



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:45 PM GMT

PDB ID : 3S1A
Title : Crystal structure of the phosphorylation-site double mutant S431E/T432E of the KaiC circadian clock protein
Authors : Pattanayek, R.; Williams, D.W.; Rossi, G.; Weigand, S.; Mori, T.; Johnson, C.H.; Stewart, P.L.; Egli, M.
Deposited on : 2011-05-14
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

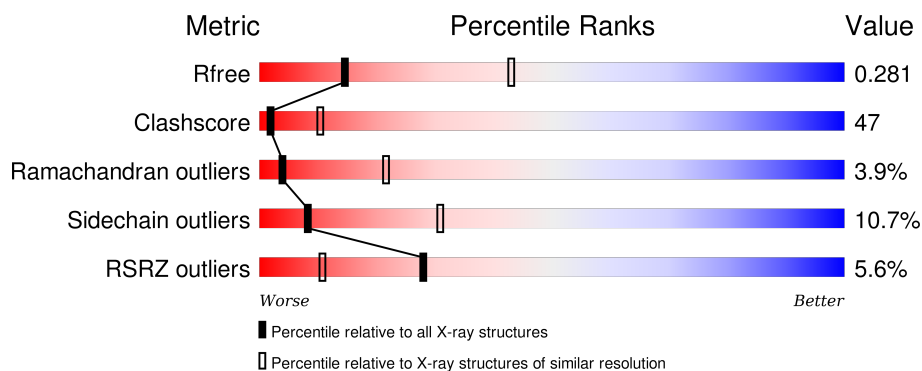
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



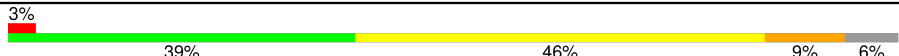
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	525	<div> <div>10%</div> <div>37% 50% 9%</div> </div>
1	F	525	<div> <div>6%</div> <div>39% 48% 9%</div> </div>
2	B	525	<div> <div>7%</div> <div>31% 53% 9% 6%</div> </div>
2	C	525	<div> <div>4%</div> <div>35% 49% 9% 7%</div> </div>
2	D	525	<div> <div>2%</div> <div>39% 46% 6% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	525	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	320	-	-	X	-
1	SEP	F	320	-	-	X	-
4	MG	A	526	-	-	-	X
4	MG	D	701	-	-	-	X
4	MG	D	801	-	-	-	X
4	MG	F	702	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23898 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3994	2512	701	765	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3994	2512	701	765	1	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
A	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
A	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
F	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
F	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	525	HIS	-	EXPRESSION TAG	UNP Q79PF4

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	491	Total	C	N	O	S		0	0	0
			3875	2442	678	740	15				
2	C	488	Total	C	N	O	S		0	0	0
			3851	2428	674	734	15				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	485	Total	C	N	O	S	0	0	0
			3827	2414	671	727	15			
2	E	492	Total	C	N	O	S	0	0	0
			3883	2448	679	741	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
B	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
B	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
C	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
C	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
D	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
D	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
E	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
E	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	525	HIS	-	EXPRESSION TAG	UNP Q79PF4

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



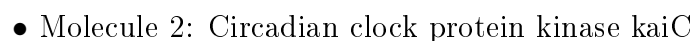
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D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

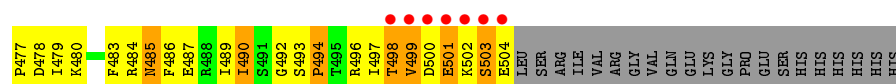
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	4	Total Mg 4 4	0	0
4	E	2	Total Mg 2 2	0	0
4	B	4	Total Mg 4 4	0	0
4	C	4	Total Mg 4 4	0	0
4	A	4	Total Mg 4 4	0	0
4	F	3	Total Mg 3 3	0	0

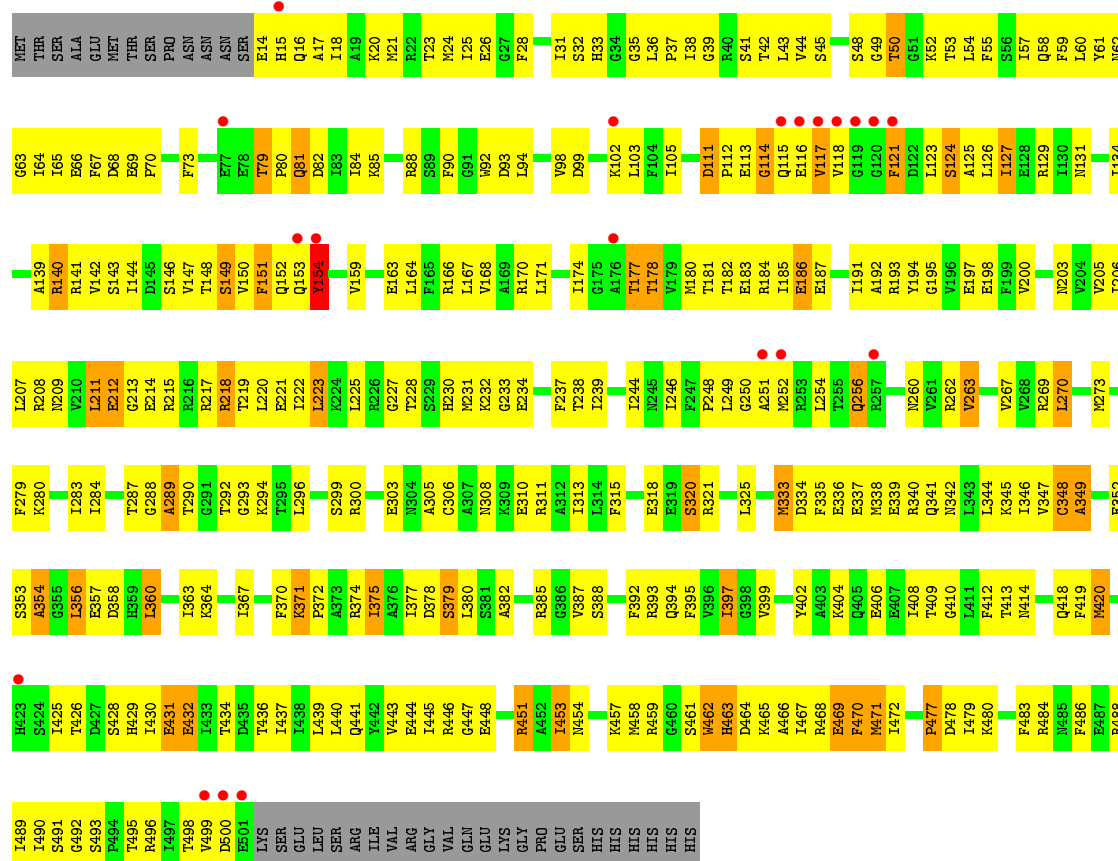
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	6	Total O 6 6	0	0
5	C	10	Total O 10 10	0	0
5	D	32	Total O 32 32	0	0
5	E	16	Total O 16 16	0	0
5	F	12	Total O 12 12	0	0

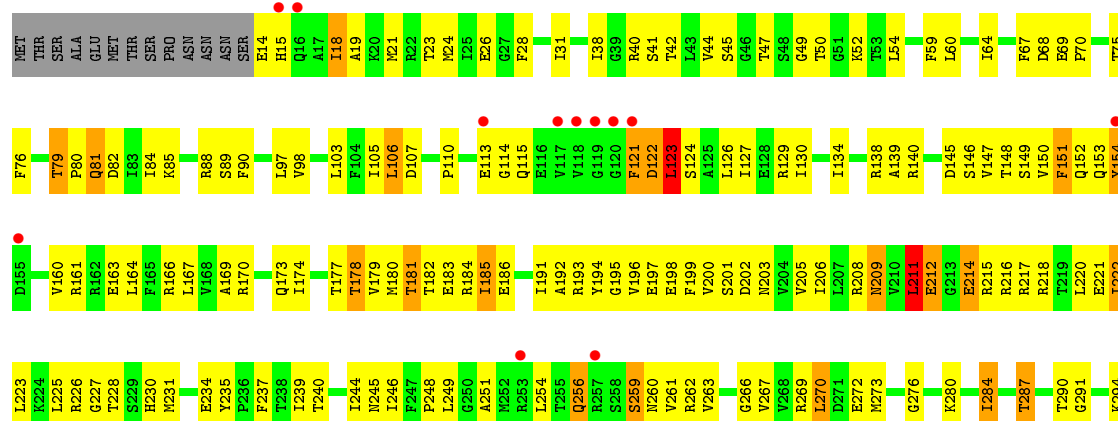


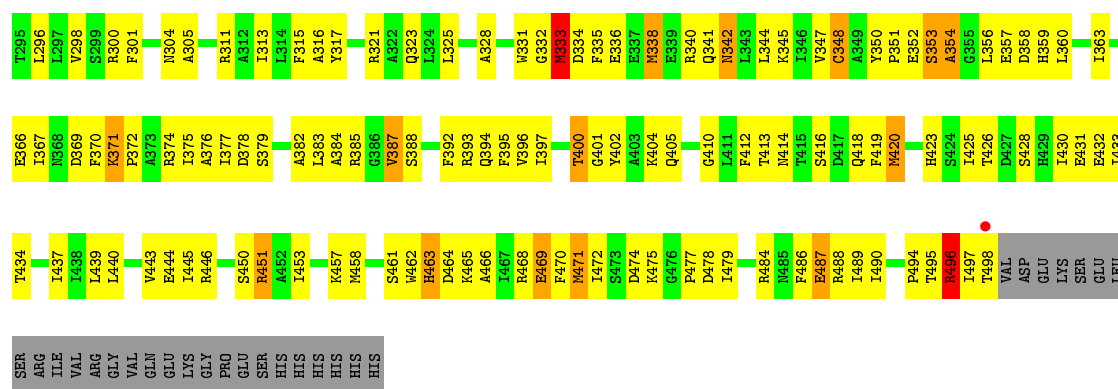


• Molecule 2: Circadian clock protein kinase kaiC

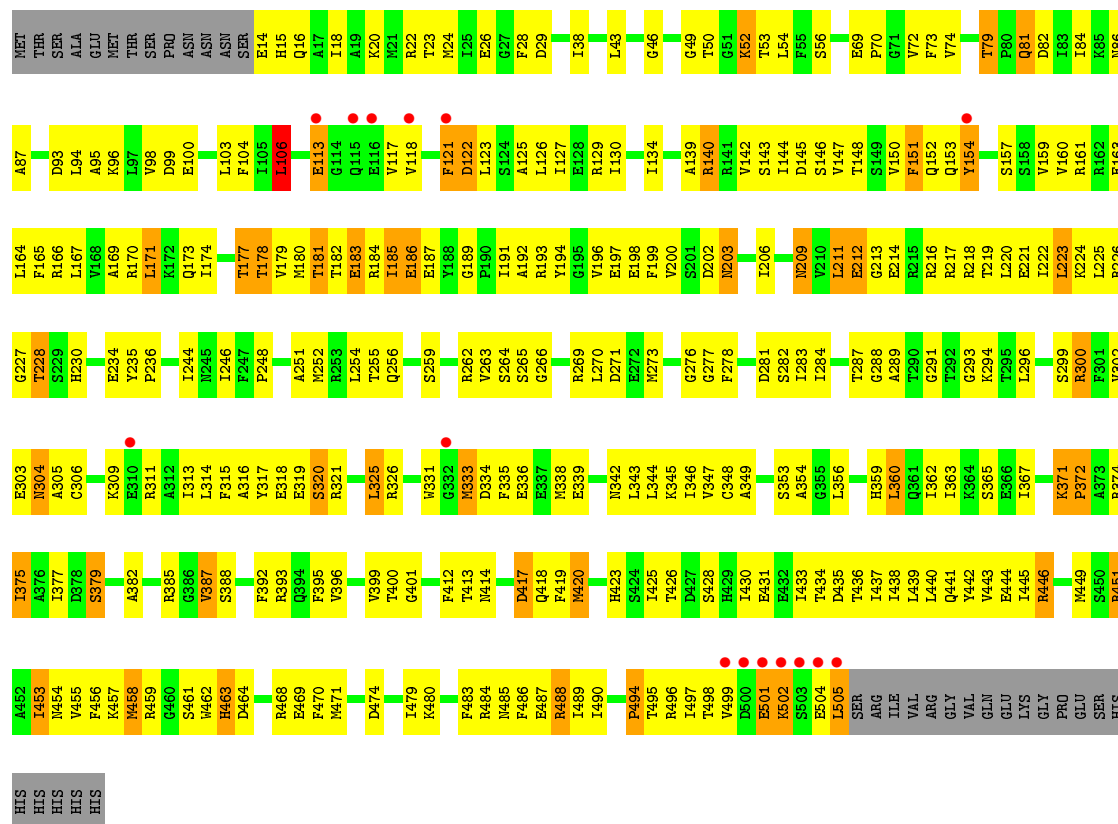


• Molecule 2: Circadian clock protein kinase kaiC





• Molecule 2: Circadian clock protein kinase kaiC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.67Å 135.49Å 204.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 3.00 16.96 – 2.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (17.00-3.00) 92.3 (16.96-2.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.87Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.288 0.239 , 0.281	Depositor DCC
R_{free} test set	6459 reflections (10.06%)	DCC
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.3	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 81280 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23898	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	0/4049	0.72	1/5453 (0.0%)
1	F	0.46	0/4049	0.73	0/5453
2	B	0.40	0/3940	0.67	0/5309
2	C	0.41	0/3916	0.69	1/5278 (0.0%)
2	D	0.50	0/3892	0.73	0/5245
2	E	0.49	0/3948	0.75	2/5320 (0.0%)
All	All	0.45	0/23794	0.72	4/32058 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	213	GLY	N-CA-C	-5.96	98.21	113.10
2	E	106	LEU	CA-CB-CG	5.81	128.67	115.30
2	C	213	GLY	N-CA-C	-5.28	99.90	113.10
1	A	380	LEU	N-CA-C	-5.23	96.88	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3994	0	3985	444	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3994	0	3983	405	0
2	B	3875	0	3863	437	0
2	C	3851	0	3839	382	0
2	D	3827	0	3819	358	0
2	E	3883	0	3875	351	0
3	A	62	0	24	7	0
3	B	62	0	24	8	0
3	C	62	0	24	5	0
3	D	62	0	24	6	0
3	E	62	0	24	11	0
3	F	62	0	24	6	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
5	A	5	0	0	0	0
5	B	6	0	0	1	0
5	C	10	0	0	2	0
5	D	32	0	0	13	0
5	E	16	0	0	0	0
5	F	12	0	0	1	0
All	All	23898	0	23508	2227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (2227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:HG12	1:A:463:HIS:CD2	1.63	1.30
1:A:320:SEP:HB2	2:B:254:LEU:O	1.42	1.17
1:A:254:LEU:CD2	1:F:320:SEP:HA	1.74	1.16
1:A:321:ARG:O	1:A:324:LEU:HB2	1.45	1.14
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.10	1.14
1:A:455:VAL:CG1	1:A:463:HIS:HD2	1.61	1.13
1:A:254:LEU:HD21	1:F:320:SEP:HA	1.15	1.13
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.21	1.13
2:D:123:LEU:HG	2:D:163:GLU:OE2	1.49	1.13
1:F:509:VAL:HG12	1:F:510:ARG:H	1.07	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ALA:HB2	2:B:374:ARG:HD2	1.33	1.11
2:E:305:ALA:HB2	2:E:374:ARG:HD2	1.26	1.11
1:A:320:SEP:CA	2:B:254:LEU:HG	1.83	1.08
2:E:263:VAL:HG12	2:E:374:ARG:HH21	1.12	1.07
1:A:14:GLU:HG3	1:A:15:HIS:H	1.19	1.07
2:B:269:ARG:HB3	2:B:479:ILE:HD13	1.37	1.06
1:A:320:SEP:HA	2:B:254:LEU:HG	1.30	1.06
2:D:123:LEU:O	2:D:127:ILE:HD13	1.54	1.05
2:B:263:VAL:HG12	2:B:374:ARG:HH21	1.20	1.05
1:A:455:VAL:HG12	1:A:463:HIS:HD2	0.88	1.04
2:C:205:VAL:HG22	2:C:222:ILE:HD13	1.38	1.04
2:B:497:ILE:HD12	2:B:499:VAL:H	1.22	1.03
1:A:455:VAL:CG1	1:A:463:HIS:CD2	2.39	1.02
2:D:445:ILE:HD13	2:D:450:SER:OG	1.58	1.02
2:D:123:LEU:HD12	2:D:166:ARG:HD2	1.41	1.02
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.39	1.02
2:D:371:LYS:HD2	2:D:371:LYS:O	1.60	1.02
1:F:18:ILE:HD12	1:F:227:GLY:HA3	1.44	0.99
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.42	0.99
2:E:313:ILE:HD12	2:E:367:ILE:HD13	1.45	0.98
1:A:41:SER:HB3	1:A:178:THR:HB	1.46	0.97
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.76	0.97
2:D:335:PHE:HA	2:D:338:MET:HG3	1.45	0.96
1:F:79:THR:HG22	1:F:82:ASP:H	1.30	0.96
2:B:325:LEU:HD23	2:B:335:PHE:CB	1.94	0.96
2:B:147:VAL:HG11	2:B:180:MET:HE3	1.47	0.96
2:B:434:THR:HG21	2:B:437:ILE:HD11	1.48	0.95
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.45	0.95
2:B:385:ARG:HG2	2:C:393:ARG:NH1	1.80	0.95
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.48	0.95
2:E:356:LEU:HD22	2:E:387:VAL:HG11	1.48	0.94
2:E:311:ARG:HD2	2:E:371:LYS:HE3	1.50	0.94
2:C:371:LYS:O	2:C:371:LYS:HD2	1.67	0.94
1:F:509:VAL:HG12	1:F:510:ARG:N	1.83	0.93
2:C:434:THR:HG23	2:C:437:ILE:HD11	1.47	0.93
2:B:285:LEU:HD23	2:B:437:ILE:HD12	1.51	0.93
2:D:146:SER:H	2:D:181:THR:HG22	1.34	0.93
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.51	0.93
2:B:73:PHE:HB3	2:B:105:ILE:HD13	1.50	0.93
2:B:325:LEU:HD23	2:B:335:PHE:HB2	1.47	0.92
2:B:170:ARG:O	2:B:174:ILE:HG12	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:MET:HE3	2:C:141:ARG:NE	1.84	0.92
2:B:54:LEU:HD23	2:B:244:ILE:HD11	1.51	0.92
1:F:263:VAL:HG12	1:F:374:ARG:NH2	1.85	0.92
1:F:508:ILE:O	1:F:509:VAL:HG23	1.69	0.91
2:D:333:MET:HA	5:D:913:HOH:O	1.70	0.91
2:C:437:ILE:CD1	2:C:457:LYS:HE2	2.01	0.91
2:E:79:THR:HG23	2:E:81:GLN:HG2	1.52	0.91
1:F:18:ILE:CD1	1:F:227:GLY:HA3	2.01	0.90
1:A:25:ILE:HD12	1:A:58:GLN:HG2	1.51	0.90
2:B:483:PHE:HB3	2:B:486:PHE:HD1	1.36	0.90
2:C:123:LEU:HD23	2:C:127:ILE:HD11	1.54	0.89
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.36	0.89
2:E:313:ILE:HB	2:E:375:ILE:HD11	1.54	0.89
1:A:462:TRP:O	1:A:463:HIS:HB3	1.73	0.89
2:B:45:SER:HB3	2:B:182:THR:HB	1.54	0.89
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.02	0.89
2:C:344:LEU:HD22	2:C:345:LYS:H	1.37	0.89
1:A:79:THR:HG23	1:A:81:GLN:HE21	1.36	0.88
2:D:79:THR:HG22	2:D:82:ASP:H	1.36	0.88
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.55	0.88
2:D:60:LEU:O	2:D:64:ILE:HD13	1.74	0.88
2:C:206:ILE:HD11	2:C:223:LEU:HB2	1.54	0.88
2:B:147:VAL:HG11	2:B:180:MET:CE	2.05	0.87
2:E:287:THR:HG23	2:E:414:ASN:HD22	1.36	0.87
2:B:148:THR:HG21	2:B:193:ARG:HD2	1.57	0.87
1:F:509:VAL:CG1	1:F:510:ARG:H	1.86	0.87
2:E:79:THR:CG2	2:E:81:GLN:HG2	2.05	0.87
1:A:396:VAL:HG11	1:A:430:ILE:HG21	1.56	0.87
2:C:182:THR:HG21	2:C:192:ALA:HB1	1.56	0.86
2:E:303:GLU:OE2	2:E:333:MET:HB3	1.76	0.86
2:C:493:SER:HB3	2:D:488:ARG:HG2	1.56	0.86
1:F:299:SER:C	1:F:333:MET:HE1	1.95	0.86
2:C:287:THR:HG21	2:C:425:ILE:O	1.76	0.85
2:C:45:SER:HB3	2:C:182:THR:HB	1.56	0.85
2:E:269:ARG:HG2	2:E:479:ILE:HB	1.55	0.85
2:C:437:ILE:HD13	2:C:457:LYS:HE2	1.58	0.85
1:A:318:GLU:OE1	2:B:432:GLU:HG2	1.76	0.85
1:F:18:ILE:HD13	1:F:40:ARG:NH1	1.91	0.85
1:A:14:GLU:CG	1:A:15:HIS:H	1.88	0.85
1:F:363:ILE:O	1:F:367:ILE:HG12	1.76	0.85
2:E:293:GLY:HA2	3:E:901:ATP:O1A	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.41	0.85
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.39	0.85
1:F:123:LEU:O	1:F:127:ILE:HD13	1.76	0.85
2:B:426:THR:HB	2:B:431:GLU:OE2	1.77	0.84
2:C:25:ILE:HG23	2:C:58:GLN:NE2	1.90	0.84
2:B:140:ARG:NH1	2:B:140:ARG:HB3	1.91	0.84
2:C:140:ARG:HB3	2:C:140:ARG:NH1	1.93	0.84
2:C:269:ARG:HB3	2:C:479:ILE:HD12	1.59	0.84
2:B:503:SER:O	2:B:504:GLU:HB2	1.74	0.84
2:E:435:ASP:HA	2:E:459:ARG:HD2	1.58	0.84
1:F:293:GLY:HA2	3:F:901:ATP:O1A	1.78	0.84
2:B:263:VAL:HG12	2:B:374:ARG:NH2	1.93	0.84
1:A:257:ARG:NH2	1:A:407:GLU:HG2	1.93	0.84
2:B:263:VAL:CG1	2:B:374:ARG:HH21	1.90	0.84
2:B:300:ARG:HA	2:B:333:MET:CE	2.07	0.83
1:F:191:ILE:HB	1:F:198:GLU:CG	2.08	0.83
1:F:313:ILE:HB	1:F:375:ILE:HD11	1.61	0.83
2:C:147:VAL:O	2:C:150:VAL:HG12	1.78	0.83
2:B:116:GLU:HG2	2:B:117:VAL:H	1.44	0.83
2:C:25:ILE:HG12	2:C:58:GLN:HE21	1.43	0.83
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.41	0.83
1:A:396:VAL:HG11	1:A:430:ILE:CG2	2.08	0.82
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.60	0.82
2:E:125:ALA:O	2:E:129:ARG:HG3	1.79	0.82
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.61	0.82
1:A:320:SEP:C	1:A:348:CYS:SG	2.68	0.82
2:B:451:ARG:HG2	2:B:451:ARG:HH11	1.43	0.82
1:A:21:MET:HB2	1:A:38:ILE:HD11	1.62	0.82
2:C:31:ILE:HD11	2:C:246:ILE:HG21	1.62	0.82
2:B:300:ARG:HA	2:B:333:MET:HE3	1.59	0.82
2:E:313:ILE:HB	2:E:375:ILE:CD1	2.10	0.81
2:B:300:ARG:N	2:B:333:MET:HE1	1.95	0.81
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.15	0.81
2:B:285:LEU:HB3	2:B:437:ILE:HD13	1.62	0.81
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.62	0.81
2:B:296:LEU:HD21	2:B:477:PRO:HD3	1.62	0.81
1:A:254:LEU:HD22	1:F:348:CYS:HB3	1.62	0.81
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.45	0.81
1:A:254:LEU:HD21	1:F:320:SEP:CA	2.04	0.81
2:E:263:VAL:HG12	2:E:374:ARG:NH2	1.95	0.81
2:D:147:VAL:HG11	2:D:180:MET:HE3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:ASP:OD1	2:B:336:GLU:HB2	1.80	0.81
2:B:169:ALA:O	2:B:173:GLN:HG3	1.81	0.81
1:A:462:TRP:O	1:A:463:HIS:CB	2.30	0.80
2:E:263:VAL:CG1	2:E:374:ARG:HH21	1.94	0.80
2:B:46:GLY:HA3	2:B:50:THR:HG21	1.64	0.80
2:E:446:ARG:NH2	2:E:496:ARG:NH2	2.29	0.80
2:B:311:ARG:HD2	2:B:371:LYS:HE3	1.63	0.80
1:A:462:TRP:CE3	1:A:463:HIS:N	2.49	0.80
2:B:479:ILE:HD12	2:B:479:ILE:H	1.44	0.80
1:A:273:MET:O	1:A:274:CYS:HB2	1.79	0.80
1:F:313:ILE:O	1:F:375:ILE:HD13	1.82	0.79
2:C:28:PHE:CE1	2:C:222:ILE:HD11	2.17	0.79
2:D:315:PHE:HB2	2:D:377:ILE:HD13	1.64	0.79
2:B:299:SER:C	2:B:333:MET:HE1	2.02	0.79
2:E:426:THR:HG21	2:E:430:ILE:HG12	1.65	0.79
1:A:318:GLU:CD	2:B:432:GLU:HG2	2.02	0.79
2:B:379:SER:HA	2:B:413:THR:HG22	1.65	0.79
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.61	0.79
1:A:320:SEP:HA	2:B:254:LEU:CG	2.12	0.79
2:C:123:LEU:HD13	2:C:166:ARG:HD2	1.65	0.79
2:E:379:SER:H	2:E:413:THR:HB	1.47	0.79
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.64	0.79
2:D:140:ARG:NH1	2:D:140:ARG:HB3	1.98	0.78
1:F:453:ILE:HG21	1:F:479:ILE:HD12	1.64	0.78
2:D:445:ILE:HD13	2:D:450:SER:HG	1.48	0.78
2:E:371:LYS:HD2	2:E:371:LYS:O	1.83	0.78
1:A:164:LEU:HD11	1:A:197:GLU:HG3	1.63	0.78
1:F:508:ILE:C	1:F:509:VAL:HG23	2.00	0.78
2:E:382:ALA:O	2:E:385:ARG:HG3	1.83	0.78
2:E:18:ILE:HD11	2:E:228:THR:OG1	1.83	0.78
2:B:191:ILE:HB	2:B:198:GLU:CG	2.14	0.78
2:D:267:VAL:HG23	2:D:300:ARG:HG2	1.65	0.78
1:A:205:VAL:HG22	1:A:222:ILE:HD13	1.63	0.78
2:E:38:ILE:HA	2:E:177:THR:HG23	1.66	0.78
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.66	0.77
1:A:147:VAL:O	1:A:150:VAL:HG12	1.83	0.77
1:A:471:MET:SD	1:A:478:ASP:HB3	2.24	0.77
1:A:227:GLY:O	1:F:89:SER:HB2	1.84	0.77
2:B:182:THR:HG21	2:B:192:ALA:HB1	1.66	0.77
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.49	0.77
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:496:ARG:HG2	2:E:487:GLU:OE1	1.85	0.77
2:D:313:ILE:HB	2:D:375:ILE:CD1	2.14	0.77
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.66	0.77
1:A:256:GLN:HG3	1:F:320:SEP:O1P	1.85	0.77
2:B:140:ARG:HH11	2:B:140:ARG:HB3	1.49	0.77
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.49	0.76
2:E:14:GLU:HG3	2:E:16:GLN:H	1.49	0.76
2:D:451:ARG:HH11	2:D:451:ARG:HG2	1.50	0.76
1:F:287:THR:CG2	1:F:414:ASN:HD22	1.98	0.76
1:F:486:PHE:CE2	1:F:496:ARG:HD2	2.19	0.76
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.49	0.76
2:E:356:LEU:CD2	2:E:387:VAL:HG11	2.16	0.76
1:A:375:ILE:HD13	1:A:408:ILE:HG21	1.68	0.76
1:F:508:ILE:O	1:F:509:VAL:CG2	2.33	0.76
2:C:170:ARG:O	2:C:174:ILE:HG12	1.86	0.76
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.00	0.76
2:C:205:VAL:CG2	2:C:222:ILE:HD13	2.16	0.75
2:D:182:THR:HG22	2:D:183:GLU:N	2.01	0.75
2:D:18:ILE:CD1	2:D:227:GLY:HA3	2.16	0.75
1:A:14:GLU:HG3	1:A:15:HIS:N	1.99	0.75
2:B:492:GLY:O	2:B:494:PRO:HD3	1.86	0.75
2:D:444:GLU:OE2	2:E:489:ILE:HD13	1.87	0.75
2:D:311:ARG:HD2	2:D:371:LYS:CE	2.17	0.75
1:A:318:GLU:OE2	2:B:432:GLU:HG2	1.86	0.75
2:E:79:THR:HG22	2:E:82:ASP:H	1.51	0.75
2:D:148:THR:OG1	2:D:182:THR:HG23	1.86	0.75
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.69	0.75
2:C:299:SER:C	2:C:333:MET:HE1	2.06	0.75
2:B:325:LEU:HD23	2:B:335:PHE:HB3	1.68	0.75
2:E:453:ILE:HG21	2:E:479:ILE:HD12	1.68	0.75
2:B:25:ILE:HG12	2:B:58:GLN:HE21	1.50	0.75
2:D:212:GLU:O	2:D:212:GLU:HG2	1.86	0.75
3:B:901:ATP:H3'	2:C:458:MET:O	1.87	0.74
2:E:273:MET:O	2:E:463:HIS:HA	1.87	0.74
2:B:356:LEU:HD13	2:B:387:VAL:HG21	1.69	0.74
2:D:18:ILE:HD12	2:D:227:GLY:HA3	1.68	0.74
1:A:25:ILE:CD1	1:A:58:GLN:HG2	2.17	0.74
2:D:443:VAL:O	2:D:445:ILE:HD12	1.88	0.74
2:E:93:ASP:OD2	2:E:96:LYS:HB2	1.87	0.74
2:E:148:THR:OG1	2:E:182:THR:HG23	1.86	0.74
2:E:123:LEU:HD23	2:E:127:ILE:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:MET:HB2	1:A:38:ILE:CD1	2.17	0.74
1:F:500:ASP:O	1:F:501:GLU:HB3	1.87	0.74
1:A:321:ARG:O	1:A:324:LEU:CB	2.32	0.74
1:A:254:LEU:HD21	1:F:319:GLU:O	1.87	0.74
2:C:335:PHE:HA	2:C:338:MET:HG3	1.68	0.74
1:A:508:ILE:H	1:A:508:ILE:HD13	1.51	0.74
1:F:170:ARG:O	1:F:174:ILE:HG12	1.88	0.74
2:B:148:THR:CG2	2:B:193:ARG:HD2	2.18	0.73
2:C:344:LEU:HD22	2:C:345:LYS:N	2.03	0.73
2:E:377:ILE:HD11	2:E:399:VAL:HG11	1.69	0.73
1:A:96:LYS:O	1:A:100:GLU:HG3	1.88	0.73
2:C:495:THR:HA	2:D:487:GLU:OE2	1.88	0.73
2:B:61:TYR:CE1	2:B:92:TRP:HB2	2.24	0.73
1:A:290:THR:HG21	2:B:425:ILE:HD12	1.69	0.73
2:B:21:MET:HB2	2:B:38:ILE:HG12	1.70	0.73
2:D:431:GLU:O	2:D:434:THR:HG22	1.87	0.73
2:B:295:THR:HG21	2:B:319:GLU:OE2	1.87	0.73
1:A:254:LEU:HD23	1:A:254:LEU:O	1.89	0.73
2:D:344:LEU:HD22	2:D:345:LYS:H	1.53	0.73
2:E:304:ASN:HB3	2:E:374:ARG:HH12	1.53	0.73
2:B:127:ILE:HG21	2:B:170:ARG:HG3	1.69	0.73
1:A:371:LYS:O	1:A:371:LYS:HD2	1.87	0.73
2:E:319:GLU:O	1:F:254:LEU:HD21	1.89	0.73
1:F:283:ILE:HG23	1:F:412:PHE:HE1	1.53	0.73
2:C:262:ARG:NH2	2:C:461:SER:HB2	2.04	0.73
1:A:266:GLY:HA3	1:A:300:ARG:O	1.88	0.73
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.23	0.73
1:F:489:ILE:HA	1:F:494:PRO:HG3	1.70	0.73
2:B:25:ILE:HG12	2:B:58:GLN:NE2	2.04	0.73
2:D:478:ASP:HB2	5:D:555:HOH:O	1.89	0.73
1:A:89:SER:HB2	2:B:227:GLY:O	1.89	0.73
1:A:320:SEP:O	1:A:348:CYS:SG	2.47	0.72
2:C:28:PHE:CZ	2:C:222:ILE:HD11	2.24	0.72
2:C:182:THR:HG22	2:C:183:GLU:N	2.04	0.72
1:F:347:VAL:O	1:F:348:CYS:HB2	1.88	0.72
2:B:493:SER:HB3	2:C:488:ARG:HG2	1.71	0.72
2:E:191:ILE:HD12	2:E:206:ILE:CD1	2.19	0.72
1:F:514:GLU:O	1:F:515:LYS:HB3	1.89	0.72
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.11	0.72
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.71	0.72
1:A:462:TRP:CD2	1:A:463:HIS:N	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:140:ARG:HB3	2:D:140:ARG:HH11	1.55	0.72
2:E:191:ILE:HB	2:E:198:GLU:CG	2.20	0.72
2:B:285:LEU:HB3	2:B:437:ILE:CD1	2.18	0.72
2:B:287:THR:HG23	2:B:414:ASN:HD22	1.55	0.72
2:E:159:VAL:O	2:E:163:GLU:HG2	1.90	0.72
1:F:379:SER:H	1:F:413:THR:HB	1.55	0.72
2:D:332:GLY:C	2:D:333:MET:HG2	2.09	0.72
2:D:446:ARG:N	2:D:496:ARG:HH12	1.87	0.71
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.72	0.71
1:F:111:ASP:OD1	1:F:112:PRO:HD2	1.90	0.71
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.72	0.71
1:F:31:ILE:HG21	1:F:222:ILE:HD13	1.73	0.71
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.71	0.71
2:B:191:ILE:HB	2:B:198:GLU:HG3	1.71	0.71
2:B:54:LEU:HD23	2:B:244:ILE:CD1	2.20	0.71
2:E:248:PRO:HB2	2:E:251:ALA:HB3	1.70	0.71
2:C:123:LEU:HD21	2:C:167:LEU:HB2	1.73	0.71
2:D:191:ILE:HB	2:D:198:GLU:CG	2.20	0.71
2:E:436:THR:HG23	2:E:458:MET:HG2	1.73	0.71
2:B:178:THR:HG22	2:B:179:VAL:H	1.55	0.71
2:C:191:ILE:HB	2:C:198:GLU:CG	2.21	0.71
2:E:313:ILE:HG13	2:E:372:PRO:CG	2.20	0.71
2:C:50:THR:HG21	2:C:207:LEU:O	1.91	0.71
2:E:426:THR:HG22	2:E:428:SER:H	1.55	0.71
2:B:284:ILE:HG23	2:B:436:THR:HB	1.71	0.71
2:B:453:ILE:HD13	2:B:454:ASN:N	2.06	0.71
1:A:116:GLU:C	1:A:117:VAL:HG23	2.09	0.71
1:F:379:SER:OG	1:F:382:ALA:HB2	1.91	0.71
2:D:446:ARG:H	2:D:496:ARG:HH12	1.39	0.71
2:E:462:TRP:CE2	2:E:463:HIS:O	2.44	0.71
2:D:439:LEU:HD12	2:D:440:LEU:N	2.06	0.71
2:D:344:LEU:HD22	2:D:345:LYS:N	2.06	0.71
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.03	0.71
2:C:140:ARG:CB	2:C:140:ARG:HH11	2.04	0.70
1:F:96:LYS:O	1:F:100:GLU:HG3	1.91	0.70
2:C:377:ILE:HD12	2:C:412:PHE:CE2	2.26	0.70
2:B:425:ILE:HD11	2:B:456:PHE:CE2	2.26	0.70
1:F:515:LYS:HG3	1:F:516:GLY:H	1.56	0.70
2:C:393:ARG:O	2:C:397:ILE:HD13	1.90	0.70
2:C:25:ILE:HG23	2:C:58:GLN:HE22	1.54	0.70
1:F:31:ILE:CG2	1:F:222:ILE:HD13	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:446:ARG:NH2	2:E:496:ARG:HH22	1.88	0.70
2:D:359:HIS:O	2:D:363:ILE:HG12	1.91	0.70
2:E:317:TYR:OH	2:E:363:ILE:HD11	1.90	0.70
2:E:453:ILE:HB	2:E:470:PHE:CD2	2.27	0.70
1:A:318:GLU:OE1	2:B:432:GLU:HB3	1.91	0.70
1:A:321:ARG:HA	1:A:324:LEU:HD12	1.71	0.70
2:E:266:GLY:HA2	2:E:304:ASN:HD22	1.55	0.70
1:F:147:VAL:O	1:F:150:VAL:HG12	1.92	0.70
1:A:458:MET:O	3:F:901:ATP:H3'	1.91	0.70
2:C:283:ILE:HD11	2:C:404:LYS:HG3	1.74	0.70
2:C:379:SER:H	2:C:413:THR:HB	1.56	0.70
2:E:418:GLN:HB2	1:F:423:HIS:O	1.91	0.70
1:F:18:ILE:HD13	1:F:40:ARG:HH12	1.53	0.69
2:B:434:THR:CG2	2:B:437:ILE:HD11	2.21	0.69
2:E:300:ARG:HA	2:E:333:MET:HE1	1.72	0.69
2:D:478:ASP:CB	5:D:555:HOH:O	2.40	0.69
1:F:317:TYR:OH	1:F:363:ILE:HD11	1.92	0.69
1:A:154:TYR:O	1:A:155:ASP:CG	2.30	0.69
2:E:43:LEU:HD11	2:E:182:THR:OG1	1.92	0.69
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.24	0.69
1:F:338:MET:HB3	1:F:344:LEU:HB3	1.74	0.69
2:D:147:VAL:O	2:D:150:VAL:HG12	1.92	0.69
2:C:221:GLU:HG3	2:C:233:GLY:O	1.92	0.69
1:F:515:LYS:HG3	1:F:516:GLY:N	2.08	0.69
2:D:284:ILE:HD12	2:D:410:GLY:O	1.92	0.69
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.74	0.69
2:B:218:ARG:CZ	2:B:239:ILE:HD12	2.22	0.69
1:F:462:TRP:O	1:F:463:HIS:CD2	2.46	0.69
2:D:269:ARG:HG2	2:D:479:ILE:HB	1.74	0.69
2:D:387:VAL:HG12	2:D:388:SER:N	2.08	0.69
2:B:84:ILE:HD12	2:B:94:LEU:HB2	1.74	0.69
2:E:294:LYS:HG2	2:E:413:THR:HG23	1.75	0.69
2:E:126:LEU:O	2:E:130:ILE:HG12	1.92	0.69
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.07	0.69
1:A:451:ARG:N	1:A:451:ARG:HD2	2.08	0.69
2:D:147:VAL:HG11	2:D:180:MET:CE	2.23	0.69
1:A:425:ILE:HD12	1:F:290:THR:HG21	1.73	0.69
2:C:94:LEU:O	2:C:98:VAL:HG23	1.92	0.69
1:F:264:SER:O	1:F:374:ARG:NH2	2.25	0.69
2:D:220:LEU:HD13	2:D:246:ILE:HD11	1.73	0.69
1:A:320:SEP:HB2	2:B:254:LEU:C	2.13	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.58	0.69
2:C:287:THR:HG23	2:C:414:ASN:ND2	2.07	0.69
2:C:218:ARG:CZ	2:C:239:ILE:HD12	2.23	0.69
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.58	0.69
2:C:419:PHE:O	2:C:420:MET:HB2	1.92	0.69
1:A:320:SEP:O1P	2:B:256:GLN:HG3	1.92	0.68
1:A:254:LEU:HD23	1:F:320:SEP:HA	1.74	0.68
2:B:51:GLY:O	2:B:54:LEU:N	2.26	0.68
1:A:396:VAL:O	1:A:400:THR:HB	1.94	0.68
2:E:320:SER:HA	1:F:254:LEU:HG	1.75	0.68
2:C:159:VAL:O	2:C:163:GLU:HG2	1.93	0.68
1:A:318:GLU:OE1	2:B:432:GLU:CG	2.42	0.68
2:B:225:LEU:HD12	2:B:230:HIS:HB3	1.74	0.68
2:C:453:ILE:HD13	2:C:454:ASN:N	2.07	0.68
1:A:264:SER:HA	1:A:271:ASP:OD1	1.94	0.68
2:E:74:VAL:HG21	2:E:130:ILE:HD12	1.76	0.68
2:B:315:PHE:CE2	2:B:347:VAL:HG21	2.29	0.68
2:B:325:LEU:CD2	2:B:335:PHE:HB3	2.23	0.68
2:C:45:SER:CB	2:C:182:THR:HB	2.23	0.68
2:E:377:ILE:HD12	2:E:412:PHE:CE2	2.28	0.68
1:A:372:PRO:O	1:A:408:ILE:HD12	1.94	0.68
1:A:191:ILE:HB	1:A:198:GLU:CG	2.24	0.68
2:D:122:ASP:O	2:D:123:LEU:HB2	1.92	0.68
1:F:508:ILE:O	1:F:509:VAL:CB	2.42	0.68
2:D:301:PHE:CZ	2:D:374:ARG:HD3	2.28	0.68
2:C:111:ASP:OD1	2:C:113:GLU:HG2	1.92	0.68
1:A:88:ARG:HH11	1:A:88:ARG:HG2	1.58	0.68
2:E:287:THR:HG23	2:E:414:ASN:ND2	2.08	0.68
2:C:447:GLY:HA2	2:D:489:ILE:HD12	1.76	0.68
2:D:347:VAL:O	2:D:348:CYS:HB2	1.94	0.68
2:E:123:LEU:O	2:E:127:ILE:HG12	1.93	0.68
2:B:502:LYS:HG3	2:B:504:GLU:O	1.94	0.68
1:A:84:ILE:HG23	1:A:94:LEU:HB2	1.76	0.68
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.74	0.68
2:D:478:ASP:CA	5:D:555:HOH:O	2.41	0.68
2:B:140:ARG:CB	2:B:140:ARG:HH11	2.07	0.67
1:F:471:MET:CG	1:F:478:ASP:HB3	2.24	0.67
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.24	0.67
2:C:470:PHE:HB2	2:C:478:ASP:O	1.94	0.67
2:D:475:LYS:HA	5:D:553:HOH:O	1.93	0.67
2:E:344:LEU:HD11	2:E:346:ILE:HG13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:ARG:HB3	2:E:140:ARG:NH1	2.09	0.67
2:E:363:ILE:O	2:E:367:ILE:HG12	1.93	0.67
2:C:431:GLU:HG2	2:C:431:GLU:O	1.94	0.67
2:E:171:LEU:HA	2:E:174:ILE:HD12	1.76	0.67
1:A:211:LEU:HB2	1:A:216:ARG:NE	2.09	0.67
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.74	0.67
2:B:56:SER:O	2:B:59:PHE:HB3	1.94	0.67
2:C:451:ARG:HG2	2:C:451:ARG:HH11	1.59	0.67
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.28	0.67
2:D:222:ILE:N	2:D:222:ILE:HD12	2.09	0.67
2:E:377:ILE:HD12	2:E:412:PHE:HE2	1.57	0.67
2:E:445:ILE:O	2:E:446:ARG:HB2	1.93	0.67
1:A:311:ARG:HA	1:A:343:LEU:O	1.95	0.67
1:A:323:GLN:HG3	1:A:324:LEU:N	2.10	0.67
2:D:81:GLN:NE2	2:D:81:GLN:H	1.93	0.67
1:F:191:ILE:HB	1:F:198:GLU:CD	2.14	0.67
2:D:287:THR:CG2	2:D:414:ASN:HD22	2.06	0.67
2:D:400:THR:HG22	2:D:401:GLY:N	2.08	0.67
2:B:497:ILE:HD12	2:B:499:VAL:N	2.03	0.66
2:C:54:LEU:HD23	2:C:244:ILE:HG12	1.77	0.66
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.58	0.66
2:C:151:PHE:C	2:C:153:GLN:H	1.95	0.66
1:F:426:THR:HG22	1:F:428:SER:H	1.61	0.66
2:E:496:ARG:O	2:E:497:ILE:HD13	1.95	0.66
2:B:79:THR:CG2	2:B:81:GLN:HG2	2.25	0.66
2:D:313:ILE:HB	2:D:375:ILE:HD13	1.76	0.66
2:B:287:THR:HG21	2:B:425:ILE:O	1.95	0.66
2:E:289:ALA:HB2	2:E:419:PHE:HA	1.77	0.66
2:B:325:LEU:CD2	2:B:335:PHE:CB	2.72	0.66
2:C:436:THR:C	2:C:437:ILE:HD12	2.16	0.66
2:B:52:LYS:N	3:B:903:ATP:O1B	2.28	0.66
1:A:359:HIS:O	1:A:363:ILE:HG12	1.95	0.66
2:C:28:PHE:HA	2:C:246:ILE:HD12	1.78	0.66
2:C:31:ILE:CD1	2:C:246:ILE:HG21	2.24	0.66
2:E:487:GLU:O	2:E:488:ARG:HB2	1.96	0.66
1:F:18:ILE:CD1	1:F:40:ARG:HH12	2.08	0.66
1:A:487:GLU:HG3	1:A:497:ILE:HD11	1.77	0.66
2:B:425:ILE:HD11	2:B:456:PHE:CD2	2.31	0.66
1:F:345:LYS:HE2	1:F:366:GLU:OE1	1.95	0.66
1:A:421:GLY:O	1:A:422:ALA:C	2.34	0.66
1:F:46:GLY:HA2	1:F:184:ARG:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:ILE:O	2:B:248:PRO:HD3	1.95	0.66
1:A:73:PHE:HB3	1:A:105:ILE:HD13	1.77	0.66
2:D:31:ILE:HG21	2:D:222:ILE:CD1	2.25	0.66
2:E:170:ARG:O	2:E:174:ILE:HG13	1.94	0.66
2:B:44:VAL:HG22	2:B:205:VAL:CG1	2.26	0.66
1:F:49:GLY:HA2	3:F:903:ATP:O2B	1.96	0.66
2:C:79:THR:CG2	2:C:82:ASP:H	2.08	0.66
1:A:406:GLU:HB3	1:A:408:ILE:HG12	1.78	0.65
2:B:462:TRP:O	2:B:463:HIS:CG	2.49	0.65
2:D:379:SER:H	2:D:413:THR:HB	1.61	0.65
2:D:21:MET:HE1	2:D:177:THR:HB	1.78	0.65
2:E:121:PHE:N	2:E:121:PHE:CD1	2.63	0.65
2:C:439:LEU:HD12	2:C:440:LEU:N	2.10	0.65
2:C:437:ILE:HD13	2:C:457:LYS:HG2	1.79	0.65
2:E:451:ARG:HD2	2:E:451:ARG:H	1.62	0.65
2:C:25:ILE:HG12	2:C:58:GLN:NE2	2.12	0.65
2:C:121:PHE:H	2:C:121:PHE:HD1	1.44	0.65
2:B:145:ASP:OD2	2:B:181:THR:HG21	1.96	0.65
2:B:43:LEU:HD11	2:B:182:THR:OG1	1.97	0.65
2:B:79:THR:HG23	2:B:81:GLN:HG2	1.78	0.65
1:F:505:LEU:O	1:F:506:SER:HB3	1.96	0.65
2:B:311:ARG:HD2	2:B:371:LYS:CE	2.26	0.65
2:B:20:LYS:HE3	2:B:228:THR:HG21	1.78	0.65
2:B:65:ILE:HG22	2:B:65:ILE:O	1.94	0.65
2:C:182:THR:HG22	2:C:183:GLU:H	1.59	0.65
2:D:18:ILE:HD13	2:D:40:ARG:NH1	2.12	0.65
2:E:147:VAL:O	2:E:150:VAL:HG12	1.97	0.65
1:F:151:PHE:C	1:F:153:GLN:H	2.00	0.65
2:E:191:ILE:HB	2:E:198:GLU:HG2	1.78	0.65
2:D:194:TYR:O	2:D:196:VAL:HG23	1.97	0.65
2:C:335:PHE:O	2:C:339:GLU:HG3	1.96	0.65
2:D:49:GLY:O	2:D:218:ARG:NH2	2.30	0.65
1:F:378:ASP:OD1	1:F:413:THR:HG21	1.97	0.65
2:E:334:ASP:OD1	2:E:336:GLU:HB2	1.97	0.65
1:F:20:LYS:HD3	1:F:35:GLY:O	1.96	0.65
2:D:170:ARG:O	2:D:174:ILE:HG13	1.97	0.65
2:E:359:HIS:HA	2:E:362:ILE:HD12	1.78	0.64
2:C:367:ILE:HG12	2:C:375:ILE:CD1	2.26	0.64
2:E:106:LEU:HD21	2:E:130:ILE:HD13	1.79	0.64
1:A:436:THR:CG2	1:A:458:MET:HG2	2.28	0.64
2:E:449:MET:HE3	1:F:490:ILE:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:MET:HB3	1:A:344:LEU:HB3	1.79	0.64
2:D:41:SER:CB	2:D:178:THR:HB	2.26	0.64
2:E:311:ARG:HD2	2:E:371:LYS:CE	2.26	0.64
1:F:79:THR:HG23	1:F:81:GLN:H	1.61	0.64
2:D:81:GLN:CD	2:D:81:GLN:H	1.98	0.64
3:E:901:ATP:H3'	1:F:458:MET:O	1.96	0.64
1:F:504:GLU:HA	1:F:507:ARG:NE	2.13	0.64
1:A:320:SEP:N	2:B:254:LEU:HG	2.12	0.64
2:D:383:LEU:HD13	2:D:395:PHE:CE2	2.31	0.64
2:C:284:ILE:HD12	2:C:410:GLY:O	1.98	0.64
2:C:448:GLU:HG2	2:D:466:ALA:HA	1.79	0.64
1:A:321:ARG:O	1:A:324:LEU:N	2.30	0.64
2:D:146:SER:N	2:D:181:THR:HG22	2.11	0.64
2:C:123:LEU:CD2	2:C:127:ILE:HD11	2.27	0.64
2:C:61:TYR:CE1	2:C:92:TRP:HB2	2.32	0.64
2:B:497:ILE:CD1	2:B:499:VAL:H	2.06	0.64
2:D:383:LEU:HD13	2:D:395:PHE:HE2	1.63	0.64
2:E:23:THR:O	2:E:24:MET:HB2	1.98	0.64
1:A:379:SER:H	1:A:413:THR:HB	1.62	0.64
2:D:197:GLU:CD	2:D:197:GLU:H	1.99	0.64
2:B:283:ILE:CD1	2:B:404:LYS:HG3	2.28	0.64
2:C:123:LEU:HD11	2:C:163:GLU:O	1.98	0.64
2:B:294:LYS:HB3	2:B:413:THR:OG1	1.98	0.63
2:E:455:VAL:HG11	2:E:463:HIS:HB2	1.80	0.63
1:F:104:PHE:CE2	1:F:106:LEU:HB2	2.33	0.63
1:A:328:ALA:O	1:A:333:MET:CG	2.46	0.63
2:B:62:ASN:O	2:B:66:GLU:HB2	1.98	0.63
2:E:94:LEU:O	2:E:98:VAL:HG23	1.98	0.63
1:F:140:ARG:HH11	1:F:140:ARG:HB3	1.61	0.63
2:C:344:LEU:HD11	2:C:346:ILE:HG13	1.79	0.63
2:E:344:LEU:HD22	2:E:345:LYS:H	1.63	0.63
2:D:328:ALA:HB2	5:D:552:HOH:O	1.97	0.63
2:D:208:ARG:NH2	2:D:221:GLU:OE2	2.31	0.63
1:F:382:ALA:O	1:F:385:ARG:HG3	1.97	0.63
2:D:446:ARG:H	2:D:496:ARG:NH1	1.97	0.63
1:A:25:ILE:HD12	1:A:58:GLN:CG	2.28	0.63
2:E:38:ILE:HA	2:E:177:THR:CG2	2.28	0.63
1:A:147:VAL:HG11	1:A:180:MET:CE	2.27	0.63
1:F:356:LEU:HD13	1:F:387:VAL:HG21	1.79	0.63
2:C:293:GLY:HA2	3:C:901:ATP:O1A	1.98	0.63
1:F:372:PRO:O	1:F:408:ILE:HD12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:447:GLY:HA2	2:D:489:ILE:CD1	2.29	0.63
1:A:218:ARG:CZ	1:A:239:ILE:HD12	2.29	0.63
2:B:273:MET:O	2:B:463:HIS:HA	1.98	0.63
2:B:147:VAL:O	2:B:150:VAL:HG12	1.98	0.63
2:B:239:ILE:HG12	2:B:244:ILE:HD13	1.81	0.63
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.80	0.63
2:E:202:ASP:HA	2:E:226:ARG:HD2	1.80	0.63
2:E:84:ILE:HG21	2:E:95:ALA:HB2	1.81	0.63
2:D:353:SER:O	2:D:354:ALA:HB2	1.98	0.63
2:B:80:PRO:O	2:B:84:ILE:HG12	1.99	0.63
2:B:387:VAL:HG12	2:B:388:SER:N	2.13	0.63
1:F:311:ARG:HD2	1:F:371:LYS:CE	2.29	0.63
2:D:123:LEU:CD1	2:D:166:ARG:HD2	2.24	0.63
2:C:313:ILE:HG12	2:C:345:LYS:HB3	1.81	0.63
2:B:360:LEU:HD22	2:B:360:LEU:O	1.97	0.63
2:C:146:SER:H	2:C:181:THR:HB	1.64	0.63
1:A:45:SER:HB3	1:A:182:THR:HB	1.80	0.62
2:C:43:LEU:HD11	2:C:182:THR:OG1	1.98	0.62
1:F:191:ILE:HB	1:F:198:GLU:HG3	1.80	0.62
2:B:203:ASN:HB3	2:B:225:LEU:HD23	1.81	0.62
2:D:114:GLY:O	2:D:115:GLN:HG3	1.98	0.62
1:A:254:LEU:HD22	1:F:348:CYS:CB	2.29	0.62
2:E:313:ILE:HG13	2:E:372:PRO:HG3	1.81	0.62
2:C:81:GLN:NE2	2:C:81:GLN:H	1.96	0.62
2:D:393:ARG:O	2:D:397:ILE:HG13	1.99	0.62
2:B:45:SER:CB	2:B:182:THR:HB	2.29	0.62
2:E:461:SER:OG	2:E:462:TRP:N	2.32	0.62
2:C:80:PRO:O	2:C:84:ILE:HG12	1.99	0.62
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.63	0.62
2:C:206:ILE:CD1	2:C:223:LEU:HB2	2.27	0.62
1:F:486:PHE:HB3	1:F:489:ILE:HD11	1.79	0.62
2:E:150:VAL:HG13	2:E:151:PHE:N	2.13	0.62
2:E:431:GLU:O	2:E:434:THR:HG22	2.00	0.62
1:A:433:ILE:HG22	1:A:433:ILE:O	1.99	0.62
1:A:273:MET:HG2	1:A:464:ASP:OD2	1.99	0.62
1:A:451:ARG:NH1	1:A:451:ARG:HG2	2.13	0.62
1:F:287:THR:HG21	1:F:425:ILE:O	1.99	0.62
2:D:231:MET:CE	2:D:251:ALA:HB2	2.30	0.62
1:A:335:PHE:O	1:A:338:MET:N	2.32	0.62
2:D:453:ILE:HG21	2:D:479:ILE:HD12	1.79	0.62
2:C:441:GLN:HE22	2:C:490:ILE:HD13	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:SEP:N	1:F:320:SEP:O2P	2.33	0.62
2:B:305:ALA:CB	2:B:374:ARG:HD2	2.21	0.62
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.80	0.62
2:B:24:MET:CB	2:B:62:ASN:HD22	2.12	0.62
1:F:186:GLU:OE2	1:F:187:GLU:N	2.32	0.62
2:B:471:MET:HE2	2:B:478:ASP:HB3	1.81	0.62
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.29	0.62
2:D:18:ILE:HD13	2:D:40:ARG:HH12	1.64	0.62
2:B:356:LEU:HD22	2:B:387:VAL:HG11	1.81	0.62
1:A:379:SER:OG	1:A:382:ALA:CB	2.48	0.62
2:E:437:ILE:CD1	2:E:457:LYS:HE2	2.29	0.62
2:E:287:THR:HG22	2:E:288:GLY:H	1.63	0.62
1:A:258:SER:OG	1:F:326:ARG:HD3	1.99	0.62
1:A:499:VAL:HG12	1:A:499:VAL:O	1.99	0.62
1:A:256:GLN:HG3	1:F:320:SEP:P	2.40	0.62
2:E:439:LEU:HD12	2:E:440:LEU:N	2.14	0.62
2:E:182:THR:HG21	2:E:192:ALA:HB1	1.82	0.62
2:D:344:LEU:HD13	2:D:344:LEU:C	2.20	0.62
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.29	0.62
1:F:298:VAL:HG22	1:F:411:LEU:HD23	1.80	0.61
1:F:315:PHE:CE1	1:F:375:ILE:HD11	2.35	0.61
1:F:134:ILE:HD11	1:F:142:VAL:CG2	2.29	0.61
2:C:232:LYS:N	2:C:232:LYS:HD2	2.14	0.61
2:C:371:LYS:CD	2:C:371:LYS:O	2.47	0.61
2:B:300:ARG:CA	2:B:333:MET:HE1	2.30	0.61
2:E:444:GLU:OE1	1:F:490:ILE:HG12	1.99	0.61
2:E:304:ASN:HB3	2:E:374:ARG:NH1	2.14	0.61
2:E:296:LEU:HD13	2:E:331:TRP:CD2	2.36	0.61
1:A:274:CYS:N	1:A:463:HIS:O	2.31	0.61
2:E:485:ASN:ND2	2:E:496:ARG:HH11	1.99	0.61
1:F:344:LEU:HD22	1:F:345:LYS:N	2.15	0.61
2:B:31:ILE:HA	2:B:231:MET:SD	2.41	0.61
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.81	0.61
2:D:445:ILE:HA	2:D:496:ARG:HH12	1.65	0.61
2:E:356:LEU:HD13	2:E:387:VAL:HG21	1.81	0.61
2:E:451:ARG:HD2	2:E:451:ARG:N	2.16	0.61
2:D:222:ILE:N	2:D:222:ILE:CD1	2.63	0.61
1:A:89:SER:CB	2:B:227:GLY:O	2.48	0.61
2:D:41:SER:HB3	2:D:178:THR:HB	1.83	0.61
1:A:364:LYS:HG2	1:A:402:TYR:CE2	2.35	0.61
1:A:148:THR:HG21	1:A:183:GLU:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:426:THR:HG21	2:D:430:ILE:HG12	1.82	0.61
1:A:327:ASN:ND2	1:A:331:TRP:CH2	2.69	0.61
1:F:311:ARG:HD2	1:F:371:LYS:HE3	1.83	0.61
1:A:183:GLU:HB2	2:B:199:PHE:CE1	2.35	0.61
2:B:117:VAL:HG12	2:B:117:VAL:O	2.01	0.61
1:A:377:ILE:HD13	1:A:412:PHE:CE2	2.36	0.61
2:C:20:LYS:HE3	2:C:228:THR:HG21	1.82	0.61
2:B:379:SER:CA	2:B:413:THR:HG22	2.31	0.61
2:D:79:THR:CG2	2:D:82:ASP:H	2.12	0.61
1:F:106:LEU:C	1:F:106:LEU:HD12	2.21	0.61
1:F:499:VAL:HG13	1:F:500:ASP:OD1	2.01	0.61
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.35	0.61
1:F:200:VAL:O	1:F:200:VAL:HG12	2.00	0.61
2:C:28:PHE:CA	2:C:246:ILE:HD12	2.31	0.61
2:E:496:ARG:HG3	2:E:497:ILE:N	2.14	0.61
2:C:469:GLU:HG3	2:C:480:LYS:HE3	1.81	0.61
1:A:441:GLN:HE22	1:A:490:ILE:HD13	1.65	0.61
2:B:335:PHE:O	2:B:339:GLU:HG3	2.01	0.60
1:F:300:ARG:N	1:F:333:MET:HE1	2.17	0.60
2:C:269:ARG:O	2:C:273:MET:HG3	2.01	0.60
1:F:170:ARG:NH1	1:F:170:ARG:HB3	2.16	0.60
2:B:284:ILE:HD12	2:B:410:GLY:O	2.01	0.60
2:B:221:GLU:HG3	2:B:233:GLY:O	2.01	0.60
1:A:316:ALA:O	1:A:348:CYS:HA	2.01	0.60
2:B:80:PRO:HB3	2:B:105:ILE:HG21	1.82	0.60
2:E:287:THR:CG2	2:E:414:ASN:HD22	2.10	0.60
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.64	0.60
1:F:451:ARG:HH11	1:F:451:ARG:HG2	1.66	0.60
2:D:433:ILE:HG22	2:D:433:ILE:O	2.00	0.60
1:A:462:TRP:O	1:A:463:HIS:ND1	2.34	0.60
2:C:418:GLN:HB2	2:D:423:HIS:O	2.01	0.60
2:C:164:LEU:HB3	2:C:200:VAL:HG11	1.83	0.60
1:A:161:ARG:NH2	1:F:149:SER:HB3	2.17	0.60
2:B:195:GLY:HA2	2:B:198:GLU:OE1	2.00	0.60
2:E:344:LEU:C	2:E:344:LEU:HD13	2.22	0.60
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.66	0.60
2:D:151:PHE:C	2:D:153:GLN:H	2.05	0.60
2:E:441:GLN:HE22	2:E:490:ILE:HD13	1.66	0.60
2:B:283:ILE:HD11	2:B:404:LYS:HG3	1.84	0.60
2:B:344:LEU:HD11	2:B:346:ILE:HD11	1.83	0.60
2:C:24:MET:HB2	2:C:62:ASN:ND2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:HD3	2:D:15:HIS:O	2.01	0.60
1:A:471:MET:HB3	1:A:480:LYS:NZ	2.15	0.60
2:B:237:PHE:CB	2:B:246:ILE:HG12	2.32	0.60
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.26	0.59
2:C:287:THR:CG2	2:C:414:ASN:HD22	2.12	0.59
2:E:164:LEU:HB3	2:E:200:VAL:HG11	1.84	0.59
2:E:284:ILE:N	2:E:284:ILE:HD12	2.17	0.59
2:E:499:VAL:HG12	2:E:499:VAL:O	2.02	0.59
2:B:382:ALA:O	2:B:385:ARG:HB2	2.02	0.59
2:C:239:ILE:HG12	2:C:244:ILE:HD13	1.84	0.59
2:E:426:THR:HG22	2:E:428:SER:N	2.17	0.59
2:D:267:VAL:CG2	2:D:300:ARG:HG2	2.30	0.59
2:D:169:ALA:O	2:D:173:GLN:HG3	2.02	0.59
2:D:47:THR:O	2:D:50:THR:HG23	2.02	0.59
2:B:219:THR:HB	2:B:234:GLU:HB3	1.84	0.59
2:C:182:THR:HG21	2:C:192:ALA:CB	2.31	0.59
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.33	0.59
1:A:98:VAL:HA	1:A:103:LEU:O	2.01	0.59
2:B:448:GLU:HG2	2:C:466:ALA:HA	1.84	0.59
2:D:130:ILE:O	2:D:134:ILE:HG12	2.02	0.59
1:A:164:LEU:CD1	1:A:197:GLU:HG3	2.32	0.59
1:A:495:THR:HG22	1:A:497:ILE:HG23	1.84	0.59
2:C:454:ASN:HB2	2:C:467:ILE:HD13	1.84	0.59
2:D:122:ASP:O	2:D:123:LEU:CB	2.51	0.59
2:E:294:LYS:HB2	3:E:901:ATP:O1B	2.02	0.59
1:A:392:PHE:HE2	1:A:430:ILE:HD11	1.67	0.59
2:C:395:PHE:O	2:C:399:VAL:HG23	2.02	0.59
2:B:377:ILE:HD13	2:B:412:PHE:CE2	2.37	0.59
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.34	0.59
2:C:437:ILE:HD11	2:C:457:LYS:HE2	1.84	0.59
1:F:461:SER:OG	1:F:462:TRP:N	2.34	0.59
2:C:471:MET:HG3	2:C:478:ASP:HB3	1.85	0.59
2:D:317:TYR:OH	2:D:363:ILE:HD11	2.02	0.59
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.83	0.59
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.28	0.59
2:E:269:ARG:O	2:E:273:MET:HG3	2.03	0.59
1:A:318:GLU:OE1	2:B:432:GLU:CB	2.50	0.59
2:D:287:THR:HG21	2:D:425:ILE:O	2.03	0.59
2:D:220:LEU:HD13	2:D:246:ILE:CD1	2.32	0.59
2:D:478:ASP:HA	5:D:555:HOH:O	2.01	0.59
2:C:387:VAL:HG12	2:C:388:SER:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:ASP:HB3	2:C:429:HIS:CE1	2.38	0.58
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.84	0.58
2:C:262:ARG:HH22	2:C:461:SER:CB	2.15	0.58
2:C:340:ARG:O	2:C:342:ASN:N	2.36	0.58
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.39	0.58
1:F:313:ILE:HD12	1:F:367:ILE:HD13	1.85	0.58
2:C:21:MET:HE3	2:C:141:ARG:CZ	2.31	0.58
1:A:325:LEU:HD23	1:A:335:PHE:CB	2.32	0.58
1:A:402:TYR:O	1:A:406:GLU:HB2	2.03	0.58
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.66	0.58
2:D:31:ILE:HG21	2:D:222:ILE:HD13	1.86	0.58
1:F:31:ILE:CD1	1:F:246:ILE:HG21	2.33	0.58
2:D:363:ILE:O	2:D:367:ILE:HG12	2.03	0.58
2:D:161:ARG:HD2	2:D:196:VAL:HG13	1.85	0.58
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.16	0.58
1:A:371:LYS:N	1:A:372:PRO:HD3	2.17	0.58
2:C:70:PRO:HD2	2:C:140:ARG:HG2	1.85	0.58
2:E:184:ARG:C	2:E:185:ILE:HD13	2.24	0.58
2:C:79:THR:HG22	2:C:82:ASP:HB2	1.86	0.58
1:A:284:ILE:H	1:A:284:ILE:HD12	1.67	0.58
1:F:375:ILE:O	1:F:410:GLY:HA2	2.04	0.58
2:B:451:ARG:HG2	2:B:451:ARG:NH1	2.12	0.58
2:C:311:ARG:HD2	2:C:371:LYS:HE3	1.86	0.58
2:C:313:ILE:HD11	2:C:370:PHE:HB3	1.84	0.58
2:D:79:THR:CG2	2:D:81:GLN:HG2	2.33	0.58
2:B:300:ARG:HA	2:B:333:MET:HE1	1.84	0.58
2:E:344:LEU:HD22	2:E:345:LYS:N	2.18	0.58
1:A:265:SER:O	1:A:301:PHE:HA	2.04	0.58
1:F:484:ARG:HB3	1:F:484:ARG:HH11	1.68	0.58
2:D:396:VAL:O	2:D:400:THR:HB	2.04	0.58
1:F:148:THR:HG21	1:F:193:ARG:HD2	1.84	0.58
2:D:182:THR:HG22	2:D:183:GLU:H	1.67	0.58
2:C:451:ARG:NH1	2:C:451:ARG:HG2	2.18	0.58
1:A:305:ALA:CB	1:A:374:ARG:HD2	2.25	0.58
2:B:151:PHE:C	2:B:153:GLN:H	2.07	0.58
1:F:426:THR:HB	1:F:431:GLU:OE2	2.03	0.58
2:E:140:ARG:HB3	2:E:140:ARG:HH11	1.68	0.58
1:A:127:ILE:HD11	1:A:167:LEU:CD1	2.33	0.58
2:D:418:GLN:HB2	2:E:423:HIS:O	2.04	0.58
2:B:51:GLY:N	3:B:903:ATP:O1B	2.36	0.58
2:E:377:ILE:CD1	2:E:399:VAL:HG11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:GLU:HG3	1:F:358:ASP:N	2.18	0.58
1:F:280:LYS:NZ	1:F:407:GLU:HB3	2.19	0.58
1:F:352:GLU:H	1:F:352:GLU:CD	2.07	0.58
2:B:496:ARG:HG2	2:B:498:THR:HG23	1.86	0.58
1:F:287:THR:HG23	1:F:414:ASN:ND2	2.14	0.58
2:D:192:ALA:HB3	2:D:197:GLU:OE2	2.04	0.58
2:D:266:GLY:O	2:D:300:ARG:HG3	2.04	0.58
1:A:64:ILE:HG22	1:A:65:ILE:HD13	1.86	0.58
1:A:272:GLU:C	1:A:273:MET:O	2.36	0.57
2:B:305:ALA:HB2	2:B:374:ARG:CD	2.21	0.57
2:E:123:LEU:CD2	2:E:127:ILE:HD11	2.33	0.57
2:E:50:THR:HG22	2:E:209:ASN:HB2	1.86	0.57
1:A:371:LYS:O	1:A:371:LYS:CD	2.52	0.57
2:B:285:LEU:HD23	2:B:437:ILE:CD1	2.31	0.57
2:C:147:VAL:HG11	2:C:180:MET:HE3	1.85	0.57
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.44	0.57
2:D:218:ARG:CZ	2:D:239:ILE:HD12	2.34	0.57
1:A:379:SER:OG	1:A:382:ALA:HB2	2.04	0.57
2:B:194:TYR:O	2:B:196:VAL:HG23	2.05	0.57
2:E:283:ILE:HG23	2:E:412:PHE:CE1	2.39	0.57
2:D:191:ILE:HB	2:D:198:GLU:HG3	1.85	0.57
2:E:140:ARG:HH11	2:E:140:ARG:CB	2.17	0.57
2:C:79:THR:HG23	2:C:82:ASP:H	1.69	0.57
2:C:353:SER:O	2:C:354:ALA:HB2	2.04	0.57
1:A:254:LEU:HD22	1:F:348:CYS:SG	2.45	0.57
2:B:191:ILE:HB	2:B:198:GLU:CD	2.25	0.57
1:A:150:VAL:HG13	1:A:151:PHE:N	2.18	0.57
2:D:47:THR:HG22	2:D:184:ARG:O	2.03	0.57
2:C:486:PHE:CB	2:C:489:ILE:HD11	2.34	0.57
1:F:118:VAL:O	1:F:118:VAL:HG13	2.03	0.57
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.40	0.57
1:A:363:ILE:O	1:A:367:ILE:HG12	2.05	0.57
2:D:79:THR:HG22	2:D:82:ASP:N	2.15	0.57
1:F:74:VAL:HB	1:F:144:ILE:HD13	1.86	0.57
2:D:31:ILE:HD11	2:D:246:ILE:HG21	1.85	0.57
2:D:183:GLU:HB2	2:E:199:PHE:CE1	2.39	0.57
2:C:334:ASP:OD1	2:C:336:GLU:HB2	2.05	0.57
2:C:14:GLU:HG3	2:C:16:GLN:H	1.69	0.57
2:D:79:THR:HG23	2:D:81:GLN:HG2	1.86	0.57
1:F:148:THR:OG1	1:F:182:THR:HG23	2.04	0.57
2:D:296:LEU:HD12	2:D:296:LEU:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:PHE:O	1:F:109:SER:HA	2.04	0.57
1:F:321:ARG:O	1:F:325:LEU:HD12	2.05	0.57
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.35	0.57
2:D:182:THR:CG2	2:D:183:GLU:N	2.67	0.57
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.39	0.57
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.86	0.57
1:A:266:GLY:CA	1:A:300:ARG:HG3	2.35	0.57
2:C:377:ILE:HD12	2:C:412:PHE:HE2	1.68	0.57
2:B:81:GLN:H	2:B:81:GLN:CD	2.08	0.57
2:C:353:SER:O	2:C:354:ALA:CB	2.53	0.57
1:A:302:VAL:HG12	1:A:303:GLU:N	2.20	0.57
1:A:313:ILE:CD1	1:A:372:PRO:HG2	2.34	0.57
2:B:294:LYS:N	3:B:901:ATP:O1B	2.37	0.57
2:B:334:ASP:O	2:B:338:MET:HG2	2.04	0.57
2:E:441:GLN:NE2	2:E:490:ILE:HD13	2.20	0.57
2:E:214:GLU:HB3	1:F:234:GLU:HB2	1.86	0.57
2:C:397:ILE:H	2:C:397:ILE:HD13	1.69	0.57
2:E:379:SER:N	2:E:413:THR:HB	2.17	0.57
2:D:296:LEU:HA	2:D:331:TRP:CZ3	2.40	0.57
2:B:264:SER:HA	2:B:271:ASP:OD1	2.05	0.57
1:A:439:LEU:HD12	1:A:440:LEU:N	2.20	0.56
2:B:150:VAL:O	2:B:153:GLN:HG3	2.05	0.56
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.70	0.56
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.18	0.56
1:F:371:LYS:CD	1:F:371:LYS:O	2.54	0.56
2:E:287:THR:HG21	2:E:425:ILE:O	2.06	0.56
2:D:31:ILE:CG2	2:D:222:ILE:CD1	2.84	0.56
1:A:487:GLU:HG3	1:A:497:ILE:CD1	2.34	0.56
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.87	0.56
2:E:163:GLU:HA	2:E:163:GLU:OE2	2.05	0.56
2:E:302:VAL:CG1	2:E:344:LEU:HD23	2.35	0.56
2:E:441:GLN:HE22	2:E:490:ILE:HA	1.70	0.56
1:A:479:ILE:H	1:A:479:ILE:HD12	1.69	0.56
2:C:33:HIS:CD2	2:C:230:HIS:HA	2.41	0.56
2:C:431:GLU:HA	2:C:434:THR:HG22	1.87	0.56
1:F:273:MET:O	1:F:463:HIS:HA	2.05	0.56
2:D:487:GLU:OE1	2:D:497:ILE:HD13	2.05	0.56
2:E:23:THR:OG1	2:E:29:ASP:OD1	2.24	0.56
2:B:264:SER:HB3	2:B:304:ASN:HD21	1.70	0.56
1:A:271:ASP:C	1:A:273:MET:O	2.44	0.56
1:A:41:SER:HA	1:A:178:THR:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:148:THR:CG2	2:E:193:ARG:HD2	2.35	0.56
2:B:248:PRO:HB2	2:B:251:ALA:HB3	1.87	0.56
1:F:504:GLU:O	1:F:505:LEU:HB2	2.03	0.56
1:A:328:ALA:O	1:A:333:MET:HG2	2.05	0.56
1:F:484:ARG:CB	1:F:484:ARG:NH1	2.68	0.56
1:F:352:GLU:N	1:F:352:GLU:CD	2.59	0.56
2:B:88:ARG:HG2	2:B:88:ARG:HH11	1.70	0.56
1:A:463:HIS:O	1:A:464:ASP:HB3	2.06	0.56
2:B:205:VAL:CG2	2:B:222:ILE:HD13	2.35	0.56
2:C:444:GLU:OE2	2:D:489:ILE:HG13	2.06	0.56
2:B:444:GLU:OE2	2:C:489:ILE:HG12	2.05	0.56
2:B:41:SER:OG	2:B:168:VAL:HG13	2.05	0.56
1:A:14:GLU:CG	1:A:15:HIS:N	2.60	0.56
1:A:153:GLN:O	1:A:154:TYR:HD2	1.87	0.56
2:B:418:GLN:HG3	2:B:418:GLN:O	2.06	0.56
2:E:497:ILE:HG22	2:E:498:THR:H	1.70	0.56
2:C:18:ILE:HB	2:C:228:THR:HG23	1.88	0.56
2:E:356:LEU:CD1	2:E:387:VAL:HG21	2.36	0.56
2:C:283:ILE:HD13	2:C:404:LYS:HE3	1.87	0.56
1:F:134:ILE:HD13	1:F:139:ALA:HB3	1.88	0.56
2:E:70:PRO:HB2	2:E:139:ALA:HA	1.88	0.56
2:B:185:ILE:H	2:B:185:ILE:HD12	1.71	0.56
2:C:393:ARG:NH2	2:C:429:HIS:HB2	2.21	0.56
2:E:462:TRP:CD2	2:E:463:HIS:O	2.59	0.56
1:F:144:ILE:CG2	1:F:147:VAL:HG12	2.36	0.56
2:D:347:VAL:HG12	2:D:348:CYS:N	2.20	0.56
1:A:88:ARG:NH1	1:A:88:ARG:HG2	2.20	0.56
2:B:196:VAL:O	2:B:200:VAL:HG23	2.06	0.55
2:C:54:LEU:CD2	2:C:244:ILE:HG12	2.36	0.55
2:D:76:PHE:CZ	2:D:126:LEU:HD21	2.41	0.55
1:A:347:VAL:O	1:A:348:CYS:HB2	2.06	0.55
2:B:462:TRP:O	2:B:463:HIS:CD2	2.60	0.55
2:C:238:THR:HG22	2:C:239:ILE:N	2.21	0.55
1:F:344:LEU:HD13	1:F:344:LEU:C	2.27	0.55
2:B:64:ILE:HG21	2:B:97:LEU:HD13	1.88	0.55
2:C:21:MET:O	2:C:35:GLY:HA3	2.07	0.55
1:A:471:MET:CE	1:A:478:ASP:HB3	2.36	0.55
2:E:191:ILE:HD12	2:E:206:ILE:HD11	1.87	0.55
1:A:333:MET:O	1:A:334:ASP:HB2	2.06	0.55
1:F:291:GLY:HA3	1:F:442:TYR:OH	2.07	0.55
2:D:340:ARG:O	2:D:342:ASN:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:O	1:A:125:ALA:HB2	2.05	0.55
1:A:323:GLN:CB	2:B:258:SER:OG	2.54	0.55
2:C:238:THR:HG22	2:C:239:ILE:H	1.70	0.55
1:F:191:ILE:CB	1:F:198:GLU:CG	2.84	0.55
2:E:396:VAL:HG11	2:E:430:ILE:HG21	1.89	0.55
2:B:90:PHE:HB2	2:B:92:TRP:CE2	2.41	0.55
2:D:191:ILE:CD1	2:D:198:GLU:HG2	2.36	0.55
2:D:76:PHE:HZ	2:D:126:LEU:HD21	1.70	0.55
2:D:89:SER:HB2	2:E:227:GLY:O	2.07	0.55
2:B:150:VAL:HG13	2:B:151:PHE:N	2.22	0.55
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.36	0.55
2:E:150:VAL:CG1	2:E:151:PHE:N	2.69	0.55
2:E:193:ARG:NH2	1:F:195:GLY:O	2.32	0.55
2:C:471:MET:CG	2:C:478:ASP:HB3	2.37	0.55
2:C:67:PHE:HB2	2:C:69:GLU:HG3	1.88	0.55
1:A:18:ILE:CD1	1:F:85:LYS:HG3	2.36	0.55
1:A:317:TYR:OH	1:A:363:ILE:HD11	2.07	0.55
2:E:348:CYS:HB3	1:F:254:LEU:HD23	1.89	0.55
1:F:443:VAL:CG1	1:F:445:ILE:HD11	2.37	0.55
2:C:225:LEU:HD12	2:C:230:HIS:HB3	1.89	0.55
1:F:316:ALA:O	1:F:348:CYS:HA	2.06	0.55
1:F:508:ILE:O	1:F:509:VAL:HB	2.06	0.55
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.68	0.55
2:C:336:GLU:OE1	2:C:336:GLU:HA	2.07	0.55
1:F:371:LYS:HD2	1:F:371:LYS:O	2.07	0.55
2:E:313:ILE:HG13	2:E:372:PRO:HG2	1.89	0.55
2:B:313:ILE:HG13	2:B:372:PRO:CG	2.37	0.55
2:E:20:LYS:HE3	2:E:228:THR:HG21	1.88	0.55
1:A:505:LEU:O	1:A:508:ILE:HD11	2.06	0.55
2:C:340:ARG:C	2:C:342:ASN:H	2.09	0.55
2:E:294:LYS:N	3:E:901:ATP:O1B	2.39	0.55
1:A:400:THR:HG22	1:A:401:GLY:N	2.22	0.55
1:F:501:GLU:HG3	1:F:502:LYS:N	2.22	0.55
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.89	0.55
1:F:336:GLU:HB3	1:F:340:ARG:NH2	2.21	0.55
2:C:397:ILE:N	2:C:397:ILE:CD1	2.69	0.55
2:E:451:ARG:HH11	2:E:451:ARG:HG2	1.72	0.55
2:E:336:GLU:HA	2:E:336:GLU:OE1	2.05	0.55
2:E:145:ASP:OD2	2:E:181:THR:HG21	2.06	0.55
1:A:448:GLU:HG2	2:B:466:ALA:HB2	1.89	0.55
1:A:322:ALA:HB3	2:B:256:GLN:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:443:VAL:HG12	2:D:445:ILE:HD11	1.89	0.54
2:E:86:ASN:OD1	1:F:18:ILE:HD11	2.06	0.54
1:F:486:PHE:HB2	1:F:489:ILE:HD11	1.89	0.54
1:A:296:LEU:HD22	1:A:472:ILE:HD12	1.87	0.54
2:D:387:VAL:CG1	2:D:388:SER:N	2.70	0.54
2:B:205:VAL:HG23	2:B:222:ILE:HD13	1.89	0.54
2:B:81:GLN:H	2:B:81:GLN:NE2	2.04	0.54
1:F:280:LYS:HZ3	1:F:407:GLU:HB3	1.73	0.54
2:D:215:ARG:HA	2:D:215:ARG:NE	2.22	0.54
2:B:265:SER:HB2	2:B:270:LEU:HD13	1.90	0.54
1:A:200:VAL:O	1:A:200:VAL:HG12	2.07	0.54
2:E:347:VAL:HG12	2:E:348:CYS:N	2.21	0.54
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.07	0.54
2:E:79:THR:HG21	2:E:81:GLN:HG2	1.88	0.54
2:C:206:ILE:N	2:C:206:ILE:HD12	2.22	0.54
1:F:169:ALA:O	1:F:173:GLN:HG3	2.07	0.54
2:B:129:ARG:O	2:B:132:TYR:HB3	2.07	0.54
1:F:23:THR:HB	1:F:25:ILE:HG12	1.88	0.54
2:B:93:ASP:OD1	2:B:95:ALA:HB3	2.07	0.54
2:D:484:ARG:HH11	2:D:484:ARG:HB3	1.72	0.54
2:B:202:ASP:HA	2:B:226:ARG:HD2	1.89	0.54
2:B:479:ILE:HD12	2:B:479:ILE:N	2.20	0.54
2:E:169:ALA:O	2:E:173:GLN:HG3	2.07	0.54
2:D:323:GLN:NE2	2:E:459:ARG:HD3	2.22	0.54
2:D:426:THR:HG22	2:D:428:SER:H	1.72	0.54
2:B:286:ALA:HA	2:B:438:ILE:O	2.08	0.54
2:C:464:ASP:OD1	2:C:465:LYS:N	2.40	0.54
2:D:443:VAL:CG1	2:D:445:ILE:HD11	2.38	0.54
2:C:426:THR:HG22	2:C:428:SER:H	1.72	0.54
2:C:437:ILE:N	2:C:437:ILE:HD12	2.22	0.54
2:C:127:ILE:CD1	2:C:167:LEU:HD13	2.37	0.54
2:C:461:SER:OG	2:C:462:TRP:N	2.39	0.54
2:B:178:THR:HG22	2:B:179:VAL:N	2.22	0.54
2:C:111:ASP:O	2:C:113:GLU:N	2.34	0.54
1:F:117:VAL:O	1:F:118:VAL:HB	2.07	0.54
1:A:56:SER:HB2	1:A:143:SER:HB3	1.89	0.54
2:B:273:MET:O	2:B:464:ASP:N	2.36	0.54
2:C:127:ILE:HD13	2:C:127:ILE:N	2.23	0.54
2:D:195:GLY:HA2	2:D:198:GLU:OE1	2.08	0.54
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.22	0.54
2:E:54:LEU:HD23	2:E:244:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:GLN:HE21	2:B:404:LYS:HB3	1.72	0.54
1:F:126:LEU:O	1:F:130:ILE:HG12	2.06	0.54
1:A:508:ILE:N	1:A:508:ILE:HD13	2.19	0.54
2:B:24:MET:HB2	2:B:62:ASN:HD22	1.72	0.54
1:F:45:SER:HB2	1:F:182:THR:HB	1.89	0.54
1:A:455:VAL:HG11	1:A:463:HIS:CD2	2.40	0.54
2:B:46:GLY:CA	2:B:50:THR:HG21	2.35	0.54
2:D:31:ILE:CG2	2:D:222:ILE:HD13	2.38	0.54
2:B:38:ILE:HA	2:B:177:THR:CG2	2.38	0.54
2:B:21:MET:CB	2:B:38:ILE:HG12	2.37	0.54
2:D:394:GLN:HA	2:D:397:ILE:HD12	1.88	0.54
1:F:469:GLU:HG3	1:F:470:PHE:N	2.23	0.54
1:A:502:LYS:O	1:A:503:SER:HB3	2.08	0.54
1:F:313:ILE:HB	1:F:375:ILE:CD1	2.35	0.54
1:F:197:GLU:H	1:F:197:GLU:CD	2.11	0.54
2:B:372:PRO:O	2:B:408:ILE:HD12	2.08	0.54
2:B:31:ILE:HD13	2:B:231:MET:SD	2.47	0.54
2:D:443:VAL:O	2:D:445:ILE:CD1	2.54	0.54
1:A:296:LEU:HD13	1:A:331:TRP:CE2	2.42	0.54
1:A:470:PHE:HE1	1:A:472:ILE:HD11	1.73	0.54
2:B:264:SER:HB3	2:B:304:ASN:ND2	2.22	0.54
2:B:67:PHE:HB2	2:B:69:GLU:HG3	1.89	0.54
1:F:294:LYS:N	3:F:901:ATP:O1B	2.41	0.53
2:E:127:ILE:CD1	2:E:167:LEU:HD13	2.38	0.53
2:D:225:LEU:HD12	2:D:230:HIS:HB3	1.90	0.53
2:E:325:LEU:CD2	2:E:335:PHE:HB2	2.38	0.53
1:A:20:LYS:HD3	1:A:35:GLY:O	2.07	0.53
2:C:31:ILE:HA	2:C:231:MET:SD	2.48	0.53
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.43	0.53
1:A:378:ASP:O	1:A:379:SER:CB	2.57	0.53
2:E:152:GLN:HG3	1:F:161:ARG:HH11	1.73	0.53
1:A:372:PRO:HB2	1:A:375:ILE:CD1	2.38	0.53
2:E:347:VAL:O	2:E:348:CYS:HB2	2.08	0.53
2:C:283:ILE:CD1	2:C:404:LYS:HG3	2.37	0.53
1:A:123:LEU:O	1:A:127:ILE:HG12	2.09	0.53
2:D:106:LEU:CD1	2:D:129:ARG:NH2	2.72	0.53
2:D:419:PHE:O	2:D:420:MET:HB2	2.08	0.53
2:D:256:GLN:HG3	2:D:404:LYS:HD3	1.90	0.53
1:A:462:TRP:O	1:A:463:HIS:CG	2.61	0.53
1:A:41:SER:CB	1:A:178:THR:HB	2.29	0.53
2:E:79:THR:CG2	2:E:82:ASP:H	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:414:ASN:ND2	1:F:426:THR:HG23	2.23	0.53
2:D:151:PHE:O	2:D:153:GLN:N	2.38	0.53
2:E:449:MET:HE3	1:F:467:ILE:HD11	1.90	0.53
1:A:336:GLU:O	1:A:339:GLU:HB2	2.08	0.53
1:F:178:THR:HG22	1:F:179:VAL:N	2.23	0.53
2:D:80:PRO:O	2:D:84:ILE:HG12	2.08	0.53
2:B:206:ILE:N	2:B:206:ILE:HD12	2.24	0.53
2:C:248:PRO:HB2	2:C:251:ALA:HB3	1.90	0.53
2:B:469:GLU:HG3	2:B:470:PHE:N	2.23	0.53
2:B:483:PHE:HB3	2:B:486:PHE:CD1	2.29	0.53
2:B:84:ILE:HA	2:B:94:LEU:HD12	1.89	0.53
1:A:183:GLU:CB	2:B:199:PHE:CE1	2.91	0.53
1:A:374:ARG:O	1:A:375:ILE:HD12	2.08	0.53
2:B:191:ILE:CB	2:B:198:GLU:HG3	2.39	0.53
2:E:287:THR:HG22	2:E:288:GLY:N	2.23	0.53
1:F:125:ALA:O	1:F:129:ARG:HG3	2.07	0.53
1:F:443:VAL:O	1:F:445:ILE:HD12	2.07	0.53
2:D:178:THR:HG22	2:D:179:VAL:N	2.23	0.53
2:C:356:LEU:HD22	2:C:387:VAL:HG11	1.91	0.53
1:F:56:SER:HB2	1:F:143:SER:HB3	1.90	0.53
2:D:468:ARG:HH11	2:D:468:ARG:HG2	1.74	0.53
1:A:376:ALA:HA	1:A:411:LEU:O	2.09	0.53
2:D:446:ARG:H	2:D:496:ARG:HH22	1.57	0.53
1:A:327:ASN:OD1	2:B:459:ARG:O	2.27	0.53
2:B:18:ILE:HB	2:B:228:THR:CG2	2.38	0.53
2:C:308:ASN:O	2:C:310:GLU:HG3	2.08	0.53
1:A:170:ARG:O	1:A:174:ILE:HG12	2.09	0.53
2:C:123:LEU:HA	2:C:127:ILE:CD1	2.39	0.53
2:D:150:VAL:O	2:D:153:GLN:HG3	2.09	0.53
2:D:21:MET:HE3	2:D:59:PHE:CZ	2.44	0.53
2:B:123:LEU:O	2:B:123:LEU:HD13	2.09	0.53
2:D:31:ILE:HG21	2:D:222:ILE:HD11	1.90	0.53
2:C:347:VAL:O	2:C:348:CYS:HB2	2.08	0.53
1:A:31:ILE:HD11	1:A:246:ILE:CG2	2.30	0.53
2:D:150:VAL:HG13	2:D:151:PHE:N	2.23	0.53
2:D:315:PHE:HE1	2:D:375:ILE:HD12	1.73	0.53
2:D:140:ARG:HH11	2:D:140:ARG:CB	2.20	0.53
1:A:296:LEU:CD2	1:A:472:ILE:HD12	2.39	0.53
2:C:378:ASP:O	2:C:379:SER:HB3	2.09	0.53
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.89	0.53
1:F:504:GLU:HA	1:F:507:ARG:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:O	1:A:409:THR:OG1	2.23	0.53
2:E:259:SER:N	2:E:281:ASP:OD2	2.42	0.53
2:C:123:LEU:HD12	2:C:163:GLU:OE2	2.09	0.52
2:C:126:LEU:O	2:C:129:ARG:HB2	2.10	0.52
2:C:182:THR:CG2	2:C:183:GLU:N	2.72	0.52
2:B:220:LEU:HD13	2:B:246:ILE:HD13	1.91	0.52
2:B:64:ILE:HG22	2:B:65:ILE:HD13	1.90	0.52
2:C:42:THR:HA	2:C:203:ASN:HB2	1.91	0.52
1:A:320:SEP:O1P	2:B:256:GLN:CG	2.57	0.52
2:B:318:GLU:OE2	2:C:432:GLU:HG2	2.10	0.52
1:F:467:ILE:HG22	1:F:467:ILE:O	2.09	0.52
1:F:338:MET:HB3	1:F:344:LEU:CB	2.37	0.52
2:C:146:SER:HA	2:C:181:THR:O	2.08	0.52
2:C:18:ILE:HD12	2:C:18:ILE:N	2.24	0.52
2:C:486:PHE:CE2	2:C:496:ARG:HG2	2.44	0.52
1:F:115:GLN:HG3	1:F:116:GLU:N	2.23	0.52
2:B:298:VAL:HG11	2:B:314:LEU:HD11	1.89	0.52
2:E:72:VAL:HG21	2:E:134:ILE:HD13	1.91	0.52
2:D:266:GLY:HA3	2:D:300:ARG:O	2.08	0.52
2:D:451:ARG:HH11	2:D:451:ARG:CG	2.19	0.52
1:A:306:CYS:SG	1:A:338:MET:SD	3.08	0.52
2:D:468:ARG:NH1	2:D:468:ARG:HG2	2.25	0.52
2:B:320:SER:HA	2:C:254:LEU:HG	1.91	0.52
2:C:267:VAL:HB	2:C:270:LEU:HB2	1.92	0.52
2:B:379:SER:N	2:B:413:THR:HG22	2.24	0.52
1:F:303:GLU:OE2	1:F:333:MET:HB3	2.10	0.52
1:F:468:ARG:NH1	1:F:468:ARG:HG2	2.25	0.52
1:A:153:GLN:O	1:A:154:TYR:HB3	2.10	0.52
2:C:262:ARG:NE	2:C:279:PHE:CE2	2.77	0.52
2:D:470:PHE:CE1	2:D:472:ILE:HD11	2.44	0.52
1:F:170:ARG:HD2	1:F:173:GLN:OE1	2.10	0.52
3:D:903:ATP:O3'	2:E:224:LYS:HB2	2.09	0.52
1:F:291:GLY:HA3	1:F:442:TYR:HH	1.75	0.52
2:B:89:SER:HB2	2:C:227:GLY:O	2.09	0.52
2:C:73:PHE:HD1	2:C:143:SER:HB2	1.74	0.52
1:A:379:SER:OG	1:A:382:ALA:N	2.43	0.52
2:C:356:LEU:CD2	2:C:387:VAL:HG11	2.39	0.52
1:A:510:ARG:HA	1:A:510:ARG:NE	2.25	0.52
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.92	0.52
2:E:439:LEU:HD12	2:E:440:LEU:H	1.74	0.52
1:F:445:ILE:HD13	1:F:450:SER:OG	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ILE:HA	2:B:177:THR:HG23	1.92	0.52
2:C:111:ASP:CG	2:C:113:GLU:HG2	2.30	0.52
2:B:220:LEU:HD13	2:B:246:ILE:CD1	2.40	0.52
2:C:79:THR:HG22	2:C:82:ASP:CB	2.39	0.52
2:E:437:ILE:HD11	2:E:457:LYS:HE2	1.92	0.52
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.92	0.52
2:C:348:CYS:HB3	2:D:254:LEU:HB3	1.89	0.52
2:C:142:VAL:O	2:C:178:THR:HA	2.09	0.52
2:B:471:MET:HB3	2:B:480:LYS:HZ1	1.75	0.52
1:A:45:SER:CB	1:A:182:THR:HB	2.40	0.52
1:A:82:ASP:O	1:A:85:LYS:HB3	2.10	0.52
2:D:301:PHE:CE1	2:D:374:ARG:HD3	2.44	0.52
2:E:203:ASN:HB3	2:E:225:LEU:HD23	1.91	0.52
1:A:479:ILE:HD12	1:A:479:ILE:N	2.25	0.52
1:F:23:THR:CB	1:F:25:ILE:HG12	2.39	0.52
1:A:320:SEP:O	1:A:324:LEU:HD12	2.10	0.52
2:B:51:GLY:O	2:B:52:LYS:C	2.47	0.52
2:E:469:GLU:HB3	2:E:483:PHE:CZ	2.44	0.52
1:A:471:MET:HB3	1:A:480:LYS:HZ1	1.73	0.52
1:F:500:ASP:O	1:F:501:GLU:CB	2.57	0.52
2:E:184:ARG:HD2	2:E:191:ILE:O	2.10	0.52
1:A:456:PHE:HE2	1:F:290:THR:HG23	1.73	0.52
2:B:289:ALA:HB2	2:B:419:PHE:HA	1.92	0.52
1:A:206:ILE:N	1:A:206:ILE:HD12	2.24	0.52
2:B:209:ASN:HD21	2:B:216:ARG:HB3	1.74	0.52
2:E:299:SER:O	2:E:333:MET:HE2	2.09	0.52
2:B:145:ASP:HA	2:B:181:THR:HB	1.92	0.52
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.92	0.52
2:B:232:LYS:N	2:B:232:LYS:HD2	2.24	0.52
2:E:160:VAL:HG21	2:E:194:TYR:CD2	2.44	0.52
2:E:313:ILE:HG22	2:E:314:LEU:N	2.25	0.52
2:C:150:VAL:HG13	2:C:151:PHE:N	2.24	0.52
1:F:74:VAL:HG21	1:F:130:ILE:HD12	1.91	0.52
1:F:191:ILE:CB	1:F:198:GLU:HG3	2.39	0.52
1:A:151:PHE:C	1:A:153:GLN:H	2.14	0.52
2:C:65:ILE:N	2:C:65:ILE:HD12	2.25	0.52
1:A:218:ARG:NH1	1:A:239:ILE:HD12	2.25	0.52
1:A:284:ILE:HB	1:A:411:LEU:HD12	1.91	0.51
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.91	0.51
2:C:182:THR:CG2	2:C:183:GLU:H	2.23	0.51
2:E:153:GLN:C	1:F:158:SER:HB2	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:516:GLY:N	1:F:517:PRO:HD2	2.24	0.51
2:C:61:TYR:CD2	2:C:65:ILE:HD13	2.46	0.51
1:A:254:LEU:O	1:A:254:LEU:CD2	2.57	0.51
2:E:413:THR:HG22	2:E:414:ASN:N	2.25	0.51
1:F:462:TRP:CE3	1:F:463:HIS:N	2.73	0.51
1:A:415:THR:HB	2:B:432:GLU:OE1	2.11	0.51
2:C:495:THR:HG22	2:D:487:GLU:OE2	2.10	0.51
1:F:220:LEU:C	1:F:220:LEU:HD23	2.30	0.51
2:B:316:ALA:O	2:B:348:CYS:HA	2.11	0.51
1:A:377:ILE:N	1:A:377:ILE:HD12	2.25	0.51
2:E:98:VAL:HA	2:E:103:LEU:O	2.10	0.51
2:E:454:ASN:HD21	2:E:456:PHE:HA	1.75	0.51
2:C:48:SER:HB2	2:D:199:PHE:CE1	2.46	0.51
1:A:446:ARG:HA	1:A:496:ARG:NH2	2.25	0.51
1:F:360:LEU:O	1:F:360:LEU:HD22	2.10	0.51
2:C:123:LEU:CD2	2:C:167:LEU:HB2	2.38	0.51
1:F:104:PHE:HE2	1:F:106:LEU:HB2	1.76	0.51
2:E:496:ARG:C	2:E:497:ILE:HD13	2.31	0.51
1:A:425:ILE:HD13	1:A:437:ILE:HD13	1.92	0.51
2:B:315:PHE:CD2	2:B:347:VAL:HG21	2.46	0.51
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.40	0.51
2:D:203:ASN:HB3	2:D:225:LEU:HD23	1.92	0.51
1:A:467:ILE:N	1:A:467:ILE:HD12	2.25	0.51
1:A:87:ALA:O	1:A:92:TRP:CD1	2.62	0.51
1:F:315:PHE:HE1	1:F:375:ILE:HD11	1.74	0.51
2:D:145:ASP:OD2	2:D:181:THR:HG21	2.11	0.51
1:F:270:LEU:O	1:F:273:MET:HB2	2.10	0.51
2:B:371:LYS:N	2:B:372:PRO:HD3	2.25	0.51
2:E:151:PHE:C	2:E:153:GLN:H	2.14	0.51
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.46	0.51
1:F:380:LEU:O	1:F:382:ALA:N	2.43	0.51
2:C:21:MET:HB2	2:C:38:ILE:HG12	1.93	0.51
2:C:206:ILE:HD12	2:C:206:ILE:H	1.76	0.51
2:C:54:LEU:O	2:C:57:ILE:N	2.44	0.51
2:E:127:ILE:HD12	2:E:167:LEU:CD1	2.41	0.51
1:F:73:PHE:HB3	1:F:105:ILE:HD13	1.91	0.51
1:A:279:PHE:HB2	1:A:282:SER:HB3	1.93	0.51
2:B:240:THR:HG21	2:B:361:GLN:HE22	1.76	0.51
2:D:185:ILE:H	2:D:185:ILE:HD12	1.76	0.51
2:C:220:LEU:C	2:C:220:LEU:HD23	2.31	0.51
2:D:461:SER:OG	2:D:462:TRP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:445:ILE:N	2:D:445:ILE:HD12	2.26	0.51
2:B:80:PRO:CB	2:B:105:ILE:HG21	2.41	0.51
1:F:468:ARG:HH11	1:F:468:ARG:HG2	1.75	0.51
2:D:31:ILE:HA	2:D:231:MET:SD	2.51	0.51
2:C:121:PHE:CD1	2:C:121:PHE:N	2.79	0.51
2:B:18:ILE:HB	2:B:228:THR:HG23	1.93	0.51
2:B:469:GLU:HB2	2:B:483:PHE:CZ	2.46	0.51
2:B:187:GLU:O	2:B:208:ARG:HD3	2.11	0.51
2:B:161:ARG:NH2	2:B:199:PHE:HB2	2.26	0.51
2:E:52:LYS:HD3	2:E:182:THR:O	2.10	0.51
1:F:451:ARG:HB3	1:F:470:PHE:CE2	2.46	0.51
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.25	0.51
1:A:463:HIS:O	1:A:464:ASP:CB	2.59	0.51
1:A:254:LEU:HD11	1:F:319:GLU:O	2.11	0.51
2:E:359:HIS:O	2:E:363:ILE:HG12	2.10	0.51
2:C:431:GLU:O	2:C:432:GLU:HB2	2.09	0.51
2:C:151:PHE:C	2:C:153:GLN:N	2.63	0.51
2:B:381:SER:HB3	2:B:414:ASN:OD1	2.10	0.51
2:C:184:ARG:HG2	2:C:191:ILE:O	2.11	0.51
1:A:470:PHE:CE1	1:A:472:ILE:HD11	2.45	0.51
1:A:433:ILE:O	1:A:433:ILE:CG2	2.59	0.51
1:F:284:ILE:HD12	1:F:410:GLY:O	2.11	0.51
1:F:320:SEP:O	1:F:324:LEU:HB2	2.10	0.51
2:B:451:ARG:CG	2:B:451:ARG:NH1	2.74	0.51
2:C:252:MET:HE3	2:C:397:ILE:HG22	1.92	0.51
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.93	0.51
2:C:214:GLU:OE2	2:D:217:ARG:NH1	2.44	0.51
2:D:437:ILE:CD1	2:D:457:LYS:HE2	2.41	0.51
1:A:140:ARG:HH11	1:A:140:ARG:CB	2.23	0.50
2:E:123:LEU:HD23	2:E:127:ILE:CD1	2.37	0.50
1:F:148:THR:HG21	1:F:183:GLU:HG3	1.93	0.50
2:E:28:PHE:N	2:E:246:ILE:HD12	2.26	0.50
1:F:312:ALA:HA	1:F:374:ARG:O	2.12	0.50
2:D:214:GLU:HA	2:E:234:GLU:OE1	2.12	0.50
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.93	0.50
1:A:320:SEP:CB	2:B:254:LEU:O	2.36	0.50
2:C:28:PHE:HE1	2:C:222:ILE:HD11	1.71	0.50
2:D:446:ARG:HB3	2:E:484:ARG:HG3	1.93	0.50
1:F:79:THR:HG23	1:F:81:GLN:HG2	1.92	0.50
2:B:147:VAL:HG11	2:B:180:MET:HE2	1.90	0.50
2:C:38:ILE:HA	2:C:177:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:VAL:CG1	2:D:151:PHE:N	2.75	0.50
1:F:203:ASN:HB3	1:F:225:LEU:CD2	2.40	0.50
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.45	0.50
2:B:440:LEU:CD2	2:B:453:ILE:HG12	2.40	0.50
2:D:385:ARG:HG2	2:E:393:ARG:NH1	2.26	0.50
2:B:280:LYS:NZ	2:B:407:GLU:HB3	2.26	0.50
2:D:371:LYS:CD	2:D:371:LYS:O	2.48	0.50
2:C:360:LEU:HA	2:C:363:ILE:HD12	1.93	0.50
1:A:79:THR:HG22	1:A:82:ASP:H	1.76	0.50
2:D:323:GLN:HE22	2:E:459:ARG:HD3	1.75	0.50
2:E:191:ILE:HD12	2:E:206:ILE:HG13	1.93	0.50
1:A:116:GLU:O	1:A:117:VAL:HG23	2.10	0.50
2:D:211:LEU:HA	2:D:216:ARG:HD3	1.93	0.50
1:A:148:THR:HG21	1:A:183:GLU:CG	2.41	0.50
1:A:118:VAL:HG23	1:A:153:GLN:OE1	2.11	0.50
2:D:161:ARG:HB2	2:D:196:VAL:CG1	2.41	0.50
1:F:140:ARG:CB	1:F:140:ARG:HH11	2.24	0.50
2:D:402:TYR:O	2:D:405:GLN:HG2	2.12	0.50
2:B:485:ASN:N	2:B:485:ASN:OD1	2.44	0.50
1:A:271:ASP:O	1:A:273:MET:O	2.30	0.50
1:F:313:ILE:HG13	1:F:372:PRO:CG	2.41	0.50
1:F:123:LEU:O	1:F:123:LEU:HD13	2.10	0.50
1:F:151:PHE:O	1:F:153:GLN:N	2.42	0.50
1:A:335:PHE:O	1:A:336:GLU:C	2.48	0.50
1:A:456:PHE:CE2	1:F:290:THR:HG23	2.46	0.50
2:B:249:LEU:CD1	2:B:394:GLN:HG2	2.42	0.50
2:E:255:THR:O	2:E:255:THR:HG22	2.11	0.50
2:E:118:VAL:HG12	2:E:118:VAL:O	2.12	0.50
2:D:446:ARG:H	2:D:496:ARG:NH2	2.10	0.50
1:F:18:ILE:HD11	1:F:227:GLY:HA3	1.87	0.50
1:F:462:TRP:CD2	1:F:463:HIS:N	2.80	0.50
2:E:148:THR:HG21	2:E:183:GLU:CG	2.42	0.50
1:A:435:ASP:HA	1:A:459:ARG:HD2	1.93	0.50
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.94	0.50
2:D:334:ASP:OD1	2:D:336:GLU:HB2	2.11	0.50
1:F:79:THR:CG2	1:F:81:GLN:HG2	2.42	0.50
2:C:393:ARG:HH21	2:C:429:HIS:CB	2.22	0.50
2:E:440:LEU:CD2	2:E:453:ILE:HG12	2.41	0.50
1:F:425:ILE:HD11	1:F:456:PHE:CD2	2.46	0.50
2:B:237:PHE:HB2	2:B:246:ILE:HG12	1.93	0.50
2:B:248:PRO:O	2:B:251:ALA:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HD12	1:A:102:LYS:HB3	1.94	0.50
2:E:54:LEU:HD23	2:E:244:ILE:CD1	2.42	0.50
2:B:68:ASP:OD1	2:B:102:LYS:NZ	2.44	0.50
2:B:106:LEU:HD12	2:B:106:LEU:C	2.32	0.50
2:B:433:ILE:O	2:B:433:ILE:HG22	2.12	0.50
1:F:317:TYR:CD2	1:F:383:LEU:HD21	2.47	0.50
2:C:127:ILE:HD13	2:C:127:ILE:H	1.77	0.50
2:C:54:LEU:HD13	2:C:90:PHE:CZ	2.47	0.50
1:F:151:PHE:C	1:F:153:GLN:N	2.65	0.50
1:A:153:GLN:O	1:A:154:TYR:CD2	2.64	0.50
2:C:41:SER:OG	2:C:168:VAL:HG13	2.11	0.50
1:F:353:SER:O	1:F:354:ALA:HB2	2.11	0.50
2:B:358:ASP:O	2:B:362:ILE:HG12	2.11	0.50
2:D:127:ILE:HD11	2:D:167:LEU:HD13	1.94	0.49
1:A:45:SER:HA	1:A:182:THR:O	2.12	0.49
2:D:81:GLN:CD	2:D:81:GLN:N	2.66	0.49
2:E:385:ARG:HA	1:F:393:ARG:NH1	2.27	0.49
1:F:504:GLU:HA	1:F:507:ARG:CG	2.41	0.49
1:A:467:ILE:HD13	1:F:447:GLY:C	2.32	0.49
2:C:214:GLU:C	2:C:215:ARG:HE	2.15	0.49
2:C:116:GLU:O	2:C:117:VAL:HB	2.11	0.49
1:A:136:LYS:HD3	1:A:137:TYR:CE1	2.47	0.49
2:C:313:ILE:HD12	2:C:372:PRO:HG2	1.93	0.49
2:C:52:LYS:HD2	2:C:182:THR:O	2.12	0.49
2:E:396:VAL:HG11	2:E:430:ILE:CG2	2.42	0.49
1:A:484:ARG:CB	1:A:484:ARG:NH1	2.74	0.49
1:A:419:PHE:O	1:A:420:MET:HB2	2.12	0.49
1:F:49:GLY:CA	3:F:903:ATP:O2B	2.59	0.49
2:C:117:VAL:HG12	2:C:117:VAL:O	2.11	0.49
2:C:252:MET:CE	2:C:397:ILE:HG22	2.42	0.49
1:A:426:THR:HG22	1:A:428:SER:H	1.77	0.49
2:C:52:LYS:N	3:C:903:ATP:O1B	2.45	0.49
1:F:287:THR:HG23	1:F:414:ASN:HB3	1.93	0.49
1:A:436:THR:HG23	1:A:457:LYS:O	2.12	0.49
1:F:514:GLU:HG2	1:F:519:SER:HB3	1.93	0.49
2:C:289:ALA:HB2	2:C:419:PHE:HA	1.93	0.49
1:A:377:ILE:HG22	1:A:379:SER:O	2.13	0.49
2:C:18:ILE:HG21	2:C:37:PRO:HB3	1.95	0.49
1:F:33:HIS:CD2	1:F:229:SER:OG	2.65	0.49
2:D:121:PHE:O	2:D:124:SER:OG	2.26	0.49
2:E:309:LYS:HA	2:E:343:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:333:MET:CG	5:D:910:HOH:O	2.60	0.49
1:F:144:ILE:HG22	1:F:147:VAL:HG12	1.94	0.49
2:C:191:ILE:HB	2:C:198:GLU:HG3	1.91	0.49
2:E:140:ARG:HH11	2:E:140:ARG:CA	2.25	0.49
1:A:218:ARG:O	1:A:236:PRO:HA	2.12	0.49
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.43	0.49
2:C:486:PHE:HB2	2:C:489:ILE:HD11	1.94	0.49
1:A:448:GLU:HG2	2:B:466:ALA:CB	2.43	0.49
2:B:126:LEU:HD12	2:B:129:ARG:HD3	1.95	0.49
2:B:340:ARG:C	2:B:342:ASN:H	2.15	0.49
2:B:162:ARG:HB2	2:B:162:ARG:NH1	2.27	0.49
1:A:284:ILE:N	1:A:284:ILE:HD12	2.26	0.49
2:B:318:GLU:HG3	5:B:528:HOH:O	2.13	0.49
1:A:436:THR:HG23	1:A:458:MET:HG2	1.93	0.49
1:A:344:LEU:HD13	1:A:344:LEU:C	2.33	0.49
2:D:191:ILE:HG12	2:D:206:ILE:HD11	1.95	0.49
2:C:149:SER:HB3	2:D:161:ARG:NH2	2.26	0.49
2:D:179:VAL:HG12	2:D:179:VAL:O	2.12	0.49
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.77	0.49
2:D:273:MET:CE	2:D:468:ARG:HD2	2.41	0.49
2:B:376:ALA:HA	2:B:411:LEU:O	2.13	0.49
2:B:273:MET:CE	2:B:468:ARG:HD2	2.42	0.49
2:D:446:ARG:N	2:D:496:ARG:NH1	2.57	0.49
2:C:397:ILE:H	2:C:397:ILE:CD1	2.25	0.49
2:E:79:THR:HG23	2:E:81:GLN:H	1.77	0.49
2:C:163:GLU:HA	2:C:163:GLU:OE2	2.13	0.49
2:C:147:VAL:HG11	2:C:180:MET:CE	2.41	0.49
2:D:67:PHE:HB2	2:D:69:GLU:HG3	1.93	0.49
2:E:262:ARG:NH2	2:E:461:SER:HB2	2.28	0.49
2:B:344:LEU:HD11	2:B:346:ILE:CD1	2.42	0.49
2:B:23:THR:O	2:B:24:MET:HB2	2.12	0.49
1:A:441:GLN:NE2	1:A:490:ILE:HD13	2.27	0.49
2:B:377:ILE:HD12	2:B:377:ILE:N	2.28	0.49
2:B:486:PHE:CE2	2:B:496:ARG:HB2	2.48	0.49
2:E:315:PHE:CE2	2:E:363:ILE:HD13	2.48	0.49
2:D:60:LEU:O	2:D:64:ILE:CD1	2.55	0.49
2:C:334:ASP:O	2:C:338:MET:HG2	2.13	0.49
2:C:121:PHE:HB3	2:C:125:ALA:HB3	1.94	0.49
2:C:340:ARG:C	2:C:342:ASN:N	2.65	0.49
1:A:284:ILE:HD12	1:A:410:GLY:O	2.13	0.49
2:D:335:PHE:HA	2:D:338:MET:CG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:TYR:O	2:B:196:VAL:N	2.46	0.49
2:C:218:ARG:NH1	2:C:239:ILE:HD12	2.27	0.49
2:C:98:VAL:HA	2:C:103:LEU:O	2.12	0.49
2:B:209:ASN:ND2	2:B:216:ARG:HD2	2.28	0.49
2:C:211:LEU:HD12	2:C:215:ARG:O	2.13	0.49
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.95	0.49
2:D:412:PHE:N	2:D:412:PHE:CD1	2.80	0.49
1:A:244:ILE:HG22	1:A:246:ILE:CD1	2.43	0.49
1:A:82:ASP:O	1:A:83:ILE:C	2.51	0.49
2:D:79:THR:HG22	2:D:82:ASP:HB2	1.94	0.49
2:E:273:MET:O	2:E:463:HIS:CA	2.60	0.49
1:F:218:ARG:CZ	1:F:239:ILE:HD12	2.43	0.49
2:E:123:LEU:HD23	2:E:127:ILE:CG1	2.43	0.49
1:F:507:ARG:CD	1:F:507:ARG:O	2.61	0.49
1:F:21:MET:HE3	1:F:141:ARG:CZ	2.43	0.49
1:F:245:ASN:HD22	1:F:361:GLN:HE21	1.60	0.49
2:E:387:VAL:HG12	2:E:388:SER:N	2.28	0.48
2:D:237:PHE:HB3	2:D:246:ILE:HG12	1.95	0.48
1:F:393:ARG:O	1:F:397:ILE:HG13	2.12	0.48
1:A:205:VAL:HG22	1:A:222:ILE:CD1	2.37	0.48
2:D:85:LYS:NZ	2:E:14:GLU:HB3	2.27	0.48
2:B:436:THR:HG23	2:B:458:MET:HG3	1.95	0.48
2:E:302:VAL:HG13	2:E:344:LEU:HD23	1.94	0.48
2:C:93:ASP:OD1	2:C:93:ASP:C	2.50	0.48
1:A:237:PHE:HB3	1:A:246:ILE:HG13	1.95	0.48
2:D:231:MET:HB3	2:D:235:TYR:OH	2.13	0.48
2:E:486:PHE:HA	2:E:495:THR:O	2.13	0.48
1:A:338:MET:HB3	1:A:344:LEU:CB	2.42	0.48
2:E:93:ASP:OD2	2:E:96:LYS:CB	2.59	0.48
2:E:96:LYS:O	2:E:100:GLU:HG3	2.12	0.48
2:D:21:MET:CE	2:D:177:THR:HB	2.42	0.48
2:D:385:ARG:NH2	2:E:433:ILE:HD11	2.27	0.48
2:E:271:ASP:OD1	2:E:277:GLY:HA2	2.13	0.48
1:F:284:ILE:N	1:F:284:ILE:HD12	2.28	0.48
2:D:445:ILE:CA	2:D:496:ARG:HH12	2.27	0.48
2:D:336:GLU:OE1	2:D:336:GLU:HA	2.13	0.48
2:C:239:ILE:CG1	2:C:244:ILE:HD13	2.44	0.48
2:E:299:SER:C	2:E:333:MET:HE2	2.33	0.48
1:F:197:GLU:N	1:F:197:GLU:OE2	2.41	0.48
2:E:53:THR:OG1	3:E:903:ATP:O2G	2.31	0.48
1:F:182:THR:HG22	1:F:183:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:GLN:CG	1:F:116:GLU:N	2.74	0.48
1:F:325:LEU:HD23	1:F:335:PHE:HB2	1.96	0.48
2:D:121:PHE:CD1	2:D:121:PHE:N	2.81	0.48
2:D:486:PHE:CE2	2:D:496:ARG:HB3	2.49	0.48
2:C:123:LEU:O	2:C:124:SER:C	2.51	0.48
1:F:220:LEU:HD21	1:F:222:ILE:CD1	2.43	0.48
2:D:433:ILE:CG2	2:D:433:ILE:O	2.60	0.48
2:C:214:GLU:HB3	2:D:234:GLU:HB2	1.95	0.48
1:A:186:GLU:HB3	1:A:189:GLY:HA3	1.94	0.48
1:F:305:ALA:O	1:F:310:GLU:HB2	2.13	0.48
2:E:316:ALA:O	2:E:348:CYS:HA	2.14	0.48
2:E:81:GLN:NE2	2:E:81:GLN:H	2.10	0.48
2:C:123:LEU:O	2:C:126:LEU:N	2.46	0.48
2:C:54:LEU:O	2:C:55:PHE:C	2.52	0.48
2:E:303:GLU:HB2	2:E:333:MET:CE	2.43	0.48
2:E:49:GLY:O	2:E:218:ARG:NH2	2.47	0.48
2:C:454:ASN:CB	2:C:467:ILE:HD13	2.43	0.48
1:F:484:ARG:HB3	1:F:484:ARG:NH1	2.27	0.48
2:D:149:SER:HA	2:D:152:GLN:HB2	1.95	0.48
2:C:364:LYS:HE2	2:C:402:TYR:CD1	2.49	0.48
1:A:106:LEU:HD12	1:A:106:LEU:C	2.34	0.48
1:F:380:LEU:C	1:F:382:ALA:H	2.16	0.48
2:D:451:ARG:N	2:D:451:ARG:HD2	2.28	0.48
2:E:148:THR:HG21	2:E:193:ARG:HD2	1.94	0.48
2:B:222:ILE:HG22	2:B:230:HIS:CE1	2.49	0.48
2:B:56:SER:HB2	2:B:143:SER:HB3	1.96	0.48
1:F:182:THR:CG2	1:F:192:ALA:HB1	2.44	0.48
1:F:23:THR:O	1:F:24:MET:HB2	2.14	0.48
1:A:256:GLN:CG	1:F:320:SEP:P	3.01	0.48
2:C:218:ARG:HB3	5:C:528:HOH:O	2.13	0.48
1:F:431:GLU:O	1:F:434:THR:HG22	2.13	0.48
2:B:438:ILE:HG23	2:B:453:ILE:HD11	1.94	0.48
2:B:237:PHE:HB3	2:B:246:ILE:HG12	1.94	0.48
2:D:262:ARG:HD2	2:D:276:GLY:O	2.14	0.48
1:A:313:ILE:HD12	1:A:367:ILE:HD13	1.94	0.48
1:F:509:VAL:CG1	1:F:510:ARG:N	2.54	0.48
2:B:503:SER:O	2:B:504:GLU:CB	2.55	0.48
2:D:443:VAL:C	2:D:445:ILE:HD12	2.34	0.48
2:D:197:GLU:OE2	2:D:197:GLU:N	2.35	0.48
1:F:446:ARG:H	1:F:496:ARG:NH2	2.12	0.48
2:E:148:THR:HG21	2:E:183:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:LEU:HD23	2:D:270:LEU:O	2.13	0.48
2:C:371:LYS:N	2:C:372:PRO:HD3	2.28	0.48
2:C:431:GLU:CG	2:C:431:GLU:O	2.61	0.48
2:E:273:MET:CE	2:E:468:ARG:HD2	2.44	0.48
2:D:212:GLU:CG	2:D:212:GLU:O	2.60	0.48
2:C:284:ILE:H	2:C:284:ILE:HD12	1.79	0.48
2:B:215:ARG:NH2	2:C:234:GLU:O	2.47	0.48
1:A:317:TYR:CD2	1:A:383:LEU:HD21	2.49	0.48
2:C:434:THR:CG2	2:C:437:ILE:HD11	2.31	0.48
3:E:901:ATP:O3'	1:F:457:LYS:HB2	2.14	0.48
2:D:182:THR:CG2	2:D:183:GLU:H	2.24	0.48
2:D:352:GLU:C	2:D:354:ALA:H	2.18	0.48
2:C:464:ASP:OD1	2:C:464:ASP:C	2.52	0.48
2:B:72:VAL:HG23	2:B:139:ALA:CB	2.44	0.48
2:B:184:ARG:NH2	2:B:186:GLU:O	2.47	0.47
1:F:302:VAL:HG12	1:F:303:GLU:N	2.28	0.47
1:F:283:ILE:HD11	1:F:404:LYS:HG3	1.96	0.47
2:B:296:LEU:HD21	2:B:477:PRO:CD	2.38	0.47
2:D:151:PHE:C	2:D:153:GLN:N	2.67	0.47
2:E:485:ASN:OD1	2:E:485:ASN:N	2.47	0.47
1:A:150:VAL:CG1	1:A:151:PHE:N	2.76	0.47
1:A:344:LEU:HD13	1:A:345:LYS:N	2.29	0.47
2:E:336:GLU:O	2:E:339:GLU:HB2	2.14	0.47
1:F:20:LYS:HB3	1:F:35:GLY:O	2.13	0.47
2:E:203:ASN:ND2	2:E:203:ASN:N	2.61	0.47
1:F:452:ALA:HA	1:F:469:GLU:HA	1.96	0.47
2:C:249:LEU:HD13	2:C:394:GLN:O	2.14	0.47
2:D:68:ASP:O	2:D:68:ASP:OD1	2.31	0.47
1:A:320:SEP:O	1:A:324:LEU:CD1	2.63	0.47
1:A:294:LYS:N	3:A:901:ATP:O1B	2.47	0.47
1:A:425:ILE:CD1	1:F:290:THR:HG21	2.42	0.47
1:A:162:ARG:NH1	1:F:116:GLU:HG2	2.29	0.47
2:B:125:ALA:O	2:B:129:ARG:HG3	2.13	0.47
2:D:334:ASP:O	2:D:338:MET:HG2	2.14	0.47
2:D:315:PHE:CE1	2:D:375:ILE:HD12	2.50	0.47
2:D:266:GLY:O	2:D:300:ARG:CG	2.62	0.47
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.95	0.47
2:C:462:TRP:CE2	2:C:463:HIS:O	2.68	0.47
2:D:451:ARG:HG2	2:D:451:ARG:NH1	2.23	0.47
2:E:49:GLY:N	3:E:903:ATP:O2B	2.48	0.47
2:E:167:LEU:HG	2:E:171:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.96	0.47
2:B:284:ILE:N	2:B:284:ILE:HD12	2.29	0.47
1:F:338:MET:CB	1:F:344:LEU:HB3	2.43	0.47
2:E:344:LEU:HD11	2:E:346:ILE:CG1	2.42	0.47
2:C:197:GLU:CD	2:C:197:GLU:H	2.14	0.47
1:A:249:LEU:HD12	1:A:394:GLN:OE1	2.15	0.47
1:F:370:PHE:C	1:F:372:PRO:HD3	2.34	0.47
2:D:370:PHE:O	2:D:371:LYS:HG3	2.13	0.47
1:A:111:ASP:CG	1:A:112:PRO:HD2	2.34	0.47
2:D:332:GLY:O	2:D:333:MET:O	2.31	0.47
2:D:64:ILE:HD12	2:D:64:ILE:N	2.29	0.47
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.76	0.47
1:F:106:LEU:HD13	1:F:129:ARG:CZ	2.44	0.47
2:D:304:ASN:OD1	2:D:374:ARG:NH2	2.47	0.47
1:F:336:GLU:OE1	1:F:336:GLU:HA	2.14	0.47
2:B:419:PHE:O	2:B:420:MET:HB2	2.14	0.47
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.49	0.47
2:D:385:ARG:HH22	2:E:433:ILE:CD1	2.28	0.47
2:B:104:PHE:HD2	2:B:133:ALA:HB1	1.79	0.47
1:A:457:LYS:HB2	3:F:901:ATP:O3'	2.14	0.47
2:D:425:ILE:CD1	2:D:439:LEU:HD22	2.45	0.47
2:B:371:LYS:O	2:B:371:LYS:HD2	2.14	0.47
2:E:52:LYS:HE3	3:E:903:ATP:O1B	2.14	0.47
2:C:191:ILE:HB	2:C:198:GLU:HG2	1.96	0.47
1:A:467:ILE:HD11	1:F:449:MET:HG2	1.95	0.47
2:D:110:PRO:HD2	2:E:165:PHE:CE2	2.49	0.47
2:E:142:VAL:HB	2:E:178:THR:HG23	1.96	0.47
1:A:462:TRP:CG	1:A:463:HIS:N	2.76	0.47
2:B:73:PHE:HD2	2:B:105:ILE:HD12	1.80	0.47
2:D:231:MET:HE1	2:D:251:ALA:HB2	1.96	0.47
1:A:154:TYR:O	1:A:155:ASP:CB	2.62	0.47
2:B:25:ILE:HG23	2:B:58:GLN:NE2	2.29	0.47
2:E:147:VAL:HG23	2:E:148:THR:N	2.30	0.47
2:E:123:LEU:HD13	2:E:166:ARG:HD2	1.96	0.47
2:E:127:ILE:HD12	2:E:167:LEU:HD13	1.96	0.47
2:C:334:ASP:OD1	2:C:336:GLU:N	2.48	0.47
1:F:31:ILE:HD11	1:F:246:ILE:HG21	1.95	0.47
3:A:901:ATP:O3'	2:B:457:LYS:HB2	2.14	0.47
2:C:419:PHE:O	2:C:420:MET:CB	2.61	0.47
1:A:421:GLY:O	1:A:422:ALA:O	2.32	0.47
2:B:22:ARG:NH2	2:B:24:MET:SD	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:225:LEU:HB2	2:D:230:HIS:HD2	1.79	0.47
2:D:42:THR:HA	2:D:203:ASN:HB2	1.97	0.47
2:D:98:VAL:HA	2:D:103:LEU:O	2.15	0.47
1:A:370:PHE:C	1:A:372:PRO:HD3	2.35	0.47
1:A:262:ARG:O	1:A:263:VAL:HG22	2.15	0.47
1:A:256:GLN:CG	1:F:320:SEP:O1P	2.60	0.47
2:E:371:LYS:N	2:E:372:PRO:HD3	2.29	0.47
2:B:150:VAL:CG1	2:B:151:PHE:N	2.77	0.47
2:C:437:ILE:HD13	2:C:457:LYS:CE	2.38	0.47
2:B:184:ARG:HG2	2:B:191:ILE:O	2.14	0.47
2:B:313:ILE:CD1	2:B:372:PRO:HG2	2.45	0.47
2:C:419:PHE:CG	2:C:419:PHE:O	2.67	0.47
2:D:328:ALA:CA	5:D:552:HOH:O	2.62	0.47
2:C:294:LYS:HB2	3:C:901:ATP:O1B	2.15	0.47
1:F:430:ILE:O	1:F:432:GLU:N	2.47	0.47
2:E:417:ASP:O	1:F:424:SER:HB3	2.15	0.47
2:B:118:VAL:HG12	2:B:121:PHE:HB2	1.96	0.47
2:C:263:VAL:HG21	2:C:280:LYS:HA	1.96	0.47
1:F:380:LEU:C	1:F:382:ALA:N	2.68	0.47
2:B:269:ARG:O	2:B:273:MET:HG3	2.15	0.47
1:A:244:ILE:HG22	1:A:246:ILE:HD11	1.96	0.47
2:B:350:TYR:HE1	2:C:252:MET:HG2	1.80	0.47
2:B:80:PRO:HG3	2:B:105:ILE:CG2	2.44	0.47
1:F:269:ARG:CG	1:F:479:ILE:HB	2.40	0.47
2:D:451:ARG:NH1	2:D:451:ARG:CG	2.75	0.47
2:D:18:ILE:CD1	2:D:40:ARG:HH12	2.27	0.47
2:E:150:VAL:CG1	2:E:151:PHE:H	2.28	0.47
2:C:294:LYS:N	3:C:901:ATP:O1B	2.46	0.47
1:F:61:TYR:O	1:F:64:ILE:N	2.48	0.47
2:E:344:LEU:HD13	2:E:345:LYS:N	2.29	0.47
1:F:504:GLU:OE2	1:F:505:LEU:HD13	2.15	0.47
1:F:507:ARG:HD3	1:F:507:ARG:O	2.15	0.47
1:F:115:GLN:CG	1:F:116:GLU:H	2.27	0.47
1:A:452:ALA:HA	1:A:468:ARG:O	2.15	0.47
1:F:98:VAL:HA	1:F:103:LEU:O	2.15	0.47
2:B:217:ARG:HG3	2:B:357:GLU:OE2	2.15	0.47
1:A:270:LEU:O	1:A:273:MET:O	2.33	0.47
2:B:501:GLU:HB2	2:B:502:LYS:H	1.36	0.47
2:C:313:ILE:HD11	2:C:370:PHE:CB	2.45	0.47
1:F:458:MET:SD	1:F:461:SER:HB3	2.55	0.47
1:F:287:THR:CG2	1:F:414:ASN:ND2	2.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:LEU:HD11	1:F:197:GLU:HG3	1.96	0.47
1:A:134:ILE:HA	1:A:139:ALA:HB3	1.97	0.47
2:B:74:VAL:HG13	2:B:106:LEU:HG	1.97	0.47
1:A:313:ILE:HG13	1:A:372:PRO:CG	2.45	0.46
1:F:315:PHE:CE1	1:F:375:ILE:CD1	2.97	0.46
2:B:193:ARG:NH2	2:C:195:GLY:O	2.42	0.46
1:A:237:PHE:CB	1:A:246:ILE:HG13	2.44	0.46
2:B:170:ARG:HH12	2:B:174:ILE:HD11	1.80	0.46
2:C:144:ILE:HD11	2:C:171:LEU:HD11	1.96	0.46
2:C:144:ILE:HD13	2:C:167:LEU:HD21	1.97	0.46
1:A:79:THR:HB	1:A:82:ASP:OD2	2.14	0.46
2:E:468:ARG:HG2	2:E:468:ARG:HH11	1.80	0.46
1:A:28:PHE:CE1	1:A:222:ILE:HD11	2.50	0.46
2:B:222:ILE:O	2:B:230:HIS:CE1	2.69	0.46
1:A:65:ILE:HD11	1:A:97:LEU:HD21	1.97	0.46
2:B:463:HIS:ND1	2:B:463:HIS:C	2.68	0.46
2:D:486:PHE:CE2	2:D:496:ARG:HD3	2.51	0.46
2:C:315:PHE:CE2	2:C:363:ILE:HA	2.50	0.46
2:B:52:LYS:HE2	3:B:903:ATP:O1B	2.16	0.46
2:E:453:ILE:HB	2:E:470:PHE:HD2	1.80	0.46
2:D:147:VAL:CG2	2:D:148:THR:N	2.77	0.46
1:A:153:GLN:O	1:A:154:TYR:CB	2.63	0.46
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.45	0.46
2:D:211:LEU:HD12	2:D:215:ARG:O	2.15	0.46
2:C:249:LEU:HD12	2:C:394:GLN:OE1	2.15	0.46
2:E:318:GLU:OE2	1:F:432:GLU:HB3	2.15	0.46
2:B:327:ASN:HD21	2:C:459:ARG:HB3	1.79	0.46
1:A:357:GLU:HG3	1:A:358:ASP:N	2.29	0.46
2:D:181:THR:HG22	2:D:181:THR:O	2.14	0.46
1:F:436:THR:OG1	1:F:458:MET:HG2	2.15	0.46
2:C:49:GLY:O	2:C:218:ARG:NH2	2.48	0.46
2:D:348:CYS:HB3	2:E:254:LEU:HB3	1.98	0.46
2:C:64:ILE:CD1	2:C:103:LEU:HB2	2.46	0.46
2:C:215:ARG:HA	2:C:215:ARG:NE	2.30	0.46
1:A:340:ARG:C	1:A:342:ASN:H	2.18	0.46
2:E:219:THR:HA	2:E:235:TYR:O	2.15	0.46
1:F:255:THR:O	1:F:255:THR:HG22	2.15	0.46
2:B:269:ARG:HG2	2:B:479:ILE:HB	1.96	0.46
2:B:127:ILE:HG22	2:B:127:ILE:O	2.16	0.46
2:B:184:ARG:HH22	2:B:187:GLU:C	2.19	0.46
2:B:208:ARG:O	2:B:218:ARG:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:GLY:CA	3:C:903:ATP:O2B	2.63	0.46
1:F:147:VAL:HG11	1:F:180:MET:HE3	1.97	0.46
2:D:28:PHE:HA	2:D:31:ILE:HD12	1.98	0.46
2:B:313:ILE:HG13	2:B:372:PRO:HG3	1.97	0.46
1:F:471:MET:O	1:F:471:MET:HE2	2.16	0.46
2:C:333:MET:H	2:C:333:MET:HG2	1.42	0.46
2:E:191:ILE:HG23	2:E:206:ILE:CD1	2.45	0.46
2:B:454:ASN:HB2	2:B:467:ILE:HD13	1.96	0.46
1:A:68:ASP:CG	1:A:102:LYS:HZ2	2.18	0.46
2:E:281:ASP:O	2:E:282:SER:HB3	2.16	0.46
2:E:221:GLU:HG3	2:E:222:ILE:N	2.31	0.46
2:B:469:GLU:HG2	2:B:480:LYS:HB2	1.97	0.46
1:F:455:VAL:HG12	1:F:463:HIS:ND1	2.31	0.46
1:F:414:ASN:HD21	1:F:426:THR:HG23	1.80	0.46
2:B:387:VAL:CG1	2:B:388:SER:N	2.78	0.46
2:E:191:ILE:HD12	2:E:206:ILE:CG1	2.45	0.46
1:F:207:LEU:HD21	1:F:220:LEU:HD12	1.96	0.46
1:A:292:THR:HB	1:A:440:LEU:HB3	1.96	0.46
1:A:440:LEU:HD22	1:A:470:PHE:CE2	2.51	0.46
1:F:505:LEU:O	1:F:506:SER:CB	2.63	0.46
2:C:232:LYS:N	2:C:232:LYS:CD	2.79	0.46
2:D:185:ILE:N	2:D:185:ILE:HD12	2.31	0.46
1:A:423:HIS:O	1:F:418:GLN:HB2	2.16	0.46
1:A:145:ASP:OD2	1:A:181:THR:HG21	2.15	0.46
2:B:353:SER:HA	2:C:250:GLY:O	2.16	0.46
2:C:357:GLU:HG3	2:C:358:ASP:N	2.30	0.46
1:F:319:GLU:HA	1:F:320:SEP:O2P	2.16	0.46
2:C:31:ILE:HD11	2:C:246:ILE:CG2	2.41	0.46
2:B:489:ILE:O	2:B:492:GLY:N	2.49	0.46
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.97	0.46
2:E:453:ILE:O	2:E:453:ILE:HG23	2.15	0.46
2:E:396:VAL:O	2:E:400:THR:HB	2.16	0.46
2:E:283:ILE:HG13	2:E:400:THR:HG23	1.98	0.46
1:F:149:SER:HA	1:F:152:GLN:HB2	1.96	0.46
2:E:454:ASN:ND2	2:E:456:PHE:HA	2.30	0.46
2:B:122:ASP:C	2:B:124:SER:H	2.19	0.46
1:F:315:PHE:CE2	1:F:347:VAL:HG21	2.50	0.46
3:B:901:ATP:O3'	2:C:457:LYS:HB2	2.15	0.46
2:C:38:ILE:HG22	2:C:39:GLY:N	2.31	0.46
1:A:392:PHE:HE2	1:A:430:ILE:CD1	2.29	0.46
1:F:514:GLU:CB	1:F:519:SER:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:THR:HG23	2:B:82:ASP:H	1.80	0.46
1:A:333:MET:O	1:A:334:ASP:CB	2.63	0.46
2:B:265:SER:CB	2:B:270:LEU:HD13	2.46	0.46
2:B:213:GLY:O	2:B:214:GLU:HB2	2.16	0.46
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.98	0.46
2:B:363:ILE:HG22	2:B:367:ILE:HD11	1.98	0.46
2:D:123:LEU:HA	2:D:123:LEU:HD22	1.83	0.46
2:C:430:ILE:O	2:C:432:GLU:N	2.48	0.46
1:F:270:LEU:CD2	1:F:274:CYS:SG	3.04	0.46
2:E:269:ARG:NH2	2:E:468:ARG:NH2	2.64	0.46
2:C:283:ILE:N	2:C:283:ILE:HD12	2.31	0.46
2:D:356:LEU:HD13	2:D:387:VAL:HG21	1.98	0.46
2:B:57:ILE:C	2:B:59:PHE:N	2.69	0.46
2:B:360:LEU:HD23	2:B:399:VAL:CG2	2.46	0.46
1:F:484:ARG:CZ	1:F:484:ARG:HB2	2.46	0.46
2:D:294:LYS:N	3:D:901:ATP:O1B	2.46	0.46
2:E:223:LEU:HD22	2:E:223:LEU:O	2.16	0.46
1:A:393:ARG:NH1	1:F:385:ARG:HA	2.31	0.46
2:B:462:TRP:CE3	2:B:463:HIS:N	2.84	0.46
1:A:231:MET:CE	1:A:251:ALA:HB2	2.45	0.46
1:A:207:LEU:HD22	1:A:237:PHE:HE2	1.81	0.46
1:F:122:ASP:O	1:F:126:LEU:HB2	2.16	0.46
1:F:191:ILE:CG2	1:F:198:GLU:HG3	2.46	0.46
2:E:46:GLY:HA2	2:E:184:ARG:HD3	1.97	0.46
1:A:191:ILE:CG2	1:A:198:GLU:HG3	2.46	0.46
2:B:20:LYS:HG2	2:B:35:GLY:O	2.16	0.46
2:D:211:LEU:O	2:D:215:ARG:O	2.34	0.46
2:C:249:LEU:HD12	2:C:394:GLN:HG2	1.97	0.46
2:E:501:GLU:O	2:E:502:LYS:HG3	2.16	0.46
1:A:375:ILE:O	1:A:410:GLY:HA2	2.15	0.46
2:C:150:VAL:O	2:C:153:GLN:HG3	2.16	0.46
2:D:287:THR:HG23	2:D:414:ASN:ND2	2.22	0.46
2:E:123:LEU:HD22	2:E:166:ARG:HD2	1.98	0.46
2:C:197:GLU:N	2:C:197:GLU:OE2	2.39	0.46
2:D:382:ALA:O	2:D:385:ARG:HG3	2.16	0.46
1:A:364:LYS:HG2	1:A:402:TYR:CD2	2.50	0.45
2:C:50:THR:HA	5:C:528:HOH:O	2.15	0.45
2:E:262:ARG:HH22	2:E:461:SER:HB2	1.81	0.45
2:D:191:ILE:HD12	2:D:198:GLU:HG2	1.98	0.45
1:A:116:GLU:O	1:A:117:VAL:CB	2.63	0.45
1:F:387:VAL:CG1	1:F:388:SER:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:HD3	2:D:15:HIS:C	2.36	0.45
1:F:292:THR:HB	1:F:440:LEU:HB3	1.98	0.45
1:F:420:MET:HE3	1:F:492:GLY:HA3	1.98	0.45
1:A:185:ILE:HD12	1:A:185:ILE:N	2.31	0.45
2:B:84:ILE:HG23	2:B:94:LEU:HB2	1.97	0.45
2:B:123:LEU:HD12	2:B:166:ARG:HD2	1.98	0.45
2:E:495:THR:HA	1:F:487:GLU:OE1	2.17	0.45
2:E:385:ARG:HA	1:F:393:ARG:HH12	1.81	0.45
2:E:504:GLU:HG2	2:E:505:LEU:N	2.30	0.45
1:F:284:ILE:HB	1:F:411:LEU:HD12	1.97	0.45
2:D:313:ILE:HG21	2:D:315:PHE:CZ	2.50	0.45
2:C:462:TRP:CD2	2:C:463:HIS:O	2.69	0.45
2:C:334:ASP:C	2:C:334:ASP:OD1	2.55	0.45
2:D:471:MET:HE2	2:D:478:ASP:HB2	1.98	0.45
1:F:222:ILE:HD12	1:F:222:ILE:N	2.31	0.45
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.98	0.45
1:A:420:MET:O	1:A:422:ALA:N	2.41	0.45
1:F:356:LEU:CD1	1:F:387:VAL:HG21	2.44	0.45
1:A:262:ARG:NH2	1:A:461:SER:HB2	2.31	0.45
2:E:315:PHE:CE2	2:E:347:VAL:HG21	2.51	0.45
2:B:379:SER:H	2:B:413:THR:HG22	1.81	0.45
2:C:150:VAL:CG1	2:C:151:PHE:N	2.80	0.45
2:B:140:ARG:CB	2:B:140:ARG:NH1	2.69	0.45
2:E:74:VAL:CG2	2:E:130:ILE:HD12	2.46	0.45
1:A:496:ARG:HG3	2:B:487:GLU:OE1	2.16	0.45
1:A:295:THR:HB	3:A:901:ATP:PA	2.57	0.45
2:D:218:ARG:NH1	2:D:239:ILE:HD12	2.31	0.45
1:F:134:ILE:HD11	1:F:142:VAL:HG22	1.97	0.45
2:D:298:VAL:HG13	2:D:376:ALA:HB1	1.98	0.45
2:E:56:SER:OG	2:E:73:PHE:HE1	1.99	0.45
2:E:392:PHE:O	2:E:395:PHE:N	2.49	0.45
1:A:286:ALA:HA	1:A:438:ILE:O	2.16	0.45
1:A:311:ARG:O	1:A:373:ALA:N	2.40	0.45
2:D:445:ILE:HA	2:D:496:ARG:NH1	2.32	0.45
2:B:218:ARG:NH2	2:B:239:ILE:HD12	2.31	0.45
2:C:127:ILE:HG21	2:C:170:ARG:HG3	1.97	0.45
2:C:127:ILE:HD12	2:C:167:LEU:HD13	1.98	0.45
1:F:299:SER:CB	1:F:333:MET:HE1	2.46	0.45
1:F:122:ASP:O	1:F:126:LEU:N	2.50	0.45
1:A:293:GLY:HA2	3:A:901:ATP:O1A	2.16	0.45
2:E:140:ARG:HH11	2:E:140:ARG:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:LEU:O	2:C:61:TYR:C	2.52	0.45
1:A:380:LEU:N	1:A:413:THR:O	2.48	0.45
1:A:387:VAL:HG12	1:A:388:SER:N	2.31	0.45
1:F:296:LEU:HD13	1:F:331:TRP:CE2	2.51	0.45
2:E:145:ASP:O	2:E:146:SER:OG	2.32	0.45
2:C:73:PHE:HB3	2:C:105:ILE:HD13	1.97	0.45
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.46	0.45
2:C:287:THR:HG22	2:C:288:GLY:N	2.31	0.45
2:E:400:THR:HG22	2:E:401:GLY:N	2.30	0.45
2:E:283:ILE:HG23	2:E:412:PHE:HE1	1.79	0.45
1:A:164:LEU:HD11	1:A:197:GLU:CG	2.41	0.45
2:E:14:GLU:HG3	2:E:16:GLN:N	2.26	0.45
2:E:193:ARG:HH11	2:E:193:ARG:HG2	1.82	0.45
1:F:31:ILE:HG22	1:F:222:ILE:HD13	1.97	0.45
1:A:287:THR:HG21	1:A:425:ILE:O	2.16	0.45
2:D:263:VAL:HG21	2:D:280:LYS:HA	1.98	0.45
1:F:387:VAL:HG12	1:F:388:SER:N	2.32	0.45
1:A:246:ILE:O	1:A:248:PRO:HD3	2.17	0.45
2:B:314:LEU:HB3	2:B:346:ILE:HD13	1.98	0.45
2:D:316:ALA:O	2:D:348:CYS:HA	2.16	0.45
2:C:300:ARG:N	2:C:333:MET:HE1	2.31	0.45
2:B:356:LEU:HD21	2:B:392:PHE:HA	1.99	0.45
1:A:296:LEU:HA	1:A:331:TRP:CZ3	2.51	0.45
2:E:121:PHE:O	2:E:122:ASP:C	2.55	0.45
1:A:18:ILE:HD11	1:F:85:LYS:HG3	1.99	0.45
1:F:497:ILE:HG13	1:F:497:ILE:O	2.14	0.45
2:D:259:SER:OG	2:D:261:VAL:HG23	2.17	0.45
2:B:445:ILE:HD12	2:B:486:PHE:CZ	2.52	0.45
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.98	0.45
2:B:147:VAL:CG2	2:B:148:THR:N	2.79	0.45
2:B:284:ILE:H	2:B:284:ILE:HD12	1.81	0.45
1:A:211:LEU:HB2	1:A:216:ARG:CD	2.46	0.45
1:F:178:THR:CG2	1:F:179:VAL:N	2.79	0.45
2:B:122:ASP:C	2:B:124:SER:N	2.70	0.45
2:C:406:GLU:O	2:C:408:ILE:HG13	2.17	0.45
1:F:256:GLN:HG2	1:F:256:GLN:H	1.50	0.45
1:A:268:VAL:O	1:A:271:ASP:HB2	2.17	0.45
2:D:333:MET:HG2	5:D:910:HOH:O	2.17	0.45
1:F:129:ARG:O	1:F:132:TYR:HB3	2.17	0.45
2:B:140:ARG:CA	2:B:140:ARG:HH11	2.30	0.45
2:B:116:GLU:HG2	2:B:117:VAL:N	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.52	0.45
1:F:471:MET:SD	1:F:478:ASP:HB3	2.56	0.45
2:C:79:THR:HG22	2:C:82:ASP:H	1.79	0.45
1:A:127:ILE:HD11	1:A:167:LEU:HD13	1.98	0.45
1:A:489:ILE:HD13	1:A:494:PRO:HB3	1.99	0.45
2:B:88:ARG:HG2	2:B:88:ARG:NH1	2.32	0.45
2:D:202:ASP:HA	2:D:226:ARG:HD2	1.99	0.45
2:B:212:GLU:HG2	2:B:212:GLU:O	2.16	0.45
1:A:352:GLU:CD	1:A:352:GLU:N	2.70	0.45
1:A:183:GLU:OE2	2:B:161:ARG:NH1	2.49	0.45
2:B:298:VAL:HG12	2:B:299:SER:N	2.32	0.45
2:E:144:ILE:HD11	2:E:171:LEU:HD11	1.98	0.45
1:F:131:ASN:OD1	1:F:174:ILE:HD12	2.16	0.45
1:F:504:GLU:HB2	1:F:505:LEU:H	1.48	0.45
2:D:23:THR:O	2:D:24:MET:HB2	2.17	0.45
1:F:379:SER:HA	1:F:413:THR:HG22	1.99	0.44
2:B:492:GLY:C	2:B:494:PRO:HD3	2.36	0.44
1:A:207:LEU:HD22	1:A:237:PHE:CE2	2.52	0.44
2:D:67:PHE:CB	2:D:69:GLU:HG3	2.47	0.44
1:A:428:SER:OG	1:A:430:ILE:HD11	2.17	0.44
2:B:302:VAL:HG13	2:B:344:LEU:HD23	1.98	0.44
1:F:514:GLU:O	1:F:515:LYS:CB	2.60	0.44
1:F:231:MET:SD	1:F:251:ALA:HB2	2.56	0.44
1:A:311:ARG:NH1	1:A:371:LYS:HE3	2.32	0.44
1:F:315:PHE:HE1	1:F:375:ILE:CD1	2.30	0.44
2:E:315:PHE:CD2	2:E:363:ILE:HD13	2.52	0.44
2:B:105:ILE:O	2:B:105:ILE:HG22	2.16	0.44
1:A:182:THR:HG22	1:A:183:GLU:N	2.32	0.44
2:B:295:THR:HG23	2:B:378:ASP:OD2	2.18	0.44
2:E:191:ILE:CB	2:E:198:GLU:HG2	2.46	0.44
1:F:515:LYS:HG3	1:F:517:PRO:HD2	1.98	0.44
2:D:191:ILE:HB	2:D:198:GLU:HG2	1.97	0.44
3:A:901:ATP:H3'	2:B:458:MET:O	2.17	0.44
2:B:57:ILE:C	2:B:59:PHE:H	2.20	0.44
1:A:24:MET:N	1:A:29:ASP:OD2	2.44	0.44
2:C:337:GLU:OE1	2:C:340:ARG:NH1	2.50	0.44
1:A:146:SER:H	1:A:181:THR:HG22	1.81	0.44
2:C:68:ASP:CG	2:C:102:LYS:HZ1	2.20	0.44
1:F:121:PHE:HD2	1:F:121:PHE:HA	1.69	0.44
2:E:161:ARG:CA	2:E:196:VAL:HG11	2.47	0.44
1:A:313:ILE:HG13	1:A:372:PRO:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:LYS:O	2:B:371:LYS:CD	2.66	0.44
1:A:44:VAL:HG22	1:A:205:VAL:HB	1.99	0.44
2:B:44:VAL:HA	2:B:205:VAL:O	2.17	0.44
2:B:360:LEU:HD23	2:B:399:VAL:HG23	1.99	0.44
1:A:441:GLN:O	1:A:441:GLN:HG3	2.18	0.44
2:D:47:THR:HG22	2:D:184:ARG:C	2.36	0.44
1:F:116:GLU:O	1:F:117:VAL:HB	2.16	0.44
1:A:462:TRP:C	1:A:463:HIS:HD1	2.21	0.44
1:F:80:PRO:HB2	1:F:81:GLN:NE2	2.32	0.44
1:F:123:LEU:HD12	1:F:166:ARG:HD2	1.99	0.44
2:E:130:ILE:O	2:E:134:ILE:HG12	2.17	0.44
2:E:443:VAL:HG12	2:E:445:ILE:HG13	2.00	0.44
2:E:489:ILE:HD12	2:E:489:ILE:N	2.32	0.44
2:C:469:GLU:CG	2:C:480:LYS:HE3	2.47	0.44
2:B:79:THR:HG22	2:B:82:ASP:OD2	2.17	0.44
2:D:378:ASP:O	2:D:379:SER:HB3	2.18	0.44
2:D:340:ARG:C	2:D:342:ASN:N	2.71	0.44
2:B:126:LEU:C	2:B:128:GLU:H	2.19	0.44
2:C:263:VAL:CG2	2:C:280:LYS:HA	2.47	0.44
2:D:464:ASP:OD1	2:D:465:LYS:N	2.50	0.44
1:A:320:SEP:C	1:A:348:CYS:HG	2.27	0.44
1:A:31:ILE:HD13	1:A:220:LEU:HD22	1.98	0.44
2:C:126:LEU:O	2:C:129:ARG:N	2.50	0.44
1:F:106:LEU:HD13	1:F:129:ARG:NH2	2.32	0.44
2:E:104:PHE:CE2	2:E:106:LEU:HB2	2.53	0.44
1:A:420:MET:CE	2:B:490:ILE:HG21	2.48	0.44
1:F:504:GLU:HB3	1:F:507:ARG:NH2	2.32	0.44
2:D:41:SER:HB2	2:D:178:THR:HB	1.98	0.44
2:C:284:ILE:HD11	2:C:409:THR:HG22	2.00	0.44
2:B:497:ILE:HD12	2:B:498:THR:N	2.33	0.44
2:D:311:ARG:CD	2:D:371:LYS:HE3	2.29	0.44
2:B:47:THR:O	2:B:50:THR:HB	2.17	0.44
1:F:191:ILE:HD13	1:F:198:GLU:HG2	1.99	0.44
2:D:353:SER:O	2:D:354:ALA:CB	2.61	0.44
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.99	0.44
2:C:41:SER:HA	2:C:178:THR:O	2.18	0.44
2:D:385:ARG:NH2	2:E:433:ILE:CD1	2.80	0.44
2:B:461:SER:OG	2:B:462:TRP:N	2.50	0.44
2:E:451:ARG:HH11	2:E:451:ARG:CG	2.30	0.44
1:F:468:ARG:HD3	1:F:479:ILE:HG22	1.99	0.44
2:D:148:THR:HG21	2:D:193:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:469:GLU:CB	2:E:483:PHE:CZ	3.01	0.44
1:F:504:GLU:HA	1:F:507:ARG:HE	1.81	0.44
2:E:202:ASP:HB2	2:E:203:ASN:ND2	2.33	0.44
2:D:458:MET:HB2	2:D:463:HIS:HD2	1.83	0.44
2:B:280:LYS:HZ3	2:B:407:GLU:HB3	1.83	0.44
1:F:21:MET:HE3	1:F:141:ARG:NE	2.33	0.44
2:D:291:GLY:CA	3:D:901:ATP:O2B	2.65	0.44
1:A:418:GLN:HB2	2:B:423:HIS:O	2.17	0.44
2:E:212:GLU:HG2	2:E:212:GLU:O	2.17	0.44
2:D:495:THR:HA	2:E:487:GLU:OE2	2.18	0.44
2:B:194:TYR:C	2:B:196:VAL:N	2.67	0.44
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.92	0.44
1:F:462:TRP:O	1:F:463:HIS:CG	2.70	0.44
2:C:239:ILE:HG12	2:C:244:ILE:CD1	2.48	0.44
2:E:451:ARG:HB3	2:E:470:PHE:CE2	2.53	0.44
2:B:266:GLY:O	2:B:300:ARG:CG	2.66	0.44
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.47	0.44
2:C:284:ILE:N	2:C:284:ILE:HD12	2.33	0.44
2:B:327:ASN:ND2	2:C:459:ARG:HB3	2.33	0.44
1:F:313:ILE:HG13	1:F:372:PRO:HG2	2.00	0.44
2:B:500:ASP:C	2:B:501:GLU:HG3	2.38	0.44
2:B:84:ILE:HD12	2:B:94:LEU:CB	2.44	0.44
2:D:333:MET:CA	5:D:913:HOH:O	2.44	0.44
2:C:140:ARG:CA	2:C:140:ARG:HH11	2.31	0.44
2:E:489:ILE:HA	2:E:494:PRO:HG3	1.99	0.44
2:E:192:ALA:HB3	2:E:197:GLU:OE2	2.18	0.44
2:D:426:THR:HB	2:D:431:GLU:OE2	2.18	0.44
2:C:420:MET:HE3	2:C:492:GLY:HA3	2.00	0.44
2:B:44:VAL:HG22	2:B:205:VAL:HG12	1.99	0.44
1:A:448:GLU:HG2	2:B:466:ALA:HA	2.00	0.44
2:B:353:SER:O	2:B:354:ALA:HB2	2.17	0.44
2:E:504:GLU:CG	2:E:505:LEU:H	2.30	0.44
1:F:44:VAL:O	1:F:181:THR:HA	2.18	0.44
2:B:199:PHE:CD2	2:B:199:PHE:N	2.86	0.43
1:F:445:ILE:HG22	1:F:446:ARG:HD2	2.00	0.43
2:E:148:THR:HG1	2:E:182:THR:HG23	1.83	0.43
1:F:231:MET:CE	1:F:251:ALA:HB2	2.48	0.43
2:B:93:ASP:OD2	2:B:96:LYS:HB2	2.18	0.43
2:D:19:ALA:HB1	2:D:38:ILE:HD12	1.99	0.43
1:A:124:SER:O	1:A:128:GLU:HG3	2.18	0.43
1:F:513:GLN:HA	1:F:513:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:ILE:HG12	2:B:400:THR:HG23	2.00	0.43
2:D:123:LEU:HD21	2:D:163:GLU:HB3	2.00	0.43
1:F:127:ILE:CD1	1:F:167:LEU:HD13	2.48	0.43
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.99	0.43
1:F:111:ASP:HA	1:F:112:PRO:HD3	1.92	0.43
2:E:419:PHE:O	2:E:420:MET:HB2	2.18	0.43
2:C:164:LEU:HD11	2:C:197:GLU:HG3	2.00	0.43
1:A:486:PHE:CB	1:A:489:ILE:HD11	2.48	0.43
2:B:126:LEU:C	2:B:128:GLU:N	2.71	0.43
2:D:273:MET:O	2:D:463:HIS:HA	2.17	0.43
1:F:185:ILE:N	1:F:185:ILE:HD13	2.33	0.43
1:F:406:GLU:HB3	1:F:408:ILE:HG12	1.99	0.43
2:E:313:ILE:HB	2:E:375:ILE:HD13	1.94	0.43
2:B:87:ALA:HB1	2:B:92:TRP:CD1	2.53	0.43
2:C:453:ILE:C	2:C:453:ILE:HD13	2.38	0.43
2:C:81:GLN:CD	2:C:81:GLN:H	2.20	0.43
2:C:292:THR:HB	2:C:440:LEU:HB3	1.99	0.43
2:B:146:SER:H	2:B:181:THR:CG2	2.31	0.43
1:A:377:ILE:HD13	1:A:412:PHE:CD2	2.53	0.43
2:D:350:TYR:CE1	2:E:252:MET:HE2	2.53	0.43
2:E:438:ILE:N	2:E:438:ILE:HD12	2.33	0.43
2:B:131:ASN:OD1	2:B:174:ILE:HD12	2.18	0.43
2:C:131:ASN:OD1	2:C:174:ILE:HD12	2.17	0.43
2:B:426:THR:HG22	2:B:429:HIS:H	1.83	0.43
2:E:444:GLU:O	2:E:494:PRO:HD2	2.17	0.43
1:F:496:ARG:HD3	1:F:496:ARG:N	2.33	0.43
2:B:377:ILE:HB	2:B:412:PHE:HD2	1.82	0.43
2:C:387:VAL:CG1	2:C:388:SER:N	2.82	0.43
2:D:350:TYR:O	2:D:351:PRO:C	2.56	0.43
1:A:305:ALA:O	1:A:310:GLU:HB2	2.19	0.43
1:A:312:ALA:HA	1:A:374:ARG:O	2.19	0.43
1:A:274:CYS:HA	1:A:463:HIS:HB2	1.99	0.43
1:F:284:ILE:HD12	1:F:284:ILE:H	1.83	0.43
2:C:392:PHE:CE2	2:C:430:ILE:HD11	2.54	0.43
1:A:153:GLN:C	1:A:154:TYR:CD2	2.92	0.43
1:A:471:MET:HE2	1:A:471:MET:O	2.18	0.43
2:E:184:ARG:CD	2:E:191:ILE:O	2.66	0.43
1:A:211:LEU:HD21	2:B:188:TYR:HE2	1.84	0.43
2:C:79:THR:HG23	2:C:81:GLN:HG2	2.01	0.43
2:C:121:PHE:O	2:C:125:ALA:HB3	2.18	0.43
2:E:22:ARG:HB3	2:E:29:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.19	0.43
2:C:66:GLU:C	2:C:67:PHE:CD1	2.92	0.43
1:F:281:ASP:OD1	1:F:407:GLU:OE1	2.37	0.43
1:A:136:LYS:HD3	1:A:137:TYR:HE1	1.83	0.43
2:C:318:GLU:OE2	2:D:432:GLU:HG2	2.19	0.43
1:A:72:VAL:HB	1:A:142:VAL:HG22	2.00	0.43
2:E:313:ILE:CD1	2:E:372:PRO:HG2	2.48	0.43
2:B:123:LEU:O	2:B:127:ILE:HG13	2.19	0.43
2:B:164:LEU:HD11	2:B:197:GLU:HG3	2.00	0.43
2:B:52:LYS:HD2	2:B:182:THR:O	2.19	0.43
2:D:387:VAL:CG1	2:D:388:SER:H	2.32	0.43
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.48	0.43
2:C:256:GLN:HG2	2:C:256:GLN:H	1.54	0.43
2:B:51:GLY:H	3:B:903:ATP:PB	2.42	0.43
2:D:148:THR:HG23	2:D:193:ARG:HD2	1.99	0.43
2:C:471:MET:HB3	2:C:480:LYS:NZ	2.34	0.43
2:B:79:THR:HG21	2:B:81:GLN:HG2	1.99	0.43
2:D:296:LEU:HD11	2:D:477:PRO:HD3	2.01	0.43
2:D:203:ASN:CB	2:D:225:LEU:HD23	2.49	0.43
1:F:464:ASP:OD2	1:F:466:ALA:HB3	2.19	0.43
2:B:455:VAL:HG11	2:B:463:HIS:HB2	2.01	0.43
2:D:446:ARG:H	2:D:496:ARG:CZ	2.31	0.43
1:F:455:VAL:HG11	1:F:463:HIS:CB	2.40	0.43
1:F:126:LEU:HD11	1:F:130:ILE:HD11	2.01	0.43
2:B:333:MET:HG2	2:B:333:MET:H	1.34	0.43
2:E:486:PHE:CB	2:E:489:ILE:HD11	2.49	0.43
2:B:92:TRP:HD1	2:B:92:TRP:O	2.02	0.43
1:A:65:ILE:HG12	1:A:65:ILE:H	1.62	0.43
1:F:109:SER:HA	1:F:110:PRO:HD3	1.84	0.43
1:A:18:ILE:HG21	1:A:37:PRO:HB3	2.00	0.43
2:D:230:HIS:HD1	2:D:230:HIS:C	2.22	0.43
2:B:89:SER:CB	2:C:227:GLY:O	2.67	0.43
2:B:136:LYS:HE2	2:B:137:TYR:CE1	2.54	0.43
2:B:142:VAL:HG23	2:B:176:ALA:HB1	2.01	0.43
2:C:44:VAL:HA	2:C:205:VAL:O	2.18	0.43
2:D:469:GLU:HG3	2:D:470:PHE:N	2.31	0.43
2:B:21:MET:HB2	2:B:38:ILE:CG1	2.43	0.43
1:F:248:PRO:HB2	1:F:251:ALA:CB	2.45	0.43
1:F:94:LEU:O	1:F:97:LEU:N	2.51	0.43
1:F:247:PHE:HB3	1:F:249:LEU:HD21	2.01	0.43
1:A:317:TYR:CE2	1:A:383:LEU:HD21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ILE:HD13	2:B:170:ARG:HG3	2.01	0.43
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.49	0.43
2:C:127:ILE:N	2:C:127:ILE:CD1	2.82	0.43
1:A:471:MET:H	1:A:471:MET:HG3	1.67	0.43
1:F:515:LYS:CG	1:F:517:PRO:HD2	2.49	0.43
1:F:93:ASP:OD2	1:F:96:LYS:HB2	2.18	0.43
2:C:113:GLU:O	2:C:114:GLY:C	2.58	0.43
2:C:61:TYR:CG	2:C:65:ILE:HD13	2.53	0.43
1:F:329:TYR:C	1:F:331:TRP:N	2.72	0.43
2:C:446:ARG:HG2	2:C:496:ARG:CZ	2.49	0.43
1:A:137:TYR:N	1:A:137:TYR:CD1	2.86	0.43
1:A:126:LEU:HG	1:A:130:ILE:CD1	2.49	0.43
2:D:209:ASN:HD22	2:D:209:ASN:HA	1.61	0.43
1:A:267:VAL:CG1	1:A:270:LEU:HB2	2.48	0.42
1:F:380:LEU:O	1:F:383:LEU:N	2.50	0.42
2:E:147:VAL:CG2	2:E:148:THR:N	2.82	0.42
1:A:356:LEU:HD23	1:A:395:PHE:HB2	2.01	0.42
2:C:348:CYS:O	2:C:349:ALA:HB2	2.19	0.42
2:B:162:ARG:HH11	2:B:162:ARG:CB	2.31	0.42
2:C:483:PHE:N	2:C:483:PHE:CD1	2.87	0.42
1:F:375:ILE:HD13	1:F:375:ILE:HA	1.87	0.42
2:C:44:VAL:HG12	2:C:44:VAL:O	2.19	0.42
2:E:371:LYS:CD	2:E:371:LYS:O	2.62	0.42
2:C:425:ILE:H	2:C:425:ILE:HD12	1.84	0.42
2:E:296:LEU:HD13	2:E:331:TRP:CE3	2.54	0.42
2:D:471:MET:HE2	2:D:478:ASP:CB	2.49	0.42
1:A:379:SER:H	1:A:413:THR:CB	2.32	0.42
1:F:387:VAL:CG1	1:F:391:ALA:HB3	2.49	0.42
2:D:394:GLN:NE2	5:D:530:HOH:O	2.51	0.42
1:F:134:ILE:CD1	1:F:139:ALA:HB3	2.50	0.42
1:F:289:ALA:O	1:F:292:THR:HG23	2.18	0.42
1:A:340:ARG:O	1:A:342:ASN:N	2.53	0.42
1:A:304:ASN:O	1:A:304:ASN:OD1	2.38	0.42
2:B:451:ARG:HB3	2:B:470:PHE:CE2	2.54	0.42
1:A:82:ASP:O	1:A:85:LYS:N	2.52	0.42
1:F:164:LEU:O	1:F:167:LEU:N	2.52	0.42
2:D:18:ILE:HD12	2:D:227:GLY:CA	2.42	0.42
2:C:378:ASP:O	2:C:379:SER:CB	2.66	0.42
2:E:69:GLU:HA	2:E:70:PRO:HD3	1.89	0.42
2:D:385:ARG:HG2	2:E:393:ARG:CZ	2.48	0.42
2:C:443:VAL:HG12	2:C:445:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:472:ILE:HD12	2:C:472:ILE:N	2.34	0.42
1:F:212:GLU:OE2	1:F:212:GLU:O	2.36	0.42
1:F:313:ILE:CD1	1:F:372:PRO:HG2	2.49	0.42
2:B:451:ARG:HD2	2:B:451:ARG:N	2.34	0.42
1:F:18:ILE:HB	1:F:228:THR:CG2	2.48	0.42
2:E:348:CYS:O	2:E:349:ALA:HB2	2.19	0.42
2:D:64:ILE:HG21	2:D:97:LEU:HD13	2.00	0.42
2:E:331:TRP:NE1	3:E:901:ATP:N7	2.59	0.42
2:E:462:TRP:O	2:E:463:HIS:CD2	2.72	0.42
1:A:266:GLY:C	1:A:300:ARG:HG3	2.39	0.42
2:E:289:ALA:CB	2:E:419:PHE:HA	2.46	0.42
1:A:64:ILE:CD1	1:A:70:PRO:HA	2.48	0.42
2:C:486:PHE:HE2	2:C:496:ARG:HG2	1.84	0.42
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.87	0.42
2:B:98:VAL:HA	2:B:103:LEU:O	2.19	0.42
2:D:244:ILE:HG22	2:D:245:ASN:N	2.34	0.42
1:A:212:GLU:CG	1:A:212:GLU:O	2.68	0.42
2:B:393:ARG:O	2:B:397:ILE:HG13	2.19	0.42
1:A:320:SEP:O2P	2:B:256:GLN:O	2.37	0.42
2:E:315:PHE:CD2	2:E:347:VAL:HG21	2.54	0.42
2:E:445:ILE:HD11	2:E:483:PHE:CE2	2.54	0.42
1:A:336:GLU:OE1	1:A:336:GLU:HA	2.19	0.42
2:D:52:LYS:N	3:D:903:ATP:O1B	2.43	0.42
1:F:484:ARG:HH11	1:F:484:ARG:CB	2.29	0.42
2:D:420:MET:HE3	2:D:420:MET:HB3	1.83	0.42
2:E:223:LEU:HD23	2:E:223:LEU:HA	1.45	0.42
1:F:47:THR:O	1:F:50:THR:HG23	2.20	0.42
2:D:127:ILE:CD1	2:D:167:LEU:HD13	2.50	0.42
2:B:73:PHE:CD2	2:B:105:ILE:HD12	2.54	0.42
1:F:191:ILE:HG21	1:F:198:GLU:HG3	2.02	0.42
3:A:901:ATP:O2G	2:B:459:ARG:NH2	2.51	0.42
2:B:36:LEU:HD12	2:B:59:PHE:CE1	2.54	0.42
2:D:52:LYS:HB2	2:D:52:LYS:HE3	1.85	0.42
2:B:24:MET:HB3	2:B:62:ASN:HD22	1.84	0.42
1:F:484:ARG:HB2	1:F:484:ARG:NH1	2.34	0.42
2:C:486:PHE:HB3	2:C:489:ILE:HD11	2.01	0.42
2:B:204:VAL:HG23	2:B:224:LYS:HG2	2.00	0.42
2:D:160:VAL:O	2:D:164:LEU:HB2	2.19	0.42
1:F:367:ILE:HD11	1:F:375:ILE:HG13	2.00	0.42
1:A:393:ARG:HH12	1:F:385:ARG:HA	1.85	0.42
2:C:363:ILE:HG22	2:C:367:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:OG1	1:A:182:THR:HG23	2.20	0.42
2:B:164:LEU:HB3	2:B:200:VAL:HG11	2.02	0.42
2:E:413:THR:CG2	2:E:414:ASN:N	2.83	0.42
1:F:269:ARG:O	1:F:272:GLU:HB2	2.20	0.42
1:A:325:LEU:HD22	1:A:336:GLU:HG2	2.02	0.42
2:B:453:ILE:HD13	2:B:454:ASN:H	1.83	0.42
2:D:367:ILE:HG23	2:D:372:PRO:HD2	2.01	0.42
2:C:208:ARG:NH2	2:C:221:GLU:OE2	2.52	0.42
2:D:384:ALA:HB2	2:D:392:PHE:CE1	2.54	0.42
2:C:186:GLU:OE2	2:C:187:GLU:N	2.53	0.42
1:A:485:ASN:N	1:A:485:ASN:OD1	2.48	0.42
1:A:311:ARG:CZ	1:A:371:LYS:HE3	2.50	0.42
1:A:348:CYS:HB3	2:B:254:LEU:HD23	2.02	0.42
2:B:445:ILE:HD11	2:B:494:PRO:HG2	2.01	0.42
1:A:81:GLN:H	1:A:81:GLN:NE2	2.18	0.42
1:A:306:CYS:HB2	1:A:338:MET:SD	2.59	0.42
2:C:439:LEU:C	2:C:439:LEU:HD12	2.40	0.42
2:E:23:THR:O	2:E:24:MET:CB	2.68	0.42
1:A:382:ALA:O	1:A:385:ARG:HG3	2.20	0.42
2:E:225:LEU:HD12	2:E:230:HIS:HB3	2.00	0.42
2:E:220:LEU:C	2:E:220:LEU:HD23	2.40	0.42
2:D:325:LEU:CD2	2:D:335:PHE:HB2	2.50	0.42
2:D:332:GLY:O	2:D:333:MET:HG2	2.19	0.42
2:E:106:LEU:HD13	2:E:129:ARG:NH2	2.34	0.42
2:E:445:ILE:HG22	2:E:445:ILE:O	2.20	0.42
2:E:486:PHE:HB2	2:E:489:ILE:HD11	2.00	0.42
1:A:166:ARG:HG3	1:F:112:PRO:O	2.20	0.42
2:B:436:THR:HG23	2:B:458:MET:CG	2.50	0.42
2:E:344:LEU:CD1	2:E:346:ILE:HG13	2.48	0.42
2:C:62:ASN:O	2:C:66:GLU:N	2.47	0.42
2:E:164:LEU:HD23	2:E:164:LEU:HA	1.81	0.42
2:E:326:ARG:HD3	1:F:258:SER:OG	2.20	0.42
2:E:217:ARG:HH21	2:E:236:PRO:HB3	1.85	0.42
1:F:433:ILE:N	1:F:433:ILE:HD12	2.34	0.42
2:E:360:LEU:HD22	2:E:360:LEU:O	2.20	0.42
1:A:319:GLU:O	2:B:254:LEU:HD21	2.20	0.42
1:A:348:CYS:O	1:A:349:ALA:HB2	2.20	0.42
2:B:350:TYR:CE1	2:C:252:MET:HE2	2.55	0.42
1:A:426:THR:HB	1:A:431:GLU:OE1	2.20	0.42
2:C:54:LEU:HD23	2:C:244:ILE:CG1	2.47	0.42
1:A:451:ARG:N	1:A:451:ARG:CD	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:451:ARG:NH1	1:F:451:ARG:HG2	2.33	0.42
1:F:117:VAL:O	1:F:118:VAL:CB	2.67	0.42
1:A:367:ILE:HD12	1:A:375:ILE:HD11	2.01	0.41
1:A:323:GLN:HA	2:B:258:SER:OG	2.19	0.41
2:B:282:SER:C	2:B:283:ILE:HD12	2.41	0.41
1:F:371:LYS:N	1:F:372:PRO:HD3	2.35	0.41
2:B:471:MET:HB3	2:B:480:LYS:NZ	2.34	0.41
2:B:50:THR:HG22	2:B:52:LYS:HE2	2.02	0.41
1:F:150:VAL:O	1:F:153:GLN:HG3	2.20	0.41
2:D:439:LEU:HD12	2:D:439:LEU:C	2.40	0.41
2:E:489:ILE:H	2:E:489:ILE:HD12	1.85	0.41
2:D:70:PRO:HG2	2:D:138:ARG:O	2.20	0.41
2:B:61:TYR:CZ	2:B:92:TRP:HB2	2.55	0.41
1:F:344:LEU:HD13	1:F:344:LEU:O	2.20	0.41
1:F:49:GLY:O	1:F:218:ARG:NH2	2.52	0.41
2:D:54:LEU:HD13	2:D:90:PHE:CZ	2.55	0.41
2:B:125:ALA:O	2:B:128:GLU:HB2	2.20	0.41
2:C:142:VAL:HG12	2:C:178:THR:HG23	2.02	0.41
2:D:19:ALA:CB	2:D:38:ILE:HD12	2.49	0.41
1:F:249:LEU:HD12	1:F:394:GLN:CD	2.39	0.41
1:F:438:ILE:O	1:F:438:ILE:HG22	2.19	0.41
2:B:73:PHE:HE2	2:B:83:ILE:HD13	1.85	0.41
1:F:486:PHE:HD2	1:F:494:PRO:HB2	1.84	0.41
1:A:283:ILE:HD12	1:A:412:PHE:CE1	2.55	0.41
2:E:200:VAL:O	2:E:200:VAL:CG1	2.67	0.41
1:F:161:ARG:HB2	1:F:196:VAL:CG1	2.49	0.41
3:A:903:ATP:O3'	2:B:224:LYS:HB2	2.21	0.41
2:C:290:THR:HG23	2:C:290:THR:O	2.21	0.41
2:E:180:MET:HB3	2:E:180:MET:HE2	1.82	0.41
1:A:244:ILE:CG2	1:A:246:ILE:HD11	2.50	0.41
1:A:79:THR:HG23	1:A:81:GLN:NE2	2.17	0.41
2:B:336:GLU:OE1	2:B:336:GLU:HA	2.21	0.41
2:E:443:VAL:HG11	2:E:445:ILE:HD11	2.02	0.41
2:D:106:LEU:HD11	2:D:129:ARG:CZ	2.50	0.41
2:C:42:THR:HG23	2:C:203:ASN:HB2	2.01	0.41
2:B:249:LEU:HD13	2:B:394:GLN:HG2	2.02	0.41
1:F:21:MET:HE1	1:F:141:ARG:HG2	2.02	0.41
1:F:433:ILE:HG22	1:F:433:ILE:O	2.19	0.41
2:C:32:SER:OG	2:C:35:GLY:HA2	2.20	0.41
2:B:51:GLY:C	3:B:903:ATP:O1B	2.59	0.41
2:C:25:ILE:CG1	2:C:58:GLN:HE21	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:SER:HB3	2:D:182:THR:HB	2.02	0.41
2:E:49:GLY:HA2	3:E:903:ATP:O2B	2.21	0.41
1:F:220:LEU:HD21	1:F:222:ILE:HD11	2.03	0.41
1:A:20:LYS:HE3	1:A:228:THR:HG21	2.01	0.41
2:C:219:THR:O	2:C:237:PHE:HE2	2.04	0.41
2:C:380:LEU:HA	2:C:380:LEU:HD23	1.90	0.41
2:B:452:ALA:O	2:B:470:PHE:HE2	2.03	0.41
2:B:499:VAL:C	2:B:501:GLU:H	2.23	0.41
2:B:182:THR:HG21	2:B:192:ALA:CB	2.41	0.41
2:B:194:TYR:O	2:B:195:GLY:C	2.57	0.41
2:C:70:PRO:HB2	2:C:139:ALA:HA	2.02	0.41
2:D:344:LEU:HD13	2:D:345:LYS:N	2.36	0.41
1:A:489:ILE:HD13	1:A:494:PRO:CG	2.50	0.41
1:F:396:VAL:O	1:F:400:THR:HB	2.19	0.41
2:C:382:ALA:O	2:C:385:ARG:HG3	2.19	0.41
1:F:312:ALA:HB2	1:F:374:ARG:HB2	2.01	0.41
2:B:471:MET:HG2	2:B:480:LYS:HZ3	1.84	0.41
2:B:73:PHE:HB3	2:B:105:ILE:CD1	2.36	0.41
2:C:63:GLY:CA	2:C:141:ARG:CZ	2.98	0.41
1:A:396:VAL:O	1:A:400:THR:CB	2.67	0.41
1:F:266:GLY:HA3	1:F:300:ARG:HG3	2.02	0.41
2:E:468:ARG:NH1	2:E:468:ARG:HG2	2.36	0.41
2:E:18:ILE:O	2:E:18:ILE:HD12	2.21	0.41
2:B:347:VAL:O	2:B:348:CYS:HB2	2.21	0.41
2:B:36:LEU:HD12	2:B:59:PHE:CZ	2.56	0.41
2:D:328:ALA:N	5:D:552:HOH:O	2.53	0.41
2:B:326:ARG:HG3	2:C:260:ASN:ND2	2.35	0.41
2:D:88:ARG:HD3	2:E:15:HIS:O	2.20	0.41
2:E:353:SER:O	2:E:354:ALA:HB2	2.20	0.41
1:A:323:GLN:HA	2:B:258:SER:CB	2.51	0.41
1:A:319:GLU:OE1	1:A:324:LEU:HD23	2.21	0.41
2:B:151:PHE:C	2:B:153:GLN:N	2.74	0.41
2:B:80:PRO:HA	2:B:83:ILE:HD12	2.03	0.41
2:B:182:THR:HG22	2:B:183:GLU:H	1.86	0.41
1:F:299:SER:HB3	1:F:333:MET:HE1	2.01	0.41
2:B:311:ARG:CD	2:B:371:LYS:HE3	2.41	0.41
1:A:94:LEU:HD22	1:A:103:LEU:CD2	2.51	0.41
2:D:49:GLY:CA	3:D:903:ATP:O2B	2.68	0.41
2:C:61:TYR:CZ	2:C:92:TRP:HB2	2.56	0.41
1:A:36:LEU:HD12	1:A:59:PHE:CE1	2.56	0.41
1:A:448:GLU:HG2	2:B:466:ALA:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:GLN:HG3	1:F:161:ARG:NH1	2.34	0.41
2:D:84:ILE:HD11	2:D:105:ILE:CD1	2.51	0.41
2:C:468:ARG:HG2	2:C:468:ARG:NH1	2.35	0.41
2:E:211:LEU:HA	2:E:211:LEU:HD12	1.88	0.41
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.86	0.41
1:A:461:SER:OG	1:A:462:TRP:N	2.54	0.41
1:A:320:SEP:CB	2:B:254:LEU:HG	2.46	0.41
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.61	0.41
2:B:51:GLY:O	2:B:54:LEU:HB3	2.21	0.41
2:C:127:ILE:HD11	2:C:167:LEU:HD13	2.02	0.41
2:E:269:ARG:HH22	2:E:468:ARG:NH2	2.18	0.41
2:C:23:THR:O	2:C:24:MET:HB2	2.21	0.41
1:A:64:ILE:HG21	1:A:97:LEU:HD22	2.02	0.41
2:E:325:LEU:HD23	2:E:335:PHE:HB2	2.03	0.41
2:D:106:LEU:C	2:D:106:LEU:HD12	2.41	0.41
1:A:467:ILE:HD13	1:F:447:GLY:O	2.20	0.41
2:E:291:GLY:C	2:E:442:TYR:OH	2.59	0.41
1:A:284:ILE:HG22	1:A:438:ILE:HD13	2.03	0.41
2:E:264:SER:O	2:E:374:ARG:NH2	2.53	0.41
2:B:479:ILE:CD1	2:B:479:ILE:H	2.21	0.41
2:C:231:MET:CE	2:C:251:ALA:HB2	2.51	0.41
2:E:362:ILE:O	2:E:365:SER:HB3	2.21	0.41
2:B:161:ARG:HB2	2:B:196:VAL:HG11	2.01	0.41
2:B:45:SER:HB3	2:B:182:THR:CB	2.39	0.41
1:F:299:SER:C	1:F:333:MET:CE	2.79	0.41
2:E:269:ARG:CG	2:E:479:ILE:HB	2.40	0.41
2:D:246:ILE:O	2:D:248:PRO:HD3	2.20	0.41
2:E:445:ILE:O	2:E:446:ARG:CB	2.65	0.41
2:B:92:TRP:CD1	2:B:92:TRP:O	2.74	0.41
2:D:387:VAL:HG12	2:D:388:SER:H	1.83	0.41
2:E:419:PHE:O	2:E:420:MET:O	2.39	0.41
2:D:21:MET:CE	2:D:59:PHE:HZ	2.33	0.41
2:D:54:LEU:CD2	2:D:239:ILE:HG23	2.51	0.41
2:C:448:GLU:HG2	2:D:466:ALA:CA	2.48	0.41
2:E:84:ILE:O	2:E:87:ALA:HB3	2.20	0.41
2:C:20:LYS:HE2	2:C:228:THR:OG1	2.21	0.41
1:A:162:ARG:O	1:A:165:PHE:HB3	2.20	0.41
2:B:76:PHE:CZ	2:B:126:LEU:HD21	2.56	0.41
2:B:96:LYS:O	2:B:100:GLU:HG3	2.21	0.41
2:D:294:LYS:O	2:D:298:VAL:HG23	2.20	0.41
2:E:265:SER:HB3	2:E:278:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:VAL:HG12	2:C:118:VAL:O	2.21	0.41
2:B:111:ASP:O	2:B:113:GLU:N	2.54	0.41
2:B:451:ARG:NH1	2:B:472:ILE:HD12	2.35	0.41
1:A:23:THR:OG1	1:A:25:ILE:HG12	2.21	0.41
2:C:53:THR:O	2:C:57:ILE:HG12	2.20	0.41
1:F:126:LEU:O	1:F:127:ILE:C	2.58	0.41
2:B:116:GLU:HG2	2:B:154:TYR:HE2	1.86	0.41
2:E:443:VAL:CG1	2:E:494:PRO:HG2	2.50	0.41
1:F:443:VAL:HG12	1:F:445:ILE:HD11	2.03	0.41
1:F:194:TYR:O	1:F:195:GLY:C	2.58	0.41
1:A:116:GLU:O	1:A:117:VAL:HB	2.21	0.41
2:B:211:LEU:O	2:B:215:ARG:O	2.39	0.41
2:B:213:GLY:O	2:B:214:GLU:CB	2.68	0.41
2:D:443:VAL:HG12	2:D:445:ILE:CD1	2.51	0.40
2:C:21:MET:HE3	2:C:141:ARG:CD	2.51	0.40
1:A:80:PRO:HD2	1:A:81:GLN:NE2	2.36	0.40
2:E:451:ARG:CG	2:E:451:ARG:NH1	2.84	0.40
2:B:429:HIS:HA	2:B:431:GLU:OE2	2.20	0.40
1:A:496:ARG:O	1:A:497:ILE:HG23	2.21	0.40
2:E:148:THR:HG23	2:E:193:ARG:HD2	2.03	0.40
1:A:296:LEU:HD21	1:A:477:PRO:HD3	2.03	0.40
1:A:116:GLU:C	1:A:117:VAL:CG2	2.79	0.40
2:B:81:GLN:N	2:B:81:GLN:CD	2.73	0.40
2:D:484:ARG:NH1	2:D:484:ARG:CB	2.84	0.40
1:F:21:MET:CE	1:F:59:PHE:CE1	3.04	0.40
2:E:392:PHE:O	2:E:395:PHE:HB3	2.20	0.40
1:A:443:VAL:CG1	1:A:445:ILE:HD11	2.51	0.40
2:E:306:CYS:SG	2:E:338:MET:SD	3.20	0.40
2:C:194:TYR:CD1	2:C:194:TYR:N	2.89	0.40
2:C:352:GLU:N	2:C:352:GLU:CD	2.74	0.40
2:C:296:LEU:HD21	2:C:477:PRO:HB3	2.03	0.40
2:B:497:ILE:O	2:B:498:THR:C	2.59	0.40
1:A:237:PHE:HA	1:A:245:ASN:O	2.21	0.40
1:A:112:PRO:O	2:B:166:ARG:HG3	2.21	0.40
2:B:161:ARG:HB2	2:B:196:VAL:CG1	2.50	0.40
2:C:153:GLN:O	2:C:154:TYR:CB	2.69	0.40
2:D:64:ILE:HD12	2:D:69:GLU:O	2.20	0.40
1:F:393:ARG:NH2	5:F:527:HOH:O	2.45	0.40
1:A:420:MET:HE1	2:B:490:ILE:HG21	2.02	0.40
2:D:49:GLY:HA2	3:D:903:ATP:O2B	2.21	0.40
1:A:24:MET:CB	1:A:62:ASN:HD22	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:320:SER:HA	2:D:254:LEU:HG	2.02	0.40
2:D:200:VAL:O	2:D:200:VAL:HG12	2.20	0.40
2:E:143:SER:HA	2:E:179:VAL:O	2.20	0.40
2:C:28:PHE:N	2:C:246:ILE:HD12	2.36	0.40
1:F:18:ILE:HD12	1:F:227:GLY:CA	2.33	0.40
1:A:237:PHE:C	1:A:237:PHE:CD1	2.94	0.40
2:B:47:THR:HG23	2:B:187:GLU:OE2	2.21	0.40
2:C:123:LEU:HA	2:C:127:ILE:HD13	2.02	0.40
2:D:472:ILE:N	2:D:472:ILE:HD12	2.37	0.40
2:B:25:ILE:HG23	2:B:58:GLN:HE22	1.86	0.40
2:D:396:VAL:HG11	2:D:430:ILE:CG2	2.51	0.40
1:A:489:ILE:HD13	1:A:494:PRO:HG3	2.04	0.40
2:B:267:VAL:HB	2:B:270:LEU:HB2	2.04	0.40
2:B:249:LEU:HD12	2:B:394:GLN:HG2	2.02	0.40
1:A:340:ARG:C	1:A:342:ASN:N	2.75	0.40
2:B:326:ARG:HG3	2:C:260:ASN:HD21	1.87	0.40
2:C:468:ARG:HG2	2:C:468:ARG:HH11	1.85	0.40
1:F:362:ILE:O	1:F:365:SER:HB3	2.21	0.40
2:D:75:THR:HG22	2:D:107:ASP:HA	2.04	0.40
2:C:484:ARG:HB3	2:C:484:ARG:NH1	2.35	0.40
2:E:262:ARG:HD2	2:E:276:GLY:O	2.21	0.40
1:F:425:ILE:HD13	1:F:437:ILE:HG21	2.03	0.40
2:D:315:PHE:HA	2:D:347:VAL:HB	2.04	0.40
1:A:487:GLU:OE1	1:F:496:ARG:HG2	2.22	0.40
1:A:290:THR:CG2	2:B:425:ILE:HD12	2.44	0.40
2:E:436:THR:HG23	2:E:458:MET:CG	2.47	0.40
2:C:149:SER:HA	2:C:152:GLN:HB2	2.03	0.40
1:F:357:GLU:CG	1:F:358:ASP:N	2.84	0.40
2:B:134:ILE:HA	2:B:139:ALA:HB3	2.02	0.40
2:E:186:GLU:OE2	2:E:187:GLU:N	2.54	0.40
2:E:333:MET:HE3	2:E:333:MET:HB2	1.96	0.40
2:E:428:SER:CB	2:E:430:ILE:HD11	2.51	0.40
2:E:428:SER:OG	2:E:430:ILE:HD11	2.22	0.40
2:D:44:VAL:HG12	2:D:44:VAL:O	2.21	0.40
2:E:49:GLY:CA	3:E:903:ATP:O2B	2.70	0.40
2:D:269:ARG:O	2:D:272:GLU:HB2	2.20	0.40
2:C:111:ASP:OD2	2:C:113:GLU:HG2	2.21	0.40
2:C:121:PHE:HB3	2:C:125:ALA:CB	2.51	0.40
2:C:65:ILE:HG22	2:C:65:ILE:O	2.21	0.40
2:D:249:LEU:CD1	2:D:394:GLN:HG2	2.51	0.40
2:B:119:GLY:C	2:B:121:PHE:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ILE:O	2:B:367:ILE:HG13	2.21	0.40
1:F:172:LYS:HE3	1:F:172:LYS:HB2	1.92	0.40
2:D:357:GLU:HG3	2:D:358:ASP:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	503/525 (96%)	406 (81%)	76 (15%)	21 (4%)	3	20
1	F	503/525 (96%)	422 (84%)	61 (12%)	20 (4%)	4	21
2	B	489/525 (93%)	389 (80%)	82 (17%)	18 (4%)	4	23
2	C	486/525 (93%)	419 (86%)	45 (9%)	22 (4%)	3	18
2	D	483/525 (92%)	415 (86%)	52 (11%)	16 (3%)	5	26
2	E	490/525 (93%)	402 (82%)	69 (14%)	19 (4%)	4	21
All	All	2954/3150 (94%)	2453 (83%)	385 (13%)	116 (4%)	4	21

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	TYR
1	A	334	ASP
1	A	462	TRP
1	A	463	HIS
1	A	503	SER
2	B	52	LYS
2	B	154	TYR
2	B	211	LEU
2	C	17	ALA

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Mol	Chain	Res	Type
2	C	117	VAL
2	C	154	TYR
2	C	354	ALA
2	C	432	GLU
2	C	463	HIS
2	D	113	GLU
2	D	154	TYR
2	D	211	LEU
2	D	463	HIS
2	E	122	ASP
2	E	154	TYR
2	E	157	SER
2	E	211	LEU
2	E	387	VAL
1	F	118	VAL
1	F	154	TYR
1	F	211	LEU
1	F	431	GLU
1	F	504	GLU
1	F	506	SER
1	F	509	VAL
1	A	117	VAL
1	A	155	ASP
1	A	322	ALA
1	A	422	ALA
2	B	119	GLY
2	B	341	GLN
2	B	484	ARG
2	C	112	PRO
2	C	124	SER
2	C	211	LEU
2	C	341	GLN
2	C	431	GLU
2	D	123	LEU
2	D	333	MET
2	D	341	GLN
2	D	354	ALA
2	D	494	PRO
2	E	420	MET
2	E	463	HIS
2	E	494	PRO
2	E	502	LYS

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Mol	Chain	Res	Type
1	F	117	VAL
1	F	214	GLU
1	F	420	MET
1	F	500	ASP
1	F	501	GLU
1	A	341	GLN
1	A	387	VAL
1	A	464	ASP
1	A	500	ASP
2	B	420	MET
2	C	379	SER
2	D	214	GLU
2	E	304	ASN
2	E	446	ARG
1	F	189	GLY
1	F	379	SER
1	F	381	SER
1	A	157	SER
1	A	379	SER
2	B	149	SER
2	B	348	CYS
2	B	379	SER
2	B	498	THR
2	C	289	ALA
2	C	349	ALA
2	D	353	SER
2	D	387	VAL
2	D	420	MET
2	D	496	ARG
2	E	52	LYS
2	E	189	GLY
2	E	379	SER
1	F	152	GLN
1	F	515	LYS
2	B	17	ALA
2	B	87	ALA
2	B	112	PRO
2	B	167	LEU
2	C	114	GLY
2	C	115	GLN
2	C	149	SER
2	C	348	CYS

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Mol	Chain	Res	Type
2	D	348	CYS
2	E	372	PRO
2	E	480	LYS
2	E	488	ARG
1	F	157	SER
1	F	348	CYS
1	F	517	PRO
1	A	48	SER
1	A	349	ALA
1	A	421	GLY
1	A	509	VAL
2	B	494	PRO
2	C	212	GLU
2	C	420	MET
2	E	113	GLU
2	C	477	PRO
2	E	117	VAL
2	B	117	VAL
1	A	65	ILE
1	A	497	ILE
2	B	195	GLY
2	C	499	VAL
2	D	18	ILE

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	431/449 (96%)	389 (90%)	42 (10%)	10	37
1	F	431/449 (96%)	383 (89%)	48 (11%)	8	29
2	B	419/450 (93%)	370 (88%)	49 (12%)	7	27
2	C	416/450 (92%)	374 (90%)	42 (10%)	9	34
2	D	413/450 (92%)	367 (89%)	46 (11%)	8	29
2	E	420/450 (93%)	377 (90%)	43 (10%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2530/2698 (94%)	2260 (89%)	270 (11%)	8	31

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	33	HIS
1	A	65	ILE
1	A	79	THR
1	A	81	GLN
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	118	VAL
1	A	121	PHE
1	A	123	LEU
1	A	151	PHE
1	A	181	THR
1	A	185	ILE
1	A	186	GLU
1	A	212	GLU
1	A	218	ARG
1	A	223	LEU
1	A	238	THR
1	A	256	GLN
1	A	263	VAL
1	A	270	LEU
1	A	284	ILE
1	A	287	THR
1	A	302	VAL
1	A	303	GLU
1	A	323	GLN
1	A	342	ASN
1	A	360	LEU
1	A	371	LYS
1	A	400	THR
1	A	428	SER
1	A	430	ILE
1	A	431	GLU
1	A	434	THR
1	A	451	ARG
1	A	469	GLU

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Mol	Chain	Res	Type
1	A	471	MET
1	A	496	ARG
1	A	508	ILE
1	A	509	VAL
1	A	518	GLU
2	B	26	GLU
2	B	52	LYS
2	B	81	GLN
2	B	92	TRP
2	B	99	ASP
2	B	106	LEU
2	B	111	ASP
2	B	112	PRO
2	B	123	LEU
2	B	128	GLU
2	B	140	ARG
2	B	151	PHE
2	B	154	TYR
2	B	178	THR
2	B	181	THR
2	B	183	GLU
2	B	185	ILE
2	B	186	GLU
2	B	198	GLU
2	B	209	ASN
2	B	212	GLU
2	B	223	LEU
2	B	256	GLN
2	B	270	LEU
2	B	284	ILE
2	B	303	GLU
2	B	320	SER
2	B	333	MET
2	B	360	LEU
2	B	366	GLU
2	B	369	ASP
2	B	371	LYS
2	B	375	ILE
2	B	380	LEU
2	B	413	THR
2	B	432	GLU
2	B	450	SER

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Mol	Chain	Res	Type
2	B	451	ARG
2	B	453	ILE
2	B	462	TRP
2	B	463	HIS
2	B	469	GLU
2	B	471	MET
2	B	474	ASP
2	B	485	ASN
2	B	490	ILE
2	B	499	VAL
2	B	501	GLU
2	B	503	SER
2	C	15	HIS
2	C	26	GLU
2	C	50	THR
2	C	79	THR
2	C	81	GLN
2	C	99	ASP
2	C	111	ASP
2	C	121	PHE
2	C	127	ILE
2	C	140	ARG
2	C	151	PHE
2	C	154	TYR
2	C	177	THR
2	C	178	THR
2	C	185	ILE
2	C	186	GLU
2	C	209	ASN
2	C	212	GLU
2	C	217	ARG
2	C	218	ARG
2	C	223	LEU
2	C	256	GLN
2	C	263	VAL
2	C	270	LEU
2	C	303	GLU
2	C	320	SER
2	C	321	ARG
2	C	333	MET
2	C	356	LEU
2	C	360	LEU

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Mol	Chain	Res	Type
2	C	371	LYS
2	C	375	ILE
2	C	397	ILE
2	C	451	ARG
2	C	453	ILE
2	C	462	TRP
2	C	469	GLU
2	C	470	PHE
2	C	471	MET
2	C	491	SER
2	C	498	THR
2	C	500	ASP
2	D	26	GLU
2	D	79	THR
2	D	81	GLN
2	D	106	LEU
2	D	121	PHE
2	D	122	ASP
2	D	123	LEU
2	D	151	PHE
2	D	154	TYR
2	D	178	THR
2	D	181	THR
2	D	185	ILE
2	D	186	GLU
2	D	201	SER
2	D	209	ASN
2	D	211	LEU
2	D	212	GLU
2	D	222	ILE
2	D	223	LEU
2	D	228	THR
2	D	240	THR
2	D	256	GLN
2	D	259	SER
2	D	260	ASN
2	D	270	LEU
2	D	284	ILE
2	D	287	THR
2	D	290	THR
2	D	321	ARG
2	D	333	MET

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Mol	Chain	Res	Type
2	D	338	MET
2	D	342	ASN
2	D	360	LEU
2	D	366	GLU
2	D	369	ASP
2	D	371	LYS
2	D	400	THR
2	D	416	SER
2	D	451	ARG
2	D	469	GLU
2	D	471	MET
2	D	474	ASP
2	D	487	GLU
2	D	490	ILE
2	D	496	ARG
2	D	498	THR
2	E	26	GLU
2	E	79	THR
2	E	81	GLN
2	E	99	ASP
2	E	106	LEU
2	E	113	GLU
2	E	121	PHE
2	E	140	ARG
2	E	151	PHE
2	E	154	TYR
2	E	171	LEU
2	E	177	THR
2	E	178	THR
2	E	181	THR
2	E	183	GLU
2	E	185	ILE
2	E	186	GLU
2	E	203	ASN
2	E	209	ASN
2	E	212	GLU
2	E	216	ARG
2	E	223	LEU
2	E	228	THR
2	E	256	GLN
2	E	270	LEU
2	E	300	ARG

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Mol	Chain	Res	Type
2	E	320	SER
2	E	321	ARG
2	E	325	LEU
2	E	333	MET
2	E	342	ASN
2	E	360	LEU
2	E	371	LYS
2	E	375	ILE
2	E	417	ASP
2	E	451	ARG
2	E	453	ILE
2	E	458	MET
2	E	464	ASP
2	E	471	MET
2	E	474	ASP
2	E	501	GLU
2	E	505	LEU
1	F	26	GLU
1	F	33	HIS
1	F	45	SER
1	F	77	GLU
1	F	79	THR
1	F	99	ASP
1	F	106	LEU
1	F	116	GLU
1	F	121	PHE
1	F	123	LEU
1	F	140	ARG
1	F	151	PHE
1	F	154	TYR
1	F	181	THR
1	F	183	GLU
1	F	184	ARG
1	F	185	ILE
1	F	186	GLU
1	F	198	GLU
1	F	203	ASN
1	F	212	GLU
1	F	223	LEU
1	F	256	GLN
1	F	287	THR
1	F	300	ARG

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Mol	Chain	Res	Type
1	F	302	VAL
1	F	314	LEU
1	F	321	ARG
1	F	325	LEU
1	F	333	MET
1	F	342	ASN
1	F	360	LEU
1	F	369	ASP
1	F	371	LYS
1	F	375	ILE
1	F	381	SER
1	F	417	ASP
1	F	451	ARG
1	F	458	MET
1	F	462	TRP
1	F	469	GLU
1	F	471	MET
1	F	496	ARG
1	F	501	GLU
1	F	504	GLU
1	F	507	ARG
1	F	514	GLU
1	F	515	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	33	HIS
1	A	62	ASN
1	A	81	GLN
1	A	209	ASN
1	A	304	ASN
1	A	368	ASN
1	A	414	ASN
1	A	441	GLN
1	A	463	HIS
2	B	58	GLN
2	B	62	ASN
2	B	81	GLN
2	B	209	ASN
2	B	256	GLN

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Mol	Chain	Res	Type
2	B	260	ASN
2	B	323	GLN
2	B	361	GLN
2	B	368	ASN
2	B	414	ASN
2	B	441	GLN
2	B	454	ASN
2	C	33	HIS
2	C	58	GLN
2	C	81	GLN
2	C	209	ASN
2	C	256	GLN
2	C	260	ASN
2	C	304	ASN
2	C	368	ASN
2	C	389	ASN
2	C	414	ASN
2	C	429	HIS
2	C	441	GLN
2	D	33	HIS
2	D	81	GLN
2	D	209	ASN
2	D	327	ASN
2	D	414	ASN
2	E	81	GLN
2	E	203	ASN
2	E	209	ASN
2	E	256	GLN
2	E	304	ASN
2	E	361	GLN
2	E	368	ASN
2	E	414	ASN
2	E	441	GLN
2	E	454	ASN
1	F	16	GLN
1	F	33	HIS
1	F	81	GLN
1	F	209	ASN
1	F	260	ASN
1	F	323	GLN
1	F	361	GLN
1	F	368	ASN

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Mol	Chain	Res	Type
1	F	414	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	SEP	A	320	1	8,9,10	1.81	2 (25%)	8,12,14	2.69	1 (12%)
1	SEP	F	320	1	8,9,10	2.06	3 (37%)	8,12,14	2.81	3 (37%)

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	SEP	A	320	1	-	0/6/8/10	0/0/0/0
1	SEP	F	320	1	-	0/6/8/10	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	SEP	P-O3P	2.01	1.61	1.54
1	F	320	SEP	CB-CA	2.50	1.59	1.52
1	F	320	SEP	P-O2P	2.86	1.65	1.54
1	F	320	SEP	P-O1P	4.20	1.65	1.51
1	A	320	SEP	P-O1P	4.54	1.66	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	320	SEP	OG-CB-CA	-6.36	102.85	108.27
1	F	320	SEP	O2P-P-O1P	-2.09	103.86	110.58
1	F	320	SEP	O3P-P-OG	3.75	117.36	106.56
1	A	320	SEP	OG-CB-CA	6.74	114.02	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	320	SEP	16	0
1	F	320	SEP	11	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 33 ligands modelled in this entry, 21 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	24,33,33	1.31	3 (12%)	31,52,52	2.59	7 (22%)
3	ATP	A	903	4	24,33,33	1.24	3 (12%)	31,52,52	2.60	6 (19%)
3	ATP	B	901	4	24,33,33	1.31	4 (16%)	31,52,52	2.57	6 (19%)
3	ATP	B	903	4	24,33,33	1.35	4 (16%)	31,52,52	2.62	7 (22%)
3	ATP	C	901	4	24,33,33	1.34	2 (8%)	31,52,52	2.61	6 (19%)
3	ATP	C	903	4	24,33,33	1.12	2 (8%)	31,52,52	2.73	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	D	901	4	24,33,33	1.28	2 (8%)	31,52,52	2.63	6 (19%)
3	ATP	D	903	4	24,33,33	1.07	1 (4%)	31,52,52	2.71	6 (19%)
3	ATP	E	901	4	24,33,33	1.32	4 (16%)	31,52,52	2.57	6 (19%)
3	ATP	E	903	-	24,33,33	1.29	2 (8%)	31,52,52	2.68	8 (25%)
3	ATP	F	901	4	24,33,33	1.32	4 (16%)	31,52,52	2.54	8 (25%)
3	ATP	F	903	4	24,33,33	1.36	2 (8%)	31,52,52	2.60	6 (19%)

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	-	0/18/38/38	0/3/3/3
3	ATP	A	903	4	-	0/18/38/38	0/3/3/3
3	ATP	B	901	4	-	0/18/38/38	0/3/3/3
3	ATP	B	903	4	-	0/18/38/38	0/3/3/3
3	ATP	C	901	4	-	0/18/38/38	0/3/3/3
3	ATP	C	903	4	-	0/18/38/38	0/3/3/3
3	ATP	D	901	4	-	0/18/38/38	0/3/3/3
3	ATP	D	903	4	-	0/18/38/38	0/3/3/3
3	ATP	E	901	4	-	0/18/38/38	0/3/3/3
3	ATP	E	903	-	-	0/18/38/38	0/3/3/3
3	ATP	F	901	4	-	0/18/38/38	0/3/3/3
3	ATP	F	903	4	-	0/18/38/38	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	903	ATP	C2'-C3'	-2.18	1.47	1.53
3	C	903	ATP	O4'-C4'	-2.10	1.40	1.45
3	F	901	ATP	C4-N3	2.02	1.38	1.35
3	B	901	ATP	C4-N3	2.08	1.38	1.35
3	A	901	ATP	C2-N1	2.09	1.37	1.33
3	E	901	ATP	O4'-C1'	2.12	1.43	1.41
3	B	903	ATP	C2-N1	2.16	1.38	1.33
3	E	901	ATP	C4-N3	2.16	1.38	1.35
3	B	903	ATP	C4-N3	2.16	1.38	1.35
3	A	903	ATP	C2-N1	2.18	1.38	1.33
3	E	901	ATP	C2-N1	2.23	1.38	1.33
3	F	901	ATP	C2-N1	2.32	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	ATP	O4'-C1'	2.37	1.44	1.41
3	B	901	ATP	C2-N1	2.47	1.38	1.33
3	F	903	ATP	C2-N1	2.50	1.38	1.33
3	D	901	ATP	O4'-C1'	2.63	1.44	1.41
3	A	903	ATP	O4'-C1'	2.67	1.44	1.41
3	B	901	ATP	O4'-C1'	2.73	1.44	1.41
3	F	901	ATP	O4'-C1'	2.91	1.44	1.41
3	A	901	ATP	O4'-C1'	2.99	1.45	1.41
3	C	903	ATP	C2-N3	3.02	1.37	1.32
3	D	903	ATP	C2-N3	3.05	1.37	1.32
3	B	903	ATP	O4'-C1'	3.35	1.45	1.41
3	A	903	ATP	C2-N3	3.38	1.38	1.32
3	D	901	ATP	C2-N3	3.39	1.38	1.32
3	B	901	ATP	C2-N3	3.40	1.38	1.32
3	B	903	ATP	C2-N3	3.60	1.38	1.32
3	E	903	ATP	C2-N3	3.69	1.38	1.32
3	F	901	ATP	C2-N3	3.74	1.38	1.32
3	A	901	ATP	C2-N3	3.79	1.38	1.32
3	E	901	ATP	C2-N3	3.84	1.39	1.32
3	C	901	ATP	C2-N3	3.99	1.39	1.32
3	F	903	ATP	C2-N3	4.31	1.39	1.32

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ATP	N3-C2-N1	-12.03	119.69	128.89
3	C	903	ATP	N3-C2-N1	-11.99	119.71	128.89
3	C	901	ATP	N3-C2-N1	-11.66	119.97	128.89
3	B	903	ATP	N3-C2-N1	-11.54	120.06	128.89
3	B	901	ATP	N3-C2-N1	-11.51	120.08	128.89
3	A	903	ATP	N3-C2-N1	-11.36	120.19	128.89
3	D	903	ATP	N3-C2-N1	-11.29	120.25	128.89
3	E	901	ATP	N3-C2-N1	-11.16	120.35	128.89
3	F	903	ATP	N3-C2-N1	-11.14	120.37	128.89
3	F	901	ATP	N3-C2-N1	-11.04	120.44	128.89
3	A	901	ATP	N3-C2-N1	-10.94	120.51	128.89
3	E	903	ATP	N3-C2-N1	-10.85	120.59	128.89
3	D	903	ATP	C4-C5-N7	-5.36	104.55	109.48
3	E	901	ATP	C4-C5-N7	-5.07	104.81	109.48
3	A	901	ATP	C4-C5-N7	-4.90	104.97	109.48
3	E	903	ATP	C4-C5-N7	-4.81	105.06	109.48
3	F	901	ATP	C4-C5-N7	-4.77	105.09	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	ATP	C4-C5-N7	-4.68	105.17	109.48
3	C	903	ATP	C4-C5-N7	-4.54	105.30	109.48
3	F	903	ATP	C4-C5-N7	-4.53	105.31	109.48
3	C	901	ATP	C4-C5-N7	-4.47	105.37	109.48
3	B	901	ATP	C4-C5-N7	-4.46	105.38	109.48
3	A	903	ATP	C4-C5-N7	-4.40	105.43	109.48
3	D	901	ATP	C4-C5-N7	-4.18	105.64	109.48
3	B	903	ATP	PB-O3B-PG	-2.70	123.60	132.67
3	E	901	ATP	N6-C6-N1	-2.55	113.74	119.20
3	D	903	ATP	N6-C6-N1	-2.54	113.76	119.20
3	A	901	ATP	N6-C6-N1	-2.47	113.89	119.20
3	B	903	ATP	N6-C6-N1	-2.42	114.01	119.20
3	F	901	ATP	N6-C6-N1	-2.40	114.06	119.20
3	C	903	ATP	N6-C6-N1	-2.31	114.25	119.20
3	A	903	ATP	PB-O3B-PG	-2.29	125.00	132.67
3	A	903	ATP	N6-C6-N1	-2.28	114.31	119.20
3	F	901	ATP	PB-O3B-PG	-2.20	125.28	132.67
3	F	903	ATP	N6-C6-N1	-2.19	114.49	119.20
3	B	901	ATP	N6-C6-N1	-2.09	114.72	119.20
3	A	901	ATP	PB-O3B-PG	-2.08	125.70	132.67
3	E	903	ATP	N6-C6-N1	-2.04	114.83	119.20
3	E	903	ATP	PB-O3B-PG	-2.03	125.86	132.67
3	D	901	ATP	N6-C6-N1	-2.03	114.85	119.20
3	C	903	ATP	O2B-PB-O3B	2.04	114.35	105.09
3	F	903	ATP	O2B-PB-O3B	2.05	114.41	105.09
3	E	903	ATP	O2B-PB-O3A	2.06	114.46	105.09
3	F	901	ATP	O2'-C2'-C3'	2.07	118.55	111.83
3	A	901	ATP	O2B-PB-O3B	2.09	114.58	105.09
3	B	901	ATP	O3A-PA-O5'	2.10	108.51	102.94
3	F	901	ATP	O2B-PB-O3B	2.12	114.72	105.09
3	D	901	ATP	O3A-PA-O5'	2.14	108.61	102.94
3	C	901	ATP	C2'-C1'-N9	2.18	117.62	114.29
3	D	903	ATP	O2B-PB-O3B	2.19	115.03	105.09
3	E	901	ATP	O2'-C2'-C3'	2.19	118.96	111.83
3	E	901	ATP	O2B-PB-O3B	2.20	115.08	105.09
3	B	901	ATP	O2B-PB-O3B	2.21	115.14	105.09
3	B	903	ATP	O2'-C2'-C3'	2.30	119.30	111.83
3	F	901	ATP	O3A-PA-O5'	2.31	109.07	102.94
3	D	901	ATP	O2B-PB-O3B	2.38	115.89	105.09
3	E	903	ATP	PA-O3A-PB	2.54	139.86	132.73
3	A	901	ATP	O3A-PA-O5'	2.56	109.72	102.94
3	C	901	ATP	O2'-C2'-C3'	2.58	120.23	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	ATP	O3A-PA-O5'	2.63	109.92	102.94
3	C	901	ATP	O2B-PB-O3B	2.70	117.34	105.09
3	C	901	ATP	O3A-PA-O5'	2.99	110.86	102.94
3	B	903	ATP	C2'-C1'-N9	2.99	118.86	114.29
3	A	903	ATP	O3A-PA-O5'	2.99	110.87	102.94
3	E	901	ATP	C2'-C1'-N9	3.02	118.91	114.29
3	F	903	ATP	O3A-PA-O5'	3.10	111.16	102.94
3	C	903	ATP	O3A-PA-O5'	3.32	111.74	102.94
3	B	901	ATP	C2'-C1'-N9	3.47	119.60	114.29
3	D	901	ATP	C2'-C1'-N9	3.52	119.67	114.29
3	F	901	ATP	C2'-C1'-N9	3.63	119.83	114.29
3	D	903	ATP	O3A-PA-O5'	3.71	112.78	102.94
3	A	903	ATP	C2'-C1'-N9	3.89	120.23	114.29
3	C	903	ATP	C2'-C1'-N9	3.93	120.30	114.29
3	F	903	ATP	C2'-C1'-N9	4.04	120.47	114.29
3	A	901	ATP	C2'-C1'-N9	4.07	120.50	114.29
3	E	903	ATP	O3A-PA-O5'	4.13	113.90	102.94
3	D	903	ATP	C2'-C1'-N9	4.73	121.51	114.29
3	E	903	ATP	C2'-C1'-N9	5.24	122.30	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ATP	6	0
3	A	903	ATP	1	0
3	B	901	ATP	3	0
3	B	903	ATP	5	0
3	C	901	ATP	3	0
3	C	903	ATP	2	0
3	D	901	ATP	2	0
3	D	903	ATP	4	0
3	E	901	ATP	6	0
3	E	903	ATP	5	0
3	F	901	ATP	4	0
3	F	903	ATP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	505/525 (96%)	0.20	53 (10%) 8 3	31, 77, 121, 154	0
1	F	505/525 (96%)	-0.07	31 (6%) 25 9	18, 66, 113, 145	0
2	B	491/525 (93%)	0.15	35 (7%) 19 7	43, 82, 126, 158	0
2	C	488/525 (92%)	-0.15	20 (4%) 41 16	30, 69, 122, 160	0
2	D	485/525 (92%)	-0.35	13 (2%) 58 28	20, 53, 106, 152	0
2	E	492/525 (93%)	-0.24	15 (3%) 54 25	15, 59, 104, 148	0
All	All	2966/3150 (94%)	-0.08	167 (5%) 28 11	15, 69, 117, 160	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	118	VAL	8.1
1	F	516	GLY	7.2
2	D	119	GLY	6.1
2	D	117	VAL	6.0
1	A	509	VAL	5.9
1	F	506	SER	5.7
1	F	517	PRO	5.6
2	D	121	PHE	5.6
2	B	500	ASP	5.5
1	A	258	SER	5.3
1	F	500	ASP	5.3
2	C	117	VAL	5.2
2	E	500	ASP	5.1
1	F	507	ARG	5.1
1	A	519	SER	5.1
1	F	515	LYS	4.8
1	A	500	ASP	4.8
1	F	509	VAL	4.8
1	A	513	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	504	GLU	4.8
1	A	506	SER	4.8
2	C	119	GLY	4.7
1	F	154	TYR	4.7
2	B	255	THR	4.7
2	B	503	SER	4.7
1	A	16	GLN	4.6
1	A	120	GLY	4.6
2	C	118	VAL	4.5
1	A	257	ARG	4.4
2	B	15	HIS	4.4
2	B	117	VAL	4.4
1	A	503	SER	4.4
1	A	507	ARG	4.4
2	D	120	GLY	4.3
2	B	501	GLU	4.3
1	F	508	ILE	4.2
2	E	154	TYR	4.2
2	C	120	GLY	4.1
2	B	254	LEU	4.0
1	A	511	GLY	4.0
2	C	499	VAL	4.0
1	F	121	PHE	4.0
1	A	517	PRO	4.0
1	A	518	GLU	3.9
1	F	519	SER	3.9
2	E	501	GLU	3.9
2	B	251	ALA	3.8
1	A	508	ILE	3.8
2	E	504	GLU	3.8
1	A	117	VAL	3.7
1	A	254	LEU	3.7
2	B	157	SER	3.7
2	E	121	PHE	3.6
1	F	511	GLY	3.6
1	F	501	GLU	3.6
2	C	251	ALA	3.5
2	B	119	GLY	3.4
2	E	503	SER	3.4
2	B	158	SER	3.4
2	C	154	TYR	3.4
2	B	307	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	115	GLN	3.4
1	A	516	GLY	3.4
2	E	499	VAL	3.3
2	D	154	TYR	3.3
2	B	257	ARG	3.3
1	A	121	PHE	3.3
2	D	498	THR	3.3
2	B	498	THR	3.2
2	E	505	LEU	3.2
1	F	498	THR	3.2
2	B	499	VAL	3.2
1	A	510	ARG	3.2
2	B	175	GLY	3.2
1	A	334	ASP	3.1
1	F	518	GLU	3.1
2	C	116	GLU	3.1
1	F	255	THR	3.1
2	B	153	GLN	3.1
1	A	498	THR	3.1
2	C	500	ASP	3.1
1	F	512	VAL	3.1
1	F	257	ARG	3.0
2	D	113	GLU	3.0
2	E	118	VAL	3.0
1	A	505	LEU	3.0
1	F	514	GLU	3.0
2	E	113	GLU	3.0
1	F	513	GLN	3.0
1	A	502	LYS	2.9
1	A	251	ALA	2.9
2	B	407	GLU	2.9
2	B	135	GLN	2.9
2	C	252	MET	2.9
1	A	241	ASP	2.9
2	B	504	GLU	2.8
1	A	253	ARG	2.8
1	F	117	VAL	2.8
2	C	15	HIS	2.8
2	D	16	GLN	2.8
1	A	116	GLU	2.8
2	C	77	GLU	2.7
2	E	116	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	118	VAL	2.7
2	B	132	TYR	2.7
2	B	502	LYS	2.7
1	F	504	GLU	2.7
1	A	337	GLU	2.7
2	C	257	ARG	2.6
1	F	155	ASP	2.6
2	B	116	GLU	2.6
1	A	256	GLN	2.6
1	F	311	ARG	2.6
1	A	499	VAL	2.6
2	D	15	HIS	2.6
1	A	17	ALA	2.6
2	E	332	GLY	2.6
1	A	255	THR	2.6
2	C	121	PHE	2.6
1	A	152	GLN	2.5
2	D	155	ASP	2.5
1	F	510	ARG	2.5
1	A	71	GLY	2.5
2	B	16	GLN	2.5
2	C	423	HIS	2.5
1	A	475	LYS	2.5
2	B	154	TYR	2.5
2	C	115	GLN	2.5
2	B	121	PHE	2.5
1	F	503	SER	2.5
1	A	112	PRO	2.5
1	A	153	GLN	2.4
1	A	154	TYR	2.4
2	B	253	ARG	2.4
1	A	113	GLU	2.4
1	A	368	ASN	2.4
2	C	501	GLU	2.4
2	B	250	GLY	2.4
1	A	311	ARG	2.3
2	D	257	ARG	2.3
1	A	310	GLU	2.3
1	F	251	ALA	2.3
1	A	515	LYS	2.3
2	E	310	GLU	2.3
1	F	502	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	114	GLY	2.3
1	F	256	GLN	2.3
2	C	102	LYS	2.3
1	F	499	VAL	2.3
2	B	115	GLN	2.2
2	C	153	GLN	2.2
2	C	176	ALA	2.2
2	B	14	GLU	2.2
1	F	341	GLN	2.2
2	E	115	GLN	2.1
2	B	342	ASN	2.1
1	A	312	ALA	2.1
2	B	120	GLY	2.1
2	E	502	LYS	2.1
2	D	253	ARG	2.1
1	A	340	ARG	2.1
1	A	342	ASN	2.0
2	B	113	GLU	2.0
1	A	252	MET	2.0
1	A	514	GLU	2.0
1	A	512	VAL	2.0
2	B	341	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	F	320	10/11	0.61	0.38	-	45,57,63,66	0
1	SEP	A	320	10/11	0.58	0.54	-	49,59,66,68	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	D	701	1/1	0.86	0.34	6.35	59,59,59,59	0
4	MG	F	702	1/1	0.96	0.24	3.74	68,68,68,68	0
4	MG	A	526	1/1	0.74	0.49	2.96	58,58,58,58	0
4	MG	D	801	1/1	0.94	0.34	2.54	44,44,44,44	0
4	MG	C	701	1/1	0.82	0.26	1.69	70,70,70,70	0
4	MG	A	802	1/1	0.94	0.31	1.21	82,82,82,82	0
4	MG	B	702	1/1	0.88	0.25	0.96	79,79,79,79	0
4	MG	B	701	1/1	0.82	0.23	0.70	58,58,58,58	0
3	ATP	C	903	31/31	0.92	0.19	0.60	42,52,85,85	0
3	ATP	D	903	31/31	0.95	0.15	0.28	26,35,60,62	0
3	ATP	B	901	31/31	0.92	0.20	0.16	67,70,85,87	0
3	ATP	D	901	31/31	0.95	0.17	-0.05	50,54,60,62	0
3	ATP	C	901	31/31	0.96	0.17	-0.11	36,47,56,56	0
4	MG	C	802	1/1	0.96	0.17	-0.28	41,41,41,41	0
3	ATP	E	903	31/31	0.96	0.14	-0.33	22,28,60,62	0
3	ATP	A	903	31/31	0.92	0.18	-0.33	61,66,76,77	0
3	ATP	F	903	31/31	0.94	0.15	-0.42	44,48,62,62	0
3	ATP	F	901	31/31	0.94	0.18	-0.46	74,83,88,89	0
4	MG	E	802	1/1	0.95	0.18	-0.52	46,46,46,46	0
4	MG	B	802	1/1	0.98	0.19	-0.60	64,64,64,64	0
3	ATP	A	901	31/31	0.93	0.19	-0.72	84,86,89,90	0
3	ATP	E	901	31/31	0.95	0.16	-0.74	65,72,81,81	0
3	ATP	B	903	31/31	0.91	0.17	-0.84	77,81,94,95	0
4	MG	B	801	1/1	0.66	0.12	-1.98	45,45,45,45	0
4	MG	F	802	1/1	0.93	0.26	-	53,53,53,53	0
4	MG	D	802	1/1	0.96	0.12	-	17,17,17,17	0
4	MG	C	702	1/1	0.85	0.44	-	65,65,65,65	0
4	MG	C	801	1/1	0.98	0.08	-	25,25,25,25	0
4	MG	D	702	1/1	0.94	0.24	-	49,49,49,49	0
4	MG	E	801	1/1	0.95	0.17	-	38,38,38,38	0
4	MG	A	801	1/1	0.94	0.14	-	46,46,46,46	0
4	MG	A	701	1/1	0.94	0.35	-	63,63,63,63	0
4	MG	F	701	1/1	0.89	0.18	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.