	1:C:630:GLU:CB	2.41	0.49
1:C:105:ARG:HD2	1:C:148:PRO:HB2	1.93	0.49
1:B:355:GLN:O	1:B:357:ALA:N	2.46	0.49
1:E:548:GLN:OE1	1:E:548:GLN:N	2.46	0.49
1:C:525:GLY:O	1:C:527:GLU:N	2.46	0.49
1:A:214:GLU:O	1:A:218:GLY:HA2	2.11	0.49
1:F:294:TYR:HB2	1:F:296:PRO:CD	2.42	0.49
1:C:265:LEU:HG	1:C:266:ASN:N	2.28	0.49
1:D:229:VAL:CG2	1:D:230:GLN:H	2.09	0.49
1:D:223:LEU:O	1:D:231:TRP:CH2	2.66	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:80:PRO:CB	1:B:83:MET:HB2	2.36	0.49
1:D:653:GLU:O	1:D:657:LEU:HD13	2.12	0.49
1:E:460:ARG:C	1:E:462:ASN:H	2.16	0.49
1:B:431:GLY:C	1:B:433:VAL:H	2.15	0.49
1:E:644:VAL:O	1:E:647:GLN:HB2	2.12	0.49
1:A:123:LEU:HD12	1:A:307:LEU:HD13	1.94	0.49
1:B:265:LEU:HD23	1:B:265:LEU:N	2.27	0.49
1:D:559:THR:HB	1:D:604:LYS:HZ1	1.78	0.49
1:F:341:GLN:HA	1:F:345:GLY:O	2.12	0.49
1:C:463:SER:HA	1:C:467:LYS:HB3	1.93	0.49
1:E:536:ARG:HH11	1:E:536:ARG:HG2	1.77	0.49
1:C:490:ILE:HG13	1:C:650:ARG:HB3	1.95	0.49
1:A:626:LEU:HB3	1:A:627:PRO:HD3	1.95	0.49
1:A:412:CYS:O	1:A:415:GLN:HB3	2.13	0.49
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.78	0.49
1:D:419:ARG:HH11	1:D:588:GLN:NE2	2.10	0.49
1:A:341:GLN:HA	1:A:345:GLY:O	2.12	0.49
1:E:49:GLU:HG3	1:E:89:ASN:ND2	2.26	0.49
1:E:49:GLU:H	1:E:89:ASN:ND2	2.11	0.49
1:D:458:LEU:HD11	1:D:544:ILE:HG21	1.94	0.49
1:F:117:LEU:HD23	1:F:119:GLU:OE1	2.13	0.49
1:F:577:LYS:HG3	1:F:578:PRO:CD	2.40	0.49
1:B:477:GLN:HE21	1:C:477:GLN:HE21	1.59	0.49
1:F:51:SER:O	1:F:55:ARG:HG3	2.12	0.49
1:E:474:SER:O	1:E:477:GLN:HG2	2.12	0.49
1:B:366:PRO:CB	1:B:368:THR:HG23	2.20	0.49
1:E:20:ARG:HB2	1:E:23:THR:HB	1.94	0.49
1:E:170:ALA:O	1:E:171:LYS:HB2	2.13	0.49
1:D:241:VAL:HG12	1:D:278:GLN:HG2	1.95	0.49
1:D:496:LYS:HD2	1:E:655:TRP:CG	2.47	0.49
1:D:490:ILE:HG21	1:D:517:MET:CE	2.43	0.49
1:B:421:LEU:N	1:B:421:LEU:HD12	2.28	0.49
1:B:621:LYS:O	1:B:625:LEU:HD12	2.13	0.49
1:E:537:MET:C	1:E:537:MET:SD	2.91	0.49
1:F:356:GLU:OE2	1:F:384:MET:HG3	2.13	0.49
1:D:103:ASP:O	1:D:104:LEU:C	2.51	0.49
1:B:220:ARG:N	1:B:221:PRO:CD	2.73	0.49
1:A:481:ALA:HB3	1:F:482:LYS:HD2	1.93	0.49
1:B:105:ARG:HD3	1:B:149:GLU:CD	2.33	0.49
1:D:310:LYS:H	1:D:310:LYS:HZ2	1.59	0.49
1:F:387:VAL:HG21	1:F:449:GLN:O	2.12	0.49
1:B:22:GLY:N	1:B:165:ILE:HG21	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:579:ARG:O	1:A:580:ASP:HB3	2.11	0.49
1:D:268:VAL:O	1:D:272:ARG:HB2	2.12	0.49
1:F:242:ASP:OD2	1:F:257:SER:HB3	2.13	0.49
1:B:279:LEU:C	1:B:281:LEU:H	2.15	0.49
1:A:170:ALA:HB3	1:A:178:LEU:HD12	1.95	0.49
1:F:527:GLU:HG3	1:F:528:ASN:N	2.28	0.49
1:C:77:ARG:N	1:C:96:MET:HA	2.27	0.49
1:A:105:ARG:CD	1:A:148:PRO:HB2	2.43	0.49
1:C:43:ILE:HD12	1:C:43:ILE:N	2.28	0.49
1:E:350:ASP:HB2	1:E:391:ASP:H	1.78	0.49
1:E:285:PRO:O	1:E:290:THR:OG1	2.31	0.48
1:C:418:LYS:O	1:C:419:ARG:CB	2.55	0.48
1:F:294:TYR:CD2	1:F:296:PRO:HD2	2.48	0.48
1:F:298:GLY:O	1:F:299:CYS:C	2.51	0.48
1:C:286:ARG:O	1:C:290:THR:N	2.46	0.48
1:F:419:ARG:NH1	1:F:588:GLN:HA	2.28	0.48
1:B:186:LEU:O	1:B:188:TYR:N	2.46	0.48
1:B:212:ALA:O	1:B:216:ILE:HG13	2.12	0.48
1:F:467:LYS:HD3	1:F:541:GLN:CD	2.33	0.48
1:D:279:LEU:C	1:D:281:LEU:H	2.15	0.48
1:A:356:GLU:HA	1:A:453:ALA:HB1	1.95	0.48
1:B:310:LYS:H	1:B:310:LYS:HZ2	1.60	0.48
1:C:536:ARG:CZ	1:C:625:LEU:HD13	2.42	0.48
1:F:350:ASP:CB	1:F:391:ASP:HB2	2.43	0.48
1:C:194:LEU:HB3	1:C:196:GLN:HE22	1.77	0.48
1:C:265:LEU:HG	1:C:266:ASN:H	1.77	0.48
1:D:213:PHE:CD2	1:D:221:PRO:HG2	2.48	0.48
1:A:60:LEU:O	1:A:64:ILE:HG12	2.13	0.48
1:E:422:ALA:O	1:E:585:GLY:HA3	2.12	0.48
1:E:103:ASP:O	1:E:106:LYS:N	2.42	0.48
1:F:501:THR:HG23	1:F:505:ILE:CG2	2.43	0.48
1:F:43:ILE:N	1:F:43:ILE:HD12	2.27	0.48
1:D:262:PRO:HB2	1:D:432:GLN:NE2	2.28	0.48
1:B:16:GLU:OE2	1:B:83:MET:HE3	2.12	0.48
1:D:418:LYS:C	1:D:419:ARG:HG3	2.34	0.48
1:E:418:LYS:HZ1	1:E:421:LEU:HD22	1.78	0.48
1:E:107:TYR:CE2	1:E:153:LEU:HD22	2.47	0.48
1:B:89:ASN:C	1:B:91:LEU:H	2.16	0.48
1:C:572:ARG:O	1:C:576:GLU:HB2	2.13	0.48
1:A:431:GLY:O	1:A:433:VAL:N	2.46	0.48
1:F:572:ARG:O	1:F:576:GLU:HB2	2.13	0.48
1:C:594:LEU:HD13	1:C:594:LEU:C	2.34	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:248:ASP:O	1:B:249:LEU:C	2.51	0.48
1:B:319:THR:HG23	1:B:320:GLY:N	2.22	0.48
1:A:205:TYR:CD1	1:A:290:THR:HG23	2.42	0.48
1:C:268:VAL:O	1:C:272:ARG:HB2	2.13	0.48
1:F:462:ASN:C	1:F:464:CYS:H	2.17	0.48
1:D:284:HIS:HB3	1:D:285:PRO:HD3	1.95	0.48
1:F:227:GLN:HG3	1:F:231:TRP:CZ3	2.48	0.48
1:D:168:GLY:O	1:D:179:CYS:SG	2.71	0.48
1:D:416:GLU:C	1:D:418:LYS:N	2.67	0.48
1:B:362:ILE:HG13	1:E:37:THR:HG22	1.96	0.48
1:D:279:LEU:HD11	1:D:290:THR:O	2.13	0.48
1:A:234:LYS:HE2	1:A:253:VAL:HG11	1.96	0.48
1:B:577:LYS:HG3	1:B:578:PRO:HD2	1.96	0.48
1:A:72:ASN:HA	1:A:163:LYS:HA	1.96	0.48
1:B:531:LYS:HB3	1:B:531:LYS:NZ	2.28	0.48
1:C:486:PHE:CE1	1:C:647:GLN:CB	2.91	0.48
1:B:496:LYS:HG2	1:C:655:TRP:CD1	2.49	0.48
1:F:285:PRO:O	1:F:290:THR:HB	2.14	0.48
1:F:429:VAL:O	1:F:433:VAL:HG23	2.14	0.48
1:B:286:ARG:CA	1:B:290:THR:HG21	2.40	0.48
1:E:294:TYR:CD2	1:E:294:TYR:N	2.79	0.48
1:D:168:GLY:O	1:D:170:ALA:N	2.47	0.48
1:B:172:GLU:HG3	1:B:175:GLN:N	2.20	0.48
1:C:394:LYS:HG2	1:C:394:LYS:O	2.13	0.48
1:C:316:ASN:HA	1:C:388:PHE:CE1	2.48	0.48
1:A:89:ASN:HD22	1:A:89:ASN:N	2.08	0.48
1:C:117:LEU:HB3	1:C:119:GLU:OE1	2.13	0.48
1:C:357:ALA:HB3	1:C:359:LEU:HD11	1.96	0.48
1:E:79:VAL:HG23	1:E:84:GLN:HG2	1.96	0.48
1:D:145:ASP:HA	1:D:189:LEU:HD11	1.94	0.48
1:F:18:LYS:HB3	1:F:19:GLU:CD	2.34	0.48
1:B:23:THR:HA	1:B:29:VAL:HG22	1.94	0.48
1:B:55:ARG:NH1	1:B:91:LEU:HD11	2.28	0.48
1:E:128:ASP:HB3	1:E:162:HIS:HB2	1.96	0.48
1:A:431:GLY:C	1:A:433:VAL:H	2.16	0.48
1:A:463:SER:HA	1:A:467:LYS:HB3	1.95	0.48
1:A:594:LEU:HD13	1:A:594:LEU:O	2.14	0.48
1:B:366:PRO:C	1:B:368:THR:N	2.66	0.48
1:D:641:LYS:HD2	1:D:645:ARG:NH1	2.29	0.48
1:B:478:GLN:HG3	1:C:481:ALA:HB2	1.95	0.48
1:C:55:ARG:HH11	1:C:91:LEU:HD11	1.76	0.48
1:E:152:VAL:HG13	1:E:165:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:22:GLY:N	1:F:165:ILE:HG21	2.29	0.48
1:C:462:ASN:C	1:C:464:CYS:H	2.16	0.48
1:E:118:ARG:HA	1:E:264:ASN:O	2.14	0.48
1:A:369:GLN:O	1:A:370:CYS:HB3	2.13	0.48
1:B:336:LEU:HD23	1:B:340:ILE:HG23	1.96	0.48
1:A:394:LYS:CD	1:A:401:ILE:HG13	2.44	0.48
1:C:240:GLU:OE1	1:C:241:VAL:N	2.47	0.48
1:B:77:ARG:HD2	1:B:78:ASP:H	1.79	0.48
1:D:570:LEU:H	1:D:570:LEU:HD12	1.77	0.48
1:D:74:VAL:HG23	1:D:164:ILE:O	2.14	0.48
1:A:160:LEU:N	1:A:160:LEU:HD12	2.29	0.48
1:D:571:TYR:HB3	1:D:575:ARG:NH2	2.13	0.48
1:F:16:GLU:N	1:F:16:GLU:OE2	2.47	0.48
1:F:80:PRO:HB2	1:F:83:MET:CB	2.34	0.48
1:C:22:GLY:N	1:C:165:ILE:HG21	2.29	0.48
1:E:410:VAL:O	1:E:411:SER:HB3	2.13	0.48
1:D:496:LYS:HD2	1:E:655:TRP:HA	1.96	0.48
1:D:657:LEU:HA	1:D:660:ILE:HG22	1.95	0.48
1:E:657:LEU:HA	1:E:660:ILE:HG22	1.95	0.48
1:C:139:ASN:O	1:C:141:ILE:HD12	2.14	0.48
1:E:105:ARG:NH2	1:E:188:TYR:OH	2.46	0.48
1:A:306:ILE:O	1:A:309:LEU:HD23	2.13	0.48
1:E:125:LEU:HA	1:E:162:HIS:CD2	2.49	0.48
1:A:125:LEU:C	1:A:125:LEU:HD13	2.33	0.48
1:D:311:LEU:O	1:D:311:LEU:HD12	2.14	0.48
1:A:217:THR:HB	1:A:260:PRO:HG3	1.96	0.48
1:A:415:GLN:NE2	1:A:419:ARG:HB3	2.29	0.48
1:F:354:LEU:CD2	1:F:457:ASN:HB2	2.42	0.48
1:E:430:TRP:HZ3	1:E:570:LEU:HB3	1.76	0.48
1:D:431:GLY:C	1:D:433:VAL:H	2.16	0.48
1:B:213:PHE:HE2	1:B:217:THR:HG21	1.78	0.48
1:C:410:VAL:HA	1:C:413:ILE:CG2	2.43	0.48
1:B:394:LYS:HZ1	1:B:402:SER:HB3	1.78	0.48
1:A:103:ASP:O	1:A:105:ARG:N	2.47	0.48
1:E:191:PRO:O	1:E:194:LEU:HB2	2.14	0.48
1:F:169:TYR:CD1	1:F:179:CYS:SG	3.05	0.48
1:B:517:MET:HG2	1:B:650:ARG:CZ	2.43	0.48
1:C:145:ASP:HA	1:C:189:LEU:HD11	1.96	0.48
1:A:577:LYS:HG2	1:A:581:GLN:HB2	1.96	0.48
1:B:249:LEU:CD1	1:B:414:LEU:HD21	2.43	0.48
1:E:212:ALA:O	1:E:216:ILE:HG13	2.13	0.48
1:E:284:HIS:O	1:E:285:PRO:C	2.52	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:434:TRP:HB3	1:B:571:TYR:CE1	2.49	0.48
1:C:268:VAL:HG13	1:C:269:LEU:N	2.29	0.48
1:E:111:PHE:CE1	1:E:575:ARG:HB3	2.49	0.48
1:F:587:SER:O	1:F:591:VAL:HG23	2.14	0.48
1:D:223:LEU:HD13	1:D:224:PRO:CD	2.43	0.48
1:E:21:LEU:HG	1:E:165:ILE:CD1	2.43	0.48
1:F:89:ASN:C	1:F:91:LEU:H	2.16	0.48
1:D:635:LEU:O	1:D:639:ASP:HB3	2.14	0.48
1:A:128:ASP:HB3	1:A:162:HIS:HB2	1.96	0.48
1:A:247:GLU:HG2	1:A:247:GLU:O	2.13	0.48
1:F:74:VAL:HG23	1:F:164:ILE:O	2.14	0.48
1:A:579:ARG:CD	1:A:579:ARG:H	2.13	0.47
1:E:497:TYR:HA	1:E:500:GLN:HB2	1.96	0.47
1:D:241:VAL:HG12	1:D:278:GLN:CG	2.44	0.47
1:A:460:ARG:HH11	1:A:460:ARG:HG2	1.78	0.47
1:B:460:ARG:HG2	1:B:460:ARG:HH11	1.79	0.47
1:C:531:LYS:HB3	1:C:531:LYS:NZ	2.29	0.47
1:A:145:ASP:HA	1:A:189:LEU:HD11	1.96	0.47
1:C:594:LEU:HD13	1:C:594:LEU:O	2.14	0.47
1:A:601:PHE:O	1:A:605:VAL:HG23	2.14	0.47
1:F:534:VAL:O	1:F:538:MET:HB2	2.13	0.47
1:F:144:ARG:HD2	1:F:171:LYS:HB2	1.96	0.47
1:E:313:HIS:ND1	1:E:324:THR:HG22	2.29	0.47
1:C:433:VAL:O	1:C:436:SER:HB3	2.15	0.47
1:A:220:ARG:O	1:A:221:PRO:O	2.31	0.47
1:C:236:ARG:HH22	1:C:283:TRP:HE3	1.61	0.47
1:E:21:LEU:HB3	1:E:165:ILE:CG2	2.39	0.47
1:D:282:MET:HB2	1:D:286:ARG:NH1	2.29	0.47
1:F:653:GLU:O	1:F:657:LEU:HD13	2.13	0.47
1:C:367:ALA:C	1:C:369:GLN:N	2.68	0.47
1:F:644:VAL:O	1:F:647:GLN:HB2	2.14	0.47
1:D:566:GLN:O	1:D:569:GLU:HB2	2.15	0.47
1:C:128:ASP:HB3	1:C:162:HIS:HB2	1.96	0.47
1:F:134:ARG:HG2	1:F:300:PHE:CD1	2.49	0.47
1:B:72:ASN:HA	1:B:163:LYS:HA	1.96	0.47
1:D:472:MET:O	1:D:475:MET:HG3	2.14	0.47
1:E:259:LEU:HD22	1:E:274:GLU:CG	2.36	0.47
1:F:227:GLN:CB	1:F:228:PRO:HD3	2.44	0.47
1:F:165:ILE:HG22	1:F:166:ASP:N	2.17	0.47
1:D:117:LEU:HD12	1:D:215:CYS:O	2.15	0.47
1:F:472:MET:O	1:F:475:MET:HG3	2.14	0.47
1:B:173:LEU:HD12	1:B:174:ASP:N	2.28	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:462:ASN:C	1:D:464:CYS:H	2.18	0.47
1:C:160:LEU:HD12	1:C:160:LEU:N	2.29	0.47
1:D:160:LEU:N	1:D:160:LEU:HD12	2.29	0.47
1:B:410:VAL:HA	1:B:413:ILE:CG2	2.41	0.47
1:C:408:GLU:O	1:C:409:SER:OG	2.25	0.47
1:D:346:ILE:HD13	1:D:388:PHE:HZ	1.79	0.47
1:F:357:ALA:O	1:F:456:MET:HG2	2.13	0.47
1:F:431:GLY:CA	1:F:571:TYR:CE2	2.96	0.47
1:F:430:TRP:NE1	1:F:587:SER:HA	2.24	0.47
1:D:587:SER:O	1:D:591:VAL:HG23	2.15	0.47
1:B:190:ALA:HB3	1:B:203:VAL:HG23	1.95	0.47
1:B:213:PHE:CZ	1:B:243:ILE:HB	2.49	0.47
1:A:165:ILE:HG22	1:A:166:ASP:N	2.17	0.47
1:A:655:TRP:HD1	1:F:500:GLN:CG	2.27	0.47
1:C:394:LYS:HB2	1:C:401:ILE:CB	2.43	0.47
1:A:353:LEU:HD12	1:A:353:LEU:N	2.29	0.47
1:C:366:PRO:C	1:C:368:THR:N	2.67	0.47
1:A:185:THR:C	1:A:187:GLN:H	2.18	0.47
1:C:360:ALA:O	1:F:37:THR:HG22	2.13	0.47
1:E:517:MET:HB3	1:E:650:ARG:NH2	2.29	0.47
1:E:621:LYS:O	1:E:625:LEU:HD12	2.14	0.47
1:F:601:PHE:O	1:F:605:VAL:HG23	2.14	0.47
1:F:285:PRO:O	1:F:286:ARG:HG3	2.15	0.47
1:F:142:ILE:HG23	1:F:204:ASP:OD2	2.15	0.47
1:F:152:VAL:HG13	1:F:165:ILE:HD11	1.95	0.47
1:F:467:LYS:NZ	1:F:541:GLN:HG2	2.29	0.47
1:A:570:LEU:HD12	1:A:570:LEU:H	1.78	0.47
1:C:460:ARG:C	1:C:462:ASN:H	2.17	0.47
1:C:118:ARG:HH22	1:C:438:GLN:CG	2.26	0.47
1:B:392:ASN:ND2	1:B:393:SER:H	2.11	0.47
1:F:617:VAL:O	1:F:621:LYS:HB2	2.13	0.47
1:C:371:ILE:HG12	1:C:384:MET:HE3	1.96	0.47
1:F:517:MET:O	1:F:521:VAL:HG23	2.15	0.47
1:B:499:GLU:OE1	1:C:659:LYS:HE2	2.14	0.47
1:F:261:TYR:HB3	1:F:409:SER:CB	2.45	0.47
1:F:245:VAL:HA	1:F:255:PHE:HA	1.96	0.47
1:E:631:GLU:HG3	1:E:632:VAL:N	2.30	0.47
1:E:649:LYS:HA	1:E:652:LYS:HE3	1.95	0.47
1:B:463:SER:HA	1:B:467:LYS:HB3	1.96	0.47
1:F:77:ARG:N	1:F:96:MET:HA	2.30	0.47
1:B:635:LEU:O	1:B:639:ASP:HB3	2.13	0.47
1:C:355:GLN:HB3	1:C:359:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:70:HIS:HE1	1:C:132:ALA:HA	1.78	0.47
1:E:151:ILE:HD12	1:E:211:LEU:HD11	1.96	0.47
1:C:294:TYR:O	1:C:301:LYS:HD3	2.15	0.47
1:B:490:ILE:HD11	1:B:651:GLN:CG	2.40	0.47
1:C:472:MET:O	1:C:475:MET:HG3	2.15	0.47
1:E:145:ASP:HA	1:E:189:LEU:HD11	1.97	0.47
1:C:416:GLU:HB2	1:D:405:PRO:HB3	1.97	0.47
1:F:294:TYR:HE1	1:F:301:LYS:NZ	2.12	0.47
1:E:357:ALA:HB3	1:E:359:LEU:HD11	1.97	0.47
1:E:571:TYR:HB3	1:E:575:ARG:NH2	2.11	0.47
1:D:272:ARG:HG3	1:D:272:ARG:NH1	2.29	0.47
1:F:49:GLU:OE1	1:F:91:LEU:HD21	2.14	0.47
1:E:190:ALA:HB3	1:E:203:VAL:HG23	1.96	0.47
1:C:346:ILE:HD13	1:C:388:PHE:HZ	1.78	0.47
1:E:241:VAL:HA	1:E:286:ARG:HH22	1.80	0.47
1:A:490:ILE:HG21	1:A:518:GLU:CB	2.40	0.47
1:E:353:LEU:HD12	1:E:353:LEU:N	2.30	0.47
1:E:385:ASP:CG	1:E:386:LEU:N	2.67	0.47
1:E:457:ASN:HA	1:E:460:ARG:HG3	1.97	0.47
1:B:408:GLU:CG	1:B:409:SER:H	2.26	0.47
1:D:77:ARG:HD2	1:D:78:ASP:H	1.80	0.47
1:A:91:LEU:HA	1:A:92:PRO:HD3	1.73	0.47
1:A:77:ARG:N	1:A:96:MET:HA	2.29	0.47
1:C:103:ASP:O	1:C:104:LEU:C	2.53	0.47
1:B:357:ALA:HB3	1:B:359:LEU:HD11	1.96	0.47
1:B:445:ASN:HA	1:B:448:GLN:HB2	1.97	0.47
1:C:635:LEU:O	1:C:639:ASP:HB3	2.14	0.47
1:D:350:ASP:CB	1:D:391:ASP:HB2	2.45	0.47
1:D:70:HIS:HE1	1:D:132:ALA:HA	1.79	0.47
1:B:246:SER:OG	1:B:247:GLU:N	2.46	0.47
1:E:43:ILE:N	1:E:43:ILE:HD12	2.30	0.47
1:E:566:GLN:O	1:E:569:GLU:HB2	2.14	0.47
1:B:572:ARG:O	1:B:576:GLU:HB2	2.15	0.47
1:A:443:ASP:HA	1:A:446:ARG:HG3	1.96	0.47
1:F:566:GLN:O	1:F:569:GLU:HB2	2.15	0.47
1:A:485:PHE:CD1	1:A:485:PHE:C	2.88	0.47
1:C:272:ARG:HG3	1:C:272:ARG:NH1	2.29	0.47
1:C:190:ALA:HB3	1:C:203:VAL:HG23	1.96	0.47
1:D:418:LYS:NZ	1:D:421:LEU:CD1	2.77	0.47
1:B:558:GLY:CA	1:B:562:ASP:HB2	2.43	0.47
1:E:77:ARG:N	1:E:96:MET:HA	2.29	0.47
1:B:392:ASN:CG	1:B:393:SER:N	2.67	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:355:GLN:HB3	1:D:359:LEU:CD1	2.44	0.47
1:F:189:LEU:N	1:F:189:LEU:HD22	2.30	0.47
1:E:475:MET:O	1:E:478:GLN:HB3	2.15	0.47
1:F:460:ARG:HG2	1:F:460:ARG:HH11	1.80	0.47
1:E:430:TRP:O	1:E:571:TYR:HE2	1.97	0.47
1:D:283:TRP:CZ3	1:D:285:PRO:HD2	2.50	0.47
1:D:217:THR:HA	1:D:263:ASN:CG	2.36	0.47
1:E:17:MET:O	1:E:18:LYS:HG2	2.15	0.47
1:E:169:TYR:OH	1:E:183:VAL:HB	2.13	0.47
1:A:460:ARG:C	1:A:462:ASN:H	2.18	0.47
1:E:635:LEU:O	1:E:639:ASP:HB3	2.14	0.47
1:D:517:MET:O	1:D:521:VAL:HG23	2.15	0.47
1:E:416:GLU:C	1:E:418:LYS:N	2.69	0.47
1:D:655:TRP:NE1	1:E:496:LYS:HD2	2.30	0.47
1:C:577:LYS:CD	1:C:581:GLN:HE22	2.28	0.47
1:F:169:TYR:HA	1:F:179:CYS:HB3	1.95	0.47
1:F:128:ASP:HB3	1:F:162:HIS:HB2	1.96	0.47
1:C:657:LEU:HA	1:C:660:ILE:HG22	1.96	0.47
1:C:431:GLY:O	1:C:433:VAL:N	2.48	0.47
1:D:192:GLU:H	1:D:192:GLU:HG3	1.42	0.47
1:F:216:ILE:HD12	1:F:277:LEU:HD22	1.95	0.47
1:B:221:PRO:O	1:B:222:PHE:CB	2.61	0.47
1:B:229:VAL:C	1:B:231:TRP:H	2.18	0.47
1:C:153:LEU:HD12	1:C:153:LEU:N	2.30	0.47
1:E:165:ILE:CG2	1:E:166:ASP:H	2.12	0.47
1:C:548:GLN:OE1	1:C:548:GLN:N	2.47	0.47
1:D:408:GLU:HG3	1:D:413:ILE:HD13	1.95	0.47
1:B:369:GLN:O	1:B:369:GLN:HG3	2.15	0.47
1:E:229:VAL:HG13	1:E:230:GLN:N	2.30	0.47
1:A:531:LYS:HB3	1:A:531:LYS:NZ	2.29	0.47
1:F:631:GLU:HG3	1:F:632:VAL:N	2.30	0.47
1:D:84:GLN:CD	1:D:85:ASN:N	2.68	0.47
1:D:460:ARG:C	1:D:462:ASN:H	2.17	0.47
1:C:168:GLY:O	1:C:178:LEU:HD22	2.14	0.47
1:C:355:GLN:HB3	1:C:359:LEU:CD1	2.45	0.47
1:A:594:LEU:HD13	1:A:594:LEU:C	2.35	0.47
1:C:341:GLN:HA	1:C:345:GLY:O	2.15	0.47
1:D:477:GLN:OE1	1:E:475:MET:HA	2.15	0.46
1:B:284:HIS:C	1:B:286:ARG:H	2.18	0.46
1:B:60:LEU:O	1:B:64:ILE:HG12	2.15	0.46
1:B:341:GLN:HA	1:B:345:GLY:O	2.15	0.46
1:D:421:LEU:O	1:D:422:ALA:O	2.32	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:89:ASN:N	1:B:89:ASN:HD22	2.11	0.46
1:B:259:LEU:H	1:B:274:GLU:HG3	1.80	0.46
1:B:306:ILE:O	1:B:309:LEU:HB2	2.15	0.46
1:B:170:ALA:N	1:B:178:LEU:HD12	2.30	0.46
1:B:566:GLN:O	1:B:569:GLU:HB2	2.14	0.46
1:A:626:LEU:HD23	1:A:626:LEU:C	2.36	0.46
1:F:431:GLY:C	1:F:433:VAL:H	2.17	0.46
1:E:410:VAL:HA	1:E:413:ILE:CG2	2.42	0.46
1:A:490:ILE:HG22	1:A:518:GLU:CD	2.35	0.46
1:E:583:THR:O	1:E:584:GLU:O	2.33	0.46
1:B:114:CYS:SG	1:B:431:GLY:HA3	2.55	0.46
1:C:631:GLU:HG3	1:C:632:VAL:H	1.80	0.46
1:B:55:ARG:HH11	1:B:91:LEU:HD11	1.80	0.46
1:B:517:MET:HG2	1:B:650:ARG:NE	2.31	0.46
1:D:473:ALA:HB2	1:D:633:VAL:HG11	1.97	0.46
1:D:72:ASN:HA	1:D:163:LYS:HA	1.97	0.46
1:A:566:GLN:O	1:A:569:GLU:HB2	2.15	0.46
1:A:623:LEU:O	1:A:623:LEU:HD23	2.15	0.46
1:E:186:LEU:CD1	1:E:189:LEU:HB2	2.45	0.46
1:C:217:THR:HA	1:C:263:ASN:ND2	2.29	0.46
1:F:419:ARG:NE	1:F:591:VAL:HG21	2.30	0.46
1:D:105:ARG:HH22	1:D:220:ARG:HH21	1.62	0.46
1:A:319:THR:HG23	1:A:320:GLY:N	2.20	0.46
1:B:123:LEU:HD12	1:B:307:LEU:HD13	1.96	0.46
1:B:312:VAL:HG12	1:B:325:TYR:O	2.15	0.46
1:D:17:MET:C	1:D:18:LYS:HD2	2.35	0.46
1:C:310:LYS:H	1:C:310:LYS:HZ2	1.63	0.46
1:D:476:SER:HB2	1:D:636:MET:HE3	1.97	0.46
1:B:43:ILE:HD12	1:B:43:ILE:N	2.31	0.46
1:E:221:PRO:HG3	1:E:243:ILE:O	2.15	0.46
1:E:261:TYR:N	1:E:262:PRO:HD2	2.29	0.46
1:F:265:LEU:HD23	1:F:265:LEU:N	2.27	0.46
1:F:433:VAL:O	1:F:436:SER:HB3	2.15	0.46
1:E:295:GLY:H	1:E:296:PRO:CD	2.17	0.46
1:F:139:ASN:O	1:F:141:ILE:HD12	2.15	0.46
1:A:481:ALA:HB1	1:F:482:LYS:HZ1	1.75	0.46
1:B:353:LEU:HD12	1:B:353:LEU:N	2.29	0.46
1:D:385:ASP:CG	1:D:386:LEU:N	2.69	0.46
1:B:141:ILE:HG22	1:B:142:ILE:N	2.30	0.46
1:C:103:ASP:O	1:C:106:LYS:N	2.47	0.46
1:A:151:ILE:HD12	1:A:211:LEU:HD11	1.98	0.46
1:B:649:LYS:HA	1:B:652:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:265:LEU:HD21	1:E:270:ALA:HB2	1.98	0.46
1:B:21:LEU:C	1:B:165:ILE:HD13	2.36	0.46
1:D:577:LYS:HG3	1:D:578:PRO:HD2	1.95	0.46
1:A:633:VAL:HA	1:A:636:MET:HE2	1.97	0.46
1:F:68:LEU:HD13	1:F:139:ASN:OD1	2.15	0.46
1:F:474:SER:O	1:F:477:GLN:HG2	2.16	0.46
1:C:313:HIS:ND1	1:C:324:THR:HG22	2.30	0.46
1:B:501:THR:HA	1:B:505:ILE:CG2	2.45	0.46
1:D:72:ASN:C	1:D:163:LYS:HA	2.36	0.46
1:E:641:LYS:HD2	1:E:645:ARG:NH1	2.31	0.46
1:E:534:VAL:O	1:E:538:MET:HB2	2.16	0.46
1:F:462:ASN:ND2	1:F:544:ILE:CD1	2.79	0.46
1:D:229:VAL:O	1:D:231:TRP:N	2.47	0.46
1:E:18:LYS:HB2	1:E:31:ARG:HB3	1.97	0.46
1:F:21:LEU:HG	1:F:165:ILE:CD1	2.44	0.46
1:A:530:VAL:HG13	1:A:633:VAL:HG12	1.98	0.46
1:E:142:ILE:HG12	1:E:201:VAL:HG13	1.97	0.46
1:A:67:ARG:NH2	1:A:68:LEU:HD12	2.22	0.46
1:B:360:ALA:O	1:E:37:THR:HA	2.16	0.46
1:A:77:ARG:HD2	1:A:78:ASP:H	1.81	0.46
1:F:537:MET:SD	1:F:537:MET:C	2.94	0.46
1:C:452:ARG:C	1:C:452:ARG:HD3	2.35	0.46
1:D:394:LYS:HZ1	1:D:402:SER:HB2	1.81	0.46
1:E:355:GLN:O	1:E:357:ALA:N	2.48	0.46
1:E:431:GLY:N	1:E:571:TYR:HE2	2.13	0.46
1:D:284:HIS:HB3	1:D:285:PRO:CD	2.45	0.46
1:D:243:ILE:HG13	1:D:244:VAL:N	2.31	0.46
1:B:243:ILE:HG13	1:B:244:VAL:H	1.80	0.46
1:B:284:HIS:O	1:B:286:ARG:N	2.45	0.46
1:B:285:PRO:C	1:B:290:THR:HG21	2.36	0.46
1:A:103:ASP:O	1:A:104:LEU:C	2.53	0.46
1:D:636:MET:C	1:D:638:GLU:N	2.69	0.46
1:B:594:LEU:HD13	1:B:594:LEU:O	2.16	0.46
1:A:142:ILE:HG12	1:A:201:VAL:HG13	1.97	0.46
1:D:445:ASN:HA	1:D:448:GLN:HB2	1.97	0.46
1:C:649:LYS:HA	1:C:652:LYS:HE3	1.98	0.46
1:E:475:MET:SD	1:E:479:LEU:HD23	2.56	0.46
1:F:80:PRO:HB3	1:F:83:MET:SD	2.56	0.46
1:A:152:VAL:HG13	1:A:165:ILE:HD11	1.97	0.46
1:E:533:LEU:HD11	1:E:632:VAL:HG21	1.98	0.46
1:F:103:ASP:O	1:F:106:LYS:N	2.42	0.46
1:E:105:ARG:HD3	1:E:149:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:547:LEU:HB2	1:B:548:GLN:OE1	2.16	0.46
1:A:248:ASP:O	1:A:249:LEU:C	2.54	0.46
1:C:189:LEU:N	1:C:189:LEU:HD22	2.31	0.46
1:A:17:MET:C	1:A:18:LYS:HD2	2.36	0.46
1:E:572:ARG:HD2	1:E:572:ARG:O	2.16	0.46
1:C:534:VAL:O	1:C:538:MET:HB2	2.15	0.46
1:A:662:CYS:C	1:A:664:LYS:H	2.19	0.46
1:E:219:PHE:O	1:E:220:ARG:HB3	2.16	0.46
1:A:298:GLY:O	1:A:299:CYS:C	2.54	0.46
1:F:370:CYS:C	1:F:371:ILE:HD12	2.36	0.46
1:C:116:GLY:HA3	1:C:217:THR:O	2.16	0.46
1:D:213:PHE:CZ	1:D:221:PRO:HB2	2.50	0.46
1:D:221:PRO:O	1:D:222:PHE:CB	2.64	0.46
1:B:294:TYR:OH	1:B:298:GLY:HA2	2.16	0.46
1:F:107:TYR:CE2	1:F:153:LEU:HD22	2.51	0.46
1:A:655:TRP:HZ2	1:F:499:GLU:OE1	1.98	0.46
1:C:186:LEU:CG	1:C:228:PRO:HG2	2.44	0.46
1:A:355:GLN:NE2	1:A:370:CYS:HA	2.27	0.46
1:C:125:LEU:HD13	1:C:125:LEU:C	2.35	0.46
1:A:99:CYS:HB3	1:A:154:GLN:HB2	1.97	0.46
1:A:291:ASP:C	1:A:293:THR:N	2.70	0.46
1:B:227:GLN:HB2	1:B:227:GLN:HE21	1.58	0.46
1:B:227:GLN:O	1:B:229:VAL:HG22	2.16	0.46
1:A:500:GLN:OE1	1:A:502:GLU:HG3	2.15	0.46
1:D:496:LYS:CG	1:E:655:TRP:CD1	2.99	0.46
1:D:658:LEU:HD11	1:E:657:LEU:HB3	1.97	0.46
1:D:657:LEU:HB3	1:E:658:LEU:HD11	1.98	0.46
1:E:123:LEU:HD12	1:E:307:LEU:HD13	1.97	0.46
1:E:415:GLN:O	1:E:415:GLN:HG2	2.16	0.46
1:D:16:GLU:CA	1:D:33:HIS:H	2.28	0.46
1:D:310:LYS:NZ	1:D:310:LYS:HB2	2.31	0.46
1:D:82:GLY:O	1:D:84:GLN:N	2.49	0.46
1:F:406:GLN:NE2	1:F:439:THR:HG22	2.31	0.46
1:D:151:ILE:HD12	1:D:211:LEU:HD11	1.97	0.46
1:D:356:GLU:HA	1:D:453:ALA:HB2	1.97	0.46
1:D:260:PRO:C	1:D:262:PRO:HD2	2.37	0.45
1:D:113:ASN:OD1	1:D:117:LEU:HA	2.16	0.45
1:A:327:VAL:HG21	1:A:367:ALA:HB1	1.98	0.45
1:F:531:LYS:HB3	1:F:531:LYS:NZ	2.30	0.45
1:C:636:MET:C	1:C:638:GLU:N	2.70	0.45
1:E:517:MET:O	1:E:521:VAL:HG23	2.16	0.45
1:F:191:PRO:O	1:F:194:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:531:LYS:NZ	1:D:531:LYS:HB3	2.31	0.45
1:C:415:GLN:HG2	1:C:415:GLN:O	2.16	0.45
1:C:537:MET:SD	1:C:537:MET:C	2.95	0.45
1:E:243:ILE:HG22	1:E:281:LEU:HD23	1.98	0.45
1:B:641:LYS:HD2	1:B:645:ARG:NH1	2.30	0.45
1:A:533:LEU:CD1	1:A:629:VAL:HG12	2.46	0.45
1:C:434:TRP:HB3	1:C:571:TYR:CE1	2.50	0.45
1:E:356:GLU:HB2	1:E:449:GLN:HE21	1.81	0.45
1:A:111:PHE:CE1	1:A:575:ARG:HD2	2.51	0.45
1:D:103:ASP:O	1:D:105:ARG:N	2.48	0.45
1:B:236:ARG:HD3	1:B:283:TRP:CH2	2.51	0.45
1:D:500:GLN:CB	1:D:505:ILE:HG12	2.44	0.45
1:A:462:ASN:C	1:A:464:CYS:H	2.19	0.45
1:E:153:LEU:HD12	1:E:153:LEU:N	2.32	0.45
1:A:173:LEU:O	1:A:173:LEU:HG	2.16	0.45
1:B:363:PRO:HG2	1:B:364:ASP:H	1.81	0.45
1:C:74:VAL:HG13	1:C:97:GLU:CG	2.46	0.45
1:B:128:ASP:HB3	1:B:162:HIS:HB2	1.97	0.45
1:C:234:LYS:HD2	1:C:237:GLN:OE1	2.17	0.45
1:B:517:MET:O	1:B:521:VAL:HG23	2.16	0.45
1:B:246:SER:O	1:B:253:VAL:HA	2.16	0.45
1:B:452:ARG:C	1:B:452:ARG:HD3	2.36	0.45
1:D:601:PHE:O	1:D:605:VAL:HG23	2.16	0.45
1:F:284:HIS:CE1	1:F:285:PRO:HD3	2.52	0.45
1:C:231:TRP:CD1	1:C:231:TRP:C	2.89	0.45
1:E:356:GLU:HB2	1:E:449:GLN:NE2	2.32	0.45
1:D:434:TRP:HB3	1:D:571:TYR:CE1	2.51	0.45
1:D:22:GLY:N	1:D:165:ILE:HG21	2.31	0.45
1:D:105:ARG:HG2	1:D:105:ARG:HH11	1.81	0.45
1:C:51:SER:O	1:C:55:ARG:HG3	2.16	0.45
1:E:294:TYR:HE1	1:E:301:LYS:HB3	1.81	0.45
1:D:169:TYR:CD2	1:D:181:GLU:HG2	2.51	0.45
1:A:547:LEU:HB2	1:A:548:GLN:OE1	2.16	0.45
1:E:192:GLU:CG	1:E:283:TRP:HB3	2.44	0.45
1:B:140:ARG:HB3	1:B:173:LEU:CD1	2.43	0.45
1:E:226:TRP:CD2	1:E:228:PRO:HD2	2.51	0.45
1:C:174:ASP:O	1:C:175:GLN:HB2	2.16	0.45
1:F:445:ASN:HA	1:F:448:GLN:HB2	1.98	0.45
1:D:572:ARG:O	1:D:576:GLU:HB2	2.17	0.45
1:F:160:LEU:HD12	1:F:160:LEU:N	2.31	0.45
1:A:416:GLU:N	1:A:417:PRO:CD	2.80	0.45
1:C:213:PHE:CZ	1:C:221:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:36:GLU:CD	1:F:460:ARG:HE	2.19	0.45
1:F:548:GLN:OE1	1:F:548:GLN:N	2.49	0.45
1:A:114:CYS:C	1:A:116:GLY:N	2.69	0.45
1:F:20:ARG:HB2	1:F:23:THR:HB	1.97	0.45
1:B:290:THR:HG23	1:B:296:PRO:O	2.17	0.45
1:F:410:VAL:HA	1:F:413:ILE:CG2	2.44	0.45
1:A:475:MET:O	1:A:478:GLN:HB3	2.16	0.45
1:A:22:GLY:N	1:A:165:ILE:HG21	2.32	0.45
1:E:142:ILE:HG22	1:E:144:ARG:HG3	1.98	0.45
1:D:654:LEU:HD23	1:E:654:LEU:CD2	2.41	0.45
1:F:463:SER:HA	1:F:467:LYS:HB3	1.98	0.45
1:E:578:PRO:O	1:E:579:ARG:HB2	2.17	0.45
1:A:117:LEU:CD1	1:A:215:CYS:O	2.62	0.45
1:A:477:GLN:CD	1:F:478:GLN:HE21	2.20	0.45
1:F:573:ARG:O	1:F:577:LYS:HB2	2.17	0.45
1:E:62:ILE:HG13	1:E:94:LEU:HD13	1.98	0.45
1:F:350:ASP:OD2	1:F:350:ASP:N	2.48	0.45
1:F:365:LYS:CD	1:F:366:PRO:HD2	2.47	0.45
1:B:241:VAL:O	1:B:241:VAL:HG12	2.16	0.45
1:B:587:SER:O	1:B:591:VAL:HG23	2.17	0.45
1:F:284:HIS:ND1	1:F:285:PRO:HD3	2.31	0.45
1:F:419:ARG:HB3	1:F:419:ARG:NH1	2.32	0.45
1:F:213:PHE:CD1	1:F:221:PRO:HD3	2.51	0.45
1:B:191:PRO:O	1:B:194:LEU:HB2	2.16	0.45
1:F:190:ALA:HB3	1:F:203:VAL:HG23	1.97	0.45
1:F:657:LEU:HA	1:F:660:ILE:HG22	1.98	0.45
1:C:336:LEU:HD23	1:C:340:ILE:HG23	1.99	0.45
1:D:20:ARG:HB2	1:D:23:THR:HB	1.99	0.45
1:C:526:ARG:HD3	1:C:529:GLU:CG	2.46	0.45
1:A:393:SER:O	1:A:394:LYS:HB2	2.17	0.45
1:E:638:GLU:O	1:E:643:VAL:HG23	2.16	0.45
1:C:621:LYS:O	1:C:625:LEU:HD12	2.16	0.45
1:A:350:ASP:OD2	1:A:350:ASP:N	2.49	0.45
1:B:143:HIS:O	1:B:145:ASP:N	2.49	0.45
1:C:467:LYS:HD3	1:C:541:GLN:NE2	2.32	0.45
1:B:485:PHE:CD1	1:C:485:PHE:CD1	3.04	0.45
1:A:537:MET:SD	1:A:537:MET:C	2.95	0.45
1:A:279:LEU:O	1:A:281:LEU:N	2.45	0.45
1:F:34:ASN:O	1:F:35:GLN:C	2.54	0.45
1:F:102:GLY:HA3	1:F:152:VAL:HG12	1.97	0.45
1:E:140:ARG:NH2	1:E:174:ASP:OD2	2.50	0.45
1:A:460:ARG:O	1:A:464:CYS:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:548:GLN:OE1	1:A:548:GLN:N	2.50	0.45
1:F:467:LYS:HD3	1:F:541:GLN:NE2	2.32	0.45
1:A:480:LYS:CD	1:A:527:GLU:HB2	2.46	0.45
1:E:418:LYS:HZ2	1:E:421:LEU:HD13	1.81	0.45
1:B:310:LYS:HB2	1:B:310:LYS:NZ	2.32	0.45
1:F:631:GLU:HG3	1:F:632:VAL:H	1.81	0.45
1:A:621:LYS:O	1:A:625:LEU:HD12	2.17	0.45
1:B:646:LEU:O	1:B:646:LEU:HD12	2.16	0.45
1:B:368:THR:C	1:B:370:CYS:N	2.70	0.45
1:B:490:ILE:N	1:B:490:ILE:HD12	2.32	0.45
1:A:216:ILE:HD12	1:A:277:LEU:HD22	1.99	0.45
1:F:449:GLN:HE22	1:F:452:ARG:HD2	1.81	0.45
1:F:419:ARG:NH2	1:F:587:SER:OG	2.50	0.45
1:D:283:TRP:HB2	1:D:284:HIS:H	1.44	0.45
1:D:102:GLY:HA3	1:D:153:LEU:H	1.81	0.45
1:D:429:VAL:O	1:D:433:VAL:HG23	2.17	0.45
1:E:631:GLU:HG3	1:E:632:VAL:H	1.81	0.45
1:E:540:LEU:HD21	1:E:622:ALA:HB2	1.99	0.45
1:D:368:THR:O	1:D:371:ILE:HG12	2.17	0.45
1:B:570:LEU:H	1:B:570:LEU:HD12	1.82	0.45
1:C:353:LEU:N	1:C:353:LEU:HD12	2.32	0.45
1:D:60:LEU:HD21	1:D:175:GLN:HB2	1.97	0.45
1:C:242:ASP:OD1	1:C:255:PHE:HB3	2.17	0.45
1:C:309:LEU:HD12	1:C:309:LEU:C	2.37	0.45
1:B:494:LEU:O	1:B:494:LEU:HD13	2.16	0.45
1:F:394:LYS:HG2	1:F:401:ILE:HG22	1.98	0.45
1:A:533:LEU:CG	1:A:629:VAL:HG12	2.46	0.45
1:F:570:LEU:H	1:F:570:LEU:HD12	1.82	0.45
1:D:223:LEU:HD21	1:D:226:TRP:CE3	2.52	0.45
1:D:431:GLY:O	1:D:433:VAL:N	2.50	0.45
1:F:186:LEU:C	1:F:188:TYR:N	2.70	0.45
1:F:226:TRP:HB3	1:F:227:GLN:H	1.42	0.45
1:A:473:ALA:HB1	1:A:530:VAL:CG1	2.37	0.45
1:A:460:ARG:NH1	1:A:460:ARG:HG2	2.31	0.45
1:A:369:GLN:O	1:A:370:CYS:CB	2.65	0.45
1:D:18:LYS:CB	1:D:31:ARG:HD3	2.47	0.45
1:F:310:LYS:HB2	1:F:310:LYS:NZ	2.31	0.45
1:D:451:GLN:HA	1:D:454:ALA:CB	2.47	0.45
1:E:328:THR:H	1:E:331:GLU:HG3	1.82	0.45
1:F:311:LEU:O	1:F:311:LEU:HD12	2.16	0.45
1:A:303:LEU:HD11	1:A:307:LEU:HD23	1.98	0.45
1:B:350:ASP:CB	1:B:391:ASP:HB2	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:350:ASP:CB	1:E:391:ASP:HB2	2.46	0.45
1:C:229:VAL:O	1:C:230:GLN:HB3	2.16	0.45
1:D:319:THR:O	1:D:321:THR:N	2.50	0.45
1:D:341:GLN:HA	1:D:345:GLY:O	2.17	0.45
1:F:249:LEU:HB3	1:F:250:ASN:H	1.50	0.45
1:F:213:PHE:HE2	1:F:217:THR:HG21	1.81	0.45
1:B:283:TRP:HB2	1:B:284:HIS:H	1.42	0.45
1:A:530:VAL:HG22	1:A:632:VAL:HG12	1.99	0.45
1:A:655:TRP:HB2	1:F:496:LYS:NZ	2.31	0.45
1:E:103:ASP:O	1:E:104:LEU:C	2.54	0.45
1:D:368:THR:OG1	1:D:369:GLN:N	2.49	0.45
1:E:89:ASN:HB3	1:E:91:LEU:HD22	1.99	0.45
1:F:70:HIS:CE1	1:F:132:ALA:HA	2.43	0.45
1:E:113:ASN:HD21	1:E:117:LEU:HG	1.81	0.45
1:C:105:ARG:CD	1:C:148:PRO:HB2	2.47	0.45
1:D:336:LEU:HD23	1:D:340:ILE:HG23	1.98	0.45
1:B:556:GLN:HE21	1:B:556:GLN:HB3	1.63	0.45
1:E:490:ILE:N	1:E:490:ILE:HD12	2.32	0.45
1:A:62:ILE:HA	1:A:94:LEU:HD13	1.98	0.45
1:C:463:SER:HA	1:C:467:LYS:CB	2.47	0.45
1:F:74:VAL:HG13	1:F:97:GLU:CG	2.47	0.45
1:B:665:VAL:HG13	1:C:665:VAL:O	2.16	0.45
1:E:189:LEU:N	1:E:189:LEU:HD22	2.32	0.45
1:E:213:PHE:CZ	1:E:243:ILE:HB	2.52	0.45
1:E:262:PRO:O	1:E:263:ASN:HB2	2.17	0.45
1:E:272:ARG:HG3	1:E:272:ARG:NH1	2.32	0.45
1:D:316:ASN:HA	1:D:388:PHE:CD1	2.51	0.45
1:F:456:MET:CE	1:F:459:LEU:HD22	2.47	0.45
1:C:282:MET:HB3	1:C:286:ARG:HG3	1.98	0.45
1:F:231:TRP:CD1	1:F:231:TRP:C	2.90	0.45
1:A:475:MET:SD	1:A:479:LEU:HD23	2.57	0.45
1:D:533:LEU:CD2	1:D:629:VAL:HG12	2.38	0.45
1:F:89:ASN:HD22	1:F:91:LEU:CB	2.29	0.45
1:B:416:GLU:N	1:B:417:PRO:CD	2.80	0.45
1:F:316:ASN:HA	1:F:388:PHE:CD1	2.51	0.45
1:D:312:VAL:HG12	1:D:325:TYR:O	2.16	0.45
1:E:547:LEU:HB2	1:E:548:GLN:OE1	2.17	0.45
1:D:460:ARG:HG2	1:D:460:ARG:HH11	1.82	0.45
1:B:501:THR:HA	1:B:505:ILE:HG21	1.99	0.45
1:B:534:VAL:O	1:B:538:MET:HB2	2.17	0.45
1:B:240:GLU:OE1	1:B:241:VAL:HG23	2.17	0.45
1:F:443:ASP:HA	1:F:446:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:641:LYS:HD2	1:F:645:ARG:NH1	2.32	0.45
1:E:594:LEU:HD13	1:E:594:LEU:O	2.17	0.45
1:A:235:VAL:HG12	1:A:236:ARG:N	2.32	0.44
1:F:114:CYS:O	1:F:116:GLY:N	2.51	0.44
1:C:90:ASP:C	1:C:91:LEU:HD22	2.38	0.44
1:D:658:LEU:HD21	1:E:657:LEU:HD23	1.99	0.44
1:B:460:ARG:HG2	1:B:460:ARG:NH1	2.32	0.44
1:E:606:ARG:HG3	1:E:606:ARG:HH21	1.81	0.44
1:F:313:HIS:ND1	1:F:324:THR:HG22	2.32	0.44
1:B:636:MET:C	1:B:638:GLU:N	2.71	0.44
1:C:587:SER:O	1:C:591:VAL:HG23	2.17	0.44
1:C:34:ASN:O	1:C:35:GLN:C	2.56	0.44
1:D:537:MET:C	1:D:537:MET:SD	2.96	0.44
1:D:155:GLN:HA	1:D:155:GLN:OE1	2.16	0.44
1:C:490:ILE:HG12	1:C:650:ARG:CB	2.48	0.44
1:E:279:LEU:O	1:E:281:LEU:N	2.47	0.44
1:E:570:LEU:H	1:E:570:LEU:HD12	1.80	0.44
1:F:173:LEU:N	1:F:173:LEU:HD12	2.32	0.44
1:F:185:THR:HG22	1:F:186:LEU:N	2.32	0.44
1:B:219:PHE:O	1:B:220:ARG:HB3	2.17	0.44
1:A:475:MET:SD	1:A:636:MET:HE1	2.58	0.44
1:B:497:TYR:HA	1:B:500:GLN:HB2	1.98	0.44
1:A:60:LEU:HD22	1:A:175:GLN:HG2	1.99	0.44
1:A:490:ILE:HD12	1:A:490:ILE:N	2.32	0.44
1:D:290:THR:HA	1:D:296:PRO:HA	1.99	0.44
1:B:239:SER:HB3	1:B:255:PHE:CD1	2.51	0.44
1:A:356:GLU:HA	1:A:453:ALA:HB2	1.99	0.44
1:A:103:ASP:O	1:A:106:LYS:N	2.45	0.44
1:A:191:PRO:O	1:A:194:LEU:HB2	2.16	0.44
1:B:448:GLN:HE21	1:B:552:MET:CE	2.29	0.44
1:F:416:GLU:N	1:F:417:PRO:CD	2.80	0.44
1:B:657:LEU:HA	1:B:660:ILE:HG22	1.99	0.44
1:C:490:ILE:CG2	1:C:517:MET:HE2	2.47	0.44
1:A:292:PRO:CG	1:A:297:ASN:HD22	2.19	0.44
1:F:357:ALA:HB3	1:F:359:LEU:HD11	1.98	0.44
1:F:361:LEU:HD22	1:F:369:GLN:NE2	2.32	0.44
1:F:571:TYR:HB3	1:F:575:ARG:NH2	2.15	0.44
1:A:229:VAL:C	1:A:231:TRP:H	2.21	0.44
1:B:86:LEU:CD1	1:B:87:ALA:H	2.30	0.44
1:F:139:ASN:C	1:F:141:ILE:HD12	2.38	0.44
1:B:360:ALA:HB3	1:E:36:GLU:CG	2.39	0.44
1:F:652:LYS:C	1:F:654:LEU:H	2.20	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:606:ARG:HH21	1:D:606:ARG:HG3	1.82	0.44
1:D:313:HIS:ND1	1:D:324:THR:HG22	2.32	0.44
1:B:578:PRO:O	1:B:580:ASP:N	2.41	0.44
1:D:212:ALA:O	1:D:216:ILE:HG13	2.18	0.44
1:D:355:GLN:HB3	1:D:359:LEU:HD13	1.99	0.44
1:C:490:ILE:HD12	1:C:490:ILE:N	2.32	0.44
1:C:416:GLU:N	1:C:417:PRO:CD	2.80	0.44
1:F:229:VAL:C	1:F:231:TRP:N	2.71	0.44
1:F:209:GLY:O	1:F:277:LEU:HD11	2.17	0.44
1:B:192:GLU:O	1:B:196:GLN:HB2	2.18	0.44
1:A:320:GLY:HA2	1:A:405:PRO:CG	2.47	0.44
1:F:303:LEU:HD11	1:F:307:LEU:HD23	1.99	0.44
1:A:659:LYS:HB2	1:F:500:GLN:HE22	1.83	0.44
1:C:68:LEU:HD13	1:C:139:ASN:CG	2.38	0.44
1:A:486:PHE:CE2	1:A:521:VAL:HB	2.52	0.44
1:D:490:ILE:HG12	1:D:650:ARG:HB3	1.99	0.44
1:A:531:LYS:O	1:A:535:GLU:HG3	2.17	0.44
1:C:328:THR:H	1:C:331:GLU:HG3	1.81	0.44
1:C:487:LYS:HB3	1:C:487:LYS:HE2	1.83	0.44
1:D:292:PRO:C	1:D:294:TYR:H	2.20	0.44
1:B:180:THR:O	1:B:180:THR:HG22	2.17	0.44
1:D:319:THR:HG23	1:D:320:GLY:N	2.24	0.44
1:A:192:GLU:HG3	1:A:192:GLU:H	1.48	0.44
1:F:285:PRO:C	1:F:286:ARG:HG3	2.38	0.44
1:A:415:GLN:O	1:A:415:GLN:HG2	2.17	0.44
1:B:21:LEU:HG	1:B:165:ILE:CD1	2.46	0.44
1:F:32:TRP:HZ3	1:F:83:MET:CB	2.22	0.44
1:B:268:VAL:CG1	1:B:269:LEU:N	2.80	0.44
1:D:533:LEU:HD13	1:D:629:VAL:CB	2.47	0.44
1:B:68:LEU:HD13	1:B:139:ASN:OD1	2.17	0.44
1:B:316:ASN:HA	1:B:388:PHE:CD1	2.52	0.44
1:D:416:GLU:N	1:D:417:PRO:CD	2.80	0.44
1:F:649:LYS:HA	1:F:652:LYS:HE3	2.00	0.44
1:B:238:LYS:HB3	1:B:239:SER:H	1.56	0.44
1:B:103:ASP:O	1:B:104:LEU:C	2.56	0.44
1:B:105:ARG:HG2	1:B:105:ARG:HH11	1.82	0.44
1:D:312:VAL:HG22	1:D:313:HIS:N	2.32	0.44
1:C:601:PHE:O	1:C:605:VAL:HG23	2.16	0.44
1:C:579:ARG:HH11	1:C:579:ARG:HG3	1.83	0.44
1:C:237:GLN:O	1:C:238:LYS:C	2.56	0.44
1:B:534:VAL:HG13	1:B:535:GLU:N	2.32	0.44
1:A:247:GLU:HG3	1:A:251:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:490:ILE:HD11	1:C:651:GLN:HG2	1.98	0.44
1:C:192:GLU:H	1:C:192:GLU:HG3	1.49	0.44
1:E:430:TRP:CH2	1:E:570:LEU:HD23	2.52	0.44
1:A:457:ASN:HA	1:A:460:ARG:HG3	1.98	0.44
1:C:319:THR:O	1:C:321:THR:N	2.51	0.44
1:E:105:ARG:HH11	1:E:105:ARG:HG2	1.82	0.44
1:B:361:LEU:HD22	1:B:367:ALA:HB1	1.99	0.44
1:B:19:GLU:C	1:B:20:ARG:HD3	2.38	0.44
1:D:87:ALA:C	1:D:89:ASN:H	2.21	0.44
1:F:328:THR:H	1:F:331:GLU:HG3	1.82	0.44
1:B:631:GLU:HG3	1:B:632:VAL:N	2.33	0.44
1:D:65:MET:HG3	1:D:94:LEU:HD21	1.99	0.44
1:C:350:ASP:CB	1:C:391:ASP:HB2	2.48	0.44
1:B:145:ASP:HA	1:B:189:LEU:HD11	2.00	0.44
1:E:594:LEU:HD13	1:E:594:LEU:C	2.38	0.44
1:E:268:VAL:O	1:E:272:ARG:HB2	2.18	0.44
1:E:312:VAL:HG12	1:E:325:TYR:O	2.17	0.44
1:A:190:ALA:HB3	1:A:203:VAL:HG23	1.99	0.44
1:D:490:ILE:HD11	1:D:651:GLN:HG2	1.99	0.44
1:E:531:LYS:O	1:E:535:GLU:HG3	2.17	0.44
1:F:105:ARG:HG2	1:F:105:ARG:HH11	1.83	0.44
1:B:429:VAL:O	1:B:433:VAL:HG23	2.18	0.44
1:A:143:HIS:O	1:A:145:ASP:N	2.50	0.44
1:B:181:GLU:C	1:B:183:VAL:H	2.21	0.44
1:E:341:GLN:HA	1:E:345:GLY:O	2.18	0.44
1:F:151:ILE:HD12	1:F:211:LEU:HD11	1.99	0.44
1:C:261:TYR:OH	1:C:407:PRO:HG3	2.17	0.44
1:A:419:ARG:HB2	1:A:419:ARG:HH11	1.82	0.44
1:F:421:LEU:N	1:F:421:LEU:HD13	2.33	0.44
1:F:81:GLU:OE1	1:F:81:GLU:HA	2.18	0.44
1:E:18:LYS:HB2	1:E:31:ARG:HD3	1.99	0.44
1:E:223:LEU:HD13	1:E:223:LEU:C	2.38	0.44
1:C:60:LEU:CD1	1:C:175:GLN:HG2	2.47	0.44
1:B:102:GLY:HA3	1:B:153:LEU:H	1.83	0.44
1:B:77:ARG:N	1:B:96:MET:HA	2.29	0.44
1:D:60:LEU:HD11	1:D:175:GLN:HG3	2.00	0.44
1:C:25:GLY:HA2	1:C:169:TYR:CZ	2.52	0.44
1:B:265:LEU:HD21	1:B:270:ALA:CB	2.48	0.44
1:A:36:GLU:CG	1:A:37:THR:H	2.29	0.44
1:A:72:ASN:C	1:A:163:LYS:HA	2.37	0.44
1:D:189:LEU:N	1:D:189:LEU:HD22	2.32	0.44
1:A:482:LYS:O	1:A:485:PHE:HD2	2.01	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:97:GLU:OE2	1:D:163:LYS:HE2	2.18	0.44
1:C:16:GLU:N	1:C:32:TRP:HE1	2.15	0.44
1:E:336:LEU:HD23	1:E:340:ILE:HG23	1.98	0.44
1:D:404:ARG:N	1:D:404:ARG:CD	2.80	0.44
1:C:213:PHE:HE2	1:C:217:THR:HG21	1.83	0.44
1:F:16:GLU:HB2	1:F:17:MET:H	1.56	0.44
1:F:220:ARG:HE	1:F:221:PRO:HD2	1.81	0.44
1:A:319:THR:O	1:A:321:THR:N	2.51	0.44
1:A:544:ILE:HG13	1:A:545:VAL:N	2.33	0.44
1:A:313:HIS:ND1	1:A:324:THR:HG22	2.33	0.44
1:D:36:GLU:CG	1:D:37:THR:H	2.28	0.44
1:B:404:ARG:HH22	1:B:406:GLN:HB3	1.83	0.44
1:E:445:ASN:HA	1:E:448:GLN:HB2	1.99	0.44
1:C:419:ARG:CD	1:C:419:ARG:N	2.78	0.43
1:C:422:ALA:O	1:C:426:LEU:HD23	2.18	0.43
1:A:283:TRP:CG	1:A:284:HIS:N	2.86	0.43
1:D:243:ILE:HG13	1:D:244:VAL:HG23	2.00	0.43
1:B:294:TYR:CE2	1:B:301:LYS:HB3	2.53	0.43
1:E:34:ASN:O	1:E:35:GLN:C	2.57	0.43
1:A:631:GLU:HG3	1:A:632:VAL:N	2.33	0.43
1:E:139:ASN:O	1:E:141:ILE:HD12	2.18	0.43
1:F:89:ASN:C	1:F:91:LEU:N	2.70	0.43
1:F:353:LEU:HD12	1:F:353:LEU:N	2.33	0.43
1:D:18:LYS:HB3	1:D:19:GLU:H	1.57	0.43
1:B:153:LEU:N	1:B:153:LEU:HD12	2.33	0.43
1:D:245:VAL:O	1:D:245:VAL:HG12	2.17	0.43
1:F:82:GLY:C	1:F:84:GLN:N	2.71	0.43
1:F:636:MET:C	1:F:638:GLU:N	2.71	0.43
1:F:569:GLU:HA	1:F:569:GLU:OE1	2.18	0.43
1:F:125:LEU:HA	1:F:162:HIS:CD2	2.53	0.43
1:A:507:SER:C	1:A:509:LYS:N	2.71	0.43
1:A:572:ARG:O	1:A:576:GLU:HB2	2.18	0.43
1:D:449:GLN:HE22	1:D:452:ARG:HD2	1.82	0.43
1:C:291:ASP:C	1:C:293:THR:H	2.22	0.43
1:F:404:ARG:HG2	1:F:605:VAL:HG21	2.00	0.43
1:A:286:ARG:HA	1:A:290:THR:HB	2.00	0.43
1:E:456:MET:HE3	1:E:459:LEU:HD22	2.01	0.43
1:D:223:LEU:CG	1:D:226:TRP:HE3	2.31	0.43
1:D:430:TRP:HE1	1:D:587:SER:HB3	1.82	0.43
1:F:186:LEU:O	1:F:188:TYR:N	2.51	0.43
1:B:34:ASN:O	1:B:35:GLN:C	2.56	0.43
1:F:346:ILE:HD13	1:F:388:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:649:LYS:HA	1:D:652:LYS:HE3	1.98	0.43
1:A:172:GLU:CG	1:A:175:GLN:H	2.31	0.43
1:D:463:SER:HA	1:D:467:LYS:HB3	2.00	0.43
1:F:103:ASP:O	1:F:105:ARG:N	2.51	0.43
1:F:472:MET:C	1:F:474:SER:H	2.21	0.43
1:B:606:ARG:HG3	1:B:606:ARG:HH21	1.83	0.43
1:E:404:ARG:HD3	1:E:404:ARG:N	2.33	0.43
1:D:631:GLU:HG3	1:D:632:VAL:H	1.83	0.43
1:B:45:GLN:OE1	1:B:88:PRO:HD3	2.18	0.43
1:C:350:ASP:N	1:C:350:ASP:OD2	2.50	0.43
1:C:359:LEU:HD12	1:C:359:LEU:N	2.32	0.43
1:F:350:ASP:HB2	1:F:391:ASP:HB2	1.99	0.43
1:D:292:PRO:O	1:D:294:TYR:N	2.46	0.43
1:F:40:GLN:O	1:F:98:TYR:HB3	2.18	0.43
1:A:227:GLN:HA	1:A:227:GLN:OE1	2.18	0.43
1:E:443:ASP:HA	1:E:446:ARG:HG3	1.99	0.43
1:E:213:PHE:HE2	1:E:217:THR:HG21	1.78	0.43
1:C:283:TRP:HD1	1:C:284:HIS:H	1.55	0.43
1:A:404:ARG:N	1:A:404:ARG:HD3	2.34	0.43
1:F:268:VAL:HG13	1:F:269:LEU:N	2.33	0.43
1:D:231:TRP:O	1:D:232:HIS:C	2.55	0.43
1:A:524:CYS:HB2	1:A:639:ASP:OD1	2.18	0.43
1:E:139:ASN:C	1:E:141:ILE:HD12	2.38	0.43
1:E:236:ARG:O	1:E:238:LYS:N	2.51	0.43
1:C:460:ARG:HG2	1:C:460:ARG:HH11	1.84	0.43
1:D:328:THR:H	1:D:331:GLU:HG3	1.81	0.43
1:D:631:GLU:HG3	1:D:632:VAL:N	2.32	0.43
1:B:624:GLU:HG3	1:B:625:LEU:HG	2.00	0.43
1:F:145:ASP:HA	1:F:189:LEU:HD11	2.01	0.43
1:C:617:VAL:O	1:C:621:LYS:HB2	2.18	0.43
1:D:361:LEU:HD22	1:D:370:CYS:HB3	2.00	0.43
1:D:356:GLU:HA	1:D:453:ALA:CB	2.48	0.43
1:E:213:PHE:CD1	1:E:221:PRO:HD3	2.53	0.43
1:D:402:SER:N	1:D:403:PRO:CD	2.79	0.43
1:A:283:TRP:HD1	1:A:284:HIS:H	1.59	0.43
1:A:286:ARG:CA	1:A:290:THR:OG1	2.66	0.43
1:C:279:LEU:O	1:C:281:LEU:N	2.46	0.43
1:E:431:GLY:C	1:E:433:VAL:H	2.22	0.43
1:C:447:LEU:CD2	1:C:609:TYR:HE1	2.21	0.43
1:A:649:LYS:HA	1:A:652:LYS:HE3	2.01	0.43
1:A:655:TRP:NE1	1:F:500:GLN:HG2	2.34	0.43
1:B:385:ASP:CG	1:B:386:LEU:N	2.69	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:368:THR:HG23	1:E:369:GLN:N	2.29	0.43
1:A:117:LEU:HD12	1:A:215:CYS:HA	2.01	0.43
1:C:105:ARG:HG2	1:C:105:ARG:HH11	1.83	0.43
1:B:350:ASP:OD2	1:B:350:ASP:N	2.51	0.43
1:D:452:ARG:HD3	1:D:452:ARG:C	2.39	0.43
1:D:298:GLY:O	1:D:299:CYS:C	2.56	0.43
1:C:475:MET:SD	1:C:479:LEU:HD23	2.59	0.43
1:C:422:ALA:HB1	1:C:426:LEU:HB3	1.99	0.43
1:F:282:MET:CB	1:F:286:ARG:HB2	2.48	0.43
1:F:238:LYS:HB3	1:F:239:SER:H	1.59	0.43
1:B:79:VAL:HB	1:B:84:GLN:NE2	2.33	0.43
1:B:192:GLU:HG2	1:B:283:TRP:HB3	2.00	0.43
1:E:168:GLY:O	1:E:178:LEU:HB3	2.19	0.43
1:E:68:LEU:HD13	1:E:139:ASN:OD1	2.19	0.43
1:A:655:TRP:HZ2	1:F:499:GLU:OE2	2.01	0.43
1:E:103:ASP:O	1:E:105:ARG:N	2.51	0.43
1:E:389:LEU:HD21	1:E:454:ALA:CB	2.49	0.43
1:E:354:LEU:HD13	1:E:454:ALA:HA	2.00	0.43
1:A:394:LYS:HD2	1:A:613:SER:OG	2.19	0.43
1:A:606:ARG:HG3	1:A:606:ARG:HH21	1.82	0.43
1:A:186:LEU:O	1:A:187:GLN:C	2.57	0.43
1:B:49:GLU:HG2	1:B:89:ASN:HB2	2.00	0.43
1:A:84:GLN:NE2	1:A:93:LEU:HD12	2.33	0.43
1:A:155:GLN:OE1	1:A:155:GLN:HA	2.18	0.43
1:E:475:MET:HB2	1:E:478:GLN:NE2	2.34	0.43
1:B:472:MET:O	1:B:475:MET:HG3	2.18	0.43
1:C:244:VAL:CG2	1:C:260:PRO:HD3	2.49	0.43
1:B:36:GLU:CG	1:B:37:THR:H	2.28	0.43
1:E:459:LEU:HD12	1:E:459:LEU:N	2.34	0.43
1:A:236:ARG:HH11	1:A:236:ARG:HG3	1.82	0.43
1:F:221:PRO:HB3	1:F:243:ILE:O	2.19	0.43
1:A:500:GLN:NE2	1:A:501:THR:N	2.67	0.43
1:F:67:ARG:NH2	1:F:68:LEU:HD12	2.22	0.43
1:D:422:ALA:O	1:D:585:GLY:CA	2.66	0.43
1:C:524:CYS:HB2	1:C:639:ASP:OD2	2.19	0.43
1:C:291:ASP:C	1:C:293:THR:N	2.71	0.43
1:E:265:LEU:CG	1:E:266:ASN:N	2.65	0.43
1:F:452:ARG:HD3	1:F:452:ARG:C	2.39	0.43
1:E:357:ALA:O	1:E:456:MET:CG	2.66	0.43
1:E:359:LEU:HD12	1:E:359:LEU:N	2.33	0.43
1:D:152:VAL:CG1	1:D:165:ILE:HD11	2.48	0.43
1:F:187:GLN:HA	1:F:227:GLN:CD	2.39	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:225:ASN:O	1:F:226:TRP:C	2.57	0.43
1:B:276:TRP:CD1	1:B:302:ALA:HB1	2.54	0.43
1:A:636:MET:C	1:A:638:GLU:N	2.71	0.43
1:E:652:LYS:C	1:E:654:LEU:H	2.21	0.43
1:E:104:LEU:O	1:E:107:TYR:HB2	2.18	0.43
1:A:113:ASN:ND2	1:A:117:LEU:HD23	2.33	0.43
1:C:460:ARG:O	1:C:464:CYS:HB2	2.18	0.43
1:D:460:ARG:O	1:D:464:CYS:HB2	2.19	0.43
1:C:572:ARG:HD2	1:C:572:ARG:O	2.19	0.43
1:A:433:VAL:O	1:A:436:SER:HB3	2.19	0.43
1:E:601:PHE:O	1:E:605:VAL:HG23	2.19	0.43
1:A:86:LEU:O	1:A:86:LEU:HD23	2.19	0.43
1:D:623:LEU:O	1:D:623:LEU:HD23	2.18	0.43
1:C:479:LEU:HD11	1:C:641:LYS:CG	2.22	0.43
1:F:355:GLN:O	1:F:357:ALA:N	2.52	0.43
1:F:358:GLY:CA	1:F:456:MET:HB3	2.49	0.43
1:C:36:GLU:CG	1:C:37:THR:H	2.29	0.43
1:B:193:LEU:O	1:B:195:GLU:N	2.51	0.43
1:B:261:TYR:N	1:B:262:PRO:CD	2.79	0.43
1:B:34:ASN:CG	1:B:83:MET:SD	2.97	0.43
1:A:500:GLN:HG2	1:A:502:GLU:HG3	2.01	0.43
1:B:460:ARG:O	1:B:464:CYS:HB2	2.19	0.43
1:B:486:PHE:HZ	1:B:647:GLN:HB3	1.77	0.43
1:E:119:GLU:HG2	1:E:121:ALA:H	1.83	0.43
1:B:541:GLN:HA	1:B:541:GLN:OE1	2.18	0.43
1:A:102:GLY:HA3	1:A:153:LEU:H	1.81	0.43
1:D:336:LEU:HD12	1:D:367:ALA:HB1	2.00	0.43
1:D:62:ILE:HA	1:D:94:LEU:HD13	2.00	0.43
1:C:392:ASN:CG	1:C:393:SER:N	2.72	0.43
1:E:51:SER:O	1:E:55:ARG:HG3	2.19	0.43
1:C:74:VAL:HG13	1:C:97:GLU:HG2	2.01	0.43
1:A:350:ASP:CB	1:A:391:ASP:HB2	2.48	0.43
1:B:72:ASN:C	1:B:163:LYS:HA	2.39	0.43
1:D:531:LYS:O	1:D:535:GLU:HG3	2.18	0.43
1:B:494:LEU:C	1:B:494:LEU:HD13	2.39	0.43
1:B:665:VAL:HB	1:C:503:PHE:CE2	2.54	0.43
1:C:664:LYS:O	1:C:665:VAL:C	2.57	0.43
1:A:449:GLN:HE22	1:A:452:ARG:HD2	1.83	0.43
1:C:445:ASN:HA	1:C:448:GLN:HB2	1.99	0.43
1:F:394:LYS:HA	1:F:613:SER:OG	2.19	0.43
1:F:418:LYS:O	1:F:419:ARG:HB2	2.17	0.43
1:F:80:PRO:O	1:F:81:GLU:C	2.55	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:213:PHE:CE1	1:F:221:PRO:HG3	2.54	0.43
1:B:231:TRP:C	1:B:233:SER:H	2.22	0.43
1:B:244:VAL:CG2	1:B:260:PRO:HD3	2.49	0.43
1:C:102:GLY:HA3	1:C:152:VAL:HG12	2.01	0.43
1:C:165:ILE:HG22	1:C:166:ASP:N	2.16	0.43
1:E:294:TYR:HD2	1:E:294:TYR:N	2.16	0.43
1:A:502:GLU:HB2	1:A:503:PHE:H	1.68	0.43
1:C:18:LYS:HG3	1:C:31:ARG:CG	2.49	0.43
1:A:652:LYS:C	1:A:654:LEU:H	2.21	0.43
1:A:410:VAL:HA	1:A:413:ILE:CG2	2.45	0.43
1:D:467:LYS:HD3	1:D:541:GLN:HE22	1.79	0.43
1:E:416:GLU:N	1:E:417:PRO:CD	2.82	0.43
1:A:367:ALA:C	1:A:369:GLN:H	2.22	0.43
1:E:408:GLU:HG3	1:E:409:SER:H	1.84	0.43
1:C:420:ASN:CG	1:C:421:LEU:N	2.72	0.43
1:A:221:PRO:O	1:A:222:PHE:HB2	2.18	0.43
1:C:214:GLU:O	1:C:218:GLY:HA2	2.18	0.43
1:D:192:GLU:O	1:D:196:GLN:HB2	2.18	0.43
1:D:223:LEU:O	1:D:231:TRP:CZ3	2.72	0.43
1:D:231:TRP:CD1	1:D:232:HIS:N	2.86	0.43
1:E:141:ILE:HG22	1:E:142:ILE:N	2.33	0.43
1:D:419:ARG:CZ	1:D:420:ASN:HB2	2.49	0.43
1:D:421:LEU:HB3	1:D:422:ALA:H	1.70	0.43
1:F:104:LEU:HB3	1:F:148:PRO:O	2.18	0.43
1:D:372:SER:H	1:D:384:MET:CE	2.27	0.43
1:B:328:THR:H	1:B:331:GLU:HG3	1.84	0.43
1:F:434:TRP:CZ3	1:F:564:GLU:OE1	2.71	0.43
1:D:125:LEU:HA	1:D:162:HIS:CD2	2.54	0.43
1:E:446:ARG:HG2	1:E:446:ARG:NH1	2.33	0.43
1:C:490:ILE:CG1	1:C:650:ARG:CB	2.96	0.42
1:A:272:ARG:NH1	1:A:272:ARG:HG3	2.34	0.42
1:D:21:LEU:C	1:D:165:ILE:HD13	2.39	0.42
1:A:231:TRP:CD1	1:A:235:VAL:HG21	2.54	0.42
1:F:319:THR:O	1:F:321:THR:N	2.52	0.42
1:D:490:ILE:HD12	1:D:490:ILE:N	2.34	0.42
1:C:60:LEU:HD13	1:C:175:GLN:HG2	2.00	0.42
1:F:276:TRP:CD1	1:F:302:ALA:HB1	2.54	0.42
1:A:34:ASN:O	1:A:35:GLN:C	2.56	0.42
1:D:412:CYS:O	1:D:415:GLN:HB3	2.19	0.42
1:D:594:LEU:C	1:D:594:LEU:HD13	2.39	0.42
1:C:420:ASN:HD22	1:C:421:LEU:H	1.65	0.42
1:A:213:PHE:HE2	1:A:217:THR:HG21	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:261:TYR:HB3	1:F:409:SER:HB3	2.01	0.42
1:D:213:PHE:HE2	1:D:217:THR:HG21	1.83	0.42
1:B:79:VAL:HB	1:B:84:GLN:CG	2.49	0.42
1:B:220:ARG:H	1:B:221:PRO:HD3	1.80	0.42
1:C:500:GLN:HE22	1:C:504:GLY:CA	2.18	0.42
1:A:479:LEU:HD12	1:A:640:GLU:HG3	1.96	0.42
1:B:344:THR:O	1:B:345:GLY:C	2.57	0.42
1:E:309:LEU:C	1:E:309:LEU:HD13	2.39	0.42
1:B:451:GLN:HA	1:B:454:ALA:CB	2.48	0.42
1:E:626:LEU:N	1:E:627:PRO:CD	2.82	0.42
1:A:117:LEU:HD12	1:A:215:CYS:CA	2.48	0.42
1:A:355:GLN:O	1:A:357:ALA:N	2.53	0.42
1:D:547:LEU:O	1:D:549:ARG:NH2	2.52	0.42
1:D:548:GLN:O	1:D:549:ARG:NH2	2.51	0.42
1:D:480:LYS:HE2	1:D:527:GLU:OE1	2.19	0.42
1:A:185:THR:OG1	1:A:187:GLN:HG2	2.19	0.42
1:F:62:ILE:HA	1:F:94:LEU:HD13	2.00	0.42
1:A:65:MET:HG3	1:A:94:LEU:HD21	2.01	0.42
1:E:408:GLU:CG	1:E:409:SER:N	2.82	0.42
1:B:525:GLY:C	1:B:527:GLU:H	2.22	0.42
1:E:40:GLN:HE21	1:E:40:GLN:HA	1.83	0.42
1:C:652:LYS:C	1:C:654:LEU:H	2.22	0.42
1:B:475:MET:SD	1:B:479:LEU:HD23	2.59	0.42
1:C:219:PHE:O	1:C:220:ARG:C	2.57	0.42
1:C:231:TRP:NE1	1:C:235:VAL:HG21	2.34	0.42
1:D:432:GLN:HG2	1:D:432:GLN:H	1.68	0.42
1:F:217:THR:HG22	1:F:260:PRO:HD2	2.01	0.42
1:B:86:LEU:H	1:B:86:LEU:HG	1.67	0.42
1:C:547:LEU:HB2	1:C:548:GLN:OE1	2.20	0.42
1:F:192:GLU:H	1:F:192:GLU:HG3	1.48	0.42
1:D:249:LEU:HD22	1:D:418:LYS:HZ1	1.84	0.42
1:E:460:ARG:HH11	1:E:460:ARG:HG2	1.83	0.42
1:A:167:LEU:O	1:A:169:TYR:N	2.52	0.42
1:C:577:LYS:HB3	1:C:582:ARG:HH22	1.84	0.42
1:B:125:LEU:HA	1:B:162:HIS:CD2	2.54	0.42
1:D:139:ASN:C	1:D:141:ILE:HD12	2.40	0.42
1:B:572:ARG:O	1:B:572:ARG:HD2	2.19	0.42
1:D:449:GLN:NE2	1:D:452:ARG:HD2	2.34	0.42
1:F:140:ARG:HH11	1:F:140:ARG:HG3	1.84	0.42
1:B:370:CYS:O	1:B:371:ILE:HB	2.20	0.42
1:A:279:LEU:HD11	1:A:291:ASP:CB	2.48	0.42
1:D:219:PHE:O	1:D:221:PRO:N	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:239:SER:HB2	1:F:242:ASP:HB2	2.02	0.42
1:C:21:LEU:C	1:C:165:ILE:HD13	2.38	0.42
1:D:652:LYS:C	1:D:654:LEU:H	2.22	0.42
1:E:389:LEU:HD21	1:E:454:ALA:HB2	2.01	0.42
1:E:460:ARG:O	1:E:464:CYS:HB2	2.18	0.42
1:F:118:ARG:HD3	1:F:435:HIS:NE2	2.35	0.42
1:A:253:VAL:CG2	1:A:254:LYS:N	2.82	0.42
1:C:62:ILE:HA	1:C:94:LEU:HD13	2.01	0.42
1:F:74:VAL:HG13	1:F:97:GLU:HG2	2.01	0.42
1:D:134:ARG:HG2	1:D:300:PHE:CD1	2.55	0.42
1:B:652:LYS:C	1:B:654:LEU:H	2.22	0.42
1:A:296:PRO:O	1:A:297:ASN:ND2	2.53	0.42
1:F:460:ARG:NH1	1:F:460:ARG:HG2	2.35	0.42
1:E:587:SER:O	1:E:591:VAL:HG23	2.20	0.42
1:B:223:LEU:HD22	1:B:226:TRP:CG	2.55	0.42
1:B:290:THR:N	1:B:298:GLY:N	2.68	0.42
1:B:299:CYS:O	1:B:300:PHE:C	2.57	0.42
1:C:497:TYR:CE1	1:C:505:ILE:HG22	2.54	0.42
1:E:183:VAL:O	1:E:183:VAL:HG12	2.20	0.42
1:E:319:THR:O	1:E:321:THR:N	2.52	0.42
1:A:658:LEU:HA	1:F:658:LEU:HD13	2.00	0.42
1:C:394:LYS:HE2	1:C:612:LEU:HD12	2.00	0.42
1:B:462:ASN:C	1:B:464:CYS:N	2.72	0.42
1:D:110:GLN:HB2	1:D:113:ASN:HB2	2.01	0.42
1:B:533:LEU:HD13	1:B:629:VAL:HG12	2.01	0.42
1:E:392:ASN:ND2	1:E:393:SER:H	2.18	0.42
1:C:385:ASP:CG	1:C:386:LEU:N	2.72	0.42
1:E:249:LEU:HD13	1:E:414:LEU:CG	2.46	0.42
1:E:617:VAL:O	1:E:621:LYS:HB2	2.19	0.42
1:C:577:LYS:HD2	1:C:581:GLN:HE22	1.84	0.42
1:A:442:GLU:O	1:A:446:ARG:HG3	2.19	0.42
1:C:146:LEU:HB3	1:C:207:SER:HB3	2.01	0.42
1:F:279:LEU:HD21	1:F:291:ASP:CA	2.46	0.42
1:F:358:GLY:HA3	1:F:456:MET:CG	2.50	0.42
1:E:424:PHE:HD1	1:E:582:ARG:NE	2.17	0.42
1:F:272:ARG:HG3	1:F:272:ARG:HH11	1.84	0.42
1:D:192:GLU:CG	1:D:283:TRP:HB3	2.39	0.42
1:D:426:LEU:HD11	1:D:574:LEU:HD11	2.02	0.42
1:B:228:PRO:HA	1:B:231:TRP:CB	2.49	0.42
1:E:17:MET:CB	1:E:32:TRP:HA	2.50	0.42
1:E:296:PRO:HG2	1:E:297:ASN:H	1.84	0.42
1:E:123:LEU:N	1:E:123:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:617:VAL:O	1:D:621:LYS:HB2	2.18	0.42
1:A:385:ASP:CG	1:A:386:LEU:N	2.73	0.42
1:E:236:ARG:NH2	1:E:283:TRP:HE1	2.14	0.42
1:B:528:ASN:H	1:B:528:ASN:ND2	2.11	0.42
1:A:456:MET:HE3	1:A:459:LEU:HD22	2.01	0.42
1:A:507:SER:C	1:A:509:LYS:H	2.21	0.42
1:C:142:ILE:HG12	1:C:201:VAL:HG13	2.01	0.42
1:D:447:LEU:HD23	1:D:609:TYR:HE1	1.85	0.42
1:C:566:GLN:O	1:C:569:GLU:HB2	2.19	0.42
1:B:537:MET:C	1:B:537:MET:SD	2.98	0.42
1:A:296:PRO:HG2	1:A:297:ASN:H	1.84	0.42
1:A:118:ARG:C	1:A:264:ASN:O	2.58	0.42
1:C:497:TYR:HA	1:C:500:GLN:HB2	2.01	0.42
1:D:505:ILE:HD12	1:D:506:THR:N	2.19	0.42
1:A:479:LEU:HD12	1:A:640:GLU:CB	2.50	0.42
1:E:36:GLU:CG	1:E:37:THR:H	2.31	0.42
1:B:18:LYS:HB3	1:B:19:GLU:CD	2.40	0.42
1:D:547:LEU:O	1:D:549:ARG:NH1	2.53	0.42
1:E:110:GLN:HB2	1:E:113:ASN:HB3	2.01	0.42
1:D:525:GLY:O	1:D:527:GLU:N	2.47	0.42
1:B:103:ASP:O	1:B:106:LYS:N	2.47	0.42
1:F:264:ASN:ND2	1:F:264:ASN:O	2.52	0.42
1:C:119:GLU:HG2	1:C:121:ALA:H	1.85	0.42
1:B:118:ARG:HD3	1:B:435:HIS:CE1	2.54	0.42
1:F:36:GLU:CG	1:F:37:THR:H	2.30	0.42
1:B:559:THR:HG21	1:B:604:LYS:NZ	2.35	0.42
1:C:480:LYS:HE2	1:C:527:GLU:OE2	2.20	0.42
1:B:531:LYS:HZ3	1:B:531:LYS:HB3	1.85	0.42
1:F:125:LEU:HD13	1:F:125:LEU:C	2.39	0.42
1:A:142:ILE:HG23	1:A:204:ASP:OD2	2.19	0.42
1:D:146:LEU:HB3	1:D:207:SER:HB3	2.02	0.42
1:F:146:LEU:HB3	1:F:207:SER:HB3	2.02	0.42
1:E:265:LEU:HD23	1:E:265:LEU:N	2.35	0.42
1:D:236:ARG:NH2	1:D:283:TRP:CD1	2.86	0.42
1:D:578:PRO:C	1:D:580:ASP:N	2.73	0.42
1:D:104:LEU:O	1:D:107:TYR:HB2	2.20	0.42
1:F:17:MET:C	1:F:18:LYS:HD2	2.39	0.42
1:F:219:PHE:N	1:F:219:PHE:CD2	2.86	0.42
1:F:220:ARG:HG3	1:F:221:PRO:N	2.34	0.42
1:F:242:ASP:O	1:F:243:ILE:HG23	2.20	0.42
1:B:286:ARG:HH11	1:B:286:ARG:HG2	1.84	0.42
1:E:25:GLY:HA3	1:E:166:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:458:LEU:CD2	1:F:619:LYS:CA	2.96	0.42
1:D:190:ALA:HB3	1:D:203:VAL:HG23	2.02	0.42
1:E:423:PHE:O	1:E:583:THR:O	2.37	0.42
1:D:117:LEU:HD23	1:D:119:GLU:OE2	2.20	0.42
1:A:430:TRP:HE1	1:A:587:SER:CA	2.32	0.42
1:E:463:SER:HA	1:E:467:LYS:CB	2.49	0.42
1:D:526:ARG:HD3	1:D:635:LEU:HB2	2.01	0.42
1:B:51:SER:O	1:B:55:ARG:HG3	2.18	0.42
1:C:577:LYS:HA	1:C:578:PRO:HD3	1.79	0.42
1:C:355:GLN:O	1:C:357:ALA:N	2.53	0.42
1:F:74:VAL:HG22	1:F:99:CYS:SG	2.59	0.42
1:C:125:LEU:HA	1:C:162:HIS:CD2	2.54	0.42
1:B:526:ARG:HH11	1:B:526:ARG:N	2.16	0.42
1:E:83:MET:O	1:E:83:MET:SD	2.78	0.42
1:C:429:VAL:O	1:C:433:VAL:HG23	2.20	0.42
1:F:294:TYR:CE1	1:F:301:LYS:NZ	2.88	0.42
1:C:283:TRP:CG	1:C:284:HIS:N	2.87	0.42
1:D:202:THR:HG21	1:D:284:HIS:O	2.19	0.42
1:F:33:HIS:O	1:F:35:GLN:N	2.53	0.42
1:F:219:PHE:HB2	1:F:223:LEU:HD13	2.00	0.42
1:E:19:GLU:N	1:E:19:GLU:CD	2.73	0.42
1:F:107:TYR:CD2	1:F:153:LEU:HD13	2.55	0.42
1:F:103:ASP:O	1:F:104:LEU:C	2.59	0.42
1:A:432:GLN:H	1:A:432:GLN:HG2	1.62	0.42
1:E:249:LEU:HB3	1:E:250:ASN:H	1.70	0.42
1:C:531:LYS:O	1:C:535:GLU:HG3	2.20	0.42
1:F:572:ARG:HD2	1:F:572:ARG:O	2.19	0.42
1:B:181:GLU:C	1:B:183:VAL:N	2.73	0.42
1:C:517:MET:O	1:C:521:VAL:HG23	2.20	0.42
1:B:641:LYS:O	1:B:645:ARG:HB2	2.20	0.42
1:B:575:ARG:HB2	1:B:575:ARG:HE	1.78	0.42
1:A:403:PRO:C	1:A:404:ARG:HG3	2.41	0.42
1:D:227:GLN:N	1:D:227:GLN:CD	2.70	0.42
1:B:184:GLY:O	1:B:186:LEU:HD22	2.20	0.42
1:C:500:GLN:HE21	1:C:500:GLN:C	2.23	0.42
1:E:140:ARG:NH1	1:E:174:ASP:OD2	2.52	0.42
1:E:316:ASN:HA	1:E:388:PHE:CD1	2.55	0.42
1:D:353:LEU:HD12	1:D:353:LEU:N	2.35	0.42
1:C:456:MET:HE3	1:C:459:LEU:HD22	2.01	0.42
1:F:171:LYS:HD3	1:F:199:TYR:OH	2.20	0.42
1:B:601:PHE:O	1:B:605:VAL:HG23	2.20	0.42
1:B:664:LYS:C	1:B:664:LYS:HD3	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:494:LEU:O	1:D:494:LEU:HD13	2.20	0.42
1:E:187:GLN:HG3	1:E:220:ARG:HE	1.83	0.41
1:C:416:GLU:O	1:C:418:LYS:N	2.53	0.41
1:F:359:LEU:N	1:F:359:LEU:HD12	2.35	0.41
1:F:459:LEU:HD12	1:F:459:LEU:N	2.35	0.41
1:E:449:GLN:HE22	1:E:452:ARG:HD2	1.85	0.41
1:D:219:PHE:HD1	1:D:221:PRO:HG3	1.84	0.41
1:F:245:VAL:HG22	1:F:255:PHE:HB3	2.02	0.41
1:B:16:GLU:OE2	1:B:35:GLN:OE1	2.38	0.41
1:B:33:HIS:O	1:B:35:GLN:N	2.53	0.41
1:A:472:MET:O	1:A:475:MET:HG3	2.19	0.41
1:E:321:THR:O	1:E:322:ILE:O	2.38	0.41
1:F:606:ARG:HH21	1:F:606:ARG:HG3	1.84	0.41
1:C:104:LEU:O	1:C:107:TYR:HB2	2.20	0.41
1:D:488:THR:CG2	1:E:648:GLU:HB3	2.49	0.41
1:D:460:ARG:HG2	1:D:460:ARG:NH1	2.35	0.41
1:B:89:ASN:CG	1:B:91:LEU:HB2	2.41	0.41
1:B:659:LYS:HE2	1:C:499:GLU:CD	2.40	0.41
1:A:141:ILE:HG22	1:A:142:ILE:N	2.35	0.41
1:F:611:GLN:O	1:F:615:THR:HG23	2.20	0.41
1:B:443:ASP:HA	1:B:446:ARG:HG3	2.02	0.41
1:D:142:ILE:HG12	1:D:201:VAL:HG13	2.01	0.41
1:A:40:GLN:HA	1:A:40:GLN:HE21	1.85	0.41
1:E:266:ASN:HD21	1:E:313:HIS:HE1	1.68	0.41
1:D:316:ASN:HA	1:D:388:PHE:HE1	1.85	0.41
1:A:209:GLY:O	1:A:277:LEU:HD11	2.20	0.41
1:E:433:VAL:O	1:E:437:ILE:HG13	2.20	0.41
1:E:426:LEU:CD1	1:E:574:LEU:HD11	2.48	0.41
1:F:431:GLY:CA	1:F:571:TYR:HE2	2.33	0.41
1:F:427:ARG:NE	1:F:575:ARG:HG3	2.12	0.41
1:F:594:LEU:HD13	1:F:598:ILE:HD11	2.02	0.41
1:F:19:GLU:CD	1:F:19:GLU:N	2.73	0.41
1:B:222:PHE:O	1:B:223:LEU:HB2	2.20	0.41
1:B:223:LEU:HA	1:B:224:PRO:HD2	1.85	0.41
1:D:497:TYR:HA	1:D:500:GLN:HB2	2.02	0.41
1:D:501:THR:HA	1:D:505:ILE:HD11	2.02	0.41
1:A:530:VAL:HG11	1:A:633:VAL:HG12	2.02	0.41
1:E:139:ASN:O	1:E:140:ARG:HB2	2.20	0.41
1:D:622:ALA:O	1:D:626:LEU:HB2	2.18	0.41
1:A:517:MET:O	1:A:521:VAL:HG23	2.20	0.41
1:E:223:LEU:HD22	1:E:223:LEU:O	2.19	0.41
1:E:113:ASN:OD1	1:E:117:LEU:HA	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:451:GLN:HA	1:C:454:ALA:CB	2.46	0.41
1:D:60:LEU:HD22	1:D:175:GLN:HB3	2.02	0.41
1:A:316:ASN:HA	1:A:388:PHE:CD1	2.55	0.41
1:D:526:ARG:HD3	1:D:635:LEU:CB	2.49	0.41
1:A:240:GLU:HG3	1:A:241:VAL:HG23	2.00	0.41
1:E:646:LEU:HD12	1:E:646:LEU:O	2.19	0.41
1:E:186:LEU:HG	1:E:187:GLN:N	2.35	0.41
1:C:422:ALA:O	1:C:585:GLY:HA2	2.20	0.41
1:C:424:PHE:O	1:C:426:LEU:N	2.54	0.41
1:A:286:ARG:C	1:A:290:THR:OG1	2.58	0.41
1:F:460:ARG:O	1:F:464:CYS:HB2	2.20	0.41
1:F:462:ASN:C	1:F:464:CYS:N	2.73	0.41
1:A:115:CYS:HB2	1:A:435:HIS:CD2	2.54	0.41
1:F:419:ARG:HH12	1:F:588:GLN:HA	1.85	0.41
1:E:144:ARG:HD3	1:E:169:TYR:O	2.20	0.41
1:A:481:ALA:CB	1:F:482:LYS:HZ1	2.32	0.41
1:D:541:GLN:HA	1:D:541:GLN:OE1	2.20	0.41
1:E:192:GLU:HG3	1:E:192:GLU:H	1.48	0.41
1:E:462:ASN:C	1:E:464:CYS:H	2.22	0.41
1:A:328:THR:H	1:A:331:GLU:HG3	1.85	0.41
1:A:644:VAL:O	1:A:644:VAL:HG12	2.21	0.41
1:D:128:ASP:CB	1:D:162:HIS:HB2	2.51	0.41
1:A:617:VAL:O	1:A:621:LYS:HB2	2.19	0.41
1:A:213:PHE:CD1	1:A:221:PRO:HB2	2.52	0.41
1:F:290:THR:N	1:F:298:GLY:N	2.68	0.41
1:F:291:ASP:HA	1:F:292:PRO:HD3	1.87	0.41
1:F:449:GLN:NE2	1:F:452:ARG:HD2	2.36	0.41
1:F:356:GLU:C	1:F:452:ARG:NH1	2.74	0.41
1:C:263:ASN:O	1:C:265:LEU:CD2	2.69	0.41
1:C:265:LEU:O	1:C:266:ASN:HB2	2.20	0.41
1:B:165:ILE:O	1:B:166:ASP:C	2.59	0.41
1:D:168:GLY:C	1:D:170:ALA:N	2.73	0.41
1:D:496:LYS:HG2	1:E:655:TRP:CD1	2.55	0.41
1:C:139:ASN:C	1:C:141:ILE:HD12	2.41	0.41
1:E:227:GLN:HE21	1:E:227:GLN:HB2	1.62	0.41
1:B:313:HIS:ND1	1:B:324:THR:HG22	2.36	0.41
1:C:19:GLU:CD	1:C:19:GLU:N	2.73	0.41
1:C:19:GLU:C	1:C:20:ARG:HD3	2.40	0.41
1:B:463:SER:HA	1:B:467:LYS:CB	2.50	0.41
1:A:105:ARG:HH11	1:A:105:ARG:HG2	1.84	0.41
1:C:299:CYS:O	1:C:300:PHE:C	2.58	0.41
1:A:463:SER:HA	1:A:467:LYS:CB	2.49	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:315:LEU:O	1:C:317:MET:N	2.53	0.41
1:E:247:GLU:HA	1:E:252:THR:O	2.20	0.41
1:C:418:LYS:NZ	1:C:421:LEU:CD1	2.75	0.41
1:F:261:TYR:O	1:F:263:ASN:N	2.54	0.41
1:B:21:LEU:HD23	1:B:165:ILE:HG23	2.03	0.41
1:D:284:HIS:CD2	1:D:285:PRO:HD3	2.56	0.41
1:D:268:VAL:CG1	1:D:269:LEU:N	2.84	0.41
1:B:230:GLN:O	1:B:233:SER:HB3	2.20	0.41
1:B:260:PRO:C	1:B:262:PRO:CD	2.85	0.41
1:E:33:HIS:O	1:E:35:GLN:N	2.53	0.41
1:D:496:LYS:CD	1:E:655:TRP:CD1	3.01	0.41
1:E:227:GLN:CA	1:E:231:TRP:HB2	2.50	0.41
1:E:226:TRP:CZ3	1:E:228:PRO:HB2	2.54	0.41
1:E:276:TRP:CD1	1:E:302:ALA:HB1	2.56	0.41
1:B:62:ILE:HA	1:B:94:LEU:HD13	2.02	0.41
1:F:145:ASP:OD1	1:F:147:LYS:HG2	2.20	0.41
1:F:366:PRO:HG2	1:F:368:THR:HG23	2.03	0.41
1:E:594:LEU:HD13	1:E:598:ILE:HD11	2.01	0.41
1:A:445:ASN:HA	1:A:448:GLN:HB2	2.01	0.41
1:E:147:LYS:HE2	1:E:184:GLY:HA3	2.01	0.41
1:A:213:PHE:CZ	1:A:221:PRO:HB2	2.55	0.41
1:F:426:LEU:CD1	1:F:574:LEU:HD11	2.49	0.41
1:D:433:VAL:O	1:D:436:SER:HB3	2.20	0.41
1:D:430:TRP:HE1	1:D:587:SER:CB	2.34	0.41
1:E:18:LYS:HB3	1:E:19:GLU:H	1.54	0.41
1:A:497:TYR:HA	1:A:500:GLN:HB2	2.02	0.41
1:E:282:MET:CE	1:E:286:ARG:HH21	2.33	0.41
1:E:231:TRP:HA	1:E:235:VAL:HG23	2.03	0.41
1:A:140:ARG:HH11	1:A:140:ARG:HG3	1.86	0.41
1:B:140:ARG:HG3	1:B:140:ARG:HH11	1.85	0.41
1:A:359:LEU:N	1:A:359:LEU:HD12	2.36	0.41
1:F:306:ILE:HA	1:F:309:LEU:HD23	2.03	0.41
1:D:524:CYS:HB2	1:D:639:ASP:OD1	2.20	0.41
1:D:526:ARG:O	1:D:530:VAL:HG23	2.21	0.41
1:B:65:MET:HG3	1:B:94:LEU:HD21	2.03	0.41
1:E:55:ARG:HB3	1:E:55:ARG:NH1	2.35	0.41
1:C:61:GLU:OE1	1:C:168:GLY:HA2	2.20	0.41
1:B:350:ASP:HB3	1:B:391:ASP:HB2	2.02	0.41
1:D:350:ASP:HB2	1:D:391:ASP:HB2	2.02	0.41
1:B:531:LYS:O	1:B:535:GLU:HG3	2.21	0.41
1:F:442:GLU:O	1:F:446:ARG:HG3	2.20	0.41
1:B:181:GLU:O	1:B:183:VAL:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:475:MET:HE3	1:D:637:ASN:HD21	1.85	0.41
1:F:294:TYR:CD1	1:F:294:TYR:N	2.88	0.41
1:F:367:ALA:O	1:F:369:GLN:N	2.53	0.41
1:E:426:LEU:HD22	1:E:586:ASP:O	2.20	0.41
1:A:263:ASN:OD1	1:A:265:LEU:CD2	2.65	0.41
1:A:223:LEU:HG	1:A:226:TRP:HD1	1.86	0.41
1:E:19:GLU:C	1:E:20:ARG:HD3	2.39	0.41
1:E:482:LYS:O	1:E:485:PHE:HD2	2.03	0.41
1:A:500:GLN:HE21	1:A:501:THR:N	2.15	0.41
1:E:190:ALA:HB2	1:E:206:TRP:HB3	2.03	0.41
1:E:193:LEU:O	1:E:195:GLU:N	2.52	0.41
1:A:420:ASN:HB3	1:B:345:GLY:N	2.36	0.41
1:D:624:GLU:HG3	1:D:625:LEU:HG	2.02	0.41
1:E:231:TRP:HA	1:E:235:VAL:CG2	2.51	0.41
1:E:332:SER:HA	1:E:366:PRO:HB3	2.01	0.41
1:D:119:GLU:HG2	1:D:121:ALA:H	1.86	0.41
1:A:340:ILE:HG13	1:A:341:GLN:N	2.36	0.41
1:C:626:LEU:HB3	1:C:627:PRO:HD3	2.01	0.41
1:A:89:ASN:C	1:A:91:LEU:H	2.23	0.41
1:A:424:PHE:C	1:A:426:LEU:N	2.73	0.41
1:A:145:ASP:OD1	1:A:147:LYS:HG2	2.21	0.41
1:E:572:ARG:O	1:E:576:GLU:HB2	2.21	0.41
1:D:415:GLN:O	1:D:415:GLN:HG2	2.20	0.41
1:C:332:SER:HB2	1:C:334:GLN:HG2	2.02	0.41
1:B:249:LEU:HD23	1:B:418:LYS:NZ	2.34	0.41
1:B:412:CYS:SG	1:B:413:ILE:N	2.94	0.41
1:B:649:LYS:C	1:B:651:GLN:H	2.22	0.41
1:D:641:LYS:O	1:D:645:ARG:HB2	2.21	0.41
1:F:452:ARG:O	1:F:456:MET:HB2	2.21	0.41
1:B:79:VAL:HB	1:B:84:GLN:HG3	2.02	0.41
1:C:447:LEU:HD12	1:C:447:LEU:H	1.86	0.41
1:D:51:SER:O	1:D:55:ARG:HG3	2.20	0.41
1:A:357:ALA:HB3	1:A:359:LEU:HD11	2.01	0.41
1:F:583:THR:HB	1:F:584:GLU:H	1.63	0.41
1:E:403:PRO:O	1:E:404:ARG:HB3	2.20	0.41
1:F:647:GLN:OE1	1:F:647:GLN:HA	2.20	0.41
1:A:276:TRP:CD1	1:A:302:ALA:HB1	2.56	0.41
1:E:65:MET:HG3	1:E:94:LEU:HD21	2.03	0.41
1:E:350:ASP:OD2	1:E:350:ASP:N	2.50	0.41
1:C:569:GLU:HA	1:C:569:GLU:OE1	2.21	0.41
1:E:130:ALA:C	1:E:134:ARG:HD3	2.41	0.41
1:F:623:LEU:HD23	1:F:623:LEU:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:623:LEU:HD23	1:B:623:LEU:O	2.21	0.41
1:F:394:LYS:HG3	1:F:401:ILE:HG22	2.02	0.41
1:C:231:TRP:C	1:C:233:SER:N	2.74	0.41
1:F:547:LEU:HB2	1:F:548:GLN:OE1	2.21	0.41
1:E:452:ARG:C	1:E:452:ARG:HD3	2.41	0.41
1:E:430:TRP:O	1:E:571:TYR:CE2	2.74	0.41
1:F:430:TRP:O	1:F:433:VAL:HB	2.21	0.41
1:F:224:PRO:HG2	1:F:225:ASN:H	1.86	0.41
1:B:190:ALA:HA	1:B:191:PRO:HD3	1.96	0.41
1:A:421:LEU:HD22	1:A:585:GLY:O	2.20	0.41
1:E:22:GLY:H	1:E:165:ILE:HG21	1.86	0.41
1:E:64:ILE:O	1:E:67:ARG:HG3	2.20	0.41
1:D:410:VAL:HA	1:D:413:ILE:CG2	2.44	0.41
1:D:190:ALA:HB2	1:D:206:TRP:HB3	2.03	0.41
1:C:68:LEU:HD13	1:C:139:ASN:OD1	2.21	0.41
1:E:303:LEU:HD11	1:E:307:LEU:HD23	2.03	0.41
1:C:344:THR:HG23	1:D:418:LYS:HB2	2.02	0.41
1:C:320:GLY:HA3	1:D:417:PRO:CA	2.41	0.41
1:D:463:SER:HA	1:D:467:LYS:CB	2.51	0.41
1:E:104:LEU:HD23	1:E:148:PRO:HB3	2.02	0.41
1:C:506:THR:HG22	1:C:507:SER:N	2.29	0.41
1:C:462:ASN:C	1:C:464:CYS:N	2.73	0.41
1:B:626:LEU:HD23	1:B:626:LEU:C	2.41	0.41
1:B:431:GLY:O	1:B:433:VAL:N	2.52	0.41
1:D:19:GLU:N	1:D:19:GLU:CD	2.73	0.41
1:F:119:GLU:HG2	1:F:121:ALA:H	1.86	0.41
1:E:544:ILE:HG13	1:E:545:VAL:N	2.36	0.41
1:C:80:PRO:O	1:C:84:GLN:HG2	2.21	0.41
1:C:310:LYS:HB2	1:C:310:LYS:NZ	2.33	0.41
1:B:65:MET:CE	1:B:167:LEU:HB2	2.51	0.41
1:B:55:ARG:NH1	1:B:91:LEU:HD21	2.36	0.41
1:F:392:ASN:ND2	1:F:393:SER:H	2.19	0.41
1:A:171:LYS:O	1:A:171:LYS:HG2	2.19	0.41
1:A:310:LYS:H	1:A:310:LYS:HZ2	1.68	0.41
1:E:624:GLU:HG3	1:E:625:LEU:HG	2.02	0.41
1:A:51:SER:O	1:A:55:ARG:HG3	2.21	0.41
1:C:72:ASN:CA	1:C:163:LYS:HA	2.51	0.41
1:B:74:VAL:HG13	1:B:97:GLU:CG	2.51	0.41
1:C:191:PRO:O	1:C:194:LEU:HB2	2.21	0.41
1:E:79:VAL:HG21	1:E:84:GLN:CD	2.41	0.41
1:B:517:MET:HB3	1:B:650:ARG:NH2	2.36	0.41
1:A:18:LYS:HB2	1:A:31:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:449:GLN:HE22	1:B:452:ARG:HD2	1.86	0.41
1:D:443:ASP:HA	1:D:446:ARG:HG3	2.03	0.41
1:C:112:GLU:OE2	1:C:112:GLU:N	2.54	0.41
1:D:34:ASN:O	1:D:35:GLN:C	2.59	0.41
1:C:528:ASN:O	1:C:532:LEU:HD23	2.20	0.41
1:B:249:LEU:HG	1:B:414:LEU:HG	2.03	0.41
1:C:496:LYS:CE	1:C:654:LEU:HD11	2.50	0.41
1:D:475:MET:SD	1:D:479:LEU:HD23	2.61	0.41
1:B:319:THR:O	1:B:405:PRO:HD3	2.21	0.41
1:F:451:GLN:HG3	1:F:612:LEU:HD23	2.03	0.41
1:A:111:PHE:CD1	1:A:575:ARG:HD2	2.56	0.41
1:F:426:LEU:HD11	1:F:574:LEU:CD1	2.50	0.41
1:D:165:ILE:O	1:D:166:ASP:C	2.59	0.41
1:D:21:LEU:HD13	1:D:98:TYR:CD1	2.55	0.41
1:F:239:SER:HA	1:F:242:ASP:OD1	2.21	0.41
1:C:55:ARG:NH1	1:C:55:ARG:HB3	2.36	0.41
1:D:500:GLN:HB3	1:D:505:ILE:CG1	2.46	0.41
1:A:631:GLU:HG3	1:A:632:VAL:H	1.86	0.41
1:E:171:LYS:HZ1	1:E:173:LEU:HD23	1.85	0.41
1:B:64:ILE:O	1:B:67:ARG:HG3	2.21	0.41
1:A:649:LYS:C	1:A:651:GLN:H	2.24	0.41
1:F:500:GLN:HE21	1:F:500:GLN:C	2.24	0.41
1:A:64:ILE:O	1:A:67:ARG:HG3	2.21	0.41
1:B:346:ILE:HD13	1:B:388:PHE:HZ	1.86	0.41
1:C:316:ASN:HA	1:C:388:PHE:CD1	2.56	0.41
1:E:346:ILE:HD13	1:E:388:PHE:HZ	1.86	0.41
1:E:367:ALA:O	1:E:368:THR:C	2.59	0.41
1:E:421:LEU:O	1:E:422:ALA:O	2.38	0.41
1:B:303:LEU:HD11	1:B:307:LEU:HD23	2.03	0.41
1:B:239:SER:HB2	1:B:242:ASP:CB	2.51	0.41
1:A:19:GLU:C	1:A:20:ARG:HD3	2.42	0.41
1:A:167:LEU:C	1:A:169:TYR:H	2.23	0.41
1:B:104:LEU:O	1:B:107:TYR:HB2	2.21	0.41
1:A:107:TYR:CD2	1:A:153:LEU:HD22	2.56	0.41
1:A:451:GLN:HA	1:A:454:ALA:CB	2.48	0.41
1:B:359:LEU:HD12	1:B:359:LEU:N	2.36	0.41
1:B:631:GLU:HG3	1:B:632:VAL:H	1.85	0.41
1:B:617:VAL:O	1:B:621:LYS:HB2	2.21	0.41
1:E:549:ARG:HB2	1:E:550:SER:H	1.62	0.41
1:A:55:ARG:HB3	1:A:55:ARG:NH1	2.36	0.41
1:F:490:ILE:HD12	1:F:490:ILE:N	2.36	0.41
1:C:33:HIS:O	1:C:35:GLN:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:472:MET:O	1:E:475:MET:HG3	2.20	0.40
1:A:294:TYR:O	1:A:301:LYS:CD	2.64	0.40
1:F:433:VAL:CG1	1:F:594:LEU:HB2	2.51	0.40
1:F:419:ARG:HE	1:F:591:VAL:HG21	1.86	0.40
1:F:594:LEU:HD13	1:F:594:LEU:C	2.42	0.40
1:B:294:TYR:CD2	1:B:295:GLY:N	2.90	0.40
1:C:165:ILE:O	1:C:166:ASP:C	2.59	0.40
1:E:190:ALA:HA	1:E:206:TRP:CD1	2.56	0.40
1:F:463:SER:HA	1:F:467:LYS:CB	2.51	0.40
1:E:362:ILE:N	1:E:362:ILE:CD1	2.76	0.40
1:B:408:GLU:CG	1:B:409:SER:N	2.84	0.40
1:B:432:GLN:HG2	1:B:432:GLN:H	1.65	0.40
1:B:105:ARG:HD2	1:B:148:PRO:HB2	2.03	0.40
1:D:85:ASN:C	1:D:87:ALA:H	2.24	0.40
1:D:350:ASP:N	1:D:350:ASP:OD2	2.51	0.40
1:A:452:ARG:HD3	1:A:452:ARG:C	2.41	0.40
1:D:594:LEU:O	1:D:594:LEU:HD13	2.21	0.40
1:C:583:THR:O	1:C:584:GLU:C	2.59	0.40
1:C:247:GLU:HG2	1:C:247:GLU:O	2.21	0.40
1:A:74:VAL:HG13	1:A:97:GLU:CG	2.51	0.40
1:B:368:THR:C	1:B:370:CYS:H	2.24	0.40
1:C:649:LYS:C	1:C:651:GLN:H	2.24	0.40
1:F:403:PRO:C	1:F:404:ARG:HG3	2.42	0.40
1:A:259:LEU:N	1:A:259:LEU:CD1	2.83	0.40
1:A:419:ARG:NH1	1:A:419:ARG:C	2.75	0.40
1:F:433:VAL:O	1:F:437:ILE:HG13	2.21	0.40
1:A:479:LEU:HD12	1:A:640:GLU:HB3	2.03	0.40
1:F:89:ASN:O	1:F:91:LEU:N	2.55	0.40
1:D:241:VAL:HG12	1:D:241:VAL:O	2.20	0.40
1:E:315:LEU:HD12	1:E:321:THR:HA	2.02	0.40
1:E:577:LYS:HA	1:E:578:PRO:HD3	1.91	0.40
1:E:416:GLU:O	1:E:418:LYS:N	2.54	0.40
1:A:110:GLN:HB2	1:A:113:ASN:HB2	2.03	0.40
1:C:457:ASN:ND2	1:C:619:LYS:NZ	2.63	0.40
1:B:430:TRP:O	1:B:433:VAL:HB	2.22	0.40
1:E:636:MET:C	1:E:638:GLU:N	2.73	0.40
1:D:462:ASN:C	1:D:464:CYS:N	2.75	0.40
1:C:392:ASN:C	1:C:393:SER:OG	2.60	0.40
1:C:65:MET:CE	1:C:167:LEU:HB2	2.50	0.40
1:B:487:LYS:HB3	1:B:487:LYS:HE2	1.86	0.40
1:A:84:GLN:OE1	1:A:84:GLN:O	2.39	0.40
1:A:74:VAL:HG13	1:A:97:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:496:LYS:HZ2	1:C:658:LEU:HD23	1.86	0.40
1:D:637:ASN:HA	1:D:641:LYS:HB2	2.04	0.40
1:D:40:GLN:O	1:D:98:TYR:HB3	2.21	0.40
1:A:231:TRP:CD1	1:A:231:TRP:C	2.93	0.40
1:D:497:TYR:CE1	1:D:505:ILE:HD13	2.56	0.40
1:D:240:GLU:HG3	1:D:241:VAL:CG2	2.38	0.40
1:A:320:GLY:HA2	1:A:405:PRO:CD	2.51	0.40
1:E:321:THR:HG21	1:E:447:LEU:CD1	2.42	0.40
1:E:652:LYS:HD2	1:E:652:LYS:C	2.42	0.40
1:E:241:VAL:H	1:E:286:ARG:NH2	2.19	0.40
1:B:647:GLN:HA	1:B:647:GLN:OE1	2.20	0.40
1:A:331:GLU:HB2	1:A:367:ALA:HB2	2.03	0.40
1:C:626:LEU:C	1:C:626:LEU:HD23	2.42	0.40
1:C:606:ARG:HG3	1:C:606:ARG:HH21	1.85	0.40
1:C:276:TRP:CD1	1:C:302:ALA:HB1	2.56	0.40
1:F:143:HIS:O	1:F:145:ASP:N	2.51	0.40
1:F:350:ASP:HB3	1:F:391:ASP:HB2	2.03	0.40
1:D:299:CYS:O	1:D:300:PHE:C	2.59	0.40
1:F:252:THR:O	1:F:254:LYS:HG3	2.21	0.40
1:E:71:PRO:C	1:E:73:VAL:H	2.24	0.40
1:C:151:ILE:HD12	1:C:211:LEU:HD11	2.04	0.40
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.85	0.40
1:F:646:LEU:HD12	1:F:646:LEU:O	2.20	0.40
1:B:412:CYS:O	1:B:415:GLN:HB3	2.22	0.40
1:A:213:PHE:CG	1:A:221:PRO:HD2	2.56	0.40
1:A:259:LEU:HB2	1:A:260:PRO:HD2	2.01	0.40
1:A:284:HIS:CB	1:A:285:PRO:CD	2.98	0.40
1:A:418:LYS:HB3	1:B:344:THR:OG1	2.21	0.40
1:F:104:LEU:HD23	1:F:148:PRO:CB	2.43	0.40
1:E:460:ARG:NH1	1:E:460:ARG:HG2	2.37	0.40
1:D:547:LEU:HB2	1:D:548:GLN:OE1	2.22	0.40
1:F:422:ALA:O	1:F:585:GLY:CA	2.68	0.40
1:C:65:MET:HG3	1:C:94:LEU:HD21	2.03	0.40
1:C:580:ASP:OD1	1:C:581:GLN:HG3	2.22	0.40
1:A:261:TYR:N	1:A:262:PRO:CD	2.84	0.40
1:D:350:ASP:HB3	1:D:391:ASP:HB2	2.04	0.40
1:E:442:GLU:O	1:E:446:ARG:HG3	2.22	0.40
1:C:40:GLN:O	1:C:98:TYR:HB3	2.22	0.40
1:C:604:LYS:O	1:C:608:ILE:HG12	2.20	0.40
1:B:481:ALA:HB1	1:C:478:GLN:HG3	1.99	0.40
1:B:481:ALA:HB3	1:C:478:GLN:HG3	1.99	0.40
1:C:296:PRO:HG2	1:C:297:ASN:HD22	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:227:GLN:H	1:F:228:PRO:CD	2.35	0.40
1:D:626:LEU:HB3	1:D:627:PRO:HD3	2.01	0.40
1:F:89:ASN:HD22	1:F:91:LEU:CG	2.35	0.40
1:E:510:LEU:HB3	1:E:653:GLU:OE2	2.21	0.40
1:E:412:CYS:O	1:E:415:GLN:HB3	2.21	0.40
1:A:139:ASN:O	1:A:140:ARG:HB2	2.21	0.40
1:B:237:GLN:O	1:B:238:LYS:C	2.60	0.40
1:D:548:GLN:N	1:D:548:GLN:OE1	2.55	0.40
1:D:357:ALA:HB3	1:D:359:LEU:HD11	2.03	0.40
1:C:72:ASN:C	1:C:163:LYS:HA	2.40	0.40
1:B:452:ARG:O	1:B:456:MET:HB2	2.21	0.40
1:C:662:CYS:O	1:C:665:VAL:HG13	2.21	0.40
1:A:33:HIS:O	1:A:35:GLN:N	2.55	0.40
1:D:447:LEU:HD12	1:D:447:LEU:H	1.87	0.40
1:E:642:THR:O	1:E:646:LEU:HD23	2.22	0.40
1:F:415:GLN:O	1:F:415:GLN:HG2	2.22	0.40
1:C:250:ASN:ND2	1:C:250:ASN:N	2.70	0.40
1:F:604:LYS:O	1:F:608:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	614/669 (92%)	427 (70%)	112 (18%)	75 (12%)	1	14
1	B	624/669 (93%)	411 (66%)	133 (21%)	80 (13%)	0	13
1	C	614/669 (92%)	423 (69%)	117 (19%)	74 (12%)	1	14
1	D	614/669 (92%)	421 (69%)	119 (19%)	74 (12%)	1	14
1	E	614/669 (92%)	417 (68%)	121 (20%)	76 (12%)	1	14
1	F	614/669 (92%)	421 (69%)	120 (20%)	73 (12%)	1	14
All	All	3694/4014 (92%)	2520 (68%)	722 (20%)	452 (12%)	1	14

All (452) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	35	GLN
1	A	92	PRO
1	A	166	ASP
1	A	182	PHE
1	A	183	VAL
1	A	221	PRO
1	A	250	ASN
1	A	299	CYS
1	A	300	PHE
1	A	302	ALA
1	A	319	THR
1	A	322	ILE
1	A	323	HIS
1	A	356	GLU
1	A	370	CYS
1	A	392	ASN
1	A	408	GLU
1	A	580	ASP
1	A	587	SER
1	A	641	LYS
1	B	35	GLN
1	B	68	LEU
1	B	84	GLN
1	B	86	LEU
1	B	104	LEU
1	B	166	ASP
1	B	186	LEU
1	B	187	GLN
1	B	188	TYR
1	B	222	PHE
1	B	224	PRO
1	B	283	TRP
1	B	299	CYS
1	B	300	PHE
1	B	302	ALA
1	B	319	THR
1	B	322	ILE
1	B	323	HIS
1	B	356	GLU
1	B	392	ASN
1	B	501	THR

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Mol	Chain	Res	Type
1	B	505	ILE
1	B	550	SER
1	B	587	SER
1	B	641	LYS
1	C	35	GLN
1	C	37	THR
1	C	68	LEU
1	C	85	ASN
1	C	166	ASP
1	C	177	GLU
1	C	222	PHE
1	C	299	CYS
1	C	300	PHE
1	C	302	ALA
1	C	319	THR
1	C	322	ILE
1	C	323	HIS
1	C	356	GLU
1	C	371	ILE
1	C	402	SER
1	C	419	ARG
1	C	501	THR
1	C	505	ILE
1	C	578	PRO
1	C	583	THR
1	C	587	SER
1	C	641	LYS
1	D	34	ASN
1	D	35	GLN
1	D	37	THR
1	D	68	LEU
1	D	81	GLU
1	D	83	MET
1	D	166	ASP
1	D	170	ALA
1	D	224	PRO
1	D	299	CYS
1	D	300	PHE
1	D	302	ALA
1	D	319	THR
1	D	322	ILE
1	D	323	HIS

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Mol	Chain	Res	Type
1	D	356	GLU
1	D	392	ASN
1	D	419	ARG
1	D	421	LEU
1	D	422	ALA
1	D	501	THR
1	D	581	GLN
1	D	587	SER
1	D	641	LYS
1	E	35	GLN
1	E	37	THR
1	E	68	LEU
1	E	86	LEU
1	E	166	ASP
1	E	263	ASN
1	E	285	PRO
1	E	294	TYR
1	E	299	CYS
1	E	300	PHE
1	E	302	ALA
1	E	319	THR
1	E	322	ILE
1	E	323	HIS
1	E	356	GLU
1	E	368	THR
1	E	421	LEU
1	E	422	ALA
1	E	501	THR
1	E	583	THR
1	E	584	GLU
1	E	587	SER
1	E	641	LYS
1	F	34	ASN
1	F	35	GLN
1	F	37	THR
1	F	68	LEU
1	F	114	CYS
1	F	118	ARG
1	F	166	ASP
1	F	221	PRO
1	F	225	ASN
1	F	227	GLN

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Mol	Chain	Res	Type
1	F	229	VAL
1	F	243	ILE
1	F	296	PRO
1	F	299	CYS
1	F	300	PHE
1	F	302	ALA
1	F	319	THR
1	F	322	ILE
1	F	323	HIS
1	F	356	GLU
1	F	372	SER
1	F	501	THR
1	F	502	GLU
1	F	585	GLY
1	F	587	SER
1	F	641	LYS
1	A	34	ASN
1	A	37	THR
1	A	68	LEU
1	A	83	MET
1	A	104	LEU
1	A	157	GLU
1	A	188	TYR
1	A	197	GLN
1	A	224	PRO
1	A	243	ILE
1	A	298	GLY
1	A	320	GLY
1	A	330	ASP
1	A	368	THR
1	A	369	GLN
1	A	410	VAL
1	A	509	LYS
1	A	579	ARG
1	B	34	ASN
1	B	37	THR
1	B	88	PRO
1	B	157	GLU
1	B	197	GLN
1	B	221	PRO
1	B	228	PRO
1	B	295	GLY

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Mol	Chain	Res	Type
1	B	320	GLY
1	B	330	ASP
1	B	345	GLY
1	B	364	ASP
1	B	367	ALA
1	B	410	VAL
1	B	509	LYS
1	B	584	GLU
1	C	34	ASN
1	C	104	LEU
1	C	157	GLU
1	C	168	GLY
1	C	175	GLN
1	C	197	GLN
1	C	221	PRO
1	C	320	GLY
1	C	330	ASP
1	C	345	GLY
1	C	392	ASN
1	C	407	PRO
1	C	408	GLU
1	C	410	VAL
1	C	422	ALA
1	C	507	SER
1	C	509	LYS
1	D	19	GLU
1	D	82	GLY
1	D	104	LEU
1	D	157	GLU
1	D	169	TYR
1	D	188	TYR
1	D	197	GLN
1	D	222	PHE
1	D	238	LYS
1	D	320	GLY
1	D	330	ASP
1	D	393	SER
1	D	410	VAL
1	D	503	PHE
1	D	505	ILE
1	D	509	LYS
1	E	34	ASN

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Mol	Chain	Res	Type
1	E	82	GLY
1	E	104	LEU
1	E	157	GLU
1	E	174	ASP
1	E	197	GLN
1	E	237	GLN
1	E	284	HIS
1	E	298	GLY
1	E	320	GLY
1	E	330	ASP
1	E	410	VAL
1	E	505	ILE
1	E	509	LYS
1	E	578	PRO
1	F	86	LEU
1	F	104	LEU
1	F	157	GLU
1	F	197	GLN
1	F	226	TRP
1	F	238	LYS
1	F	250	ASN
1	F	263	ASN
1	F	266	ASN
1	F	320	GLY
1	F	330	ASP
1	F	392	ASN
1	F	409	SER
1	F	410	VAL
1	F	509	LYS
1	F	578	PRO
1	A	36	GLU
1	A	187	GLN
1	A	189	LEU
1	A	249	LEU
1	A	280	MET
1	A	293	THR
1	A	321	THR
1	A	357	ALA
1	A	366	PRO
1	A	393	SER
1	A	402	SER
1	A	407	PRO

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Mol	Chain	Res	Type
1	A	432	GLN
1	A	466	SER
1	B	36	GLU
1	B	81	GLU
1	B	189	LEU
1	B	280	MET
1	B	321	THR
1	B	357	ALA
1	B	407	PRO
1	B	422	ALA
1	B	425	GLN
1	B	432	GLN
1	C	36	GLU
1	C	178	LEU
1	C	189	LEU
1	C	226	TRP
1	C	232	HIS
1	C	280	MET
1	C	321	THR
1	C	357	ALA
1	C	393	SER
1	C	432	GLN
1	C	466	SER
1	C	526	ARG
1	D	36	GLU
1	D	92	PRO
1	D	189	LEU
1	D	229	VAL
1	D	230	GLN
1	D	232	HIS
1	D	265	LEU
1	D	280	MET
1	D	357	ALA
1	D	417	PRO
1	D	418	LYS
1	D	425	GLN
1	D	432	GLN
1	D	466	SER
1	D	583	THR
1	D	626	LEU
1	E	36	GLU
1	E	84	GLN

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Mol	Chain	Res	Type
1	E	159	ARG
1	E	171	LYS
1	E	189	LEU
1	E	222	PHE
1	E	223	LEU
1	E	227	GLN
1	E	280	MET
1	E	321	THR
1	E	357	ALA
1	E	392	ASN
1	E	425	GLN
1	E	502	GLU
1	E	508	ASP
1	F	17	MET
1	F	36	GLU
1	F	175	GLN
1	F	189	LEU
1	F	224	PRO
1	F	260	PRO
1	F	280	MET
1	F	357	ALA
1	F	368	THR
1	F	369	GLN
1	F	371	ILE
1	F	421	LEU
1	F	432	GLN
1	F	466	SER
1	A	159	ARG
1	A	170	ALA
1	A	223	LEU
1	A	270	ALA
1	A	284	HIS
1	A	292	PRO
1	A	425	GLN
1	B	159	ARG
1	B	170	ALA
1	B	175	GLN
1	B	177	GLU
1	B	182	PHE
1	B	194	LEU
1	B	223	LEU
1	B	238	LYS

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Mol	Chain	Res	Type
1	B	249	LEU
1	B	270	ALA
1	B	298	GLY
1	B	368	THR
1	B	461	ASN
1	B	466	SER
1	B	579	ARG
1	C	159	ARG
1	C	186	LEU
1	C	249	LEU
1	C	263	ASN
1	C	270	ALA
1	C	369	GLN
1	C	425	GLN
1	D	159	ARG
1	D	223	LEU
1	D	251	GLY
1	D	270	ALA
1	D	298	GLY
1	D	321	THR
1	D	345	GLY
1	D	402	SER
1	D	578	PRO
1	D	579	ARG
1	E	19	GLU
1	E	221	PRO
1	E	296	PRO
1	E	345	GLY
1	E	385	ASP
1	E	432	GLN
1	E	461	ASN
1	E	466	SER
1	E	507	SER
1	F	83	MET
1	F	159	ARG
1	F	174	ASP
1	F	219	PHE
1	F	230	GLN
1	F	270	ALA
1	A	21	LEU
1	A	114	CYS
1	A	194	LEU

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Mol	Chain	Res	Type
1	A	294	TYR
1	A	346	ILE
1	A	409	SER
1	A	626	LEU
1	B	227	GLN
1	B	285	PRO
1	B	346	ILE
1	B	626	LEU
1	C	194	LEU
1	C	265	LEU
1	C	298	GLY
1	C	346	ILE
1	C	420	ASN
1	C	584	GLU
1	C	626	LEU
1	D	185	THR
1	D	384	MET
1	D	507	SER
1	E	21	LEU
1	E	170	ALA
1	E	194	LEU
1	E	265	LEU
1	E	270	ALA
1	E	346	ILE
1	F	117	LEU
1	F	194	LEU
1	F	346	ILE
1	F	461	ASN
1	A	18	LYS
1	A	176	GLY
1	A	238	LYS
1	A	345	GLY
1	B	91	LEU
1	B	265	LEU
1	B	366	PRO
1	B	393	SER
1	B	502	GLU
1	C	238	LYS
1	C	417	PRO
1	D	221	PRO
1	D	346	ILE
1	D	420	ASN

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Mol	Chain	Res	Type
1	E	198	LYS
1	E	403	PRO
1	F	21	LEU
1	F	321	THR
1	F	525	GLY
1	C	92	PRO
1	C	241	VAL
1	C	585	GLY
1	E	245	VAL
1	A	165	ILE
1	B	229	VAL
1	B	371	ILE
1	E	165	ILE
1	F	345	GLY
1	B	585	GLY
1	C	82	GLY
1	D	165	ILE
1	E	228	PRO
1	E	405	PRO
1	F	92	PRO
1	F	165	ILE
1	A	525	GLY
1	B	165	ILE
1	C	165	ILE
1	D	245	VAL
1	E	417	PRO
1	E	585	GLY
1	F	183	VAL
1	A	241	VAL
1	A	578	PRO
1	B	557	GLY
1	C	245	VAL

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	567/601 (94%)	491 (87%)	76 (13%)	6 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	572/601 (95%)	485 (85%)	87 (15%)	4	30
1	C	567/601 (94%)	490 (86%)	77 (14%)	5	36
1	D	567/601 (94%)	488 (86%)	79 (14%)	5	35
1	E	567/601 (94%)	492 (87%)	75 (13%)	6	37
1	F	567/601 (94%)	478 (84%)	89 (16%)	4	28
All	All	3407/3606 (94%)	2924 (86%)	483 (14%)	5	34

All (483) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	20	ARG
1	A	23	THR
1	A	26	PHE
1	A	37	THR
1	A	89	ASN
1	A	103	ASP
1	A	105	ARG
1	A	119	GLU
1	A	124	THR
1	A	152	VAL
1	A	178	LEU
1	A	182	PHE
1	A	183	VAL
1	A	185	THR
1	A	192	GLU
1	A	194	LEU
1	A	210	THR
1	A	213	PHE
1	A	222	PHE
1	A	225	ASN
1	A	226	TRP
1	A	229	VAL
1	A	236	ARG
1	A	243	ILE
1	A	248	ASP
1	A	257	SER
1	A	259	LEU
1	A	261	TYR
1	A	294	TYR

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Mol	Chain	Res	Type
1	A	304	ASP
1	A	307	LEU
1	A	310	LYS
1	A	311	LEU
1	A	319	THR
1	A	334	GLN
1	A	359	LEU
1	A	364	ASP
1	A	371	ILE
1	A	385	ASP
1	A	388	PHE
1	A	390	PHE
1	A	404	ARG
1	A	415	GLN
1	A	418	LYS
1	A	419	ARG
1	A	421	LEU
1	A	424	PHE
1	A	432	GLN
1	A	434	TRP
1	A	448	GLN
1	A	452	ARG
1	A	472	MET
1	A	475	MET
1	A	478	GLN
1	A	483	LEU
1	A	485	PHE
1	A	486	PHE
1	A	499	GLU
1	A	500	GLN
1	A	502	GLU
1	A	511	LEU
1	A	514	TRP
1	A	517	MET
1	A	529	GLU
1	A	543	ASP
1	A	548	GLN
1	A	549	ARG
1	A	564	GLU
1	A	575	ARG
1	A	579	ARG
1	A	595	LEU

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Mol	Chain	Res	Type
1	A	631	GLU
1	A	648	GLU
1	A	651	GLN
1	A	652	LYS
1	B	16	GLU
1	B	20	ARG
1	B	23	THR
1	B	26	PHE
1	B	37	THR
1	B	53	ARG
1	B	86	LEU
1	B	89	ASN
1	B	103	ASP
1	B	105	ARG
1	B	119	GLU
1	B	124	THR
1	B	152	VAL
1	B	173	LEU
1	B	182	PHE
1	B	187	GLN
1	B	192	GLU
1	B	194	LEU
1	B	210	THR
1	B	213	PHE
1	B	227	GLN
1	B	236	ARG
1	B	238	LYS
1	B	242	ASP
1	B	248	ASP
1	B	249	LEU
1	B	263	ASN
1	B	283	TRP
1	B	284	HIS
1	B	286	ARG
1	B	290	THR
1	B	304	ASP
1	B	307	LEU
1	B	308	ASN
1	B	310	LYS
1	B	311	LEU
1	B	319	THR
1	B	334	GLN

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Mol	Chain	Res	Type
1	B	359	LEU
1	B	362	ILE
1	B	369	GLN
1	B	384	MET
1	B	385	ASP
1	B	388	PHE
1	B	390	PHE
1	B	394	LYS
1	B	404	ARG
1	B	419	ARG
1	B	421	LEU
1	B	424	PHE
1	B	432	GLN
1	B	434	TRP
1	B	448	GLN
1	B	452	ARG
1	B	472	MET
1	B	475	MET
1	B	478	GLN
1	B	483	LEU
1	B	485	PHE
1	B	486	PHE
1	B	493	ASP
1	B	499	GLU
1	B	500	GLN
1	B	502	GLU
1	B	503	PHE
1	B	511	LEU
1	B	514	TRP
1	B	517	MET
1	B	526	ARG
1	B	527	GLU
1	B	528	ASN
1	B	529	GLU
1	B	543	ASP
1	B	548	GLN
1	B	549	ARG
1	B	552	MET
1	B	556	GLN
1	B	564	GLU
1	B	575	ARG
1	B	579	ARG

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Mol	Chain	Res	Type
1	B	583	THR
1	B	595	LEU
1	B	631	GLU
1	B	648	GLU
1	B	651	GLN
1	B	652	LYS
1	B	664	LYS
1	C	20	ARG
1	C	23	THR
1	C	26	PHE
1	C	37	THR
1	C	53	ARG
1	C	103	ASP
1	C	105	ARG
1	C	119	GLU
1	C	124	THR
1	C	152	VAL
1	C	169	TYR
1	C	174	ASP
1	C	178	LEU
1	C	181	GLU
1	C	186	LEU
1	C	192	GLU
1	C	194	LEU
1	C	210	THR
1	C	213	PHE
1	C	225	ASN
1	C	231	TRP
1	C	236	ARG
1	C	243	ILE
1	C	247	GLU
1	C	250	ASN
1	C	253	VAL
1	C	257	SER
1	C	304	ASP
1	C	307	LEU
1	C	309	LEU
1	C	310	LYS
1	C	311	LEU
1	C	319	THR
1	C	334	GLN
1	C	359	LEU

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Mol	Chain	Res	Type
1	C	362	ILE
1	C	368	THR
1	C	385	ASP
1	C	388	PHE
1	C	390	PHE
1	C	394	LYS
1	C	401	ILE
1	C	404	ARG
1	C	419	ARG
1	C	424	PHE
1	C	432	GLN
1	C	434	TRP
1	C	448	GLN
1	C	452	ARG
1	C	472	MET
1	C	475	MET
1	C	478	GLN
1	C	483	LEU
1	C	485	PHE
1	C	486	PHE
1	C	493	ASP
1	C	499	GLU
1	C	500	GLN
1	C	502	GLU
1	C	503	PHE
1	C	511	LEU
1	C	514	TRP
1	C	517	MET
1	C	528	ASN
1	C	529	GLU
1	C	543	ASP
1	C	548	GLN
1	C	549	ARG
1	C	559	THR
1	C	564	GLU
1	C	575	ARG
1	C	581	GLN
1	C	595	LEU
1	C	631	GLU
1	C	648	GLU
1	C	651	GLN
1	C	652	LYS

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Mol	Chain	Res	Type
1	D	20	ARG
1	D	23	THR
1	D	26	PHE
1	D	37	THR
1	D	85	ASN
1	D	103	ASP
1	D	105	ARG
1	D	115	CYS
1	D	118	ARG
1	D	119	GLU
1	D	124	THR
1	D	152	VAL
1	D	169	TYR
1	D	182	PHE
1	D	187	GLN
1	D	192	GLU
1	D	194	LEU
1	D	210	THR
1	D	213	PHE
1	D	219	PHE
1	D	222	PHE
1	D	223	LEU
1	D	225	ASN
1	D	226	TRP
1	D	230	GLN
1	D	236	ARG
1	D	238	LYS
1	D	248	ASP
1	D	253	VAL
1	D	273	LEU
1	D	283	TRP
1	D	304	ASP
1	D	307	LEU
1	D	310	LYS
1	D	311	LEU
1	D	319	THR
1	D	334	GLN
1	D	359	LEU
1	D	368	THR
1	D	385	ASP
1	D	388	PHE
1	D	390	PHE

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Mol	Chain	Res	Type
1	D	404	ARG
1	D	408	GLU
1	D	419	ARG
1	D	420	ASN
1	D	421	LEU
1	D	424	PHE
1	D	432	GLN
1	D	434	TRP
1	D	448	GLN
1	D	452	ARG
1	D	472	MET
1	D	475	MET
1	D	478	GLN
1	D	483	LEU
1	D	485	PHE
1	D	486	PHE
1	D	493	ASP
1	D	499	GLU
1	D	500	GLN
1	D	502	GLU
1	D	505	ILE
1	D	511	LEU
1	D	514	TRP
1	D	517	MET
1	D	526	ARG
1	D	529	GLU
1	D	543	ASP
1	D	548	GLN
1	D	549	ARG
1	D	564	GLU
1	D	575	ARG
1	D	582	ARG
1	D	595	LEU
1	D	631	GLU
1	D	648	GLU
1	D	651	GLN
1	D	652	LYS
1	E	20	ARG
1	E	23	THR
1	E	26	PHE
1	E	37	THR
1	E	84	GLN

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Mol	Chain	Res	Type
1	E	91	LEU
1	E	103	ASP
1	E	105	ARG
1	E	119	GLU
1	E	124	THR
1	E	152	VAL
1	E	169	TYR
1	E	172	GLU
1	E	175	GLN
1	E	178	LEU
1	E	182	PHE
1	E	192	GLU
1	E	194	LEU
1	E	210	THR
1	E	213	PHE
1	E	222	PHE
1	E	223	LEU
1	E	227	GLN
1	E	230	GLN
1	E	236	ARG
1	E	258	SER
1	E	261	TYR
1	E	283	TRP
1	E	284	HIS
1	E	285	PRO
1	E	286	ARG
1	E	294	TYR
1	E	304	ASP
1	E	307	LEU
1	E	309	LEU
1	E	310	LYS
1	E	311	LEU
1	E	319	THR
1	E	334	GLN
1	E	359	LEU
1	E	373	ASP
1	E	385	ASP
1	E	388	PHE
1	E	390	PHE
1	E	404	ARG
1	E	424	PHE
1	E	432	GLN

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Mol	Chain	Res	Type
1	E	434	TRP
1	E	448	GLN
1	E	452	ARG
1	E	472	MET
1	E	475	MET
1	E	478	GLN
1	E	483	LEU
1	E	485	PHE
1	E	486	PHE
1	E	499	GLU
1	E	500	GLN
1	E	503	PHE
1	E	511	LEU
1	E	514	TRP
1	E	517	MET
1	E	526	ARG
1	E	529	GLU
1	E	543	ASP
1	E	548	GLN
1	E	549	ARG
1	E	559	THR
1	E	564	GLU
1	E	575	ARG
1	E	595	LEU
1	E	631	GLU
1	E	648	GLU
1	E	651	GLN
1	E	652	LYS
1	F	16	GLU
1	F	23	THR
1	F	26	PHE
1	F	37	THR
1	F	53	ARG
1	F	81	GLU
1	F	84	GLN
1	F	90	ASP
1	F	91	LEU
1	F	103	ASP
1	F	105	ARG
1	F	119	GLU
1	F	124	THR
1	F	152	VAL

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Mol	Chain	Res	Type
1	F	169	TYR
1	F	182	PHE
1	F	183	VAL
1	F	186	LEU
1	F	192	GLU
1	F	194	LEU
1	F	210	THR
1	F	213	PHE
1	F	219	PHE
1	F	220	ARG
1	F	222	PHE
1	F	226	TRP
1	F	227	GLN
1	F	231	TRP
1	F	236	ARG
1	F	238	LYS
1	F	243	ILE
1	F	247	GLU
1	F	252	THR
1	F	255	PHE
1	F	261	TYR
1	F	283	TRP
1	F	293	THR
1	F	294	TYR
1	F	304	ASP
1	F	307	LEU
1	F	310	LYS
1	F	311	LEU
1	F	319	THR
1	F	323	HIS
1	F	334	GLN
1	F	359	LEU
1	F	362	ILE
1	F	368	THR
1	F	385	ASP
1	F	388	PHE
1	F	390	PHE
1	F	404	ARG
1	F	419	ARG
1	F	421	LEU
1	F	424	PHE
1	F	432	GLN

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Mol	Chain	Res	Type
1	F	434	TRP
1	F	448	GLN
1	F	452	ARG
1	F	472	MET
1	F	475	MET
1	F	478	GLN
1	F	483	LEU
1	F	485	PHE
1	F	486	PHE
1	F	493	ASP
1	F	499	GLU
1	F	500	GLN
1	F	502	GLU
1	F	503	PHE
1	F	507	SER
1	F	511	LEU
1	F	514	TRP
1	F	517	MET
1	F	526	ARG
1	F	527	GLU
1	F	529	GLU
1	F	543	ASP
1	F	548	GLN
1	F	564	GLU
1	F	575	ARG
1	F	580	ASP
1	F	581	GLN
1	F	582	ARG
1	F	595	LEU
1	F	631	GLU
1	F	648	GLU
1	F	651	GLN
1	F	652	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	89	ASN
1	A	113	ASN
1	A	175	GLN
1	A	196	GLN

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Mol	Chain	Res	Type
1	A	225	ASN
1	A	278	GLN
1	A	284	HIS
1	A	297	ASN
1	A	334	GLN
1	A	355	GLN
1	A	369	GLN
1	A	415	GLN
1	A	420	ASN
1	A	432	GLN
1	A	449	GLN
1	A	478	GLN
1	A	500	GLN
1	A	581	GLN
1	A	651	GLN
1	B	40	GLN
1	B	70	HIS
1	B	72	ASN
1	B	89	ASN
1	B	113	ASN
1	B	187	GLN
1	B	196	GLN
1	B	227	GLN
1	B	264	ASN
1	B	308	ASN
1	B	334	GLN
1	B	406	GLN
1	B	415	GLN
1	B	432	GLN
1	B	448	GLN
1	B	449	GLN
1	B	457	ASN
1	B	477	GLN
1	B	478	GLN
1	B	500	GLN
1	B	528	ASN
1	B	556	GLN
1	B	581	GLN
1	B	651	GLN
1	C	40	GLN
1	C	70	HIS
1	C	72	ASN

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Mol	Chain	Res	Type
1	C	84	GLN
1	C	85	ASN
1	C	230	GLN
1	C	237	GLN
1	C	250	ASN
1	C	278	GLN
1	C	297	ASN
1	C	334	GLN
1	C	355	GLN
1	C	420	ASN
1	C	432	GLN
1	C	449	GLN
1	C	457	ASN
1	C	478	GLN
1	C	500	GLN
1	D	40	GLN
1	D	70	HIS
1	D	72	ASN
1	D	84	GLN
1	D	85	ASN
1	D	89	ASN
1	D	137	HIS
1	D	187	GLN
1	D	196	GLN
1	D	225	ASN
1	D	278	GLN
1	D	284	HIS
1	D	334	GLN
1	D	432	GLN
1	D	449	GLN
1	D	457	ASN
1	D	478	GLN
1	D	500	GLN
1	D	588	GLN
1	D	651	GLN
1	E	40	GLN
1	E	89	ASN
1	E	137	HIS
1	E	196	GLN
1	E	278	GLN
1	E	334	GLN
1	E	432	GLN

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Mol	Chain	Res	Type
1	E	449	GLN
1	E	478	GLN
1	E	500	GLN
1	E	528	ASN
1	E	651	GLN
1	F	40	GLN
1	F	70	HIS
1	F	72	ASN
1	F	89	ASN
1	F	187	GLN
1	F	263	ASN
1	F	278	GLN
1	F	297	ASN
1	F	334	GLN
1	F	369	GLN
1	F	415	GLN
1	F	432	GLN
1	F	449	GLN
1	F	457	ASN
1	F	478	GLN
1	F	500	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	624/669 (93%)	0.38	14 (2%) 59 45	56, 129, 201, 287	0
1	B	632/669 (94%)	0.29	5 (0%) 83 70	56, 130, 204, 256	0
1	C	624/669 (93%)	0.25	9 (1%) 72 57	64, 133, 201, 267	0
1	D	624/669 (93%)	0.23	11 (1%) 65 52	62, 132, 201, 286	0
1	E	624/669 (93%)	0.36	18 (2%) 49 39	63, 134, 205, 264	0
1	F	624/669 (93%)	0.35	21 (3%) 43 35	64, 144, 206, 256	0
All	All	3752/4014 (93%)	0.31	78 (2%) 60 47	56, 133, 204, 287	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	510	LEU	8.9
1	A	505	ILE	6.3
1	A	497	TYR	5.6
1	B	510	LEU	4.9
1	A	494	LEU	4.1
1	D	665	VAL	3.9
1	A	487	LYS	3.5
1	A	491	GLN	3.5
1	F	49	GLU	3.5
1	A	495	GLU	3.5
1	E	510	LEU	3.4
1	D	509	LYS	3.3
1	F	650	ARG	3.3
1	C	16	GLU	3.1
1	A	650	ARG	3.1
1	D	482	LYS	3.0
1	B	557	GLY	2.9
1	F	497	TYR	2.9
1	C	93	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	510	LEU	2.9
1	F	88	PRO	2.8
1	E	654	LEU	2.8
1	F	215	CYS	2.8
1	F	535	GLU	2.8
1	E	516	GLU	2.8
1	B	551	PRO	2.8
1	F	404	ARG	2.8
1	D	479	LEU	2.7
1	F	510	LEU	2.7
1	E	408	GLU	2.6
1	F	31	ARG	2.6
1	A	483	LEU	2.5
1	E	261	TYR	2.5
1	E	524	CYS	2.5
1	A	530	VAL	2.5
1	A	94	LEU	2.5
1	A	510	LEU	2.5
1	C	521	VAL	2.4
1	E	662	CYS	2.4
1	C	655	TRP	2.4
1	D	329	GLU	2.4
1	C	94	LEU	2.4
1	A	498	SER	2.4
1	F	477	GLN	2.4
1	D	640	GLU	2.3
1	E	509	LYS	2.3
1	E	658	LEU	2.3
1	B	482	LYS	2.3
1	F	93	LEU	2.3
1	F	94	LEU	2.3
1	D	550	SER	2.3
1	F	655	TRP	2.3
1	F	46	CYS	2.3
1	F	657	LEU	2.3
1	D	658	LEU	2.3
1	E	660	ILE	2.3
1	F	313	HIS	2.2
1	E	497	TYR	2.2
1	E	640	GLU	2.2
1	C	232	HIS	2.2
1	E	514	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	199	TYR	2.2
1	D	514	TRP	2.2
1	E	407	PRO	2.2
1	E	499	GLU	2.2
1	E	651	GLN	2.1
1	C	61	GLU	2.1
1	F	40	GLN	2.1
1	F	489	SER	2.1
1	A	492	ILE	2.1
1	F	41	ILE	2.1
1	A	480	LYS	2.1
1	F	658	LEU	2.1
1	D	507	SER	2.0
1	E	231	TRP	2.0
1	F	623	LEU	2.0
1	E	657	LEU	2.0
1	B	658	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.