



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:26 PM GMT

PDB ID : 3K0C
Title : Crystal structure of the phosphorylation-site double mutant S431A/T432E of the KaiC circadian clock protein
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on : 2009-09-24
Resolution : 3.30 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>

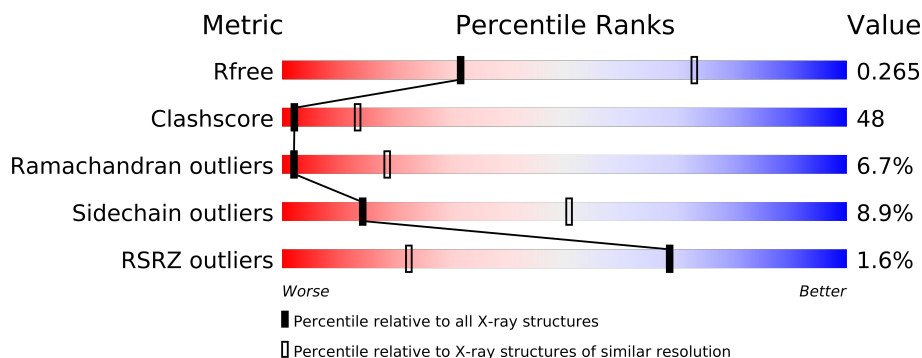
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.30 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	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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	519	
1	B	519	
1	E	519	
1	F	519	
2	C	519	
2	D	519	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	520	-	X
4	MG	A	701	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	802	-	X
4	MG	B	701	-	X
4	MG	C	701	-	X
4	MG	C	702	-	X
4	MG	C	801	-	X
4	MG	C	802	-	X
4	MG	D	701	-	X
4	MG	D	702	-	X
4	MG	D	801	-	X
4	MG	E	520	-	X
4	MG	F	701	-	X
4	MG	F	702	-	X
4	MG	F	802	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23919 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3990	2510	701	763	1	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3875	2440	678	741	1	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3883	2446	679	742	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3990	2510	701	763	1	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ALA	SER	ENGINEERED	UNP Q79PF4
A	432	GLU	THR	ENGINEERED	UNP Q79PF4
B	431	ALA	SER	ENGINEERED	UNP Q79PF4
B	432	GLU	THR	ENGINEERED	UNP Q79PF4
E	431	ALA	SER	ENGINEERED	UNP Q79PF4
E	432	GLU	THR	ENGINEERED	UNP Q79PF4
F	431	ALA	SER	ENGINEERED	UNP Q79PF4
F	432	GLU	THR	ENGINEERED	UNP Q79PF4

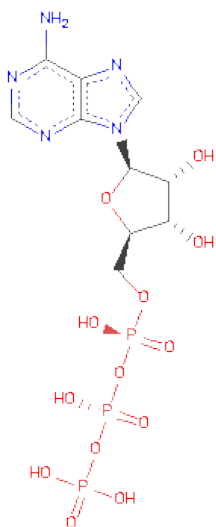
- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	488	Total	C	N	O	S	0	0	0
			3847	2426	674	732	15			
2	D	485	Total	C	N	O	S	0	0	0
			3823	2412	671	725	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	431	ALA	SER	ENGINEERED	UNP Q79PF4
C	432	GLU	THR	ENGINEERED	UNP Q79PF4
D	431	ALA	SER	ENGINEERED	UNP Q79PF4
D	432	GLU	THR	ENGINEERED	UNP Q79PF4

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	4	Total	Mg	0	0
			4	4		
4	E	3	Total	Mg	0	0
			3	3		
4	B	3	Total	Mg	0	0
			3	3		
4	C	4	Total	Mg	0	0
			4	4		
4	A	5	Total	Mg	0	0
			5	5		
4	F	3	Total	Mg	0	0
			3	3		

- Molecule 5 is water.

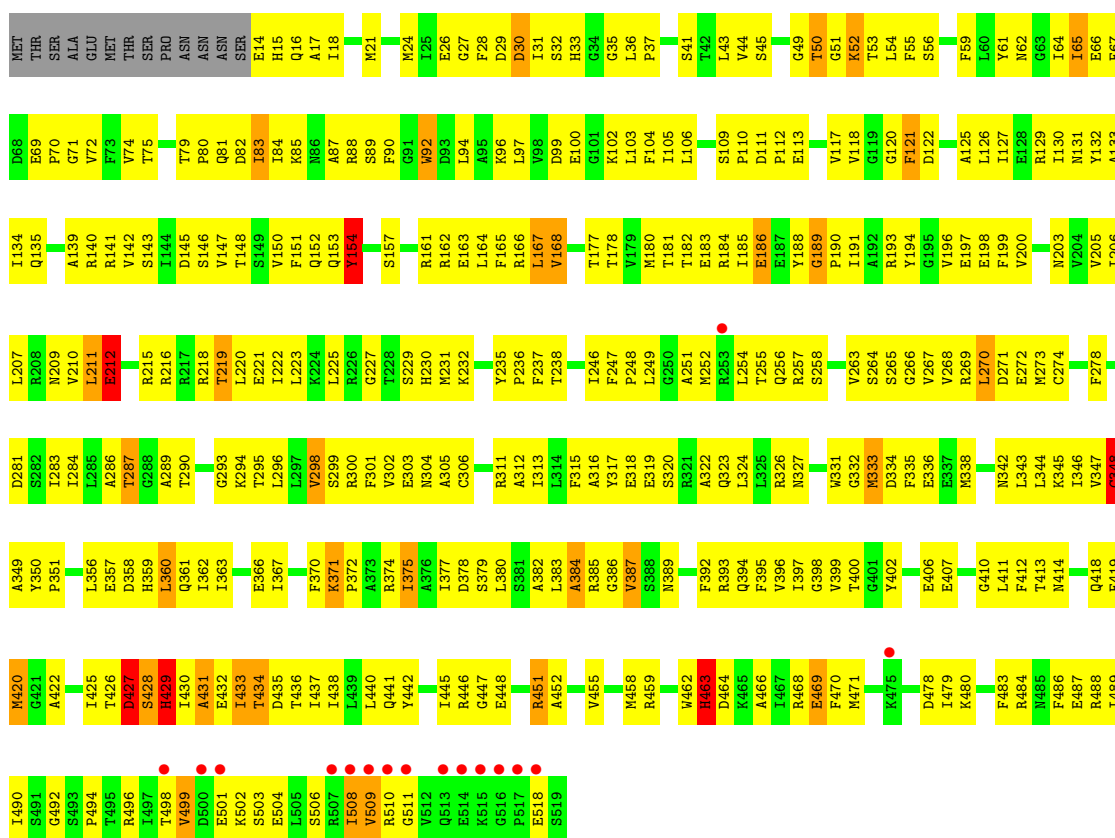
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	18	Total	O	0	0
			18	18		
5	C	22	Total	O	0	0
			22	22		
5	D	31	Total	O	0	0
			31	31		
5	E	13	Total	O	0	0
			13	13		
5	F	21	Total	O	0	0
			21	21		

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.

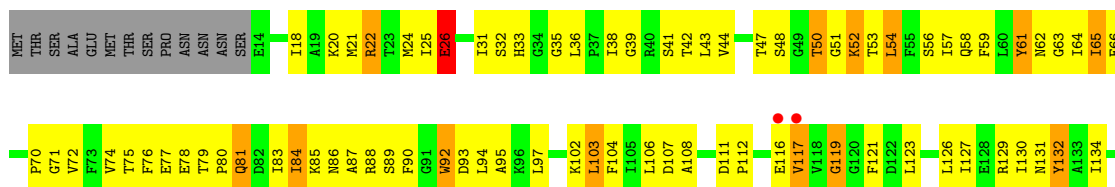
- Molecule 1: Circadian clock protein kinase KaiC

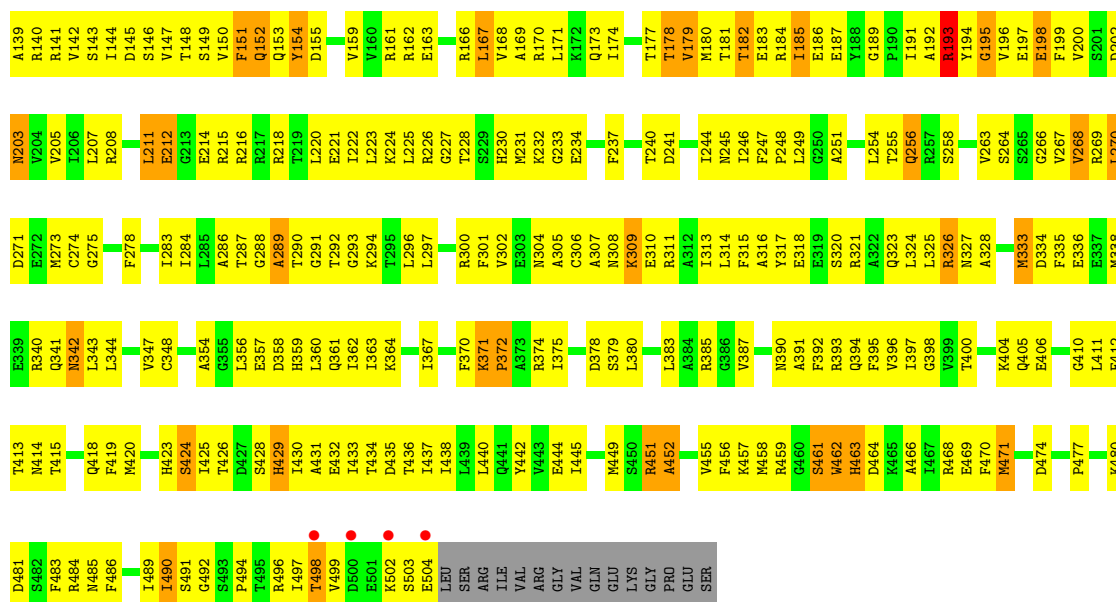
Chain A: 



- Molecule 1: Circadian clock protein kinase KaiC

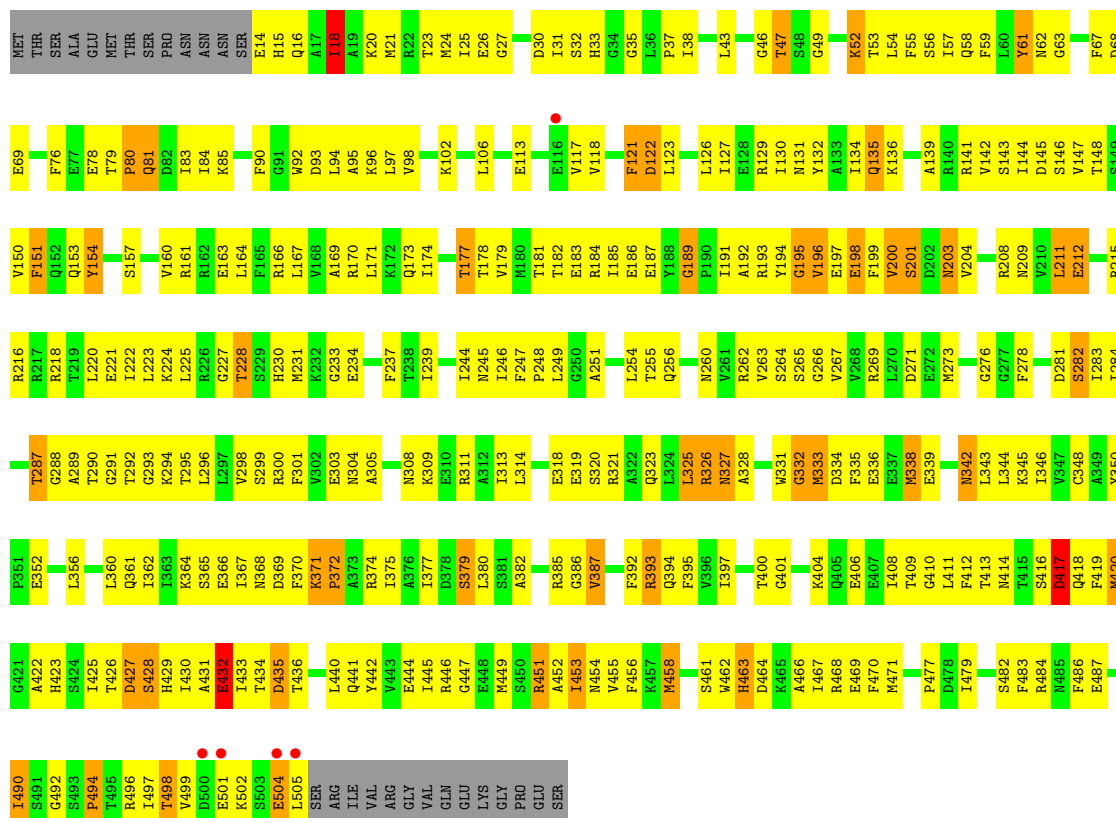
Chain B: 





• Molecule 1: Circadian clock protein kinase KaiC

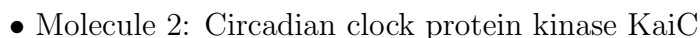
Chain E:



• Molecule 1: Circadian clock protein kinase KaiC

Chain F:





Chain D:

MET	B69	A139	L211	S353	F419	S483
THR	P70	R140	E212	A354	M420	P494
SER	G71	R141	G213	G355	H423	T495
ALA	V74	V142	E214	L356	H423	R496
GLU	T75	S143	R215	E357	S424	I497
MET	F76	V147	R216	D358	I425	T498
THR	E77	T148	R217	H359	T426	VAL
SER	E78	S148	R218	L360	H429	ASP
PRO	T79	V150	T219	G361	I430	GLU
ASN	P80	F151	L220	L362	I430	LYS
ASN	Q81	Q152	E221	L297	A431	SER
ASN	D82	Q153	L222	V298	T434	GLU
SER	I83	Y154	L223	S299	D435	LEU
E14	R84	A155	R224	R300	I436	SER
H15	K85	A156	L225	F301	I437	ARG
Q16	N86	S157	R226	E303	K371	ILE
A17	A87	S158	H230	N304	R374	VAL
I18	R88	V159	M231	A305	I375	ARG
M21	S89	V160	K232	C306	R376	GLY
R22	P90	R161	G233	A307	I377	GLY
T23	G91	R162	E234	N308	A376	VAL
M24	W92	E163	Y235	K309	I377	GLN
I25	D93	L164	F236	E310	D378	GLU
E26	L94	L167	F237	R311	S379	LYS
D30	A95	R170	T238	A312	L380	GLY
I31	K96	I174	I239	I313	S381	PRO
G35	V98	T177	T246	L314	A382	GLU
L36	D99	T178	F247	A315	A383	SER
P37	E100	T179	P248	A316	A384	
I38	L103	M180	L249	Y317	R385	
G39	F104	I105	G250	E318	G386	
R40	I106	T181	A251	R321	V387	
S41	D107	E183	L254	A322	S388	
V44	E113	R184	Q255	L324	N389	
S45	G114	Q115	Q256	R325	N390	
G46	Q116	S48	R262	R326	A391	
T47	V117	G195	V263	N327	F392	
Q49	G120	F121	S264	A328	R393	
K52	F122	D123	S265	W331	Q394	
T53	L124	S124	G266	G332	F395	
L54	A125	E126	V267	M333	V396	
F55	L126	L127	V268	D334	I397	
S56	F59	E128	R269	F335	G398	
I57	L128	N203	D271	E336	V399	
Q58	L129	V204	E272	M338	T400	
F59	E130	L206	G273	L343	G401	
L60	Y131	L207	G274	L344	Y402	
Y61	Y132	R208	G275	K345	E406	
I64	I133	N209	G276	I346	F407	
T65	A134	I210	G277	V347	I408	
E66	F67	D68	K280	C348	L411	
			D281	A349	F412	
			I283	Y350	T413	
					I414	
					T415	
					S416	
					D417	
					Q418	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.28Å 135.03Å 204.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (30.00-3.30) 90.8 (30.07-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.269 0.239 , 0.265	Depositor DCC
R_{free} test set	5141 reflections (10.20%)	DCC
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 19.2	EDS
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 54452 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23919	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MG, ATP

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	0.39	0/4044	0.67	0/5446
1	B	0.37	0/3928	0.64	0/5291
1	E	0.48	0/3936	0.72	2/5302 (0.0%)
1	F	0.45	0/4044	0.71	1/5446 (0.0%)
2	C	0.41	0/3912	0.67	0/5273
2	D	0.45	0/3888	0.70	0/5240
All	All	0.43	0/23752	0.69	3/31998 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	16	GLN	N-CA-C	-5.61	95.85	111.00
1	E	332	GLY	N-CA-C	-5.09	100.38	113.10
1	E	380	LEU	N-CA-C	-5.04	97.38	111.00

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	3990	0	3983	403	0
1	B	3875	0	3861	411	0
1	E	3883	0	3871	375	0
1	F	3990	0	3982	462	0
2	C	3847	0	3839	418	0
2	D	3823	0	3819	359	0
3	A	62	0	24	6	0
3	B	62	0	24	8	0
3	C	62	0	24	8	0
3	D	62	0	24	5	0
3	E	62	0	24	9	0
3	F	62	0	24	4	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
5	A	12	0	0	1	0
5	B	18	0	0	2	0
5	C	22	0	0	4	0
5	D	31	0	0	6	0
5	E	13	0	0	3	0
5	F	21	0	0	5	0
All	All	23919	0	23499	2276	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 48.

All (2276) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:425:ILE:O	1:A:426:TPO:HG22	1.25	1.24
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.26	1.14
1:B:300:ARG:HA	1:B:333:MET:HE1	1.16	1.14
1:A:299:SER:HB3	1:A:333:MET:HE1	1.33	1.10
2:D:379:SER:H	2:D:413:THR:HB	0.97	1.09
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.30	1.07
1:F:426:TPO:CG2	1:F:430:ILE:H	1.66	1.07
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.38	1.06
1:F:191:ILE:HG13	1:F:206:ILE:HD11	1.35	1.04
1:A:379:SER:H	1:A:413:THR:HB	1.19	1.04
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.18	1.04
2:C:25:ILE:HG12	2:C:58:GLN:HE21	1.24	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:45:SER:HB3	2:C:182:THR:HB	1.41	1.03
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.39	1.02
1:A:211:LEU:O	1:A:212:GLU:HB3	1.58	1.02
1:A:425:ILE:O	1:A:426:TPO:CG2	2.08	1.01
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.42	1.01
1:A:380:LEU:HD11	1:A:412:PHE:CD2	1.96	1.00
2:C:215:ARG:HA	2:C:215:ARG:HE	1.26	1.00
2:D:379:SER:N	2:D:413:THR:HB	1.76	1.00
1:F:426:TPO:HG21	1:F:430:ILE:N	1.77	1.00
1:E:18:ILE:HD11	1:E:227:GLY:HA3	1.43	0.98
1:F:426:TPO:HG21	1:F:430:ILE:H	1.26	0.98
1:B:25:ILE:HG12	1:B:58:GLN:HE21	1.27	0.97
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.29	0.97
1:F:127:ILE:HD11	1:F:167:LEU:HA	1.44	0.97
1:A:14:GLU:HG3	1:A:15:HIS:H	1.30	0.96
1:F:283:ILE:HG23	1:F:412:PHE:HE1	1.31	0.96
1:E:320:SER:HA	1:F:254:LEU:HG	1.47	0.96
1:B:147:VAL:HG11	1:B:180:MET:HE2	1.48	0.95
1:B:273:MET:O	1:B:463:HIS:HA	1.66	0.95
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.46	0.95
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.49	0.94
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.46	0.94
2:C:70:PRO:HB2	2:C:139:ALA:HA	1.51	0.93
1:F:486:PHE:HE2	1:F:496:ARG:HH11	1.10	0.92
1:B:25:ILE:HG23	1:B:58:GLN:HE22	1.32	0.92
1:F:299:SER:HB3	1:F:333:MET:HE1	1.51	0.92
1:E:356:LEU:HD11	1:E:387:VAL:HG21	1.52	0.92
1:E:426:TPO:HG21	1:E:431:ALA:H	1.34	0.91
1:A:380:LEU:HD11	1:A:412:PHE:HD2	1.36	0.90
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.54	0.89
1:B:300:ARG:CA	1:B:333:MET:HE1	2.01	0.88
1:F:515:LYS:HG3	1:F:516:GLY:H	1.39	0.88
1:E:266:GLY:HA2	1:E:304:ASN:HD22	1.37	0.88
1:B:221:GLU:HG3	1:B:233:GLY:O	1.74	0.88
1:E:344:LEU:HD22	1:E:345:LYS:H	1.36	0.88
1:A:350:TYR:CZ	1:B:254:LEU:HD13	2.09	0.88
1:E:426:TPO:HG21	1:E:431:ALA:N	1.89	0.88
1:A:265:SER:O	1:A:301:PHE:HA	1.73	0.88
1:A:429:HIS:HB3	5:F:522:HOH:O	1.73	0.87
1:E:263:VAL:HG12	1:E:374:ARG:NH2	1.89	0.87
2:D:148:THR:HG21	2:D:193:ARG:HD2	1.55	0.87
1:A:441:GLN:HE22	1:A:490:ILE:HD13	1.38	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:261:VAL:HG12	2:C:262:ARG:H	1.39	0.86
1:A:266:GLY:HA3	1:A:300:ARG:O	1.76	0.86
1:B:146:SER:H	1:B:181:THR:HB	1.39	0.86
1:B:497:ILE:HD12	1:B:498:THR:N	1.91	0.86
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.58	0.85
1:B:218:ARG:HD3	1:B:237:PHE:CE1	2.10	0.85
1:B:426:TPO:O1P	1:B:429:HIS:HA	1.77	0.85
1:A:147:VAL:O	1:A:150:VAL:HG12	1.75	0.85
1:F:312:ALA:HA	1:F:372:PRO:HB3	1.58	0.85
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.42	0.85
1:A:263:VAL:CG1	1:A:374:ARG:HH21	1.90	0.84
2:C:220:LEU:HD13	2:C:246:ILE:HD11	1.59	0.84
1:F:313:ILE:HG13	1:F:372:PRO:HG2	1.58	0.84
2:C:451:ARG:HH11	2:C:451:ARG:HG2	1.41	0.84
2:D:147:VAL:HG11	2:D:180:MET:HE3	1.58	0.84
1:F:500:ASP:O	1:F:501:GLU:HB3	1.75	0.84
1:F:171:LEU:HD13	1:F:178:THR:HG21	1.58	0.84
1:E:379:SER:H	1:E:413:THR:HB	1.43	0.84
1:B:140:ARG:NH1	1:B:140:ARG:HB3	1.92	0.84
1:F:170:ARG:HH12	1:F:174:ILE:HG12	1.42	0.83
1:A:264:SER:HA	1:A:271:ASP:OD1	1.78	0.83
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.13	0.82
1:F:142:VAL:HB	1:F:178:THR:HG23	1.61	0.82
1:A:323:GLN:HG2	1:A:327:ASN:HD21	1.42	0.82
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.60	0.82
1:E:294:LYS:HB2	3:E:901:ATP:O1B	1.79	0.82
2:C:182:THR:HG22	2:C:183:GLU:H	1.45	0.82
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.44	0.82
1:A:211:LEU:HG	1:A:212:GLU:H	1.43	0.82
1:A:65:ILE:O	1:A:66:GLU:HG2	1.79	0.82
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.93	0.82
2:D:52:LYS:HB2	5:D:550:HOH:O	1.80	0.81
1:A:451:ARG:N	1:A:451:ARG:HD2	1.95	0.81
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.59	0.81
2:D:18:ILE:HD12	2:D:18:ILE:H	1.42	0.81
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.63	0.81
1:E:418:GLN:HB2	1:F:423:HIS:O	1.81	0.81
2:C:45:SER:CB	2:C:182:THR:HB	2.11	0.81
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.11	0.81
2:C:431:ALA:O	2:C:434:THR:HG22	1.79	0.81
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.62	0.81
2:C:287:THR:HG21	2:C:425:ILE:O	1.81	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:436:THR:HG23	2:D:458:MET:HG2	1.62	0.81
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.46	0.81
2:C:409:THR:HA	5:C:539:HOH:O	1.80	0.81
3:B:901:ATP:H3'	2:C:458:MET:O	1.82	0.80
2:C:344:LEU:HD22	2:C:345:LYS:H	1.46	0.80
1:B:300:ARG:HA	1:B:333:MET:CE	2.08	0.80
1:A:72:VAL:HB	1:A:142:VAL:HG22	1.64	0.80
1:E:14:GLU:HG3	1:E:16:GLN:H	1.47	0.80
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.63	0.80
1:E:293:GLY:HA2	3:E:901:ATP:O1A	1.81	0.80
1:E:283:ILE:HG13	1:E:400:THR:HG23	1.63	0.80
1:B:25:ILE:HG23	1:B:58:GLN:NE2	1.97	0.79
2:C:384:ALA:HB2	2:C:392:PHE:CE1	2.16	0.79
2:D:31:ILE:HA	2:D:231:MET:SD	2.23	0.79
2:C:446:ARG:HG2	2:C:496:ARG:NH2	1.97	0.79
2:D:419:PHE:CE2	1:E:425:ILE:HG13	2.16	0.79
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.12	0.79
1:F:303:GLU:OE2	1:F:333:MET:HB3	1.82	0.79
1:F:344:LEU:HD22	1:F:345:LYS:H	1.47	0.79
1:A:446:ARG:HA	1:A:496:ARG:NH2	1.98	0.79
2:C:315:PHE:CE2	2:C:363:ILE:HA	2.19	0.78
1:E:263:VAL:CG1	1:E:374:ARG:HH21	1.95	0.78
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.63	0.78
5:D:538:HOH:O	1:E:432:GLU:HG2	1.84	0.78
1:F:377:ILE:HD11	1:F:399:VAL:HG11	1.66	0.78
1:F:383:LEU:HD13	1:F:395:PHE:CE2	2.18	0.78
2:D:347:VAL:HG12	2:D:348:CYS:N	1.98	0.78
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.65	0.78
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.49	0.78
2:D:294:LYS:O	2:D:298:VAL:HG23	1.83	0.78
1:E:382:ALA:O	1:E:385:ARG:HG3	1.84	0.78
1:F:393:ARG:O	1:F:397:ILE:HG12	1.84	0.77
2:D:267:VAL:CG2	2:D:300:ARG:HG2	2.14	0.77
2:D:170:ARG:O	2:D:174:ILE:HG12	1.84	0.77
1:A:14:GLU:CG	1:A:15:HIS:H	1.97	0.77
2:C:72:VAL:HG22	2:C:104:PHE:HB3	1.65	0.77
2:C:42:THR:HA	2:C:203:ASN:HB2	1.66	0.77
1:B:492:GLY:O	1:B:494:PRO:HD3	1.83	0.77
1:E:313:ILE:CD1	1:E:372:PRO:HG2	2.15	0.77
1:E:445:ILE:HG22	1:E:446:ARG:HD2	1.67	0.77
1:E:497:ILE:HG22	1:E:498:THR:H	1.48	0.77
2:C:371:LYS:HD2	2:C:371:LYS:O	1.84	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:464:ASP:OD2	1:E:466:ALA:HB3	1.83	0.77
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.67	0.77
2:D:212:GLU:O	2:D:212:GLU:HG2	1.84	0.77
1:B:116:GLU:HG2	1:B:117:VAL:H	1.50	0.77
2:C:182:THR:HG22	2:C:183:GLU:N	2.00	0.77
1:A:64:ILE:HD11	1:A:103:LEU:HB2	1.65	0.77
2:D:377:ILE:O	2:D:377:ILE:HG22	1.84	0.77
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.00	0.76
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.20	0.76
1:E:24:MET:HA	1:E:24:MET:HE3	1.65	0.76
1:B:25:ILE:HG12	1:B:58:GLN:NE2	1.99	0.76
1:A:16:GLN:O	1:F:88:ARG:HD2	1.85	0.76
1:E:326:ARG:HD3	1:F:258:SER:OG	1.85	0.76
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.68	0.76
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.16	0.76
1:E:294:LYS:HB3	1:E:413:THR:HG23	1.67	0.76
1:E:504:GLU:HG2	1:E:505:LEU:H	1.51	0.76
1:A:320:SER:HA	1:B:254:LEU:HG	1.68	0.75
2:C:245:ASN:HD22	2:C:245:ASN:C	1.88	0.75
2:C:422:ALA:HB1	5:C:536:HOH:O	1.86	0.75
1:F:344:LEU:HD22	1:F:345:LYS:N	2.00	0.75
2:D:214:GLU:HB3	1:E:234:GLU:HB2	1.67	0.75
2:D:371:LYS:HD2	2:D:371:LYS:O	1.85	0.75
1:F:381:SER:HB3	1:F:414:ASN:OD1	1.87	0.75
1:A:425:ILE:C	1:A:426:TPO:O1P	2.24	0.75
1:E:323:GLN:HE21	1:F:459:ARG:HD3	1.50	0.75
1:E:191:ILE:HB	1:E:198:GLU:CG	2.16	0.75
1:B:191:ILE:HB	1:B:198:GLU:CG	2.16	0.75
2:C:261:VAL:HG12	2:C:262:ARG:N	2.01	0.75
1:A:323:GLN:HG2	1:A:327:ASN:ND2	2.01	0.75
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.69	0.75
1:A:386:GLY:HA2	1:B:390:ASN:OD1	1.86	0.75
1:B:52:LYS:H	1:B:207:LEU:HD12	1.51	0.74
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.51	0.74
1:E:148:THR:OG1	1:E:182:THR:HG23	1.85	0.74
1:B:56:SER:O	1:B:59:PHE:HB3	1.87	0.74
1:A:207:LEU:HD21	1:A:220:LEU:HD12	1.70	0.74
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.17	0.74
1:B:358:ASP:O	1:B:362:ILE:HG12	1.88	0.74
1:B:50:THR:HB	1:B:207:LEU:HB3	1.68	0.74
1:B:426:TPO:O1P	1:B:429:HIS:CA	2.35	0.74
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.53	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.69	0.74
1:E:461:SER:OG	1:E:462:TRP:N	2.19	0.74
1:A:50:THR:HG22	1:A:209:ASN:HB2	1.70	0.74
1:E:20:LYS:HE3	1:E:228:THR:HG21	1.70	0.74
1:B:263:VAL:HG12	1:B:374:ARG:NH2	2.03	0.73
1:B:379:SER:H	1:B:413:THR:HB	1.53	0.73
1:E:304:ASN:HB3	1:E:374:ARG:HH12	1.53	0.73
1:A:425:ILE:C	1:A:426:TPO:HG22	2.07	0.73
2:C:140:ARG:HB3	2:C:140:ARG:NH1	2.01	0.73
1:F:20:LYS:HE2	1:F:228:THR:HG21	1.69	0.73
1:B:214:GLU:HB3	2:C:234:GLU:HB2	1.70	0.73
2:D:304:ASN:HB3	2:D:374:ARG:HH12	1.51	0.73
2:D:221:GLU:HG3	2:D:233:GLY:O	1.88	0.73
2:D:220:LEU:HD23	2:D:221:GLU:N	2.02	0.73
1:B:196:VAL:O	1:B:200:VAL:HG23	1.89	0.73
1:B:316:ALA:HA	1:B:378:ASP:HB3	1.70	0.73
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.68	0.73
2:D:497:ILE:O	2:D:497:ILE:HD12	1.89	0.73
2:C:296:LEU:HD21	2:C:477:PRO:HB3	1.70	0.73
2:C:232:LYS:N	2:C:232:LYS:HD2	2.02	0.73
1:B:458:MET:HB2	1:B:463:HIS:HD2	1.54	0.73
1:F:514:GLU:CD	1:F:515:LYS:H	1.92	0.72
1:B:21:MET:HB2	1:B:38:ILE:HG12	1.71	0.72
2:C:446:ARG:HG2	2:C:496:ARG:CZ	2.18	0.72
2:C:215:ARG:HA	2:C:215:ARG:NE	2.03	0.72
1:F:383:LEU:HD13	1:F:395:PHE:HE2	1.53	0.72
1:B:195:GLY:HA2	1:B:198:GLU:OE2	1.88	0.72
1:F:336:GLU:HB3	1:F:340:ARG:NH2	2.04	0.72
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.04	0.72
1:B:318:GLU:OE2	2:C:432:GLU:HB3	1.90	0.72
2:D:18:ILE:N	2:D:18:ILE:HD12	2.04	0.72
1:F:79:THR:HG23	1:F:81:GLN:H	1.54	0.72
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.53	0.72
1:B:503:SER:O	1:B:504:GLU:HB2	1.88	0.72
2:D:114:GLY:O	2:D:115:GLN:HG3	1.89	0.72
1:E:134:ILE:HG23	1:E:139:ALA:HB3	1.72	0.72
1:A:436:THR:CG2	1:A:458:MET:HG2	2.19	0.72
1:B:140:ARG:HH11	1:B:140:ARG:HB3	1.54	0.72
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.54	0.72
1:B:184:ARG:HD2	1:B:191:ILE:O	1.89	0.72
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.72	0.71
1:E:123:LEU:HD13	1:E:163:GLU:OE2	1.90	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:258:SER:OG	1:F:326:ARG:HD3	1.89	0.71
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.25	0.71
1:A:84:ILE:HG23	1:A:94:LEU:HB2	1.73	0.71
1:E:436:THR:HG23	1:E:458:MET:HG2	1.72	0.71
2:C:300:ARG:N	2:C:333:MET:HE1	2.06	0.71
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.72	0.71
1:F:497:ILE:O	1:F:497:ILE:HG13	1.88	0.71
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.91	0.71
1:A:447:GLY:HA2	1:B:489:ILE:CD1	2.20	0.71
1:F:191:ILE:HG13	1:F:206:ILE:CD1	2.18	0.71
1:E:344:LEU:HD22	1:E:345:LYS:N	2.06	0.71
1:B:84:ILE:HA	1:B:94:LEU:HD12	1.72	0.71
2:D:67:PHE:HB3	2:D:69:GLU:HG3	1.72	0.71
1:B:169:ALA:O	1:B:173:GLN:HG3	1.91	0.71
1:B:183:GLU:HB2	2:C:199:PHE:CE1	2.25	0.70
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.55	0.70
1:F:148:THR:HG21	1:F:193:ARG:HD2	1.73	0.70
2:D:64:ILE:HG21	2:D:97:LEU:HD13	1.71	0.70
2:C:146:SER:H	2:C:181:THR:HB	1.55	0.70
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.56	0.70
1:A:379:SER:N	1:A:413:THR:HB	2.02	0.70
1:B:191:ILE:HB	1:B:198:GLU:CD	2.12	0.70
2:C:483:PHE:HB2	2:C:489:ILE:HD13	1.74	0.70
1:A:126:LEU:O	1:A:130:ILE:HG13	1.92	0.70
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.73	0.70
2:C:293:GLY:HA2	3:C:901:ATP:O1A	1.90	0.70
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.22	0.70
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.06	0.70
1:B:341:GLN:O	1:B:343:LEU:HG	1.92	0.70
1:F:106:LEU:HD11	1:F:129:ARG:CZ	2.22	0.70
1:B:379:SER:HA	1:B:413:THR:O	1.92	0.69
1:A:44:VAL:HG22	1:A:205:VAL:HB	1.72	0.69
2:D:287:THR:HG21	2:D:425:ILE:O	1.92	0.69
2:C:41:SER:HB3	2:C:178:THR:HB	1.73	0.69
2:C:220:LEU:HD13	2:C:246:ILE:CD1	2.21	0.69
1:A:148:THR:OG1	1:A:182:THR:HG23	1.92	0.69
1:A:438:ILE:HD11	1:A:455:VAL:HG22	1.74	0.69
1:A:79:THR:HG23	1:A:80:PRO:HD2	1.74	0.69
1:F:325:LEU:HD23	1:F:335:PHE:HB2	1.74	0.69
2:D:21:MET:HE3	2:D:59:PHE:HZ	1.57	0.69
1:B:75:THR:O	1:B:108:ALA:HB3	1.92	0.69
1:F:78:GLU:HB3	1:F:83:ILE:HD11	1.75	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.05	0.69
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.23	0.69
1:A:65:ILE:O	1:A:65:ILE:HG22	1.92	0.69
1:F:336:GLU:HB3	1:F:340:ARG:HH21	1.57	0.69
2:C:50:THR:HG21	2:C:207:LEU:C	2.13	0.69
1:A:43:LEU:HD11	1:A:182:THR:OG1	1.92	0.69
2:C:269:ARG:O	2:C:273:MET:HG3	1.91	0.69
2:D:354:ALA:HB3	2:D:359:HIS:NE2	2.06	0.69
1:A:488:ARG:HE	1:F:488:ARG:HH12	1.41	0.69
1:B:161:ARG:NH2	1:B:199:PHE:HB2	2.07	0.69
1:A:487:GLU:OE1	1:F:495:THR:HA	1.92	0.69
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.57	0.69
1:B:426:TPO:O1P	1:B:430:ILE:N	2.26	0.69
2:D:64:ILE:HG22	2:D:65:ILE:HD13	1.75	0.69
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.56	0.68
2:C:451:ARG:NH1	2:C:451:ARG:HG2	2.08	0.68
1:B:56:SER:HB2	1:B:143:SER:HB3	1.75	0.68
1:F:49:GLY:O	1:F:218:ARG:NH2	2.26	0.68
2:C:214:GLU:OE2	2:D:217:ARG:NH1	2.26	0.68
1:B:194:TYR:O	1:B:196:VAL:HG23	1.93	0.68
2:D:56:SER:HB2	2:D:143:SER:HB3	1.75	0.68
2:D:387:VAL:HG12	2:D:388:SER:N	2.08	0.68
1:A:210:VAL:HG12	1:A:211:LEU:O	1.93	0.68
1:B:130:ILE:O	1:B:134:ILE:HG13	1.92	0.68
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.58	0.68
1:E:462:TRP:O	1:E:463:HIS:O	2.11	0.68
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.23	0.68
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.75	0.68
2:D:347:VAL:O	2:D:348:CYS:HB2	1.94	0.68
1:F:426:TPO:O1P	1:F:431:ALA:HB3	1.94	0.68
2:C:52:LYS:HD2	2:C:182:THR:O	1.93	0.68
1:F:516:GLY:N	1:F:517:PRO:HD2	2.08	0.68
1:A:371:LYS:O	1:A:371:LYS:HD2	1.92	0.68
1:F:266:GLY:HA3	1:F:300:ARG:HG3	1.76	0.68
2:C:308:ASN:O	2:C:310:GLU:HG3	1.92	0.68
2:C:488:ARG:HH22	2:D:488:ARG:HH21	1.41	0.68
1:E:281:ASP:O	1:E:282:SER:HB3	1.91	0.68
1:B:155:ASP:OD1	1:B:159:VAL:HG11	1.93	0.68
1:E:147:VAL:O	1:E:150:VAL:HG12	1.94	0.68
1:B:293:GLY:HA2	3:B:901:ATP:O1A	1.93	0.68
2:C:50:THR:HB	2:C:207:LEU:HB3	1.74	0.68
1:B:184:ARG:HH22	1:B:187:GLU:C	1.98	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:221:GLU:HG3	1:E:233:GLY:O	1.94	0.68
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.73	0.68
2:D:152:GLN:HG3	1:E:161:ARG:NH1	2.09	0.68
2:C:214:GLU:HB3	2:D:234:GLU:HB2	1.76	0.68
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.58	0.68
2:C:164:LEU:HD11	2:C:197:GLU:HG3	1.76	0.68
1:E:319:GLU:O	1:F:254:LEU:HD21	1.94	0.67
1:B:315:PHE:CE2	1:B:347:VAL:HG21	2.29	0.67
1:F:79:THR:HG22	1:F:82:ASP:H	1.58	0.67
1:F:47:THR:HG22	1:F:50:THR:CG2	2.24	0.67
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.75	0.67
1:F:170:ARG:HH22	1:F:174:ILE:HD11	1.57	0.67
1:F:353:SER:O	1:F:354:ALA:HB2	1.93	0.67
1:F:464:ASP:OD2	1:F:466:ALA:HB3	1.94	0.67
1:F:44:VAL:HG22	1:F:205:VAL:HB	1.76	0.67
3:E:901:ATP:H3'	1:F:458:MET:O	1.94	0.67
2:D:88:ARG:HD3	1:E:15:HIS:O	1.94	0.67
1:E:131:ASN:O	1:E:135:GLN:HB2	1.93	0.67
2:D:496:ARG:HG2	1:E:487:GLU:OE1	1.94	0.67
1:E:21:MET:HE1	1:E:141:ARG:HG2	1.76	0.67
2:D:220:LEU:HD13	2:D:246:ILE:CD1	2.25	0.67
1:B:326:ARG:HG3	2:C:260:ASN:ND2	2.10	0.67
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.59	0.67
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.76	0.67
2:C:488:ARG:NH2	2:D:488:ARG:HH21	1.93	0.67
1:E:304:ASN:HB3	1:E:374:ARG:NH1	2.10	0.67
2:D:89:SER:HB2	1:E:227:GLY:O	1.95	0.67
1:A:348:CYS:SG	1:B:254:LEU:HD23	2.35	0.67
1:B:129:ARG:O	1:B:132:TYR:HB3	1.95	0.67
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.77	0.67
1:E:309:LYS:HA	1:E:343:LEU:HD13	1.75	0.67
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.77	0.67
1:B:81:GLN:H	1:B:81:GLN:HE21	1.42	0.67
2:C:25:ILE:HG23	2:C:58:GLN:NE2	2.09	0.66
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.76	0.66
2:D:332:GLY:O	2:D:333:MET:HG2	1.94	0.66
1:E:289:ALA:CB	1:E:419:PHE:HA	2.25	0.66
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.59	0.66
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.59	0.66
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.78	0.66
1:F:338:MET:HB3	1:F:344:LEU:HB3	1.78	0.66
2:D:267:VAL:HG23	2:D:300:ARG:HG2	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:GLU:HG3	1:A:15:HIS:N	2.08	0.66
2:C:70:PRO:HD2	2:C:140:ARG:HG2	1.78	0.66
1:E:431:ALA:O	1:E:434:THR:HG22	1.94	0.66
1:B:246:ILE:O	1:B:248:PRO:HD3	1.95	0.66
1:A:274:CYS:HG	1:A:278:PHE:HE2	1.39	0.66
1:B:304:ASN:HB3	1:B:374:ARG:HH12	1.61	0.66
1:F:260:ASN:HA	1:F:279:PHE:HE2	1.61	0.66
1:E:94:LEU:O	1:E:98:VAL:HG23	1.96	0.66
3:C:903:ATP:HO2'	2:D:230:HIS:CE1	2.12	0.66
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.76	0.66
2:C:21:MET:HB2	2:C:38:ILE:HG13	1.78	0.66
1:E:194:TYR:O	1:E:196:VAL:N	2.29	0.66
1:F:197:GLU:N	1:F:197:GLU:OE2	2.25	0.66
1:E:305:ALA:HB2	1:E:374:ARG:CD	2.18	0.66
1:F:96:LYS:O	1:F:100:GLU:HG3	1.96	0.66
2:D:344:LEU:HD13	2:D:344:LEU:C	2.16	0.66
1:F:313:ILE:CG1	1:F:372:PRO:HG2	2.26	0.66
1:F:299:SER:CB	1:F:333:MET:HE1	2.25	0.66
1:E:313:ILE:HG22	1:E:314:LEU:N	2.10	0.66
2:D:221:GLU:HG3	2:D:233:GLY:C	2.16	0.66
1:A:45:SER:CB	1:A:182:THR:HB	2.26	0.66
2:D:178:THR:HG22	2:D:179:VAL:N	2.11	0.66
1:B:334:ASP:OD1	1:B:336:GLU:HB2	1.96	0.66
1:F:263:VAL:HG12	1:F:374:ARG:NH2	2.12	0.65
1:A:431:ALA:O	1:A:434:THR:HB	1.97	0.65
1:E:504:GLU:HG2	1:E:505:LEU:N	2.10	0.65
1:B:178:THR:HG22	1:B:179:VAL:H	1.60	0.65
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.31	0.65
1:F:118:VAL:HG22	1:F:122:ASP:OD1	1.96	0.65
2:C:221:GLU:HG3	2:C:233:GLY:O	1.96	0.65
1:A:191:ILE:N	1:A:191:ILE:HD12	2.11	0.65
1:F:144:ILE:HD13	1:F:167:LEU:HD21	1.79	0.65
1:A:14:GLU:HG3	1:A:16:GLN:OE1	1.96	0.65
1:F:377:ILE:CD1	1:F:399:VAL:HG11	2.26	0.65
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.24	0.65
2:C:202:ASP:HA	2:C:226:ARG:HD2	1.77	0.65
1:A:227:GLY:O	1:F:89:SER:HB2	1.96	0.65
2:C:52:LYS:N	3:C:903:ATP:O1B	2.29	0.65
1:E:446:ARG:HH21	1:E:496:ARG:HH22	1.45	0.65
1:E:225:LEU:HB2	1:E:230:HIS:HD2	1.61	0.65
1:F:370:PHE:HD2	1:F:372:PRO:HG3	1.61	0.65
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.31	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:123:LEU:O	1:E:127:ILE:HG13	1.96	0.65
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.79	0.65
1:E:142:VAL:HB	1:E:178:THR:HG23	1.77	0.65
1:F:313:ILE:HG13	1:F:372:PRO:CG	2.26	0.65
1:A:161:ARG:HD2	1:A:196:VAL:HG13	1.79	0.65
1:E:452:ALA:HA	1:E:469:GLU:HA	1.78	0.65
1:F:509:VAL:HG12	1:F:510:ARG:H	1.61	0.65
1:A:425:ILE:HG23	1:F:419:PHE:CE2	2.30	0.65
2:D:436:THR:CG2	2:D:458:MET:HG2	2.27	0.65
2:C:444:GLU:OE2	2:D:489:ILE:HG12	1.97	0.65
2:D:486:PHE:CE2	2:D:496:ARG:HD3	2.32	0.65
1:B:80:PRO:HA	1:B:83:ILE:HD13	1.79	0.65
1:F:46:GLY:HA2	1:F:184:ARG:HD2	1.79	0.65
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.61	0.65
1:A:426:TPO:O	1:A:427:ASP:HB2	1.97	0.64
1:E:212:GLU:HG2	1:E:212:GLU:O	1.96	0.64
1:A:31:ILE:HA	1:A:231:MET:SD	2.37	0.64
1:F:400:THR:HG21	1:F:433:ILE:CG2	2.27	0.64
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.12	0.64
2:D:194:TYR:O	2:D:196:VAL:HG23	1.96	0.64
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.33	0.64
1:E:451:ARG:HD2	1:E:451:ARG:H	1.62	0.64
1:E:367:ILE:HG12	1:E:375:ILE:HD11	1.79	0.64
1:F:452:ALA:HA	1:F:469:GLU:HA	1.79	0.64
1:A:164:LEU:HD11	1:A:197:GLU:HG3	1.79	0.64
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.10	0.64
2:D:225:LEU:HB2	2:D:230:HIS:HD2	1.62	0.64
2:D:225:LEU:HD12	2:D:230:HIS:HB3	1.80	0.64
1:A:273:MET:O	1:A:463:HIS:HA	1.97	0.64
1:B:147:VAL:HG11	1:B:180:MET:CE	2.27	0.64
1:A:327:ASN:HB3	5:A:531:HOH:O	1.96	0.64
1:E:425:ILE:HG22	1:E:425:ILE:O	1.97	0.64
1:E:24:MET:CE	1:E:24:MET:HA	2.26	0.64
1:E:393:ARG:O	1:E:397:ILE:HG12	1.96	0.64
2:D:267:VAL:HG22	2:D:300:ARG:HG2	1.79	0.64
1:A:130:ILE:O	1:A:134:ILE:HG13	1.97	0.64
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.79	0.64
1:E:427:ASP:O	1:E:428:SER:HB3	1.96	0.64
1:A:161:ARG:NH1	1:F:183:GLU:OE2	2.26	0.64
1:E:199:PHE:C	1:E:201:SER:H	2.01	0.64
1:B:191:ILE:HB	1:B:198:GLU:HG3	1.79	0.64
2:C:21:MET:HE1	2:C:141:ARG:HG2	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:123:LEU:O	1:B:123:LEU:HD13	1.98	0.64
2:C:25:ILE:CG1	2:C:58:GLN:HE21	2.07	0.64
1:A:436:THR:HG23	1:A:458:MET:HG2	1.80	0.64
1:A:488:ARG:HE	1:F:488:ARG:NH1	1.95	0.64
1:F:298:VAL:O	1:F:301:PHE:HB3	1.98	0.64
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.79	0.64
1:B:145:ASP:OD2	1:B:181:THR:HG21	1.98	0.64
2:D:18:ILE:CD1	2:D:18:ILE:H	2.11	0.64
1:A:27:GLY:O	1:A:30:ASP:HB2	1.98	0.63
1:A:356:LEU:HD11	1:A:387:VAL:HG21	1.80	0.63
2:C:17:ALA:C	2:C:18:ILE:HD12	2.19	0.63
1:B:151:PHE:C	1:B:153:GLN:H	2.02	0.63
1:B:426:TPO:O3P	1:B:426:TPO:O	2.16	0.63
1:E:294:LYS:N	3:E:901:ATP:O1B	2.30	0.63
1:F:458:MET:SD	1:F:461:SER:HB3	2.37	0.63
1:E:146:SER:H	1:E:181:THR:HB	1.61	0.63
1:E:332:GLY:O	1:E:333:MET:HG2	1.99	0.63
1:B:123:LEU:HD12	1:B:166:ARG:HD2	1.80	0.63
1:A:41:SER:HA	1:A:178:THR:O	1.98	0.63
1:F:293:GLY:HA2	3:F:901:ATP:O1A	1.98	0.63
1:E:18:ILE:HD11	1:E:227:GLY:CA	2.25	0.63
1:F:317:TYR:HA	1:F:349:ALA:O	1.97	0.63
2:C:380:LEU:HD11	2:C:412:PHE:HD2	1.63	0.63
1:F:453:ILE:HG12	1:F:454:ASN:H	1.63	0.63
1:A:166:ARG:HG3	1:F:112:PRO:O	1.97	0.63
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.62	0.63
1:E:458:MET:SD	1:E:461:SER:HB3	2.38	0.63
1:E:323:GLN:HG2	1:E:327:ASN:HD21	1.63	0.63
1:F:61:TYR:CZ	1:F:65:ILE:HG13	2.34	0.63
2:C:54:LEU:HD23	2:C:244:ILE:HG13	1.81	0.63
2:C:74:VAL:HG22	2:C:106:LEU:HD23	1.80	0.63
1:F:461:SER:OG	1:F:462:TRP:N	2.30	0.63
1:A:183:GLU:HB2	1:B:199:PHE:CZ	2.34	0.63
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.99	0.63
2:D:283:ILE:HG13	2:D:400:THR:HG23	1.79	0.63
1:A:231:MET:HB3	1:A:235:TYR:OH	1.99	0.63
2:C:344:LEU:HD22	2:C:345:LYS:N	2.13	0.63
1:B:192:ALA:O	1:B:194:TYR:N	2.32	0.63
2:D:496:ARG:HD2	5:D:546:HOH:O	1.97	0.63
1:F:315:PHE:CE1	1:F:375:ILE:HD11	2.34	0.63
1:A:360:LEU:O	1:A:360:LEU:HD22	1.98	0.63
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:88:ARG:HH11	1:B:88:ARG:HG2	1.64	0.63
1:A:442:TYR:HE1	1:B:456:PHE:CZ	2.17	0.62
1:F:247:PHE:HB3	1:F:249:LEU:CD2	2.29	0.62
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.34	0.62
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.81	0.62
2:D:379:SER:HA	2:D:413:THR:O	1.98	0.62
1:F:80:PRO:HG2	1:F:107:ASP:HB2	1.80	0.62
2:C:299:SER:C	2:C:333:MET:HE1	2.20	0.62
1:F:264:SER:O	1:F:374:ARG:NH2	2.31	0.62
2:C:316:ALA:O	2:C:348:CYS:HA	1.98	0.62
2:C:211:LEU:O	2:C:212:GLU:HB3	1.99	0.62
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.30	0.62
1:B:18:ILE:HB	1:B:228:THR:CG2	2.30	0.62
1:A:50:THR:CG2	1:A:209:ASN:HB2	2.28	0.62
1:F:168:VAL:HG12	1:F:169:ALA:N	2.14	0.62
1:E:294:LYS:HB3	1:E:413:THR:CG2	2.30	0.62
2:D:60:LEU:HD22	2:D:71:GLY:HA3	1.82	0.62
2:D:79:THR:HG22	2:D:82:ASP:OD2	2.00	0.62
1:F:445:ILE:HG13	1:F:483:PHE:HE2	1.63	0.62
1:F:147:VAL:O	1:F:150:VAL:HG12	2.00	0.62
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.81	0.62
2:D:196:VAL:O	2:D:200:VAL:HG23	1.99	0.62
2:C:25:ILE:HG23	2:C:58:GLN:HE22	1.64	0.62
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.30	0.62
1:E:301:PHE:HZ	1:E:409:THR:HG22	1.65	0.62
1:A:284:ILE:HD12	1:A:436:THR:HB	1.82	0.62
2:C:137:TYR:O	2:C:138:ARG:HB2	1.98	0.62
1:B:469:GLU:HB3	1:B:483:PHE:CZ	2.35	0.62
2:D:266:GLY:HA3	2:D:300:ARG:O	2.00	0.62
2:D:446:ARG:HB3	1:E:484:ARG:HG3	1.82	0.62
1:E:284:ILE:HB	1:E:411:LEU:HD12	1.82	0.62
2:C:46:GLY:HA2	2:C:184:ARG:HD2	1.79	0.62
1:B:36:LEU:HD12	1:B:59:PHE:CZ	2.35	0.62
1:B:315:PHE:CD2	1:B:347:VAL:HG21	2.34	0.62
1:A:356:LEU:HD23	1:A:395:PHE:HB2	1.80	0.62
1:E:52:LYS:HB3	1:E:181:THR:HG23	1.80	0.62
1:F:504:GLU:O	1:F:505:LEU:HB2	1.98	0.62
1:A:427:ASP:O	1:A:429:HIS:ND1	2.31	0.61
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.30	0.61
2:C:311:ARG:HD2	2:C:371:LYS:HE3	1.81	0.61
1:E:311:ARG:HD2	1:E:371:LYS:HE3	1.81	0.61
2:C:121:PHE:O	2:C:125:ALA:HB3	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:400:THR:HG21	1:A:433:ILE:HG22	1.82	0.61
2:C:41:SER:HA	2:C:178:THR:O	2.00	0.61
1:B:297:LEU:HD12	1:B:440:LEU:HD11	1.83	0.61
2:D:147:VAL:CG2	2:D:148:THR:N	2.63	0.61
1:B:220:LEU:HD13	1:B:246:ILE:CD1	2.30	0.61
2:C:87:ALA:C	2:C:89:SER:H	2.04	0.61
2:D:334:ASP:OD1	2:D:336:GLU:N	2.33	0.61
2:C:461:SER:OG	2:C:462:TRP:N	2.33	0.61
2:C:24:MET:HB2	2:C:62:ASN:ND2	2.15	0.61
1:B:31:ILE:HA	1:B:231:MET:SD	2.41	0.61
2:D:127:ILE:HG12	2:D:167:LEU:HD13	1.81	0.61
1:E:27:GLY:O	1:E:30:ASP:HB2	2.01	0.61
2:C:182:THR:CG2	2:C:183:GLU:H	2.11	0.61
2:C:267:VAL:HB	2:C:270:LEU:HB2	1.82	0.61
1:B:461:SER:OG	1:B:462:TRP:N	2.34	0.61
1:A:79:THR:HB	1:A:82:ASP:OD2	2.01	0.61
1:F:171:LEU:CD1	1:F:178:THR:HG21	2.31	0.61
1:E:184:ARG:HD2	1:E:191:ILE:O	2.01	0.61
2:C:98:VAL:HG13	2:C:103:LEU:O	2.01	0.61
1:E:38:ILE:HA	1:E:177:THR:HG23	1.81	0.61
2:D:80:PRO:HG2	2:D:107:ASP:HB2	1.82	0.61
2:D:273:MET:SD	2:D:468:ARG:HD2	2.39	0.61
2:C:347:VAL:O	2:C:348:CYS:HB2	1.99	0.61
1:A:24:MET:N	1:A:29:ASP:OD2	2.33	0.61
1:B:170:ARG:O	1:B:174:ILE:HG12	1.99	0.61
2:D:23:THR:HB	2:D:25:ILE:HG13	1.82	0.61
2:D:375:ILE:HG13	2:D:408:ILE:HG21	1.82	0.61
1:A:508:ILE:HD13	1:A:508:ILE:H	1.65	0.61
2:D:218:ARG:HG3	2:D:237:PHE:O	2.00	0.61
1:B:187:GLU:OE2	1:B:208:ARG:HA	2.01	0.61
1:A:45:SER:HB2	1:A:182:THR:HB	1.83	0.61
1:F:115:GLN:CG	1:F:116:GLU:H	2.13	0.61
1:F:363:ILE:O	1:F:367:ILE:HG13	2.00	0.61
1:F:313:ILE:CD1	1:F:372:PRO:HG2	2.31	0.61
1:E:469:GLU:HB3	1:E:483:PHE:CE1	2.36	0.61
2:D:123:LEU:O	2:D:127:ILE:HG13	2.00	0.61
1:E:93:ASP:OD1	1:E:95:ALA:HB3	2.01	0.61
1:E:31:ILE:HA	1:E:231:MET:HG3	1.83	0.61
1:B:112:PRO:O	2:C:166:ARG:HG3	2.01	0.61
2:C:170:ARG:O	2:C:174:ILE:HG12	2.01	0.61
1:F:484:ARG:HH11	1:F:484:ARG:HB3	1.66	0.61
2:C:283:ILE:HG13	2:C:400:THR:HG23	1.81	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:315:PHE:HA	2:C:347:VAL:HB	1.83	0.60
1:F:64:ILE:HG22	1:F:65:ILE:HD13	1.82	0.60
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.66	0.60
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.36	0.60
2:C:488:ARG:O	2:C:491:SER:HB3	2.01	0.60
1:B:326:ARG:HD3	2:C:259:SER:O	2.01	0.60
1:F:194:TYR:O	1:F:196:VAL:HG23	2.00	0.60
1:B:414:ASN:ND2	1:B:426:TPO:HG23	2.17	0.60
1:A:191:ILE:HB	1:A:198:GLU:CG	2.31	0.60
1:A:418:GLN:HB2	1:B:423:HIS:O	2.02	0.60
1:E:170:ARG:O	1:E:174:ILE:HG12	2.01	0.60
1:A:79:THR:HG22	1:A:81:GLN:HG2	1.83	0.60
2:C:315:PHE:HE2	2:C:363:ILE:HA	1.62	0.60
2:C:48:SER:HB2	2:D:199:PHE:CE1	2.36	0.60
1:B:311:ARG:HD2	1:B:371:LYS:HE3	1.84	0.60
1:A:52:LYS:HD2	1:A:181:THR:HG23	1.84	0.60
2:D:48:SER:HA	5:D:526:HOH:O	2.01	0.60
1:A:32:SER:OG	1:A:35:GLY:N	2.34	0.60
1:B:202:ASP:HA	1:B:226:ARG:HD2	1.82	0.60
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.36	0.60
2:C:156:ALA:O	2:C:160:VAL:HG23	2.01	0.60
2:D:380:LEU:N	2:D:413:THR:O	2.32	0.60
2:C:70:PRO:HG2	2:C:138:ARG:O	2.02	0.60
1:E:455:VAL:HG11	1:E:463:HIS:HB2	1.82	0.60
1:F:269:ARG:O	1:F:272:GLU:HB2	2.01	0.60
1:A:273:MET:O	1:A:464:ASP:N	2.30	0.60
2:C:393:ARG:NH2	2:C:429:HIS:HB2	2.17	0.60
1:E:52:LYS:HB3	1:E:181:THR:CG2	2.31	0.60
1:F:247:PHE:HB3	1:F:249:LEU:HD21	1.81	0.60
1:F:451:ARG:HH11	1:F:451:ARG:HG2	1.67	0.60
2:D:81:GLN:H	2:D:81:GLN:CD	2.05	0.60
2:D:163:GLU:HA	2:D:163:GLU:OE2	2.01	0.60
2:C:389:ASN:HD21	2:C:428:SER:HB2	1.67	0.60
1:E:283:ILE:HD12	1:E:412:PHE:HE1	1.66	0.60
1:F:248:PRO:C	1:F:250:GLY:H	2.06	0.60
1:F:260:ASN:HA	1:F:279:PHE:CE2	2.36	0.60
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.32	0.60
1:F:329:TYR:HA	1:F:332:GLY:O	2.01	0.60
1:B:294:LYS:HB3	1:B:413:THR:HG23	1.83	0.60
1:F:197:GLU:H	1:F:197:GLU:CD	2.03	0.60
1:E:153:GLN:C	1:F:158:SER:HB2	2.22	0.60
1:E:392:PHE:O	1:E:395:PHE:N	2.35	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:62:ASN:O	1:B:66:GLU:HB2	2.02	0.59
1:F:53:THR:OG1	1:F:145:ASP:OD1	2.20	0.59
1:A:230:HIS:CE1	1:A:232:LYS:HG3	2.37	0.59
1:A:147:VAL:HG11	1:A:180:MET:CE	2.32	0.59
2:C:464:ASP:OD1	2:C:466:ALA:N	2.35	0.59
2:C:386:GLY:HA2	2:D:390:ASN:HD21	1.66	0.59
1:E:164:LEU:HD11	1:E:197:GLU:HG3	1.85	0.59
1:A:446:ARG:HA	1:A:496:ARG:HH22	1.67	0.59
1:F:47:THR:CG2	1:F:50:THR:CG2	2.80	0.59
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.82	0.59
1:B:52:LYS:O	1:B:53:THR:C	2.41	0.59
1:F:82:ASP:HA	1:F:85:LYS:HB3	1.84	0.59
1:F:78:GLU:CB	1:F:83:ILE:HD11	2.32	0.59
1:B:31:ILE:HG23	1:B:231:MET:HB2	1.85	0.59
1:E:153:GLN:O	1:F:158:SER:HB2	2.02	0.59
2:C:358:ASP:O	2:C:362:ILE:HG12	2.02	0.59
1:A:448:GLU:HG2	1:B:466:ALA:HB2	1.84	0.59
1:F:311:ARG:HD2	1:F:371:LYS:CE	2.33	0.59
1:B:221:GLU:HG2	1:B:222:ILE:N	2.15	0.59
2:D:152:GLN:HG3	1:E:161:ARG:HH11	1.67	0.59
1:B:415:THR:HB	2:C:432:GLU:OE2	2.02	0.59
1:B:490:ILE:HG22	1:B:491:SER:N	2.18	0.59
1:E:467:ILE:O	1:E:467:ILE:HG22	2.02	0.59
1:B:123:LEU:O	1:B:127:ILE:HG13	2.02	0.59
2:D:155:ASP:OD1	2:D:159:VAL:HG11	2.01	0.59
1:A:469:GLU:HG3	1:A:470:PHE:N	2.18	0.59
1:E:267:VAL:HG21	1:E:477:PRO:HG3	1.85	0.59
1:B:50:THR:HB	1:B:207:LEU:CB	2.33	0.59
1:F:501:GLU:HG3	1:F:502:LYS:N	2.17	0.59
2:D:81:GLN:NE2	2:D:81:GLN:H	2.01	0.59
1:E:501:GLU:O	1:E:502:LYS:HG3	2.03	0.59
2:D:262:ARG:NH1	2:D:275:GLY:O	2.36	0.59
1:A:211:LEU:CG	1:A:212:GLU:H	2.08	0.59
1:B:148:THR:C	1:B:150:VAL:H	2.07	0.59
1:E:419:PHE:CE2	1:F:425:ILE:HG13	2.37	0.59
1:F:453:ILE:HG12	1:F:454:ASN:N	2.18	0.59
1:B:363:ILE:O	1:B:367:ILE:HG13	2.03	0.59
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.84	0.58
1:F:315:PHE:CE2	1:F:347:VAL:HG21	2.38	0.58
1:A:18:ILE:HD12	1:A:18:ILE:N	2.18	0.58
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.67	0.58
1:B:140:ARG:CB	1:B:140:ARG:HH11	2.15	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:184:ARG:NH2	1:E:187:GLU:O	2.36	0.58
1:E:385:ARG:HA	1:F:393:ARG:NH1	2.19	0.58
1:B:36:LEU:HD12	1:B:59:PHE:CE1	2.38	0.58
1:F:187:GLU:OE2	1:F:208:ARG:HA	2.03	0.58
2:D:86:ASN:O	2:D:88:ARG:N	2.36	0.58
1:E:342:ASN:O	1:E:343:LEU:HD23	2.02	0.58
1:B:185:ILE:N	1:B:185:ILE:HD13	2.19	0.58
1:F:370:PHE:C	1:F:372:PRO:HD3	2.23	0.58
1:F:294:LYS:HB3	1:F:413:THR:HG23	1.83	0.58
1:F:150:VAL:HG13	1:F:151:PHE:N	2.17	0.58
1:B:193:ARG:NH2	2:C:196:VAL:HG23	2.19	0.58
1:E:344:LEU:HD13	1:E:345:LYS:N	2.19	0.58
2:C:220:LEU:HD23	2:C:221:GLU:N	2.17	0.58
2:C:379:SER:H	2:C:413:THR:HB	1.68	0.58
1:F:220:LEU:C	1:F:220:LEU:HD23	2.23	0.58
1:A:286:ALA:HA	1:A:438:ILE:O	2.03	0.58
2:D:150:VAL:O	2:D:153:GLN:HG3	2.02	0.58
1:E:81:GLN:NE2	1:E:81:GLN:H	2.02	0.58
1:E:21:MET:HE3	1:E:141:ARG:NE	2.18	0.58
1:F:191:ILE:HB	1:F:198:GLU:CG	2.32	0.58
1:A:348:CYS:SG	1:B:254:LEU:CD2	2.91	0.58
1:E:420:MET:SD	1:F:490:ILE:HG13	2.44	0.58
2:C:185:ILE:HD13	2:C:185:ILE:N	2.19	0.58
1:B:150:VAL:O	1:B:153:GLN:HG3	2.04	0.58
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.69	0.58
1:E:492:GLY:O	1:E:494:PRO:HD3	2.03	0.58
1:A:85:LYS:HE3	1:B:18:ILE:HD13	1.85	0.58
2:C:311:ARG:HD3	2:C:370:PHE:O	2.04	0.58
1:B:341:GLN:O	1:B:342:ASN:C	2.41	0.58
2:C:106:LEU:CD2	2:C:130:ILE:HG12	2.34	0.58
2:C:493:SER:OG	2:D:488:ARG:HG2	2.04	0.58
1:E:311:ARG:HD2	1:E:371:LYS:CE	2.33	0.58
1:A:254:LEU:HG	1:F:320:SER:HA	1.86	0.58
2:C:344:LEU:HD11	2:C:346:ILE:HG13	1.85	0.58
1:E:126:LEU:O	1:E:130:ILE:HG13	2.04	0.58
1:F:248:PRO:O	1:F:250:GLY:N	2.36	0.58
2:D:83:ILE:HD12	2:D:83:ILE:H	1.67	0.58
2:D:312:ALA:O	2:D:344:LEU:HD22	2.04	0.58
1:B:462:TRP:O	1:B:463:HIS:O	2.21	0.58
1:E:33:HIS:HD2	1:E:230:HIS:HA	1.69	0.58
2:D:318:GLU:OE2	1:E:432:GLU:HB3	2.03	0.58
2:D:182:THR:HG22	2:D:183:GLU:N	2.18	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:323:GLN:HG2	1:E:327:ASN:ND2	2.19	0.58
2:D:21:MET:HE2	2:D:177:THR:HG21	1.86	0.58
2:D:21:MET:O	2:D:35:GLY:HA3	2.03	0.58
1:F:231:MET:CE	1:F:251:ALA:HB2	2.34	0.58
1:A:360:LEU:HD21	1:A:398:GLY:O	2.03	0.58
1:B:31:ILE:O	1:B:231:MET:HG3	2.04	0.58
2:D:367:ILE:HD11	2:D:375:ILE:CD1	2.34	0.58
1:E:200:VAL:O	1:E:200:VAL:HG12	2.04	0.58
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.69	0.58
2:C:486:PHE:CE2	2:C:496:ARG:HG2	2.39	0.58
1:B:24:MET:CB	1:B:62:ASN:HD22	2.17	0.58
1:F:353:SER:O	1:F:354:ALA:CB	2.51	0.58
2:C:38:ILE:H	2:C:38:ILE:HD12	1.68	0.58
2:D:147:VAL:HG11	2:D:180:MET:CE	2.32	0.57
2:C:265:SER:O	2:C:301:PHE:HA	2.04	0.57
2:C:147:VAL:O	2:C:150:VAL:HG12	2.04	0.57
1:B:81:GLN:H	1:B:81:GLN:NE2	2.01	0.57
1:A:316:ALA:O	1:A:348:CYS:HA	2.04	0.57
2:D:151:PHE:C	2:D:153:GLN:H	2.07	0.57
2:C:38:ILE:HG22	2:C:39:GLY:N	2.18	0.57
1:F:406:GLU:O	1:F:408:ILE:HG13	2.04	0.57
1:B:147:VAL:O	1:B:150:VAL:HG12	2.03	0.57
2:D:294:LYS:N	3:D:901:ATP:O1B	2.36	0.57
2:C:493:SER:OG	2:D:488:ARG:HA	2.05	0.57
1:A:274:CYS:SG	1:A:278:PHE:HE2	2.27	0.57
1:A:284:ILE:CD1	1:A:436:THR:HB	2.34	0.57
1:E:291:GLY:C	1:E:442:TYR:OH	2.42	0.57
1:A:152:GLN:HG3	1:B:161:ARG:HH11	1.70	0.57
2:C:71:GLY:O	2:C:104:PHE:N	2.37	0.57
2:C:182:THR:CG2	2:C:183:GLU:N	2.68	0.57
2:D:305:ALA:O	2:D:310:GLU:O	2.22	0.57
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.34	0.57
2:C:298:VAL:O	2:C:301:PHE:HB3	2.04	0.57
2:D:332:GLY:O	2:D:333:MET:O	2.22	0.57
1:E:132:TYR:HE2	1:E:136:LYS:HD2	1.69	0.57
2:C:497:ILE:HD12	2:C:497:ILE:O	2.04	0.57
2:D:225:LEU:HB2	2:D:230:HIS:CD2	2.40	0.57
1:F:311:ARG:HD2	1:F:371:LYS:HE3	1.86	0.57
2:C:70:PRO:HB2	2:C:139:ALA:CA	2.30	0.57
1:A:27:GLY:O	1:A:30:ASP:N	2.33	0.57
2:C:389:ASN:O	2:C:392:PHE:N	2.38	0.57
2:D:31:ILE:HA	2:D:231:MET:CG	2.35	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:23:THR:O	1:E:24:MET:HB2	2.04	0.57
2:D:214:GLU:HG2	1:E:234:GLU:OE1	2.04	0.57
1:F:435:ASP:OD1	1:F:459:ARG:NH1	2.37	0.57
1:B:191:ILE:N	1:B:191:ILE:HD12	2.20	0.57
2:C:294:LYS:O	2:C:298:VAL:HG23	2.04	0.57
2:C:296:LEU:CD2	2:C:477:PRO:HB3	2.35	0.57
1:B:436:THR:HA	1:B:457:LYS:O	2.04	0.57
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.40	0.57
1:F:379:SER:OG	1:F:382:ALA:HB2	2.04	0.57
1:F:515:LYS:HG3	1:F:516:GLY:N	2.14	0.57
1:F:344:LEU:HD13	1:F:344:LEU:C	2.25	0.57
2:D:295:THR:HA	2:D:298:VAL:CG2	2.35	0.57
2:C:149:SER:HB3	2:D:161:ARG:NH2	2.19	0.57
1:F:52:LYS:HB3	1:F:181:THR:HG23	1.86	0.57
1:A:191:ILE:HD13	1:A:198:GLU:OE2	2.04	0.57
1:A:70:PRO:HA	1:A:102:LYS:O	2.04	0.57
2:D:249:LEU:HD12	2:D:394:GLN:OE1	2.04	0.57
1:F:446:ARG:H	1:F:496:ARG:NH2	2.03	0.57
1:B:126:LEU:HD12	1:B:129:ARG:HD3	1.87	0.57
2:C:212:GLU:HG2	2:C:212:GLU:O	2.04	0.57
1:B:431:ALA:HA	1:B:434:THR:HG22	1.86	0.57
2:C:323:GLN:NE2	2:D:459:ARG:HD3	2.20	0.57
1:E:445:ILE:HG22	1:E:445:ILE:O	2.04	0.57
1:F:435:ASP:HA	1:F:459:ARG:HD2	1.87	0.57
1:E:287:THR:CG2	1:E:414:ASN:HD22	2.18	0.57
2:D:353:SER:O	2:D:354:ALA:HB2	2.05	0.57
1:A:458:MET:O	3:F:901:ATP:H3'	2.05	0.56
2:D:151:PHE:O	2:D:153:GLN:N	2.32	0.56
1:E:283:ILE:HD12	1:E:412:PHE:CE1	2.40	0.56
1:B:435:ASP:HA	1:B:459:ARG:HD2	1.87	0.56
2:C:231:MET:CE	2:C:251:ALA:HB2	2.35	0.56
1:A:299:SER:CB	1:A:333:MET:HE1	2.22	0.56
1:F:305:ALA:HB2	1:F:374:ARG:CD	2.28	0.56
1:B:294:LYS:N	3:B:901:ATP:O1B	2.38	0.56
1:B:36:LEU:HD22	1:B:42:THR:HG21	1.86	0.56
2:C:357:GLU:HG3	2:C:358:ASP:N	2.20	0.56
1:F:103:LEU:HD12	1:F:103:LEU:C	2.26	0.56
1:E:273:MET:SD	1:E:479:ILE:HD13	2.45	0.56
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.70	0.56
2:D:382:ALA:O	2:D:385:ARG:HG3	2.04	0.56
1:E:266:GLY:HA3	1:E:300:ARG:HG3	1.86	0.56
1:F:379:SER:H	1:F:413:THR:HB	1.70	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:444:GLU:OE1	1:F:489:ILE:HB	2.05	0.56
2:C:24:MET:CB	2:C:62:ASN:HD22	2.16	0.56
2:C:425:ILE:H	2:C:425:ILE:HD12	1.70	0.56
1:E:451:ARG:HD2	1:E:451:ARG:N	2.20	0.56
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.86	0.56
2:D:461:SER:OG	2:D:462:TRP:N	2.39	0.56
1:E:364:LYS:O	1:E:368:ASN:ND2	2.38	0.56
2:D:96:LYS:O	2:D:100:GLU:HG3	2.05	0.56
1:A:298:VAL:HG23	1:A:411:LEU:HD23	1.88	0.56
1:A:188:TYR:HE2	1:F:211:LEU:HD23	1.69	0.56
1:B:379:SER:N	1:B:413:THR:HB	2.21	0.56
2:C:488:ARG:HH22	2:D:488:ARG:NH2	2.03	0.56
1:A:191:ILE:HB	1:A:198:GLU:HG2	1.87	0.56
1:B:308:ASN:O	1:B:310:GLU:HG3	2.05	0.56
1:B:192:ALA:HB3	1:B:197:GLU:OE2	2.05	0.56
2:D:170:ARG:HH12	2:D:174:ILE:HD11	1.70	0.56
1:F:45:SER:HB3	1:F:182:THR:HB	1.87	0.56
2:C:404:LYS:C	2:C:406:GLU:H	2.09	0.56
1:F:426:TPO:C	1:F:428:SER:H	2.19	0.56
2:C:150:VAL:HG13	2:C:151:PHE:N	2.20	0.56
1:F:111:ASP:OD1	1:F:112:PRO:HD2	2.04	0.56
1:A:509:VAL:O	1:A:511:GLY:N	2.37	0.56
2:C:191:ILE:H	2:C:191:ILE:HD12	1.70	0.56
1:A:14:GLU:CG	1:A:15:HIS:N	2.66	0.56
1:B:150:VAL:CG1	1:B:151:PHE:N	2.69	0.56
1:B:150:VAL:HG13	1:B:151:PHE:N	2.20	0.56
2:C:315:PHE:HB3	2:C:317:TYR:HE1	1.69	0.56
1:B:117:VAL:O	1:B:117:VAL:HG12	2.06	0.56
1:B:347:VAL:O	1:B:348:CYS:HB2	2.06	0.56
1:B:334:ASP:O	1:B:338:MET:HG2	2.06	0.56
1:E:146:SER:HA	1:E:181:THR:O	2.06	0.56
2:C:261:VAL:CG1	2:C:262:ARG:H	2.16	0.56
1:E:379:SER:N	1:E:413:THR:HB	2.19	0.56
1:B:130:ILE:HG22	1:B:134:ILE:HD11	1.86	0.56
1:F:192:ALA:HB3	1:F:197:GLU:OE2	2.06	0.56
1:A:471:MET:CG	1:A:478:ASP:HB3	2.35	0.56
2:D:346:ILE:CG2	2:D:347:VAL:N	2.68	0.56
1:A:64:ILE:CD1	1:A:103:LEU:HB2	2.34	0.56
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.46	0.56
1:E:221:GLU:HG2	1:E:222:ILE:N	2.19	0.56
1:B:64:ILE:HG21	1:B:97:LEU:HD13	1.86	0.56
1:E:371:LYS:HD2	1:E:371:LYS:O	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:123:LEU:HG	1:B:163:GLU:HB3	1.87	0.56
1:A:219:THR:HA	1:A:235:TYR:O	2.06	0.56
1:B:502:LYS:HG3	1:B:504:GLU:O	2.06	0.56
2:C:20:LYS:C	2:C:38:ILE:HD11	2.27	0.56
2:D:468:ARG:HH11	2:D:468:ARG:HG2	1.71	0.56
1:F:484:ARG:HB3	1:F:484:ARG:NH1	2.19	0.56
1:F:396:VAL:HG11	1:F:430:ILE:HD12	1.88	0.55
1:F:514:GLU:O	1:F:515:LYS:HB2	2.05	0.55
1:F:439:LEU:HD23	1:F:454:ASN:HD22	1.71	0.55
2:D:294:LYS:HD3	2:D:294:LYS:H	1.71	0.55
1:A:254:LEU:HD23	1:F:348:CYS:SG	2.46	0.55
1:F:362:ILE:O	1:F:365:SER:HB3	2.06	0.55
2:D:350:TYR:CE1	1:E:254:LEU:HD13	2.42	0.55
2:C:471:MET:SD	2:C:478:ASP:HB3	2.46	0.55
1:A:318:GLU:OE2	1:B:432:GLU:HB3	2.05	0.55
1:E:417:ASP:OD2	1:F:429:HIS:CE1	2.60	0.55
1:F:191:ILE:HB	1:F:198:GLU:HG2	1.88	0.55
1:F:514:GLU:O	1:F:515:LYS:CB	2.53	0.55
1:B:237:PHE:HB2	1:B:246:ILE:HG12	1.88	0.55
1:B:486:PHE:CE2	1:B:496:ARG:HB2	2.41	0.55
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.46	0.55
1:B:325:LEU:O	1:B:328:ALA:HB3	2.06	0.55
1:E:311:ARG:HD3	1:E:370:PHE:CE1	2.40	0.55
1:A:426:TPO:O3P	1:A:426:TPO:CG2	2.55	0.55
1:A:344:LEU:C	1:A:344:LEU:HD13	2.26	0.55
1:E:167:LEU:HG	1:E:171:LEU:HD12	1.89	0.55
1:A:199:PHE:CZ	1:F:183:GLU:HB2	2.41	0.55
2:C:71:GLY:O	2:C:103:LEU:HA	2.05	0.55
1:F:45:SER:CB	1:F:182:THR:HB	2.37	0.55
2:C:63:GLY:HA3	2:C:141:ARG:CZ	2.36	0.55
1:A:483:PHE:HB2	1:A:489:ILE:CD1	2.36	0.55
1:F:408:ILE:O	1:F:408:ILE:HG22	2.06	0.55
2:C:191:ILE:HD12	2:C:191:ILE:N	2.21	0.55
2:D:334:ASP:O	2:D:338:MET:HG2	2.07	0.55
1:F:515:LYS:HB3	1:F:517:PRO:HD2	1.89	0.55
2:C:311:ARG:HA	2:C:343:LEU:O	2.06	0.55
2:C:142:VAL:O	2:C:178:THR:HA	2.07	0.55
2:D:358:ASP:O	2:D:361:GLN:N	2.40	0.55
1:F:323:GLN:HG2	1:F:327:ASN:HD21	1.71	0.55
1:A:414:ASN:ND2	1:A:426:TPO:HA	2.21	0.55
1:A:350:TYR:OH	1:B:254:LEU:HD13	2.07	0.55
2:D:220:LEU:HD13	2:D:246:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:170:ARG:HD2	1:E:173:GLN:OE1	2.07	0.55
1:A:362:ILE:O	1:A:366:GLU:HB2	2.07	0.55
1:A:317:TYR:HA	1:A:349:ALA:O	2.06	0.55
2:D:347:VAL:CG1	2:D:348:CYS:N	2.70	0.55
2:C:261:VAL:O	2:C:262:ARG:HG2	2.07	0.55
2:C:262:ARG:NH2	2:C:461:SER:HB2	2.22	0.55
1:A:52:LYS:HB3	1:A:181:THR:HG23	1.88	0.55
2:D:354:ALA:HB3	2:D:359:HIS:CE1	2.40	0.55
1:B:383:LEU:HD13	1:B:395:PHE:CE2	2.42	0.55
2:C:94:LEU:O	2:C:98:VAL:HG23	2.06	0.55
1:E:441:GLN:HE22	1:E:490:ILE:HA	1.71	0.55
1:B:284:ILE:CD1	1:B:436:THR:HB	2.37	0.55
1:F:508:ILE:HD12	1:F:508:ILE:H	1.71	0.55
2:C:217:ARG:O	2:C:217:ARG:HG3	2.06	0.55
2:D:387:VAL:CG1	2:D:388:SER:N	2.68	0.55
1:E:417:ASP:O	1:F:424:SER:HB3	2.06	0.55
2:C:252:MET:HE3	2:C:397:ILE:HG22	1.89	0.55
2:D:23:THR:O	2:D:24:MET:HB2	2.07	0.55
2:C:31:ILE:HG23	2:C:231:MET:HB2	1.89	0.55
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.22	0.55
1:B:291:GLY:HA3	1:B:442:TYR:OH	2.06	0.55
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.72	0.55
1:F:203:ASN:OD1	1:F:225:LEU:HA	2.06	0.55
2:D:315:PHE:HB3	2:D:317:TYR:HE1	1.72	0.54
1:A:211:LEU:O	1:A:212:GLU:CB	2.44	0.54
2:D:147:VAL:O	2:D:150:VAL:HG12	2.07	0.54
1:B:284:ILE:HD12	1:B:436:THR:HB	1.88	0.54
1:A:483:PHE:HB2	1:A:489:ILE:HD11	1.88	0.54
1:A:379:SER:O	1:A:382:ALA:HB3	2.08	0.54
1:F:183:GLU:HG3	1:F:193:ARG:HE	1.72	0.54
1:E:203:ASN:CB	1:E:225:LEU:HD23	2.29	0.54
1:E:451:ARG:CG	1:E:451:ARG:HH11	2.18	0.54
1:B:167:LEU:O	1:B:170:ARG:N	2.40	0.54
1:A:363:ILE:O	1:A:367:ILE:HG13	2.07	0.54
1:F:471:MET:O	1:F:471:MET:HE2	2.07	0.54
1:A:419:PHE:CD2	1:B:425:ILE:HD12	2.43	0.54
2:C:379:SER:HA	2:C:413:THR:O	2.07	0.54
1:E:54:LEU:HD13	1:E:90:PHE:CE1	2.42	0.54
1:E:294:LYS:CB	1:E:413:THR:HG23	2.37	0.54
1:F:397:ILE:CD1	1:F:433:ILE:HG12	2.38	0.54
2:D:399:VAL:O	2:D:400:THR:C	2.45	0.54
1:A:442:TYR:CE1	1:B:456:PHE:CZ	2.95	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:354:ALA:HB1	2:C:358:ASP:HB2	1.90	0.54
1:A:501:GLU:O	1:A:503:SER:N	2.39	0.54
1:E:290:THR:HG21	1:F:431:ALA:HB1	1.88	0.54
1:B:51:GLY:O	1:B:54:LEU:HB3	2.08	0.54
1:E:132:TYR:CE2	1:E:136:LYS:HD2	2.42	0.54
2:C:418:GLN:HB2	2:D:423:HIS:O	2.07	0.54
2:D:94:LEU:O	2:D:98:VAL:HG23	2.07	0.54
1:A:389:ASN:ND2	1:A:428:SER:HB2	2.23	0.54
1:A:87:ALA:HB1	1:A:92:TRP:CD1	2.42	0.54
2:D:31:ILE:HA	2:D:231:MET:HG3	1.89	0.54
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.88	0.54
1:F:418:GLN:NE2	1:F:421:GLY:O	2.40	0.54
1:E:499:VAL:HG12	1:E:499:VAL:O	2.07	0.54
2:C:462:TRP:O	2:C:463:HIS:O	2.26	0.54
1:B:451:ARG:N	1:B:451:ARG:HD2	2.23	0.54
1:F:436:THR:HG23	1:F:458:MET:HG2	1.89	0.54
2:C:426:THR:HG22	2:C:427:ASP:N	2.23	0.54
2:C:72:VAL:HG13	2:C:104:PHE:HD2	1.72	0.54
1:A:218:ARG:O	1:A:236:PRO:HA	2.07	0.54
2:D:273:MET:CE	2:D:468:ARG:HD2	2.37	0.54
1:B:121:PHE:HD1	1:B:121:PHE:H	1.54	0.54
2:D:313:ILE:HG12	2:D:345:LYS:HB3	1.89	0.54
1:F:426:TPO:HG21	1:F:429:HIS:CA	2.38	0.54
1:B:193:ARG:NH2	2:C:195:GLY:O	2.41	0.54
1:B:293:GLY:O	1:B:296:LEU:HB3	2.08	0.54
3:A:903:ATP:O3'	1:B:224:LYS:HA	2.07	0.54
1:F:78:GLU:HB3	1:F:83:ILE:CD1	2.38	0.54
1:B:131:ASN:HA	1:B:134:ILE:HD12	1.90	0.54
2:C:95:ALA:O	2:C:99:ASP:HB2	2.08	0.54
2:D:347:VAL:HG12	2:D:348:CYS:H	1.71	0.54
1:E:106:LEU:HD11	1:E:129:ARG:CZ	2.38	0.54
1:B:48:SER:OG	2:C:224:LYS:HD3	2.07	0.54
1:A:426:TPO:O3P	1:A:426:TPO:HG21	2.08	0.54
1:A:429:HIS:CD2	1:F:417:ASP:CG	2.81	0.54
1:B:25:ILE:CG1	1:B:58:GLN:HE21	2.12	0.54
1:E:447:GLY:HA2	1:F:467:ILE:HD12	1.90	0.54
2:C:87:ALA:O	2:C:89:SER:N	2.40	0.54
1:E:169:ALA:O	1:E:173:GLN:HG3	2.06	0.54
1:F:21:MET:HE3	1:F:59:PHE:CE1	2.43	0.54
1:F:163:GLU:OE2	1:F:163:GLU:HA	2.07	0.54
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.37	0.54
2:D:486:PHE:HE2	2:D:496:ARG:HD3	1.70	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:318:GLU:OE2	1:F:432:GLU:OE1	2.26	0.53
1:F:170:ARG:HD2	1:F:173:GLN:OE1	2.08	0.53
2:D:49:GLY:HA2	1:E:224:LYS:HB3	1.90	0.53
2:C:144:ILE:HG22	2:C:147:VAL:HG12	1.89	0.53
2:C:20:LYS:HE3	2:C:228:THR:HG21	1.91	0.53
2:D:178:THR:CG2	2:D:179:VAL:N	2.71	0.53
1:F:504:GLU:HA	1:F:507:ARG:HG3	1.89	0.53
1:B:287:THR:HG21	1:B:425:ILE:O	2.08	0.53
1:A:272:GLU:O	1:A:462:TRP:HZ3	1.91	0.53
1:E:435:ASP:N	1:E:435:ASP:OD1	2.41	0.53
2:D:370:PHE:O	2:D:371:LYS:HG3	2.08	0.53
1:F:486:PHE:CE2	1:F:496:ARG:HD2	2.43	0.53
1:E:504:GLU:CG	1:E:505:LEU:H	2.14	0.53
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.89	0.53
2:C:21:MET:HE3	2:C:141:ARG:CZ	2.39	0.53
2:C:38:ILE:HG23	2:C:177:THR:OG1	2.08	0.53
1:F:64:ILE:HG21	1:F:97:LEU:HD13	1.90	0.53
2:C:471:MET:HE2	2:C:478:ASP:H	1.72	0.53
1:F:256:GLN:HB3	1:F:405:GLN:HA	1.90	0.53
1:F:453:ILE:CG1	1:F:454:ASN:H	2.21	0.53
2:C:54:LEU:O	2:C:57:ILE:N	2.42	0.53
1:A:315:PHE:HE1	1:A:375:ILE:HG12	1.74	0.53
1:A:89:SER:HB2	1:B:227:GLY:O	2.08	0.53
1:E:67:PHE:O	1:E:69:GLU:HG3	2.09	0.53
2:C:218:ARG:HD2	5:C:526:HOH:O	2.08	0.53
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.39	0.53
1:E:194:TYR:O	1:E:196:VAL:HB	2.09	0.53
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.91	0.53
1:E:497:ILE:HG22	1:E:498:THR:N	2.21	0.53
2:C:310:GLU:O	2:C:343:LEU:HB3	2.08	0.53
1:F:52:LYS:HB3	1:F:181:THR:CG2	2.39	0.53
1:A:459:ARG:NH1	1:F:319:GLU:HG2	2.23	0.53
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.74	0.53
2:C:38:ILE:HG22	2:C:39:GLY:H	1.73	0.53
1:F:316:ALA:HB2	1:F:324:LEU:HD11	1.89	0.53
1:F:437:ILE:HD12	1:F:457:LYS:HG2	1.90	0.53
1:B:247:PHE:HZ	1:B:361:GLN:HG3	1.74	0.53
2:D:264:SER:HA	2:D:271:ASP:OD1	2.08	0.53
1:A:24:MET:CB	1:A:62:ASN:HD22	2.21	0.53
2:C:248:PRO:O	2:C:250:GLY:N	2.42	0.53
1:A:188:TYR:HE2	1:F:211:LEU:CD2	2.22	0.53
2:D:44:VAL:HG22	2:D:205:VAL:CB	2.39	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:47:THR:HG22	1:F:50:THR:HG22	1.89	0.53
1:F:44:VAL:O	1:F:181:THR:HA	2.08	0.53
2:D:443:VAL:HG13	2:D:494:PRO:HG2	1.89	0.53
2:C:386:GLY:CA	2:D:390:ASN:HD21	2.21	0.53
1:F:262:ARG:HD2	1:F:276:GLY:O	2.08	0.53
1:E:406:GLU:O	1:E:408:ILE:HG13	2.09	0.53
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.90	0.53
2:C:23:THR:O	2:C:24:MET:HB2	2.08	0.53
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.90	0.53
1:F:147:VAL:HG23	1:F:148:THR:N	2.24	0.53
1:E:262:ARG:HD2	1:E:276:GLY:O	2.09	0.53
1:F:118:VAL:O	1:F:118:VAL:HG13	2.08	0.53
1:E:220:LEU:HD13	1:E:246:ILE:HD11	1.91	0.53
2:C:170:ARG:HB3	2:C:170:ARG:NH1	2.24	0.53
2:C:248:PRO:O	2:C:251:ALA:N	2.42	0.53
1:B:286:ALA:HA	1:B:438:ILE:O	2.09	0.53
1:A:396:VAL:HG21	1:A:430:ILE:HD12	1.91	0.53
1:B:43:LEU:HD12	1:B:180:MET:HB2	1.92	0.53
2:C:71:GLY:N	2:C:102:LYS:O	2.41	0.53
1:A:375:ILE:O	1:A:410:GLY:HA2	2.09	0.53
1:F:451:ARG:HD2	1:F:451:ARG:N	2.24	0.53
2:D:451:ARG:H	2:D:451:ARG:HD2	1.74	0.53
1:E:303:GLU:OE2	1:E:333:MET:HB3	2.09	0.52
1:B:50:THR:HG21	1:B:207:LEU:O	2.09	0.52
2:D:52:LYS:HE3	5:D:550:HOH:O	2.07	0.52
2:C:426:THR:HG22	2:C:428:SER:H	1.73	0.52
1:E:313:ILE:HD12	1:E:372:PRO:HG2	1.90	0.52
2:C:151:PHE:C	2:C:153:GLN:H	2.12	0.52
2:C:334:ASP:O	2:C:338:MET:HG2	2.09	0.52
2:D:468:ARG:NH1	2:D:468:ARG:HG2	2.23	0.52
1:A:379:SER:HA	1:A:413:THR:O	2.09	0.52
1:F:127:ILE:CD1	1:F:167:LEU:HD12	2.39	0.52
1:F:514:GLU:OE1	1:F:515:LYS:N	2.42	0.52
1:E:497:ILE:O	1:E:498:THR:OG1	2.21	0.52
1:E:451:ARG:HG2	1:E:470:PHE:CE1	2.45	0.52
2:C:50:THR:HG21	2:C:207:LEU:O	2.08	0.52
1:A:251:ALA:O	1:A:252:MET:C	2.47	0.52
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.90	0.52
2:C:464:ASP:C	2:C:464:ASP:OD1	2.47	0.52
1:A:257:ARG:NH2	1:A:407:GLU:HG2	2.23	0.52
1:A:162:ARG:O	1:A:165:PHE:HB3	2.09	0.52
1:F:73:PHE:HE2	1:F:75:THR:HB	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:131:ASN:O	1:F:135:GLN:HB2	2.09	0.52
1:F:127:ILE:HD13	1:F:167:LEU:HD12	1.91	0.52
1:E:416:SER:C	1:E:418:GLN:H	2.12	0.52
1:B:316:ALA:O	1:B:348:CYS:HA	2.09	0.52
2:C:469:GLU:HG3	2:C:480:LYS:HE3	1.92	0.52
1:E:47:THR:HG23	5:E:527:HOH:O	2.09	0.52
1:F:94:LEU:O	1:F:98:VAL:HG23	2.10	0.52
1:A:296:LEU:HD13	1:A:331:TRP:CE2	2.45	0.52
1:E:266:GLY:HA2	1:E:304:ASN:ND2	2.15	0.52
1:A:436:THR:OG1	1:A:458:MET:HG2	2.08	0.52
1:F:436:THR:CG2	1:F:458:MET:HG2	2.39	0.52
1:B:385:ARG:NH1	2:C:397:ILE:HD11	2.24	0.52
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.90	0.52
2:C:123:LEU:CD2	2:C:167:LEU:HB2	2.40	0.52
2:C:323:GLN:HE22	2:D:459:ARG:HD3	1.75	0.52
2:D:74:VAL:HA	2:D:106:LEU:HB3	1.91	0.52
2:D:296:LEU:HD12	2:D:296:LEU:O	2.08	0.52
1:F:289:ALA:O	1:F:292:THR:HG23	2.09	0.52
1:F:150:VAL:CG1	1:F:151:PHE:N	2.72	0.52
1:B:497:ILE:HD12	1:B:498:THR:H	1.71	0.52
1:F:270:LEU:O	1:F:273:MET:N	2.42	0.52
2:D:183:GLU:HB2	1:E:199:PHE:CE1	2.44	0.52
2:C:395:PHE:O	2:C:399:VAL:HG23	2.09	0.52
2:C:98:VAL:HA	2:C:103:LEU:O	2.10	0.52
1:E:313:ILE:CG1	1:E:372:PRO:HG2	2.39	0.52
2:C:296:LEU:HD13	2:C:331:TRP:CE2	2.44	0.52
1:F:115:GLN:CG	1:F:116:GLU:N	2.72	0.52
1:F:418:GLN:HE21	1:F:421:GLY:C	2.13	0.52
2:D:313:ILE:HG21	2:D:315:PHE:CZ	2.44	0.52
2:C:42:THR:HG23	2:C:203:ASN:CB	2.40	0.52
1:E:346:ILE:HG22	1:E:348:CYS:SG	2.49	0.52
1:A:344:LEU:HD13	1:A:345:LYS:N	2.25	0.52
1:B:74:VAL:HG13	1:B:106:LEU:HG	1.90	0.52
2:C:14:GLU:OE2	2:C:16:GLN:HB2	2.10	0.52
1:A:199:PHE:CE1	1:F:183:GLU:HB2	2.44	0.52
2:C:363:ILE:O	2:C:367:ILE:HG13	2.10	0.52
1:A:371:LYS:N	1:A:372:PRO:HD3	2.24	0.52
2:C:174:ILE:HG22	2:C:174:ILE:O	2.10	0.52
1:B:320:SER:HB3	2:C:256:GLN:HG2	1.91	0.52
1:B:152:GLN:NE2	1:B:194:TYR:OH	2.43	0.52
1:A:44:VAL:HA	1:A:205:VAL:O	2.10	0.52
2:C:357:GLU:CG	2:C:358:ASP:N	2.73	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.45	0.52
1:E:255:THR:O	1:E:255:THR:HG22	2.08	0.52
2:D:371:LYS:CD	2:D:371:LYS:O	2.56	0.52
1:E:339:GLU:HG2	1:E:344:LEU:HD12	1.91	0.52
2:C:313:ILE:HG12	2:C:345:LYS:HB3	1.90	0.52
1:A:148:THR:HG1	1:A:182:THR:HG23	1.75	0.52
1:B:326:ARG:C	1:B:328:ALA:H	2.12	0.52
2:C:53:THR:HG23	2:C:145:ASP:OD1	2.10	0.52
2:D:206:ILE:HD11	2:D:223:LEU:HD12	1.92	0.52
1:A:385:ARG:HG2	1:B:393:ARG:CZ	2.40	0.52
1:F:379:SER:O	1:F:382:ALA:HB3	2.10	0.52
1:A:31:ILE:HG23	1:A:231:MET:HB2	1.92	0.52
1:A:147:VAL:HG11	1:A:180:MET:HE2	1.92	0.52
2:D:219:THR:HA	2:D:235:TYR:O	2.10	0.52
2:C:72:VAL:HG13	2:C:104:PHE:CD2	2.44	0.52
1:E:313:ILE:HG13	1:E:372:PRO:HG2	1.88	0.52
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.90	0.52
1:F:47:THR:N	1:F:50:THR:HG21	2.25	0.52
1:E:21:MET:O	1:E:35:GLY:HA3	2.10	0.52
1:A:230:HIS:HE1	1:A:232:LYS:HG3	1.74	0.52
2:C:56:SER:O	2:C:59:PHE:HB3	2.09	0.52
1:B:404:LYS:C	1:B:406:GLU:H	2.14	0.52
1:E:325:LEU:HD21	1:E:336:GLU:H	1.75	0.52
2:C:387:VAL:HG12	2:C:388:SER:O	2.10	0.52
2:C:140:ARG:CB	2:C:140:ARG:HH11	2.20	0.51
1:B:83:ILE:HD12	1:B:83:ILE:H	1.76	0.51
1:E:43:LEU:HD23	1:E:204:VAL:HG13	1.92	0.51
1:B:148:THR:O	1:B:150:VAL:N	2.42	0.51
1:F:302:VAL:HG12	1:F:303:GLU:N	2.25	0.51
1:E:199:PHE:O	1:E:201:SER:N	2.44	0.51
1:F:80:PRO:CG	1:F:107:ASP:HB2	2.40	0.51
2:C:50:THR:HB	2:C:207:LEU:CB	2.39	0.51
1:F:274:CYS:HG	1:F:278:PHE:HE2	1.57	0.51
2:C:419:PHE:O	2:C:420:MET:HB2	2.10	0.51
2:C:320:SER:HB3	2:D:256:GLN:HG2	1.92	0.51
1:B:220:LEU:HD13	1:B:246:ILE:HD11	1.91	0.51
2:C:60:LEU:O	2:C:61:TYR:C	2.47	0.51
1:F:20:LYS:CE	1:F:228:THR:HG21	2.39	0.51
1:F:20:LYS:HB3	1:F:35:GLY:O	2.09	0.51
1:B:418:GLN:HB2	2:C:423:HIS:O	2.10	0.51
2:C:32:SER:HB3	2:C:222:ILE:HD11	1.92	0.51
1:E:444:GLU:O	1:E:494:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:261:VAL:CG1	2:C:262:ARG:N	2.73	0.51
1:B:53:THR:HB	3:B:903:ATP:PA	2.50	0.51
1:E:321:ARG:HG2	1:E:348:CYS:SG	2.51	0.51
1:B:486:PHE:HE2	1:B:496:ARG:HB2	1.75	0.51
2:C:359:HIS:O	2:C:363:ILE:HG13	2.10	0.51
1:B:194:TYR:O	1:B:196:VAL:N	2.44	0.51
2:D:21:MET:HE3	2:D:59:PHE:CZ	2.41	0.51
1:B:65:ILE:HG22	1:B:65:ILE:O	2.10	0.51
1:F:207:LEU:HD21	1:F:220:LEU:HD12	1.91	0.51
1:A:317:TYR:CD2	1:A:349:ALA:O	2.63	0.51
1:B:321:ARG:NH1	5:B:535:HOH:O	2.44	0.51
1:E:56:SER:HB2	1:E:143:SER:HB3	1.91	0.51
2:D:164:LEU:CD1	2:D:197:GLU:HG3	2.41	0.51
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.92	0.51
1:B:237:PHE:CB	1:B:246:ILE:HG12	2.40	0.51
1:F:273:MET:O	1:F:463:HIS:HB2	2.10	0.51
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.93	0.51
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.91	0.51
1:B:360:LEU:C	1:B:360:LEU:HD13	2.31	0.51
1:E:335:PHE:HA	1:E:338:MET:HG3	1.91	0.51
1:B:72:VAL:HB	1:B:142:VAL:HG13	1.93	0.51
1:B:268:VAL:O	1:B:271:ASP:N	2.44	0.51
1:B:54:LEU:CD2	1:B:244:ILE:HG13	2.40	0.51
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.92	0.51
1:E:25:ILE:HG23	1:E:58:GLN:NE2	2.25	0.51
1:F:430:ILE:O	1:F:432:GLU:N	2.44	0.51
2:C:245:ASN:ND2	2:C:245:ASN:C	2.60	0.51
1:A:94:LEU:HD22	1:A:103:LEU:CD2	2.40	0.51
1:B:294:LYS:H	1:B:294:LYS:HD3	1.74	0.51
1:F:334:ASP:OD1	1:F:336:GLU:HB2	2.10	0.51
2:C:295:THR:HG22	2:C:331:TRP:CH2	2.46	0.51
1:B:39:GLY:H	1:B:177:THR:CB	2.24	0.51
1:A:164:LEU:HD11	1:A:197:GLU:CG	2.41	0.51
1:F:211:LEU:HD12	1:F:215:ARG:O	2.10	0.51
1:B:247:PHE:HE2	1:B:364:LYS:HD2	1.76	0.51
1:F:329:TYR:O	1:F:332:GLY:N	2.36	0.51
1:B:145:ASP:HA	1:B:181:THR:HB	1.92	0.51
2:D:67:PHE:O	2:D:68:ASP:HB3	2.11	0.51
1:E:453:ILE:HG22	1:E:470:PHE:HD2	1.76	0.51
1:B:65:ILE:O	1:B:66:GLU:HG2	2.11	0.51
1:A:164:LEU:CD1	1:A:197:GLU:HG3	2.39	0.51
2:D:323:GLN:O	2:D:326:ARG:HB3	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:TYR:CE1	1:B:92:TRP:HB2	2.45	0.51
2:C:90:PHE:CD1	2:C:90:PHE:N	2.78	0.51
1:E:97:LEU:N	1:E:97:LEU:HD23	2.25	0.51
1:E:265:SER:HB3	1:E:278:PHE:CZ	2.46	0.51
1:E:194:TYR:O	1:E:195:GLY:C	2.49	0.51
1:E:292:THR:N	1:E:442:TYR:OH	2.43	0.51
1:A:483:PHE:CD1	1:A:483:PHE:N	2.79	0.51
1:F:316:ALA:O	1:F:348:CYS:HA	2.11	0.51
2:D:393:ARG:O	2:D:397:ILE:HG12	2.11	0.51
1:F:149:SER:O	1:F:152:GLN:HB2	2.11	0.50
1:B:357:GLU:CG	1:B:358:ASP:N	2.74	0.50
1:F:38:ILE:H	1:F:38:ILE:HD12	1.76	0.50
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.41	0.50
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.76	0.50
1:A:21:MET:HE1	1:A:59:PHE:HZ	1.74	0.50
1:F:311:ARG:HG3	1:F:371:LYS:NZ	2.26	0.50
1:B:183:GLU:HG3	1:B:193:ARG:HD2	1.94	0.50
2:D:182:THR:CG2	2:D:183:GLU:N	2.74	0.50
1:B:197:GLU:O	1:B:200:VAL:N	2.39	0.50
2:D:64:ILE:CD1	2:D:97:LEU:HD13	2.41	0.50
1:A:52:LYS:HB2	3:A:903:ATP:O1B	2.11	0.50
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.45	0.50
1:F:505:LEU:O	1:F:506:SER:HB3	2.11	0.50
2:C:82:ASP:O	2:C:85:LYS:N	2.44	0.50
1:E:451:ARG:CG	1:E:451:ARG:NH1	2.72	0.50
1:B:79:THR:O	1:B:83:ILE:HD12	2.11	0.50
1:F:56:SER:O	1:F:59:PHE:HB3	2.11	0.50
1:A:131:ASN:HD21	1:A:135:GLN:NE2	2.09	0.50
2:D:184:ARG:HG2	2:D:191:ILE:O	2.11	0.50
1:F:370:PHE:HB3	1:F:372:PRO:HD3	1.94	0.50
1:B:193:ARG:NH1	5:B:525:HOH:O	2.44	0.50
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.31	0.50
1:F:486:PHE:HB2	1:F:489:ILE:HD11	1.94	0.50
1:F:515:LYS:CB	1:F:517:PRO:HD2	2.41	0.50
1:B:248:PRO:O	1:B:251:ALA:N	2.44	0.50
2:D:445:ILE:HA	2:D:496:ARG:HH12	1.75	0.50
1:A:359:HIS:O	1:A:363:ILE:HG13	2.11	0.50
1:B:287:THR:HG22	1:B:288:GLY:N	2.27	0.50
2:D:484:ARG:NH1	2:D:484:ARG:CB	2.75	0.50
2:D:152:GLN:HB3	1:E:161:ARG:HD3	1.93	0.50
1:E:425:ILE:HD12	1:E:456:PHE:CE2	2.45	0.50
1:E:441:GLN:HG3	1:E:441:GLN:O	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:39:GLY:N	2:D:177:THR:HG23	2.25	0.50
1:F:357:GLU:HG3	1:F:358:ASP:N	2.27	0.50
1:B:273:MET:O	1:B:464:ASP:N	2.45	0.50
1:B:53:THR:HA	1:B:145:ASP:OD1	2.11	0.50
1:B:146:SER:N	1:B:181:THR:HB	2.18	0.50
1:B:161:ARG:HH21	1:B:199:PHE:HB2	1.77	0.50
1:E:445:ILE:HG13	1:E:483:PHE:HE2	1.77	0.50
2:D:486:PHE:HB3	2:D:489:ILE:CD1	2.41	0.50
1:F:59:PHE:CE1	1:F:141:ARG:HD3	2.46	0.50
1:E:303:GLU:OE1	1:E:333:MET:HE3	2.11	0.50
2:C:263:VAL:HG12	2:C:374:ARG:HH21	1.77	0.50
1:E:61:TYR:CZ	1:E:92:TRP:CD1	3.00	0.50
1:E:323:GLN:CG	1:E:327:ASN:HD21	2.25	0.50
1:A:145:ASP:O	1:A:146:SER:OG	2.26	0.50
1:A:52:LYS:O	1:A:55:PHE:N	2.45	0.50
1:E:178:THR:HG22	1:E:179:VAL:N	2.27	0.50
1:F:103:LEU:HD12	1:F:104:PHE:N	2.27	0.50
1:A:326:ARG:HD3	1:B:258:SER:OG	2.11	0.50
2:C:49:GLY:O	2:C:218:ARG:NH2	2.45	0.50
1:B:426:TPO:O3P	1:B:426:TPO:C	2.60	0.50
1:E:313:ILE:CG2	1:E:314:LEU:N	2.75	0.50
2:D:425:ILE:HD11	2:D:456:PHE:CE2	2.47	0.50
2:C:54:LEU:O	2:C:56:SER:N	2.44	0.50
1:F:471:MET:HE3	1:F:472:ILE:C	2.32	0.50
2:D:451:ARG:N	2:D:451:ARG:HD2	2.27	0.50
1:B:232:LYS:H	1:B:232:LYS:HD2	1.77	0.50
1:E:303:GLU:OE2	1:E:333:MET:CB	2.60	0.50
2:D:222:ILE:CG2	2:D:225:LEU:HG	2.42	0.50
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.27	0.50
1:A:82:ASP:O	1:A:83:ILE:C	2.49	0.50
1:E:418:GLN:CB	1:F:423:HIS:O	2.57	0.50
2:D:270:LEU:HD23	2:D:270:LEU:O	2.12	0.50
1:F:467:ILE:HG22	1:F:467:ILE:O	2.12	0.50
2:C:193:ARG:NH2	2:D:199:PHE:HE2	2.10	0.50
2:D:425:ILE:HG22	2:D:426:THR:HG23	1.94	0.50
1:F:59:PHE:CZ	1:F:141:ARG:HD3	2.47	0.50
1:A:153:GLN:O	1:A:154:TYR:HB3	2.12	0.50
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.12	0.49
1:A:294:LYS:HB3	1:A:413:THR:HG23	1.94	0.49
1:A:183:GLU:OE2	1:B:161:ARG:NH2	2.44	0.49
1:B:182:THR:HG21	1:B:192:ALA:CB	2.37	0.49
1:E:262:ARG:HH12	1:E:461:SER:HB2	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:452:ALA:HA	2:C:469:GLU:HA	1.92	0.49
2:D:103:LEU:HD12	2:D:104:PHE:N	2.26	0.49
1:A:426:TPO:O2P	1:A:429:HIS:HA	2.11	0.49
1:F:294:LYS:N	3:F:901:ATP:O1B	2.46	0.49
1:F:516:GLY:N	1:F:517:PRO:CD	2.74	0.49
2:D:332:GLY:C	2:D:333:MET:HG2	2.33	0.49
1:F:360:LEU:HD13	1:F:360:LEU:C	2.32	0.49
2:D:82:ASP:O	2:D:83:ILE:C	2.49	0.49
2:C:87:ALA:HB1	2:C:92:TRP:CD1	2.47	0.49
2:D:191:ILE:HB	2:D:198:GLU:CG	2.41	0.49
1:E:299:SER:C	1:E:333:MET:HE1	2.33	0.49
1:F:52:LYS:HB2	3:F:903:ATP:O1B	2.13	0.49
1:F:298:VAL:HA	1:F:411:LEU:CD2	2.42	0.49
2:D:121:PHE:N	2:D:121:PHE:CD1	2.80	0.49
2:D:437:ILE:O	2:D:437:ILE:HG22	2.12	0.49
2:D:412:PHE:N	2:D:412:PHE:CD1	2.79	0.49
1:B:284:ILE:N	1:B:410:GLY:O	2.34	0.49
1:E:215:ARG:HD3	5:F:528:HOH:O	2.11	0.49
1:A:191:ILE:N	1:A:191:ILE:CD1	2.76	0.49
2:D:164:LEU:HD11	2:D:197:GLU:HG3	1.95	0.49
2:D:202:ASP:HA	2:D:226:ARG:HD2	1.94	0.49
1:E:386:GLY:O	1:E:387:VAL:O	2.30	0.49
2:C:295:THR:HB	3:C:901:ATP:O3A	2.12	0.49
2:C:469:GLU:HB3	2:C:483:PHE:CE1	2.47	0.49
2:C:217:ARG:CG	2:C:217:ARG:O	2.59	0.49
1:A:87:ALA:HB1	1:A:92:TRP:HD1	1.77	0.49
1:E:433:ILE:HD12	1:E:433:ILE:N	2.28	0.49
1:A:430:ILE:O	1:A:431:ALA:C	2.51	0.49
1:E:344:LEU:C	1:E:344:LEU:HD13	2.33	0.49
1:B:445:ILE:HD12	1:B:486:PHE:CE1	2.47	0.49
2:D:52:LYS:HD2	2:D:182:THR:O	2.13	0.49
2:C:311:ARG:CD	2:C:371:LYS:HE3	2.43	0.49
1:B:75:THR:HG21	1:B:78:GLU:O	2.12	0.49
2:C:21:MET:O	2:C:35:GLY:HA3	2.13	0.49
1:F:27:GLY:O	1:F:31:ILE:HG13	2.12	0.49
1:E:245:ASN:ND2	1:E:247:PHE:CE2	2.81	0.49
2:D:262:ARG:HD2	2:D:276:GLY:O	2.13	0.49
1:A:215:ARG:NH2	1:B:234:GLU:O	2.46	0.49
1:A:402:TYR:O	1:A:406:GLU:HB2	2.13	0.49
1:F:426:TPO:HG21	1:F:429:HIS:C	2.30	0.49
2:D:21:MET:CE	2:D:177:THR:HB	2.43	0.49
1:F:463:HIS:CE1	1:F:465:LYS:HD3	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:462:TRP:O	1:F:463:HIS:O	2.31	0.49
1:E:148:THR:CG2	1:E:193:ARG:HD2	2.43	0.49
1:A:371:LYS:O	1:A:371:LYS:CD	2.59	0.49
1:F:83:ILE:HD12	1:F:83:ILE:N	2.28	0.49
1:F:47:THR:HG23	1:F:48:SER:N	2.27	0.49
1:E:311:ARG:HD2	1:E:371:LYS:NZ	2.28	0.49
2:D:271:ASP:O	2:D:277:GLY:N	2.36	0.49
1:F:379:SER:HA	1:F:413:THR:O	2.12	0.49
2:C:215:ARG:HE	2:C:215:ARG:CA	2.11	0.49
1:A:199:PHE:HE2	1:F:193:ARG:NH2	2.11	0.49
2:C:197:GLU:CD	2:C:197:GLU:H	2.13	0.49
1:F:486:PHE:HE2	1:F:496:ARG:NH1	1.93	0.49
1:B:52:LYS:H	1:B:207:LEU:CD1	2.24	0.49
1:A:61:TYR:CZ	1:A:65:ILE:HG13	2.48	0.49
1:A:64:ILE:HG21	1:A:97:LEU:HD22	1.95	0.49
1:A:356:LEU:HB3	1:A:395:PHE:HD1	1.78	0.49
1:A:18:ILE:HD11	1:F:86:ASN:HA	1.94	0.49
1:B:317:TYR:CD2	1:B:383:LEU:HD21	2.48	0.49
1:E:54:LEU:HD13	1:E:90:PHE:CZ	2.48	0.49
2:D:264:SER:OG	2:D:265:SER:N	2.46	0.49
2:D:130:ILE:O	2:D:134:ILE:HG13	2.12	0.49
2:C:453:ILE:HG12	2:C:454:ASN:N	2.28	0.49
1:E:295:THR:O	1:E:298:VAL:HB	2.13	0.48
1:F:164:LEU:O	1:F:167:LEU:N	2.46	0.48
1:B:385:ARG:HD3	2:C:393:ARG:HD3	1.94	0.48
1:A:207:LEU:CD2	1:A:220:LEU:HD12	2.41	0.48
1:B:215:ARG:NH2	2:C:234:GLU:O	2.46	0.48
2:C:149:SER:HB3	2:D:161:ARG:CZ	2.43	0.48
1:F:31:ILE:CD1	1:F:246:ILE:HG21	2.43	0.48
2:D:60:LEU:O	2:D:61:TYR:C	2.52	0.48
2:C:121:PHE:N	2:C:121:PHE:CD1	2.81	0.48
1:A:357:GLU:HG3	1:A:358:ASP:N	2.28	0.48
2:C:73:PHE:HD1	2:C:143:SER:HB2	1.78	0.48
1:A:379:SER:OG	1:A:382:ALA:HB2	2.14	0.48
1:E:289:ALA:O	1:E:292:THR:HG23	2.13	0.48
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.43	0.48
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.94	0.48
1:A:483:PHE:HD1	1:A:483:PHE:H	1.60	0.48
1:E:167:LEU:O	1:E:171:LEU:HB2	2.12	0.48
2:D:268:VAL:O	2:D:271:ASP:HB2	2.13	0.48
3:C:903:ATP:O2'	2:D:230:HIS:CE1	2.65	0.48
1:B:32:SER:HB3	1:B:222:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:212:GLU:CG	2:D:212:GLU:O	2.58	0.48
1:F:20:LYS:HD3	1:F:35:GLY:O	2.13	0.48
1:B:127:ILE:HG22	1:B:127:ILE:O	2.12	0.48
1:A:448:GLU:HG2	1:B:466:ALA:CB	2.43	0.48
1:B:380:LEU:HB3	1:B:392:PHE:HZ	1.78	0.48
2:D:411:LEU:HD12	2:D:412:PHE:N	2.29	0.48
1:E:294:LYS:HG2	1:E:413:THR:HG23	1.93	0.48
2:C:396:VAL:HG11	2:C:430:ILE:CG2	2.43	0.48
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.49	0.48
1:E:32:SER:OG	1:E:35:GLY:N	2.45	0.48
2:D:314:LEU:O	2:D:314:LEU:HG	2.13	0.48
1:B:387:VAL:HG12	1:B:391:ALA:HB3	1.95	0.48
1:E:265:SER:O	1:E:301:PHE:HA	2.13	0.48
2:C:184:ARG:NH1	2:C:187:GLU:O	2.47	0.48
1:A:273:MET:HA	1:A:464:ASP:HB2	1.95	0.48
2:C:384:ALA:HB2	2:C:392:PHE:CZ	2.47	0.48
1:B:21:MET:CB	1:B:38:ILE:HG12	2.42	0.48
2:C:123:LEU:HD12	2:C:163:GLU:OE2	2.14	0.48
1:F:23:THR:O	1:F:24:MET:HB2	2.13	0.48
2:C:281:ASP:OD1	2:C:407:GLU:HA	2.14	0.48
1:A:104:PHE:HD2	1:A:133:ALA:HB1	1.79	0.48
2:C:304:ASN:HB3	2:C:374:ARG:HH12	1.77	0.48
1:B:25:ILE:CG1	1:B:58:GLN:NE2	2.75	0.48
1:A:161:ARG:HD3	1:F:152:GLN:HB3	1.95	0.48
1:B:146:SER:H	1:B:181:THR:CB	2.17	0.48
1:B:220:LEU:HD13	1:B:246:ILE:HD13	1.96	0.48
2:C:237:PHE:CB	2:C:246:ILE:HA	2.43	0.48
2:D:486:PHE:CB	2:D:489:ILE:HD11	2.43	0.48
1:F:16:GLN:NE2	1:F:33:HIS:HB3	2.27	0.48
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.49	0.48
1:A:426:TPO:O3P	1:A:431:ALA:HB2	2.14	0.48
1:B:197:GLU:CD	1:B:197:GLU:H	2.17	0.48
1:B:64:ILE:O	1:B:66:GLU:N	2.44	0.48
2:C:42:THR:HG22	2:C:43:LEU:N	2.28	0.48
2:C:42:THR:HG23	2:C:203:ASN:HB2	1.95	0.48
2:D:147:VAL:HG23	2:D:148:THR:N	2.29	0.48
1:F:273:MET:SD	1:F:468:ARG:HD2	2.53	0.48
1:E:308:ASN:O	1:E:309:LYS:HB2	2.14	0.48
1:E:311:ARG:HB3	1:E:370:PHE:CE2	2.49	0.48
1:F:154:TYR:HD1	1:F:154:TYR:O	1.97	0.48
1:A:366:GLU:HA	1:A:366:GLU:OE2	2.13	0.48
1:F:426:TPO:HG23	1:F:429:HIS:N	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:377:ILE:HD11	1:A:399:VAL:HG11	1.96	0.48
2:C:483:PHE:HB2	2:C:489:ILE:CD1	2.43	0.48
2:C:334:ASP:OD1	2:C:336:GLU:HB2	2.14	0.48
2:C:123:LEU:O	2:C:127:ILE:HG13	2.14	0.48
2:D:269:ARG:O	2:D:272:GLU:HB2	2.13	0.48
2:C:53:THR:HG22	2:C:53:THR:O	2.14	0.48
2:C:419:PHE:O	2:C:419:PHE:CG	2.67	0.48
1:A:306:CYS:SG	1:A:338:MET:SD	3.12	0.48
1:A:426:TPO:O	1:A:427:ASP:CB	2.60	0.48
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.44	0.48
1:F:191:ILE:HB	1:F:198:GLU:CD	2.33	0.48
1:A:458:MET:HB2	1:A:463:HIS:HD2	1.78	0.48
1:B:273:MET:O	1:B:463:HIS:CA	2.52	0.48
1:B:52:LYS:HB2	3:B:903:ATP:O1B	2.14	0.48
1:A:90:PHE:HB2	1:A:92:TRP:NE1	2.29	0.48
2:D:484:ARG:NH1	2:D:484:ARG:HB2	2.28	0.48
2:D:380:LEU:O	2:D:382:ALA:N	2.47	0.47
1:B:183:GLU:HB2	2:C:199:PHE:CZ	2.48	0.47
1:B:211:LEU:HD13	1:B:216:ARG:NE	2.28	0.47
2:C:246:ILE:HG22	2:C:247:PHE:N	2.28	0.47
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.37	0.47
1:A:220:LEU:C	1:A:220:LEU:HD23	2.34	0.47
1:B:371:LYS:O	1:B:371:LYS:CD	2.62	0.47
1:E:31:ILE:HA	1:E:231:MET:CG	2.43	0.47
1:B:437:ILE:HD12	1:B:457:LYS:HG2	1.96	0.47
2:C:353:SER:O	2:C:354:ALA:HB2	2.14	0.47
1:E:362:ILE:O	1:E:365:SER:HB3	2.14	0.47
1:B:87:ALA:C	1:B:89:SER:H	2.18	0.47
2:C:340:ARG:O	2:C:342:ASN:N	2.47	0.47
3:E:903:ATP:O3'	1:F:224:LYS:HB2	2.14	0.47
1:F:263:VAL:CG1	1:F:374:ARG:NH2	2.69	0.47
1:F:296:LEU:HD13	1:F:331:TRP:CE2	2.49	0.47
2:C:389:ASN:O	2:C:390:ASN:C	2.52	0.47
1:B:323:GLN:HG3	1:B:326:ARG:NH2	2.30	0.47
1:E:183:GLU:OE2	1:F:161:ARG:NH1	2.40	0.47
1:F:504:GLU:HA	1:F:507:ARG:HE	1.80	0.47
2:C:256:GLN:HG3	2:C:404:LYS:HD3	1.96	0.47
1:B:304:ASN:HB3	1:B:374:ARG:NH1	2.26	0.47
1:B:148:THR:HG21	1:B:193:ARG:HD2	1.95	0.47
1:B:269:ARG:O	1:B:273:MET:HG3	2.13	0.47
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.79	0.47
1:E:199:PHE:C	1:E:201:SER:N	2.66	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:344:LEU:HD13	2:C:345:LYS:N	2.28	0.47
2:D:67:PHE:CB	2:D:69:GLU:HG3	2.41	0.47
2:D:25:ILE:HG23	2:D:58:GLN:NE2	2.29	0.47
1:E:160:VAL:HG21	1:E:194:TYR:CD2	2.48	0.47
1:E:446:ARG:HE	1:E:496:ARG:HH22	1.62	0.47
2:C:54:LEU:O	2:C:55:PHE:C	2.52	0.47
1:A:332:GLY:O	1:A:333:MET:O	2.32	0.47
1:B:264:SER:HA	1:B:271:ASP:OD1	2.14	0.47
1:F:312:ALA:HA	1:F:374:ARG:O	2.15	0.47
1:A:393:ARG:NH1	1:F:385:ARG:HA	2.30	0.47
1:B:51:GLY:O	1:B:52:LYS:C	2.53	0.47
1:E:294:LYS:CB	3:E:901:ATP:O1B	2.57	0.47
2:C:64:ILE:HG12	2:C:69:GLU:O	2.14	0.47
1:E:313:ILE:CG1	1:E:372:PRO:CG	2.89	0.47
1:F:79:THR:HG22	1:F:82:ASP:OD2	2.14	0.47
1:E:53:THR:O	1:E:54:LEU:C	2.52	0.47
2:D:484:ARG:HH11	2:D:484:ARG:CB	2.28	0.47
2:C:340:ARG:C	2:C:342:ASN:N	2.68	0.47
1:B:148:THR:HA	1:B:151:PHE:CE1	2.49	0.47
1:F:446:ARG:H	1:F:496:ARG:HH22	1.63	0.47
1:E:356:LEU:CD2	1:E:392:PHE:HA	2.44	0.47
1:B:32:SER:OG	1:B:35:GLY:HA2	2.15	0.47
1:F:334:ASP:O	1:F:338:MET:HG2	2.14	0.47
1:E:446:ARG:HE	1:E:496:ARG:NH2	2.13	0.47
1:B:326:ARG:O	1:B:328:ALA:N	2.48	0.47
1:F:65:ILE:HD11	1:F:97:LEU:HD11	1.97	0.47
2:C:248:PRO:HB2	2:C:251:ALA:HB3	1.96	0.47
1:E:404:LYS:C	1:E:406:GLU:H	2.17	0.47
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.28	0.47
2:D:431:ALA:O	2:D:434:THR:HG23	2.15	0.47
1:E:352:GLU:H	1:E:352:GLU:CD	2.17	0.47
2:D:383:LEU:HD13	2:D:395:PHE:CE2	2.49	0.47
1:A:211:LEU:CG	1:A:212:GLU:N	2.78	0.47
2:C:197:GLU:OE2	2:C:197:GLU:N	2.26	0.47
2:D:151:PHE:CE1	2:D:160:VAL:HG13	2.50	0.47
1:E:469:GLU:HB3	1:E:483:PHE:CZ	2.49	0.47
1:B:315:PHE:HE1	1:B:375:ILE:HD11	1.80	0.47
2:D:21:MET:HE1	2:D:177:THR:HB	1.96	0.47
1:E:31:ILE:HG22	1:E:222:ILE:CD1	2.45	0.47
1:E:21:MET:HB2	1:E:38:ILE:HG12	1.97	0.47
1:E:371:LYS:CD	1:E:371:LYS:O	2.63	0.47
1:A:420:MET:CE	1:B:490:ILE:HG21	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:72:VAL:HG23	1:B:139:ALA:CB	2.45	0.47
1:B:63:GLY:HA3	1:B:141:ARG:HD2	1.97	0.47
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.96	0.47
1:B:344:LEU:C	1:B:344:LEU:HD13	2.35	0.47
1:A:320:SER:O	1:A:324:LEU:HG	2.15	0.47
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.47	0.47
1:B:284:ILE:HG23	1:B:436:THR:HB	1.97	0.47
1:F:31:ILE:HD11	1:F:246:ILE:HG21	1.96	0.47
1:A:418:GLN:CB	1:B:423:HIS:O	2.63	0.47
1:B:119:GLY:C	1:B:121:PHE:H	2.18	0.47
1:A:104:PHE:C	1:A:104:PHE:CD1	2.86	0.47
1:F:371:LYS:N	1:F:372:PRO:HD3	2.29	0.47
1:E:313:ILE:CD1	1:E:372:PRO:CG	2.91	0.47
1:E:58:GLN:HG2	1:E:62:ASN:ND2	2.30	0.47
2:D:44:VAL:HA	2:D:205:VAL:O	2.15	0.47
1:F:325:LEU:CD2	1:F:335:PHE:HB2	2.44	0.47
1:F:76:PHE:O	1:F:109:SER:HA	2.15	0.47
1:E:183:GLU:H	1:E:183:GLU:HG2	1.56	0.47
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.97	0.47
1:B:283:ILE:HD13	1:B:410:GLY:HA3	1.96	0.47
1:B:240:THR:HG21	1:B:361:GLN:HE22	1.79	0.47
1:A:498:THR:O	1:A:499:VAL:C	2.54	0.47
2:D:30:ASP:N	2:D:30:ASP:OD2	2.48	0.47
1:E:417:ASP:HB2	1:E:427:ASP:OD2	2.14	0.47
1:A:382:ALA:O	1:A:385:ARG:HG3	2.15	0.47
1:A:273:MET:HE3	1:A:468:ARG:HD2	1.97	0.47
1:F:486:PHE:HD2	1:F:494:PRO:HB2	1.80	0.47
1:A:266:GLY:C	1:A:300:ARG:HG3	2.35	0.47
1:E:61:TYR:C	1:E:63:GLY:N	2.66	0.47
1:F:115:GLN:HG3	1:F:116:GLU:N	2.29	0.47
1:F:315:PHE:HE1	1:F:375:ILE:HD11	1.76	0.47
1:F:98:VAL:HA	1:F:103:LEU:O	2.15	0.47
2:D:106:LEU:HD11	2:D:129:ARG:HH21	1.80	0.47
1:E:264:SER:O	1:E:374:ARG:NH2	2.48	0.46
2:C:299:SER:C	2:C:333:MET:CE	2.82	0.46
2:D:328:ALA:O	2:D:332:GLY:O	2.34	0.46
1:A:229:SER:O	1:A:230:HIS:HB3	2.14	0.46
1:E:246:ILE:HG22	1:E:247:PHE:N	2.29	0.46
1:F:484:ARG:CB	1:F:484:ARG:NH1	2.78	0.46
1:F:211:LEU:O	1:F:212:GLU:HB3	2.15	0.46
2:C:191:ILE:H	2:C:191:ILE:CD1	2.28	0.46
2:D:316:ALA:O	2:D:348:CYS:HA	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:148:THR:C	1:B:150:VAL:N	2.68	0.46
1:B:455:VAL:HG11	1:B:463:HIS:HB2	1.96	0.46
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.97	0.46
1:A:451:ARG:H	1:A:451:ARG:HD2	1.75	0.46
1:F:453:ILE:CG1	1:F:454:ASN:N	2.77	0.46
2:C:315:PHE:CZ	2:C:363:ILE:HG23	2.51	0.46
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.45	0.46
2:D:445:ILE:O	2:D:446:ARG:HB2	2.15	0.46
1:F:204:VAL:HG23	1:F:224:LYS:HG2	1.98	0.46
2:C:111:ASP:O	2:C:113:GLU:N	2.43	0.46
1:A:440:LEU:HA	1:A:452:ALA:O	2.15	0.46
1:B:290:THR:O	1:B:442:TYR:HE1	1.99	0.46
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.48	0.46
2:D:58:GLN:OE1	2:D:92:TRP:HH2	1.99	0.46
1:A:162:ARG:HH11	1:A:162:ARG:HG3	1.80	0.46
2:D:121:PHE:O	2:D:124:SER:OG	2.26	0.46
1:F:356:LEU:HD13	1:F:387:VAL:HG21	1.98	0.46
1:A:121:PHE:HD1	1:A:122:ASP:N	2.14	0.46
1:A:426:TPO:HG21	1:A:431:ALA:H	1.80	0.46
1:A:283:ILE:HD12	1:A:412:PHE:CE1	2.51	0.46
1:F:144:ILE:HG21	1:F:147:VAL:HG12	1.97	0.46
2:D:436:THR:HA	2:D:457:LYS:O	2.16	0.46
2:D:492:GLY:O	2:D:494:PRO:HD3	2.16	0.46
2:D:90:PHE:CD1	2:D:90:PHE:N	2.83	0.46
1:F:29:ASP:O	1:F:34:GLY:N	2.45	0.46
2:D:313:ILE:HD11	2:D:370:PHE:HB3	1.96	0.46
1:A:237:PHE:HB3	1:A:246:ILE:HG12	1.96	0.46
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.97	0.46
1:E:24:MET:HB2	1:E:62:ASN:HB3	1.98	0.46
1:F:20:LYS:C	1:F:38:ILE:CD1	2.84	0.46
1:A:51:GLY:O	1:A:52:LYS:C	2.54	0.46
1:F:218:ARG:HG3	1:F:237:PHE:O	2.14	0.46
1:F:47:THR:HB	5:F:523:HOH:O	2.15	0.46
1:F:146:SER:H	1:F:181:THR:HB	1.79	0.46
1:F:247:PHE:CE1	1:F:360:LEU:HD12	2.51	0.46
1:E:27:GLY:HA3	1:E:246:ILE:HB	1.97	0.46
2:C:123:LEU:HD11	2:C:163:GLU:HA	1.97	0.46
2:C:53:THR:HG21	2:C:78:GLU:OE2	2.15	0.46
1:E:186:GLU:OE1	1:E:189:GLY:N	2.48	0.46
1:E:211:LEU:CD1	1:E:216:ARG:HG2	2.45	0.46
2:D:37:PRO:HD2	2:D:203:ASN:ND2	2.31	0.46
1:B:428:SER:O	1:B:429:HIS:HB2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:396:VAL:HG11	2:C:430:ILE:HG23	1.96	0.46
1:E:382:ALA:O	1:E:385:ARG:CG	2.59	0.46
1:B:371:LYS:N	1:B:372:PRO:HD3	2.30	0.46
2:D:324:LEU:C	2:D:326:ARG:H	2.18	0.46
2:C:88:ARG:NH2	2:D:15:HIS:ND1	2.64	0.46
2:C:448:GLU:HA	2:D:466:ALA:HA	1.98	0.46
1:A:96:LYS:O	1:A:100:GLU:HG3	2.14	0.46
1:B:44:VAL:HG22	1:B:205:VAL:HG11	1.98	0.46
2:D:346:ILE:HG22	2:D:347:VAL:N	2.29	0.46
2:D:222:ILE:HG21	2:D:225:LEU:HG	1.97	0.46
1:F:425:ILE:HG21	1:F:439:LEU:HD13	1.98	0.46
2:D:49:GLY:O	2:D:218:ARG:NH2	2.48	0.46
1:E:326:ARG:O	1:E:328:ALA:N	2.48	0.46
2:C:232:LYS:N	2:C:232:LYS:CD	2.76	0.46
1:F:266:GLY:HA3	1:F:300:ARG:O	2.16	0.46
1:F:231:MET:SD	1:F:251:ALA:HB2	2.55	0.46
1:A:227:GLY:O	1:F:89:SER:CB	2.64	0.46
1:F:451:ARG:NH1	1:F:451:ARG:HG2	2.30	0.46
2:C:404:LYS:O	2:C:406:GLU:N	2.49	0.46
1:E:332:GLY:O	1:E:333:MET:O	2.33	0.46
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.98	0.46
1:E:392:PHE:O	1:E:395:PHE:HB3	2.16	0.46
2:D:193:ARG:HH11	2:D:193:ARG:HG2	1.80	0.46
1:E:296:LEU:HD13	1:E:331:TRP:CE2	2.51	0.46
1:B:194:TYR:C	1:B:196:VAL:N	2.68	0.46
1:E:446:ARG:NH2	1:E:496:ARG:HH22	2.11	0.46
1:A:129:ARG:O	1:A:132:TYR:HB3	2.15	0.46
2:D:358:ASP:O	2:D:360:LEU:N	2.49	0.46
1:B:65:ILE:HD11	1:B:97:LEU:HD11	1.98	0.46
2:D:420:MET:HE3	2:D:492:GLY:O	2.15	0.46
1:B:245:ASN:ND2	1:B:247:PHE:CZ	2.84	0.46
1:A:302:VAL:HG12	1:A:303:GLU:N	2.30	0.46
1:E:218:ARG:NH1	1:E:239:ILE:HD12	2.31	0.46
1:A:429:HIS:CD2	1:F:417:ASP:OD2	2.68	0.46
1:A:332:GLY:O	1:A:333:MET:C	2.54	0.46
1:B:211:LEU:O	1:B:212:GLU:HB3	2.15	0.46
2:C:311:ARG:HH11	2:C:371:LYS:HG3	1.81	0.46
1:B:191:ILE:CB	1:B:198:GLU:HG3	2.46	0.46
1:E:453:ILE:CG2	1:E:470:PHE:HD2	2.28	0.46
2:C:96:LYS:O	2:C:99:ASP:N	2.49	0.46
1:E:377:ILE:HG22	1:E:377:ILE:O	2.14	0.46
1:A:161:ARG:NH1	1:F:152:GLN:HG3	2.30	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:18:ILE:HB	1:B:228:THR:HG23	1.96	0.46
1:E:191:ILE:HG21	1:E:198:GLU:HG3	1.98	0.46
2:C:469:GLU:CG	2:C:480:LYS:HE3	2.46	0.46
2:D:38:ILE:HG23	2:D:39:GLY:N	2.31	0.46
1:B:166:ARG:O	1:B:170:ARG:HG2	2.16	0.46
1:F:367:ILE:HD11	1:F:375:ILE:CD1	2.46	0.46
1:A:21:MET:CE	1:A:59:PHE:HZ	2.28	0.46
2:D:396:VAL:HG11	2:D:430:ILE:HG21	1.98	0.46
1:B:162:ARG:NH1	1:B:162:ARG:HB2	2.31	0.46
1:A:200:VAL:HG12	1:A:200:VAL:O	2.16	0.46
1:A:396:VAL:O	1:A:397:ILE:C	2.55	0.45
1:E:197:GLU:O	1:E:199:PHE:N	2.49	0.45
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.98	0.45
1:E:367:ILE:HG22	1:E:367:ILE:O	2.16	0.45
2:C:440:LEU:CD2	2:C:453:ILE:HG13	2.46	0.45
1:F:426:TPO:HG23	1:F:430:ILE:H	1.70	0.45
1:A:266:GLY:O	1:A:300:ARG:HG3	2.16	0.45
2:C:335:PHE:HA	2:C:338:MET:HG3	1.99	0.45
1:F:298:VAL:HA	1:F:411:LEU:HD23	1.98	0.45
1:A:442:TYR:HE1	1:B:456:PHE:CE2	2.34	0.45
2:C:211:LEU:O	2:C:212:GLU:CB	2.64	0.45
2:D:94:LEU:HD23	2:D:94:LEU:N	2.31	0.45
2:C:435:ASP:HA	2:C:459:ARG:HD2	1.97	0.45
2:D:317:TYR:CD2	2:D:383:LEU:HD21	2.50	0.45
2:D:315:PHE:HA	2:D:347:VAL:HB	1.98	0.45
1:F:294:LYS:O	1:F:295:THR:C	2.54	0.45
1:F:514:GLU:HG2	1:F:519:SER:HB3	1.98	0.45
1:E:416:SER:O	1:E:418:GLN:N	2.49	0.45
2:C:64:ILE:HG22	2:C:65:ILE:HD13	1.97	0.45
2:D:67:PHE:HD1	2:D:141:ARG:NH2	2.14	0.45
1:F:161:ARG:NH2	1:F:199:PHE:HB2	2.32	0.45
2:D:471:MET:CG	2:D:478:ASP:HB3	2.46	0.45
2:C:123:LEU:HD11	2:C:163:GLU:O	2.16	0.45
1:A:188:TYR:CE2	1:F:211:LEU:HD23	2.50	0.45
1:F:256:GLN:HG2	1:F:256:GLN:H	1.58	0.45
1:B:93:ASP:OD1	1:B:95:ALA:HB3	2.16	0.45
1:E:118:VAL:O	1:E:118:VAL:HG12	2.17	0.45
1:F:379:SER:CB	1:F:382:ALA:HB2	2.46	0.45
1:E:350:TYR:CE1	1:F:254:LEU:HD13	2.51	0.45
1:B:151:PHE:O	1:B:153:GLN:N	2.45	0.45
1:F:170:ARG:HB3	1:F:170:ARG:NH1	2.32	0.45
1:A:61:TYR:CE1	1:A:97:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:220:LEU:HD13	2:D:246:ILE:HD13	1.97	0.45
1:F:367:ILE:O	1:F:367:ILE:HG22	2.16	0.45
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.97	0.45
2:D:406:GLU:HB3	2:D:408:ILE:HG13	1.98	0.45
2:C:191:ILE:HB	2:C:198:GLU:CG	2.47	0.45
1:F:418:GLN:O	1:F:418:GLN:HG3	2.17	0.45
1:B:247:PHE:CE2	1:B:364:LYS:HD2	2.51	0.45
2:C:116:GLU:C	2:C:118:VAL:H	2.20	0.45
1:B:71:GLY:O	1:B:103:LEU:HA	2.17	0.45
1:F:293:GLY:O	1:F:296:LEU:HB3	2.17	0.45
1:B:20:LYS:HG2	1:B:35:GLY:O	2.16	0.45
1:A:28:PHE:H	1:A:246:ILE:HD12	1.82	0.45
2:C:392:PHE:O	2:C:395:PHE:HB3	2.15	0.45
1:B:311:ARG:HA	1:B:343:LEU:O	2.17	0.45
1:B:311:ARG:HG2	1:B:343:LEU:HA	1.98	0.45
2:C:87:ALA:C	2:C:89:SER:N	2.70	0.45
1:A:165:PHE:CE2	1:F:110:PRO:HB2	2.52	0.45
1:B:74:VAL:HB	1:B:144:ILE:HG23	1.98	0.45
1:B:70:PRO:HA	1:B:102:LYS:O	2.17	0.45
1:F:430:ILE:HG22	1:F:430:ILE:O	2.16	0.45
1:F:127:ILE:CD1	1:F:167:LEU:HA	2.31	0.45
1:B:216:ARG:NE	2:C:221:GLU:OE1	2.41	0.45
1:F:170:ARG:HH12	1:F:174:ILE:CG1	2.19	0.45
2:C:287:THR:HG22	2:C:288:GLY:N	2.32	0.45
2:D:358:ASP:O	2:D:359:HIS:C	2.54	0.45
1:E:21:MET:CE	1:E:141:ARG:HG2	2.46	0.45
1:F:504:GLU:HA	1:F:507:ARG:CG	2.47	0.45
1:A:254:LEU:HD11	5:F:535:HOH:O	2.15	0.45
1:F:73:PHE:C	1:F:73:PHE:CD2	2.90	0.45
2:C:126:LEU:O	2:C:129:ARG:N	2.50	0.45
2:C:381:SER:C	2:C:383:LEU:N	2.70	0.45
1:F:420:MET:HE2	1:F:492:GLY:HA3	1.99	0.45
2:D:203:ASN:HB3	2:D:225:LEU:HD23	1.98	0.45
1:B:305:ALA:CB	1:B:374:ARG:HD2	2.29	0.45
1:B:458:MET:HB2	1:B:463:HIS:CD2	2.43	0.45
1:E:386:GLY:O	1:E:387:VAL:C	2.55	0.45
1:A:267:VAL:CG1	1:A:270:LEU:HB2	2.47	0.45
1:B:371:LYS:O	1:B:371:LYS:HD2	2.16	0.45
1:A:45:SER:HB3	1:A:182:THR:HB	1.96	0.45
1:E:281:ASP:O	1:E:282:SER:CB	2.63	0.45
1:F:384:ALA:HB2	1:F:392:PHE:CE1	2.51	0.45
2:C:382:ALA:O	2:C:385:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:426:TPO:OG1	1:A:427:ASP:N	2.50	0.45
2:C:46:GLY:HA2	2:C:184:ARG:CD	2.47	0.45
1:E:33:HIS:HD2	1:E:230:HIS:CA	2.30	0.45
1:A:80:PRO:HB3	1:A:105:ILE:HG21	1.99	0.45
2:D:152:GLN:CB	1:E:161:ARG:HD3	2.45	0.45
2:C:312:ALA:N	2:C:343:LEU:O	2.43	0.45
1:E:84:ILE:O	1:E:85:LYS:C	2.54	0.45
1:B:283:ILE:HD12	1:B:412:PHE:CE1	2.52	0.45
1:E:247:PHE:HZ	1:E:361:GLN:HG3	1.82	0.45
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.98	0.45
1:B:359:HIS:O	1:B:360:LEU:C	2.56	0.45
1:A:21:MET:HE2	1:A:177:THR:HG21	1.99	0.45
1:B:232:LYS:N	1:B:232:LYS:HD2	2.32	0.45
1:B:274:CYS:HG	1:B:278:PHE:HE2	1.62	0.45
1:A:425:ILE:O	1:A:425:ILE:HG13	2.15	0.45
2:D:387:VAL:CG1	2:D:388:SER:H	2.29	0.45
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.47	0.45
1:B:216:ARG:HH21	2:C:221:GLU:CD	2.19	0.45
2:D:52:LYS:N	3:D:903:ATP:O1B	2.47	0.45
1:A:52:LYS:HB3	1:A:181:THR:CG2	2.46	0.45
2:C:54:LEU:HD23	2:C:244:ILE:CG1	2.45	0.45
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.99	0.45
1:A:290:THR:O	1:A:290:THR:HG23	2.17	0.45
2:C:360:LEU:HD23	2:C:360:LEU:O	2.16	0.45
2:D:334:ASP:OD1	2:D:334:ASP:C	2.55	0.45
1:E:301:PHE:O	1:E:374:ARG:NH1	2.49	0.45
1:F:426:TPO:HG21	1:F:429:HIS:HA	1.99	0.45
2:C:263:VAL:HG12	2:C:374:ARG:NH2	2.32	0.45
1:A:273:MET:O	1:A:463:HIS:CA	2.64	0.45
1:F:332:GLY:O	1:F:333:MET:O	2.35	0.45
1:E:323:GLN:NE2	1:F:459:ARG:CD	2.78	0.45
1:B:335:PHE:O	1:B:336:GLU:C	2.56	0.45
1:E:52:LYS:O	1:E:55:PHE:HB3	2.16	0.45
1:A:167:LEU:O	1:A:168:VAL:C	2.56	0.45
1:F:361:GLN:O	1:F:362:ILE:C	2.56	0.45
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.47	0.45
1:F:252:MET:CE	1:F:401:GLY:HA3	2.46	0.45
1:A:293:GLY:HA2	3:A:901:ATP:O1A	2.16	0.45
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.81	0.44
1:E:18:ILE:CD1	1:E:227:GLY:HA3	2.31	0.44
1:E:46:GLY:HA2	1:E:184:ARG:HD3	1.99	0.44
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:295:THR:HB	3:C:901:ATP:PA	2.57	0.44
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.44	0.44
1:E:150:VAL:HG13	1:E:151:PHE:N	2.32	0.44
1:B:326:ARG:C	1:B:328:ALA:N	2.71	0.44
1:F:61:TYR:O	1:F:64:ILE:HB	2.17	0.44
2:D:484:ARG:HH11	2:D:484:ARG:HB3	1.82	0.44
2:C:468:ARG:HA	2:C:481:ASP:O	2.17	0.44
1:F:351:PRO:HD2	1:F:352:GLU:OE1	2.17	0.44
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.98	0.44
1:A:247:PHE:O	1:A:249:LEU:N	2.50	0.44
2:D:99:ASP:HA	5:D:545:HOH:O	2.17	0.44
1:B:393:ARG:O	1:B:397:ILE:HG12	2.17	0.44
1:B:451:ARG:HG2	1:B:451:ARG:NH1	2.27	0.44
2:D:64:ILE:HD12	2:D:97:LEU:HD13	1.99	0.44
1:A:356:LEU:N	1:A:356:LEU:HD12	2.32	0.44
1:A:184:ARG:NH2	1:A:186:GLU:O	2.50	0.44
1:A:344:LEU:HD11	1:A:346:ILE:HG13	1.97	0.44
1:A:154:TYR:HD1	1:A:154:TYR:O	2.00	0.44
1:A:430:ILE:O	1:A:432:GLU:N	2.51	0.44
1:E:266:GLY:CA	1:E:300:ARG:HG3	2.47	0.44
1:E:193:ARG:NH2	1:F:195:GLY:O	2.48	0.44
1:A:52:LYS:HD3	1:A:182:THR:O	2.17	0.44
1:F:160:VAL:HG21	1:F:194:TYR:CD2	2.51	0.44
1:E:375:ILE:O	1:E:410:GLY:HA2	2.16	0.44
2:D:402:TYR:O	2:D:406:GLU:HB2	2.18	0.44
2:D:140:ARG:HB3	2:D:140:ARG:NH1	2.31	0.44
1:F:382:ALA:O	1:F:385:ARG:HG3	2.17	0.44
2:C:315:PHE:HB3	2:C:317:TYR:CE1	2.50	0.44
2:C:295:THR:HG22	2:C:331:TRP:HH2	1.83	0.44
2:D:64:ILE:HD12	2:D:97:LEU:CD1	2.48	0.44
1:F:269:ARG:HG2	1:F:479:ILE:CG2	2.47	0.44
1:B:106:LEU:O	1:B:107:ASP:C	2.55	0.44
1:E:211:LEU:HA	1:E:211:LEU:HD12	1.72	0.44
2:D:315:PHE:CE2	2:D:347:VAL:HG21	2.52	0.44
1:A:351:PRO:CG	1:A:382:ALA:O	2.66	0.44
1:B:464:ASP:OD2	1:B:468:ARG:NE	2.50	0.44
2:C:220:LEU:C	2:C:220:LEU:HD23	2.38	0.44
1:B:182:THR:CG2	1:B:192:ALA:HB1	2.43	0.44
2:C:72:VAL:HA	2:C:104:PHE:O	2.18	0.44
1:B:357:GLU:HG3	1:B:358:ASP:N	2.33	0.44
1:B:418:GLN:HG3	1:B:418:GLN:O	2.17	0.44
1:A:56:SER:O	1:A:59:PHE:HB3	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:191:ILE:HB	2:D:198:GLU:HG2	1.97	0.44
2:D:302:VAL:HG21	2:D:314:LEU:HB2	1.99	0.44
1:F:380:LEU:C	1:F:382:ALA:N	2.71	0.44
1:F:148:THR:HG21	1:F:183:GLU:CG	2.48	0.44
1:F:486:PHE:CE2	1:F:496:ARG:CD	3.00	0.44
1:F:303:GLU:CD	1:F:333:MET:HB3	2.38	0.44
1:A:82:ASP:O	1:A:85:LYS:N	2.51	0.44
3:D:901:ATP:O2'	1:E:463:HIS:NE2	2.46	0.44
1:F:65:ILE:HG22	1:F:65:ILE:O	2.17	0.44
2:D:272:GLU:O	2:D:275:GLY:N	2.45	0.44
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.52	0.44
1:A:189:GLY:O	1:A:190:PRO:C	2.56	0.44
1:A:118:VAL:HG23	1:A:118:VAL:O	2.18	0.44
1:A:221:GLU:HG2	1:A:222:ILE:N	2.32	0.44
1:B:237:PHE:C	1:B:237:PHE:CD1	2.90	0.44
2:C:396:VAL:O	2:C:400:THR:HB	2.17	0.44
1:B:480:LYS:HB3	1:B:481:ASP:H	1.62	0.44
1:B:86:ASN:HD21	2:C:40:ARG:HH22	1.64	0.44
2:C:111:ASP:OD2	2:C:113:GLU:HG2	2.18	0.44
1:A:492:GLY:O	1:A:494:PRO:HD3	2.17	0.44
1:A:458:MET:HB2	1:A:463:HIS:CD2	2.53	0.44
1:A:194:TYR:O	1:A:196:VAL:HG23	2.18	0.44
1:B:151:PHE:C	1:B:153:GLN:N	2.68	0.44
1:B:452:ALA:HA	1:B:469:GLU:HA	2.00	0.44
2:D:52:LYS:HE3	2:D:52:LYS:HB2	1.84	0.44
1:E:192:ALA:HB3	1:E:197:GLU:OE2	2.18	0.44
1:F:79:THR:CG2	1:F:82:ASP:H	2.26	0.44
2:C:21:MET:HB2	2:C:38:ILE:CG1	2.47	0.44
1:B:171:LEU:HA	1:B:174:ILE:HG12	2.00	0.44
1:A:166:ARG:O	1:A:167:LEU:C	2.56	0.44
1:F:61:TYR:CE2	1:F:65:ILE:HG13	2.53	0.44
1:B:88:ARG:HG2	1:B:88:ARG:NH1	2.31	0.44
1:A:322:ALA:HB3	1:B:256:GLN:O	2.18	0.44
1:E:468:ARG:HG2	1:E:468:ARG:HH11	1.83	0.44
1:F:380:LEU:C	1:F:382:ALA:H	2.19	0.44
2:D:150:VAL:CG1	2:D:151:PHE:N	2.81	0.44
1:B:54:LEU:HD13	1:B:90:PHE:CE1	2.53	0.44
1:F:142:VAL:HB	1:F:178:THR:CG2	2.41	0.44
1:E:24:MET:CE	1:E:24:MET:CA	2.92	0.44
1:F:20:LYS:C	1:F:38:ILE:HD11	2.39	0.44
1:F:38:ILE:N	1:F:38:ILE:HD12	2.32	0.44
1:A:311:ARG:HA	1:A:343:LEU:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:397:ILE:O	1:E:401:GLY:N	2.35	0.44
2:C:86:ASN:O	2:C:87:ALA:C	2.56	0.44
1:B:44:VAL:HG22	1:B:205:VAL:CG1	2.47	0.44
2:C:80:PRO:HB3	2:C:105:ILE:HG21	1.99	0.44
1:A:163:GLU:HA	1:A:163:GLU:OE2	2.18	0.44
1:E:386:GLY:HA2	1:F:390:ASN:OD1	2.18	0.43
1:B:414:ASN:ND2	1:B:426:TPO:CG2	2.81	0.43
1:E:294:LYS:CG	1:E:413:THR:HG23	2.48	0.43
2:D:52:LYS:CD	2:D:182:THR:O	2.66	0.43
2:C:294:LYS:HB2	3:C:901:ATP:O1B	2.17	0.43
2:C:232:LYS:H	2:C:232:LYS:HD2	1.80	0.43
1:E:123:LEU:HD21	1:E:166:ARG:HG2	2.00	0.43
1:F:116:GLU:O	1:F:117:VAL:CB	2.66	0.43
1:F:154:TYR:CD1	1:F:154:TYR:O	2.71	0.43
1:F:408:ILE:O	1:F:409:THR:C	2.56	0.43
1:E:144:ILE:HD11	1:E:171:LEU:HD11	1.99	0.43
1:B:25:ILE:CG2	1:B:58:GLN:NE2	2.75	0.43
2:D:46:GLY:O	2:D:183:GLU:HA	2.18	0.43
2:C:430:ILE:O	2:C:431:ALA:C	2.56	0.43
2:D:21:MET:HE2	2:D:177:THR:CG2	2.48	0.43
1:F:507:ARG:O	1:F:508:ILE:O	2.36	0.43
2:C:340:ARG:C	2:C:342:ASN:H	2.21	0.43
1:E:121:PHE:CD1	1:E:121:PHE:N	2.87	0.43
1:F:124:SER:OG	1:F:166:ARG:NH1	2.51	0.43
1:B:273:MET:C	1:B:275:GLY:H	2.20	0.43
2:D:263:VAL:CG2	2:D:280:LYS:HA	2.48	0.43
1:E:392:PHE:O	1:E:394:GLN:N	2.50	0.43
1:B:483:PHE:O	1:B:485:ASN:N	2.51	0.43
1:E:416:SER:C	1:E:418:GLN:N	2.71	0.43
2:C:347:VAL:HG12	2:C:348:CYS:N	2.33	0.43
2:C:311:ARG:HD2	2:C:371:LYS:CD	2.49	0.43
1:B:36:LEU:CD1	1:B:59:PHE:CE1	3.01	0.43
2:D:161:ARG:CB	2:D:196:VAL:HG11	2.46	0.43
2:D:21:MET:HE2	2:D:177:THR:CB	2.48	0.43
2:D:38:ILE:HA	2:D:177:THR:HG23	2.00	0.43
1:E:150:VAL:CG1	1:E:151:PHE:N	2.81	0.43
1:B:64:ILE:C	1:B:66:GLU:H	2.21	0.43
1:F:246:ILE:HG22	1:F:247:PHE:N	2.34	0.43
2:C:79:THR:HG23	2:C:82:ASP:H	1.84	0.43
2:C:118:VAL:O	2:C:118:VAL:HG12	2.18	0.43
1:E:102:LYS:HD3	1:E:102:LYS:HA	1.55	0.43
1:A:487:GLU:OE1	1:F:496:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:198:GLU:O	1:E:224:LYS:HE2	2.19	0.43
1:B:437:ILE:HB	1:B:456:PHE:HB3	2.00	0.43
2:D:78:GLU:HB3	2:D:83:ILE:HD11	2.01	0.43
1:F:98:VAL:HG22	1:F:103:LEU:HG	1.99	0.43
2:D:223:LEU:HD23	2:D:223:LEU:O	2.18	0.43
2:C:126:LEU:O	2:C:129:ARG:HB2	2.18	0.43
2:C:302:VAL:HG12	2:C:303:GLU:N	2.33	0.43
1:A:425:ILE:HD12	1:A:437:ILE:HG21	2.00	0.43
1:A:426:TPO:O1P	1:A:426:TPO:N	2.51	0.43
2:D:338:MET:HB3	2:D:344:LEU:HB3	2.00	0.43
1:F:430:ILE:C	1:F:432:GLU:H	2.20	0.43
2:C:70:PRO:CG	2:C:138:ARG:O	2.66	0.43
1:B:52:LYS:N	3:B:903:ATP:O1B	2.51	0.43
1:F:169:ALA:O	1:F:173:GLN:HG3	2.18	0.43
1:A:451:ARG:HH11	1:A:451:ARG:CG	2.28	0.43
1:B:419:PHE:CD2	2:C:425:ILE:HD12	2.53	0.43
2:D:31:ILE:O	2:D:231:MET:HG3	2.18	0.43
2:C:64:ILE:O	2:C:68:ASP:HA	2.19	0.43
2:D:67:PHE:CD1	2:D:141:ARG:NH2	2.86	0.43
2:D:446:ARG:HB3	1:E:484:ARG:CG	2.46	0.43
2:D:443:VAL:HG13	2:D:494:PRO:CG	2.49	0.43
2:D:332:GLY:O	2:D:333:MET:CG	2.65	0.43
2:C:31:ILE:HA	2:C:231:MET:SD	2.58	0.43
1:F:212:GLU:OE2	1:F:212:GLU:O	2.37	0.43
1:F:21:MET:HE3	1:F:59:PHE:HE1	1.83	0.43
1:A:269:ARG:O	1:A:272:GLU:HB2	2.19	0.43
2:C:435:ASP:OD1	2:C:459:ARG:NH1	2.51	0.43
2:C:329:TYR:CD2	2:C:329:TYR:O	2.71	0.43
1:A:299:SER:C	1:A:301:PHE:N	2.71	0.43
1:F:191:ILE:CG1	1:F:206:ILE:HD11	2.26	0.43
2:C:194:TYR:HD1	2:C:197:GLU:OE1	2.01	0.43
1:A:441:GLN:O	1:A:441:GLN:HG3	2.18	0.43
1:B:291:GLY:O	1:B:293:GLY:N	2.52	0.43
1:E:446:ARG:O	1:E:447:GLY:C	2.57	0.43
1:F:33:HIS:CD2	1:F:229:SER:OG	2.72	0.43
1:B:380:LEU:O	1:B:383:LEU:HB2	2.18	0.43
1:B:103:LEU:HD12	1:B:104:PHE:N	2.34	0.43
1:A:334:ASP:OD1	1:A:336:GLU:HB2	2.18	0.43
2:D:315:PHE:CE1	2:D:363:ILE:HG23	2.54	0.43
1:E:37:PRO:HG2	1:E:225:LEU:HD22	2.01	0.43
2:D:151:PHE:C	2:D:153:GLN:N	2.71	0.43
1:A:71:GLY:O	1:A:103:LEU:HA	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:191:ILE:HB	1:E:198:GLU:HG3	1.98	0.43
1:A:52:LYS:O	1:A:53:THR:C	2.56	0.43
2:C:127:ILE:HG12	2:C:167:LEU:HD13	2.01	0.43
1:F:22:ARG:HA	1:F:29:ASP:OD2	2.18	0.43
1:B:145:ASP:HA	1:B:181:THR:CB	2.48	0.43
1:B:451:ARG:HB3	1:B:452:ALA:H	1.69	0.43
1:E:292:THR:HB	1:E:440:LEU:HB3	2.01	0.43
2:C:400:THR:O	2:C:402:TYR:N	2.52	0.43
2:C:316:ALA:HB2	2:C:324:LEU:HD11	2.01	0.43
2:D:295:THR:HA	2:D:298:VAL:HG23	2.00	0.43
1:B:116:GLU:HG2	1:B:117:VAL:N	2.27	0.43
1:E:61:TYR:O	1:E:63:GLY:N	2.51	0.43
1:F:181:THR:HG22	1:F:182:THR:N	2.34	0.43
1:A:248:PRO:HB2	1:A:251:ALA:CB	2.46	0.43
1:F:116:GLU:O	1:F:117:VAL:HG23	2.18	0.43
2:D:122:ASP:O	2:D:123:LEU:C	2.57	0.43
2:C:378:ASP:O	2:C:379:SER:HB3	2.19	0.43
1:A:358:ASP:O	1:A:361:GLN:N	2.52	0.43
1:F:256:GLN:HE21	1:F:404:LYS:HB3	1.82	0.43
1:B:26:GLU:HB3	1:B:245:ASN:OD1	2.19	0.43
1:A:153:GLN:O	1:A:154:TYR:CB	2.66	0.43
2:C:278:PHE:CE1	2:C:284:ILE:HG21	2.54	0.43
2:D:418:GLN:HB2	1:E:423:HIS:O	2.19	0.43
1:A:109:SER:HA	1:A:110:PRO:HD3	1.80	0.43
1:E:360:LEU:C	1:E:360:LEU:HD13	2.39	0.43
1:A:206:ILE:HD11	1:A:223:LEU:CD1	2.49	0.43
2:D:384:ALA:HB2	2:D:392:PHE:CE1	2.54	0.43
2:D:304:ASN:O	2:D:308:ASN:ND2	2.44	0.43
1:E:430:ILE:O	1:E:431:ALA:C	2.56	0.43
1:B:50:THR:O	1:B:207:LEU:HD13	2.19	0.43
3:D:901:ATP:H3'	1:E:458:MET:O	2.19	0.43
2:C:294:LYS:NZ	2:C:415:THR:HG23	2.34	0.43
1:F:452:ALA:CB	1:F:469:GLU:HA	2.49	0.43
2:C:211:LEU:HA	2:C:216:ARG:HD3	2.00	0.43
2:D:79:THR:HG23	2:D:79:THR:O	2.18	0.43
1:A:504:GLU:C	1:A:506:SER:H	2.22	0.43
1:A:425:ILE:N	1:A:426:TPO:O1P	2.52	0.43
1:F:289:ALA:HB2	1:F:419:PHE:HA	2.00	0.43
1:A:379:SER:CB	1:A:382:ALA:HB2	2.49	0.43
2:C:311:ARG:NE	2:C:371:LYS:HE3	2.34	0.43
1:A:447:GLY:HA2	1:B:489:ILE:HD13	2.00	0.43
2:C:323:GLN:HE21	2:C:327:ASN:HD21	1.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:364:LYS:O	1:F:365:SER:C	2.55	0.43
1:B:240:THR:CG2	1:B:361:GLN:HE22	2.32	0.43
1:F:262:ARG:HA	1:F:278:PHE:O	2.18	0.43
1:E:194:TYR:CD1	1:E:194:TYR:N	2.87	0.42
1:B:54:LEU:HD21	1:B:244:ILE:HG13	2.01	0.42
1:E:191:ILE:CB	1:E:198:GLU:CG	2.93	0.42
1:B:191:ILE:N	1:B:191:ILE:CD1	2.83	0.42
1:A:52:LYS:N	3:A:903:ATP:O1B	2.52	0.42
2:D:443:VAL:CG1	2:D:494:PRO:HG2	2.49	0.42
1:F:471:MET:HG2	1:F:480:LYS:HE2	2.01	0.42
1:F:222:ILE:HG21	1:F:225:LEU:HG	2.01	0.42
1:F:29:ASP:OD1	1:F:29:ASP:N	2.51	0.42
2:C:208:ARG:HG3	5:C:535:HOH:O	2.18	0.42
2:C:43:LEU:HD11	2:C:182:THR:OG1	2.18	0.42
1:A:199:PHE:CE2	1:F:193:ARG:NH2	2.86	0.42
1:E:356:LEU:N	1:E:356:LEU:HD12	2.34	0.42
1:F:500:ASP:O	1:F:501:GLU:CB	2.54	0.42
2:C:400:THR:HG22	2:C:401:GLY:N	2.34	0.42
2:D:291:GLY:CA	3:D:901:ATP:O2B	2.68	0.42
1:B:42:THR:O	1:B:179:VAL:HA	2.19	0.42
2:C:483:PHE:N	2:C:483:PHE:CD1	2.87	0.42
1:B:335:PHE:HA	1:B:338:MET:CG	2.49	0.42
2:C:170:ARG:HH11	2:C:170:ARG:HB3	1.82	0.42
2:C:404:LYS:C	2:C:406:GLU:N	2.72	0.42
1:A:389:ASN:HD21	1:A:428:SER:HB2	1.85	0.42
1:B:359:HIS:O	1:B:361:GLN:N	2.51	0.42
2:D:451:ARG:HH11	2:D:451:ARG:HG2	1.84	0.42
1:B:22:ARG:O	1:B:141:ARG:NH2	2.52	0.42
1:B:396:VAL:C	1:B:398:GLY:N	2.73	0.42
1:A:299:SER:C	1:A:301:PHE:H	2.22	0.42
1:E:266:GLY:O	1:E:300:ARG:NE	2.52	0.42
2:C:263:VAL:CG1	2:C:374:ARG:HH21	2.32	0.42
1:F:294:LYS:HD3	1:F:294:LYS:H	1.84	0.42
2:D:305:ALA:CB	2:D:374:ARG:HD2	2.33	0.42
1:B:451:ARG:CG	1:B:451:ARG:NH1	2.80	0.42
1:B:179:VAL:O	1:B:179:VAL:HG12	2.20	0.42
1:F:129:ARG:O	1:F:132:TYR:HB3	2.19	0.42
2:C:163:GLU:HA	2:C:163:GLU:OE2	2.19	0.42
1:B:423:HIS:O	1:B:424:SER:HB3	2.19	0.42
2:D:81:GLN:N	2:D:81:GLN:CD	2.71	0.42
1:B:490:ILE:HA	1:B:490:ILE:HD13	1.82	0.42
2:C:185:ILE:CD1	2:C:185:ILE:N	2.81	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:248:PRO:C	2:C:250:GLY:N	2.72	0.42
1:A:184:ARG:HH22	1:A:188:TYR:CA	2.32	0.42
1:B:317:TYR:CE2	1:B:383:LEU:HD21	2.54	0.42
1:A:435:ASP:HA	1:A:459:ARG:HD2	2.01	0.42
2:C:73:PHE:HE2	2:C:83:ILE:HD13	1.83	0.42
1:E:352:GLU:N	1:E:352:GLU:CD	2.72	0.42
1:F:356:LEU:CD1	1:F:387:VAL:HG21	2.49	0.42
1:F:312:ALA:HB2	1:F:374:ARG:HB2	2.00	0.42
1:B:148:THR:HA	1:B:151:PHE:HE1	1.84	0.42
1:B:193:ARG:NH1	1:B:193:ARG:HG2	2.33	0.42
1:F:485:ASN:O	1:F:486:PHE:CD1	2.72	0.42
2:C:364:LYS:HE2	2:C:402:TYR:CD1	2.54	0.42
2:C:425:ILE:HD12	2:C:425:ILE:N	2.32	0.42
2:C:148:THR:C	2:C:150:VAL:H	2.21	0.42
2:D:361:GLN:O	2:D:364:LYS:N	2.52	0.42
2:C:202:ASP:CA	2:C:226:ARG:HD2	2.47	0.42
2:C:204:VAL:HG21	2:C:224:LYS:HE2	2.02	0.42
1:E:67:PHE:O	1:E:68:ASP:C	2.58	0.42
1:E:78:GLU:HB2	1:E:83:ILE:HD11	2.02	0.42
2:D:380:LEU:O	2:D:383:LEU:N	2.52	0.42
2:D:385:ARG:O	2:D:387:VAL:HG23	2.20	0.42
2:D:219:THR:HB	2:D:234:GLU:HB3	2.00	0.42
3:B:901:ATP:O3'	2:C:457:LYS:HB2	2.19	0.42
1:A:146:SER:H	1:A:181:THR:HB	1.85	0.42
1:F:47:THR:HG22	1:F:50:THR:HG21	2.00	0.42
1:B:284:ILE:O	1:B:411:LEU:HA	2.19	0.42
1:F:360:LEU:HD13	1:F:360:LEU:O	2.19	0.42
1:E:121:PHE:O	1:E:122:ASP:C	2.58	0.42
1:F:271:ASP:OD1	1:F:277:GLY:HA2	2.19	0.42
1:A:111:ASP:C	1:A:113:GLU:H	2.22	0.42
1:E:298:VAL:O	1:E:301:PHE:HB3	2.20	0.42
1:F:311:ARG:HG3	1:F:371:LYS:HZ1	1.85	0.42
1:B:90:PHE:HA	1:B:241:ASP:O	2.19	0.42
1:B:445:ILE:CD1	1:B:494:PRO:HG2	2.50	0.42
2:C:24:MET:CB	2:C:62:ASN:ND2	2.79	0.42
1:E:58:GLN:CG	1:E:62:ASN:ND2	2.83	0.42
1:A:51:GLY:O	1:A:54:LEU:HB3	2.18	0.42
1:A:49:GLY:HA2	3:A:903:ATP:O2B	2.20	0.42
1:E:393:ARG:NH2	5:E:524:HOH:O	2.52	0.42
2:D:123:LEU:HD11	2:D:167:LEU:HB2	2.00	0.42
2:C:123:LEU:HD13	2:C:166:ARG:HD2	2.02	0.42
1:A:419:PHE:O	1:A:420:MET:HB2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:119:GLY:C	1:B:121:PHE:N	2.72	0.42
2:C:204:VAL:CG2	2:C:224:LYS:HE2	2.49	0.42
2:C:88:ARG:CZ	2:D:15:HIS:HA	2.49	0.42
1:F:389:ASN:O	1:F:392:PHE:N	2.53	0.42
1:B:50:THR:O	1:B:237:PHE:HZ	2.02	0.42
2:C:61:TYR:CD1	2:C:97:LEU:HD11	2.54	0.42
1:F:134:ILE:HD11	1:F:142:VAL:HG21	2.01	0.42
1:A:183:GLU:H	1:A:183:GLU:HG2	1.67	0.42
1:A:209:ASN:ND2	1:A:218:ARG:HG3	2.34	0.42
2:D:161:ARG:HD2	2:D:196:VAL:HG13	2.02	0.42
2:C:146:SER:C	2:C:148:THR:H	2.23	0.42
1:A:49:GLY:CA	3:A:903:ATP:O2B	2.68	0.42
2:D:38:ILE:HA	2:D:177:THR:CG2	2.50	0.42
2:D:361:GLN:O	2:D:362:ILE:C	2.56	0.42
1:F:116:GLU:O	1:F:117:VAL:HB	2.19	0.42
2:C:123:LEU:O	2:C:124:SER:C	2.58	0.42
1:A:32:SER:OG	1:A:35:GLY:CA	2.68	0.42
1:A:420:MET:SD	1:B:490:ILE:HG13	2.60	0.42
1:E:269:ARG:HG2	1:E:479:ILE:HB	2.02	0.42
1:B:392:PHE:C	1:B:394:GLN:N	2.71	0.42
1:B:278:PHE:CD1	1:B:301:PHE:HE1	2.37	0.42
1:A:380:LEU:O	1:A:392:PHE:HE1	2.03	0.42
1:B:41:SER:O	1:B:203:ASN:ND2	2.53	0.42
1:E:249:LEU:CD1	1:E:394:GLN:HG2	2.50	0.42
1:B:51:GLY:O	1:B:54:LEU:N	2.53	0.42
1:E:331:TRP:NE1	3:E:901:ATP:N7	2.68	0.42
1:E:61:TYR:O	1:E:62:ASN:C	2.58	0.42
2:C:299:SER:CB	2:C:333:MET:HE1	2.49	0.42
1:A:191:ILE:H	1:A:191:ILE:HD12	1.83	0.42
1:F:315:PHE:CD2	1:F:347:VAL:HG21	2.55	0.42
2:C:87:ALA:HB1	2:C:92:TRP:HD1	1.82	0.42
2:C:378:ASP:O	2:C:379:SER:CB	2.67	0.42
1:B:383:LEU:HA	1:B:383:LEU:HD23	1.82	0.42
1:A:306:CYS:CB	1:A:338:MET:SD	3.07	0.42
1:F:387:VAL:HG13	1:F:391:ALA:HB3	2.02	0.42
2:C:169:ALA:O	2:C:172:LYS:HB3	2.20	0.42
2:D:344:LEU:C	2:D:344:LEU:CD1	2.86	0.42
1:B:266:GLY:O	1:B:300:ARG:CG	2.68	0.42
1:E:300:ARG:N	1:E:333:MET:HE1	2.35	0.42
1:A:383:LEU:C	1:A:385:ARG:H	2.23	0.42
2:D:304:ASN:O	2:D:304:ASN:OD1	2.37	0.42
1:E:431:ALA:O	1:E:432:GLU:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:52:LYS:HE3	1:B:52:LYS:HB2	1.81	0.42
1:B:52:LYS:HE3	3:B:903:ATP:O3B	2.20	0.42
1:A:94:LEU:O	1:A:97:LEU:N	2.52	0.42
2:C:384:ALA:HB2	2:C:392:PHE:CD1	2.54	0.42
1:B:215:ARG:HA	1:B:215:ARG:NE	2.33	0.42
1:F:140:ARG:CB	1:F:140:ARG:HH11	2.30	0.42
1:B:284:ILE:HB	1:B:411:LEU:HD12	2.01	0.42
2:C:123:LEU:HD21	2:C:167:LEU:HB2	2.01	0.42
1:B:356:LEU:N	1:B:356:LEU:CD1	2.82	0.42
2:D:14:GLU:CD	2:D:15:HIS:H	2.23	0.42
2:D:317:TYR:HE2	2:D:383:LEU:HD21	1.80	0.42
2:C:196:VAL:HG12	2:C:197:GLU:N	2.34	0.42
1:E:288:GLY:O	1:E:294:LYS:NZ	2.48	0.42
1:F:79:THR:HA	1:F:80:PRO:HD3	1.87	0.42
1:A:508:ILE:HD13	1:A:508:ILE:N	2.33	0.42
2:C:191:ILE:HB	2:C:198:GLU:HG2	2.02	0.42
1:F:437:ILE:HD11	1:F:457:LYS:HE2	2.01	0.42
2:C:73:PHE:CD1	2:C:143:SER:HB2	2.55	0.42
2:C:75:THR:HB	2:C:83:ILE:HD11	2.02	0.42
1:E:49:GLY:HA2	3:E:903:ATP:O2B	2.20	0.42
2:D:396:VAL:HG11	2:D:430:ILE:CG2	2.50	0.42
2:D:128:GLU:O	2:D:132:TYR:N	2.49	0.42
2:C:445:ILE:O	2:C:445:ILE:HG22	2.19	0.42
2:C:316:ALA:HB3	2:C:348:CYS:SG	2.60	0.41
1:E:123:LEU:C	1:E:123:LEU:HD23	2.40	0.41
2:C:480:LYS:HB2	2:C:480:LYS:HE3	1.93	0.41
1:A:356:LEU:CD1	1:A:356:LEU:N	2.83	0.41
1:A:445:ILE:HD12	1:A:486:PHE:CE2	2.54	0.41
1:A:184:ARG:O	1:A:185:ILE:HD13	2.19	0.41
1:A:281:ASP:OD1	1:A:407:GLU:OE1	2.38	0.41
1:F:388:SER:O	1:F:389:ASN:C	2.57	0.41
2:D:441:GLN:HE22	2:D:490:ILE:HD12	1.85	0.41
2:D:76:PHE:CZ	2:D:126:LEU:CD2	3.03	0.41
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.81	0.41
1:F:60:LEU:HA	1:F:60:LEU:HD23	1.73	0.41
1:F:426:TPO:CG2	1:F:429:HIS:CA	2.99	0.41
1:F:377:ILE:HD12	1:F:412:PHE:CD2	2.55	0.41
2:C:164:LEU:HB3	2:C:200:VAL:HG11	2.02	0.41
2:C:60:LEU:O	2:C:62:ASN:N	2.53	0.41
1:F:170:ARG:O	1:F:174:ILE:HG12	2.20	0.41
1:A:264:SER:HB3	1:A:304:ASN:ND2	2.36	0.41
2:D:237:PHE:HE1	2:D:239:ILE:HG13	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:496:ARG:O	1:E:497:ILE:HD13	2.20	0.41
1:A:448:GLU:HA	1:B:466:ALA:HA	2.02	0.41
1:E:404:LYS:C	1:E:406:GLU:N	2.73	0.41
1:B:76:PHE:HE1	1:B:144:ILE:CG2	2.33	0.41
2:D:323:GLN:HG2	2:D:327:ASN:ND2	2.35	0.41
1:A:384:ALA:HB2	1:A:392:PHE:CE1	2.55	0.41
2:C:245:ASN:ND2	2:C:247:PHE:CZ	2.88	0.41
2:C:344:LEU:HD13	2:C:344:LEU:C	2.40	0.41
1:B:38:ILE:HA	1:B:177:THR:CG2	2.51	0.41
2:D:78:GLU:HB3	2:D:83:ILE:CD1	2.50	0.41
1:F:504:GLU:HB2	1:F:505:LEU:H	1.49	0.41
2:D:54:LEU:HD13	2:D:90:PHE:CZ	2.55	0.41
2:C:261:VAL:C	2:C:262:ARG:HG2	2.40	0.41
1:B:218:ARG:HD3	1:B:237:PHE:CZ	2.53	0.41
1:F:462:TRP:CE3	1:F:463:HIS:N	2.88	0.41
1:A:65:ILE:HD11	1:A:97:LEU:HD21	2.03	0.41
1:E:283:ILE:HG23	1:E:412:PHE:CE1	2.55	0.41
2:C:317:TYR:CD1	2:C:317:TYR:N	2.88	0.41
1:F:145:ASP:O	1:F:146:SER:OG	2.30	0.41
1:F:61:TYR:O	1:F:64:ILE:N	2.41	0.41
2:C:166:ARG:O	2:C:166:ARG:HG2	2.19	0.41
1:E:54:LEU:CD2	1:E:244:ILE:HG13	2.50	0.41
3:E:903:ATP:O3G	1:F:224:LYS:NZ	2.44	0.41
2:D:76:PHE:HZ	2:D:126:LEU:CD2	2.34	0.41
2:C:107:ASP:OD1	2:C:107:ASP:C	2.59	0.41
1:F:312:ALA:CA	1:F:372:PRO:HB3	2.40	0.41
1:E:184:ARG:C	1:E:185:ILE:HD13	2.41	0.41
2:C:252:MET:CE	2:C:397:ILE:HG22	2.49	0.41
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.49	0.41
2:C:335:PHE:O	2:C:339:GLU:HG3	2.20	0.41
1:B:425:ILE:H	1:B:425:ILE:HD12	1.85	0.41
2:C:111:ASP:HA	2:C:112:PRO:HD3	1.93	0.41
1:A:256:GLN:O	1:F:322:ALA:HB3	2.20	0.41
2:D:344:LEU:HD13	2:D:345:LYS:N	2.36	0.41
1:E:348:CYS:HB3	1:F:254:LEU:HD23	2.03	0.41
2:D:306:CYS:C	2:D:308:ASN:N	2.74	0.41
2:D:182:THR:HG21	2:D:192:ALA:CB	2.51	0.41
1:E:470:PHE:C	1:E:470:PHE:CD1	2.94	0.41
1:A:129:ARG:O	1:A:130:ILE:C	2.59	0.41
1:B:311:ARG:O	1:B:372:PRO:HA	2.20	0.41
1:F:218:ARG:HB2	1:F:237:PHE:CE2	2.55	0.41
2:D:487:GLU:O	2:D:494:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:486:PHE:CB	2:D:489:ILE:CD1	2.98	0.41
1:F:117:VAL:HA	1:F:154:TYR:OH	2.20	0.41
1:B:167:LEU:O	1:B:170:ARG:HB2	2.21	0.41
1:F:317:TYR:OH	1:F:363:ILE:HD11	2.20	0.41
2:C:54:LEU:C	2:C:56:SER:N	2.74	0.41
1:A:18:ILE:CD1	1:A:18:ILE:N	2.83	0.41
1:F:490:ILE:HG12	1:F:490:ILE:H	1.61	0.41
2:C:320:SER:HA	2:D:254:LEU:HG	2.03	0.41
1:E:218:ARG:HG3	1:E:237:PHE:O	2.20	0.41
1:E:334:ASP:HA	5:E:525:HOH:O	2.19	0.41
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.94	0.41
1:F:426:TPO:HG23	1:F:429:HIS:H	1.86	0.41
1:A:267:VAL:HG22	1:A:300:ARG:HG2	2.02	0.41
1:B:451:ARG:HB2	1:B:470:PHE:O	2.21	0.41
1:A:27:GLY:O	1:A:28:PHE:C	2.58	0.41
1:A:71:GLY:HA2	1:A:141:ARG:O	2.20	0.41
2:D:208:ARG:O	2:D:218:ARG:HA	2.21	0.41
1:A:313:ILE:HD12	1:A:372:PRO:HG2	2.03	0.41
1:B:503:SER:O	1:B:504:GLU:CB	2.66	0.41
2:C:150:VAL:CG1	2:C:151:PHE:N	2.82	0.41
1:F:153:GLN:O	1:F:154:TYR:CB	2.69	0.41
1:F:284:ILE:HB	1:F:411:LEU:HA	2.03	0.41
2:D:53:THR:C	2:D:55:PHE:N	2.73	0.41
1:F:295:THR:HA	1:F:378:ASP:OD2	2.20	0.41
2:D:303:GLU:C	2:D:305:ALA:H	2.23	0.41
1:A:79:THR:O	1:A:82:ASP:HB2	2.20	0.41
1:F:171:LEU:O	1:F:174:ILE:HB	2.20	0.41
1:E:81:GLN:HE21	1:E:81:GLN:H	1.66	0.41
2:C:64:ILE:HG23	2:C:102:LYS:HB3	2.03	0.41
1:A:125:ALA:O	1:A:129:ARG:HG3	2.20	0.41
1:B:340:ARG:C	1:B:342:ASN:H	2.24	0.41
2:D:358:ASP:C	2:D:360:LEU:N	2.74	0.41
1:F:47:THR:N	5:F:523:HOH:O	2.54	0.41
1:A:162:ARG:HG3	1:A:162:ARG:NH1	2.36	0.41
1:F:67:PHE:CB	1:F:69:GLU:HG3	2.51	0.41
2:D:356:LEU:HD23	2:D:391:ALA:O	2.20	0.41
2:D:392:PHE:O	2:D:395:PHE:HB3	2.21	0.41
1:F:426:TPO:CG2	1:F:429:HIS:N	2.84	0.41
2:C:187:GLU:OE2	2:C:208:ARG:HA	2.21	0.41
2:C:46:GLY:O	2:C:52:LYS:HD3	2.21	0.41
1:F:371:LYS:HD2	1:F:371:LYS:C	2.41	0.41
1:A:392:PHE:O	1:A:393:ARG:C	2.57	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:306:CYS:C	2:D:308:ASN:H	2.23	0.41
1:F:489:ILE:O	1:F:491:SER:N	2.54	0.41
1:A:147:VAL:HG21	1:A:180:MET:CE	2.50	0.41
2:C:451:ARG:NH1	2:C:451:ARG:CG	2.74	0.41
1:E:80:PRO:HB2	1:E:81:GLN:NE2	2.36	0.41
1:F:425:ILE:HD12	1:F:425:ILE:N	2.36	0.41
2:D:208:ARG:NE	2:D:234:GLU:OE2	2.54	0.41
2:D:267:VAL:HG12	2:D:270:LEU:H	1.86	0.41
1:B:195:GLY:HA2	1:B:198:GLU:CD	2.39	0.41
1:B:57:ILE:C	1:B:59:PHE:N	2.74	0.41
2:C:295:THR:HG22	2:C:296:LEU:N	2.34	0.41
2:C:153:GLN:O	2:C:154:TYR:HB3	2.21	0.41
1:F:208:ARG:O	1:F:218:ARG:HA	2.20	0.41
1:F:237:PHE:HA	1:F:245:ASN:O	2.21	0.41
1:B:64:ILE:HG22	1:B:65:ILE:N	2.35	0.41
1:F:76:PHE:HB2	1:F:146:SER:HG	1.85	0.41
2:D:486:PHE:HB3	2:D:489:ILE:HD11	2.02	0.41
2:D:496:ARG:NH2	1:E:486:PHE:O	2.54	0.41
2:D:331:TRP:O	2:D:333:MET:HG2	2.20	0.41
2:D:265:SER:N	2:D:271:ASP:OD1	2.52	0.41
2:C:289:ALA:HB2	2:C:419:PHE:HA	2.02	0.41
2:D:324:LEU:C	2:D:326:ARG:N	2.74	0.41
1:E:362:ILE:O	1:E:365:SER:N	2.51	0.41
1:A:96:LYS:HE2	1:A:100:GLU:OE1	2.21	0.41
1:A:249:LEU:HD13	1:A:394:GLN:HG2	2.02	0.41
1:E:57:ILE:HD13	1:E:57:ILE:HA	1.85	0.41
2:D:75:THR:HG23	2:D:75:THR:O	2.21	0.41
1:F:419:PHE:O	1:F:420:MET:O	2.39	0.41
1:F:191:ILE:CD1	1:F:191:ILE:N	2.84	0.41
2:C:239:ILE:HG22	3:C:903:ATP:N3	2.36	0.41
1:A:150:VAL:HG13	1:A:151:PHE:N	2.35	0.41
2:C:50:THR:CB	2:C:207:LEU:HB3	2.47	0.41
1:E:131:ASN:OD1	1:E:135:GLN:NE2	2.54	0.41
1:A:191:ILE:H	1:A:191:ILE:CD1	2.33	0.41
1:A:361:GLN:O	1:A:362:ILE:C	2.58	0.41
1:F:21:MET:CE	1:F:59:PHE:CZ	3.04	0.41
2:D:376:ALA:HA	2:D:411:LEU:O	2.21	0.41
2:C:42:THR:HG23	2:C:203:ASN:HB3	2.03	0.40
1:A:211:LEU:HA	1:A:216:ARG:HD3	2.03	0.40
1:F:294:LYS:CB	1:F:413:THR:HG23	2.48	0.40
1:B:273:MET:HA	1:B:464:ASP:HB2	2.03	0.40
1:E:426:TPO:O3P	1:E:429:HIS:HA	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:441:GLN:NE2	1:A:490:ILE:HD13	2.21	0.40
1:A:147:VAL:HG11	1:A:180:MET:HE3	2.02	0.40
1:F:170:ARG:CA	1:F:170:ARG:HH11	2.34	0.40
1:E:191:ILE:CB	1:E:198:GLU:HG2	2.42	0.40
2:D:44:VAL:HG22	2:D:205:VAL:CG1	2.52	0.40
1:E:21:MET:CE	1:E:59:PHE:CZ	3.04	0.40
2:D:299:SER:HB3	2:D:333:MET:CE	2.51	0.40
1:B:306:CYS:CB	1:B:338:MET:SD	3.09	0.40
1:F:117:VAL:O	1:F:118:VAL:HB	2.20	0.40
1:B:167:LEU:O	1:B:168:VAL:C	2.59	0.40
1:E:145:ASP:O	1:E:146:SER:OG	2.37	0.40
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.86	0.40
1:B:313:ILE:HG22	1:B:314:LEU:N	2.36	0.40
2:D:444:GLU:HA	2:D:448:GLU:O	2.21	0.40
1:F:70:PRO:HA	1:F:102:LYS:O	2.21	0.40
1:B:397:ILE:HG22	1:B:397:ILE:O	2.20	0.40
2:D:225:LEU:CB	2:D:230:HIS:HD2	2.31	0.40
1:F:371:LYS:CD	1:F:371:LYS:O	2.69	0.40
1:A:273:MET:HE1	1:A:479:ILE:HG21	2.03	0.40
1:F:378:ASP:OD1	1:F:413:THR:HG21	2.21	0.40
1:A:161:ARG:HH11	1:F:152:GLN:HG3	1.86	0.40
2:C:393:ARG:O	2:C:396:VAL:N	2.54	0.40
1:F:433:ILE:HD12	1:F:433:ILE:N	2.36	0.40
2:C:64:ILE:CD1	2:C:103:LEU:HB2	2.52	0.40
1:A:69:GLU:HB3	1:A:140:ARG:HB2	2.02	0.40
2:C:48:SER:HB2	2:D:199:PHE:CD1	2.55	0.40
2:C:57:ILE:HA	2:C:57:ILE:HD13	1.94	0.40
1:A:312:ALA:O	1:A:344:LEU:HD22	2.21	0.40
1:F:256:GLN:NE2	1:F:404:LYS:HB3	2.36	0.40
1:B:86:ASN:O	1:B:89:SER:N	2.48	0.40
1:A:121:PHE:CD1	1:A:122:ASP:N	2.89	0.40
1:B:307:ALA:C	1:B:309:LYS:H	2.24	0.40
1:B:449:MET:CE	2:C:467:ILE:HD11	2.52	0.40
1:F:209:ASN:O	1:F:216:ARG:NH1	2.54	0.40
1:A:287:THR:HG23	1:A:414:ASN:HB3	2.03	0.40
1:F:263:VAL:HG12	1:F:264:SER:H	1.86	0.40
1:A:438:ILE:HD13	1:A:455:VAL:HA	2.04	0.40
1:F:440:LEU:HD23	1:F:453:ILE:HG13	2.03	0.40
1:E:454:ASN:ND2	1:E:456:PHE:HD1	2.19	0.40
1:F:47:THR:CG2	1:F:50:THR:HG22	2.51	0.40
2:D:85:LYS:O	2:D:86:ASN:C	2.60	0.40
1:F:248:PRO:C	1:F:250:GLY:N	2.74	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:47:THR:O	1:E:52:LYS:HE2	2.21	0.40
2:C:412:PHE:N	2:C:412:PHE:CD1	2.89	0.40
2:C:231:MET:HE3	2:C:251:ALA:HB2	2.03	0.40
1:B:356:LEU:HD23	1:B:395:PHE:HB2	2.04	0.40
1:E:360:LEU:HD13	1:E:360:LEU:O	2.22	0.40
2:C:443:VAL:HG12	2:C:445:ILE:HG12	2.04	0.40
1:B:449:MET:HE3	2:C:467:ILE:HD11	2.03	0.40
2:D:311:ARG:HA	2:D:343:LEU:O	2.20	0.40
1:B:266:GLY:O	1:B:300:ARG:HG2	2.20	0.40
1:E:356:LEU:H	1:E:356:LEU:CD1	2.35	0.40
1:A:31:ILE:HD11	1:A:246:ILE:CG2	2.40	0.40
1:A:180:MET:HE2	1:A:180:MET:HB3	1.93	0.40
1:E:262:ARG:NH1	1:E:461:SER:HB2	2.36	0.40
2:C:370:PHE:O	2:C:371:LYS:HG3	2.21	0.40
1:A:488:ARG:HA	1:F:493:SER:HB2	2.02	0.40
2:D:443:VAL:HG11	2:D:483:PHE:CE2	2.57	0.40
1:E:311:ARG:HA	1:E:343:LEU:O	2.21	0.40
2:D:41:SER:HA	2:D:178:THR:O	2.22	0.40
1:F:452:ALA:CA	1:F:469:GLU:HA	2.50	0.40
2:C:106:LEU:HG	2:C:106:LEU:O	2.21	0.40
1:B:400:THR:HG21	1:B:433:ILE:CG2	2.51	0.40
2:D:80:PRO:HA	2:D:83:ILE:HD13	2.03	0.40
1:B:87:ALA:C	1:B:89:SER:N	2.74	0.40
1:A:88:ARG:HH11	1:A:88:ARG:HG2	1.86	0.40
1:A:255:THR:O	1:A:255:THR:HG22	2.22	0.40
1:F:420:MET:HE2	1:F:492:GLY:CA	2.52	0.40
2:C:208:ARG:O	2:C:218:ARG:HA	2.22	0.40
2:D:263:VAL:CG1	2:D:374:ARG:HH21	2.34	0.40
1:E:160:VAL:O	1:E:161:ARG:C	2.58	0.40
2:D:193:ARG:NH2	1:E:195:GLY:O	2.45	0.40
1:B:444:GLU:O	1:B:494:PRO:HD2	2.22	0.40
2:C:451:ARG:NH1	2:C:472:ILE:HD12	2.37	0.40
1:B:39:GLY:N	1:B:177:THR:OG1	2.39	0.40
2:C:18:ILE:HD12	2:C:18:ILE:N	2.37	0.40
1:E:67:PHE:CB	1:E:69:GLU:HG3	2.51	0.40
1:A:59:PHE:HD2	1:A:143:SER:OG	2.05	0.40
2:D:211:LEU:HD12	2:D:215:ARG:O	2.22	0.40
1:B:255:THR:O	1:B:255:THR:HG22	2.21	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	503/519 (97%)	377 (75%)	92 (18%)	34 (7%)	2	18
1	B	488/519 (94%)	365 (75%)	82 (17%)	41 (8%)	1	12
1	E	489/519 (94%)	375 (77%)	79 (16%)	35 (7%)	2	16
1	F	503/519 (97%)	399 (79%)	70 (14%)	34 (7%)	2	18
2	C	486/519 (94%)	373 (77%)	81 (17%)	32 (7%)	2	19
2	D	483/519 (93%)	392 (81%)	69 (14%)	22 (5%)	4	31
All	All	2952/3114 (95%)	2281 (77%)	473 (16%)	198 (7%)	2	18

All (198) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	65	ILE
1	A	154	TYR
1	A	212	GLU
1	A	333	MET
1	A	427	ASP
1	A	499	VAL
1	A	502	LYS
1	A	510	ARG
1	B	52	LYS
1	B	65	ILE
1	B	154	TYR
1	B	193	ARG
1	B	461	SER
1	B	463	HIS
2	C	17	ALA
2	C	88	ARG
2	C	117	VAL
2	C	154	TYR
2	C	333	MET
2	C	463	HIS

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Mol	Chain	Res	Type
2	D	87	ALA
2	D	122	ASP
2	D	154	TYR
2	D	333	MET
1	E	122	ASP
1	E	154	TYR
1	E	157	SER
1	E	195	GLY
1	E	333	MET
1	E	372	PRO
1	E	387	VAL
1	E	428	SER
1	E	463	HIS
1	F	26	GLU
1	F	117	VAL
1	F	118	VAL
1	F	154	TYR
1	F	249	LEU
1	F	333	MET
1	F	354	ALA
1	F	431	ALA
1	F	463	HIS
1	F	504	GLU
1	F	506	SER
1	F	507	ARG
1	F	508	ILE
1	F	515	LYS
1	A	17	ALA
1	A	167	LEU
1	A	189	GLY
1	A	387	VAL
1	A	420	MET
1	A	429	HIS
1	A	431	ALA
1	A	463	HIS
1	B	26	GLU
1	B	119	GLY
1	B	132	TYR
1	B	149	SER
1	B	249	LEU
1	B	292	THR
1	B	342	ASN

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Mol	Chain	Res	Type
1	B	370	PHE
1	B	372	PRO
1	B	420	MET
1	B	484	ARG
2	C	47	THR
2	C	115	GLN
2	C	149	SER
2	C	193	ARG
2	C	249	LEU
2	C	405	GLN
2	D	17	ALA
2	D	152	GLN
2	D	211	LEU
2	D	381	SER
2	D	400	THR
1	E	117	VAL
1	E	198	GLU
1	E	200	VAL
1	E	282	SER
1	E	327	ASN
1	E	393	ARG
1	E	417	ASP
1	E	420	MET
1	E	422	ALA
1	E	427	ASP
1	E	494	PRO
1	E	498	THR
1	E	504	GLU
1	F	47	THR
1	F	189	GLY
1	F	420	MET
1	F	501	GLU
1	A	157	SER
1	A	422	ALA
1	A	480	LYS
1	B	22	ARG
1	B	61	TYR
1	B	211	LEU
1	B	327	ASN
1	B	354	ALA
1	B	424	SER
1	B	429	HIS

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Mol	Chain	Res	Type
2	C	55	PHE
2	C	61	TYR
2	C	96	LYS
2	C	97	LEU
2	C	107	ASP
2	C	112	PRO
2	C	114	GLY
2	C	157	SER
2	C	341	GLN
2	C	398	GLY
2	D	86	ASN
2	D	123	LEU
2	D	420	MET
1	E	211	LEU
1	E	326	ARG
1	E	342	ASN
1	E	432	GLU
1	F	52	LYS
1	F	490	ILE
1	A	347	VAL
1	A	384	ALA
1	A	428	SER
1	B	167	LEU
1	B	189	GLY
1	B	326	ARG
1	B	405	GLN
1	B	452	ALA
1	B	498	THR
2	C	197	GLU
2	C	289	ALA
2	C	477	PRO
2	D	325	LEU
2	D	429	HIS
1	E	18	ILE
1	E	47	THR
1	E	52	LYS
1	E	379	SER
1	E	482	SER
1	E	490	ILE
1	F	61	TYR
1	F	116	GLU
1	F	379	SER

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Mol	Chain	Res	Type
1	F	468	ARG
1	A	120	GLY
1	A	211	LEU
1	A	289	ALA
1	B	54	LEU
1	B	152	GLN
1	B	198	GLU
1	B	268	VAL
1	B	289	ALA
1	B	309	LYS
2	C	212	GLU
2	C	379	SER
2	C	386	GLY
2	D	26	GLU
2	D	212	GLU
2	D	348	CYS
2	D	463	HIS
1	E	61	TYR
1	F	157	SER
1	F	211	LEU
1	F	500	ASP
1	F	517	PRO
1	A	112	PRO
1	A	117	VAL
1	A	268	VAL
1	A	348	CYS
1	B	85	LYS
2	C	87	ALA
2	C	348	CYS
2	C	420	MET
2	D	248	PRO
2	D	354	ALA
2	D	359	HIS
1	F	152	GLN
1	F	409	THR
1	B	84	ILE
1	B	117	VAL
1	B	195	GLY
1	F	425	ILE
1	F	489	ILE
1	F	509	VAL
1	A	509	VAL

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Mol	Chain	Res	Type
2	C	196	VAL
2	D	347	VAL
1	E	80	PRO
1	A	168	VAL
1	B	179	VAL
1	F	371	LYS
1	A	433	ILE
1	A	83	ILE
1	E	189	GLY

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	430/442 (97%)	400 (93%)	30 (7%)	21	66
1	B	417/442 (94%)	387 (93%)	30 (7%)	21	64
1	E	418/442 (95%)	385 (92%)	33 (8%)	18	59
1	F	430/442 (97%)	383 (89%)	47 (11%)	9	38
2	C	415/443 (94%)	371 (89%)	44 (11%)	10	40
2	D	412/443 (93%)	372 (90%)	40 (10%)	12	45
All	All	2522/2654 (95%)	2298 (91%)	224 (9%)	14	51

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	30	ASP
1	A	33	HIS
1	A	50	THR
1	A	75	THR
1	A	92	TRP
1	A	99	ASP
1	A	121	PHE
1	A	154	TYR
1	A	186	GLU

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Mol	Chain	Res	Type
1	A	212	GLU
1	A	219	THR
1	A	238	THR
1	A	270	LEU
1	A	287	THR
1	A	298	VAL
1	A	335	PHE
1	A	342	ASN
1	A	348	CYS
1	A	360	LEU
1	A	371	LYS
1	A	375	ILE
1	A	427	ASP
1	A	429	HIS
1	A	434	THR
1	A	451	ARG
1	A	463	HIS
1	A	469	GLU
1	A	508	ILE
1	A	518	GLU
1	B	26	GLU
1	B	33	HIS
1	B	47	THR
1	B	50	THR
1	B	77	GLU
1	B	81	GLN
1	B	92	TRP
1	B	103	LEU
1	B	111	ASP
1	B	151	PHE
1	B	154	TYR
1	B	178	THR
1	B	182	THR
1	B	185	ILE
1	B	186	GLU
1	B	193	ARG
1	B	203	ASN
1	B	212	GLU
1	B	223	LEU
1	B	256	GLN
1	B	270	LEU
1	B	302	VAL

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Mol	Chain	Res	Type
1	B	333	MET
1	B	371	LYS
1	B	451	ARG
1	B	462	TRP
1	B	471	MET
1	B	474	ASP
1	B	490	ILE
1	B	499	VAL
2	C	15	HIS
2	C	26	GLU
2	C	50	THR
2	C	121	PHE
2	C	122	ASP
2	C	140	ARG
2	C	149	SER
2	C	151	PHE
2	C	154	TYR
2	C	184	ARG
2	C	185	ILE
2	C	186	GLU
2	C	196	VAL
2	C	198	GLU
2	C	209	ASN
2	C	210	VAL
2	C	212	GLU
2	C	215	ARG
2	C	218	ARG
2	C	223	LEU
2	C	228	THR
2	C	238	THR
2	C	245	ASN
2	C	256	GLN
2	C	260	ASN
2	C	263	VAL
2	C	270	LEU
2	C	290	THR
2	C	295	THR
2	C	303	GLU
2	C	317	TYR
2	C	333	MET
2	C	336	GLU
2	C	356	LEU

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Mol	Chain	Res	Type
2	C	366	GLU
2	C	371	LYS
2	C	383	LEU
2	C	451	ARG
2	C	454	ASN
2	C	470	PHE
2	C	471	MET
2	C	477	PRO
2	C	491	SER
2	C	498	THR
2	D	26	GLU
2	D	30	ASP
2	D	48	SER
2	D	80	PRO
2	D	81	GLN
2	D	106	LEU
2	D	121	PHE
2	D	122	ASP
2	D	123	LEU
2	D	154	TYR
2	D	177	THR
2	D	209	ASN
2	D	211	LEU
2	D	212	GLU
2	D	218	ARG
2	D	237	PHE
2	D	238	THR
2	D	256	GLN
2	D	263	VAL
2	D	270	LEU
2	D	281	ASP
2	D	284	ILE
2	D	290	THR
2	D	302	VAL
2	D	314	LEU
2	D	321	ARG
2	D	356	LEU
2	D	371	LYS
2	D	412	PHE
2	D	416	SER
2	D	423	HIS
2	D	434	THR

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Mol	Chain	Res	Type
2	D	451	ARG
2	D	453	ILE
2	D	463	HIS
2	D	471	MET
2	D	474	ASP
2	D	490	ILE
2	D	496	ARG
2	D	498	THR
1	E	18	ILE
1	E	26	GLU
1	E	81	GLN
1	E	113	GLU
1	E	121	PHE
1	E	135	GLN
1	E	151	PHE
1	E	154	TYR
1	E	177	THR
1	E	196	VAL
1	E	201	SER
1	E	203	ASN
1	E	209	ASN
1	E	212	GLU
1	E	223	LEU
1	E	228	THR
1	E	256	GLN
1	E	260	ASN
1	E	271	ASP
1	E	287	THR
1	E	325	LEU
1	E	338	MET
1	E	366	GLU
1	E	369	ASP
1	E	371	LYS
1	E	417	ASP
1	E	432	GLU
1	E	435	ASP
1	E	449	MET
1	E	451	ARG
1	E	453	ILE
1	E	458	MET
1	E	471	MET
1	F	15	HIS

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Mol	Chain	Res	Type
1	F	26	GLU
1	F	29	ASP
1	F	33	HIS
1	F	43	LEU
1	F	56	SER
1	F	77	GLU
1	F	79	THR
1	F	103	LEU
1	F	121	PHE
1	F	123	LEU
1	F	140	ARG
1	F	143	SER
1	F	154	TYR
1	F	178	THR
1	F	184	ARG
1	F	185	ILE
1	F	186	GLU
1	F	209	ASN
1	F	210	VAL
1	F	212	GLU
1	F	215	ARG
1	F	218	ARG
1	F	219	THR
1	F	256	GLN
1	F	285	LEU
1	F	302	VAL
1	F	325	LEU
1	F	348	CYS
1	F	366	GLU
1	F	371	LYS
1	F	387	VAL
1	F	424	SER
1	F	425	ILE
1	F	427	ASP
1	F	451	ARG
1	F	458	MET
1	F	462	TRP
1	F	468	ARG
1	F	469	GLU
1	F	471	MET
1	F	481	ASP
1	F	497	ILE

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Mol	Chain	Res	Type
1	F	501	GLU
1	F	504	GLU
1	F	509	VAL
1	F	514	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	33	HIS
1	A	62	ASN
1	A	135	GLN
1	A	152	GLN
1	A	209	ASN
1	A	327	ASN
1	A	414	ASN
1	A	441	GLN
1	B	58	GLN
1	B	62	ASN
1	B	81	GLN
1	B	152	GLN
1	B	203	ASN
1	B	209	ASN
1	B	361	GLN
2	C	33	HIS
2	C	58	GLN
2	C	62	ASN
2	C	152	GLN
2	C	209	ASN
2	C	245	ASN
2	C	260	ASN
2	C	323	GLN
2	C	389	ASN
2	C	414	ASN
2	C	418	GLN
2	D	33	HIS
2	D	81	GLN
2	D	209	ASN
2	D	323	GLN
2	D	414	ASN
2	D	441	GLN
1	E	33	HIS

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Mol	Chain	Res	Type
1	E	62	ASN
1	E	81	GLN
1	E	135	GLN
1	E	153	GLN
1	E	209	ASN
1	E	256	GLN
1	E	304	ASN
1	E	323	GLN
1	E	368	ASN
1	E	414	ASN
1	E	441	GLN
1	E	454	ASN
1	F	16	GLN
1	F	33	HIS
1	F	153	GLN
1	F	209	ASN
1	F	256	GLN
1	F	327	ASN
1	F	418	GLN
1	F	454	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	A	426	1	10,10,11	6.45	2 (20%)	12,14,16	0.93	0
1	TPO	B	426	1	10,10,11	5.77	5 (50%)	12,14,16	2.55	5 (41%)
1	TPO	E	426	1	10,10,11	5.85	2 (20%)	12,14,16	1.95	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	F	426	1	10,10,11	6.62	5 (50%)	12,14,16	3.30	7 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	426	1	-	0/9/11/13	0/0/0/0
1	TPO	B	426	1	-	0/9/11/13	0/0/0/0
1	TPO	E	426	1	-	0/9/11/13	0/0/0/0
1	TPO	F	426	1	-	0/9/11/13	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	TPO	O-C	19.91	1.25	1.11
1	F	426	TPO	O-C	19.32	1.24	1.11
1	E	426	TPO	O-C	17.84	1.23	1.11
1	B	426	TPO	O-C	16.50	1.22	1.11
1	B	426	TPO	OG1-CB	5.81	1.56	1.45
1	F	426	TPO	OG1-CB	5.66	1.56	1.45
1	F	426	TPO	CB-CA	4.66	1.60	1.53
1	E	426	TPO	OG1-CB	4.05	1.53	1.45
1	A	426	TPO	CA-C	3.73	1.55	1.48
1	B	426	TPO	CA-C	3.23	1.54	1.48
1	B	426	TPO	CG2-CB	3.01	1.59	1.51
1	F	426	TPO	CA-C	2.19	1.52	1.48
1	B	426	TPO	P-O1P	-2.15	1.44	1.51
1	F	426	TPO	P-O3P	2.01	1.62	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	426	TPO	OG1-CB-CG2	6.80	121.50	110.13
1	E	426	TPO	OG1-CB-CA	4.88	115.73	107.55
1	F	426	TPO	CB-CA-N	4.27	115.56	109.60
1	B	426	TPO	OG1-CB-CG2	4.25	117.22	110.13
1	F	426	TPO	O2P-P-OG1	4.17	119.09	107.09
1	F	426	TPO	O2P-P-O1P	-4.07	97.14	110.44
1	B	426	TPO	OG1-CB-CA	3.98	114.22	107.55
1	B	426	TPO	CG2-CB-CA	-3.79	105.42	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	TPO	O2P-P-OG1	3.48	117.13	107.09
1	F	426	TPO	CG2-CB-CA	-3.40	106.22	113.20
1	E	426	TPO	CG2-CB-CA	-3.34	106.34	113.20
1	B	426	TPO	P-OG1-CB	-3.10	106.50	120.17
1	F	426	TPO	OG1-CB-CA	2.93	112.46	107.55
1	F	426	TPO	O3P-P-O2P	2.63	117.85	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	A	901	4	33,33,33	1.12	3 (9%)	52,52,52	2.14	12 (23%)
3	ATP	A	903	4	33,33,33	1.27	5 (15%)	52,52,52	2.08	12 (23%)
3	ATP	B	901	4	33,33,33	1.05	3 (9%)	52,52,52	2.12	11 (21%)
3	ATP	B	903	4	33,33,33	1.14	4 (12%)	52,52,52	2.11	10 (19%)
3	ATP	C	901	4	33,33,33	1.25	2 (6%)	52,52,52	2.27	14 (26%)
3	ATP	C	903	4	33,33,33	1.26	3 (9%)	52,52,52	2.18	13 (25%)
3	ATP	D	901	4	33,33,33	1.19	3 (9%)	52,52,52	2.27	13 (25%)
3	ATP	D	903	4	33,33,33	1.18	3 (9%)	52,52,52	2.14	10 (19%)
3	ATP	E	901	4	33,33,33	1.10	1 (3%)	52,52,52	2.25	14 (26%)
3	ATP	E	903	4	33,33,33	1.18	3 (9%)	52,52,52	2.23	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	F	901	4	33,33,33	1.11	3 (9%)	52,52,52	2.10	12 (23%)
3	ATP	F	903	4	33,33,33	1.22	4 (12%)	52,52,52	2.16	11 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	901	4	-	0/22/38/38	0/1/3/3
3	ATP	A	903	4	-	0/22/38/38	0/1/3/3
3	ATP	B	901	4	-	0/22/38/38	0/1/3/3
3	ATP	B	903	4	-	0/22/38/38	0/1/3/3
3	ATP	C	901	4	-	0/22/38/38	0/1/3/3
3	ATP	C	903	4	-	0/22/38/38	0/1/3/3
3	ATP	D	901	4	-	0/22/38/38	0/1/3/3
3	ATP	D	903	4	-	0/22/38/38	0/1/3/3
3	ATP	E	901	4	-	0/22/38/38	0/1/3/3
3	ATP	E	903	4	-	0/22/38/38	0/1/3/3
3	ATP	F	901	4	-	0/22/38/38	0/1/3/3
3	ATP	F	903	4	-	0/22/38/38	0/1/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	ATP	C2-N3	3.47	1.39	1.32
3	F	903	ATP	C2-N3	3.46	1.39	1.32
3	C	901	ATP	C2-N3	3.42	1.38	1.32
3	A	901	ATP	C2-N3	3.41	1.38	1.32
3	F	901	ATP	C2-N3	3.34	1.38	1.32
3	B	903	ATP	C2-N3	3.32	1.38	1.32
3	E	901	ATP	C2-N3	3.23	1.38	1.32
3	D	903	ATP	C2-N3	3.22	1.38	1.32
3	C	903	ATP	C2-N3	3.20	1.38	1.32
3	A	903	ATP	C2-N3	3.11	1.38	1.32
3	E	903	ATP	C2-N3	2.94	1.38	1.32
3	C	901	ATP	PB-O3A	-2.77	1.54	1.59
3	C	903	ATP	C2'-C1'	-2.71	1.49	1.53
3	D	903	ATP	C4-N3	2.69	1.39	1.35
3	F	903	ATP	PG-O3B	2.60	1.64	1.60
3	D	903	ATP	C2'-C1'	-2.59	1.49	1.53
3	B	901	ATP	C2-N3	2.56	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	903	ATP	PB-O3A	-2.52	1.55	1.59
3	F	901	ATP	O4'-C1'	2.46	1.45	1.41
3	E	903	ATP	C4-N9	-2.45	1.34	1.37
3	A	901	ATP	O4'-C1'	2.43	1.45	1.41
3	B	903	ATP	O4'-C1'	2.42	1.45	1.41
3	F	903	ATP	C2'-C1'	-2.41	1.50	1.53
3	D	901	ATP	C2-N1	2.39	1.38	1.33
3	A	903	ATP	PB-O3A	2.27	1.64	1.59
3	F	903	ATP	C2-N1	2.26	1.38	1.33
3	F	901	ATP	C2-N1	2.26	1.38	1.33
3	A	903	ATP	C2'-C1'	-2.25	1.50	1.53
3	A	903	ATP	C2-N1	2.24	1.38	1.33
3	E	903	ATP	PB-O3B	-2.17	1.55	1.59
3	D	901	ATP	C2'-C1'	-2.12	1.50	1.53
3	B	903	ATP	C2-N1	2.11	1.38	1.33
3	A	903	ATP	PA-O3A	2.07	1.63	1.59
3	A	901	ATP	C2-N1	2.06	1.38	1.33
3	B	901	ATP	O4'-C1'	2.03	1.44	1.41
3	B	901	ATP	C2-N1	2.02	1.37	1.33
3	B	903	ATP	C4-N3	2.02	1.38	1.35

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ATP	N3-C2-N1	-10.44	119.98	128.71
3	E	901	ATP	N3-C2-N1	-10.43	119.99	128.71
3	D	903	ATP	N3-C2-N1	-10.41	120.01	128.71
3	E	903	ATP	N3-C2-N1	-10.34	120.06	128.71
3	B	903	ATP	N3-C2-N1	-10.32	120.08	128.71
3	B	901	ATP	N3-C2-N1	-10.29	120.10	128.71
3	C	903	ATP	N3-C2-N1	-10.23	120.15	128.71
3	C	901	ATP	N3-C2-N1	-10.06	120.30	128.71
3	F	901	ATP	N3-C2-N1	-10.05	120.31	128.71
3	A	903	ATP	N3-C2-N1	-9.91	120.42	128.71
3	F	903	ATP	N3-C2-N1	-9.88	120.45	128.71
3	A	901	ATP	N3-C2-N1	-9.68	120.62	128.71
3	C	901	ATP	O4'-C1'-N9	-5.83	103.01	108.44
3	B	903	ATP	C4-C5-N7	-5.52	104.79	109.52
3	C	903	ATP	C4-C5-N7	-5.42	104.88	109.52
3	D	903	ATP	C4-C5-N7	-5.35	104.94	109.52
3	F	901	ATP	C4-C5-N7	-5.30	104.98	109.52
3	C	901	ATP	C4-C5-N7	-5.27	105.01	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	903	ATP	O4'-C1'-N9	-5.23	103.58	108.44
3	A	901	ATP	C4-C5-N7	-5.19	105.08	109.52
3	B	901	ATP	C4-C5-N7	-5.15	105.11	109.52
3	F	903	ATP	C4-C5-N7	-5.12	105.14	109.52
3	D	901	ATP	O4'-C1'-N9	-5.09	103.70	108.44
3	E	903	ATP	C4-C5-N7	-5.08	105.17	109.52
3	E	901	ATP	C4-C5-N7	-4.99	105.25	109.52
3	A	903	ATP	C4-C5-N7	-4.90	105.32	109.52
3	D	901	ATP	O3A-PB-O3B	4.80	111.43	101.66
3	D	901	ATP	C4-C5-N7	-4.61	105.58	109.52
3	A	901	ATP	O4'-C1'-N9	-4.33	104.41	108.44
3	E	901	ATP	O4'-C1'-N9	-4.21	104.52	108.44
3	F	903	ATP	O4'-C1'-N9	-4.17	104.56	108.44
3	A	903	ATP	O4'-C1'-N9	-3.87	104.84	108.44
3	E	901	ATP	O3A-PB-O3B	3.78	109.34	101.66
3	B	901	ATP	O3A-PB-O3B	3.75	109.28	101.66
3	F	903	ATP	O3A-PB-O3B	3.21	108.20	101.66
3	D	903	ATP	PB-O3B-PG	-3.21	122.28	131.68
3	C	903	ATP	O4'-C1'-N9	-3.17	105.49	108.44
3	B	901	ATP	O4'-C1'-N9	-3.08	105.58	108.44
3	E	903	ATP	C2'-C1'-N9	3.01	121.00	113.27
3	F	903	ATP	N6-C6-N1	-3.00	113.47	119.36
3	B	903	ATP	N6-C6-N1	-2.95	113.57	119.36
3	D	903	ATP	C2'-C1'-N9	2.92	120.76	113.27
3	C	901	ATP	N3-C4-N9	2.88	130.63	125.43
3	E	903	ATP	C8-N9-C4	2.83	109.06	106.90
3	C	903	ATP	N6-C6-N1	-2.83	113.81	119.36
3	A	901	ATP	N6-C6-N1	-2.78	113.91	119.36
3	C	901	ATP	N6-C6-N1	-2.77	113.92	119.36
3	F	901	ATP	O3A-PB-O3B	2.77	107.29	101.66
3	E	903	ATP	N7-C8-N9	-2.76	106.55	114.36
3	D	901	ATP	N3-C4-N9	2.75	130.41	125.43
3	D	903	ATP	N6-C6-N1	-2.75	113.96	119.36
3	A	901	ATP	N3-C4-N9	2.73	130.36	125.43
3	F	903	ATP	N3-C4-N9	2.73	130.36	125.43
3	C	901	ATP	C2'-C1'-N9	2.71	120.23	113.27
3	C	903	ATP	C2'-C1'-N9	2.71	120.23	113.27
3	C	903	ATP	N7-C8-N9	-2.69	106.75	114.36
3	B	903	ATP	C5-C6-N6	2.69	126.79	120.72
3	C	903	ATP	C5-C6-N6	2.68	126.78	120.72
3	C	901	ATP	C8-N7-C5	2.67	111.87	103.58
3	D	903	ATP	O4'-C1'-N9	-2.67	105.95	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	ATP	C8-N7-C5	2.67	111.87	103.58
3	D	903	ATP	C8-N7-C5	2.67	111.86	103.58
3	F	903	ATP	C8-N7-C5	2.67	111.85	103.58
3	F	901	ATP	O4'-C1'-N9	-2.67	105.96	108.44
3	F	903	ATP	C5-C6-N6	2.65	126.71	120.72
3	B	901	ATP	C8-N7-C5	2.65	111.80	103.58
3	F	901	ATP	N6-C6-N1	-2.65	114.17	119.36
3	F	903	ATP	C2'-C1'-N9	2.64	120.04	113.27
3	B	901	ATP	C5-C6-N6	2.64	126.69	120.72
3	A	901	ATP	C5-C6-N6	2.64	126.68	120.72
3	F	901	ATP	C8-N7-C5	2.62	111.71	103.58
3	C	903	ATP	C8-N7-C5	2.62	111.69	103.58
3	E	903	ATP	N6-C6-N1	-2.61	114.24	119.36
3	A	901	ATP	C2'-C1'-N9	2.61	119.95	113.27
3	E	903	ATP	PB-O3B-PG	-2.60	124.05	131.68
3	E	901	ATP	N6-C6-N1	-2.59	114.28	119.36
3	E	903	ATP	C8-N7-C5	2.59	111.62	103.58
3	A	901	ATP	C8-N7-C5	2.59	111.61	103.58
3	E	901	ATP	N3-C4-N9	2.58	130.10	125.43
3	E	901	ATP	C8-N7-C5	2.58	111.58	103.58
3	D	903	ATP	N7-C8-N9	-2.58	107.07	114.36
3	E	901	ATP	O2'-C2'-C3'	2.57	120.18	111.83
3	D	901	ATP	C8-N7-C5	2.55	111.48	103.58
3	F	901	ATP	C5-C6-N6	2.54	126.47	120.72
3	B	903	ATP	C2'-C1'-N9	2.54	119.80	113.27
3	C	901	ATP	C5-C6-N6	2.54	126.47	120.72
3	A	901	ATP	C3'-C2'-C1'	2.53	104.87	100.91
3	F	901	ATP	N3-C4-N9	2.53	130.01	125.43
3	E	901	ATP	N7-C8-N9	-2.53	107.21	114.36
3	B	901	ATP	N6-C6-N1	-2.50	114.45	119.36
3	C	903	ATP	C3'-C2'-C1'	2.50	104.82	100.91
3	D	903	ATP	N3-C4-N9	2.50	129.95	125.43
3	C	901	ATP	N7-C8-N9	-2.48	107.36	114.36
3	C	903	ATP	C8-N9-C4	2.47	108.78	106.90
3	B	901	ATP	N7-C8-N9	-2.47	107.38	114.36
3	A	901	ATP	PB-O3B-PG	-2.46	124.48	131.68
3	A	903	ATP	N6-C6-N1	-2.45	114.56	119.36
3	F	903	ATP	N7-C8-N9	-2.44	107.45	114.36
3	D	901	ATP	C3'-C2'-C1'	2.44	104.72	100.91
3	B	903	ATP	N7-C8-N9	-2.44	107.47	114.36
3	E	901	ATP	O2B-PB-O3B	2.43	116.68	105.14
3	A	903	ATP	N7-C8-N9	-2.43	107.49	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	901	ATP	N7-C8-N9	-2.42	107.51	114.36
3	A	903	ATP	C8-N7-C5	2.42	111.07	103.58
3	D	903	ATP	C5-C6-N6	2.41	126.18	120.72
3	C	901	ATP	O2B-PB-O3B	2.41	116.57	105.14
3	E	903	ATP	C5-C6-N6	2.38	126.10	120.72
3	D	901	ATP	N7-C8-N9	-2.37	107.64	114.36
3	B	903	ATP	PB-O3B-PG	-2.37	124.72	131.68
3	A	903	ATP	C5-C6-N6	2.36	126.06	120.72
3	B	901	ATP	N3-C4-N9	2.36	129.70	125.43
3	B	901	ATP	O2B-PB-O3B	2.36	116.33	105.14
3	B	903	ATP	N3-C4-N9	2.36	129.69	125.43
3	D	901	ATP	N6-C6-N1	-2.35	114.75	119.36
3	E	901	ATP	C5-C6-N6	2.35	126.03	120.72
3	A	901	ATP	N7-C8-N9	-2.34	107.75	114.36
3	A	903	ATP	O2'-C2'-C3'	2.33	119.40	111.83
3	A	903	ATP	C2'-C1'-N9	2.32	119.23	113.27
3	D	901	ATP	C2'-C1'-N9	2.30	119.18	113.27
3	F	901	ATP	C2'-C1'-N9	2.30	119.17	113.27
3	F	901	ATP	O2'-C2'-C3'	2.27	119.23	111.83
3	D	901	ATP	O2B-PB-O3B	2.28	115.94	105.14
3	A	903	ATP	N3-C4-N9	2.27	129.53	125.43
3	E	901	ATP	C3'-C2'-C1'	2.25	104.43	100.91
3	F	903	ATP	C2'-C3'-C4'	2.20	107.04	102.65
3	C	903	ATP	N3-C4-N9	2.20	129.40	125.43
3	E	903	ATP	N3-C4-N9	2.19	129.39	125.43
3	C	903	ATP	O2B-PB-O3B	2.16	115.40	105.14
3	C	901	ATP	C3'-C2'-C1'	2.15	104.28	100.91
3	B	901	ATP	C2'-C1'-N9	2.15	118.78	113.27
3	E	901	ATP	C8-N9-C4	2.15	108.54	106.90
3	C	901	ATP	O3A-PB-O3B	2.12	105.98	101.66
3	D	901	ATP	C5-C6-N6	2.12	125.51	120.72
3	C	903	ATP	O3A-PB-O3B	2.10	105.94	101.66
3	E	903	ATP	O3A-PB-O3B	2.10	105.93	101.66
3	E	901	ATP	C2'-C1'-N9	2.09	118.63	113.27
3	C	901	ATP	C2'-C3'-C4'	2.07	106.78	102.65
3	A	901	ATP	C2'-C3'-C4'	2.06	106.77	102.65
3	B	903	ATP	O2'-C2'-C3'	2.06	118.53	111.83
3	A	903	ATP	O3A-PB-O3B	2.05	105.83	101.66
3	D	901	ATP	C2'-C3'-C4'	2.04	106.73	102.65
3	A	903	ATP	C8-N9-C4	2.04	108.46	106.90
3	F	901	ATP	O2B-PB-O3B	2.03	114.76	105.14
3	C	901	ATP	O2'-C2'-C3'	2.01	118.38	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	506/519 (97%)	0.12	16 (3%)	45 11	20, 76, 128, 156	0
1	B	491/519 (94%)	0.02	6 (1%)	75 29	31, 78, 130, 168	0
1	E	492/519 (94%)	-0.15	5 (1%)	79 33	2, 48, 110, 149	0
1	F	506/519 (97%)	-0.04	12 (2%)	56 15	2, 57, 123, 139	0
2	C	488/519 (94%)	-0.07	4 (0%)	83 39	8, 62, 129, 167	0
2	D	485/519 (93%)	-0.21	6 (1%)	75 29	5, 42, 100, 152	0
All	All	2968/3114 (95%)	-0.06	49 (1%)	68 21	2, 62, 126, 168	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	GLU	4.7
1	F	517	PRO	4.4
1	E	505	LEU	4.0
1	F	518	GLU	3.8
1	A	515	LYS	3.7
1	A	513	GLN	3.7
1	B	504	GLU	3.7
1	A	508	ILE	3.6
1	A	514	GLU	3.5
1	A	517	PRO	3.4
1	F	516	GLY	3.0
1	A	507	ARG	3.0
1	F	507	ARG	2.9
1	F	504	GLU	2.9
2	C	120	GLY	2.8
1	B	116	GLU	2.8
1	F	509	VAL	2.7
2	C	501	GLU	2.7
1	A	516	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	504	GLU	2.6
1	E	501	GLU	2.6
1	F	515	LYS	2.6
1	A	500	ASP	2.5
1	A	253	ARG	2.5
2	D	16	GLN	2.4
2	D	113	GLU	2.4
1	B	500	ASP	2.4
1	E	500	ASP	2.4
1	B	117	VAL	2.3
1	A	510	ARG	2.3
1	A	509	VAL	2.3
1	A	501	GLU	2.3
2	D	157	SER	2.3
1	F	514	GLU	2.3
1	A	511	GLY	2.3
1	A	475	LYS	2.3
1	F	511	GLY	2.2
1	A	498	THR	2.2
2	C	17	ALA	2.2
1	B	502	LYS	2.2
1	F	510	ARG	2.2
2	D	117	VAL	2.2
1	B	498	THR	2.1
2	C	119	GLY	2.1
1	E	116	GLU	2.1
1	F	513	GLN	2.1
2	D	120	GLY	2.1
2	D	14	GLU	2.1
1	F	508	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	TPO	F	426	11/12	0.32	2.30	67,68,79,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	TPO	E	426	11/12	0.32	1.30	75,89,101,102	0
1	TPO	B	426	11/12	0.26	0.46	79,85,91,92	0
1	TPO	A	426	11/12	0.26	-0.23	74,77,78,78	0

6.3 Carbohydrates i

There are no carbohydrates in this entry.

6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	A	701	1/1	0.89	16.93	70,70,70,70	0
4	MG	F	701	1/1	0.49	7.92	29,29,29,29	0
4	MG	B	701	1/1	0.52	6.78	49,49,49,49	0
4	MG	D	702	1/1	0.59	5.11	70,70,70,70	0
4	MG	C	702	1/1	0.41	3.81	67,67,67,67	0
4	MG	C	701	1/1	0.58	3.51	69,69,69,69	0
4	MG	A	520	1/1	0.48	3.45	58,58,58,58	0
4	MG	E	520	1/1	0.47	3.35	23,23,23,23	0
4	MG	C	801	1/1	0.29	3.33	6,6,6,6	0
4	MG	F	702	1/1	0.33	3.31	62,62,62,62	0
4	MG	D	701	1/1	0.37	2.81	67,67,67,67	0
4	MG	A	802	1/1	0.55	2.68	77,77,77,77	0
4	MG	D	801	1/1	0.38	2.51	72,72,72,72	0
4	MG	C	802	1/1	0.34	2.34	19,19,19,19	0
4	MG	F	802	1/1	0.37	2.17	21,21,21,21	0
4	MG	B	802	1/1	0.30	1.68	61,61,61,61	0
4	MG	A	702	1/1	0.33	1.28	76,76,76,76	0
4	MG	E	702	1/1	0.34	0.99	70,70,70,70	0
3	ATP	E	901	31/31	0.26	0.50	35,63,67,68	0
3	ATP	D	903	31/31	0.21	0.50	15,19,42,44	0
3	ATP	A	901	31/31	0.31	0.40	65,80,87,88	0
3	ATP	E	903	31/31	0.20	0.40	16,24,41,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ATP	D	901	31/31	0.24	0.37	38,43,54,55	0
3	ATP	B	903	31/31	0.24	0.32	65,69,75,76	0
3	ATP	C	901	31/31	0.19	0.31	24,28,38,40	0
3	ATP	F	901	31/31	0.24	0.31	53,79,88,88	0
3	ATP	F	903	31/31	0.19	0.19	31,36,40,40	0
3	ATP	B	901	31/31	0.22	0.18	42,47,53,54	0
3	ATP	A	903	31/31	0.24	0.18	57,64,69,70	0
3	ATP	C	903	31/31	0.20	0.11	36,41,67,68	0
4	MG	A	801	1/1	0.37	-0.48	31,31,31,31	0
4	MG	E	801	1/1	0.27	-0.55	1,1,1,1	0
4	MG	D	802	1/1	0.25	-0.90	1,1,1,1	0
4	MG	B	801	1/1	0.24	-1.00	10,10,10,10	0

6.5 Other polymers ⓘ

There are no such residues in this entry.