Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 09:18 am GMT

PDB ID	:	3ZZI
Title	:	Crystal structure of a tetrameric acetylglutamate kinase from Saccharomyces cerevisiae
Authors	:	de Cima, S.; Gil-Ortiz, F.; Crabeel, M.; Fita, I.; Rubio, V.
Deposited on	:	2011-09-01
Resolution	:	3.80 Å(reported)

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

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

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

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

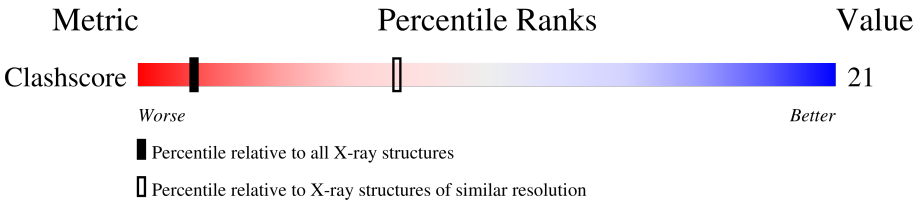
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	464	65% 27% • 6%
1	B	464	64% 29% • 6%
1	C	464	64% 29% • 6%
1	D	464	62% 32% • 6%
1	E	464	57% 35% • 6%
1	F	464	61% 33% • 6%
1	G	464	68% 25% • 6%
1	H	464	59% 34% • 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 27248 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 ACETYLGLUTAMATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3402	2167	571	655	9			
1	B	436	Total	C	N	O	S	0	0	0
			3402	2167	571	655	9			
1	C	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			
1	D	436	Total	C	N	O	S	0	0	0
			3404	2167	573	655	9			
1	E	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			
1	F	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			
1	G	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			
1	H	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	expression tag	UNP Q01217
A	51	GLY	-	expression tag	UNP Q01217
A	52	HIS	-	expression tag	UNP Q01217
A	53	HIS	-	expression tag	UNP Q01217
A	54	HIS	-	expression tag	UNP Q01217
A	55	HIS	-	expression tag	UNP Q01217
A	56	HIS	-	expression tag	UNP Q01217
A	57	HIS	-	expression tag	UNP Q01217
B	50	MET	-	expression tag	UNP Q01217
B	51	GLY	-	expression tag	UNP Q01217
B	52	HIS	-	expression tag	UNP Q01217
B	53	HIS	-	expression tag	UNP Q01217
B	54	HIS	-	expression tag	UNP Q01217

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Chain	Residue	Modelled	Actual	Comment	Reference
B	55	HIS	-	expression tag	UNP Q01217
B	56	HIS	-	expression tag	UNP Q01217
B	57	HIS	-	expression tag	UNP Q01217
C	50	MET	-	expression tag	UNP Q01217
C	51	GLY	-	expression tag	UNP Q01217
C	52	HIS	-	expression tag	UNP Q01217
C	53	HIS	-	expression tag	UNP Q01217
C	54	HIS	-	expression tag	UNP Q01217
C	55	HIS	-	expression tag	UNP Q01217
C	56	HIS	-	expression tag	UNP Q01217
C	57	HIS	-	expression tag	UNP Q01217
D	50	MET	-	expression tag	UNP Q01217
D	51	GLY	-	expression tag	UNP Q01217
D	52	HIS	-	expression tag	UNP Q01217
D	53	HIS	-	expression tag	UNP Q01217
D	54	HIS	-	expression tag	UNP Q01217
D	55	HIS	-	expression tag	UNP Q01217
D	56	HIS	-	expression tag	UNP Q01217
D	57	HIS	-	expression tag	UNP Q01217
E	50	MET	-	expression tag	UNP Q01217
E	51	GLY	-	expression tag	UNP Q01217
E	52	HIS	-	expression tag	UNP Q01217
E	53	HIS	-	expression tag	UNP Q01217
E	54	HIS	-	expression tag	UNP Q01217
E	55	HIS	-	expression tag	UNP Q01217
E	56	HIS	-	expression tag	UNP Q01217
E	57	HIS	-	expression tag	UNP Q01217
F	50	MET	-	expression tag	UNP Q01217
F	51	GLY	-	expression tag	UNP Q01217
F	52	HIS	-	expression tag	UNP Q01217
F	53	HIS	-	expression tag	UNP Q01217
F	54	HIS	-	expression tag	UNP Q01217
F	55	HIS	-	expression tag	UNP Q01217
F	56	HIS	-	expression tag	UNP Q01217
F	57	HIS	-	expression tag	UNP Q01217
G	50	MET	-	expression tag	UNP Q01217
G	51	GLY	-	expression tag	UNP Q01217
G	52	HIS	-	expression tag	UNP Q01217
G	53	HIS	-	expression tag	UNP Q01217
G	54	HIS	-	expression tag	UNP Q01217
G	55	HIS	-	expression tag	UNP Q01217
G	56	HIS	-	expression tag	UNP Q01217

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Chain	Residue	Modelled	Actual	Comment	Reference
G	57	HIS	-	expression tag	UNP Q01217
H	50	MET	-	expression tag	UNP Q01217
H	51	GLY	-	expression tag	UNP Q01217
H	52	HIS	-	expression tag	UNP Q01217
H	53	HIS	-	expression tag	UNP Q01217
H	54	HIS	-	expression tag	UNP Q01217
H	55	HIS	-	expression tag	UNP Q01217
H	56	HIS	-	expression tag	UNP Q01217
H	57	HIS	-	expression tag	UNP Q01217

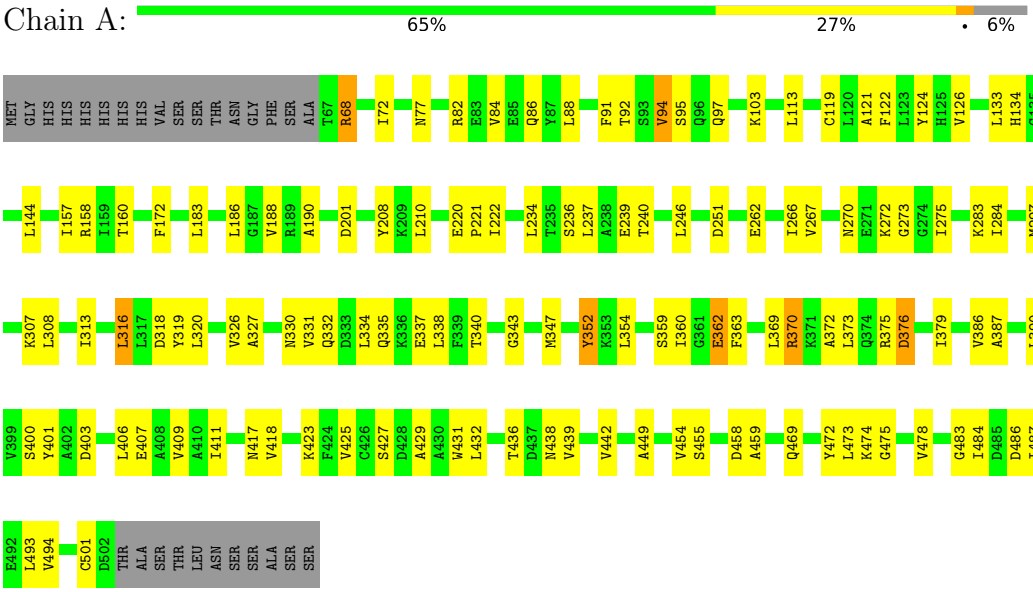
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

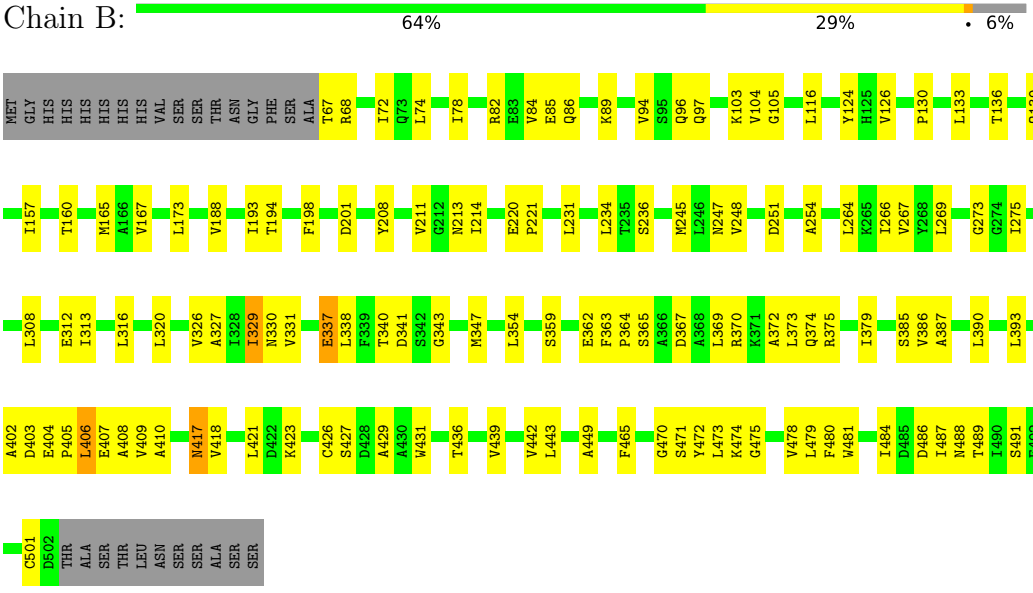
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain A:



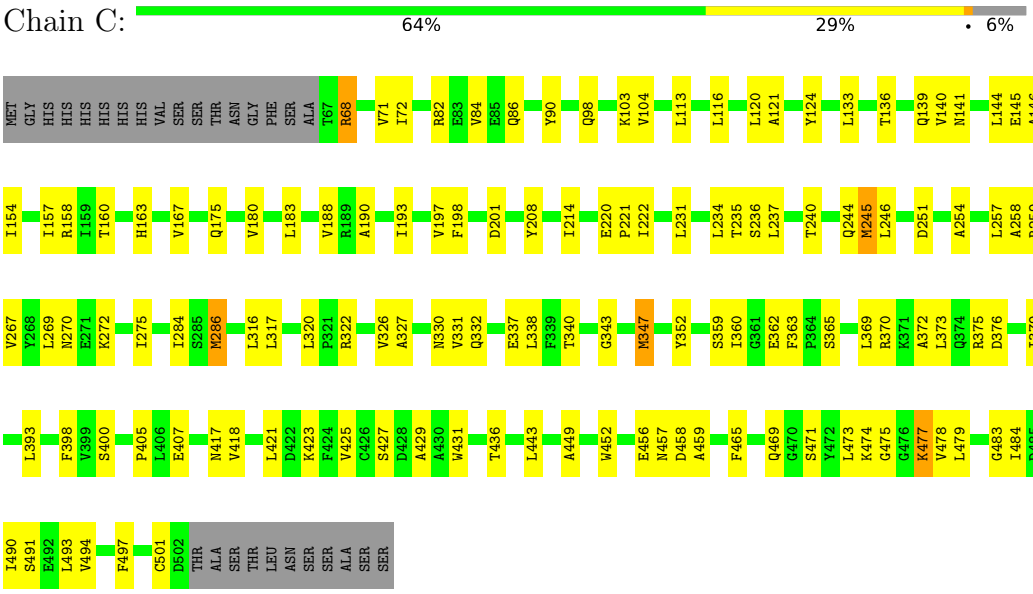
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain B:



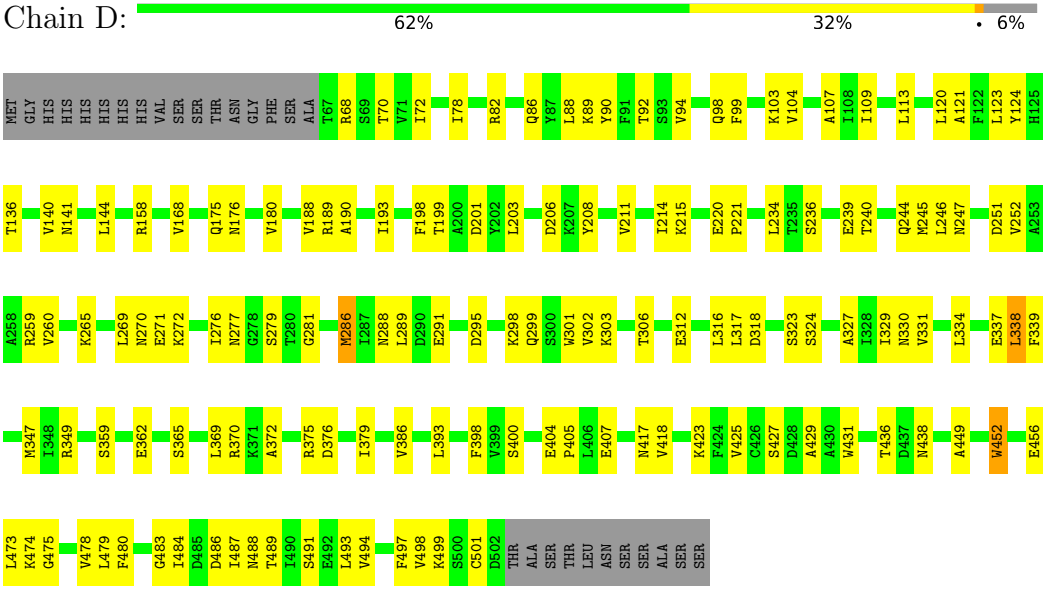
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain C:



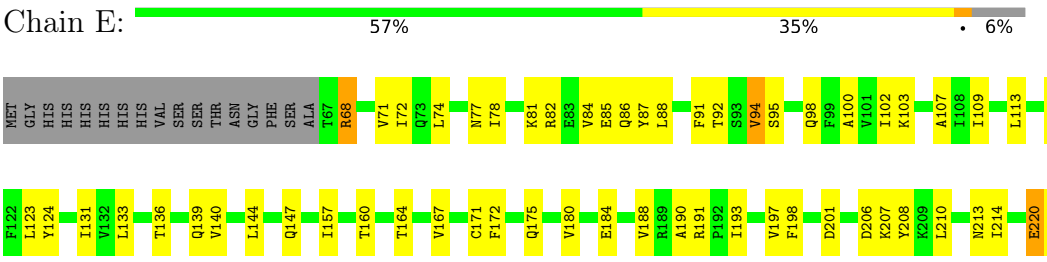
• Molecule 1: ACETYLGLUTAMATE KINASE

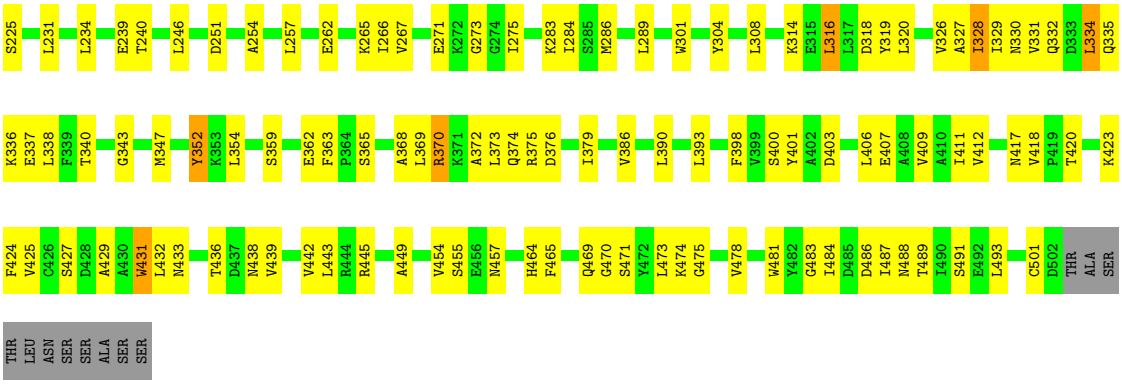
Chain D:



• Molecule 1: ACETYLGLUTAMATE KINASE

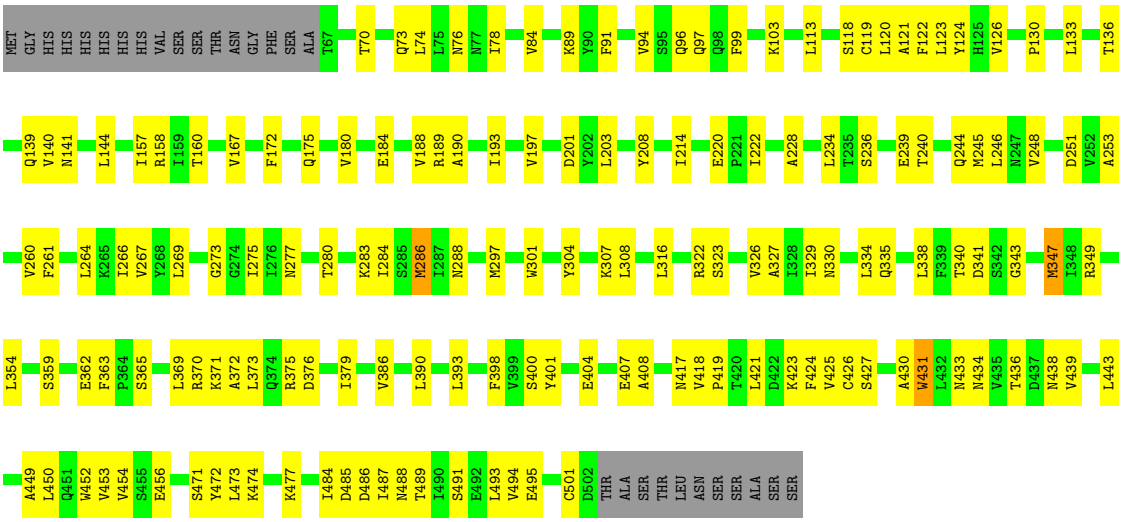
Chain E:





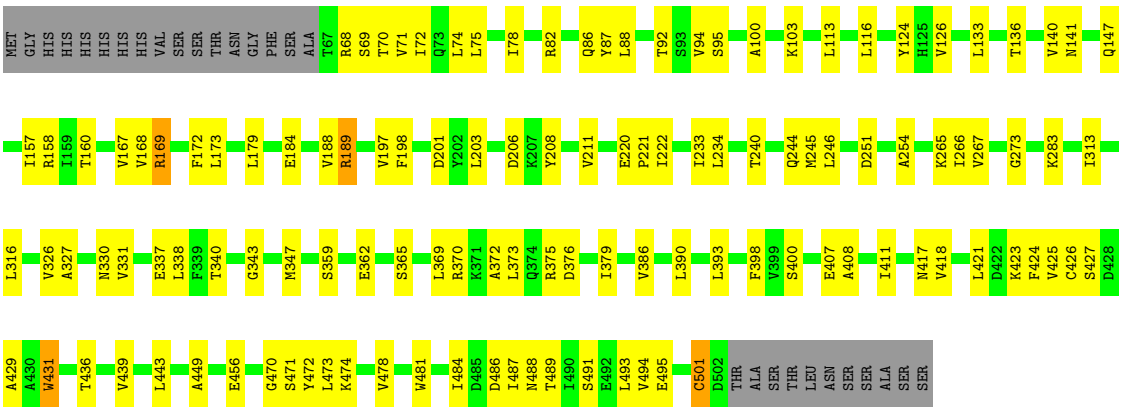
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain F:



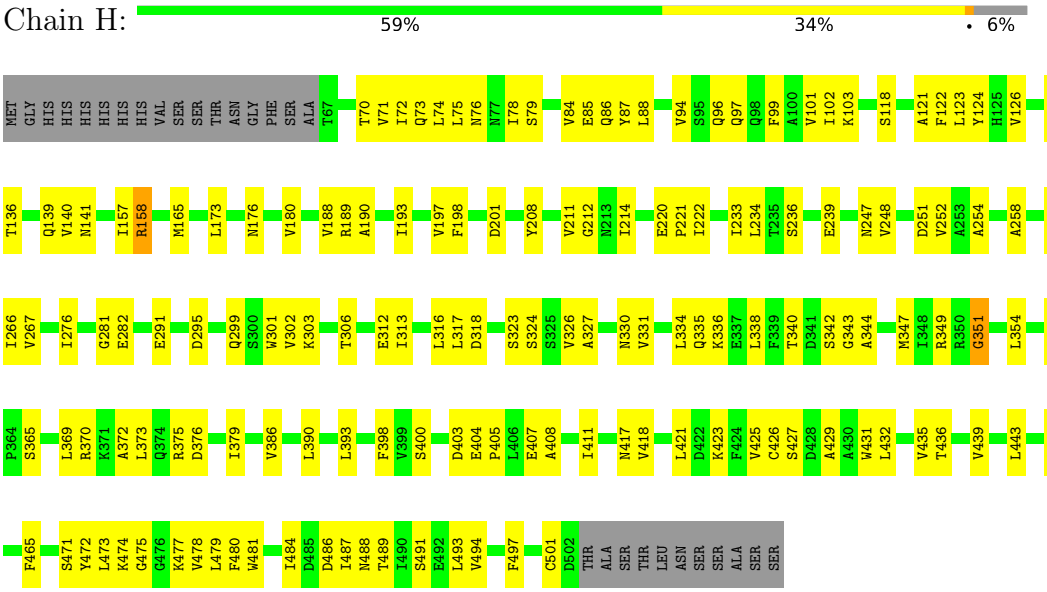
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain G:



• Molecule 1: ACETYLGLUTAMATE KINASE

Chain H:


59%
34%
6%
MET GLY HIS HIS HIS HIS HIS VAL SER SER THR ASN GLY PHE SER ALA T67 T70 V71 I72 Q73 L74 L75 N76 N77 I78 S79 V84 E85 Q86 Y87 L88 V94 S95 Q96 Q97 Q98 F99 A100 V101 I102 K103 S118 A121 F122 L123 Y124 H125 V126 I131 V132 L133
T136 Q139 V140 N141 I157 R158 M165 L173 N176 V180 V188 R189 A190 I193 V197 F198 D201 Y208 V211 G212 N213 I214 E220 P221 I222 I233 L234 T235 S236 E239 N247 V248 D251 V252 A253 A254 A258 E262 P263 L264 K265
I266 V267 I276 G281 E282 E291 D295 Q299 S300 W301 V302 K303 T306 E312 I313 L316 L317 D318 S323 S324 S325 V326 A327 N330 V331 L334 Q335 K336 E337 L338 F339 T340 D341 S342 G343 A344 M347 I348 R349 R350 G361 L354 S359 E362 F363
P364 S365 L369 R370 K371 A372 L373 Q374 R375 D376 I379 V386 L390 L393 F398 V399 S400 D403 E404 P405 L406 E407 A408 I411 N417 V418 L421 D422 K423 F424 V425 C426 S427 D428 A429 A430 W431 L432 V435 T436 V439 L443 A449 E456 N457
F465 S471 Y472 L473 K474 G475 G476 K477 V478 L479 F480 W481 I484 D485 D486 I487 N488 T489 I490 S491 E492 L493 V494 F497 C501 D502 THR ALA SER THR LEU ASN SER SER ALA SER SER

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	95.24Å 111.29Å 113.14Å 75.77° 89.29° 69.12°	Depositor
Resolution (Å)	109.11 – 3.80	Depositor
% Data completeness (in resolution range)	95.3 (109.11-3.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.236	Depositor
Wilson B-factor (Å^2)	136.5	Xtriage
Anisotropy	0.142	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27248	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.86	3/3460 (0.1%)	0.95	9/4686 (0.2%)
1	B	0.86	3/3460 (0.1%)	0.92	3/4686 (0.1%)
1	C	0.77	0/3466	0.89	9/4693 (0.2%)
1	D	0.80	2/3462 (0.1%)	0.93	8/4689 (0.2%)
1	E	0.94	6/3466 (0.2%)	1.00	12/4693 (0.3%)
1	F	0.86	5/3466 (0.1%)	0.92	2/4693 (0.0%)
1	G	0.75	2/3466 (0.1%)	0.84	1/4693 (0.0%)
1	H	0.83	4/3466 (0.1%)	0.99	11/4693 (0.2%)
All	All	0.83	25/27712 (0.1%)	0.93	55/37526 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	E	0	2
1	G	0	2
1	H	0	1
All	All	0	7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	GLU	CD-OE1	8.55	1.35	1.25
1	H	239	GLU	CD-OE1	7.00	1.33	1.25
1	H	282	GLU	CG-CD	6.51	1.61	1.51
1	H	481	TRP	CD2-CE2	6.05	1.48	1.41
1	E	223	GLU	CD-OE1	6.04	1.32	1.25
1	F	341	ASP	CB-CG	5.83	1.64	1.51
1	E	431	TRP	CD2-CE2	5.77	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	301	TRP	CD2-CE2	5.72	1.48	1.41
1	E	301	TRP	CD2-CE2	5.68	1.48	1.41
1	F	431	TRP	CD2-CE2	5.39	1.47	1.41
1	B	337	GLU	CD-OE1	5.38	1.31	1.25
1	B	312	GLU	CD-OE2	5.35	1.31	1.25
1	A	301	TRP	CD2-CE2	5.31	1.47	1.41
1	A	362	GLU	CD-OE1	5.30	1.31	1.25
1	A	239	GLU	CD-OE1	5.27	1.31	1.25
1	E	220	GLU	CD-OE2	5.26	1.31	1.25
1	B	341	ASP	CB-CG	5.25	1.62	1.51
1	F	301	TRP	CD2-CE2	5.24	1.47	1.41
1	E	239	GLU	CD-OE1	5.20	1.31	1.25
1	F	239	GLU	CD-OE2	5.19	1.31	1.25
1	E	220	GLU	CD-OE1	5.15	1.31	1.25
1	F	220	GLU	CD-OE2	5.11	1.31	1.25
1	G	431	TRP	CD2-CE2	5.07	1.47	1.41
1	D	452	TRP	CD2-CE2	5.06	1.47	1.41
1	G	189	ARG	CZ-NH2	5.02	1.39	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	316	LEU	CB-CG-CD1	-8.74	96.14	111.00
1	C	68	ARG	CB-CA-C	-7.61	95.19	110.40
1	A	316	LEU	CB-CG-CD1	-7.41	98.41	111.00
1	E	334	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	H	295	ASP	CB-CG-OD2	6.83	124.45	118.30
1	D	318	ASP	CB-CG-OD2	6.72	124.35	118.30
1	H	351	GLY	CA-C-N	-6.71	102.44	117.20
1	A	423	LYS	CD-CE-NZ	6.61	126.90	111.70
1	A	352	TYR	CB-CA-C	-6.42	97.57	110.40
1	B	67	THR	N-CA-C	-6.34	93.89	111.00
1	F	286	MET	CG-SD-CE	6.31	110.30	100.20
1	H	318	ASP	CB-CG-OD2	6.05	123.75	118.30
1	E	286	MET	CG-SD-CE	6.01	109.82	100.20
1	H	282	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	E	328	ILE	CG1-CB-CG2	-5.96	98.28	111.40
1	D	239	GLU	CG-CD-OE2	-5.79	106.72	118.30
1	F	347	MET	CG-SD-CE	5.77	109.43	100.20
1	H	264	LEU	CA-CB-CG	5.76	128.54	115.30
1	E	98	GLN	CB-CA-C	-5.75	98.91	110.40
1	H	165	MET	CG-SD-CE	-5.72	91.05	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	183	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	H	158	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	376	ASP	CB-CG-OD1	5.67	123.41	118.30
1	H	351	GLY	O-C-N	5.64	131.72	122.70
1	D	286	MET	CG-SD-CE	5.62	109.20	100.20
1	D	291	GLU	CG-CD-OE1	5.60	129.50	118.30
1	E	352	TYR	N-CA-C	5.58	126.06	111.00
1	E	68	ARG	CB-CA-C	-5.57	99.27	110.40
1	C	477	LYS	CD-CE-NZ	-5.53	98.97	111.70
1	C	286	MET	CG-SD-CE	5.50	109.00	100.20
1	C	347	MET	CG-SD-CE	5.45	108.91	100.20
1	G	169	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	E	231	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	H	291	GLU	CG-CD-OE2	-5.41	107.49	118.30
1	E	116	LEU	CA-CB-CG	5.38	127.67	115.30
1	C	245	MET	CG-SD-CE	5.35	108.75	100.20
1	H	239	GLU	CG-CD-OE2	-5.34	107.61	118.30
1	A	68	ARG	CB-CA-C	-5.34	99.72	110.40
1	A	352	TYR	N-CA-C	5.32	125.37	111.00
1	D	338	LEU	CB-CA-C	5.31	120.30	110.20
1	D	291	GLU	CG-CD-OE2	-5.28	107.75	118.30
1	E	120	LEU	CB-CG-CD2	5.26	119.94	111.00
1	D	98	GLN	CB-CA-C	-5.25	99.89	110.40
1	H	291	GLU	CG-CD-OE1	5.23	128.76	118.30
1	D	158	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	406	LEU	CB-CG-CD2	5.20	119.84	111.00
1	A	370	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	370	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	186	LEU	CB-CG-CD2	5.14	119.75	111.00
1	B	329	ILE	CB-CA-C	-5.14	101.32	111.60
1	E	370	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	259	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	98	GLN	CB-CA-C	-5.06	100.28	110.40
1	C	158	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	E	123	LEU	CB-CG-CD1	5.02	119.53	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	VAL	Peptide
1	B	417	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	94	VAL	Peptide
1	E	95	SER	Peptide
1	G	501	CYS	Peptide
1	G	95	SER	Peptide
1	H	351	GLY	Peptide

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	3402	0	3429	130	0
1	B	3402	0	3429	147	1
1	C	3408	0	3440	143	0
1	D	3404	0	3429	142	0
1	E	3408	0	3440	197	0
1	F	3408	0	3440	183	0
1	G	3408	0	3440	140	1
1	H	3408	0	3440	180	0
All	All	27248	0	27487	1169	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1169) 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:E:354:LEU:HD11	1:E:438:ASN:ND2	1.54	1.22
1:B:327:ALA:HB2	1:B:347:MET:CE	1.75	1.14
1:B:327:ALA:HB2	1:B:347:MET:HE3	1.29	1.12
1:E:418:VAL:HG21	1:E:493:LEU:HD11	1.25	1.11
1:D:418:VAL:HG21	1:D:493:LEU:HD11	1.12	1.11
1:E:267:VAL:HG21	1:E:338:LEU:HD11	1.25	1.10
1:G:327:ALA:HB2	1:G:347:MET:CE	1.82	1.10
1:A:266:ILE:HD13	1:A:316:LEU:HD21	1.34	1.09
1:D:334:LEU:HD11	1:D:338:LEU:HD12	1.32	1.09
1:E:77:ASN:ND2	1:E:335:GLN:HE21	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ASP:OD1	1:H:323:SER:HB2	1.53	1.08
1:D:334:LEU:CD1	1:D:338:LEU:HD12	1.84	1.07
1:G:267:VAL:HG21	1:G:338:LEU:HD11	1.31	1.04
1:D:334:LEU:HD11	1:D:338:LEU:CD1	1.89	1.01
1:B:267:VAL:HG21	1:B:338:LEU:HD11	1.40	1.01
1:E:267:VAL:CG2	1:E:338:LEU:HD11	1.89	1.01
1:G:327:ALA:HB2	1:G:347:MET:HE2	1.42	1.01
1:A:267:VAL:HG21	1:A:338:LEU:HD11	1.41	1.00
1:A:370:ARG:HG3	1:A:386:VAL:HG11	1.43	0.97
1:F:73:GLN:NE2	1:F:335:GLN:OE1	1.97	0.95
1:H:418:VAL:HG21	1:H:493:LEU:HD11	1.49	0.95
1:D:418:VAL:CG2	1:D:493:LEU:HD11	1.96	0.94
1:E:84:VAL:HG21	1:H:78:ILE:CG2	1.98	0.94
1:E:84:VAL:HG21	1:H:78:ILE:HG22	1.47	0.94
1:F:417:ASN:O	1:F:418:VAL:HG22	1.69	0.93
1:C:418:VAL:HG21	1:C:493:LEU:HD11	1.52	0.92
1:F:273:GLY:O	1:F:283:LYS:NZ	2.01	0.92
1:E:78:ILE:HG22	1:H:84:VAL:HG21	1.52	0.92
1:F:379:ILE:HG21	1:F:386:VAL:HG23	1.51	0.91
1:G:418:VAL:HG21	1:G:493:LEU:HD11	1.52	0.91
1:D:418:VAL:HG21	1:D:493:LEU:CD1	1.99	0.91
1:E:77:ASN:HD22	1:E:335:GLN:HE21	1.02	0.91
1:G:313:ILE:HD13	1:G:326:VAL:HG11	1.53	0.91
1:H:70:THR:HG23	1:H:122:PHE:CD1	2.05	0.90
1:B:327:ALA:CB	1:B:347:MET:HE3	2.02	0.90
1:F:97:GLN:OE1	1:F:264:LEU:HD22	1.72	0.90
1:E:354:LEU:HD11	1:E:438:ASN:HD22	1.31	0.90
1:B:417:ASN:O	1:B:418:VAL:HG22	1.72	0.90
1:E:354:LEU:CD1	1:E:438:ASN:ND2	2.36	0.89
1:C:146:ALA:HB1	1:F:323:SER:HB2	1.55	0.88
1:B:379:ILE:HG21	1:B:386:VAL:HG23	1.56	0.88
1:B:133:LEU:HD21	1:B:236:SER:HB3	1.55	0.88
1:C:136:THR:HG23	1:C:136:THR:O	1.72	0.88
1:B:103:LYS:HE3	1:B:251:ASP:OD1	1.73	0.88
1:A:417:ASN:O	1:A:418:VAL:HG22	1.73	0.88
1:C:327:ALA:HB2	1:C:347:MET:CE	2.04	0.88
1:H:97:GLN:OE1	1:H:264:LEU:HD13	1.73	0.87
1:E:418:VAL:CG2	1:E:493:LEU:HD11	2.04	0.87
1:H:313:ILE:HD13	1:H:326:VAL:HG11	1.56	0.87
1:G:234:LEU:N	1:G:234:LEU:HD12	1.89	0.86
1:E:77:ASN:ND2	1:E:335:GLN:NE2	2.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:370:ARG:HG3	1:H:386:VAL:HG11	1.58	0.86
1:E:85:GLU:HB3	1:E:432:LEU:HD22	1.55	0.86
1:E:88:LEU:HD11	1:H:76:ASN:OD1	1.76	0.85
1:E:91:PHE:HB3	1:H:72:ILE:CD1	2.06	0.85
1:B:387:ALA:HB3	1:H:262:GLU:CD	1.96	0.85
1:C:317:LEU:HD21	1:C:326:VAL:HG23	1.56	0.85
1:F:97:GLN:OE1	1:F:264:LEU:CD2	2.24	0.85
1:F:327:ALA:HB2	1:F:347:MET:CE	2.06	0.85
1:G:417:ASN:O	1:G:418:VAL:HG22	1.77	0.85
1:H:103:LYS:HE3	1:H:251:ASP:OD1	1.75	0.85
1:E:91:PHE:HB3	1:H:72:ILE:HD13	1.59	0.84
1:F:288:ASN:HD22	1:F:438:ASN:ND2	1.74	0.84
1:H:86:GLN:OE1	1:H:340:THR:CB	2.26	0.84
1:B:157:ILE:HD12	1:B:208:TYR:CE1	2.13	0.84
1:B:387:ALA:HB3	1:H:262:GLU:OE2	1.78	0.83
1:C:147:GLN:HG3	1:F:322:ARG:HB3	1.60	0.83
1:B:385:SER:HB3	1:H:262:GLU:OE1	1.78	0.83
1:E:144:LEU:HD21	1:E:164:THR:HG23	1.60	0.83
1:E:418:VAL:HG21	1:E:493:LEU:CD1	2.08	0.83
1:G:103:LYS:HE3	1:G:251:ASP:OD1	1.77	0.83
1:D:94:VAL:O	1:D:94:VAL:HG12	1.77	0.83
1:F:349:ARG:NH2	1:F:433:ASN:O	2.11	0.83
1:E:273:GLY:O	1:E:283:LYS:NZ	2.11	0.83
1:C:146:ALA:CB	1:F:323:SER:HB2	2.08	0.82
1:H:73:GLN:HG2	1:H:335:GLN:OE1	1.79	0.82
1:C:222:ILE:HD11	1:C:234:LEU:HD11	1.62	0.82
1:E:136:THR:HA	1:E:139:GLN:HE22	1.45	0.82
1:F:327:ALA:HB2	1:F:347:MET:HE1	1.62	0.82
1:C:103:LYS:HE3	1:C:251:ASP:OD1	1.80	0.82
1:B:213:ASN:HD22	1:B:214:ILE:N	1.78	0.82
1:A:157:ILE:HD12	1:A:208:TYR:CE1	2.15	0.81
1:B:273:GLY:O	1:B:283:LYS:NZ	2.14	0.81
1:G:267:VAL:CG2	1:G:338:LEU:HD11	2.10	0.81
1:B:363:PHE:CG	1:B:369:LEU:HD12	2.16	0.81
1:D:176:ASN:O	1:D:180:VAL:HG23	1.81	0.81
1:G:234:LEU:N	1:G:234:LEU:CD1	2.43	0.80
1:A:474:LYS:NZ	1:A:501:CYS:SG	2.54	0.80
1:C:68:ARG:O	1:C:72:ILE:CD1	2.30	0.80
1:G:370:ARG:HG3	1:G:386:VAL:HG11	1.61	0.79
1:A:487:ILE:HD11	1:D:491:SER:HA	1.63	0.79
1:F:379:ILE:HD11	1:F:423:LYS:NZ	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HE3	1:A:251:ASP:OD1	1.82	0.79
1:E:376:ASP:HB2	1:E:425:VAL:HG22	1.65	0.79
1:B:213:ASN:HD22	1:B:213:ASN:C	1.86	0.79
1:D:90:TYR:OH	1:D:265:LYS:NZ	2.15	0.79
1:C:68:ARG:O	1:C:72:ILE:HD12	1.83	0.79
1:F:495:GLU:HG3	1:G:487:ILE:HD13	1.65	0.79
1:E:82:ARG:HD2	1:E:432:LEU:O	1.83	0.78
1:F:103:LYS:HE3	1:F:251:ASP:OD1	1.84	0.78
1:D:103:LYS:HE3	1:D:251:ASP:OD1	1.83	0.78
1:D:193:ILE:HB	1:D:234:LEU:HD13	1.65	0.78
1:E:370:ARG:HG3	1:E:386:VAL:HG11	1.66	0.78
1:F:120:LEU:HA	1:F:123:LEU:HD12	1.67	0.77
1:H:342:SER:O	1:H:344:ALA:N	2.17	0.77
1:F:157:ILE:HD12	1:F:208:TYR:CE1	2.19	0.77
1:E:136:THR:HA	1:E:139:GLN:NE2	2.00	0.76
1:C:379:ILE:HG21	1:C:386:VAL:HG23	1.66	0.76
1:H:197:VAL:HG21	1:H:234:LEU:HD21	1.66	0.76
1:A:313:ILE:HD13	1:A:326:VAL:HG11	1.68	0.76
1:B:474:LYS:NZ	1:B:501:CYS:SG	2.57	0.76
1:E:487:ILE:HD11	1:H:491:SER:HB3	1.66	0.76
1:A:417:ASN:O	1:A:418:VAL:CG2	2.34	0.76
1:F:491:SER:O	1:G:487:ILE:HD11	1.86	0.75
1:G:417:ASN:O	1:G:418:VAL:CG2	2.34	0.75
1:D:203:LEU:HD22	1:D:208:TYR:CE2	2.21	0.75
1:H:133:LEU:HD21	1:H:236:SER:HB3	1.66	0.75
1:A:97:GLN:NE2	1:A:262:GLU:O	2.20	0.75
1:D:327:ALA:HB2	1:D:347:MET:CE	2.15	0.75
1:D:379:ILE:HG21	1:D:386:VAL:HG23	1.68	0.75
1:B:370:ARG:NH2	1:H:323:SER:OG	2.19	0.74
1:F:244:GLN:HE21	1:F:245:MET:N	1.85	0.74
1:G:369:LEU:O	1:G:369:LEU:HD23	1.88	0.74
1:D:342:SER:O	1:D:344:ALA:N	2.20	0.74
1:F:140:VAL:CG1	1:F:141:ASN:N	2.50	0.74
1:A:240:THR:CG2	1:A:246:LEU:HD11	2.18	0.74
1:C:267:VAL:HG21	1:C:338:LEU:HD11	1.67	0.74
1:G:233:ILE:C	1:G:234:LEU:HD12	2.07	0.74
1:H:140:VAL:CG1	1:H:141:ASN:N	2.50	0.74
1:C:157:ILE:HD12	1:C:208:TYR:CE1	2.23	0.73
1:F:386:VAL:CG1	1:F:390:LEU:HD22	2.17	0.73
1:A:273:GLY:O	1:A:283:LYS:NZ	2.19	0.73
1:F:119:CYS:SG	1:F:335:GLN:HB3	2.27	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ALA:HB2	1:D:347:MET:HE3	1.68	0.73
1:F:487:ILE:HD11	1:G:491:SER:HA	1.70	0.73
1:H:136:THR:HG23	1:H:136:THR:O	1.87	0.73
1:H:363:PHE:CG	1:H:369:LEU:HD12	2.24	0.73
1:H:313:ILE:CD1	1:H:326:VAL:HG11	2.19	0.73
1:C:490:ILE:O	1:C:494:VAL:HG23	1.88	0.72
1:D:417:ASN:O	1:D:418:VAL:HG22	1.88	0.72
1:E:103:LYS:HE3	1:E:251:ASP:OD1	1.89	0.72
1:G:267:VAL:HG21	1:G:338:LEU:CD1	2.15	0.72
1:C:327:ALA:HB2	1:C:347:MET:HE3	1.70	0.72
1:D:256:GLU:O	1:D:260:VAL:HG12	1.89	0.72
1:F:133:LEU:HD21	1:F:236:SER:HB3	1.71	0.72
1:C:327:ALA:HB2	1:C:347:MET:HE2	1.70	0.72
1:D:120:LEU:HD23	1:D:123:LEU:HD12	1.71	0.72
1:A:491:SER:HA	1:D:487:ILE:HD11	1.70	0.72
1:G:421:LEU:HD22	1:G:443:LEU:HD21	1.71	0.72
1:A:270:ASN:ND2	1:A:272:LYS:HB2	2.04	0.71
1:C:90:TYR:CE2	1:C:264:LEU:HD12	2.25	0.71
1:F:417:ASN:O	1:F:418:VAL:CG2	2.39	0.71
1:C:133:LEU:HD21	1:C:236:SER:HB3	1.71	0.71
1:A:418:VAL:HG21	1:A:493:LEU:HD11	1.70	0.71
1:E:94:VAL:HG12	1:E:94:VAL:O	1.91	0.71
1:E:213:ASN:HD22	1:E:214:ILE:N	1.88	0.71
1:F:140:VAL:HG12	1:F:141:ASN:N	2.05	0.71
1:H:180:VAL:HG13	1:H:190:ALA:HB3	1.71	0.71
1:H:140:VAL:HG12	1:H:141:ASN:N	2.04	0.71
1:D:474:LYS:NZ	1:D:501:CYS:SG	2.63	0.70
1:H:70:THR:HG23	1:H:122:PHE:HD1	1.54	0.70
1:B:267:VAL:HG21	1:B:338:LEU:CD1	2.20	0.70
1:B:327:ALA:CB	1:B:347:MET:CE	2.62	0.70
1:B:369:LEU:HD23	1:B:373:LEU:HD11	1.73	0.70
1:H:157:ILE:HD12	1:H:208:TYR:CE1	2.25	0.70
1:B:418:VAL:HG21	1:B:493:LEU:HD11	1.74	0.70
1:A:266:ILE:HD13	1:A:316:LEU:CD2	2.19	0.70
1:G:82:ARG:O	1:G:86:GLN:HG2	1.92	0.70
1:H:122:PHE:O	1:H:126:VAL:HG22	1.91	0.70
1:E:222:ILE:HD11	1:E:234:LEU:HD11	1.73	0.69
1:F:354:LEU:HD21	1:F:439:VAL:CG2	2.22	0.69
1:C:163:HIS:NE2	1:F:404:GLU:OE2	2.24	0.69
1:A:369:LEU:CD2	1:A:373:LEU:HD11	2.22	0.69
1:E:74:LEU:CD2	1:H:71:VAL:HG13	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:379:ILE:HG21	1:G:386:VAL:HG23	1.74	0.69
1:B:417:ASN:O	1:B:418:VAL:CG2	2.39	0.69
1:A:266:ILE:CD1	1:A:316:LEU:HD21	2.19	0.69
1:D:417:ASN:O	1:D:418:VAL:CG2	2.41	0.69
1:A:157:ILE:HD12	1:A:208:TYR:CZ	2.27	0.69
1:H:267:VAL:HG21	1:H:338:LEU:HD21	1.75	0.69
1:A:363:PHE:CD1	1:A:369:LEU:HD12	2.28	0.69
1:F:286:MET:SD	1:F:434:ASN:ND2	2.65	0.68
1:F:354:LEU:HD21	1:F:439:VAL:HG23	1.75	0.68
1:A:449:ALA:HB1	1:A:484:ILE:HG22	1.74	0.68
1:G:327:ALA:CB	1:G:347:MET:CE	2.67	0.68
1:H:99:PHE:CZ	1:H:338:LEU:HD12	2.28	0.68
1:F:144:LEU:HD22	1:F:167:VAL:HG11	1.75	0.68
1:G:169:ARG:HD2	1:G:245:MET:CE	2.23	0.68
1:E:84:VAL:HG11	1:H:78:ILE:O	1.94	0.68
1:D:379:ILE:HG21	1:D:386:VAL:CG2	2.23	0.68
1:E:376:ASP:HB2	1:E:425:VAL:CG2	2.24	0.68
1:F:418:VAL:HG11	1:F:493:LEU:HD11	1.76	0.68
1:G:313:ILE:CD1	1:G:326:VAL:HG11	2.24	0.68
1:B:385:SER:CB	1:H:262:GLU:OE1	2.42	0.67
1:B:144:LEU:HD22	1:B:167:VAL:HG11	1.75	0.67
1:B:193:ILE:HB	1:B:234:LEU:HD22	1.75	0.67
1:B:369:LEU:CD2	1:B:373:LEU:HD11	2.24	0.67
1:G:157:ILE:HD12	1:G:208:TYR:CE1	2.29	0.67
1:E:157:ILE:HD12	1:E:208:TYR:CE1	2.29	0.67
1:A:84:VAL:HG21	1:D:78:ILE:HG21	1.77	0.67
1:C:144:LEU:HD22	1:C:167:VAL:HG11	1.75	0.67
1:D:82:ARG:O	1:D:86:GLN:HG2	1.94	0.67
1:H:363:PHE:CD1	1:H:369:LEU:HD12	2.30	0.67
1:D:473:LEU:HD13	1:D:478:VAL:HG22	1.77	0.67
1:E:77:ASN:HD22	1:E:335:GLN:NE2	1.81	0.67
1:E:369:LEU:CD2	1:E:373:LEU:HD11	2.25	0.67
1:E:78:ILE:CG2	1:H:84:VAL:HG21	2.23	0.67
1:H:86:GLN:OE1	1:H:340:THR:HB	1.94	0.67
1:H:417:ASN:O	1:H:418:VAL:CG2	2.43	0.67
1:F:386:VAL:HG12	1:F:390:LEU:HD22	1.77	0.66
1:G:473:LEU:HD13	1:G:478:VAL:HG22	1.78	0.66
1:E:417:ASN:O	1:E:418:VAL:HG22	1.94	0.66
1:C:370:ARG:HG3	1:C:386:VAL:HG11	1.76	0.66
1:A:267:VAL:CG2	1:A:338:LEU:HD11	2.21	0.66
1:E:213:ASN:HD22	1:E:213:ASN:C	1.98	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:THR:HG23	1:D:136:THR:O	1.95	0.66
1:E:88:LEU:CD1	1:H:76:ASN:OD1	2.42	0.66
1:H:70:THR:CG2	1:H:122:PHE:CD1	2.77	0.66
1:A:82:ARG:O	1:A:86:GLN:HG2	1.94	0.66
1:D:334:LEU:HD11	1:D:338:LEU:HD11	1.78	0.66
1:G:136:THR:O	1:G:136:THR:HG23	1.96	0.66
1:A:425:VAL:HG12	1:A:425:VAL:O	1.95	0.66
1:C:418:VAL:HG21	1:C:493:LEU:CD1	2.25	0.66
1:E:82:ARG:O	1:E:86:GLN:HG2	1.95	0.66
1:F:327:ALA:HB2	1:F:347:MET:HE2	1.78	0.66
1:E:379:ILE:HG21	1:E:386:VAL:HG23	1.76	0.66
1:E:457:ASN:ND2	1:E:457:ASN:H	1.94	0.65
1:G:94:VAL:HG12	1:G:94:VAL:O	1.95	0.65
1:G:70:THR:CG2	1:G:126:VAL:HG12	2.27	0.65
1:F:379:ILE:HD11	1:F:423:LYS:HZ2	1.61	0.65
1:E:180:VAL:HG13	1:E:190:ALA:HB3	1.78	0.65
1:E:379:ILE:HD11	1:E:423:LYS:NZ	2.12	0.65
1:F:99:PHE:HE2	1:F:123:LEU:HD22	1.60	0.65
1:H:327:ALA:HB2	1:H:347:MET:HE3	1.79	0.65
1:G:124:TYR:CG	1:G:188:VAL:HG13	2.32	0.65
1:H:393:LEU:HD22	1:H:398:PHE:CD1	2.32	0.65
1:E:484:ILE:HD11	1:E:493:LEU:HD22	1.80	0.64
1:H:176:ASN:ND2	1:H:233:ILE:HG22	2.12	0.64
1:H:323:SER:O	1:H:324:SER:C	2.35	0.64
1:C:82:ARG:O	1:C:86:GLN:HG2	1.96	0.64
1:F:94:VAL:CG1	1:F:96:GLN:NE2	2.60	0.64
1:G:169:ARG:HD2	1:G:245:MET:HE3	1.78	0.64
1:D:323:SER:O	1:D:324:SER:C	2.36	0.64
1:E:81:LYS:HG3	1:H:79:SER:O	1.98	0.64
1:A:386:VAL:HG12	1:A:387:ALA:N	2.11	0.64
1:B:354:LEU:HD21	1:B:439:VAL:HG23	1.79	0.64
1:C:469:GLN:HE21	1:C:483:GLY:H	1.44	0.64
1:D:488:ASN:HD22	1:D:489:THR:N	1.96	0.64
1:E:88:LEU:HD22	1:E:92:THR:HG23	1.80	0.64
1:F:136:THR:HG23	1:F:136:THR:O	1.97	0.64
1:G:424:PHE:HE1	1:G:439:VAL:HG11	1.63	0.64
1:C:266:ILE:HD13	1:C:316:LEU:HD21	1.80	0.64
1:A:124:TYR:CD2	1:A:188:VAL:HG22	2.32	0.63
1:B:82:ARG:O	1:B:86:GLN:HG2	1.98	0.63
1:C:327:ALA:CB	1:C:347:MET:HE3	2.28	0.63
1:E:304:TYR:CE1	1:E:308:LEU:HD13	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD11	1:A:236:SER:HB3	1.79	0.63
1:E:474:LYS:NZ	1:E:501:CYS:SG	2.67	0.63
1:F:327:ALA:CB	1:F:347:MET:HE2	2.29	0.63
1:F:327:ALA:CB	1:F:347:MET:CE	2.76	0.63
1:F:449:ALA:HB1	1:F:484:ILE:HG22	1.81	0.63
1:E:136:THR:HG23	1:E:136:THR:O	1.99	0.62
1:F:487:ILE:HD11	1:G:491:SER:CA	2.28	0.62
1:E:88:LEU:HD22	1:E:92:THR:CG2	2.29	0.62
1:F:340:THR:HG23	1:F:343:GLY:H	1.63	0.62
1:H:474:LYS:NZ	1:H:501:CYS:SG	2.69	0.62
1:C:473:LEU:HD13	1:C:478:VAL:HG22	1.81	0.62
1:H:386:VAL:CG1	1:H:390:LEU:HD22	2.30	0.62
1:C:90:TYR:HE2	1:C:264:LEU:HD12	1.63	0.62
1:A:297:MET:HE1	1:A:307:LYS:HA	1.81	0.62
1:B:213:ASN:C	1:B:213:ASN:ND2	2.53	0.62
1:E:68:ARG:O	1:E:72:ILE:HD12	2.00	0.62
1:C:68:ARG:O	1:C:72:ILE:HD13	1.99	0.61
1:F:133:LEU:C	1:F:133:LEU:HD22	2.20	0.61
1:C:473:LEU:HD13	1:C:478:VAL:CG2	2.30	0.61
1:G:266:ILE:HD13	1:G:316:LEU:HD21	1.81	0.61
1:B:68:ARG:O	1:B:72:ILE:HD12	2.00	0.61
1:B:369:LEU:HD23	1:B:373:LEU:CD1	2.30	0.61
1:B:393:LEU:HD22	1:B:398:PHE:CD1	2.36	0.61
1:F:222:ILE:HD11	1:F:234:LEU:HD11	1.80	0.61
1:F:418:VAL:HG21	1:F:493:LEU:HD11	1.83	0.61
1:H:417:ASN:O	1:H:418:VAL:HG22	2.00	0.61
1:C:474:LYS:NZ	1:C:501:CYS:SG	2.73	0.61
1:A:304:TYR:CE1	1:A:308:LEU:HD13	2.35	0.61
1:D:133:LEU:HD11	1:D:236:SER:HB3	1.82	0.61
1:F:393:LEU:HD22	1:F:398:PHE:CD1	2.35	0.61
1:A:240:THR:HG22	1:A:246:LEU:HD11	1.81	0.61
1:B:406:LEU:HD12	1:B:409:VAL:CG2	2.30	0.61
1:D:449:ALA:HB1	1:D:484:ILE:HG22	1.83	0.61
1:G:140:VAL:CG1	1:G:141:ASN:N	2.63	0.61
1:G:173:LEU:N	1:G:173:LEU:HD23	2.15	0.61
1:G:473:LEU:HD13	1:G:478:VAL:CG2	2.30	0.61
1:H:472:TYR:CD2	1:H:494:VAL:HG13	2.36	0.61
1:F:193:ILE:CG2	1:F:234:LEU:HD22	2.31	0.60
1:A:122:PHE:O	1:A:126:VAL:HG22	2.01	0.60
1:B:313:ILE:HD13	1:B:326:VAL:HG11	1.83	0.60
1:E:379:ILE:HD11	1:E:423:LYS:HZ2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HG23	1:A:136:THR:O	2.01	0.60
1:C:116:LEU:HD11	1:C:120:LEU:HD11	1.83	0.60
1:D:369:LEU:HD23	1:D:369:LEU:O	2.01	0.60
1:H:94:VAL:HG12	1:H:96:GLN:NE2	2.16	0.60
1:B:157:ILE:HD12	1:B:208:TYR:CZ	2.35	0.60
1:G:240:THR:CG2	1:G:246:LEU:HD11	2.32	0.60
1:F:160:THR:O	1:F:160:THR:HG22	2.01	0.60
1:B:363:PHE:CD1	1:B:369:LEU:CD1	2.85	0.60
1:H:87:TYR:OH	1:H:335:GLN:O	2.19	0.60
1:E:124:TYR:CD2	1:E:188:VAL:HG22	2.35	0.60
1:E:442:VAL:HG12	1:E:443:LEU:N	2.16	0.60
1:F:297:MET:HE1	1:F:307:LYS:CA	2.31	0.60
1:G:222:ILE:HD11	1:G:234:LEU:HD21	1.83	0.60
1:A:113:LEU:HD23	1:A:113:LEU:O	2.01	0.60
1:B:136:THR:O	1:B:136:THR:HG23	2.01	0.60
1:C:240:THR:CG2	1:C:246:LEU:HD11	2.31	0.60
1:E:393:LEU:HD11	1:E:411:ILE:HD13	1.84	0.60
1:A:487:ILE:HD11	1:D:491:SER:CA	2.32	0.60
1:B:387:ALA:HB3	1:H:262:GLU:OE1	2.00	0.60
1:F:94:VAL:HG11	1:F:96:GLN:NE2	2.17	0.60
1:G:169:ARG:CD	1:G:245:MET:HE3	2.31	0.60
1:H:369:LEU:CD2	1:H:373:LEU:HD11	2.31	0.60
1:E:304:TYR:CZ	1:E:308:LEU:HD13	2.37	0.60
1:E:407:GLU:OE2	1:E:429:ALA:HB3	2.00	0.59
1:C:267:VAL:HG21	1:C:338:LEU:CD1	2.32	0.59
1:A:297:MET:HE1	1:A:307:LYS:CA	2.30	0.59
1:D:286:MET:HE3	1:D:347:MET:HB3	1.83	0.59
1:E:74:LEU:HD21	1:H:71:VAL:HG13	1.84	0.59
1:F:370:ARG:HG3	1:F:386:VAL:HG11	1.84	0.59
1:C:363:PHE:CD1	1:C:369:LEU:HD12	2.36	0.59
1:D:479:LEU:HD12	1:D:480:PHE:H	1.67	0.59
1:A:262:GLU:HA	1:A:320:LEU:HD22	1.84	0.59
1:E:354:LEU:CD1	1:E:438:ASN:HD21	2.12	0.59
1:H:86:GLN:OE1	1:H:340:THR:HA	2.02	0.59
1:G:379:ILE:HD11	1:G:423:LYS:NZ	2.17	0.59
1:G:486:ASP:CB	1:G:489:THR:HG23	2.33	0.59
1:F:297:MET:HE1	1:F:307:LYS:HA	1.84	0.59
1:A:407:GLU:OE2	1:A:429:ALA:HB3	2.03	0.59
1:E:77:ASN:HD21	1:E:335:GLN:HG3	1.68	0.58
1:G:474:LYS:NZ	1:G:501:CYS:SG	2.75	0.58
1:G:386:VAL:CG1	1:G:390:LEU:HD22	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:HB2	1:B:347:MET:HE2	1.75	0.58
1:H:258:ALA:HB3	1:H:316:LEU:HD11	1.85	0.58
1:C:417:ASN:O	1:C:418:VAL:CG2	2.51	0.58
1:D:370:ARG:HG3	1:D:386:VAL:HG11	1.86	0.58
1:E:197:VAL:HG21	1:E:234:LEU:HD13	1.86	0.58
1:E:418:VAL:HG11	1:E:493:LEU:HD21	1.84	0.58
1:F:76:ASN:OD1	1:G:88:LEU:HD11	2.04	0.58
1:F:203:LEU:C	1:F:203:LEU:HD13	2.24	0.58
1:F:474:LYS:NZ	1:F:501:CYS:SG	2.72	0.58
1:G:421:LEU:HD22	1:G:443:LEU:CD2	2.33	0.58
1:H:140:VAL:HG11	1:H:158:ARG:NH2	2.18	0.58
1:C:457:ASN:H	1:C:457:ASN:ND2	1.99	0.58
1:H:489:THR:O	1:H:493:LEU:HD13	2.03	0.58
1:G:273:GLY:O	1:G:283:LYS:NZ	2.27	0.58
1:E:84:VAL:CG2	1:H:78:ILE:HG22	2.30	0.58
1:C:486:ASP:CB	1:C:489:THR:HG23	2.34	0.58
1:D:252:VAL:HG22	1:D:312:GLU:CD	2.23	0.58
1:D:479:LEU:HD12	1:D:480:PHE:N	2.19	0.58
1:H:266:ILE:HD13	1:H:316:LEU:HD21	1.86	0.58
1:B:74:LEU:CD2	1:C:71:VAL:HG13	2.34	0.57
1:G:140:VAL:HG11	1:G:158:ARG:NH2	2.19	0.57
1:C:154:ILE:HD12	1:F:371:LYS:NZ	2.19	0.57
1:C:393:LEU:HD22	1:C:398:PHE:CD1	2.40	0.57
1:B:379:ILE:HG21	1:B:386:VAL:CG2	2.31	0.57
1:E:363:PHE:CD1	1:E:369:LEU:HD12	2.39	0.57
1:H:379:ILE:HG21	1:H:386:VAL:HG23	1.86	0.57
1:D:193:ILE:HG22	1:D:193:ILE:O	2.03	0.57
1:E:417:ASN:O	1:E:418:VAL:CG2	2.53	0.57
1:F:304:TYR:CZ	1:F:308:LEU:HD13	2.39	0.57
1:A:313:ILE:CD1	1:A:326:VAL:HG11	2.34	0.57
1:D:473:LEU:HD13	1:D:478:VAL:CG2	2.34	0.57
1:E:363:PHE:CG	1:E:369:LEU:HD12	2.40	0.57
1:G:160:THR:HG22	1:G:160:THR:O	2.04	0.57
1:B:354:LEU:HD22	1:B:439:VAL:HG22	1.87	0.57
1:B:363:PHE:CD1	1:B:369:LEU:HD12	2.39	0.57
1:H:124:TYR:CG	1:H:188:VAL:HG13	2.39	0.57
1:E:136:THR:CA	1:E:139:GLN:NE2	2.68	0.57
1:E:457:ASN:ND2	1:E:457:ASN:N	2.51	0.57
1:D:334:LEU:HD12	1:D:338:LEU:HD12	1.80	0.57
1:D:379:ILE:HD11	1:D:423:LYS:NZ	2.19	0.57
1:E:160:THR:HG22	1:E:160:THR:O	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:473:LEU:HD12	1:F:474:LYS:O	2.05	0.56
1:D:70:THR:CG2	1:D:126:VAL:HG12	2.34	0.56
1:D:299:GLN:HB2	1:D:302:VAL:HG23	1.87	0.56
1:E:74:LEU:HD22	1:H:71:VAL:HG13	1.88	0.56
1:F:408:ALA:HB1	1:F:426:CYS:SG	2.44	0.56
1:G:140:VAL:HG12	1:G:141:ASN:N	2.21	0.56
1:H:407:GLU:OE2	1:H:429:ALA:HB3	2.04	0.56
1:B:364:PRO:HB3	1:H:407:GLU:OE2	2.06	0.56
1:A:469:GLN:HE21	1:A:483:GLY:H	1.53	0.56
1:B:133:LEU:HD12	1:B:254:ALA:HA	1.88	0.56
1:C:154:ILE:HD12	1:F:371:LYS:HZ3	1.70	0.56
1:D:329:ILE:HD12	1:D:337:GLU:CG	2.34	0.56
1:D:400:SER:O	1:D:400:SER:OG	2.23	0.56
1:H:198:PHE:CD1	1:H:214:ILE:HD13	2.40	0.56
1:C:327:ALA:CB	1:C:347:MET:CE	2.80	0.56
1:C:363:PHE:CG	1:C:369:LEU:HD12	2.41	0.56
1:C:449:ALA:HB1	1:C:484:ILE:HG22	1.86	0.56
1:F:260:VAL:HG12	1:F:261:PHE:CD1	2.41	0.56
1:F:400:SER:O	1:F:400:SER:OG	2.24	0.56
1:B:97:GLN:OE1	1:B:264:LEU:HD23	2.06	0.56
1:E:449:ALA:HB1	1:E:484:ILE:HG22	1.87	0.56
1:H:124:TYR:CD1	1:H:188:VAL:HG13	2.40	0.56
1:A:222:ILE:HD11	1:A:234:LEU:HD21	1.88	0.55
1:B:340:THR:HG23	1:B:343:GLY:H	1.71	0.55
1:B:400:SER:O	1:B:400:SER:OG	2.25	0.55
1:D:168:VAL:HG11	1:D:247:ASN:HD22	1.71	0.55
1:A:88:LEU:HD22	1:A:92:THR:HG23	1.88	0.55
1:D:329:ILE:CD1	1:D:337:GLU:HB2	2.36	0.55
1:E:88:LEU:HD11	1:H:76:ASN:HA	1.88	0.55
1:B:363:PHE:CE1	1:B:369:LEU:HD11	2.41	0.55
1:C:136:THR:O	1:C:136:THR:CG2	2.45	0.55
1:F:376:ASP:HB2	1:F:425:VAL:HG22	1.89	0.55
1:B:104:VAL:HG12	1:B:105:GLY:O	2.07	0.55
1:C:146:ALA:HB3	1:F:323:SER:HB2	1.89	0.55
1:H:363:PHE:CD1	1:H:369:LEU:CD1	2.90	0.55
1:A:369:LEU:CD2	1:A:373:LEU:CD1	2.84	0.55
1:B:491:SER:CB	1:C:487:ILE:HD11	2.37	0.55
1:C:145:GLU:OE2	1:F:89:LYS:HE3	2.07	0.55
1:E:139:GLN:HG3	1:E:175:GLN:HE22	1.71	0.55
1:H:86:GLN:OE1	1:H:340:THR:OG1	2.23	0.55
1:A:94:VAL:HG12	1:A:94:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLN:HB3	1:F:96:GLN:NE2	2.21	0.55
1:F:94:VAL:HG12	1:F:96:GLN:NE2	2.22	0.55
1:D:180:VAL:HG13	1:D:190:ALA:CB	2.37	0.55
1:G:393:LEU:HD22	1:G:398:PHE:CE1	2.41	0.55
1:B:374:GLN:O	1:H:96:GLN:HG3	2.07	0.55
1:B:491:SER:HA	1:C:487:ILE:HD11	1.87	0.55
1:E:193:ILE:HB	1:E:234:LEU:HD22	1.87	0.55
1:H:449:ALA:HB1	1:H:484:ILE:HG22	1.89	0.55
1:C:407:GLU:OE2	1:C:429:ALA:HB3	2.07	0.55
1:F:369:LEU:HD23	1:F:369:LEU:O	2.06	0.55
1:F:267:VAL:HG21	1:F:338:LEU:HD11	1.88	0.54
1:C:376:ASP:HB2	1:C:425:VAL:HG22	1.89	0.54
1:F:123:LEU:HD13	1:F:130:PRO:HG3	1.90	0.54
1:G:386:VAL:HG12	1:G:390:LEU:HD22	1.88	0.54
1:B:487:ILE:HD11	1:C:491:SER:O	2.07	0.54
1:C:133:LEU:HD12	1:C:254:ALA:HA	1.90	0.54
1:C:400:SER:O	1:C:400:SER:OG	2.25	0.54
1:G:68:ARG:O	1:G:71:VAL:N	2.39	0.54
1:A:360:ILE:HD11	1:A:393:LEU:HD13	1.90	0.54
1:C:160:THR:HG22	1:C:160:THR:O	2.08	0.54
1:C:180:VAL:HG13	1:C:190:ALA:HB3	1.89	0.54
1:F:240:THR:CG2	1:F:246:LEU:HD11	2.38	0.54
1:G:140:VAL:HG21	1:G:168:VAL:HG22	1.90	0.54
1:H:363:PHE:CE1	1:H:369:LEU:HD11	2.43	0.54
1:A:363:PHE:CG	1:A:369:LEU:HD12	2.43	0.54
1:F:133:LEU:C	1:F:133:LEU:CD2	2.75	0.54
1:C:486:ASP:HB3	1:C:489:THR:HG23	1.89	0.54
1:E:84:VAL:CG2	1:H:78:ILE:CG2	2.81	0.54
1:G:472:TYR:CD2	1:G:494:VAL:HG13	2.43	0.54
1:D:198:PHE:CD1	1:D:214:ILE:HD13	2.42	0.54
1:G:393:LEU:CD2	1:G:398:PHE:CD1	2.91	0.54
1:G:400:SER:O	1:G:400:SER:OG	2.25	0.54
1:C:139:GLN:CB	1:F:96:GLN:HG3	2.38	0.53
1:F:244:GLN:HE21	1:F:245:MET:H	1.56	0.53
1:G:169:ARG:CD	1:G:245:MET:CE	2.87	0.53
1:A:140:VAL:HG12	1:A:141:ASN:N	2.24	0.53
1:E:84:VAL:HG21	1:H:78:ILE:HG21	1.84	0.53
1:C:113:LEU:HD23	1:C:113:LEU:O	2.08	0.53
1:D:94:VAL:HG23	1:E:147:GLN:HG3	1.89	0.53
1:D:193:ILE:CG2	1:D:234:LEU:CD1	2.86	0.53
1:H:327:ALA:HB2	1:H:347:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:SER:O	1:E:400:SER:OG	2.23	0.53
1:A:376:ASP:HB2	1:A:425:VAL:CG2	2.39	0.53
1:D:68:ARG:O	1:D:72:ILE:HD12	2.09	0.53
1:H:336:LYS:HG2	1:H:340:THR:CG2	2.39	0.53
1:B:379:ILE:HD13	1:B:386:VAL:HG22	1.90	0.53
1:H:197:VAL:HG21	1:H:234:LEU:CD2	2.34	0.53
1:E:393:LEU:HD22	1:E:398:PHE:CE1	2.44	0.53
1:E:473:LEU:HD13	1:E:478:VAL:CG2	2.39	0.53
1:H:86:GLN:OE1	1:H:340:THR:CA	2.56	0.53
1:A:77:ASN:ND2	1:A:335:GLN:NE2	2.57	0.53
1:B:370:ARG:HG3	1:B:386:VAL:HG11	1.90	0.53
1:D:140:VAL:HG12	1:D:141:ASN:N	2.22	0.53
1:D:379:ILE:HD11	1:D:423:LYS:HZ2	1.73	0.53
1:E:486:ASP:CB	1:E:489:THR:HG23	2.39	0.53
1:F:136:THR:HA	1:F:139:GLN:NE2	2.24	0.53
1:A:234:LEU:HD12	1:A:234:LEU:N	2.24	0.52
1:A:352:TYR:CD1	1:A:352:TYR:N	2.77	0.52
1:C:157:ILE:HD12	1:C:208:TYR:CZ	2.44	0.52
1:D:486:ASP:CB	1:D:489:THR:HG23	2.39	0.52
1:E:330:ASN:OD1	1:E:331:VAL:N	2.42	0.52
1:F:124:TYR:CG	1:F:188:VAL:HG13	2.44	0.52
1:B:94:VAL:HG12	1:B:96:GLN:HE21	1.75	0.52
1:C:457:ASN:ND2	1:C:457:ASN:N	2.54	0.52
1:D:124:TYR:CG	1:D:188:VAL:HG13	2.44	0.52
1:H:317:LEU:HD13	1:H:349:ARG:HA	1.91	0.52
1:F:203:LEU:HD12	1:F:208:TYR:CD2	2.44	0.52
1:F:473:LEU:CD1	1:F:477:LYS:O	2.57	0.52
1:F:386:VAL:HG13	1:F:390:LEU:HD22	1.91	0.52
1:E:87:TYR:HB3	1:H:75:LEU:HD13	1.90	0.52
1:H:212:GLY:O	1:H:248:VAL:HG13	2.10	0.52
1:B:78:ILE:CG2	1:C:84:VAL:HG21	2.39	0.52
1:H:211:VAL:HG13	1:H:247:ASN:O	2.10	0.52
1:E:369:LEU:CD2	1:E:373:LEU:CD1	2.88	0.52
1:E:393:LEU:CD2	1:E:398:PHE:CD1	2.93	0.52
1:F:157:ILE:HD12	1:F:208:TYR:CZ	2.43	0.52
1:B:160:THR:HG22	1:B:160:THR:O	2.10	0.52
1:D:193:ILE:HB	1:D:234:LEU:CD1	2.37	0.52
1:E:240:THR:HG22	1:E:246:LEU:HD11	1.91	0.52
1:E:334:LEU:HD11	1:E:338:LEU:HD22	1.92	0.52
1:F:363:PHE:CD1	1:F:369:LEU:HD12	2.45	0.52
1:E:401:TYR:CE1	1:E:442:VAL:HG11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:479:LEU:HD12	1:H:480:PHE:H	1.75	0.52
1:A:407:GLU:HG3	1:A:427:SER:HB3	1.92	0.51
1:C:198:PHE:CD1	1:C:214:ILE:HD13	2.45	0.51
1:D:94:VAL:O	1:D:94:VAL:CG1	2.48	0.51
1:D:220:GLU:N	1:D:221:PRO:CD	2.74	0.51
1:E:107:ALA:HB1	1:E:271:GLU:OE1	2.10	0.51
1:E:222:ILE:CD1	1:E:234:LEU:HD11	2.40	0.51
1:E:354:LEU:HD21	1:E:439:VAL:HG23	1.93	0.51
1:F:94:VAL:HG12	1:F:96:GLN:CD	2.31	0.51
1:F:418:VAL:HG23	1:F:418:VAL:O	2.10	0.51
1:B:201:ASP:OD1	1:B:201:ASP:N	2.43	0.51
1:C:418:VAL:CG1	1:C:484:ILE:HG21	2.40	0.51
1:G:157:ILE:HD12	1:G:208:TYR:CZ	2.46	0.51
1:A:400:SER:O	1:A:400:SER:OG	2.24	0.51
1:E:124:TYR:CD1	1:E:188:VAL:HG13	2.44	0.51
1:F:486:ASP:CB	1:F:489:THR:HG23	2.40	0.51
1:H:418:VAL:HG21	1:H:493:LEU:CD1	2.33	0.51
1:B:68:ARG:O	1:B:72:ILE:CD1	2.58	0.51
1:B:354:LEU:HD21	1:B:439:VAL:CG2	2.40	0.51
1:E:213:ASN:C	1:E:213:ASN:ND2	2.61	0.51
1:H:484:ILE:HD11	1:H:493:LEU:HD22	1.91	0.51
1:A:133:LEU:HD12	1:A:134:HIS:N	2.25	0.51
1:G:88:LEU:HD22	1:G:92:THR:HG23	1.91	0.51
1:G:486:ASP:HB3	1:G:489:THR:HG23	1.91	0.51
1:D:203:LEU:HD22	1:D:208:TYR:CD2	2.45	0.51
1:F:487:ILE:HG21	1:G:495:GLU:OE2	2.11	0.51
1:G:197:VAL:HG12	1:G:198:PHE:CD2	2.46	0.51
1:G:376:ASP:HB2	1:G:425:VAL:HG22	1.91	0.51
1:A:369:LEU:HD23	1:A:373:LEU:CD1	2.41	0.51
1:D:240:THR:CG2	1:D:246:LEU:HD11	2.40	0.51
1:D:393:LEU:HD22	1:D:398:PHE:CD1	2.45	0.51
1:F:136:THR:HA	1:F:139:GLN:HE22	1.76	0.51
1:H:473:LEU:HD13	1:H:478:VAL:HG22	1.92	0.51
1:D:103:LYS:CE	1:D:251:ASP:OD1	2.55	0.51
1:F:91:PHE:HE1	1:F:126:VAL:HB	1.74	0.51
1:G:407:GLU:OE2	1:G:429:ALA:HB3	2.10	0.51
1:C:193:ILE:HB	1:C:234:LEU:CD2	2.40	0.51
1:D:317:LEU:HD13	1:D:349:ARG:HA	1.93	0.51
1:G:124:TYR:CD1	1:G:188:VAL:HG13	2.45	0.51
1:C:235:THR:HB	1:C:237:LEU:HD22	1.93	0.50
1:E:193:ILE:O	1:E:193:ILE:HG22	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:HG22	1:C:84:VAL:HG21	1.93	0.50
1:F:124:TYR:CD2	1:F:188:VAL:HG22	2.46	0.50
1:F:288:ASN:HD22	1:F:438:ASN:CG	2.15	0.50
1:A:140:VAL:HG11	1:A:158:ARG:NH2	2.27	0.50
1:A:340:THR:HG23	1:A:343:GLY:H	1.75	0.50
1:D:107:ALA:HB1	1:D:271:GLU:OE1	2.11	0.50
1:E:465:PHE:CD1	1:H:465:PHE:CD1	2.99	0.50
1:F:197:VAL:HG11	1:F:234:LEU:HD13	1.92	0.50
1:A:393:LEU:HD22	1:A:398:PHE:CE1	2.46	0.50
1:B:193:ILE:HB	1:B:234:LEU:CD2	2.41	0.50
1:F:354:LEU:CD2	1:F:439:VAL:HG22	2.41	0.50
1:D:407:GLU:OE2	1:D:429:ALA:HB3	2.10	0.50
1:F:203:LEU:HD12	1:F:208:TYR:CE2	2.46	0.50
1:H:479:LEU:HD12	1:H:480:PHE:N	2.26	0.50
1:A:119:CYS:SG	1:A:334:LEU:HD23	2.51	0.50
1:A:220:GLU:N	1:A:221:PRO:CD	2.75	0.50
1:E:157:ILE:HD12	1:E:208:TYR:CZ	2.46	0.50
1:E:487:ILE:HD11	1:H:491:SER:CB	2.37	0.50
1:F:99:PHE:CE2	1:F:123:LEU:HD22	2.43	0.50
1:F:297:MET:HE1	1:F:307:LYS:CB	2.42	0.50
1:B:486:ASP:CB	1:B:489:THR:HG23	2.42	0.50
1:F:471:SER:CB	1:G:471:SER:HG	2.24	0.50
1:E:193:ILE:HB	1:E:234:LEU:CD2	2.41	0.50
1:F:94:VAL:HG11	1:F:96:GLN:HE22	1.76	0.50
1:H:267:VAL:HG21	1:H:338:LEU:CD2	2.40	0.50
1:A:376:ASP:HB2	1:A:425:VAL:HG22	1.94	0.49
1:B:487:ILE:HD11	1:C:491:SER:CA	2.41	0.49
1:D:211:VAL:HG13	1:D:247:ASN:O	2.11	0.49
1:E:109:ILE:HG21	1:E:175:GLN:HG3	1.94	0.49
1:F:214:ILE:HG13	1:F:248:VAL:HG11	1.94	0.49
1:A:240:THR:HG23	1:A:246:LEU:HD11	1.92	0.49
1:C:163:HIS:CE1	1:F:404:GLU:OE2	2.66	0.49
1:D:286:MET:HE2	1:D:347:MET:SD	2.52	0.49
1:D:469:GLN:HE21	1:D:483:GLY:H	1.60	0.49
1:H:102:ILE:HD13	1:H:334:LEU:HD21	1.94	0.49
1:H:157:ILE:HD12	1:H:208:TYR:CZ	2.47	0.49
1:H:201:ASP:N	1:H:201:ASP:OD1	2.44	0.49
1:D:337:GLU:O	1:D:339:PHE:N	2.45	0.49
1:E:103:LYS:CE	1:E:251:ASP:OD1	2.58	0.49
1:E:491:SER:HA	1:H:487:ILE:HD11	1.93	0.49
1:F:201:ASP:OD1	1:F:201:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:407:GLU:HG3	1:H:427:SER:HB3	1.93	0.49
1:B:354:LEU:CD2	1:B:439:VAL:CG2	2.91	0.49
1:C:393:LEU:CD2	1:C:398:PHE:CD1	2.96	0.49
1:F:140:VAL:HG11	1:F:158:ARG:NH2	2.27	0.49
1:F:269:LEU:HD21	1:F:334:LEU:HD13	1.94	0.49
1:F:407:GLU:HG3	1:F:427:SER:HB3	1.95	0.49
1:G:379:ILE:HD11	1:G:423:LYS:HZ2	1.76	0.49
1:H:421:LEU:HD22	1:H:443:LEU:HD21	1.94	0.49
1:B:393:LEU:HD22	1:B:398:PHE:CE1	2.48	0.49
1:E:139:GLN:HE21	1:E:175:GLN:NE2	2.10	0.49
1:E:220:GLU:N	1:E:221:PRO:CD	2.76	0.49
1:E:330:ASN:ND2	1:E:332:GLN:HE21	2.11	0.49
1:F:473:LEU:HD12	1:F:474:LYS:N	2.26	0.49
1:F:486:ASP:HB3	1:F:489:THR:HG23	1.94	0.49
1:C:139:GLN:HE21	1:C:175:GLN:CD	2.16	0.49
1:E:424:PHE:HE1	1:E:439:VAL:HG11	1.76	0.49
1:F:424:PHE:HE1	1:F:439:VAL:HG11	1.77	0.49
1:A:275:ILE:HG21	1:A:284:ILE:HD12	1.95	0.49
1:C:393:LEU:HD21	1:C:398:PHE:CG	2.47	0.49
1:F:124:TYR:CD1	1:F:188:VAL:HG13	2.47	0.49
1:G:370:ARG:HG3	1:G:386:VAL:CG1	2.38	0.49
1:H:124:TYR:CD2	1:H:188:VAL:HG22	2.48	0.49
1:B:379:ILE:HD11	1:B:423:LYS:NZ	2.28	0.49
1:C:133:LEU:HD22	1:C:133:LEU:C	2.33	0.49
1:D:431:TRP:CE2	1:D:436:THR:HG21	2.48	0.49
1:E:407:GLU:HG3	1:E:427:SER:HB3	1.95	0.49
1:G:369:LEU:HD23	1:G:369:LEU:C	2.31	0.49
1:G:393:LEU:HD21	1:G:398:PHE:CG	2.48	0.49
1:G:407:GLU:HG3	1:G:427:SER:HB3	1.95	0.49
1:D:88:LEU:HD22	1:D:92:THR:CG2	2.42	0.49
1:E:354:LEU:CD2	1:E:439:VAL:CG2	2.91	0.49
1:F:266:ILE:HD13	1:F:316:LEU:HD21	1.94	0.49
1:B:364:PRO:HB3	1:H:407:GLU:CD	2.33	0.49
1:E:393:LEU:HD21	1:E:398:PHE:CG	2.47	0.49
1:H:220:GLU:N	1:H:221:PRO:CD	2.76	0.49
1:A:393:LEU:HD11	1:A:411:ILE:HD13	1.95	0.48
1:F:74:LEU:O	1:F:78:ILE:HD12	2.13	0.48
1:A:172:PHE:CE2	1:A:237:LEU:HD21	2.47	0.48
1:B:393:LEU:CD2	1:B:398:PHE:CD1	2.96	0.48
1:B:479:LEU:HD22	1:B:497:PHE:HB2	1.95	0.48
1:C:407:GLU:HG3	1:C:427:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ILE:HD13	1:E:222:ILE:HG21	1.94	0.48
1:E:198:PHE:CD1	1:E:214:ILE:HD13	2.47	0.48
1:H:400:SER:O	1:H:400:SER:OG	2.23	0.48
1:A:113:LEU:C	1:A:113:LEU:CD2	2.81	0.48
1:B:472:TYR:CD2	1:B:494:VAL:HG13	2.48	0.48
1:C:331:VAL:HG13	1:C:332:GLN:N	2.29	0.48
1:C:469:GLN:HE21	1:C:483:GLY:N	2.11	0.48
1:E:87:TYR:HB3	1:H:75:LEU:CD1	2.43	0.48
1:F:495:GLU:HG3	1:G:487:ILE:CD1	2.40	0.48
1:G:169:ARG:NE	1:G:245:MET:HE1	2.28	0.48
1:A:95:SER:CB	1:A:97:GLN:O	2.61	0.48
1:A:136:THR:HG22	1:A:172:PHE:CZ	2.48	0.48
1:A:473:LEU:HD13	1:A:478:VAL:CG2	2.43	0.48
1:A:486:ASP:O	1:A:487:ILE:C	2.50	0.48
1:B:330:ASN:OD1	1:B:331:VAL:N	2.47	0.48
1:B:354:LEU:CD2	1:B:439:VAL:HG22	2.43	0.48
1:D:180:VAL:HG13	1:D:190:ALA:HB3	1.95	0.48
1:G:208:TYR:O	1:G:211:VAL:HG23	2.13	0.48
1:G:418:VAL:HG21	1:G:493:LEU:CD1	2.33	0.48
1:B:386:VAL:HG12	1:B:390:LEU:HD22	1.96	0.48
1:B:408:ALA:HB1	1:B:426:CYS:SG	2.53	0.48
1:B:491:SER:CA	1:C:487:ILE:HD11	2.43	0.48
1:C:275:ILE:HG21	1:C:284:ILE:HD12	1.96	0.48
1:C:386:VAL:HG13	1:C:390:LEU:HD13	1.95	0.48
1:E:136:THR:HG22	1:E:172:PHE:CZ	2.49	0.48
1:E:484:ILE:CD1	1:E:493:LEU:HD22	2.43	0.48
1:G:189:ARG:HG2	1:H:189:ARG:NH1	2.28	0.48
1:A:262:GLU:HA	1:A:320:LEU:CD2	2.43	0.48
1:B:84:VAL:HG12	1:B:85:GLU:N	2.29	0.48
1:B:407:GLU:OE2	1:B:429:ALA:HB3	2.13	0.48
1:E:210:LEU:N	1:E:210:LEU:HD12	2.29	0.48
1:E:473:LEU:HD13	1:E:478:VAL:HG22	1.96	0.48
1:G:222:ILE:CD1	1:G:234:LEU:HD21	2.43	0.48
1:D:82:ARG:HG2	1:D:86:GLN:HE21	1.77	0.48
1:H:473:LEU:HD12	1:H:477:LYS:O	2.14	0.48
1:C:417:ASN:O	1:C:418:VAL:HG22	2.14	0.48
1:D:113:LEU:HD23	1:D:113:LEU:O	2.13	0.48
1:D:486:ASP:HB3	1:D:489:THR:HG23	1.96	0.48
1:E:393:LEU:HD22	1:E:398:PHE:CD1	2.49	0.48
1:H:393:LEU:CD2	1:H:398:PHE:CG	2.97	0.48
1:A:77:ASN:ND2	1:A:335:GLN:HE21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:GLU:HG3	1:B:427:SER:HB3	1.95	0.48
1:D:456:GLU:OE2	1:D:473:LEU:HD21	2.13	0.48
1:E:334:LEU:CD1	1:E:338:LEU:HD22	2.44	0.48
1:G:116:LEU:HD13	1:G:179:LEU:HD11	1.95	0.48
1:G:244:GLN:HE21	1:G:245:MET:N	2.11	0.48
1:G:431:TRP:CE2	1:G:436:THR:HG21	2.49	0.48
1:B:173:LEU:HD22	1:B:194:THR:HG21	1.96	0.48
1:C:201:ASP:N	1:C:201:ASP:OD1	2.47	0.48
1:C:244:GLN:HE21	1:C:245:MET:N	2.12	0.48
1:E:262:GLU:HA	1:E:320:LEU:HD22	1.94	0.48
1:F:121:ALA:HA	1:F:188:VAL:HG21	1.95	0.48
1:H:84:VAL:HG12	1:H:85:GLU:N	2.28	0.48
1:A:331:VAL:HG13	1:A:332:GLN:N	2.29	0.47
1:D:99:PHE:CZ	1:D:338:LEU:HD22	2.48	0.47
1:D:486:ASP:O	1:D:487:ILE:C	2.52	0.47
1:F:453:VAL:HG12	1:F:454:VAL:N	2.29	0.47
1:H:97:GLN:HB3	1:H:264:LEU:HD22	1.96	0.47
1:H:266:ILE:CD1	1:H:316:LEU:HD21	2.43	0.47
1:H:276:ILE:HG23	1:H:281:GLY:O	2.14	0.47
1:A:88:LEU:HD22	1:A:92:THR:CG2	2.43	0.47
1:A:95:SER:HB2	1:A:97:GLN:O	2.14	0.47
1:G:449:ALA:HB1	1:G:484:ILE:HG22	1.97	0.47
1:A:275:ILE:CG2	1:A:284:ILE:HD12	2.44	0.47
1:A:431:TRP:CE2	1:A:436:THR:HG21	2.49	0.47
1:C:340:THR:HG23	1:C:343:GLY:H	1.79	0.47
1:D:121:ALA:HA	1:D:188:VAL:HG21	1.97	0.47
1:E:431:TRP:CE2	1:E:436:THR:HG21	2.48	0.47
1:E:442:VAL:HG22	1:E:445:ARG:HH12	1.79	0.47
1:G:393:LEU:HD22	1:G:398:PHE:CD1	2.49	0.47
1:E:340:THR:HG23	1:E:343:GLY:H	1.79	0.47
1:G:327:ALA:CB	1:G:347:MET:HE3	2.44	0.47
1:C:140:VAL:HG13	1:C:144:LEU:HD23	1.97	0.47
1:C:456:GLU:OE2	1:C:473:LEU:HD21	2.14	0.47
1:D:329:ILE:HD13	1:D:337:GLU:HB2	1.96	0.47
1:A:330:ASN:OD1	1:A:331:VAL:N	2.47	0.47
1:B:449:ALA:HB1	1:B:484:ILE:HG22	1.97	0.47
1:B:471:SER:HG	1:C:471:SER:CB	2.27	0.47
1:G:133:LEU:HD23	1:G:254:ALA:HA	1.96	0.47
1:A:201:ASP:OD1	1:A:201:ASP:N	2.48	0.47
1:A:318:ASP:O	1:A:319:TYR:HD1	1.98	0.47
1:D:303:LYS:O	1:D:306:THR:OG1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ILE:CG2	1:H:84:VAL:CG2	2.92	0.47
1:E:454:VAL:HG12	1:E:455:SER:N	2.29	0.47
1:H:363:PHE:CE1	1:H:369:LEU:CD1	2.97	0.47
1:H:457:ASN:H	1:H:457:ASN:ND2	2.12	0.47
1:H:473:LEU:HD12	1:H:474:LYS:O	2.14	0.47
1:B:126:VAL:O	1:C:68:ARG:HG2	2.15	0.47
1:C:220:GLU:N	1:C:221:PRO:CD	2.78	0.47
1:E:121:ALA:HA	1:E:188:VAL:HG21	1.97	0.47
1:G:68:ARG:O	1:G:69:SER:C	2.52	0.47
1:A:140:VAL:CG1	1:A:141:ASN:N	2.77	0.47
1:A:354:LEU:HD21	1:A:439:VAL:HG23	1.95	0.47
1:A:369:LEU:HD21	1:A:373:LEU:HD11	1.95	0.47
1:B:266:ILE:HD11	1:B:320:LEU:CD1	2.45	0.47
1:C:139:GLN:HB2	1:F:96:GLN:HG3	1.97	0.47
1:C:197:VAL:HG12	1:C:198:PHE:CG	2.49	0.47
1:D:472:TYR:CD2	1:D:494:VAL:HG13	2.50	0.47
1:F:426:CYS:SG	1:F:436:THR:HG22	2.55	0.47
1:G:372:ALA:O	1:G:375:ARG:HG2	2.15	0.47
1:C:372:ALA:O	1:C:375:ARG:HG2	2.15	0.47
1:D:407:GLU:HG3	1:D:427:SER:HB3	1.97	0.47
1:D:479:LEU:HD22	1:D:497:PHE:HB2	1.96	0.47
1:E:147:GLN:OE1	1:E:167:VAL:HG21	2.14	0.47
1:E:327:ALA:HB2	1:E:347:MET:CE	2.45	0.47
1:F:473:LEU:HD12	1:F:477:LYS:O	2.15	0.47
1:F:486:ASP:O	1:F:487:ILE:C	2.52	0.47
1:G:201:ASP:OD1	1:G:201:ASP:N	2.46	0.47
1:B:363:PHE:CD2	1:B:369:LEU:HD12	2.49	0.46
1:D:334:LEU:HD12	1:D:334:LEU:O	2.15	0.46
1:E:68:ARG:O	1:E:72:ILE:CD1	2.63	0.46
1:F:401:TYR:CE2	1:F:443:LEU:CD1	2.98	0.46
1:B:193:ILE:CB	1:B:234:LEU:HD22	2.45	0.46
1:C:473:LEU:HD12	1:C:477:LYS:O	2.16	0.46
1:G:197:VAL:HG12	1:G:198:PHE:CG	2.50	0.46
1:G:376:ASP:HB2	1:G:425:VAL:CG2	2.45	0.46
1:H:421:LEU:HD22	1:H:443:LEU:CD2	2.45	0.46
1:C:82:ARG:HG2	1:C:86:GLN:HE21	1.80	0.46
1:D:140:VAL:CG1	1:D:141:ASN:N	2.77	0.46
1:E:147:GLN:OE1	1:E:167:VAL:CG2	2.63	0.46
1:E:486:ASP:HB3	1:E:489:THR:HG23	1.96	0.46
1:A:472:TYR:CD2	1:A:494:VAL:HG13	2.51	0.46
1:E:77:ASN:HD21	1:E:335:GLN:NE2	2.09	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:GLN:NE2	1:F:245:MET:N	2.60	0.46
1:G:197:VAL:HG21	1:G:222:ILE:HD11	1.95	0.46
1:B:393:LEU:HD21	1:B:398:PHE:CG	2.50	0.46
1:D:379:ILE:CG2	1:D:386:VAL:HG23	2.40	0.46
1:F:73:GLN:HG2	1:F:335:GLN:OE1	2.15	0.46
1:H:193:ILE:HG22	1:H:193:ILE:O	2.15	0.46
1:C:240:THR:HG22	1:C:246:LEU:HD11	1.98	0.46
1:C:393:LEU:HD22	1:C:398:PHE:CE1	2.51	0.46
1:F:97:GLN:HB3	1:F:264:LEU:HD23	1.97	0.46
1:F:425:VAL:O	1:F:425:VAL:HG12	2.16	0.46
1:H:372:ALA:O	1:H:375:ARG:HG2	2.16	0.46
1:B:104:VAL:HG21	1:B:116:LEU:HD21	1.98	0.46
1:B:198:PHE:CD1	1:B:214:ILE:HD13	2.50	0.46
1:B:465:PHE:CD1	1:C:465:PHE:CD1	3.04	0.46
1:C:133:LEU:C	1:C:133:LEU:CD2	2.84	0.46
1:C:147:GLN:HG3	1:F:322:ARG:CB	2.40	0.46
1:C:379:ILE:HG21	1:C:386:VAL:CG2	2.40	0.46
1:D:372:ALA:O	1:D:375:ARG:HG2	2.16	0.46
1:F:417:ASN:N	1:F:417:ASN:OD1	2.49	0.46
1:G:266:ILE:HD13	1:G:316:LEU:CD2	2.43	0.46
1:G:340:THR:HG23	1:G:343:GLY:H	1.81	0.46
1:G:488:ASN:HD22	1:G:489:THR:N	2.13	0.46
1:B:402:ALA:HB2	1:B:409:VAL:HG22	1.98	0.46
1:B:431:TRP:CE2	1:B:436:THR:HG21	2.51	0.46
1:C:417:ASN:O	1:C:418:VAL:HG23	2.16	0.46
1:D:498:VAL:CG1	1:D:499:LYS:N	2.79	0.46
1:G:486:ASP:O	1:G:487:ILE:C	2.54	0.46
1:H:140:VAL:HG12	1:H:141:ASN:H	1.77	0.46
1:A:372:ALA:O	1:A:375:ARG:HG2	2.16	0.46
1:E:352:TYR:CD1	1:E:352:TYR:N	2.83	0.46
1:F:197:VAL:HG11	1:F:234:LEU:CD1	2.46	0.46
1:H:340:THR:CG2	1:H:342:SER:HB3	2.46	0.46
1:A:140:VAL:HG13	1:A:144:LEU:HD12	1.98	0.46
1:A:474:LYS:CE	1:A:501:CYS:SG	3.04	0.46
1:B:234:LEU:N	1:B:234:LEU:HD23	2.30	0.46
1:B:379:ILE:HD11	1:B:423:LYS:HZ3	1.79	0.46
1:F:267:VAL:HG21	1:F:338:LEU:CD1	2.46	0.46
1:E:240:THR:CG2	1:E:246:LEU:HD11	2.47	0.45
1:E:469:GLN:HE21	1:E:483:GLY:H	1.62	0.45
1:E:471:SER:CB	1:H:471:SER:HG	2.29	0.45
1:F:379:ILE:HD13	1:F:386:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:299:GLN:HB2	1:H:302:VAL:HG23	1.97	0.45
1:A:121:ALA:HA	1:A:188:VAL:HG21	1.98	0.45
1:C:188:VAL:HG11	1:C:231:LEU:HD12	1.98	0.45
1:C:421:LEU:HD13	1:C:443:LEU:HD21	1.98	0.45
1:F:372:ALA:O	1:F:375:ARG:HG2	2.16	0.45
1:G:417:ASN:OD1	1:G:417:ASN:N	2.50	0.45
1:B:116:LEU:HD12	1:B:116:LEU:O	2.16	0.45
1:B:329:ILE:HG22	1:B:330:ASN:N	2.31	0.45
1:D:257:LEU:HA	1:D:257:LEU:HD23	1.62	0.45
1:E:336:LYS:HG2	1:E:340:THR:HG21	1.99	0.45
1:E:372:ALA:O	1:E:375:ARG:HG2	2.16	0.45
1:G:147:GLN:OE1	1:G:167:VAL:HG21	2.16	0.45
1:G:197:VAL:HG12	1:G:198:PHE:N	2.30	0.45
1:C:197:VAL:HG12	1:C:198:PHE:CD2	2.52	0.45
1:F:73:GLN:OE1	1:F:118:SER:O	2.34	0.45
1:F:193:ILE:HG21	1:F:234:LEU:HD22	1.99	0.45
1:F:485:ASP:HB3	1:G:472:TYR:OH	2.17	0.45
1:A:68:ARG:O	1:A:72:ILE:CD1	2.65	0.45
1:A:160:THR:O	1:A:160:THR:HG22	2.16	0.45
1:A:234:LEU:N	1:A:234:LEU:CD1	2.80	0.45
1:A:491:SER:CA	1:D:487:ILE:HD11	2.44	0.45
1:G:88:LEU:HA	1:G:88:LEU:HD23	1.67	0.45
1:D:240:THR:HG22	1:D:246:LEU:HD11	1.98	0.45
1:D:277:ASN:OD1	1:D:301:TRP:CE2	2.70	0.45
1:D:417:ASN:OD1	1:D:417:ASN:N	2.49	0.45
1:F:203:LEU:HD13	1:F:203:LEU:O	2.17	0.45
1:F:456:GLU:OE2	1:F:473:LEU:HD21	2.17	0.45
1:G:173:LEU:N	1:G:173:LEU:CD2	2.79	0.45
1:H:88:LEU:HD12	1:H:88:LEU:HA	1.67	0.45
1:H:386:VAL:HG12	1:H:390:LEU:HD22	1.98	0.45
1:B:484:ILE:HD11	1:B:493:LEU:HD22	1.99	0.45
1:D:120:LEU:HA	1:D:123:LEU:HD12	1.97	0.45
1:E:88:LEU:CD2	1:E:92:THR:HG23	2.46	0.45
1:E:338:LEU:HD12	1:E:338:LEU:HA	1.76	0.45
1:E:354:LEU:CD2	1:E:439:VAL:HG23	2.46	0.45
1:E:365:SER:OG	1:E:368:ALA:HB3	2.17	0.45
1:E:412:VAL:HG13	1:E:420:THR:O	2.17	0.45
1:E:454:VAL:HG21	1:E:464:HIS:CD2	2.51	0.45
1:F:103:LYS:CE	1:F:251:ASP:OD1	2.60	0.45
1:H:303:LYS:O	1:H:306:THR:OG1	2.33	0.45
1:H:330:ASN:OD1	1:H:331:VAL:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HG2	1:A:86:GLN:HE21	1.82	0.45
1:A:84:VAL:HG21	1:D:78:ILE:CG2	2.47	0.45
1:D:201:ASP:OD1	1:D:201:ASP:N	2.49	0.45
1:H:417:ASN:O	1:H:418:VAL:HG23	2.15	0.45
1:H:486:ASP:CB	1:H:489:THR:HG23	2.46	0.45
1:A:473:LEU:HD13	1:A:478:VAL:HG22	1.97	0.45
1:B:410:ALA:HB1	1:B:421:LEU:HD11	1.98	0.45
1:B:474:LYS:CE	1:B:501:CYS:SG	3.05	0.45
1:G:74:LEU:HD11	1:G:87:TYR:CE2	2.51	0.45
1:G:240:THR:HG22	1:G:246:LEU:HD11	1.98	0.45
1:H:369:LEU:HD23	1:H:373:LEU:CD1	2.47	0.45
1:B:367:ASP:CG	1:H:323:SER:HB2	2.32	0.45
1:B:479:LEU:HD12	1:B:480:PHE:H	1.82	0.45
1:C:144:LEU:HD22	1:C:167:VAL:CG1	2.46	0.45
1:C:330:ASN:OD1	1:C:331:VAL:N	2.50	0.45
1:D:270:ASN:ND2	1:D:272:LYS:HG2	2.31	0.45
1:F:193:ILE:HB	1:F:234:LEU:HD22	1.98	0.45
1:H:180:VAL:HG13	1:H:190:ALA:CB	2.41	0.45
1:E:140:VAL:HG23	1:E:171:CYS:SG	2.56	0.44
1:E:267:VAL:CG2	1:E:338:LEU:CD1	2.79	0.44
1:H:425:VAL:O	1:H:425:VAL:HG12	2.17	0.44
1:B:354:LEU:HD13	1:B:442:VAL:HG21	1.99	0.44
1:B:426:CYS:SG	1:B:436:THR:HG22	2.57	0.44
1:B:488:ASN:HD22	1:B:489:THR:N	2.16	0.44
1:B:491:SER:HB3	1:C:487:ILE:HD11	1.99	0.44
1:D:88:LEU:HD22	1:D:92:THR:HG23	2.00	0.44
1:D:286:MET:CE	1:D:347:MET:HB3	2.47	0.44
1:F:266:ILE:HB	1:F:326:VAL:HG22	1.98	0.44
1:H:411:ILE:O	1:H:421:LEU:HD12	2.17	0.44
1:B:374:GLN:CD	1:H:97:GLN:HB2	2.37	0.44
1:C:124:TYR:CD2	1:C:188:VAL:HG22	2.52	0.44
1:C:469:GLN:NE2	1:C:483:GLY:H	2.13	0.44
1:E:417:ASN:OD1	1:E:417:ASN:N	2.50	0.44
1:F:133:LEU:HD11	1:F:253:ALA:HB3	1.99	0.44
1:F:275:ILE:CG2	1:F:284:ILE:HD12	2.48	0.44
1:A:86:GLN:OE1	1:A:432:LEU:HD13	2.17	0.44
1:B:337:GLU:HG2	1:B:340:THR:O	2.18	0.44
1:D:140:VAL:HG13	1:D:144:LEU:HD12	2.00	0.44
1:E:201:ASP:N	1:E:201:ASP:OD1	2.50	0.44
1:F:373:LEU:HA	1:F:373:LEU:HD23	1.75	0.44
1:G:369:LEU:C	1:G:369:LEU:CD2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:VAL:O	1:H:101:VAL:HG12	2.15	0.44
1:H:486:ASP:O	1:H:487:ILE:C	2.55	0.44
1:B:417:ASN:OD1	1:B:417:ASN:N	2.50	0.44
1:D:199:THR:HG22	1:D:215:LYS:HB3	1.99	0.44
1:D:337:GLU:C	1:D:339:PHE:N	2.71	0.44
1:E:113:LEU:O	1:E:113:LEU:HD23	2.17	0.44
1:G:266:ILE:HB	1:G:326:VAL:HG22	1.99	0.44
1:F:419:PRO:O	1:F:450:LEU:HD12	2.17	0.44
1:H:363:PHE:CD2	1:H:369:LEU:HD12	2.53	0.44
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.70	0.44
1:G:489:THR:O	1:G:493:LEU:HD13	2.18	0.44
1:A:474:LYS:O	1:A:475:GLY:C	2.56	0.44
1:B:387:ALA:CB	1:H:262:GLU:OE1	2.66	0.44
1:B:486:ASP:HB3	1:B:489:THR:HG23	2.00	0.44
1:E:91:PHE:CB	1:H:72:ILE:HD13	2.41	0.44
1:E:359:SER:OG	1:E:362:GLU:HB2	2.17	0.44
1:F:74:LEU:HD21	1:G:75:LEU:HD11	1.99	0.44
1:G:189:ARG:HE	1:G:189:ARG:HB3	1.64	0.44
1:A:386:VAL:HG13	1:A:390:LEU:HD22	1.98	0.44
1:A:393:LEU:CD2	1:A:398:PHE:CD1	3.00	0.44
1:B:139:GLN:OE1	1:B:139:GLN:N	2.49	0.44
1:E:275:ILE:HG21	1:E:284:ILE:HD12	2.00	0.44
1:F:244:GLN:NE2	1:F:245:MET:H	2.16	0.44
1:G:408:ALA:HB1	1:G:426:CYS:SG	2.57	0.44
1:B:124:TYR:CG	1:B:188:VAL:HG13	2.52	0.43
1:B:359:SER:OG	1:B:362:GLU:HB2	2.18	0.43
1:D:295:ASP:HA	1:D:298:LYS:HG2	2.00	0.43
1:A:327:ALA:HB2	1:A:347:MET:CE	2.48	0.43
1:A:418:VAL:HG21	1:A:493:LEU:CD1	2.45	0.43
1:B:479:LEU:HD12	1:B:480:PHE:N	2.33	0.43
1:C:193:ILE:HB	1:C:234:LEU:HD23	2.00	0.43
1:C:258:ALA:O	1:C:320:LEU:HD21	2.18	0.43
1:E:486:ASP:O	1:E:487:ILE:C	2.55	0.43
1:G:203:LEU:HD22	1:G:208:TYR:CE2	2.53	0.43
1:G:369:LEU:HD21	1:G:373:LEU:HD11	1.99	0.43
1:A:68:ARG:O	1:A:72:ILE:HD12	2.18	0.43
1:A:417:ASN:N	1:A:417:ASN:OD1	2.51	0.43
1:C:104:VAL:HG11	1:C:116:LEU:CD2	2.48	0.43
1:C:352:TYR:CE2	1:C:405:PRO:HG3	2.53	0.43
1:C:359:SER:OG	1:C:362:GLU:HB2	2.19	0.43
1:D:474:LYS:CE	1:D:501:CYS:SG	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:ASN:HA	1:D:491:SER:OG	2.19	0.43
1:F:359:SER:OG	1:F:362:GLU:HB2	2.17	0.43
1:G:74:LEU:CD1	1:G:87:TYR:CE2	3.02	0.43
1:G:456:GLU:OE2	1:G:473:LEU:HD21	2.19	0.43
1:G:488:ASN:HA	1:G:491:SER:OG	2.19	0.43
1:C:270:ASN:ND2	1:C:272:LYS:HB2	2.34	0.43
1:D:286:MET:HE3	1:D:347:MET:CB	2.48	0.43
1:D:365:SER:O	1:D:365:SER:OG	2.36	0.43
1:D:418:VAL:HG11	1:D:484:ILE:HD13	1.99	0.43
1:F:474:LYS:HD2	1:F:501:CYS:SG	2.58	0.43
1:H:73:GLN:OE1	1:H:118:SER:O	2.36	0.43
1:C:486:ASP:O	1:C:487:ILE:C	2.55	0.43
1:E:406:LEU:HD12	1:E:409:VAL:CG2	2.49	0.43
1:G:365:SER:O	1:G:365:SER:OG	2.36	0.43
1:H:73:GLN:CG	1:H:335:GLN:OE1	2.60	0.43
1:A:363:PHE:CE1	1:A:369:LEU:HD12	2.52	0.43
1:B:275:ILE:HG21	1:B:284:ILE:HD12	2.00	0.43
1:E:330:ASN:HD21	1:E:332:GLN:HE21	1.65	0.43
1:F:97:GLN:OE1	1:F:264:LEU:HD23	2.12	0.43
1:F:275:ILE:HG21	1:F:284:ILE:HD12	2.01	0.43
1:F:277:ASN:ND2	1:F:280:THR:OG1	2.52	0.43
1:F:338:LEU:HD12	1:F:338:LEU:HA	1.73	0.43
1:G:393:LEU:HD11	1:G:411:ILE:HD13	2.00	0.43
1:H:408:ALA:HB3	1:H:435:VAL:HG11	1.99	0.43
1:B:308:LEU:HD23	1:B:308:LEU:O	2.18	0.43
1:D:193:ILE:HG21	1:D:234:LEU:CD1	2.47	0.43
1:D:376:ASP:HB2	1:D:425:VAL:HG22	2.00	0.43
1:D:474:LYS:HD2	1:D:501:CYS:SG	2.58	0.43
1:F:401:TYR:CD2	1:F:443:LEU:CD1	3.01	0.43
1:H:474:LYS:CE	1:H:501:CYS:SG	3.06	0.43
1:B:393:LEU:CD2	1:B:398:PHE:CG	3.01	0.43
1:C:417:ASN:OD1	1:C:417:ASN:N	2.52	0.43
1:D:133:LEU:HD23	1:D:254:ALA:HA	2.01	0.43
1:D:279:SER:HB2	1:D:301:TRP:CD1	2.54	0.43
1:E:329:ILE:HG21	1:E:329:ILE:HD13	1.75	0.43
1:F:180:VAL:HG13	1:F:190:ALA:HB3	2.00	0.43
1:G:220:GLU:N	1:G:221:PRO:CD	2.82	0.43
1:H:97:GLN:HB3	1:H:264:LEU:CD2	2.48	0.43
1:A:359:SER:OG	1:A:362:GLU:HB2	2.18	0.43
1:C:139:GLN:CA	1:F:96:GLN:HE21	2.31	0.43
1:C:140:VAL:HG12	1:C:141:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ILE:HB	1:E:326:VAL:HG22	2.01	0.43
1:G:133:LEU:CD2	1:G:254:ALA:HA	2.49	0.43
1:G:338:LEU:HD12	1:G:338:LEU:HA	1.75	0.43
1:G:359:SER:OG	1:G:362:GLU:HB2	2.19	0.43
1:G:370:ARG:CG	1:G:386:VAL:HG11	2.43	0.43
1:H:139:GLN:OE1	1:H:139:GLN:N	2.52	0.43
1:A:363:PHE:CE1	1:A:369:LEU:CD1	3.01	0.43
1:A:474:LYS:HD2	1:A:501:CYS:SG	2.59	0.43
1:A:486:ASP:CB	1:A:489:THR:HG23	2.48	0.43
1:D:180:VAL:HG13	1:D:190:ALA:HB1	2.01	0.43
1:D:259:ARG:HG3	1:D:316:LEU:CD1	2.49	0.43
1:D:452:TRP:O	1:D:479:LEU:HD12	2.19	0.43
1:E:337:GLU:HG2	1:E:340:THR:O	2.19	0.43
1:G:474:LYS:CE	1:G:501:CYS:SG	3.07	0.43
1:G:474:LYS:HD2	1:G:501:CYS:SG	2.59	0.43
1:H:432:LEU:C	1:H:432:LEU:HD12	2.38	0.43
1:B:193:ILE:CG2	1:B:234:LEU:HD22	2.49	0.42
1:D:359:SER:OG	1:D:362:GLU:HB2	2.19	0.42
1:E:491:SER:HB3	1:H:487:ILE:HD11	2.00	0.42
1:F:136:THR:HG22	1:F:172:PHE:CZ	2.53	0.42
1:F:184:GLU:HA	1:F:188:VAL:O	2.19	0.42
1:F:297:MET:CE	1:F:307:LYS:HG2	2.48	0.42
1:G:418:VAL:CG2	1:G:493:LEU:HD11	2.37	0.42
1:H:173:LEU:N	1:H:173:LEU:HD23	2.33	0.42
1:A:354:LEU:HD12	1:A:438:ASN:ND2	2.34	0.42
1:B:372:ALA:O	1:B:375:ARG:HG2	2.18	0.42
1:B:474:LYS:HD2	1:B:501:CYS:SG	2.59	0.42
1:B:487:ILE:HD11	1:C:491:SER:HA	2.01	0.42
1:C:113:LEU:CD2	1:C:113:LEU:C	2.88	0.42
1:D:109:ILE:HG21	1:D:175:GLN:HG3	2.01	0.42
1:D:276:ILE:HG23	1:D:281:GLY:O	2.18	0.42
1:E:124:TYR:CG	1:E:188:VAL:HG13	2.54	0.42
1:E:275:ILE:CG2	1:E:284:ILE:HD12	2.49	0.42
1:E:365:SER:OG	1:E:365:SER:O	2.36	0.42
1:F:488:ASN:HD22	1:F:489:THR:N	2.17	0.42
1:G:203:LEU:HD22	1:G:208:TYR:CD2	2.54	0.42
1:H:365:SER:O	1:H:365:SER:OG	2.37	0.42
1:H:417:ASN:N	1:H:417:ASN:OD1	2.52	0.42
1:A:210:LEU:N	1:A:210:LEU:HD12	2.34	0.42
1:A:308:LEU:HA	1:A:308:LEU:HD12	1.78	0.42
1:B:365:SER:O	1:B:365:SER:OG	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:SER:O	1:C:365:SER:OG	2.36	0.42
1:F:390:LEU:HD12	1:F:390:LEU:HA	1.69	0.42
1:A:91:PHE:HE1	1:A:126:VAL:O	2.02	0.42
1:A:454:VAL:HG12	1:A:455:SER:N	2.34	0.42
1:E:390:LEU:HD12	1:E:390:LEU:HA	1.89	0.42
1:E:474:LYS:O	1:E:475:GLY:C	2.58	0.42
1:F:70:THR:HG23	1:F:122:PHE:CD1	2.53	0.42
1:F:123:LEU:HD21	1:F:338:LEU:HD23	2.00	0.42
1:H:431:TRP:CE2	1:H:436:THR:HG21	2.54	0.42
1:A:403:ASP:OD1	1:A:403:ASP:N	2.52	0.42
1:C:474:LYS:CE	1:C:501:CYS:SG	3.08	0.42
1:D:337:GLU:C	1:D:339:PHE:H	2.23	0.42
1:E:91:PHE:HB3	1:H:72:ILE:HD11	1.95	0.42
1:E:197:VAL:HG21	1:E:234:LEU:CD1	2.49	0.42
1:E:206:ASP:N	1:E:206:ASP:OD1	2.53	0.42
1:E:318:ASP:O	1:E:319:TYR:HD1	2.02	0.42
1:F:84:VAL:HG21	1:G:78:ILE:HG22	2.02	0.42
1:H:376:ASP:HB2	1:H:425:VAL:HG22	2.00	0.42
1:H:474:LYS:O	1:H:475:GLY:C	2.58	0.42
1:A:401:TYR:CE1	1:A:442:VAL:HG11	2.55	0.42
1:B:470:GLY:HA3	1:B:481:TRP:CZ2	2.54	0.42
1:E:100:ALA:HA	1:E:265:LYS:O	2.19	0.42
1:E:474:LYS:CE	1:E:501:CYS:SG	3.07	0.42
1:F:119:CYS:HG	1:F:335:GLN:HB3	1.84	0.42
1:F:386:VAL:CG1	1:F:390:LEU:CD2	2.95	0.42
1:F:431:TRP:CE2	1:F:436:THR:HG21	2.54	0.42
1:H:342:SER:O	1:H:343:GLY:C	2.58	0.42
1:H:457:ASN:ND2	1:H:457:ASN:N	2.66	0.42
1:B:220:GLU:N	1:B:221:PRO:CD	2.83	0.42
1:C:104:VAL:HG11	1:C:116:LEU:HD21	2.02	0.42
1:C:234:LEU:HD12	1:C:257:LEU:HD11	2.02	0.42
1:G:184:GLU:HA	1:G:188:VAL:O	2.20	0.42
1:A:484:ILE:HG21	1:A:484:ILE:HD13	1.78	0.42
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.88	0.42
1:C:269:LEU:HD23	1:C:269:LEU:HA	1.81	0.42
1:C:337:GLU:HG2	1:C:340:THR:O	2.20	0.42
1:D:189:ARG:HE	1:D:189:ARG:HB3	1.67	0.42
1:D:330:ASN:OD1	1:D:331:VAL:N	2.52	0.42
1:E:386:VAL:CG1	1:E:390:LEU:HD22	2.49	0.42
1:F:140:VAL:HG12	1:F:141:ASN:H	1.79	0.42
1:G:208:TYR:HB3	1:G:211:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:LEU:HB3	1:C:452:TRP:HB3	2.02	0.42
1:E:207:LYS:HB3	1:E:208:TYR:CD2	2.55	0.42
1:H:474:LYS:HD2	1:H:501:CYS:SG	2.59	0.42
1:H:479:LEU:HD22	1:H:497:PHE:HB2	2.02	0.42
1:A:406:LEU:HD12	1:A:409:VAL:CG2	2.50	0.42
1:B:316:LEU:HA	1:B:316:LEU:HD12	1.76	0.42
1:C:150:GLU:N	1:F:407:GLU:OE2	2.48	0.42
1:C:373:LEU:HD23	1:C:373:LEU:HA	1.83	0.42
1:C:458:ASP:O	1:C:459:ALA:C	2.57	0.42
1:C:474:LYS:HD2	1:C:501:CYS:SG	2.60	0.42
1:E:234:LEU:HD12	1:E:257:LEU:HD11	2.02	0.42
1:E:454:VAL:HG21	1:E:464:HIS:CG	2.54	0.42
1:F:139:GLN:HG3	1:F:175:GLN:HE22	1.85	0.42
1:F:393:LEU:HD21	1:F:398:PHE:CG	2.55	0.42
1:H:197:VAL:HG12	1:H:198:PHE:CD2	2.55	0.42
1:D:86:GLN:O	1:D:89:LYS:HB2	2.20	0.41
1:E:354:LEU:CD2	1:E:439:VAL:HG22	2.50	0.41
1:G:113:LEU:O	1:G:113:LEU:HD23	2.20	0.41
1:H:252:VAL:HG22	1:H:312:GLU:CD	2.40	0.41
1:H:354:LEU:HD21	1:H:439:VAL:HG22	2.02	0.41
1:H:486:ASP:HB3	1:H:489:THR:HG23	2.02	0.41
1:C:431:TRP:CE2	1:C:436:THR:HG21	2.55	0.41
1:E:184:GLU:HA	1:E:188:VAL:O	2.19	0.41
1:F:474:LYS:CE	1:F:501:CYS:SG	3.08	0.41
1:A:469:GLN:NE2	1:A:483:GLY:H	2.17	0.41
1:B:130:PRO:HG2	1:B:231:LEU:HD22	2.02	0.41
1:D:474:LYS:O	1:D:475:GLY:C	2.59	0.41
1:F:203:LEU:C	1:F:203:LEU:CD1	2.89	0.41
1:G:116:LEU:CD1	1:G:179:LEU:HD11	2.49	0.41
1:H:386:VAL:HG13	1:H:390:LEU:HD22	2.00	0.41
1:B:211:VAL:HG13	1:B:247:ASN:O	2.20	0.41
1:C:379:ILE:HD11	1:C:423:LYS:NZ	2.35	0.41
1:E:133:LEU:HD23	1:E:254:ALA:HA	2.02	0.41
1:F:421:LEU:HB3	1:F:452:TRP:HB3	2.02	0.41
1:G:337:GLU:HG2	1:G:340:THR:O	2.20	0.41
1:H:488:ASN:HD22	1:H:489:THR:N	2.18	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.70	0.41
1:B:443:LEU:HA	1:B:443:LEU:HD12	1.66	0.41
1:C:121:ALA:HA	1:C:188:VAL:HG21	2.01	0.41
1:D:393:LEU:HA	1:D:393:LEU:HD23	1.67	0.41
1:F:113:LEU:HD23	1:F:113:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:THR:HG22	1:G:172:PHE:CZ	2.56	0.41
1:G:470:GLY:HA3	1:G:481:TRP:CZ2	2.56	0.41
1:H:403:ASP:OD1	1:H:403:ASP:N	2.53	0.41
1:H:456:GLU:OE2	1:H:473:LEU:HD21	2.20	0.41
1:B:86:GLN:O	1:B:89:LYS:HB2	2.20	0.41
1:B:370:ARG:NH1	1:H:323:SER:OG	2.52	0.41
1:E:375:ARG:HA	1:E:375:ARG:HD2	1.96	0.41
1:G:372:ALA:O	1:G:425:VAL:HG11	2.20	0.41
1:H:379:ILE:HD11	1:H:423:LYS:NZ	2.36	0.41
1:A:354:LEU:HD21	1:A:439:VAL:CG2	2.50	0.41
1:B:474:LYS:O	1:B:475:GLY:C	2.59	0.41
1:D:244:GLN:HE21	1:D:245:MET:N	2.18	0.41
1:F:144:LEU:CD2	1:F:167:VAL:HG11	2.49	0.41
1:F:189:ARG:HE	1:F:189:ARG:HB3	1.65	0.41
1:G:100:ALA:HA	1:G:265:LYS:O	2.21	0.41
1:A:337:GLU:HG2	1:A:340:THR:O	2.20	0.41
1:A:386:VAL:CG1	1:A:390:LEU:HD22	2.51	0.41
1:B:488:ASN:HA	1:B:491:SER:OG	2.21	0.41
1:E:369:LEU:HD21	1:E:373:LEU:HD11	2.00	0.41
1:E:401:TYR:CD1	1:E:442:VAL:HG11	2.56	0.41
1:F:70:THR:HG23	1:F:122:PHE:HD1	1.86	0.41
1:F:407:GLU:HG3	1:F:430:ALA:HB2	2.03	0.41
1:F:443:LEU:HA	1:F:443:LEU:HD12	1.80	0.41
1:A:91:PHE:O	1:D:68:ARG:NH1	2.53	0.41
1:A:458:ASP:O	1:A:459:ALA:C	2.58	0.41
1:B:124:TYR:CD1	1:B:188:VAL:HG13	2.56	0.41
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.90	0.41
1:B:404:GLU:N	1:B:405:PRO:CD	2.84	0.41
1:B:473:LEU:HD13	1:B:478:VAL:HG23	2.03	0.41
1:C:322:ARG:HD3	1:C:352:TYR:CZ	2.56	0.41
1:D:120:LEU:HD23	1:D:120:LEU:HA	1.66	0.41
1:D:289:LEU:HD23	1:D:289:LEU:HA	1.94	0.41
1:D:404:GLU:N	1:D:405:PRO:CD	2.83	0.41
1:E:84:VAL:CG2	1:H:78:ILE:HG21	2.47	0.41
1:F:329:ILE:HG22	1:F:330:ASN:N	2.36	0.41
1:F:365:SER:O	1:F:365:SER:OG	2.35	0.41
1:F:472:TYR:CD2	1:F:494:VAL:HG13	2.56	0.41
1:G:330:ASN:OD1	1:G:331:VAL:N	2.54	0.41
1:G:393:LEU:CD2	1:G:398:PHE:CG	3.04	0.41
1:H:99:PHE:CE2	1:H:123:LEU:HD22	2.56	0.41
1:H:121:ALA:HA	1:H:188:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:369:LEU:CD2	1:H:373:LEU:CD1	2.97	0.41
1:A:183:LEU:HD13	1:A:190:ALA:HB2	2.03	0.41
1:A:379:ILE:HD13	1:A:379:ILE:HG21	1.85	0.41
1:B:214:ILE:HG13	1:B:248:VAL:HG11	2.01	0.41
1:E:470:GLY:HA3	1:E:481:TRP:CZ2	2.56	0.41
1:H:133:LEU:HD12	1:H:254:ALA:HA	2.02	0.41
1:B:144:LEU:HD12	1:B:149:ILE:CG2	2.51	0.40
1:E:71:VAL:HG13	1:H:74:LEU:CD2	2.52	0.40
1:E:102:ILE:HG21	1:E:102:ILE:HD13	1.76	0.40
1:E:184:GLU:OE1	1:F:228:ALA:HB1	2.21	0.40
1:E:257:LEU:HD23	1:E:257:LEU:HA	1.79	0.40
1:E:316:LEU:HD12	1:E:316:LEU:HA	1.66	0.40
1:H:404:GLU:N	1:H:405:PRO:CD	2.83	0.40
1:B:313:ILE:CD1	1:B:326:VAL:HG11	2.49	0.40
1:B:379:ILE:O	1:B:379:ILE:HG22	2.21	0.40
1:C:286:MET:HA	1:C:347:MET:O	2.21	0.40
1:C:360:ILE:HD11	1:C:393:LEU:HD13	2.03	0.40
1:C:474:LYS:O	1:C:475:GLY:C	2.58	0.40
1:D:286:MET:HG3	1:D:347:MET:HB3	2.03	0.40
1:E:191:ARG:HD2	1:E:225:SER:HB2	2.03	0.40
1:E:289:LEU:HD13	1:E:314:LYS:HA	2.02	0.40
1:E:328:ILE:HG21	1:E:328:ILE:HD13	1.64	0.40
1:E:374:GLN:HE21	1:E:374:GLN:HB3	1.76	0.40
1:F:193:ILE:HB	1:F:234:LEU:CD2	2.51	0.40
1:H:408:ALA:HB1	1:H:426:CYS:SG	2.61	0.40
1:A:172:PHE:CD2	1:A:237:LEU:HD21	2.56	0.40
1:B:403:ASP:OD1	1:B:403:ASP:N	2.54	0.40
1:D:104:VAL:HG22	1:D:269:LEU:HD12	2.03	0.40
1:D:303:LYS:HA	1:D:303:LYS:HD2	1.93	0.40
1:D:334:LEU:HD12	1:D:334:LEU:C	2.41	0.40
1:E:474:LYS:HD2	1:E:501:CYS:SG	2.61	0.40
1:F:379:ILE:HG21	1:F:386:VAL:CG2	2.37	0.40
1:F:418:VAL:HG21	1:F:493:LEU:CD1	2.49	0.40
1:H:359:SER:OG	1:H:362:GLU:HB2	2.21	0.40
1:A:113:LEU:HD23	1:A:113:LEU:C	2.39	0.40
1:B:165:MET:CE	1:B:245:MET:O	2.70	0.40
1:C:473:LEU:HD13	1:C:478:VAL:HG23	2.01	0.40
1:C:479:LEU:HD22	1:C:497:PHE:HB2	2.03	0.40
1:D:206:ASP:OD1	1:D:206:ASP:N	2.54	0.40
1:E:180:VAL:HG13	1:E:190:ALA:CB	2.47	0.40
1:G:375:ARG:HA	1:G:375:ARG:HD2	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:VAL:CG1	1:H:96:GLN:NE2	2.85	0.40
1:H:131:ILE:HD13	1:H:222:ILE:HG21	2.04	0.40
1:D:175:GLN:HE21	1:D:175:GLN:HB2	1.67	0.40
1:D:288:ASN:OD1	1:D:438:ASN:ND2	2.55	0.40
1:E:289:LEU:HD23	1:E:289:LEU:HA	1.73	0.40
1:E:352:TYR:HE1	1:E:433:ASN:HD22	1.69	0.40
1:E:403:ASP:OD1	1:E:403:ASP:N	2.54	0.40
1:E:488:ASN:HA	1:E:491:SER:OG	2.21	0.40
1:F:288:ASN:ND2	1:F:438:ASN:ND2	2.55	0.40
1:G:72:ILE:HD12	1:G:72:ILE:N	2.35	0.40
1:G:206:ASP:OD1	1:G:206:ASP:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:TYR:OH	1:G:495:GLU:OE2[1_546]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.