Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 07:41 AM EDT

PDB ID	:	6QX5
Title	:	Crystal structure of T7 bacteriophage portal protein, 12mer, closed valve
Authors	:	Fabrega-Ferrer, M.; Cuervo, A.; Machon, C.; Fernandez, F.J.; Perez-Luque, R.; Pous, J.; Vega, M.C.; Carrascosa, J.L.; Coll, M.
Deposited on	:	2019-03-07
Resolution	:	3.60 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 (i) symbol.

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

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

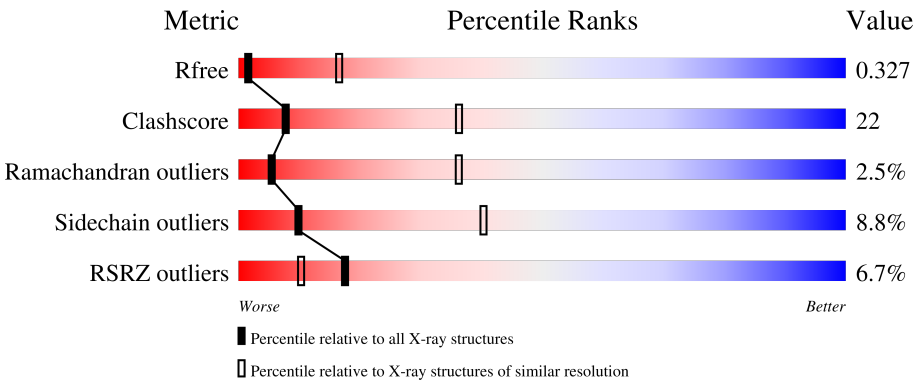
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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% 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	490	5% 61% 33% • •
1	B	490	6% 61% 32% • •
1	C	490	7% 59% 35% • •
1	D	490	7% 59% 34% 5% •
1	E	490	7% 58% 35% 5% •

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Mol	Chain	Length	Quality of chain
1	F	490	4% 59% 35%
1	G	490	10% 59% 34%
1	H	490	8% 60% 33%
1	I	490	7% 60% 34%
1	J	490	7% 60% 33% 5%
1	K	490	3% 59% 35%
1	L	490	9% 60% 33%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 45048 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 Portal protein.

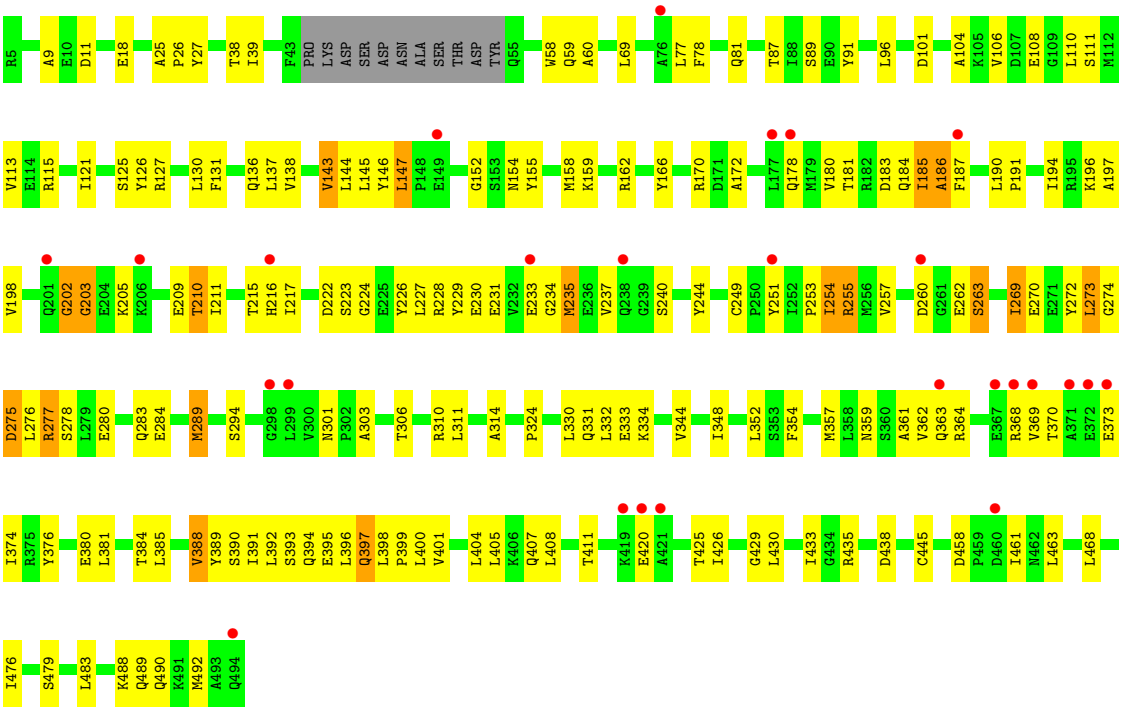
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	3754	2364	637	735	18	0	0	0
1	B	479	3754	2364	637	735	18	0	0	0
1	C	479	3754	2364	637	735	18	0	0	0
1	D	479	3754	2364	637	735	18	0	0	0
1	E	479	3754	2364	637	735	18	0	0	0
1	F	479	3754	2364	637	735	18	0	0	0
1	G	479	3754	2364	637	735	18	0	0	0
1	H	479	3754	2364	637	735	18	0	0	0
1	I	479	3754	2364	637	735	18	0	0	0
1	J	479	3754	2364	637	735	18	0	0	0
1	K	479	3754	2364	637	735	18	0	0	0
1	L	479	3754	2364	637	735	18	0	0	0

3 Residue-property plots (i)

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

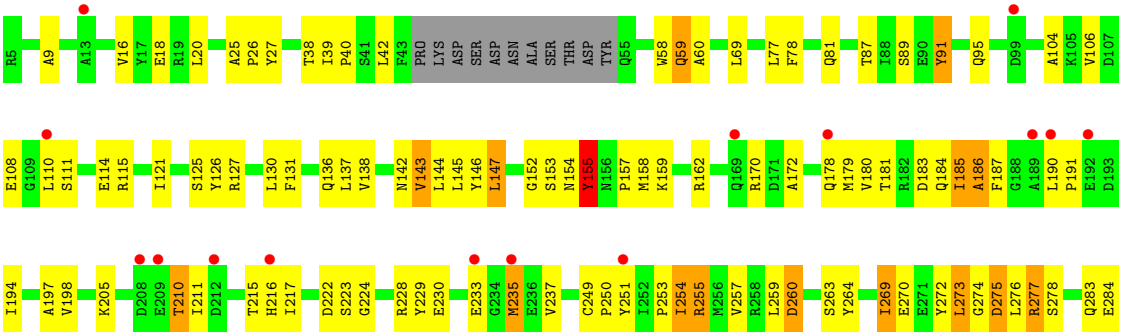
• Molecule 1: Portal protein

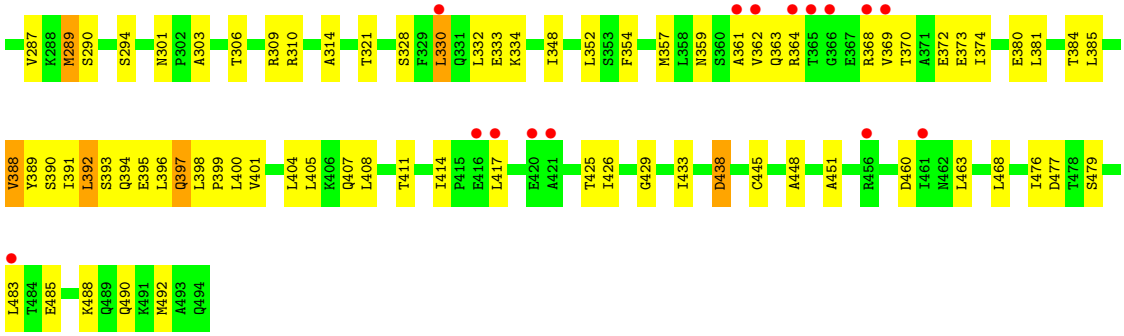
Chain A:



• Molecule 1: Portal protein

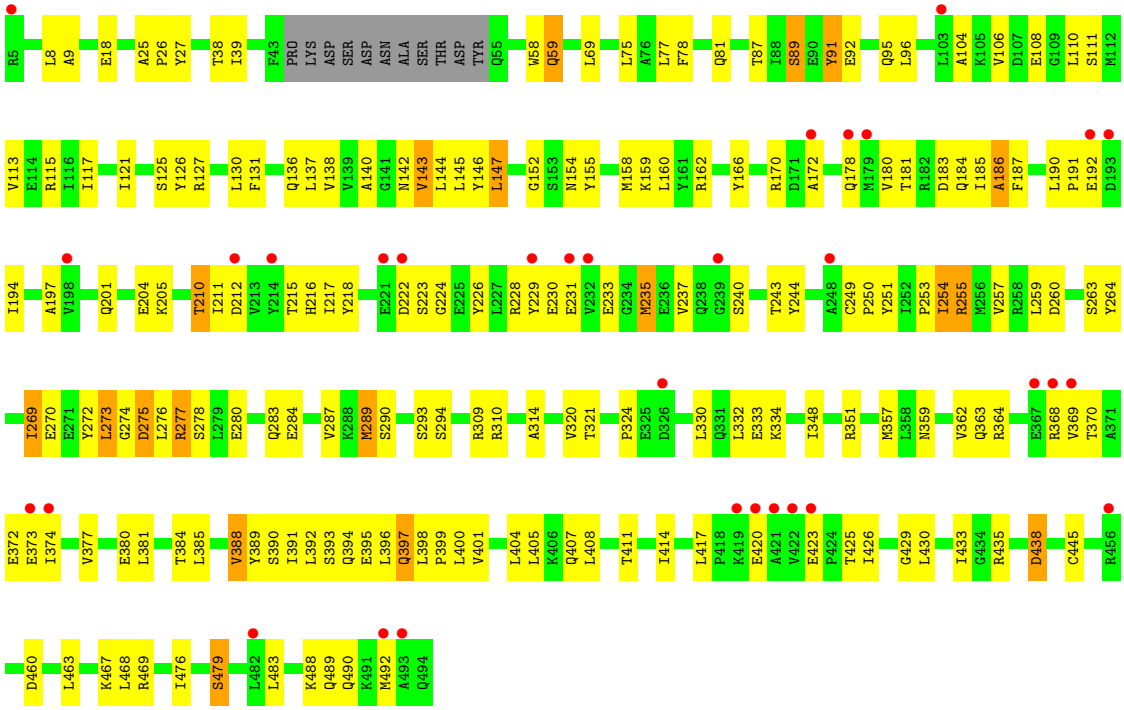
Chain B:





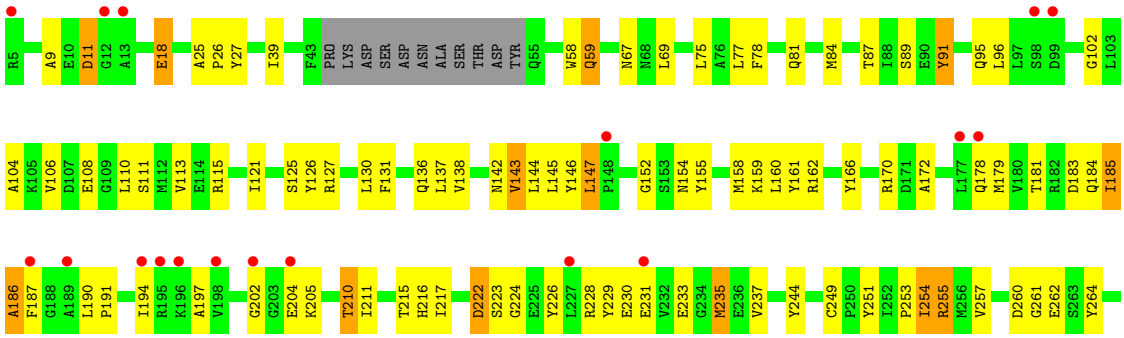
• Molecule 1: Portal protein

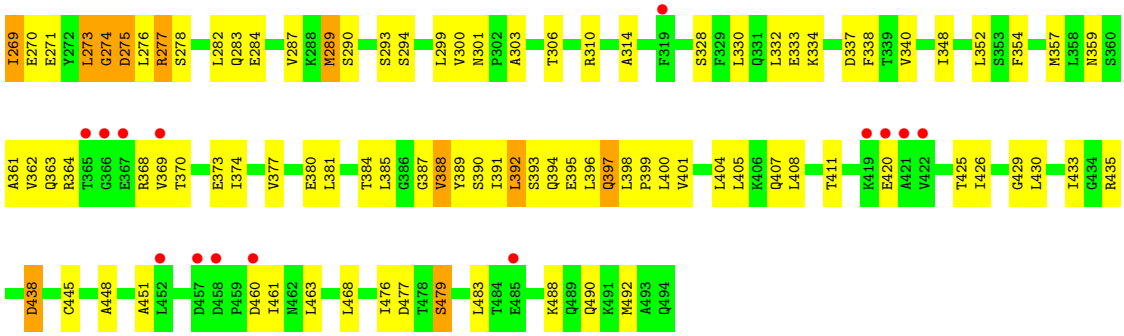
Chain C:



• Molecule 1: Portal protein

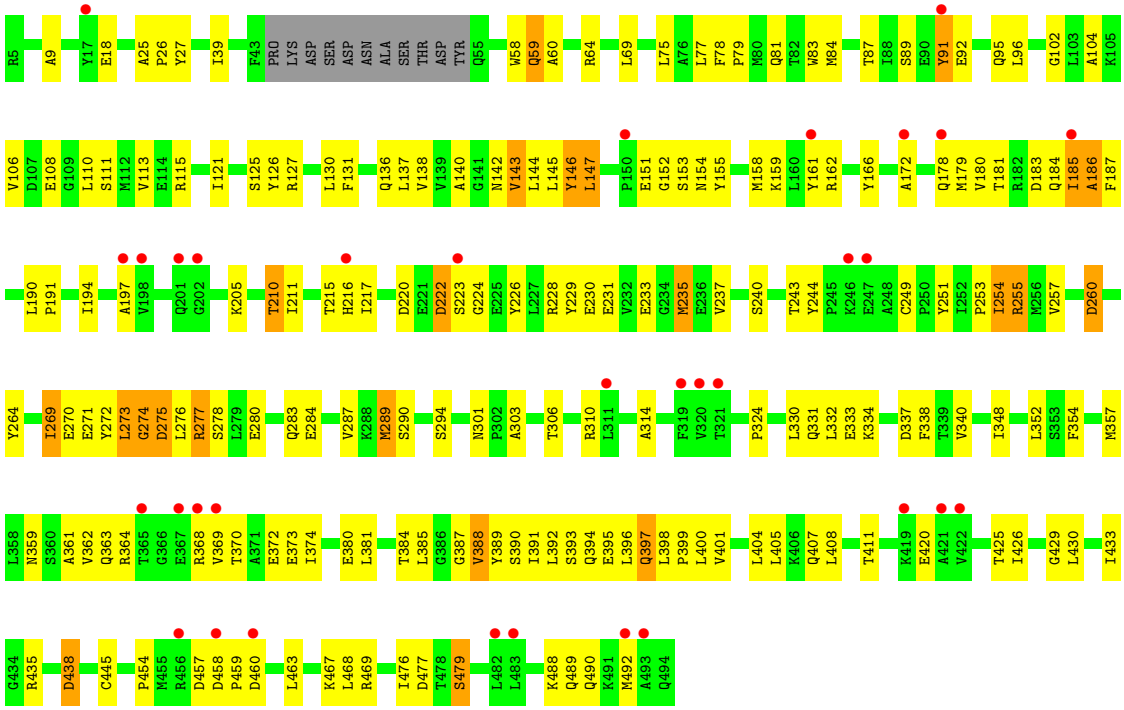
Chain D:





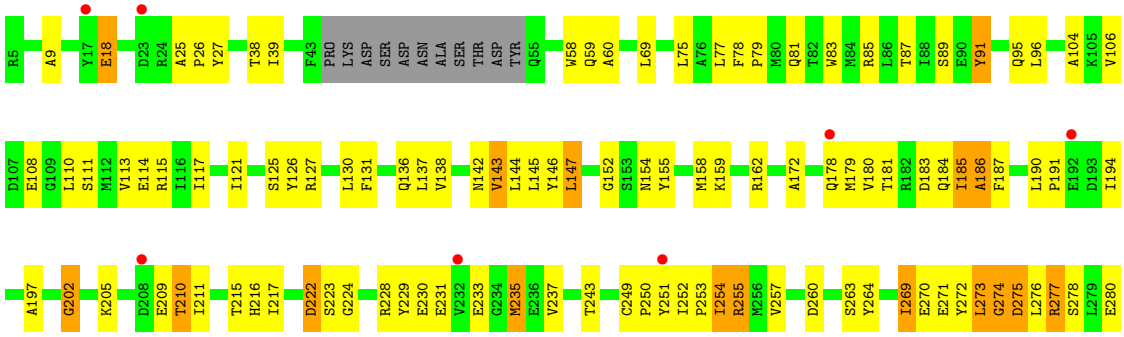
• Molecule 1: Portal protein

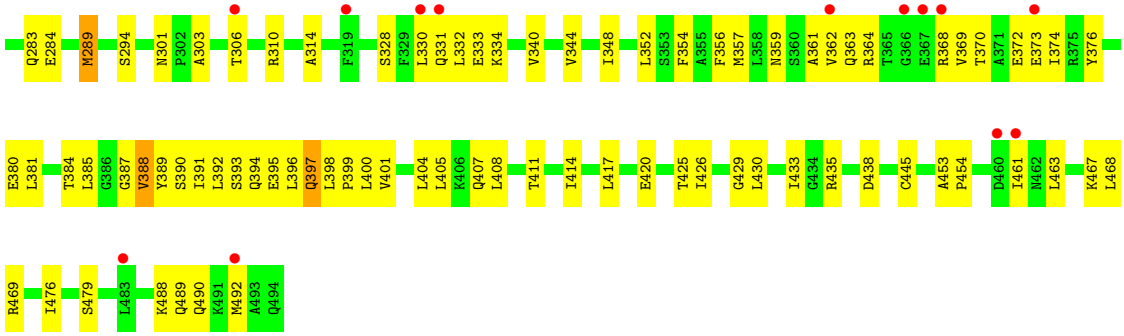
Chain E:



• Molecule 1: Portal protein

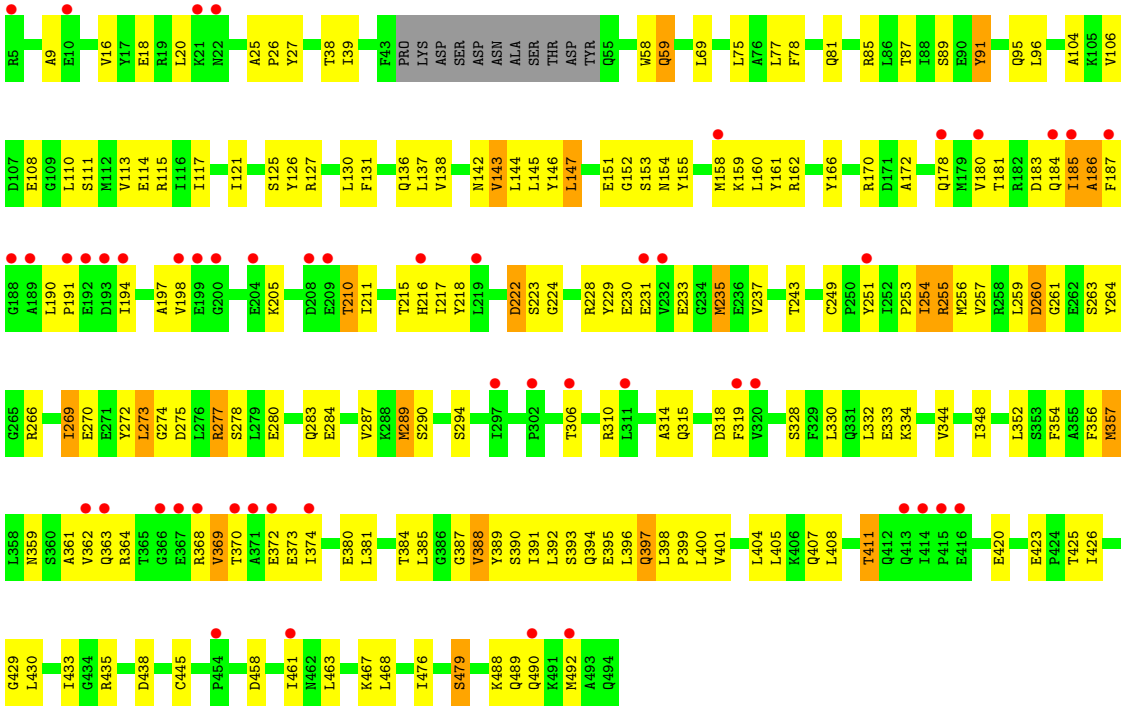
Chain F:





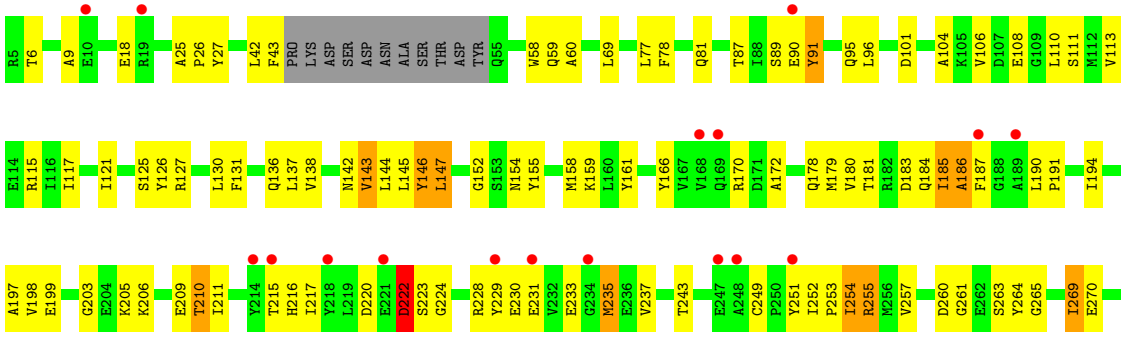
• Molecule 1: Portal protein

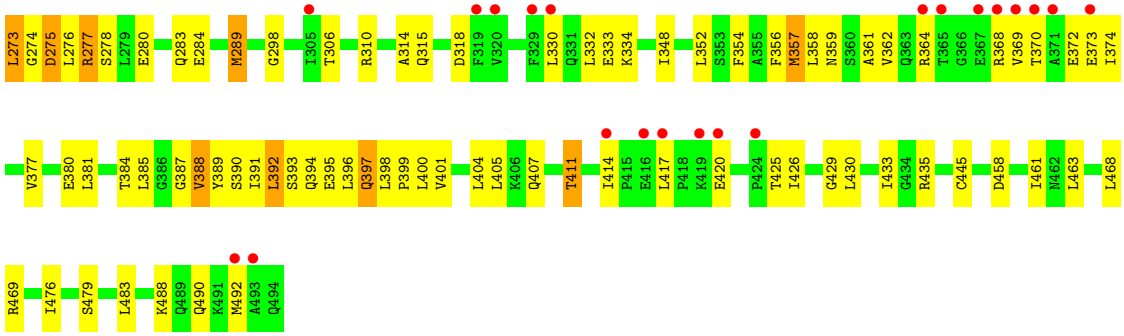
Chain G:



• Molecule 1: Portal protein

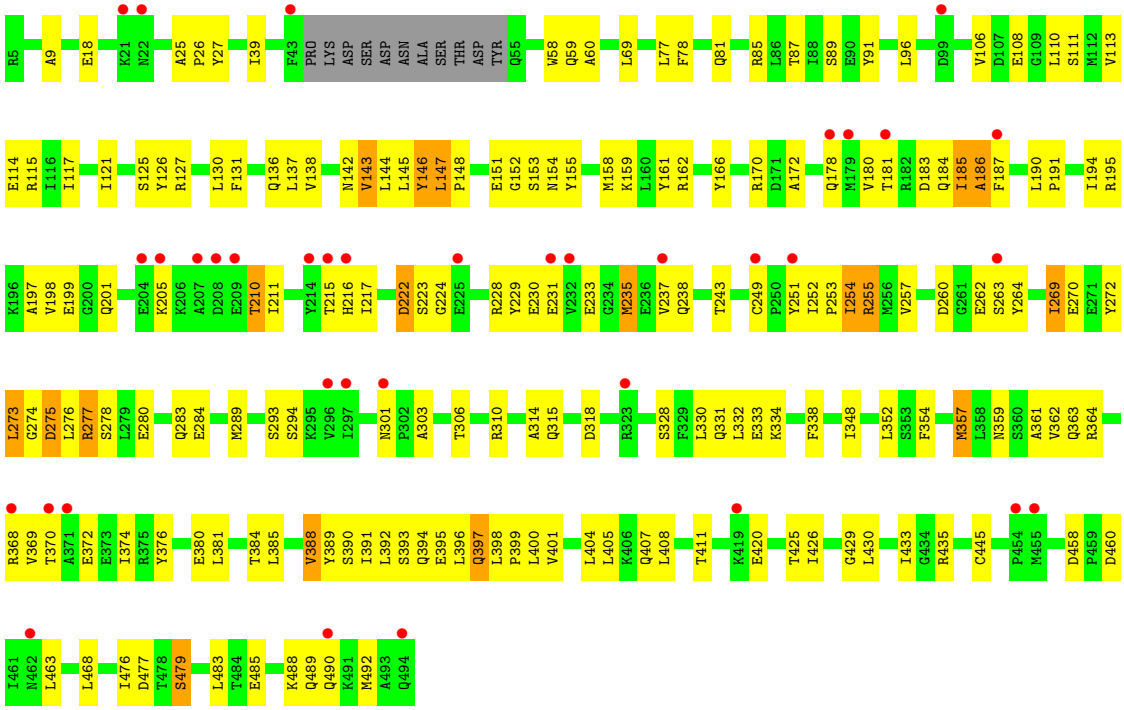
Chain H:





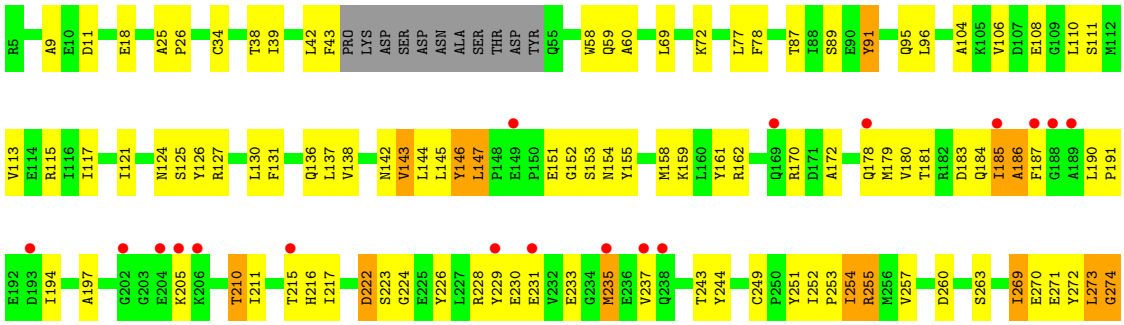
- Molecule 1: Portal protein

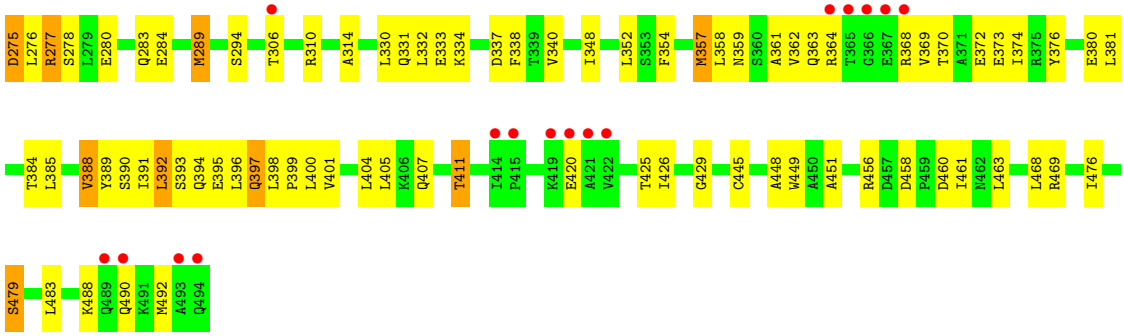
Chain I:



- Molecule 1: Portal protein

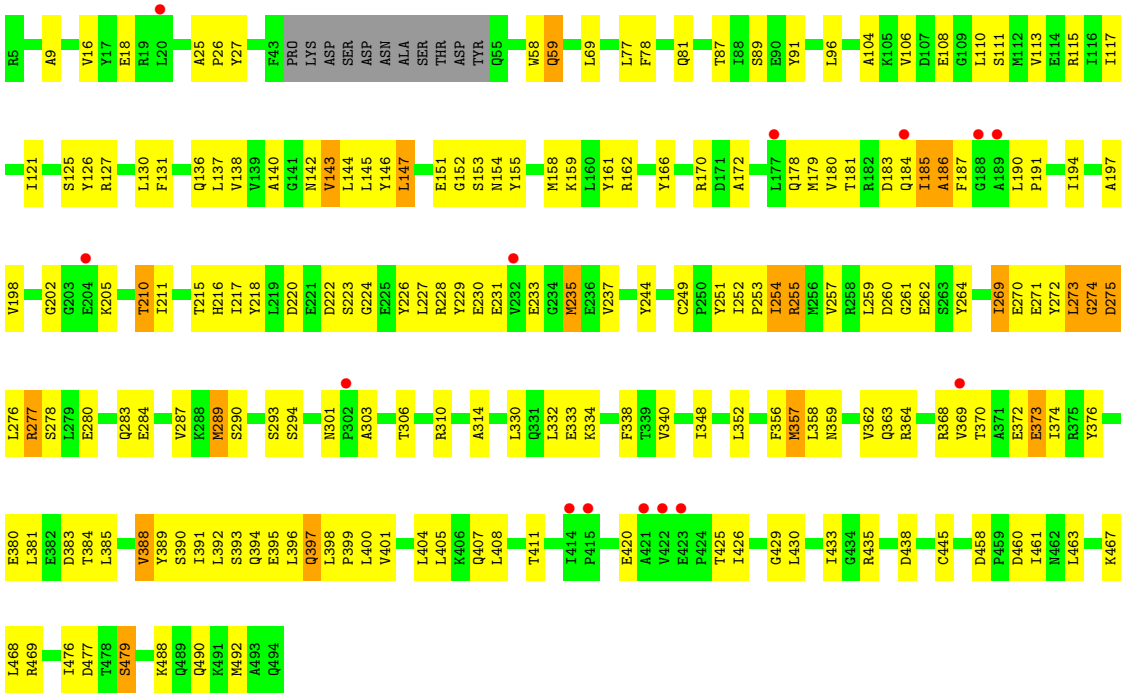
Chain J:





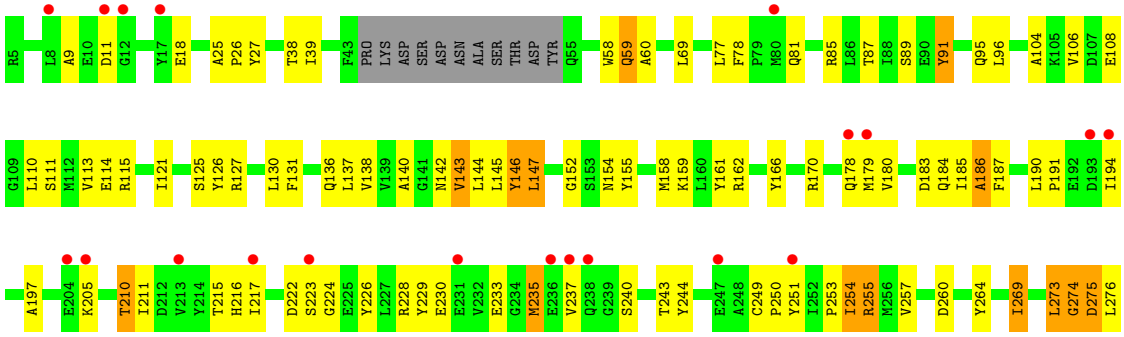
- Molecule 1: Portal protein

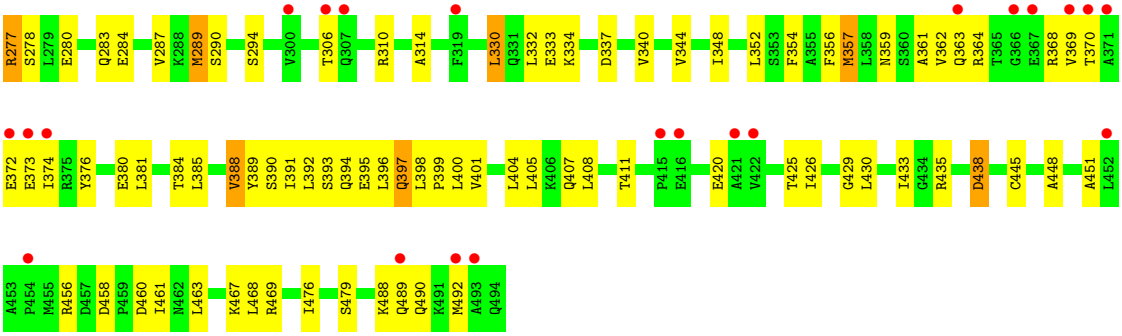
Chain K:



- Molecule 1: Portal protein

Chain L:




R277 S278 L279 E280 Q283 E284 V287 K288 M289 S290 S294 V300 T306 Q307 R310 A314 F319 L330 Q331 L332 E333 K334 D337 V340 V344 I348 L352 S353 F354 A355 F356 M357 L358 N359 S360 A361 V362 Q363 R364 T365 G366 E367 R368 V369 T370 A371
E372 E373 I374 R376 V376 E380 L381 T384 L385 V388 Y389 S390 I391 L392 S393 Q394 E395 L396 Q397 L398 P399 L400 V401 L404 L405 K406 Q407 L408 T411 P415 E416 E420 A421 V422 T425 I426 G429 L430 I433 G434 R435 D438 C445 A448 A451 L452
A453 P454 M455 R456 D457 D458 P459 D460 I461 M462 L463 K467 L468 R469 I476 S479 K488 Q489 Q490 K491 M492 A493 Q494

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	165.85Å 191.33Å 260.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.23 – 3.60 49.18 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.7 (49.23-3.60) 89.7 (49.18-3.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.284 , 0.334 0.283 , 0.327	Depositor DCC
R_{free} test set	4317 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	142.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 130.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	45048	wwPDB-VP
Average B, all atoms (Å^2)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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 (i)

5.1 Standard geometry (i)

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	0.69	0/3811	0.82	0/5156
1	B	0.69	0/3811	0.83	0/5156
1	C	0.70	0/3811	0.83	0/5156
1	D	0.69	0/3811	0.82	0/5156
1	E	0.69	0/3811	0.83	0/5156
1	F	0.69	0/3811	0.82	0/5156
1	G	0.69	0/3811	0.82	0/5156
1	H	0.69	0/3811	0.84	1/5156 (0.0%)
1	I	0.68	0/3811	0.82	0/5156
1	J	0.69	0/3811	0.82	0/5156
1	K	0.70	0/3811	0.82	0/5156
1	L	0.68	0/3811	0.82	0/5156
All	All	0.69	0/45732	0.82	1/61872 (0.0%)

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	2
1	F	0	1
1	H	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	222	ASP	OD1-CG-OD2	-12.15	100.22	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	GLY	Peptide
1	A	203	GLY	Peptide
1	F	202	GLY	Peptide
1	H	222	ASP	Sidechain

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	3754	0	3771	180	2
1	B	3754	0	3771	170	5
1	C	3754	0	3771	182	4
1	D	3754	0	3771	193	3
1	E	3754	0	3771	203	0
1	F	3754	0	3771	191	0
1	G	3754	0	3771	190	5
1	H	3754	0	3771	177	6
1	I	3754	0	3771	179	1
1	J	3754	0	3771	182	0
1	K	3754	0	3771	195	0
1	L	3754	0	3771	186	0
All	All	45048	0	45252	1971	13

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 22.

All (1971) 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:125:SER:HA	1:F:394:GLN:HE21	1.07	1.18
1:A:125:SER:HA	1:B:394:GLN:NE2	1.60	1.15
1:J:125:SER:HA	1:K:394:GLN:HE21	1.03	1.14
1:A:125:SER:HA	1:B:394:GLN:HE21	1.01	1.13
1:G:125:SER:HA	1:H:394:GLN:HE21	1.15	1.11
1:H:125:SER:HA	1:I:394:GLN:HE21	1.02	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:SER:HA	1:I:394:GLN:NE2	1.65	1.11
1:I:125:SER:HA	1:J:394:GLN:NE2	1.65	1.11
1:B:125:SER:HA	1:C:394:GLN:HE21	1.05	1.10
1:K:125:SER:HA	1:L:394:GLN:HE21	1.15	1.10
1:H:186:ALA:HA	1:H:210:THR:HA	1.34	1.10
1:A:394:GLN:HE21	1:L:125:SER:HA	1.17	1.08
1:D:125:SER:HA	1:E:394:GLN:HE21	0.91	1.07
1:K:186:ALA:HA	1:K:210:THR:HA	1.35	1.07
1:L:77:LEU:HD23	1:L:389:TYR:CE1	1.90	1.07
1:D:125:SER:HA	1:E:394:GLN:NE2	1.68	1.06
1:C:125:SER:HA	1:D:394:GLN:HE21	1.07	1.06
1:F:125:SER:HA	1:G:394:GLN:HE21	1.12	1.06
1:C:186:ALA:HA	1:C:210:THR:HA	1.37	1.06
1:D:186:ALA:HA	1:D:210:THR:HA	1.36	1.06
1:F:186:ALA:HA	1:F:210:THR:HA	1.35	1.06
1:E:186:ALA:HA	1:E:210:THR:HA	1.39	1.05
1:J:125:SER:HA	1:K:394:GLN:NE2	1.72	1.04
1:I:125:SER:HA	1:J:394:GLN:HE21	0.93	1.04
1:L:186:ALA:HA	1:L:210:THR:HA	1.37	1.04
1:G:186:ALA:HA	1:G:210:THR:HA	1.37	1.03
1:B:186:ALA:HA	1:B:210:THR:HA	1.39	1.03
1:J:186:ALA:HA	1:J:210:THR:HA	1.39	1.03
1:B:125:SER:HA	1:C:394:GLN:NE2	1.74	1.02
1:D:332:LEU:HD12	1:D:334:LYS:H	1.23	1.02
1:A:186:ALA:HA	1:A:210:THR:HA	1.37	1.02
1:C:332:LEU:HD12	1:C:334:LYS:H	1.24	1.02
1:I:186:ALA:HA	1:I:210:THR:HA	1.37	1.01
1:K:77:LEU:HD23	1:K:389:TYR:CE1	1.95	1.01
1:E:77:LEU:HD23	1:E:389:TYR:CE1	1.96	1.01
1:F:332:LEU:HD12	1:F:334:LYS:H	1.25	1.00
1:E:332:LEU:HD12	1:E:334:LYS:H	1.23	0.99
1:G:332:LEU:HD12	1:G:334:LYS:H	1.27	0.98
1:B:332:LEU:HD12	1:B:334:LYS:H	1.29	0.97
1:D:77:LEU:HD23	1:D:389:TYR:CE1	1.99	0.97
1:A:332:LEU:HD12	1:A:334:LYS:H	1.28	0.96
1:L:332:LEU:HD12	1:L:334:LYS:H	1.29	0.96
1:E:143:VAL:H	1:E:254:ILE:HD11	1.29	0.96
1:H:332:LEU:HD12	1:H:334:LYS:H	1.30	0.95
1:E:125:SER:HA	1:F:394:GLN:NE2	1.79	0.95
1:D:143:VAL:H	1:D:254:ILE:HD11	1.31	0.95
1:F:143:VAL:H	1:F:254:ILE:HD11	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:186:ALA:HA	1:H:210:THR:CA	1.95	0.95
1:C:125:SER:HA	1:D:394:GLN:NE2	1.81	0.95
1:F:125:SER:HA	1:G:394:GLN:NE2	1.82	0.95
1:G:143:VAL:H	1:G:254:ILE:HD11	1.32	0.94
1:K:332:LEU:HD12	1:K:334:LYS:H	1.28	0.94
1:J:143:VAL:H	1:J:254:ILE:HD11	1.30	0.94
1:L:395:GLU:O	1:L:399:PRO:HG2	1.66	0.94
1:F:77:LEU:HD23	1:F:389:TYR:CE1	2.02	0.94
1:G:77:LEU:HD23	1:G:389:TYR:CE1	2.01	0.94
1:K:125:SER:HA	1:L:394:GLN:NE2	1.82	0.94
1:H:77:LEU:HD23	1:H:389:TYR:CE1	2.02	0.94
1:A:395:GLU:O	1:A:399:PRO:HG2	1.67	0.93
1:C:77:LEU:HD23	1:C:389:TYR:CE1	2.02	0.93
1:H:143:VAL:H	1:H:254:ILE:HD11	1.34	0.93
1:I:332:LEU:HD12	1:I:334:LYS:H	1.31	0.93
1:B:77:LEU:HD23	1:B:389:TYR:CE1	2.03	0.93
1:D:186:ALA:HA	1:D:210:THR:CA	1.99	0.93
1:I:143:VAL:H	1:I:254:ILE:HD11	1.32	0.92
1:K:143:VAL:H	1:K:254:ILE:HD11	1.34	0.92
1:L:186:ALA:HA	1:L:210:THR:CA	1.99	0.92
1:F:186:ALA:HA	1:F:210:THR:CA	1.99	0.92
1:A:186:ALA:HA	1:A:210:THR:CA	1.98	0.92
1:K:186:ALA:HA	1:K:210:THR:CA	1.99	0.92
1:B:393:SER:O	1:B:397:GLN:HB2	1.70	0.91
1:G:186:ALA:HA	1:G:210:THR:CA	1.99	0.91
1:C:186:ALA:HA	1:C:210:THR:CA	1.99	0.91
1:F:269:ILE:O	1:F:269:ILE:HG22	1.70	0.91
1:J:332:LEU:HD12	1:J:334:LYS:H	1.34	0.91
1:K:395:GLU:O	1:K:399:PRO:HG2	1.71	0.91
1:L:143:VAL:H	1:L:254:ILE:HD11	1.33	0.91
1:B:186:ALA:HA	1:B:210:THR:CA	2.01	0.91
1:J:77:LEU:HD23	1:J:389:TYR:CE1	2.05	0.91
1:A:77:LEU:HD23	1:A:389:TYR:CE1	2.06	0.90
1:J:186:ALA:HA	1:J:210:THR:CA	2.01	0.90
1:C:143:VAL:H	1:C:254:ILE:HD11	1.37	0.90
1:A:394:GLN:NE2	1:L:125:SER:HA	1.87	0.90
1:I:186:ALA:HA	1:I:210:THR:CA	2.01	0.90
1:J:393:SER:O	1:J:397:GLN:HB2	1.71	0.90
1:D:395:GLU:O	1:D:399:PRO:HG2	1.72	0.90
1:L:393:SER:O	1:L:397:GLN:HB2	1.71	0.90
1:B:395:GLU:O	1:B:399:PRO:HG2	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:395:GLU:O	1:J:399:PRO:HG2	1.72	0.89
1:C:395:GLU:O	1:C:399:PRO:HG2	1.72	0.89
1:A:143:VAL:H	1:A:254:ILE:HD11	1.37	0.89
1:G:125:SER:HA	1:H:394:GLN:NE2	1.88	0.89
1:I:77:LEU:HD23	1:I:389:TYR:CE1	2.07	0.89
1:H:395:GLU:O	1:H:399:PRO:HG2	1.72	0.89
1:K:393:SER:O	1:K:397:GLN:HB2	1.73	0.88
1:G:393:SER:O	1:G:397:GLN:HB2	1.73	0.88
1:D:393:SER:O	1:D:397:GLN:HB2	1.74	0.88
1:G:269:ILE:HG22	1:G:269:ILE:O	1.72	0.88
1:E:395:GLU:O	1:E:399:PRO:HG2	1.73	0.87
1:E:186:ALA:HA	1:E:210:THR:CA	2.03	0.87
1:C:393:SER:O	1:C:397:GLN:HB2	1.72	0.87
1:L:401:VAL:HG11	1:L:426:ILE:HG21	1.57	0.87
1:F:395:GLU:O	1:F:399:PRO:HG2	1.74	0.87
1:K:269:ILE:O	1:K:269:ILE:HG22	1.74	0.86
1:F:401:VAL:HG11	1:F:426:ILE:HG21	1.58	0.86
1:L:395:GLU:O	1:L:399:PRO:CG	2.24	0.86
1:I:395:GLU:O	1:I:399:PRO:HG2	1.75	0.86
1:D:332:LEU:CD1	1:D:334:LYS:H	1.89	0.85
1:D:269:ILE:O	1:D:269:ILE:HG22	1.73	0.85
1:A:393:SER:O	1:A:397:GLN:HB2	1.77	0.85
1:E:269:ILE:HG22	1:E:269:ILE:O	1.76	0.85
1:E:332:LEU:HD13	1:E:334:LYS:HG2	1.58	0.85
1:F:393:SER:O	1:F:397:GLN:HB2	1.77	0.85
1:E:401:VAL:HG11	1:E:426:ILE:HG21	1.58	0.85
1:B:143:VAL:H	1:B:254:ILE:HD11	1.41	0.85
1:I:401:VAL:HG11	1:I:426:ILE:HG21	1.58	0.85
1:F:332:LEU:HD13	1:F:334:LYS:HG2	1.59	0.84
1:D:401:VAL:HG11	1:D:426:ILE:HG21	1.60	0.84
1:A:395:GLU:O	1:A:399:PRO:CG	2.25	0.84
1:A:401:VAL:HG11	1:A:426:ILE:HG21	1.59	0.84
1:I:393:SER:O	1:I:397:GLN:HB2	1.77	0.84
1:H:186:ALA:CA	1:H:210:THR:HA	2.07	0.84
1:G:187:PHE:CD2	1:G:205:LYS:HB2	2.13	0.84
1:I:269:ILE:O	1:I:269:ILE:HG22	1.77	0.84
1:L:269:ILE:O	1:L:269:ILE:HG22	1.78	0.83
1:E:332:LEU:CD1	1:E:334:LYS:H	1.90	0.83
1:F:332:LEU:CD1	1:F:334:LYS:H	1.91	0.83
1:D:332:LEU:HD13	1:D:334:LYS:HG2	1.61	0.83
1:J:269:ILE:HG22	1:J:269:ILE:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:401:VAL:HG11	1:K:426:ILE:HG21	1.58	0.83
1:H:393:SER:O	1:H:397:GLN:HB2	1.77	0.83
1:C:269:ILE:O	1:C:269:ILE:HG22	1.78	0.82
1:H:401:VAL:HG11	1:H:426:ILE:HG21	1.59	0.82
1:H:269:ILE:O	1:H:269:ILE:HG22	1.78	0.82
1:B:269:ILE:HG22	1:B:269:ILE:O	1.78	0.82
1:C:332:LEU:HD13	1:C:334:LYS:HG2	1.61	0.82
1:G:401:VAL:HG11	1:G:426:ILE:HG21	1.62	0.82
1:E:393:SER:O	1:E:397:GLN:HB2	1.78	0.82
1:A:269:ILE:O	1:A:269:ILE:HG22	1.79	0.81
1:D:186:ALA:CA	1:D:210:THR:HA	2.10	0.81
1:K:186:ALA:CA	1:K:210:THR:HA	2.10	0.81
1:F:186:ALA:CA	1:F:210:THR:HA	2.09	0.81
1:G:186:ALA:CA	1:G:210:THR:HA	2.10	0.81
1:K:395:GLU:O	1:K:399:PRO:CG	2.28	0.81
1:E:187:PHE:CD2	1:E:205:LYS:HB2	2.15	0.81
1:I:186:ALA:CA	1:I:210:THR:HA	2.10	0.81
1:K:332:LEU:CD1	1:K:334:LYS:H	1.93	0.81
1:C:401:VAL:HG11	1:C:426:ILE:HG21	1.63	0.81
1:B:332:LEU:HD13	1:B:334:LYS:HG2	1.61	0.81
1:G:332:LEU:HD13	1:G:334:LYS:HG2	1.60	0.81
1:G:395:GLU:O	1:G:399:PRO:HG2	1.79	0.81
1:C:332:LEU:CD1	1:C:334:LYS:H	1.93	0.80
1:G:332:LEU:CD1	1:G:334:LYS:H	1.93	0.80
1:L:186:ALA:CA	1:L:210:THR:HA	2.10	0.80
1:D:395:GLU:O	1:D:399:PRO:CG	2.30	0.80
1:L:332:LEU:CD1	1:L:334:LYS:H	1.95	0.80
1:C:186:ALA:CA	1:C:210:THR:HA	2.11	0.80
1:J:401:VAL:HG11	1:J:426:ILE:HG21	1.64	0.80
1:L:332:LEU:HD13	1:L:334:LYS:HG2	1.64	0.80
1:E:187:PHE:CE2	1:E:205:LYS:HB2	2.16	0.80
1:H:332:LEU:CD1	1:H:334:LYS:H	1.95	0.80
1:A:332:LEU:CD1	1:A:334:LYS:H	1.95	0.79
1:A:186:ALA:CA	1:A:210:THR:HA	2.10	0.79
1:E:186:ALA:CA	1:E:210:THR:HA	2.12	0.79
1:B:186:ALA:CA	1:B:210:THR:HA	2.13	0.79
1:H:332:LEU:HD13	1:H:334:LYS:HG2	1.64	0.79
1:A:332:LEU:HD13	1:A:334:LYS:HG2	1.64	0.79
1:B:332:LEU:CD1	1:B:334:LYS:H	1.95	0.79
1:K:332:LEU:HD13	1:K:334:LYS:HG2	1.65	0.78
1:J:186:ALA:CA	1:J:210:THR:HA	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLU:O	1:B:399:PRO:CG	2.32	0.78
1:H:395:GLU:O	1:H:399:PRO:CG	2.31	0.78
1:B:401:VAL:HG11	1:B:426:ILE:HG21	1.64	0.78
1:J:395:GLU:O	1:J:399:PRO:CG	2.30	0.77
1:K:332:LEU:HD12	1:K:333:GLU:N	1.99	0.77
1:H:230:GLU:HB2	1:H:237:VAL:HG21	1.67	0.77
1:A:230:GLU:HB2	1:A:237:VAL:CG2	2.15	0.77
1:J:230:GLU:HB2	1:J:237:VAL:CG2	2.14	0.77
1:K:230:GLU:HB2	1:K:237:VAL:HG21	1.66	0.77
1:A:230:GLU:HB2	1:A:237:VAL:HG21	1.66	0.77
1:I:332:LEU:HD13	1:I:334:LYS:HG2	1.65	0.77
1:D:230:GLU:HB2	1:D:237:VAL:HG21	1.67	0.76
1:L:230:GLU:HB2	1:L:237:VAL:HG21	1.67	0.76
1:J:230:GLU:HB2	1:J:237:VAL:HG21	1.65	0.76
1:C:395:GLU:O	1:C:399:PRO:CG	2.34	0.76
1:I:332:LEU:CD1	1:I:334:LYS:H	1.98	0.76
1:G:230:GLU:HB2	1:G:237:VAL:CG2	2.16	0.76
1:B:230:GLU:HB2	1:B:237:VAL:HG21	1.67	0.76
1:I:395:GLU:O	1:I:399:PRO:CG	2.32	0.76
1:B:230:GLU:HB2	1:B:237:VAL:CG2	2.16	0.76
1:K:230:GLU:HB2	1:K:237:VAL:CG2	2.16	0.76
1:G:187:PHE:CE2	1:G:205:LYS:HB2	2.21	0.76
1:F:230:GLU:HB2	1:F:237:VAL:HG21	1.68	0.75
1:H:230:GLU:HB2	1:H:237:VAL:CG2	2.16	0.75
1:E:395:GLU:O	1:E:399:PRO:CG	2.35	0.75
1:C:230:GLU:HB2	1:C:237:VAL:HG21	1.69	0.75
1:D:131:PHE:CG	1:E:391:ILE:HD11	2.22	0.75
1:J:332:LEU:HD13	1:J:334:LYS:HG2	1.67	0.75
1:E:131:PHE:CG	1:F:391:ILE:HD11	2.21	0.75
1:D:230:GLU:HB2	1:D:237:VAL:CG2	2.16	0.75
1:A:131:PHE:CG	1:B:391:ILE:HD11	2.22	0.74
1:F:230:GLU:HB2	1:F:237:VAL:CG2	2.18	0.74
1:G:230:GLU:HB2	1:G:237:VAL:HG21	1.67	0.74
1:C:230:GLU:HB2	1:C:237:VAL:CG2	2.17	0.74
1:G:127:ARG:HH12	1:H:394:GLN:HB2	1.53	0.74
1:I:187:PHE:CD2	1:I:205:LYS:HB2	2.23	0.74
1:L:230:GLU:HB2	1:L:237:VAL:CG2	2.17	0.74
1:J:332:LEU:CD1	1:J:334:LYS:H	2.00	0.74
1:H:384:THR:O	1:H:388:VAL:HG12	1.88	0.74
1:J:332:LEU:HD12	1:J:333:GLU:N	2.02	0.74
1:K:332:LEU:HD12	1:K:332:LEU:C	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:GLU:HB2	1:E:237:VAL:HG21	1.70	0.73
1:I:230:GLU:HB2	1:I:237:VAL:CG2	2.18	0.73
1:E:143:VAL:N	1:E:254:ILE:HD11	2.03	0.73
1:I:230:GLU:HB2	1:I:237:VAL:HG21	1.69	0.73
1:D:332:LEU:HD12	1:D:332:LEU:C	2.09	0.73
1:H:332:LEU:HD12	1:H:333:GLU:N	2.03	0.73
1:J:332:LEU:HD12	1:J:332:LEU:C	2.09	0.73
1:A:332:LEU:HD12	1:A:333:GLU:N	2.04	0.73
1:D:332:LEU:HD12	1:D:334:LYS:N	2.03	0.73
1:G:58:TRP:CD1	1:G:284:GLU:OE1	2.42	0.72
1:F:395:GLU:O	1:F:399:PRO:CG	2.36	0.72
1:F:159:LYS:HD3	1:G:172:ALA:O	1.89	0.72
1:I:58:TRP:CD1	1:I:284:GLU:OE1	2.42	0.72
1:F:269:ILE:O	1:F:269:ILE:CG2	2.38	0.72
1:F:332:LEU:HD12	1:F:333:GLU:N	2.04	0.72
1:E:230:GLU:HB2	1:E:237:VAL:CG2	2.20	0.72
1:F:143:VAL:N	1:F:254:ILE:HD11	2.04	0.72
1:K:395:GLU:O	1:K:399:PRO:CD	2.37	0.72
1:L:395:GLU:O	1:L:399:PRO:CD	2.37	0.72
1:H:332:LEU:HD12	1:H:332:LEU:C	2.09	0.72
1:I:332:LEU:HD12	1:I:333:GLU:N	2.05	0.72
1:L:357:MET:CE	1:L:384:THR:OG1	2.38	0.72
1:L:332:LEU:HD12	1:L:333:GLU:N	2.04	0.72
1:B:332:LEU:HD12	1:B:333:GLU:N	2.05	0.71
1:E:332:LEU:HD12	1:E:333:GLU:N	2.05	0.71
1:B:58:TRP:CD1	1:B:284:GLU:OE1	2.43	0.71
1:B:273:LEU:HD23	1:B:273:LEU:C	2.11	0.71
1:D:357:MET:CE	1:D:384:THR:OG1	2.39	0.71
1:J:384:THR:O	1:J:388:VAL:HG12	1.90	0.71
1:A:138:VAL:HG12	1:A:269:ILE:HD12	1.73	0.71
1:D:332:LEU:HD12	1:D:333:GLU:N	2.04	0.71
1:H:186:ALA:HA	1:H:210:THR:N	2.05	0.71
1:C:332:LEU:HD12	1:C:332:LEU:C	2.12	0.70
1:E:332:LEU:HD12	1:E:334:LYS:N	2.04	0.70
1:G:127:ARG:NH1	1:H:394:GLN:HB2	2.06	0.70
1:G:384:THR:O	1:G:388:VAL:HG12	1.91	0.70
1:L:143:VAL:N	1:L:254:ILE:HD11	2.05	0.70
1:A:186:ALA:HA	1:A:210:THR:N	2.07	0.70
1:A:332:LEU:HD12	1:A:332:LEU:C	2.12	0.70
1:I:58:TRP:CG	1:I:284:GLU:HB2	2.26	0.70
1:I:332:LEU:HD12	1:I:332:LEU:C	2.12	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:LYS:HD3	1:H:172:ALA:O	1.91	0.69
1:J:143:VAL:N	1:J:254:ILE:HD11	2.05	0.69
1:D:143:VAL:N	1:D:254:ILE:HD11	2.06	0.69
1:G:357:MET:CE	1:G:384:THR:OG1	2.40	0.69
1:I:143:VAL:N	1:I:254:ILE:HD11	2.07	0.69
1:A:395:GLU:O	1:A:399:PRO:CD	2.40	0.69
1:D:395:GLU:O	1:D:399:PRO:CD	2.40	0.69
1:F:384:THR:O	1:F:388:VAL:HG12	1.93	0.69
1:G:395:GLU:O	1:G:399:PRO:CG	2.41	0.69
1:H:138:VAL:HG12	1:H:269:ILE:HD12	1.74	0.69
1:B:332:LEU:HD12	1:B:332:LEU:C	2.13	0.69
1:B:357:MET:HE3	1:B:384:THR:OG1	1.92	0.69
1:B:357:MET:CE	1:B:384:THR:OG1	2.41	0.69
1:L:186:ALA:HA	1:L:210:THR:N	2.07	0.69
1:F:332:LEU:HD12	1:F:332:LEU:C	2.13	0.69
1:K:138:VAL:HG12	1:K:269:ILE:HD12	1.75	0.69
1:K:368:ARG:NE	1:L:368:ARG:O	2.25	0.69
1:L:332:LEU:HD12	1:L:332:LEU:C	2.14	0.69
1:C:294:SER:HA	1:D:289:MET:HE1	1.75	0.68
1:F:186:ALA:HA	1:F:210:THR:N	2.08	0.68
1:G:332:LEU:HD12	1:G:333:GLU:N	2.08	0.68
1:H:131:PHE:CG	1:I:391:ILE:HD11	2.28	0.68
1:H:143:VAL:N	1:H:254:ILE:HD11	2.08	0.68
1:G:186:ALA:HA	1:G:210:THR:N	2.08	0.68
1:H:395:GLU:O	1:H:399:PRO:CD	2.42	0.68
1:I:138:VAL:HG12	1:I:269:ILE:HD12	1.75	0.68
1:B:131:PHE:CG	1:C:391:ILE:HD11	2.28	0.68
1:C:332:LEU:HD12	1:C:333:GLU:N	2.08	0.68
1:D:58:TRP:CD1	1:D:284:GLU:OE1	2.47	0.68
1:E:332:LEU:HD12	1:E:332:LEU:C	2.14	0.68
1:I:395:GLU:O	1:I:399:PRO:CD	2.41	0.68
1:K:58:TRP:CD1	1:K:284:GLU:OE1	2.46	0.68
1:E:394:GLN:HA	1:E:398:LEU:HD23	1.76	0.68
1:F:131:PHE:CG	1:G:391:ILE:HD11	2.27	0.68
1:C:187:PHE:CD2	1:C:205:LYS:HB2	2.29	0.68
1:D:159:LYS:NZ	1:E:260:ASP:O	2.26	0.68
1:C:384:THR:O	1:C:388:VAL:HG12	1.94	0.68
1:F:332:LEU:HD12	1:F:334:LYS:N	2.05	0.68
1:I:357:MET:CE	1:I:384:THR:OG1	2.42	0.68
1:C:332:LEU:HD12	1:C:334:LYS:N	2.05	0.68
1:K:394:GLN:HA	1:K:398:LEU:HD23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:TYR:CE1	1:B:157:PRO:HB3	2.28	0.68
1:B:187:PHE:CE2	1:B:205:LYS:HB2	2.29	0.68
1:D:186:ALA:HA	1:D:210:THR:N	2.08	0.67
1:L:357:MET:HE3	1:L:384:THR:OG1	1.93	0.67
1:L:394:GLN:HA	1:L:398:LEU:HD23	1.76	0.67
1:C:186:ALA:HA	1:C:210:THR:N	2.08	0.67
1:G:143:VAL:N	1:G:254:ILE:HD11	2.06	0.67
1:J:395:GLU:O	1:J:399:PRO:CD	2.42	0.67
1:K:363:GLN:HB3	1:L:373:GLU:OE1	1.95	0.67
1:G:273:LEU:HD23	1:G:273:LEU:C	2.15	0.67
1:H:273:LEU:HD23	1:H:273:LEU:C	2.15	0.67
1:I:131:PHE:CG	1:J:391:ILE:HD11	2.29	0.67
1:J:131:PHE:CG	1:K:391:ILE:HD11	2.29	0.67
1:D:138:VAL:HG12	1:D:269:ILE:HD12	1.76	0.67
1:E:368:ARG:NE	1:F:368:ARG:O	2.25	0.67
1:D:287:VAL:O	1:D:290:SER:OG	2.12	0.67
1:A:203:GLY:HA3	1:A:205:LYS:HD3	1.77	0.67
1:E:58:TRP:CD1	1:E:284:GLU:OE1	2.47	0.67
1:E:269:ILE:O	1:E:269:ILE:CG2	2.42	0.67
1:K:186:ALA:HA	1:K:210:THR:N	2.09	0.67
1:K:384:THR:O	1:K:388:VAL:HG12	1.95	0.67
1:G:58:TRP:CG	1:G:284:GLU:HB2	2.28	0.66
1:K:187:PHE:CE2	1:K:205:LYS:HB2	2.30	0.66
1:K:357:MET:CE	1:K:384:THR:OG1	2.43	0.66
1:I:186:ALA:HA	1:I:210:THR:N	2.10	0.66
1:F:127:ARG:HH12	1:G:394:GLN:HB2	1.61	0.66
1:H:58:TRP:CG	1:H:284:GLU:HB2	2.31	0.66
1:J:186:ALA:HA	1:J:210:THR:N	2.10	0.66
1:A:391:ILE:HD11	1:L:131:PHE:CG	2.31	0.66
1:E:186:ALA:HA	1:E:210:THR:N	2.11	0.66
1:B:186:ALA:HA	1:B:210:THR:N	2.09	0.66
1:F:187:PHE:CE2	1:F:205:LYS:HB2	2.31	0.66
1:A:368:ARG:O	1:L:368:ARG:NE	2.25	0.66
1:L:138:VAL:HG12	1:L:269:ILE:HD12	1.77	0.66
1:L:77:LEU:CD2	1:L:389:TYR:CE1	2.72	0.66
1:D:159:LYS:HD3	1:E:172:ALA:O	1.95	0.66
1:A:143:VAL:N	1:A:254:ILE:HD11	2.10	0.65
1:A:394:GLN:HA	1:A:398:LEU:HD23	1.78	0.65
1:B:138:VAL:HG12	1:B:269:ILE:HD12	1.77	0.65
1:B:395:GLU:O	1:B:399:PRO:CD	2.44	0.65
1:H:58:TRP:CD1	1:H:284:GLU:OE1	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:143:VAL:N	1:K:254:ILE:HD11	2.08	0.65
1:C:138:VAL:HG12	1:C:269:ILE:HD12	1.77	0.65
1:F:138:VAL:HG12	1:F:269:ILE:HD12	1.78	0.65
1:J:58:TRP:CD1	1:J:284:GLU:OE1	2.49	0.65
1:K:269:ILE:O	1:K:269:ILE:CG2	2.43	0.65
1:F:127:ARG:NH1	1:G:394:GLN:HB2	2.11	0.65
1:G:368:ARG:NE	1:H:368:ARG:O	2.25	0.65
1:I:273:LEU:C	1:I:273:LEU:HD23	2.16	0.65
1:K:77:LEU:CD2	1:K:389:TYR:CE1	2.78	0.65
1:I:384:THR:O	1:I:388:VAL:HG12	1.95	0.65
1:L:384:THR:O	1:L:388:VAL:HG12	1.95	0.65
1:D:269:ILE:O	1:D:269:ILE:CG2	2.40	0.65
1:E:159:LYS:HD3	1:F:172:ALA:O	1.96	0.65
1:B:145:LEU:HB3	1:B:158:MET:HE2	1.77	0.65
1:D:394:GLN:HA	1:D:398:LEU:HD23	1.78	0.65
1:G:357:MET:HE3	1:G:384:THR:OG1	1.95	0.65
1:A:394:GLN:HB2	1:L:127:ARG:HH12	1.61	0.65
1:G:138:VAL:HG12	1:G:269:ILE:HD12	1.78	0.65
1:G:332:LEU:HD12	1:G:332:LEU:C	2.17	0.65
1:I:187:PHE:CE2	1:I:205:LYS:HB2	2.32	0.65
1:J:138:VAL:HG12	1:J:269:ILE:HD12	1.78	0.65
1:L:136:GLN:NE2	1:L:162:ARG:HD2	2.11	0.65
1:H:357:MET:CE	1:H:384:THR:OG1	2.45	0.65
1:H:394:GLN:HA	1:H:398:LEU:HD23	1.77	0.65
1:D:58:TRP:CG	1:D:284:GLU:HB2	2.32	0.65
1:D:273:LEU:C	1:D:273:LEU:HD23	2.17	0.65
1:G:394:GLN:HA	1:G:398:LEU:HD23	1.78	0.65
1:C:273:LEU:HD23	1:C:273:LEU:C	2.17	0.64
1:L:269:ILE:O	1:L:269:ILE:CG2	2.45	0.64
1:L:58:TRP:CD1	1:L:284:GLU:OE1	2.51	0.64
1:L:273:LEU:C	1:L:273:LEU:HD23	2.17	0.64
1:A:384:THR:O	1:A:388:VAL:HG12	1.97	0.64
1:C:269:ILE:O	1:C:269:ILE:CG2	2.46	0.64
1:C:357:MET:CE	1:C:384:THR:OG1	2.46	0.64
1:E:77:LEU:CD2	1:E:389:TYR:CE1	2.78	0.64
1:L:394:GLN:O	1:L:398:LEU:HD23	1.97	0.64
1:J:187:PHE:CE2	1:J:205:LYS:HB2	2.33	0.64
1:A:357:MET:CE	1:A:384:THR:OG1	2.46	0.64
1:C:187:PHE:CE2	1:C:205:LYS:HB2	2.32	0.64
1:E:127:ARG:HH12	1:F:394:GLN:HB2	1.63	0.64
1:E:273:LEU:HD23	1:E:273:LEU:C	2.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:394:GLN:HA	1:J:398:LEU:HD23	1.80	0.64
1:K:332:LEU:HD12	1:K:334:LYS:N	2.08	0.64
1:A:273:LEU:C	1:A:273:LEU:HD23	2.18	0.64
1:C:143:VAL:N	1:C:254:ILE:HD11	2.10	0.64
1:E:331:GLN:HE22	1:F:334:LYS:HA	1.62	0.64
1:J:273:LEU:HD23	1:J:273:LEU:C	2.19	0.64
1:K:145:LEU:HB3	1:K:158:MET:HE2	1.80	0.64
1:A:394:GLN:HB2	1:L:127:ARG:NH1	2.13	0.64
1:C:58:TRP:CG	1:C:284:GLU:HB2	2.33	0.63
1:D:359:ASN:OD1	1:E:380:GLU:HB2	1.98	0.63
1:F:145:LEU:HB3	1:F:158:MET:HE2	1.79	0.63
1:L:344:VAL:O	1:L:348:ILE:HD12	1.98	0.63
1:F:394:GLN:HA	1:F:398:LEU:HD23	1.79	0.63
1:I:294:SER:HA	1:J:289:MET:HE1	1.79	0.63
1:L:191:PRO:HD2	1:L:194:ILE:HD11	1.80	0.63
1:D:357:MET:HE3	1:D:384:THR:OG1	1.96	0.63
1:A:172:ALA:O	1:L:159:LYS:HD3	1.98	0.63
1:E:127:ARG:NH1	1:F:394:GLN:HB2	2.13	0.63
1:G:488:LYS:O	1:G:492:MET:HG2	1.98	0.63
1:B:187:PHE:CD2	1:B:205:LYS:HB2	2.34	0.63
1:E:58:TRP:CG	1:E:284:GLU:HB2	2.33	0.63
1:I:394:GLN:HA	1:I:398:LEU:HD23	1.80	0.63
1:K:197:ALA:O	1:K:235:MET:HE1	1.99	0.63
1:D:191:PRO:HD2	1:D:194:ILE:HD11	1.80	0.63
1:A:138:VAL:CG1	1:A:269:ILE:CD1	2.77	0.62
1:G:269:ILE:O	1:G:269:ILE:CG2	2.41	0.62
1:A:357:MET:HE3	1:A:384:THR:OG1	1.98	0.62
1:C:191:PRO:HD2	1:C:194:ILE:HD11	1.81	0.62
1:J:310:ARG:O	1:J:314:ALA:HB2	1.99	0.62
1:C:310:ARG:O	1:C:314:ALA:HB2	1.99	0.62
1:A:332:LEU:HD12	1:A:334:LYS:N	2.08	0.62
1:A:488:LYS:O	1:A:492:MET:HG2	1.99	0.62
1:B:394:GLN:HA	1:B:398:LEU:HD23	1.81	0.62
1:I:357:MET:HE2	1:I:384:THR:OG1	1.99	0.62
1:K:58:TRP:CG	1:K:284:GLU:HB2	2.35	0.62
1:G:131:PHE:CG	1:H:391:ILE:HD11	2.34	0.62
1:L:310:ARG:O	1:L:314:ALA:HB2	2.00	0.62
1:A:145:LEU:HB3	1:A:158:MET:CE	2.30	0.62
1:D:145:LEU:HB3	1:D:158:MET:HE2	1.82	0.62
1:F:222:ASP:OD1	1:F:223:SER:N	2.31	0.62
1:K:202:GLY:O	1:K:205:LYS:HD3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLN:HB3	1:B:283:GLN:HG2	1.81	0.62
1:G:332:LEU:HD12	1:G:334:LYS:N	2.08	0.62
1:J:58:TRP:CG	1:J:284:GLU:HB2	2.34	0.62
1:K:191:PRO:HD2	1:K:194:ILE:HD11	1.82	0.62
1:E:138:VAL:HG12	1:E:269:ILE:HD12	1.81	0.62
1:G:467:LYS:NZ	1:H:461:ILE:HD11	2.14	0.62
1:D:384:THR:O	1:D:388:VAL:HG12	1.99	0.61
1:K:301:ASN:HD21	1:K:303:ALA:HB3	1.65	0.61
1:F:357:MET:CE	1:F:384:THR:OG1	2.47	0.61
1:L:187:PHE:CD2	1:L:205:LYS:HB2	2.34	0.61
1:B:269:ILE:O	1:B:269:ILE:CG2	2.46	0.61
1:E:191:PRO:HD2	1:E:194:ILE:HD11	1.82	0.61
1:F:58:TRP:CD1	1:F:284:GLU:OE1	2.54	0.61
1:F:145:LEU:HB3	1:F:158:MET:CE	2.31	0.61
1:K:145:LEU:HB3	1:K:158:MET:CE	2.30	0.61
1:B:145:LEU:HB3	1:B:158:MET:CE	2.30	0.61
1:B:332:LEU:HD12	1:B:334:LYS:N	2.09	0.61
1:G:191:PRO:HD2	1:G:194:ILE:HD11	1.82	0.61
1:L:254:ILE:HD12	1:L:254:ILE:O	2.01	0.61
1:F:488:LYS:O	1:F:492:MET:HG2	2.01	0.61
1:G:145:LEU:HB3	1:G:158:MET:CE	2.31	0.61
1:I:191:PRO:HD2	1:I:194:ILE:HD11	1.82	0.61
1:L:58:TRP:CG	1:L:284:GLU:HB2	2.35	0.61
1:A:191:PRO:HD2	1:A:194:ILE:HD11	1.82	0.61
1:L:407:GLN:O	1:L:411:THR:HG23	2.01	0.61
1:C:394:GLN:HA	1:C:398:LEU:HD23	1.81	0.61
1:F:58:TRP:CG	1:F:284:GLU:HB2	2.35	0.61
1:G:359:ASN:OD1	1:H:380:GLU:HB2	2.00	0.61
1:F:273:LEU:HD23	1:F:273:LEU:C	2.21	0.61
1:H:269:ILE:O	1:H:269:ILE:CG2	2.47	0.61
1:H:332:LEU:HD12	1:H:334:LYS:N	2.10	0.61
1:A:310:ARG:O	1:A:314:ALA:HB2	2.00	0.61
1:F:191:PRO:HD2	1:F:194:ILE:HD11	1.81	0.61
1:J:222:ASP:OD1	1:J:223:SER:N	2.33	0.61
1:L:187:PHE:CE2	1:L:205:LYS:HB2	2.35	0.61
1:A:269:ILE:O	1:A:269:ILE:CG2	2.47	0.60
1:B:310:ARG:O	1:B:314:ALA:HB2	2.01	0.60
1:D:393:SER:OG	1:D:397:GLN:NE2	2.33	0.60
1:H:138:VAL:CG1	1:H:269:ILE:CD1	2.78	0.60
1:B:143:VAL:N	1:B:254:ILE:HD11	2.13	0.60
1:H:191:PRO:HD2	1:H:194:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:138:VAL:CG1	1:K:269:ILE:CD1	2.79	0.60
1:B:58:TRP:CG	1:B:284:GLU:HB2	2.36	0.60
1:C:488:LYS:O	1:C:492:MET:HG2	2.02	0.60
1:E:187:PHE:CD2	1:E:205:LYS:CB	2.84	0.60
1:D:77:LEU:CD2	1:D:389:TYR:CE1	2.80	0.60
1:E:488:LYS:O	1:E:492:MET:HG2	2.02	0.60
1:F:106:VAL:O	1:F:110:LEU:HD12	2.01	0.60
1:J:269:ILE:O	1:J:269:ILE:CG2	2.45	0.60
1:E:332:LEU:O	1:E:333:GLU:HG2	2.02	0.60
1:K:136:GLN:NE2	1:K:162:ARG:HD2	2.16	0.60
1:K:394:GLN:O	1:K:398:LEU:HD23	2.02	0.60
1:H:488:LYS:O	1:H:492:MET:HG2	2.01	0.60
1:I:138:VAL:CG1	1:I:269:ILE:CD1	2.79	0.60
1:J:191:PRO:HD2	1:J:194:ILE:HD11	1.83	0.60
1:K:357:MET:HE1	1:K:384:THR:OG1	2.02	0.60
1:K:310:ARG:O	1:K:314:ALA:HB2	2.02	0.60
1:B:191:PRO:HD2	1:B:194:ILE:HD11	1.84	0.59
1:F:332:LEU:O	1:F:333:GLU:HG2	2.02	0.59
1:C:145:LEU:HB3	1:C:158:MET:CE	2.31	0.59
1:I:269:ILE:O	1:I:269:ILE:CG2	2.46	0.59
1:A:331:GLN:HE22	1:B:334:LYS:HA	1.66	0.59
1:C:58:TRP:CD1	1:C:284:GLU:OE1	2.55	0.59
1:F:159:LYS:NZ	1:G:260:ASP:O	2.34	0.59
1:G:332:LEU:O	1:G:333:GLU:HG2	2.02	0.59
1:J:145:LEU:HB3	1:J:158:MET:CE	2.32	0.59
1:K:394:GLN:HA	1:K:398:LEU:CD2	2.32	0.59
1:L:138:VAL:CG1	1:L:269:ILE:CD1	2.81	0.59
1:A:394:GLN:O	1:A:398:LEU:HD23	2.03	0.59
1:G:310:ARG:O	1:G:314:ALA:HB2	2.03	0.59
1:L:394:GLN:HA	1:L:398:LEU:CD2	2.32	0.59
1:A:59:GLN:HB3	1:A:283:GLN:HG2	1.84	0.59
1:C:159:LYS:NZ	1:D:260:ASP:O	2.34	0.59
1:K:488:LYS:O	1:K:492:MET:HG2	2.02	0.59
1:D:59:GLN:HB3	1:D:283:GLN:HG2	1.84	0.59
1:E:395:GLU:O	1:E:399:PRO:CD	2.51	0.59
1:K:273:LEU:HD23	1:K:273:LEU:C	2.23	0.59
1:D:104:ALA:O	1:D:108:GLU:HG3	2.03	0.59
1:F:368:ARG:NE	1:G:368:ARG:O	2.30	0.59
1:H:145:LEU:HB3	1:H:158:MET:HE2	1.84	0.59
1:A:60:ALA:HB1	1:B:272:TYR:HD1	1.68	0.58
1:B:138:VAL:CG1	1:B:269:ILE:CD1	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:310:ARG:O	1:I:314:ALA:HB2	2.03	0.58
1:L:332:LEU:HD12	1:L:334:LYS:N	2.10	0.58
1:A:407:GLN:O	1:A:411:THR:HG23	2.03	0.58
1:H:357:MET:HE3	1:H:384:THR:OG1	2.02	0.58
1:A:145:LEU:HB3	1:A:158:MET:HE2	1.85	0.58
1:J:332:LEU:HD12	1:J:334:LYS:N	2.14	0.58
1:F:396:LEU:HD23	1:F:396:LEU:C	2.24	0.58
1:G:138:VAL:CG1	1:G:269:ILE:CD1	2.82	0.58
1:D:357:MET:HE1	1:D:384:THR:OG1	2.02	0.58
1:I:222:ASP:OD1	1:I:223:SER:N	2.36	0.58
1:J:393:SER:OG	1:J:397:GLN:NE2	2.36	0.58
1:A:58:TRP:CD1	1:A:284:GLU:OE1	2.57	0.58
1:B:488:LYS:O	1:B:492:MET:HG2	2.03	0.58
1:D:138:VAL:CG1	1:D:269:ILE:CD1	2.81	0.58
1:D:294:SER:HA	1:E:289:MET:HE1	1.85	0.58
1:E:404:LEU:O	1:E:408:LEU:HG	2.04	0.58
1:C:395:GLU:O	1:C:399:PRO:CD	2.51	0.58
1:D:145:LEU:HB3	1:D:158:MET:CE	2.34	0.58
1:D:488:LYS:O	1:D:492:MET:HG2	2.03	0.58
1:C:138:VAL:CG1	1:C:269:ILE:CD1	2.81	0.58
1:G:396:LEU:HD23	1:G:396:LEU:C	2.24	0.58
1:F:445:CYS:CB	1:F:476:ILE:HD11	2.34	0.58
1:I:194:ILE:O	1:I:198:VAL:HG23	2.04	0.58
1:J:357:MET:HE3	1:J:384:THR:OG1	2.04	0.58
1:K:396:LEU:HD23	1:K:396:LEU:C	2.25	0.57
1:L:77:LEU:HD23	1:L:389:TYR:HE1	1.62	0.57
1:B:384:THR:O	1:B:388:VAL:HG12	2.04	0.57
1:B:396:LEU:HD23	1:B:396:LEU:C	2.24	0.57
1:K:187:PHE:CD2	1:K:205:LYS:HB2	2.39	0.57
1:L:332:LEU:O	1:L:333:GLU:HG2	2.04	0.57
1:L:488:LYS:O	1:L:492:MET:HG2	2.02	0.57
1:C:357:MET:HE3	1:C:384:THR:OG1	2.05	0.57
1:C:363:GLN:HB3	1:D:373:GLU:OE1	2.03	0.57
1:K:477:ASP:HB3	1:L:469:ARG:HH12	1.68	0.57
1:L:145:LEU:HB3	1:L:158:MET:CE	2.34	0.57
1:C:159:LYS:HD3	1:D:172:ALA:O	2.04	0.57
1:J:136:GLN:NE2	1:J:162:ARG:HD2	2.20	0.57
1:J:488:LYS:O	1:J:492:MET:HG2	2.04	0.57
1:A:368:ARG:NE	1:B:368:ARG:O	2.34	0.57
1:C:127:ARG:HH12	1:D:394:GLN:HB2	1.67	0.57
1:G:178:GLN:HA	1:G:217:ILE:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:9:ALA:HB2	1:L:216:HIS:HD2	1.69	0.57
1:E:145:LEU:HB3	1:E:158:MET:CE	2.34	0.57
1:H:396:LEU:HD23	1:H:396:LEU:C	2.24	0.57
1:L:145:LEU:HB3	1:L:158:MET:HE2	1.87	0.57
1:L:357:MET:HE1	1:L:384:THR:OG1	2.04	0.57
1:B:332:LEU:O	1:B:333:GLU:HG2	2.04	0.57
1:E:121:ILE:HG23	1:E:126:TYR:HB2	1.87	0.57
1:E:310:ARG:O	1:E:314:ALA:HB2	2.05	0.57
1:J:145:LEU:HB3	1:J:158:MET:HE2	1.86	0.57
1:A:190:LEU:HD22	1:A:194:ILE:HD12	1.87	0.57
1:B:394:GLN:O	1:B:398:LEU:HD23	2.04	0.57
1:E:394:GLN:HA	1:E:398:LEU:CD2	2.35	0.57
1:F:138:VAL:CG1	1:F:269:ILE:CD1	2.83	0.57
1:F:395:GLU:O	1:F:399:PRO:CD	2.52	0.57
1:F:407:GLN:O	1:F:411:THR:HG23	2.05	0.57
1:H:445:CYS:CB	1:H:476:ILE:HD11	2.35	0.57
1:J:143:VAL:H	1:J:254:ILE:CD1	2.13	0.57
1:B:445:CYS:CB	1:B:476:ILE:HD11	2.35	0.57
1:F:197:ALA:O	1:F:235:MET:HE1	2.05	0.57
1:I:190:LEU:HD22	1:I:194:ILE:HD12	1.86	0.57
1:A:58:TRP:CG	1:A:284:GLU:HB2	2.40	0.56
1:A:483:LEU:HD12	1:B:460:ASP:HA	1.86	0.56
1:B:407:GLN:O	1:B:411:THR:HG23	2.04	0.56
1:E:359:ASN:OD1	1:F:380:GLU:HB2	2.05	0.56
1:G:190:LEU:HD22	1:G:194:ILE:HD12	1.87	0.56
1:I:184:GLN:HA	1:I:211:ILE:O	2.05	0.56
1:A:178:GLN:HA	1:A:217:ILE:O	2.05	0.56
1:C:294:SER:HA	1:D:289:MET:CE	2.34	0.56
1:F:77:LEU:CD2	1:F:389:TYR:CE1	2.84	0.56
1:I:385:LEU:HD23	1:I:385:LEU:C	2.26	0.56
1:C:59:GLN:HB3	1:C:283:GLN:HG2	1.86	0.56
1:C:145:LEU:HB3	1:C:158:MET:HE2	1.86	0.56
1:C:396:LEU:HD23	1:C:396:LEU:C	2.25	0.56
1:F:121:ILE:HG23	1:F:126:TYR:HB2	1.88	0.56
1:J:357:MET:CE	1:J:384:THR:OG1	2.52	0.56
1:K:357:MET:HE3	1:K:384:THR:OG1	2.04	0.56
1:K:407:GLN:O	1:K:411:THR:HG23	2.05	0.56
1:L:445:CYS:CB	1:L:476:ILE:HD11	2.35	0.56
1:C:197:ALA:O	1:C:235:MET:HE1	2.05	0.56
1:D:197:ALA:O	1:D:235:MET:HE1	2.05	0.56
1:E:138:VAL:CG1	1:E:269:ILE:CD1	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:GLN:HB3	1:F:373:GLU:OE1	2.04	0.56
1:K:9:ALA:HB2	1:K:216:HIS:HD2	1.71	0.56
1:A:394:GLN:HA	1:A:398:LEU:CD2	2.35	0.56
1:D:127:ARG:NH1	1:E:394:GLN:HB2	2.20	0.56
1:E:222:ASP:OD1	1:E:223:SER:N	2.38	0.56
1:F:143:VAL:H	1:F:254:ILE:CD1	2.12	0.56
1:G:77:LEU:CD2	1:G:389:TYR:CE1	2.84	0.56
1:G:394:GLN:HA	1:G:398:LEU:CD2	2.36	0.56
1:B:159:LYS:NZ	1:C:260:ASP:O	2.38	0.56
1:D:310:ARG:O	1:D:314:ALA:HB2	2.06	0.56
1:D:334:LYS:HG3	1:D:334:LYS:O	2.06	0.56
1:E:445:CYS:CB	1:E:476:ILE:HD11	2.36	0.56
1:H:483:LEU:HD12	1:I:460:ASP:HA	1.88	0.56
1:J:190:LEU:HD22	1:J:194:ILE:HD12	1.87	0.56
1:K:184:GLN:HA	1:K:211:ILE:O	2.06	0.56
1:L:352:LEU:O	1:L:356:PHE:HD2	1.89	0.56
1:D:127:ARG:HH12	1:E:394:GLN:HB2	1.69	0.56
1:D:222:ASP:OD1	1:D:223:SER:N	2.39	0.56
1:D:394:GLN:HA	1:D:398:LEU:CD2	2.35	0.56
1:F:190:LEU:HD22	1:F:194:ILE:HD12	1.87	0.56
1:F:310:ARG:O	1:F:314:ALA:HB2	2.06	0.56
1:F:385:LEU:HD23	1:F:385:LEU:C	2.26	0.56
1:G:395:GLU:O	1:G:399:PRO:CD	2.54	0.56
1:I:147:LEU:N	1:I:147:LEU:HD23	2.21	0.56
1:I:363:GLN:HB3	1:J:373:GLU:OE1	2.05	0.56
1:C:190:LEU:HD22	1:C:194:ILE:HD12	1.87	0.55
1:C:273:LEU:HD23	1:C:274:GLY:N	2.21	0.55
1:D:190:LEU:HD22	1:D:194:ILE:HD12	1.88	0.55
1:G:106:VAL:O	1:G:110:LEU:HD12	2.04	0.55
1:A:38:THR:OG1	1:A:39:ILE:N	2.38	0.55
1:D:230:GLU:O	1:D:237:VAL:HG23	2.05	0.55
1:G:87:THR:OG1	1:G:425:THR:OG1	2.24	0.55
1:G:273:LEU:HD23	1:G:274:GLY:N	2.21	0.55
1:I:331:GLN:HE22	1:J:334:LYS:HA	1.70	0.55
1:A:332:LEU:O	1:A:333:GLU:HG2	2.06	0.55
1:G:147:LEU:HD23	1:G:147:LEU:N	2.21	0.55
1:J:138:VAL:CG1	1:J:269:ILE:CD1	2.84	0.55
1:A:147:LEU:N	1:A:147:LEU:HD23	2.21	0.55
1:B:230:GLU:O	1:B:237:VAL:HG23	2.07	0.55
1:C:275:ASP:HB3	1:C:348:ILE:HG23	1.88	0.55
1:C:393:SER:OG	1:C:397:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:SER:HA	1:F:289:MET:HE1	1.87	0.55
1:F:357:MET:HE3	1:F:384:THR:OG1	2.06	0.55
1:G:59:GLN:HB3	1:G:283:GLN:HG2	1.88	0.55
1:H:394:GLN:HA	1:H:398:LEU:CD2	2.36	0.55
1:I:59:GLN:HB3	1:I:283:GLN:HG2	1.87	0.55
1:I:357:MET:HE1	1:I:384:THR:OG1	2.06	0.55
1:I:359:ASN:OD1	1:J:380:GLU:HB2	2.05	0.55
1:E:190:LEU:HD22	1:E:194:ILE:HD12	1.88	0.55
1:E:396:LEU:HD23	1:E:396:LEU:C	2.25	0.55
1:G:142:ASN:ND2	1:G:255:ARG:HG3	2.22	0.55
1:I:273:LEU:HD23	1:I:274:GLY:N	2.22	0.55
1:K:78:PHE:CE2	1:K:130:LEU:HD23	2.42	0.55
1:K:190:LEU:HD22	1:K:194:ILE:HD12	1.88	0.55
1:F:187:PHE:CD2	1:F:205:LYS:HB2	2.42	0.55
1:H:197:ALA:O	1:H:235:MET:HE1	2.05	0.55
1:I:145:LEU:HB3	1:I:158:MET:HE2	1.88	0.55
1:I:332:LEU:HD12	1:I:334:LYS:N	2.12	0.55
1:J:187:PHE:CD2	1:J:205:LYS:HB2	2.42	0.55
1:D:178:GLN:HA	1:D:217:ILE:O	2.06	0.55
1:H:273:LEU:HD23	1:H:274:GLY:N	2.21	0.55
1:I:159:LYS:NZ	1:J:260:ASP:O	2.39	0.55
1:D:273:LEU:HD23	1:D:274:GLY:N	2.21	0.55
1:E:401:VAL:HG11	1:E:426:ILE:CG2	2.36	0.55
1:H:59:GLN:HB3	1:H:283:GLN:HG2	1.89	0.55
1:C:121:ILE:HG23	1:C:126:TYR:HB2	1.89	0.55
1:D:9:ALA:HB2	1:D:216:HIS:HD2	1.72	0.55
1:E:25:ALA:N	1:E:26:PRO:HD2	2.22	0.55
1:E:254:ILE:HD12	1:E:254:ILE:O	2.06	0.55
1:H:184:GLN:HA	1:H:211:ILE:O	2.06	0.55
1:H:199:GLU:HA	1:H:203:GLY:O	2.07	0.55
1:K:131:PHE:CG	1:L:391:ILE:HD11	2.42	0.55
1:L:401:VAL:HG11	1:L:426:ILE:CG2	2.34	0.55
1:G:9:ALA:HB2	1:G:216:HIS:HD2	1.73	0.55
1:G:187:PHE:CD2	1:G:205:LYS:CB	2.89	0.55
1:H:190:LEU:HD22	1:H:194:ILE:HD12	1.88	0.55
1:I:332:LEU:O	1:I:333:GLU:HG2	2.06	0.55
1:I:394:GLN:HA	1:I:398:LEU:CD2	2.36	0.55
1:J:230:GLU:HB2	1:J:237:VAL:HG23	1.89	0.55
1:G:357:MET:HE1	1:G:384:THR:OG1	2.07	0.54
1:H:9:ALA:HB2	1:H:216:HIS:HD2	1.72	0.54
1:K:59:GLN:HB3	1:K:283:GLN:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:PHE:HZ	1:K:396:LEU:HD22	1.72	0.54
1:L:190:LEU:HD22	1:L:194:ILE:HD12	1.88	0.54
1:B:136:GLN:NE2	1:B:162:ARG:HD2	2.22	0.54
1:D:396:LEU:C	1:D:396:LEU:HD23	2.28	0.54
1:J:59:GLN:HB3	1:J:283:GLN:HG2	1.88	0.54
1:A:363:GLN:HB3	1:B:373:GLU:OE1	2.08	0.54
1:C:77:LEU:CD2	1:C:389:TYR:CE1	2.83	0.54
1:C:407:GLN:O	1:C:411:THR:HG23	2.06	0.54
1:D:363:GLN:HB3	1:E:373:GLU:OE1	2.07	0.54
1:E:77:LEU:HD23	1:E:389:TYR:HE1	1.65	0.54
1:H:77:LEU:CD2	1:H:389:TYR:CE1	2.84	0.54
1:H:186:ALA:HA	1:H:210:THR:H	1.72	0.54
1:J:121:ILE:HG23	1:J:126:TYR:HB2	1.89	0.54
1:J:230:GLU:O	1:J:237:VAL:HG23	2.07	0.54
1:L:78:PHE:HZ	1:L:396:LEU:HD22	1.72	0.54
1:B:230:GLU:HB2	1:B:237:VAL:HG23	1.90	0.54
1:D:67:ASN:ND2	1:E:272:TYR:OH	2.39	0.54
1:E:9:ALA:HB2	1:E:216:HIS:HD2	1.73	0.54
1:E:159:LYS:NZ	1:F:260:ASP:O	2.39	0.54
1:J:394:GLN:HA	1:J:398:LEU:CD2	2.38	0.54
1:L:59:GLN:HB3	1:L:283:GLN:HG2	1.89	0.54
1:E:438:ASP:N	1:E:438:ASP:OD1	2.41	0.54
1:F:147:LEU:N	1:F:147:LEU:HD23	2.22	0.54
1:G:121:ILE:HG23	1:G:126:TYR:HB2	1.88	0.54
1:K:143:VAL:H	1:K:254:ILE:CD1	2.16	0.54
1:L:186:ALA:HA	1:L:210:THR:H	1.72	0.54
1:B:190:LEU:HD22	1:B:194:ILE:HD12	1.89	0.54
1:F:357:MET:HE1	1:F:384:THR:OG1	2.08	0.54
1:G:445:CYS:CB	1:G:476:ILE:HD11	2.37	0.54
1:H:145:LEU:HB3	1:H:158:MET:CE	2.37	0.54
1:I:230:GLU:O	1:I:237:VAL:HG23	2.07	0.54
1:J:273:LEU:HD23	1:J:274:GLY:N	2.23	0.54
1:D:78:PHE:CE2	1:D:130:LEU:HD23	2.43	0.54
1:G:407:GLN:O	1:G:411:THR:HG23	2.07	0.54
1:H:230:GLU:O	1:H:237:VAL:HG23	2.08	0.54
1:J:106:VAL:O	1:J:110:LEU:HD12	2.06	0.54
1:K:178:GLN:HA	1:K:217:ILE:O	2.08	0.54
1:K:222:ASP:OD1	1:K:223:SER:N	2.41	0.54
1:C:131:PHE:CG	1:D:391:ILE:HD11	2.42	0.54
1:C:394:GLN:O	1:C:398:LEU:HD23	2.07	0.54
1:D:39:ILE:HG13	1:E:271:GLU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:SER:HA	1:F:289:MET:CE	2.38	0.54
1:H:357:MET:HE1	1:H:384:THR:OG1	2.08	0.54
1:I:145:LEU:HB3	1:I:158:MET:CE	2.38	0.54
1:B:273:LEU:HD23	1:B:274:GLY:N	2.23	0.54
1:B:309:ARG:HG3	1:B:310:ARG:N	2.23	0.54
1:D:445:CYS:CB	1:D:476:ILE:HD11	2.37	0.54
1:F:78:PHE:CE2	1:F:130:LEU:HD23	2.42	0.54
1:F:467:LYS:NZ	1:G:461:ILE:HD11	2.21	0.54
1:I:275:ASP:HB3	1:I:348:ILE:HG23	1.90	0.54
1:I:396:LEU:C	1:I:396:LEU:HD23	2.27	0.54
1:I:488:LYS:O	1:I:492:MET:HG2	2.08	0.54
1:J:368:ARG:NE	1:K:368:ARG:O	2.37	0.54
1:K:394:GLN:CA	1:K:398:LEU:HD23	2.37	0.54
1:K:445:CYS:CB	1:K:476:ILE:HD11	2.38	0.54
1:L:9:ALA:HB2	1:L:216:HIS:CD2	2.43	0.54
1:C:9:ALA:HB2	1:C:216:HIS:HD2	1.73	0.53
1:J:407:GLN:O	1:J:411:THR:HG23	2.08	0.53
1:K:359:ASN:OD1	1:L:380:GLU:HB2	2.08	0.53
1:B:77:LEU:CD2	1:B:389:TYR:CE1	2.84	0.53
1:D:187:PHE:CE2	1:D:205:LYS:HB2	2.43	0.53
1:E:59:GLN:HB3	1:E:283:GLN:HG2	1.90	0.53
1:E:145:LEU:HB3	1:E:158:MET:HE2	1.90	0.53
1:E:273:LEU:HD23	1:E:274:GLY:N	2.23	0.53
1:K:230:GLU:HB2	1:K:237:VAL:HG23	1.90	0.53
1:L:197:ALA:O	1:L:235:MET:HE1	2.08	0.53
1:C:230:GLU:HB2	1:C:237:VAL:HG23	1.90	0.53
1:C:394:GLN:HA	1:C:398:LEU:CD2	2.38	0.53
1:F:394:GLN:HA	1:F:398:LEU:CD2	2.37	0.53
1:H:121:ILE:HG23	1:H:126:TYR:HB2	1.89	0.53
1:H:310:ARG:O	1:H:314:ALA:HB2	2.08	0.53
1:H:332:LEU:O	1:H:333:GLU:HG2	2.09	0.53
1:K:294:SER:O	1:L:289:MET:HE2	2.08	0.53
1:A:445:CYS:CB	1:A:476:ILE:HD11	2.39	0.53
1:C:106:VAL:O	1:C:110:LEU:HD12	2.07	0.53
1:G:401:VAL:HG11	1:G:426:ILE:CG2	2.37	0.53
1:H:147:LEU:N	1:H:147:LEU:HD23	2.23	0.53
1:J:78:PHE:CE2	1:J:130:LEU:HD23	2.43	0.53
1:D:394:GLN:O	1:D:398:LEU:HD23	2.07	0.53
1:J:359:ASN:OD1	1:K:380:GLU:HB2	2.07	0.53
1:A:87:THR:OG1	1:A:425:THR:OG1	2.27	0.53
1:A:104:ALA:O	1:A:108:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:CG1	1:A:269:ILE:HD12	2.38	0.53
1:B:9:ALA:HB2	1:B:216:HIS:HD2	1.73	0.53
1:D:293:SER:HB3	1:E:337:ASP:HB3	1.90	0.53
1:E:106:VAL:O	1:E:110:LEU:HD12	2.08	0.53
1:H:230:GLU:HB2	1:H:237:VAL:HG23	1.90	0.53
1:J:111:SER:O	1:J:115:ARG:HD3	2.09	0.53
1:J:147:LEU:N	1:J:147:LEU:HD23	2.24	0.53
1:J:458:ASP:OD2	1:J:461:ILE:O	2.27	0.53
1:A:311:LEU:O	1:A:314:ALA:N	2.42	0.53
1:F:78:PHE:HZ	1:F:396:LEU:HD22	1.74	0.53
1:J:445:CYS:CB	1:J:476:ILE:HD11	2.38	0.53
1:K:385:LEU:HD23	1:K:385:LEU:C	2.29	0.53
1:B:87:THR:OG1	1:B:425:THR:OG1	2.27	0.53
1:D:111:SER:O	1:D:115:ARG:HD3	2.09	0.53
1:E:230:GLU:O	1:E:237:VAL:HG23	2.08	0.53
1:K:364:ARG:NE	1:K:364:ARG:HA	2.23	0.53
1:A:222:ASP:OD1	1:A:223:SER:N	2.41	0.53
1:A:275:ASP:HB3	1:A:348:ILE:HG23	1.91	0.53
1:A:396:LEU:C	1:A:396:LEU:HD23	2.29	0.53
1:C:357:MET:HE1	1:C:384:THR:OG1	2.08	0.53
1:C:445:CYS:CB	1:C:476:ILE:HD11	2.38	0.53
1:D:106:VAL:O	1:D:110:LEU:HD12	2.09	0.53
1:D:362:VAL:HG11	1:D:374:ILE:HG12	1.91	0.53
1:E:332:LEU:HD13	1:E:334:LYS:CG	2.35	0.53
1:E:359:ASN:ND2	1:F:376:TYR:CE2	2.77	0.53
1:E:385:LEU:HD23	1:E:385:LEU:C	2.29	0.53
1:F:9:ALA:HB2	1:F:216:HIS:HD2	1.74	0.53
1:I:401:VAL:HG11	1:I:426:ILE:CG2	2.35	0.53
1:A:187:PHE:CE2	1:A:205:LYS:HB2	2.44	0.53
1:A:197:ALA:O	1:A:235:MET:HE1	2.09	0.53
1:B:394:GLN:HA	1:B:398:LEU:CD2	2.38	0.53
1:E:275:ASP:HB3	1:E:348:ILE:HG23	1.90	0.53
1:G:362:VAL:HG11	1:G:374:ILE:HG12	1.91	0.52
1:K:127:ARG:HH12	1:L:394:GLN:HB2	1.74	0.52
1:L:273:LEU:HD23	1:L:274:GLY:N	2.24	0.52
1:C:127:ARG:NH1	1:D:394:GLN:HB2	2.25	0.52
1:C:293:SER:HB3	1:D:337:ASP:HB3	1.90	0.52
1:D:121:ILE:HG23	1:D:126:TYR:HB2	1.91	0.52
1:G:364:ARG:HA	1:G:364:ARG:NE	2.24	0.52
1:I:58:TRP:NE1	1:I:284:GLU:OE1	2.41	0.52
1:I:87:THR:OG1	1:I:425:THR:OG1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:CD2	1:A:389:TYR:CE1	2.89	0.52
1:B:127:ARG:NH1	1:C:394:GLN:HB2	2.25	0.52
1:D:385:LEU:C	1:D:385:LEU:HD23	2.30	0.52
1:H:407:GLN:O	1:H:411:THR:HG23	2.09	0.52
1:I:106:VAL:O	1:I:110:LEU:HD12	2.09	0.52
1:A:230:GLU:O	1:A:237:VAL:HG23	2.09	0.52
1:B:147:LEU:N	1:B:147:LEU:HD23	2.24	0.52
1:C:294:SER:O	1:D:289:MET:HE2	2.09	0.52
1:D:294:SER:HA	1:E:289:MET:CE	2.38	0.52
1:D:438:ASP:OD1	1:D:438:ASP:N	2.42	0.52
1:E:407:GLN:O	1:E:411:THR:HG23	2.09	0.52
1:F:59:GLN:HB3	1:F:283:GLN:HG2	1.91	0.52
1:G:230:GLU:HB2	1:G:237:VAL:HG23	1.90	0.52
1:G:394:GLN:O	1:G:398:LEU:HD23	2.10	0.52
1:H:78:PHE:CE2	1:H:130:LEU:HD23	2.45	0.52
1:K:368:ARG:HD2	1:L:368:ARG:HB2	1.90	0.52
1:L:184:GLN:HA	1:L:211:ILE:O	2.09	0.52
1:L:396:LEU:C	1:L:396:LEU:HD23	2.29	0.52
1:A:380:GLU:HB2	1:L:359:ASN:OD1	2.09	0.52
1:E:111:SER:O	1:E:115:ARG:HD3	2.10	0.52
1:F:332:LEU:HD13	1:F:334:LYS:CG	2.35	0.52
1:H:110:LEU:O	1:H:113:VAL:HB	2.10	0.52
1:I:294:SER:O	1:J:289:MET:HE2	2.08	0.52
1:J:87:THR:OG1	1:J:425:THR:OG1	2.27	0.52
1:K:147:LEU:N	1:K:147:LEU:HD23	2.25	0.52
1:D:184:GLN:HA	1:D:211:ILE:O	2.09	0.52
1:E:136:GLN:NE2	1:E:162:ARG:HD2	2.23	0.52
1:F:144:LEU:C	1:F:144:LEU:HD12	2.30	0.52
1:G:145:LEU:HB3	1:G:158:MET:HE2	1.91	0.52
1:H:87:THR:OG1	1:H:425:THR:OG1	2.27	0.52
1:J:362:VAL:HG11	1:J:374:ILE:HG12	1.92	0.52
1:L:222:ASP:OD1	1:L:223:SER:N	2.43	0.52
1:C:332:LEU:O	1:C:333:GLU:HG2	2.09	0.52
1:E:393:SER:OG	1:E:397:GLN:NE2	2.42	0.52
1:H:277:ARG:HG3	1:H:278:SER:N	2.25	0.52
1:B:178:GLN:HA	1:B:217:ILE:O	2.09	0.52
1:C:249:CYS:SG	1:C:251:TYR:HB3	2.50	0.52
1:I:77:LEU:CD2	1:I:389:TYR:CE1	2.90	0.52
1:I:230:GLU:HB2	1:I:237:VAL:HG23	1.91	0.52
1:L:230:GLU:HB2	1:L:237:VAL:HG23	1.91	0.52
1:B:159:LYS:HD3	1:C:172:ALA:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LEU:HD23	1:D:147:LEU:N	2.24	0.52
1:I:121:ILE:HG23	1:I:126:TYR:HB2	1.92	0.52
1:K:121:ILE:HG23	1:K:126:TYR:HB2	1.91	0.52
1:L:394:GLN:CA	1:L:398:LEU:HD23	2.38	0.52
1:A:344:VAL:O	1:A:348:ILE:HD12	2.10	0.52
1:C:111:SER:O	1:C:115:ARG:HD3	2.10	0.52
1:C:178:GLN:HA	1:C:217:ILE:O	2.10	0.52
1:F:357:MET:SD	1:F:385:LEU:HB2	2.50	0.52
1:I:362:VAL:HG11	1:I:374:ILE:HG12	1.92	0.52
1:A:9:ALA:HB2	1:A:216:HIS:HD2	1.75	0.51
1:B:332:LEU:HD13	1:B:334:LYS:CG	2.38	0.51
1:B:385:LEU:O	1:B:388:VAL:HG13	2.09	0.51
1:J:77:LEU:CD2	1:J:389:TYR:CE1	2.87	0.51
1:A:205:LYS:HD2	1:A:209:GLU:OE2	2.10	0.51
1:C:385:LEU:HD23	1:C:385:LEU:C	2.30	0.51
1:D:230:GLU:HB2	1:D:237:VAL:HG23	1.90	0.51
1:E:147:LEU:N	1:E:147:LEU:HD23	2.25	0.51
1:F:230:GLU:HB2	1:F:237:VAL:HG23	1.93	0.51
1:G:222:ASP:OD1	1:G:223:SER:N	2.43	0.51
1:J:363:GLN:HB3	1:K:373:GLU:OE1	2.09	0.51
1:K:374:ILE:HD13	1:L:372:GLU:HB2	1.93	0.51
1:A:394:GLN:CA	1:A:398:LEU:HD23	2.39	0.51
1:C:398:LEU:HD22	1:C:398:LEU:N	2.24	0.51
1:D:407:GLN:O	1:D:411:THR:HG23	2.09	0.51
1:E:362:VAL:HG11	1:E:374:ILE:HG12	1.92	0.51
1:G:184:GLN:HA	1:G:211:ILE:O	2.10	0.51
1:L:143:VAL:H	1:L:254:ILE:CD1	2.15	0.51
1:L:362:VAL:HG11	1:L:374:ILE:HG12	1.92	0.51
1:C:186:ALA:HA	1:C:210:THR:H	1.75	0.51
1:D:138:VAL:CG1	1:D:269:ILE:HD12	2.41	0.51
1:D:488:LYS:HG3	1:E:460:ASP:HB3	1.91	0.51
1:G:78:PHE:CE2	1:G:130:LEU:HD23	2.46	0.51
1:I:108:GLU:OE2	1:J:479:SER:HA	2.10	0.51
1:J:78:PHE:HZ	1:J:396:LEU:HD22	1.75	0.51
1:J:394:GLN:O	1:J:398:LEU:HD23	2.09	0.51
1:D:9:ALA:HB2	1:D:216:HIS:CD2	2.46	0.51
1:D:254:ILE:HD12	1:D:254:ILE:O	2.11	0.51
1:E:364:ARG:NE	1:E:364:ARG:HA	2.25	0.51
1:G:275:ASP:HB3	1:G:348:ILE:HG23	1.93	0.51
1:I:159:LYS:HD3	1:J:172:ALA:O	2.10	0.51
1:J:331:GLN:HE22	1:K:334:LYS:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:147:LEU:N	1:L:147:LEU:HD23	2.26	0.51
1:A:78:PHE:HZ	1:A:396:LEU:HD22	1.75	0.51
1:B:186:ALA:HA	1:B:210:THR:H	1.74	0.51
1:B:368:ARG:NE	1:C:368:ARG:O	2.35	0.51
1:A:289:MET:HE2	1:L:294:SER:O	2.11	0.51
1:A:401:VAL:HG11	1:A:426:ILE:CG2	2.35	0.51
1:C:147:LEU:N	1:C:147:LEU:HD23	2.25	0.51
1:E:357:MET:CE	1:E:384:THR:OG1	2.59	0.51
1:F:294:SER:HA	1:G:289:MET:HE1	1.93	0.51
1:F:362:VAL:HG11	1:F:374:ILE:HG12	1.92	0.51
1:G:144:LEU:HD23	1:G:166:TYR:CE1	2.46	0.51
1:G:180:VAL:HA	1:G:215:THR:O	2.10	0.51
1:H:385:LEU:HD23	1:H:385:LEU:C	2.31	0.51
1:I:136:GLN:NE2	1:I:162:ARG:HD2	2.26	0.51
1:K:9:ALA:HB2	1:K:216:HIS:CD2	2.45	0.51
1:K:287:VAL:O	1:K:290:SER:OG	2.28	0.51
1:K:393:SER:OG	1:K:397:GLN:NE2	2.44	0.51
1:A:194:ILE:O	1:A:198:VAL:HG23	2.11	0.51
1:D:186:ALA:HA	1:D:210:THR:H	1.74	0.51
1:H:111:SER:O	1:H:115:ARG:HD3	2.10	0.51
1:I:9:ALA:HB2	1:I:216:HIS:HD2	1.76	0.51
1:I:138:VAL:CG1	1:I:269:ILE:HD12	2.40	0.51
1:I:445:CYS:CB	1:I:476:ILE:HD11	2.40	0.51
1:K:186:ALA:HA	1:K:210:THR:H	1.75	0.51
1:L:230:GLU:O	1:L:237:VAL:HG23	2.10	0.51
1:A:254:ILE:HD12	1:A:254:ILE:O	2.10	0.51
1:A:294:SER:HA	1:B:289:MET:HE1	1.93	0.51
1:C:25:ALA:N	1:C:26:PRO:HD2	2.26	0.51
1:D:131:PHE:CB	1:E:391:ILE:HD11	2.41	0.51
1:E:249:CYS:SG	1:E:251:TYR:HB3	2.51	0.51
1:E:287:VAL:O	1:E:290:SER:OG	2.23	0.51
1:I:195:ARG:O	1:I:199:GLU:HG2	2.10	0.51
1:J:448:ALA:O	1:J:451:ALA:HB3	2.11	0.51
1:K:144:LEU:C	1:K:144:LEU:HD12	2.32	0.51
1:G:385:LEU:O	1:G:388:VAL:HG13	2.11	0.51
1:H:249:CYS:SG	1:H:251:TYR:HB3	2.51	0.51
1:I:394:GLN:O	1:I:398:LEU:HD23	2.11	0.51
1:J:138:VAL:CG1	1:J:269:ILE:HD12	2.41	0.51
1:K:187:PHE:CD1	1:K:190:LEU:HD12	2.46	0.51
1:L:38:THR:OG1	1:L:39:ILE:N	2.43	0.51
1:L:178:GLN:HA	1:L:217:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASN:HD21	1:B:303:ALA:HB3	1.75	0.50
1:B:398:LEU:HD22	1:B:398:LEU:N	2.26	0.50
1:C:104:ALA:O	1:C:108:GLU:HG3	2.11	0.50
1:G:136:GLN:HB3	1:G:143:VAL:HG21	1.93	0.50
1:A:198:VAL:O	1:A:202:GLY:N	2.45	0.50
1:B:389:TYR:OH	1:B:429:GLY:HA2	2.11	0.50
1:C:270:GLU:O	1:C:273:LEU:HB3	2.11	0.50
1:E:186:ALA:HA	1:E:210:THR:H	1.75	0.50
1:H:394:GLN:O	1:H:398:LEU:HD23	2.11	0.50
1:I:294:SER:HA	1:J:289:MET:CE	2.40	0.50
1:K:458:ASP:OD2	1:K:461:ILE:O	2.28	0.50
1:B:187:PHE:CD1	1:B:190:LEU:HD12	2.47	0.50
1:C:277:ARG:HG3	1:C:278:SER:N	2.27	0.50
1:C:401:VAL:HG11	1:C:426:ILE:CG2	2.39	0.50
1:F:401:VAL:CG1	1:F:426:ILE:HG21	2.37	0.50
1:G:59:GLN:HG3	1:G:280:GLU:OE1	2.10	0.50
1:I:186:ALA:HA	1:I:210:THR:H	1.75	0.50
1:K:111:SER:O	1:K:115:ARG:HD3	2.12	0.50
1:B:222:ASP:OD1	1:B:223:SER:N	2.45	0.50
1:C:136:GLN:NE2	1:C:162:ARG:HD2	2.26	0.50
1:D:332:LEU:HD13	1:D:334:LYS:CG	2.37	0.50
1:E:394:GLN:CA	1:E:398:LEU:HD23	2.42	0.50
1:G:230:GLU:O	1:G:237:VAL:HG23	2.11	0.50
1:B:364:ARG:NE	1:B:364:ARG:HA	2.26	0.50
1:C:320:VAL:O	1:D:299:LEU:HA	2.11	0.50
1:C:362:VAL:HG11	1:C:374:ILE:HG12	1.92	0.50
1:E:142:ASN:ND2	1:E:255:ARG:HG3	2.27	0.50
1:F:187:PHE:CD1	1:F:190:LEU:HD12	2.47	0.50
1:G:9:ALA:HB2	1:G:216:HIS:CD2	2.46	0.50
1:H:144:LEU:C	1:H:144:LEU:HD12	2.31	0.50
1:H:159:LYS:HD3	1:I:172:ALA:O	2.12	0.50
1:A:273:LEU:HD23	1:A:274:GLY:N	2.27	0.50
1:E:60:ALA:HB1	1:F:272:TYR:HD1	1.76	0.50
1:H:60:ALA:HB1	1:I:272:TYR:HD1	1.76	0.50
1:L:87:THR:OG1	1:L:425:THR:OG1	2.29	0.50
1:L:401:VAL:CG1	1:L:426:ILE:HG21	2.37	0.50
1:A:186:ALA:HA	1:A:210:THR:H	1.73	0.50
1:A:385:LEU:O	1:A:388:VAL:HG13	2.11	0.50
1:B:38:THR:OG1	1:B:39:ILE:N	2.45	0.50
1:B:184:GLN:HA	1:B:211:ILE:O	2.11	0.50
1:B:362:VAL:HG11	1:B:374:ILE:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:LEU:HD21	1:H:387:GLY:HA2	1.94	0.50
1:G:138:VAL:CG1	1:G:269:ILE:HD12	2.42	0.50
1:H:401:VAL:HG11	1:H:426:ILE:CG2	2.36	0.50
1:J:9:ALA:HB2	1:J:216:HIS:HD2	1.75	0.50
1:J:385:LEU:HD23	1:J:385:LEU:C	2.32	0.50
1:L:78:PHE:CE2	1:L:130:LEU:HD23	2.47	0.50
1:B:385:LEU:HD23	1:B:385:LEU:C	2.32	0.50
1:E:9:ALA:HB2	1:E:216:HIS:CD2	2.46	0.50
1:F:398:LEU:HD22	1:F:398:LEU:N	2.27	0.50
1:G:78:PHE:HZ	1:G:396:LEU:HD22	1.75	0.50
1:G:352:LEU:O	1:G:356:PHE:HD2	1.95	0.50
1:G:385:LEU:C	1:G:385:LEU:HD23	2.32	0.50
1:J:401:VAL:HG11	1:J:426:ILE:CG2	2.39	0.50
1:K:401:VAL:HG11	1:K:426:ILE:CG2	2.35	0.50
1:C:222:ASP:OD1	1:C:223:SER:N	2.44	0.50
1:G:143:VAL:H	1:G:254:ILE:CD1	2.14	0.50
1:G:197:ALA:O	1:G:235:MET:HE1	2.12	0.50
1:I:394:GLN:CA	1:I:398:LEU:HD23	2.42	0.50
1:J:187:PHE:CD1	1:J:190:LEU:HD12	2.47	0.50
1:J:197:ALA:O	1:J:235:MET:HE1	2.11	0.50
1:K:230:GLU:O	1:K:237:VAL:HG23	2.11	0.50
1:K:275:ASP:N	1:K:275:ASP:OD1	2.45	0.50
1:L:121:ILE:HG23	1:L:126:TYR:HB2	1.93	0.50
1:A:289:MET:HE1	1:L:294:SER:HA	1.94	0.49
1:E:197:ALA:O	1:E:235:MET:HE1	2.12	0.49
1:G:58:TRP:NE1	1:G:284:GLU:OE1	2.45	0.49
1:G:254:ILE:HD12	1:G:254:ILE:O	2.12	0.49
1:H:78:PHE:HZ	1:H:396:LEU:HD22	1.77	0.49
1:I:407:GLN:O	1:I:411:THR:HG23	2.12	0.49
1:K:187:PHE:HD1	1:K:190:LEU:HD12	1.76	0.49
1:K:277:ARG:HG3	1:K:278:SER:N	2.26	0.49
1:L:398:LEU:HD22	1:L:398:LEU:N	2.27	0.49
1:A:272:TYR:HD1	1:L:60:ALA:HB1	1.77	0.49
1:B:127:ARG:HH12	1:C:394:GLN:HB2	1.76	0.49
1:C:136:GLN:HB3	1:C:143:VAL:HG21	1.93	0.49
1:C:389:TYR:OH	1:C:429:GLY:HA2	2.13	0.49
1:I:170:ARG:CZ	1:I:255:ARG:HD2	2.42	0.49
1:J:294:SER:HA	1:K:289:MET:HE1	1.93	0.49
1:K:127:ARG:NH1	1:L:394:GLN:HB2	2.27	0.49
1:L:385:LEU:C	1:L:385:LEU:HD23	2.33	0.49
1:B:180:VAL:HA	1:B:215:THR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:GLN:HG3	1:E:280:GLU:OE1	2.11	0.49
1:E:187:PHE:CD1	1:E:190:LEU:HD12	2.48	0.49
1:F:186:ALA:HA	1:F:210:THR:H	1.74	0.49
1:F:187:PHE:HD1	1:F:190:LEU:HD12	1.77	0.49
1:G:186:ALA:HA	1:G:210:THR:H	1.74	0.49
1:I:78:PHE:CE2	1:I:130:LEU:HD23	2.47	0.49
1:B:249:CYS:SG	1:B:251:TYR:HB3	2.53	0.49
1:C:187:PHE:CD1	1:C:190:LEU:HD12	2.47	0.49
1:C:230:GLU:O	1:C:237:VAL:HG23	2.11	0.49
1:D:364:ARG:HA	1:D:364:ARG:NE	2.26	0.49
1:E:467:LYS:NZ	1:F:461:ILE:HD11	2.26	0.49
1:F:142:ASN:ND2	1:F:255:ARG:HG3	2.27	0.49
1:F:401:VAL:HG11	1:F:426:ILE:CG2	2.34	0.49
1:H:9:ALA:HB2	1:H:216:HIS:CD2	2.47	0.49
1:H:178:GLN:HA	1:H:217:ILE:O	2.12	0.49
1:I:143:VAL:H	1:I:254:ILE:CD1	2.15	0.49
1:J:396:LEU:HD23	1:J:396:LEU:C	2.32	0.49
1:K:362:VAL:HG11	1:K:374:ILE:HG12	1.95	0.49
1:C:77:LEU:HD23	1:C:389:TYR:HE1	1.71	0.49
1:F:9:ALA:HB2	1:F:216:HIS:CD2	2.48	0.49
1:J:186:ALA:HA	1:J:210:THR:H	1.76	0.49
1:J:187:PHE:HD1	1:J:190:LEU:HD12	1.77	0.49
1:K:477:ASP:HB3	1:L:469:ARG:NH1	2.27	0.49
1:L:144:LEU:HD12	1:L:144:LEU:C	2.33	0.49
1:A:159:LYS:HD3	1:B:172:ALA:O	2.13	0.49
1:C:78:PHE:HZ	1:C:396:LEU:HD22	1.77	0.49
1:F:138:VAL:CG1	1:F:269:ILE:HD12	2.42	0.49
1:G:136:GLN:NE2	1:G:162:ARG:HD2	2.28	0.49
1:I:78:PHE:HZ	1:I:396:LEU:HD22	1.76	0.49
1:I:127:ARG:NH1	1:J:394:GLN:HB2	2.28	0.49
1:J:483:LEU:HD12	1:K:460:ASP:HA	1.94	0.49
1:L:458:ASP:OD2	1:L:461:ILE:O	2.31	0.49
1:B:187:PHE:HD1	1:B:190:LEU:HD12	1.77	0.49
1:B:270:GLU:O	1:B:273:LEU:HB3	2.13	0.49
1:B:357:MET:HE1	1:B:384:THR:OG1	2.11	0.49
1:C:332:LEU:HD13	1:C:334:LYS:CG	2.37	0.49
1:E:78:PHE:CE2	1:E:130:LEU:HD23	2.47	0.49
1:F:230:GLU:O	1:F:237:VAL:HG23	2.12	0.49
1:I:111:SER:O	1:I:115:ARG:HD3	2.12	0.49
1:A:81:GLN:OE1	1:A:433:ILE:CG2	2.60	0.49
1:C:9:ALA:HB2	1:C:216:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:TYR:OH	1:D:429:GLY:HA2	2.11	0.49
1:F:216:HIS:HB3	1:F:229:TYR:CE1	2.48	0.49
1:H:143:VAL:H	1:H:254:ILE:CD1	2.16	0.49
1:J:60:ALA:HB1	1:K:272:TYR:HD1	1.78	0.49
1:J:181:THR:HG23	1:J:215:THR:HB	1.95	0.49
1:L:77:LEU:CD2	1:L:389:TYR:CD1	2.96	0.49
1:L:275:ASP:HB2	1:L:352:LEU:HD21	1.95	0.49
1:A:121:ILE:HG23	1:A:126:TYR:HB2	1.94	0.49
1:B:121:ILE:HG23	1:B:126:TYR:HB2	1.94	0.49
1:B:275:ASP:HB3	1:B:348:ILE:HG23	1.95	0.49
1:D:394:GLN:CA	1:D:398:LEU:HD23	2.41	0.49
1:I:197:ALA:O	1:I:235:MET:HE1	2.13	0.49
1:I:270:GLU:O	1:I:273:LEU:HB3	2.12	0.49
1:J:277:ARG:HG3	1:J:278:SER:N	2.27	0.49
1:L:187:PHE:CD1	1:L:190:LEU:HD12	2.48	0.49
1:L:254:ILE:CD1	1:L:254:ILE:C	2.81	0.49
1:B:9:ALA:HB2	1:B:216:HIS:CD2	2.47	0.49
1:E:384:THR:O	1:E:388:VAL:HG12	2.12	0.49
1:E:389:TYR:OH	1:E:429:GLY:HA2	2.12	0.49
1:F:277:ARG:HG3	1:F:278:SER:N	2.27	0.49
1:G:332:LEU:HD13	1:G:334:LYS:CG	2.37	0.49
1:G:394:GLN:CA	1:G:398:LEU:HD23	2.41	0.49
1:H:187:PHE:CD1	1:H:190:LEU:HD12	2.48	0.49
1:H:385:LEU:O	1:H:388:VAL:HG13	2.13	0.49
1:A:249:CYS:SG	1:A:251:TYR:HB3	2.53	0.48
1:A:364:ARG:NE	1:A:364:ARG:HA	2.28	0.48
1:B:393:SER:OG	1:B:397:GLN:NE2	2.46	0.48
1:C:394:GLN:CA	1:C:398:LEU:HD23	2.43	0.48
1:D:25:ALA:N	1:D:26:PRO:HD2	2.28	0.48
1:E:331:GLN:NE2	1:F:334:LYS:HA	2.28	0.48
1:H:362:VAL:HG11	1:H:374:ILE:HG12	1.94	0.48
1:I:368:ARG:NE	1:J:368:ARG:O	2.41	0.48
1:K:87:THR:OG1	1:K:425:THR:OG1	2.31	0.48
1:A:106:VAL:O	1:A:110:LEU:HD12	2.13	0.48
1:A:230:GLU:HB2	1:A:237:VAL:HG23	1.90	0.48
1:E:144:LEU:C	1:E:144:LEU:HD12	2.33	0.48
1:G:467:LYS:CE	1:H:461:ILE:HD11	2.42	0.48
1:K:59:GLN:HG3	1:K:280:GLU:OE1	2.12	0.48
1:K:77:LEU:HD23	1:K:389:TYR:HE1	1.68	0.48
1:F:364:ARG:NE	1:F:364:ARG:HA	2.27	0.48
1:J:178:GLN:HA	1:J:217:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:273:LEU:HD23	1:K:274:GLY:N	2.28	0.48
1:A:187:PHE:CD1	1:A:190:LEU:HD12	2.48	0.48
1:A:357:MET:HE1	1:A:384:THR:OG1	2.14	0.48
1:A:362:VAL:HG11	1:A:374:ILE:HG12	1.95	0.48
1:B:197:ALA:O	1:B:235:MET:HE1	2.13	0.48
1:C:184:GLN:HA	1:C:211:ILE:O	2.12	0.48
1:F:87:THR:OG1	1:F:425:THR:OG1	2.31	0.48
1:F:273:LEU:HD23	1:F:274:GLY:N	2.27	0.48
1:H:108:GLU:OE2	1:I:479:SER:HA	2.13	0.48
1:H:136:GLN:HB3	1:H:143:VAL:HG21	1.95	0.48
1:H:142:ASN:ND2	1:H:255:ARG:HG3	2.29	0.48
1:H:359:ASN:OD1	1:I:380:GLU:HB2	2.14	0.48
1:J:170:ARG:CZ	1:J:255:ARG:HD2	2.43	0.48
1:J:275:ASP:HB3	1:J:348:ILE:HG23	1.95	0.48
1:B:58:TRP:NE1	1:B:284:GLU:OE1	2.46	0.48
1:C:359:ASN:OD1	1:D:380:GLU:HB2	2.13	0.48
1:F:184:GLN:HA	1:F:211:ILE:O	2.12	0.48
1:F:404:LEU:O	1:F:408:LEU:HG	2.13	0.48
1:G:25:ALA:N	1:G:26:PRO:HD2	2.28	0.48
1:H:27:TYR:CE2	1:H:264:TYR:HB2	2.48	0.48
1:H:364:ARG:NE	1:H:364:ARG:HA	2.28	0.48
1:H:394:GLN:CA	1:H:398:LEU:HD23	2.41	0.48
1:I:354:PHE:CE2	1:I:361:ALA:HB1	2.49	0.48
1:A:78:PHE:CE2	1:A:130:LEU:HD23	2.48	0.48
1:D:401:VAL:HG11	1:D:426:ILE:CG2	2.36	0.48
1:D:479:SER:HB3	1:E:469:ARG:NH2	2.29	0.48
1:F:136:GLN:NE2	1:F:162:ARG:HD2	2.29	0.48
1:H:187:PHE:HD1	1:H:190:LEU:HD12	1.78	0.48
1:H:194:ILE:O	1:H:198:VAL:HG23	2.13	0.48
1:J:159:LYS:NZ	1:K:260:ASP:O	2.47	0.48
1:K:273:LEU:O	1:K:276:LEU:N	2.47	0.48
1:K:368:ARG:NE	1:L:368:ARG:HB2	2.28	0.48
1:L:104:ALA:O	1:L:108:GLU:HG3	2.13	0.48
1:C:87:THR:OG1	1:C:425:THR:OG1	2.31	0.48
1:D:87:THR:OG1	1:D:425:THR:OG1	2.32	0.48
1:D:136:GLN:HB3	1:D:143:VAL:HG21	1.94	0.48
1:E:374:ILE:HD13	1:F:373:GLU:N	2.28	0.48
1:K:385:LEU:O	1:K:388:VAL:HG13	2.14	0.48
1:A:277:ARG:HG3	1:A:278:SER:N	2.29	0.48
1:C:332:LEU:C	1:C:333:GLU:HG2	2.34	0.48
1:D:187:PHE:CD1	1:D:190:LEU:HD12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:CYS:SG	1:D:251:TYR:HB3	2.53	0.48
1:D:282:LEU:O	1:D:283:GLN:C	2.52	0.48
1:F:331:GLN:HE22	1:G:334:LYS:HA	1.79	0.48
1:F:394:GLN:CA	1:F:398:LEU:HD23	2.44	0.48
1:G:479:SER:HB3	1:H:469:ARG:NH2	2.28	0.48
1:I:332:LEU:HD13	1:I:334:LYS:CG	2.42	0.48
1:K:138:VAL:CG1	1:K:269:ILE:HD12	2.41	0.48
1:L:77:LEU:HD23	1:L:389:TYR:CD1	2.47	0.48
1:L:111:SER:O	1:L:115:ARG:HD3	2.13	0.48
1:A:170:ARG:CZ	1:A:255:ARG:HD2	2.44	0.48
1:G:181:THR:HG23	1:G:215:THR:HB	1.95	0.48
1:G:185:ILE:O	1:G:186:ALA:HB3	2.14	0.48
1:I:187:PHE:CD1	1:I:190:LEU:HD12	2.49	0.48
1:B:25:ALA:N	1:B:26:PRO:HD2	2.29	0.48
1:C:438:ASP:N	1:C:438:ASP:OD1	2.47	0.48
1:F:359:ASN:OD1	1:G:380:GLU:HB2	2.13	0.48
1:I:178:GLN:HA	1:I:217:ILE:O	2.13	0.48
1:J:364:ARG:NE	1:J:364:ARG:HA	2.29	0.48
1:L:254:ILE:HD12	1:L:254:ILE:C	2.34	0.48
1:A:59:GLN:HG3	1:A:280:GLU:OE1	2.14	0.47
1:D:143:VAL:H	1:D:254:ILE:CD1	2.14	0.47
1:F:275:ASP:HB3	1:F:348:ILE:HG23	1.96	0.47
1:G:187:PHE:CD1	1:G:190:LEU:HD12	2.49	0.47
1:H:25:ALA:N	1:H:26:PRO:HD2	2.29	0.47
1:L:170:ARG:CZ	1:L:255:ARG:HD2	2.43	0.47
1:B:111:SER:O	1:B:115:ARG:HD3	2.13	0.47
1:C:144:LEU:C	1:C:144:LEU:HD12	2.35	0.47
1:E:301:ASN:HD21	1:E:303:ALA:HB3	1.80	0.47
1:E:401:VAL:CG1	1:E:426:ILE:HG21	2.39	0.47
1:K:398:LEU:HD22	1:K:398:LEU:N	2.28	0.47
1:A:393:SER:OG	1:A:397:GLN:NE2	2.48	0.47
1:A:461:ILE:HD11	1:L:467:LYS:NZ	2.29	0.47
1:B:438:ASP:N	1:B:438:ASP:OD1	2.47	0.47
1:D:137:LEU:HD13	1:D:254:ILE:HD13	1.96	0.47
1:D:160:LEU:O	1:E:260:ASP:HB2	2.13	0.47
1:F:60:ALA:HB1	1:G:272:TYR:HD1	1.79	0.47
1:F:393:SER:OG	1:F:397:GLN:NE2	2.47	0.47
1:H:222:ASP:CG	1:H:223:SER:N	2.67	0.47
1:I:9:ALA:HB2	1:I:216:HIS:CD2	2.49	0.47
1:J:9:ALA:HB2	1:J:216:HIS:CD2	2.49	0.47
1:L:277:ARG:HG3	1:L:278:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:PHE:CE2	1:C:130:LEU:HD23	2.49	0.47
1:D:404:LEU:O	1:D:408:LEU:HG	2.14	0.47
1:D:479:SER:HB3	1:E:469:ARG:HH22	1.79	0.47
1:E:187:PHE:HD1	1:E:190:LEU:HD12	1.79	0.47
1:E:230:GLU:HB2	1:E:237:VAL:HG23	1.95	0.47
1:F:104:ALA:O	1:F:108:GLU:HG3	2.14	0.47
1:K:136:GLN:O	1:K:140:ALA:HB3	2.14	0.47
1:L:138:VAL:CG1	1:L:269:ILE:HD12	2.43	0.47
1:A:332:LEU:HD13	1:A:334:LYS:CG	2.39	0.47
1:A:357:MET:SD	1:A:385:LEU:HB2	2.54	0.47
1:D:78:PHE:HZ	1:D:396:LEU:HD22	1.77	0.47
1:E:78:PHE:HZ	1:E:396:LEU:HD22	1.79	0.47
1:E:136:GLN:HB3	1:E:143:VAL:HG21	1.95	0.47
1:E:143:VAL:H	1:E:254:ILE:CD1	2.12	0.47
1:E:181:THR:HG23	1:E:215:THR:HB	1.97	0.47
1:F:178:GLN:HA	1:F:217:ILE:O	2.14	0.47
1:I:138:VAL:HG12	1:I:269:ILE:CD1	2.42	0.47
1:K:275:ASP:HB3	1:K:348:ILE:HG23	1.97	0.47
1:K:374:ILE:CD1	1:L:372:GLU:HB2	2.45	0.47
1:L:275:ASP:HB3	1:L:348:ILE:HG23	1.95	0.47
1:L:448:ALA:O	1:L:451:ALA:HB3	2.15	0.47
1:A:273:LEU:HA	1:A:276:LEU:HB3	1.96	0.47
1:B:40:PRO:O	1:B:42:LEU:N	2.48	0.47
1:B:138:VAL:CG1	1:B:269:ILE:HD12	2.43	0.47
1:B:185:ILE:O	1:B:186:ALA:HB3	2.15	0.47
1:C:27:TYR:CE2	1:C:264:TYR:HB2	2.49	0.47
1:C:201:GLN:HG3	1:C:235:MET:SD	2.55	0.47
1:C:364:ARG:NE	1:C:364:ARG:HA	2.28	0.47
1:D:75:LEU:HD21	1:E:387:GLY:HA2	1.97	0.47
1:E:254:ILE:HD12	1:E:254:ILE:C	2.35	0.47
1:F:394:GLN:O	1:F:398:LEU:HD23	2.14	0.47
1:H:398:LEU:HD22	1:H:398:LEU:N	2.30	0.47
1:J:294:SER:O	1:K:289:MET:HE2	2.14	0.47
1:A:25:ALA:N	1:A:26:PRO:HD2	2.29	0.47
1:B:170:ARG:CZ	1:B:255:ARG:HD2	2.44	0.47
1:B:357:MET:SD	1:B:385:LEU:HB2	2.55	0.47
1:B:363:GLN:HB3	1:C:373:GLU:OE1	2.15	0.47
1:C:483:LEU:HD12	1:D:460:ASP:HA	1.97	0.47
1:D:108:GLU:OE2	1:E:479:SER:HA	2.14	0.47
1:D:187:PHE:HD1	1:D:190:LEU:HD12	1.79	0.47
1:D:275:ASP:HB3	1:D:348:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:PHE:CD1	1:E:340:VAL:HG13	2.49	0.47
1:D:398:LEU:HD22	1:D:398:LEU:N	2.29	0.47
1:E:277:ARG:HG3	1:E:278:SER:N	2.30	0.47
1:E:368:ARG:HD2	1:F:368:ARG:HB2	1.96	0.47
1:F:25:ALA:N	1:F:26:PRO:HD2	2.30	0.47
1:G:159:LYS:NZ	1:H:260:ASP:O	2.47	0.47
1:G:270:GLU:O	1:G:273:LEU:HB3	2.15	0.47
1:G:277:ARG:HG3	1:G:278:SER:N	2.28	0.47
1:G:401:VAL:CG1	1:G:426:ILE:HG21	2.41	0.47
1:H:275:ASP:HB2	1:H:352:LEU:HD21	1.96	0.47
1:I:127:ARG:HH12	1:J:394:GLN:HB2	1.79	0.47
1:J:25:ALA:N	1:J:26:PRO:HD2	2.29	0.47
1:J:144:LEU:C	1:J:144:LEU:HD12	2.35	0.47
1:K:359:ASN:ND2	1:L:376:TYR:CE2	2.83	0.47
1:A:194:ILE:O	1:A:198:VAL:N	2.47	0.47
1:C:170:ARG:CZ	1:C:255:ARG:HD2	2.45	0.47
1:E:110:LEU:O	1:E:113:VAL:HB	2.15	0.47
1:F:27:TYR:CE2	1:F:264:TYR:HB2	2.50	0.47
1:F:249:CYS:SG	1:F:251:TYR:HB3	2.55	0.47
1:F:254:ILE:HD12	1:F:254:ILE:O	2.14	0.47
1:I:401:VAL:CG1	1:I:426:ILE:HG21	2.38	0.47
1:J:59:GLN:HG3	1:J:280:GLU:OE1	2.14	0.47
1:K:144:LEU:HD23	1:K:166:TYR:CE1	2.50	0.47
1:K:294:SER:HA	1:L:289:MET:HE1	1.96	0.47
1:L:59:GLN:C	1:L:59:GLN:OE1	2.52	0.47
1:L:187:PHE:HD1	1:L:190:LEU:HD12	1.79	0.47
1:A:294:SER:HA	1:B:289:MET:CE	2.45	0.47
1:A:301:ASN:HD21	1:A:303:ALA:HB3	1.79	0.47
1:D:181:THR:HG23	1:D:215:THR:HB	1.97	0.47
1:E:229:TYR:HE2	1:E:231:GLU:HB2	1.79	0.47
1:F:137:LEU:HD13	1:F:254:ILE:HD13	1.95	0.47
1:J:91:TYR:O	1:J:95:GLN:HG2	2.15	0.47
1:J:104:ALA:O	1:J:108:GLU:HG3	2.15	0.47
1:A:127:ARG:NH1	1:B:394:GLN:HB2	2.30	0.47
1:F:389:TYR:OH	1:F:429:GLY:HA2	2.15	0.47
1:H:106:VAL:O	1:H:110:LEU:HD12	2.15	0.47
1:H:180:VAL:HA	1:H:215:THR:O	2.14	0.47
1:H:372:GLU:C	1:H:374:ILE:H	2.18	0.47
1:H:401:VAL:CG1	1:H:426:ILE:HG21	2.38	0.47
1:I:364:ARG:NE	1:I:364:ARG:HA	2.28	0.47
1:J:72:LYS:HG3	1:K:383:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:194:ILE:O	1:K:198:VAL:HG23	2.15	0.47
1:K:273:LEU:HA	1:K:276:LEU:HB3	1.96	0.47
1:A:187:PHE:HD1	1:A:190:LEU:HD12	1.79	0.46
1:A:254:ILE:HD12	1:A:254:ILE:C	2.36	0.46
1:B:372:GLU:C	1:B:374:ILE:H	2.18	0.46
1:C:273:LEU:HA	1:C:276:LEU:HB3	1.97	0.46
1:D:142:ASN:ND2	1:D:255:ARG:HG3	2.30	0.46
1:D:368:ARG:NE	1:E:368:ARG:O	2.41	0.46
1:F:59:GLN:HG3	1:F:280:GLU:OE1	2.15	0.46
1:J:249:CYS:SG	1:J:251:TYR:HB3	2.55	0.46
1:L:364:ARG:HA	1:L:364:ARG:NE	2.30	0.46
1:A:9:ALA:HB2	1:A:216:HIS:CD2	2.49	0.46
1:A:159:LYS:NZ	1:B:260:ASP:O	2.47	0.46
1:C:321:THR:HA	1:D:300:VAL:O	2.15	0.46
1:E:338:PHE:CD1	1:F:340:VAL:HG13	2.49	0.46
1:E:354:PHE:CE2	1:E:361:ALA:HB1	2.50	0.46
1:I:136:GLN:HB3	1:I:143:VAL:HG21	1.96	0.46
1:J:394:GLN:CA	1:J:398:LEU:HD23	2.43	0.46
1:J:398:LEU:HD22	1:J:398:LEU:N	2.31	0.46
1:K:374:ILE:HD13	1:L:373:GLU:N	2.30	0.46
1:A:81:GLN:OE1	1:A:433:ILE:HG21	2.15	0.46
1:B:77:LEU:HD23	1:B:389:TYR:HE1	1.74	0.46
1:F:180:VAL:HA	1:F:215:THR:O	2.16	0.46
1:G:144:LEU:C	1:G:144:LEU:HD12	2.35	0.46
1:H:332:LEU:HD13	1:H:334:LYS:CG	2.40	0.46
1:H:332:LEU:C	1:H:333:GLU:HG2	2.36	0.46
1:I:180:VAL:HA	1:I:215:THR:O	2.14	0.46
1:J:38:THR:OG1	1:J:39:ILE:N	2.46	0.46
1:K:332:LEU:HD13	1:K:334:LYS:CG	2.40	0.46
1:L:25:ALA:N	1:L:26:PRO:HD2	2.31	0.46
1:B:393:SER:O	1:B:397:GLN:CB	2.55	0.46
1:H:373:GLU:O	1:H:377:VAL:HG22	2.16	0.46
1:I:187:PHE:HD1	1:I:190:LEU:HD12	1.80	0.46
1:J:338:PHE:CD1	1:K:340:VAL:HG13	2.51	0.46
1:L:106:VAL:O	1:L:110:LEU:HD12	2.15	0.46
1:A:373:GLU:OE1	1:L:363:GLN:HB3	2.15	0.46
1:F:396:LEU:HD23	1:F:396:LEU:O	2.16	0.46
1:G:145:LEU:HD13	1:G:158:MET:HE1	1.97	0.46
1:G:187:PHE:HD1	1:G:190:LEU:HD12	1.80	0.46
1:G:389:TYR:OH	1:G:429:GLY:HA2	2.15	0.46
1:I:142:ASN:ND2	1:I:255:ARG:HG3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:LEU:C	1:I:144:LEU:HD12	2.35	0.46
1:I:254:ILE:HD12	1:I:254:ILE:O	2.16	0.46
1:I:430:LEU:HG	1:I:435:ARG:O	2.15	0.46
1:C:187:PHE:HD1	1:C:190:LEU:HD12	1.79	0.46
1:C:324:PRO:HD3	1:D:328:SER:HB2	1.98	0.46
1:D:277:ARG:HG3	1:D:278:SER:N	2.31	0.46
1:E:357:MET:HE3	1:E:384:THR:OG1	2.15	0.46
1:E:479:SER:HB3	1:F:469:ARG:NH2	2.31	0.46
1:F:136:GLN:HB3	1:F:143:VAL:HG21	1.96	0.46
1:G:249:CYS:SG	1:G:251:TYR:HB3	2.56	0.46
1:H:101:ASP:HB3	1:I:485:GLU:HB2	1.98	0.46
1:H:185:ILE:O	1:H:186:ALA:HB3	2.16	0.46
1:J:110:LEU:O	1:J:113:VAL:HB	2.16	0.46
1:J:254:ILE:C	1:J:254:ILE:HD12	2.36	0.46
1:A:294:SER:O	1:B:289:MET:HE2	2.15	0.46
1:A:332:LEU:C	1:A:333:GLU:HG2	2.36	0.46
1:A:463:LEU:N	1:A:463:LEU:HD23	2.31	0.46
1:B:136:GLN:HB3	1:B:143:VAL:HG21	1.98	0.46
1:E:104:ALA:O	1:E:108:GLU:HG3	2.16	0.46
1:F:75:LEU:HD21	1:G:387:GLY:HA2	1.98	0.46
1:H:222:ASP:OD2	1:H:223:SER:N	2.49	0.46
1:I:85:ARG:HG3	1:I:114:GLU:OE2	2.16	0.46
1:I:277:ARG:HG3	1:I:278:SER:N	2.30	0.46
1:K:187:PHE:HA	1:K:190:LEU:HG	1.97	0.46
1:L:59:GLN:HG3	1:L:280:GLU:OE1	2.15	0.46
1:L:249:CYS:SG	1:L:251:TYR:HB3	2.56	0.46
1:L:393:SER:OG	1:L:397:GLN:NE2	2.49	0.46
1:A:229:TYR:HE2	1:A:231:GLU:HB2	1.81	0.46
1:B:181:THR:HG23	1:B:215:THR:HB	1.98	0.46
1:E:178:GLN:HA	1:E:217:ILE:O	2.16	0.46
1:H:127:ARG:NH1	1:I:394:GLN:HB2	2.31	0.46
1:H:389:TYR:OH	1:H:429:GLY:HA2	2.16	0.46
1:I:39:ILE:HG13	1:J:271:GLU:HB3	1.96	0.46
1:I:181:THR:HG23	1:I:215:THR:HB	1.97	0.46
1:I:275:ASP:HB2	1:I:352:LEU:HD21	1.97	0.46
1:K:404:LEU:O	1:K:408:LEU:HG	2.15	0.46
1:A:401:VAL:CG1	1:A:426:ILE:HG21	2.38	0.46
1:D:170:ARG:CZ	1:D:255:ARG:HD2	2.46	0.46
1:D:187:PHE:CD2	1:D:205:LYS:HB2	2.51	0.46
1:E:27:TYR:CE2	1:E:264:TYR:HB2	2.51	0.46
1:F:96:LEU:HD11	1:F:420:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:430:LEU:HG	1:G:435:ARG:O	2.15	0.46
1:I:488:LYS:HG3	1:J:460:ASP:HB3	1.97	0.46
1:J:159:LYS:HD3	1:K:172:ALA:O	2.16	0.46
1:A:254:ILE:C	1:A:254:ILE:CD1	2.84	0.46
1:B:401:VAL:HG11	1:B:426:ILE:CG2	2.41	0.46
1:G:393:SER:OG	1:G:397:GLN:NE2	2.49	0.46
1:H:187:PHE:HA	1:H:190:LEU:HG	1.98	0.46
1:J:58:TRP:NE1	1:J:284:GLU:OE1	2.48	0.46
1:J:275:ASP:HB2	1:J:352:LEU:HD21	1.98	0.46
1:J:294:SER:HA	1:K:289:MET:CE	2.46	0.46
1:J:332:LEU:O	1:J:333:GLU:HG2	2.16	0.46
1:L:393:SER:O	1:L:397:GLN:CB	2.55	0.46
1:L:430:LEU:HG	1:L:435:ARG:O	2.16	0.46
1:B:394:GLN:CA	1:B:398:LEU:HD23	2.44	0.45
1:G:27:TYR:CE2	1:G:264:TYR:HB2	2.50	0.45
1:I:81:GLN:OE1	1:I:433:ILE:CG2	2.65	0.45
1:I:144:LEU:HD23	1:I:166:TYR:CE1	2.51	0.45
1:A:187:PHE:CD2	1:A:205:LYS:HB2	2.51	0.45
1:A:216:HIS:HB3	1:A:229:TYR:CE1	2.52	0.45
1:D:448:ALA:O	1:D:451:ALA:HB3	2.17	0.45
1:E:254:ILE:CD1	1:E:254:ILE:C	2.84	0.45
1:I:27:TYR:CE2	1:I:264:TYR:HB2	2.52	0.45
1:J:230:GLU:CB	1:J:237:VAL:HG21	2.42	0.45
1:L:144:LEU:HD23	1:L:166:TYR:CE1	2.51	0.45
1:B:332:LEU:C	1:B:333:GLU:HG2	2.37	0.45
1:C:138:VAL:CG1	1:C:269:ILE:HD12	2.43	0.45
1:D:110:LEU:O	1:D:113:VAL:HB	2.17	0.45
1:D:273:LEU:HA	1:D:276:LEU:HB3	1.99	0.45
1:E:185:ILE:O	1:E:186:ALA:HB3	2.17	0.45
1:G:142:ASN:HD21	1:G:255:ARG:HG3	1.81	0.45
1:L:394:GLN:C	1:L:398:LEU:HD23	2.36	0.45
1:A:136:GLN:HB3	1:A:143:VAL:HG21	1.98	0.45
1:A:331:GLN:NE2	1:B:334:LYS:HA	2.30	0.45
1:C:181:THR:HG23	1:C:215:THR:HB	1.97	0.45
1:C:226:TYR:HB2	1:C:244:TYR:HB2	1.98	0.45
1:D:125:SER:CA	1:E:394:GLN:NE2	2.59	0.45
1:D:392:LEU:HD23	1:D:392:LEU:HA	1.85	0.45
1:F:91:TYR:O	1:F:95:GLN:HG2	2.16	0.45
1:G:111:SER:O	1:G:115:ARG:HD3	2.17	0.45
1:G:404:LEU:O	1:G:408:LEU:HG	2.16	0.45
1:H:463:LEU:HD23	1:H:463:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:273:LEU:HA	1:J:276:LEU:HB3	1.98	0.45
1:K:372:GLU:C	1:K:374:ILE:H	2.19	0.45
1:B:483:LEU:HD12	1:C:460:ASP:HA	1.98	0.45
1:C:254:ILE:O	1:C:254:ILE:HD12	2.17	0.45
1:D:337:ASP:O	1:D:340:VAL:HB	2.17	0.45
1:K:27:TYR:CE2	1:K:264:TYR:HB2	2.51	0.45
1:K:106:VAL:O	1:K:110:LEU:HD12	2.17	0.45
1:A:101:ASP:HB3	1:B:485:GLU:HB2	1.98	0.45
1:B:273:LEU:HA	1:B:276:LEU:HB3	1.98	0.45
1:B:275:ASP:HB2	1:B:352:LEU:HD21	1.99	0.45
1:D:202:GLY:O	1:D:205:LYS:HD3	2.16	0.45
1:F:38:THR:OG1	1:F:39:ILE:N	2.48	0.45
1:G:319:PHE:HA	1:H:298:GLY:O	2.16	0.45
1:H:138:VAL:CG1	1:H:269:ILE:HD12	2.39	0.45
1:L:110:LEU:O	1:L:113:VAL:HB	2.16	0.45
1:L:180:VAL:HA	1:L:215:THR:O	2.17	0.45
1:B:230:GLU:CB	1:B:237:VAL:HG21	2.44	0.45
1:C:143:VAL:H	1:C:254:ILE:CD1	2.18	0.45
1:E:39:ILE:HG13	1:F:271:GLU:HB3	1.99	0.45
1:E:275:ASP:OD1	1:E:275:ASP:N	2.49	0.45
1:F:81:GLN:OE1	1:F:433:ILE:HG21	2.17	0.45
1:F:229:TYR:HE2	1:F:231:GLU:HB2	1.82	0.45
1:F:332:LEU:C	1:F:333:GLU:HG2	2.36	0.45
1:G:104:ALA:O	1:G:108:GLU:HG3	2.16	0.45
1:H:270:GLU:O	1:H:273:LEU:HB3	2.17	0.45
1:H:273:LEU:HA	1:H:276:LEU:HB3	1.99	0.45
1:H:430:LEU:HG	1:H:435:ARG:O	2.17	0.45
1:J:113:VAL:O	1:J:117:ILE:HG12	2.17	0.45
1:B:78:PHE:HZ	1:B:396:LEU:HD22	1.80	0.45
1:B:91:TYR:O	1:B:95:GLN:HG2	2.17	0.45
1:D:254:ILE:CD1	1:D:254:ILE:C	2.86	0.45
1:E:58:TRP:NE1	1:E:284:GLU:OE1	2.50	0.45
1:E:216:HIS:HB3	1:E:229:TYR:CE1	2.52	0.45
1:G:194:ILE:O	1:G:198:VAL:HG23	2.17	0.45
1:H:144:LEU:HB2	1:H:252:ILE:O	2.17	0.45
1:H:254:ILE:HD12	1:H:254:ILE:O	2.17	0.45
1:I:249:CYS:SG	1:I:251:TYR:HB3	2.57	0.45
1:J:389:TYR:OH	1:J:429:GLY:HA2	2.17	0.45
1:K:58:TRP:NE1	1:K:284:GLU:OE1	2.49	0.45
1:K:229:TYR:HE2	1:K:231:GLU:HB2	1.82	0.45
1:K:394:GLN:C	1:K:398:LEU:HD23	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLU:OE2	1:C:479:SER:HA	2.17	0.45
1:E:477:ASP:HB3	1:F:469:ARG:HH12	1.81	0.45
1:K:81:GLN:OE1	1:K:433:ILE:CG2	2.65	0.45
1:K:438:ASP:N	1:K:438:ASP:OD1	2.49	0.45
1:A:144:LEU:C	1:A:144:LEU:HD12	2.38	0.45
1:B:359:ASN:OD1	1:C:380:GLU:HB2	2.17	0.45
1:C:404:LEU:HD23	1:C:404:LEU:HA	1.87	0.45
1:G:170:ARG:CZ	1:G:255:ARG:HD2	2.46	0.45
1:G:332:LEU:C	1:G:333:GLU:HG2	2.37	0.45
1:I:393:SER:OG	1:I:397:GLN:NE2	2.50	0.45
1:I:398:LEU:HD22	1:I:398:LEU:N	2.31	0.45
1:J:404:LEU:HD23	1:J:404:LEU:HA	1.83	0.45
1:K:77:LEU:CD2	1:K:389:TYR:CD1	3.00	0.45
1:K:275:ASP:HB2	1:K:352:LEU:HD21	1.97	0.45
1:L:334:LYS:HG3	1:L:334:LYS:O	2.17	0.45
1:A:389:TYR:OH	1:A:429:GLY:HA2	2.16	0.44
1:C:75:LEU:HD21	1:D:387:GLY:HA2	1.99	0.44
1:F:111:SER:O	1:F:115:ARG:HD3	2.16	0.44
1:G:58:TRP:CD1	1:G:284:GLU:HB2	2.51	0.44
1:H:59:GLN:HG3	1:H:280:GLU:OE1	2.17	0.44
1:H:205:LYS:HG2	1:H:209:GLU:OE2	2.17	0.44
1:I:25:ALA:N	1:I:26:PRO:HD2	2.33	0.44
1:I:463:LEU:N	1:I:463:LEU:HD23	2.32	0.44
1:K:142:ASN:ND2	1:K:255:ARG:HG3	2.32	0.44
1:K:249:CYS:SG	1:K:251:TYR:HB3	2.57	0.44
1:K:332:LEU:O	1:K:333:GLU:HG2	2.17	0.44
1:L:332:LEU:HD13	1:L:334:LYS:CG	2.41	0.44
1:A:385:LEU:C	1:A:385:LEU:HD23	2.38	0.44
1:B:60:ALA:HB1	1:C:272:TYR:HD1	1.82	0.44
1:C:393:SER:O	1:C:397:GLN:CB	2.57	0.44
1:C:404:LEU:O	1:C:408:LEU:HG	2.16	0.44
1:C:430:LEU:HG	1:C:435:ARG:O	2.17	0.44
1:D:216:HIS:HB3	1:D:229:TYR:CE1	2.52	0.44
1:H:275:ASP:HB3	1:H:348:ILE:HG23	1.97	0.44
1:I:254:ILE:HD12	1:I:254:ILE:C	2.37	0.44
1:J:136:GLN:HB3	1:J:143:VAL:HG21	1.98	0.44
1:K:25:ALA:N	1:K:26:PRO:HD2	2.31	0.44
1:K:81:GLN:OE1	1:K:433:ILE:HG21	2.17	0.44
1:K:96:LEU:HD11	1:K:420:GLU:HG2	2.00	0.44
1:A:359:ASN:OD1	1:B:380:GLU:HB2	2.17	0.44
1:C:110:LEU:O	1:C:113:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:TYR:HB2	1:D:244:TYR:HB2	2.00	0.44
1:D:275:ASP:HB2	1:D:352:LEU:HD21	1.98	0.44
1:D:430:LEU:HG	1:D:435:ARG:O	2.17	0.44
1:E:184:GLN:HA	1:E:211:ILE:O	2.17	0.44
1:J:187:PHE:HA	1:J:190:LEU:HG	1.99	0.44
1:K:185:ILE:O	1:K:186:ALA:HB3	2.17	0.44
1:B:277:ARG:HG3	1:B:278:SER:N	2.32	0.44
1:C:180:VAL:HA	1:C:215:THR:O	2.18	0.44
1:D:463:LEU:N	1:D:463:LEU:HD23	2.33	0.44
1:E:354:PHE:CD2	1:E:361:ALA:HB1	2.52	0.44
1:G:467:LYS:HE2	1:H:461:ILE:HD11	2.00	0.44
1:I:394:GLN:O	1:I:394:GLN:HG3	2.15	0.44
1:J:254:ILE:CD1	1:J:254:ILE:C	2.86	0.44
1:K:181:THR:HG23	1:K:215:THR:HB	2.00	0.44
1:K:396:LEU:HD23	1:K:396:LEU:O	2.17	0.44
1:L:27:TYR:CE2	1:L:264:TYR:HB2	2.53	0.44
1:A:125:SER:CA	1:B:394:GLN:HE21	1.96	0.44
1:D:254:ILE:HD12	1:D:254:ILE:C	2.37	0.44
1:E:87:THR:OG1	1:E:425:THR:OG1	2.36	0.44
1:F:270:GLU:O	1:F:273:LEU:HB3	2.17	0.44
1:G:256:MET:O	1:G:266:ARG:O	2.34	0.44
1:G:463:LEU:N	1:G:463:LEU:HD23	2.32	0.44
1:K:368:ARG:CD	1:L:368:ARG:HB2	2.46	0.44
1:D:142:ASN:O	1:D:143:VAL:HG23	2.17	0.44
1:E:96:LEU:HD11	1:E:420:GLU:HG2	2.00	0.44
1:E:180:VAL:HA	1:E:215:THR:O	2.18	0.44
1:E:187:PHE:HA	1:E:190:LEU:HG	1.99	0.44
1:E:463:LEU:N	1:E:463:LEU:HD23	2.32	0.44
1:G:404:LEU:HD23	1:G:404:LEU:HA	1.87	0.44
1:I:477:ASP:HB3	1:J:469:ARG:HH12	1.82	0.44
1:J:254:ILE:HD12	1:J:254:ILE:O	2.17	0.44
1:A:144:LEU:HD23	1:A:166:TYR:CE1	2.53	0.44
1:A:145:LEU:HD13	1:A:158:MET:HE1	1.99	0.44
1:A:260:ASP:O	1:L:159:LYS:NZ	2.49	0.44
1:C:96:LEU:HD11	1:C:420:GLU:HG2	1.99	0.44
1:E:273:LEU:HA	1:E:276:LEU:HB3	1.99	0.44
1:E:385:LEU:O	1:E:388:VAL:HG13	2.18	0.44
1:F:301:ASN:HD21	1:F:303:ALA:HB3	1.83	0.44
1:G:96:LEU:HD11	1:G:420:GLU:HG2	1.98	0.44
1:G:254:ILE:HD12	1:G:254:ILE:C	2.38	0.44
1:I:293:SER:HB3	1:J:337:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:354:PHE:CD2	1:I:361:ALA:HB1	2.53	0.44
1:J:216:HIS:HB3	1:J:229:TYR:CE1	2.53	0.44
1:K:352:LEU:O	1:K:356:PHE:HD2	1.99	0.44
1:L:145:LEU:HD13	1:L:158:MET:HE1	2.00	0.44
1:A:145:LEU:HD13	1:A:158:MET:CE	2.48	0.44
1:A:398:LEU:HD22	1:A:398:LEU:N	2.32	0.44
1:B:81:GLN:OE1	1:B:433:ILE:CG2	2.66	0.44
1:B:392:LEU:HD23	1:B:392:LEU:HA	1.83	0.44
1:C:91:TYR:O	1:C:95:GLN:HG2	2.17	0.44
1:C:463:LEU:N	1:C:463:LEU:HD23	2.33	0.44
1:F:81:GLN:OE1	1:F:433:ILE:CG2	2.65	0.44
1:I:332:LEU:C	1:I:333:GLU:HG2	2.38	0.44
1:K:136:GLN:HB3	1:K:143:VAL:HG21	1.99	0.44
1:L:136:GLN:HB3	1:L:143:VAL:HG21	1.98	0.44
1:A:143:VAL:H	1:A:254:ILE:CD1	2.19	0.44
1:A:170:ARG:NE	1:A:263:SER:O	2.47	0.44
1:A:404:LEU:O	1:A:408:LEU:HG	2.18	0.44
1:B:488:LYS:HG3	1:C:460:ASP:HB3	2.00	0.44
1:C:160:LEU:O	1:D:260:ASP:HB2	2.18	0.44
1:C:216:HIS:HB3	1:C:229:TYR:CE1	2.53	0.44
1:D:91:TYR:O	1:D:95:GLN:HG2	2.18	0.44
1:D:102:GLY:O	1:D:106:VAL:HG23	2.16	0.44
1:F:110:LEU:O	1:F:113:VAL:HB	2.17	0.44
1:F:202:GLY:O	1:F:205:LYS:HD3	2.18	0.44
1:F:275:ASP:HB2	1:F:352:LEU:HD21	1.99	0.44
1:G:85:ARG:HG3	1:G:114:GLU:OE2	2.18	0.44
1:H:352:LEU:O	1:H:356:PHE:HD2	2.01	0.44
1:I:254:ILE:CD1	1:I:254:ILE:C	2.86	0.44
1:I:389:TYR:OH	1:I:429:GLY:HA2	2.18	0.44
1:J:42:LEU:O	1:J:43:PHE:CD2	2.71	0.44
1:J:142:ASN:ND2	1:J:255:ARG:HG3	2.33	0.44
1:J:151:GLU:O	1:J:153:SER:N	2.51	0.44
1:C:58:TRP:NE1	1:C:284:GLU:OE1	2.51	0.43
1:D:385:LEU:O	1:D:388:VAL:HG13	2.18	0.43
1:E:226:TYR:HB2	1:E:244:TYR:HB2	2.00	0.43
1:E:398:LEU:N	1:E:398:LEU:HD22	2.32	0.43
1:F:385:LEU:HD23	1:F:385:LEU:O	2.18	0.43
1:G:260:ASP:OD1	1:G:261:GLY:N	2.51	0.43
1:G:372:GLU:C	1:G:374:ILE:H	2.21	0.43
1:H:42:LEU:O	1:H:43:PHE:CD2	2.71	0.43
1:H:58:TRP:NE1	1:H:284:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:270:GLU:O	1:J:273:LEU:HB3	2.18	0.43
1:J:385:LEU:O	1:J:388:VAL:HG13	2.18	0.43
1:K:16:VAL:HG11	1:K:178:GLN:NE2	2.32	0.43
1:K:216:HIS:HB3	1:K:229:TYR:CE1	2.53	0.43
1:A:184:GLN:HA	1:A:211:ILE:O	2.19	0.43
1:A:438:ASP:OD1	1:A:438:ASP:N	2.51	0.43
1:E:91:TYR:O	1:E:95:GLN:HG2	2.18	0.43
1:F:79:PRO:HD2	1:F:83:TRP:CD1	2.53	0.43
1:F:142:ASN:O	1:F:143:VAL:CG2	2.66	0.43
1:F:372:GLU:C	1:F:374:ILE:H	2.21	0.43
1:G:398:LEU:HD22	1:G:398:LEU:N	2.33	0.43
1:I:385:LEU:O	1:I:388:VAL:HG13	2.17	0.43
1:J:124:ASN:HD22	1:J:124:ASN:N	2.14	0.43
1:A:458:ASP:HB3	1:A:463:LEU:HD21	2.00	0.43
1:B:404:LEU:O	1:B:408:LEU:HG	2.18	0.43
1:C:59:GLN:HG3	1:C:280:GLU:OE1	2.19	0.43
1:C:142:ASN:ND2	1:C:255:ARG:HG3	2.33	0.43
1:D:18:GLU:OE1	1:D:18:GLU:HA	2.17	0.43
1:E:151:GLU:O	1:E:153:SER:N	2.52	0.43
1:K:467:LYS:NZ	1:L:461:ILE:HD11	2.33	0.43
1:A:27:TYR:OH	1:A:262:GLU:HG3	2.18	0.43
1:C:145:LEU:HD13	1:C:158:MET:HE1	2.00	0.43
1:F:187:PHE:HA	1:F:190:LEU:HG	2.00	0.43
1:I:113:VAL:O	1:I:117:ILE:HG12	2.19	0.43
1:A:111:SER:O	1:A:115:ARG:HD3	2.18	0.43
1:A:187:PHE:HA	1:A:190:LEU:HG	2.01	0.43
1:A:194:ILE:O	1:A:198:VAL:HB	2.19	0.43
1:A:230:GLU:CB	1:A:237:VAL:HG21	2.43	0.43
1:B:111:SER:OG	1:B:114:GLU:OE2	2.33	0.43
1:C:229:TYR:HE2	1:C:231:GLU:HB2	1.84	0.43
1:E:394:GLN:O	1:E:394:GLN:HG3	2.18	0.43
1:G:159:LYS:HE3	1:G:161:TYR:CE1	2.53	0.43
1:G:229:TYR:HE2	1:G:231:GLU:HB2	1.84	0.43
1:I:359:ASN:ND2	1:J:376:TYR:CE2	2.86	0.43
1:K:430:LEU:HG	1:K:435:ARG:O	2.18	0.43
1:L:81:GLN:OE1	1:L:433:ILE:CG2	2.66	0.43
1:B:137:LEU:HD13	1:B:254:ILE:HD13	2.00	0.43
1:B:194:ILE:O	1:B:198:VAL:HG23	2.19	0.43
1:B:463:LEU:N	1:B:463:LEU:HD23	2.32	0.43
1:D:27:TYR:CE2	1:D:264:TYR:HB2	2.54	0.43
1:D:77:LEU:CD2	1:D:389:TYR:CD1	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:LEU:C	1:E:333:GLU:HG2	2.37	0.43
1:H:91:TYR:O	1:H:95:GLN:HG2	2.18	0.43
1:I:483:LEU:HD12	1:J:460:ASP:HA	1.99	0.43
1:J:96:LEU:HD11	1:J:420:GLU:HG2	2.00	0.43
1:J:127:ARG:NH1	1:K:394:GLN:HB2	2.33	0.43
1:J:137:LEU:HD13	1:J:254:ILE:HD13	2.00	0.43
1:K:113:VAL:O	1:K:117:ILE:HG12	2.18	0.43
1:K:151:GLU:HA	1:K:151:GLU:OE2	2.18	0.43
1:L:275:ASP:N	1:L:275:ASP:OD1	2.52	0.43
1:L:404:LEU:O	1:L:408:LEU:HG	2.18	0.43
1:A:180:VAL:HA	1:A:215:THR:O	2.18	0.43
1:B:254:ILE:C	1:B:254:ILE:HD12	2.39	0.43
1:C:275:ASP:OD2	1:C:351:ARG:NH1	2.35	0.43
1:D:229:TYR:HE2	1:D:231:GLU:HB2	1.83	0.43
1:E:64:ARG:HA	1:F:272:TYR:OH	2.19	0.43
1:E:137:LEU:HD13	1:E:254:ILE:HD13	2.00	0.43
1:J:181:THR:CG2	1:J:215:THR:HB	2.48	0.43
1:L:463:LEU:N	1:L:463:LEU:HD23	2.34	0.43
1:A:137:LEU:HD13	1:A:254:ILE:HD13	2.00	0.43
1:A:394:GLN:C	1:A:398:LEU:HD23	2.39	0.43
1:B:16:VAL:O	1:B:20:LEU:HG	2.19	0.43
1:B:106:VAL:O	1:B:110:LEU:HD12	2.19	0.43
1:D:142:ASN:O	1:D:143:VAL:CG2	2.67	0.43
1:D:477:ASP:HB3	1:E:469:ARG:HH12	1.83	0.43
1:E:368:ARG:NE	1:F:368:ARG:HB2	2.34	0.43
1:F:142:ASN:O	1:F:143:VAL:HG23	2.19	0.43
1:F:181:THR:HG23	1:F:215:THR:HB	2.01	0.43
1:F:230:GLU:CB	1:F:237:VAL:HG21	2.45	0.43
1:G:315:GLN:N	1:G:318:ASP:OD2	2.52	0.43
1:I:60:ALA:HB1	1:J:272:TYR:HD1	1.84	0.43
1:I:96:LEU:HD11	1:I:420:GLU:HG2	2.00	0.43
1:I:404:LEU:HD23	1:I:404:LEU:HA	1.89	0.43
1:L:11:ASP:OD1	1:L:11:ASP:N	2.52	0.43
1:L:332:LEU:C	1:L:333:GLU:HG2	2.38	0.43
1:E:430:LEU:HD12	1:E:430:LEU:HA	1.88	0.43
1:H:137:LEU:HD13	1:H:254:ILE:HD13	2.00	0.43
1:H:205:LYS:HD3	1:H:209:GLU:HG2	2.01	0.43
1:K:180:VAL:HA	1:K:215:THR:O	2.19	0.43
1:A:181:THR:HG23	1:A:215:THR:HB	2.00	0.43
1:C:287:VAL:O	1:C:290:SER:OG	2.27	0.43
1:C:393:SER:CB	1:C:397:GLN:HE21	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:LEU:HD11	1:D:420:GLU:HG2	2.00	0.43
1:D:483:LEU:HD12	1:E:460:ASP:HA	2.00	0.43
1:E:75:LEU:HD21	1:F:387:GLY:HA2	2.01	0.43
1:E:102:GLY:O	1:E:106:VAL:HG23	2.18	0.43
1:F:352:LEU:O	1:F:356:PHE:HD2	2.01	0.43
1:F:363:GLN:HB3	1:G:373:GLU:OE1	2.19	0.43
1:G:38:THR:OG1	1:G:39:ILE:N	2.49	0.43
1:I:58:TRP:CD1	1:I:284:GLU:HB2	2.53	0.43
1:I:372:GLU:C	1:I:374:ILE:H	2.22	0.43
1:A:185:ILE:O	1:A:186:ALA:HB3	2.17	0.42
1:B:259:LEU:HD23	1:B:259:LEU:HA	1.90	0.42
1:B:448:ALA:O	1:B:451:ALA:HB3	2.19	0.42
1:B:477:ASP:HB3	1:C:469:ARG:HH12	1.84	0.42
1:C:137:LEU:HD13	1:C:254:ILE:HD13	2.00	0.42
1:C:259:LEU:HD23	1:C:259:LEU:HA	1.91	0.42
1:E:372:GLU:C	1:E:374:ILE:H	2.22	0.42
1:E:394:GLN:O	1:E:398:LEU:HD23	2.19	0.42
1:F:463:LEU:N	1:F:463:LEU:HD23	2.32	0.42
1:G:151:GLU:O	1:G:153:SER:N	2.52	0.42
1:I:110:LEU:O	1:I:113:VAL:HB	2.19	0.42
1:I:151:GLU:HA	1:I:151:GLU:OE2	2.18	0.42
1:I:187:PHE:HA	1:I:190:LEU:HG	2.01	0.42
1:J:127:ARG:HH12	1:K:394:GLN:HB2	1.84	0.42
1:J:144:LEU:HB2	1:J:252:ILE:O	2.19	0.42
1:L:187:PHE:HA	1:L:190:LEU:HG	2.00	0.42
1:L:273:LEU:HA	1:L:276:LEU:HB3	1.99	0.42
1:L:389:TYR:OH	1:L:429:GLY:HA2	2.19	0.42
1:L:438:ASP:OD1	1:L:438:ASP:N	2.51	0.42
1:B:294:SER:HA	1:C:289:MET:HE1	2.02	0.42
1:C:254:ILE:HD12	1:C:254:ILE:C	2.39	0.42
1:C:373:GLU:O	1:C:377:VAL:HG22	2.19	0.42
1:D:84:MET:N	1:D:84:MET:SD	2.92	0.42
1:D:136:GLN:NE2	1:D:162:ARG:HD2	2.33	0.42
1:E:445:CYS:HB3	1:E:476:ILE:HD11	2.01	0.42
1:E:477:ASP:HB3	1:F:469:ARG:NH1	2.34	0.42
1:F:294:SER:HA	1:G:289:MET:CE	2.49	0.42
1:G:254:ILE:CD1	1:G:254:ILE:C	2.87	0.42
1:J:393:SER:O	1:J:397:GLN:CB	2.57	0.42
1:K:110:LEU:O	1:K:113:VAL:HB	2.19	0.42
1:K:260:ASP:OD1	1:K:261:GLY:N	2.52	0.42
1:L:81:GLN:OE1	1:L:433:ILE:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:250:PRO:HB3	1:L:407:GLN:HE21	1.84	0.42
1:A:226:TYR:HB2	1:A:244:TYR:HB2	2.00	0.42
1:A:458:ASP:OD2	1:A:461:ILE:O	2.37	0.42
1:D:332:LEU:CD1	1:D:334:LYS:N	2.71	0.42
1:G:344:VAL:O	1:G:348:ILE:HD12	2.20	0.42
1:G:479:SER:HB3	1:H:469:ARG:HH22	1.83	0.42
1:H:254:ILE:HD12	1:H:254:ILE:C	2.40	0.42
1:I:151:GLU:O	1:I:153:SER:N	2.52	0.42
1:I:185:ILE:O	1:I:186:ALA:HB3	2.20	0.42
1:I:186:ALA:HB2	1:I:210:THR:HG22	2.01	0.42
1:I:230:GLU:CB	1:I:237:VAL:HG21	2.46	0.42
1:I:404:LEU:O	1:I:408:LEU:HG	2.19	0.42
1:I:458:ASP:HB3	1:I:463:LEU:HD21	2.01	0.42
1:A:354:PHE:CD2	1:A:361:ALA:HB1	2.54	0.42
1:A:354:PHE:CE2	1:A:361:ALA:HB1	2.54	0.42
1:A:430:LEU:HG	1:A:435:ARG:O	2.20	0.42
1:C:113:VAL:O	1:C:117:ILE:HG12	2.18	0.42
1:C:145:LEU:HD13	1:C:158:MET:CE	2.50	0.42
1:D:81:GLN:OE1	1:D:433:ILE:CG2	2.67	0.42
1:E:92:GLU:O	1:E:96:LEU:HG	2.20	0.42
1:E:479:SER:HB3	1:F:469:ARG:HH22	1.84	0.42
1:F:254:ILE:HD12	1:F:254:ILE:C	2.39	0.42
1:G:273:LEU:C	1:G:273:LEU:CD2	2.84	0.42
1:I:273:LEU:HA	1:I:276:LEU:HB3	2.01	0.42
1:J:332:LEU:HD13	1:J:334:LYS:CG	2.44	0.42
1:J:479:SER:HB3	1:K:469:ARG:HH22	1.84	0.42
1:K:358:LEU:HD23	1:K:358:LEU:HA	1.88	0.42
1:K:458:ASP:HB3	1:K:463:LEU:HD21	2.01	0.42
1:L:456:ARG:HA	1:L:463:LEU:HD11	2.02	0.42
1:A:275:ASP:N	1:A:275:ASP:OD1	2.50	0.42
1:C:334:LYS:HG3	1:C:334:LYS:O	2.19	0.42
1:D:77:LEU:HD23	1:D:389:TYR:HE1	1.70	0.42
1:D:373:GLU:O	1:D:377:VAL:HG22	2.19	0.42
1:G:186:ALA:HB2	1:G:210:THR:HG22	2.01	0.42
1:G:396:LEU:HD23	1:G:396:LEU:O	2.18	0.42
1:H:81:GLN:OE1	1:H:433:ILE:CG2	2.68	0.42
1:H:81:GLN:OE1	1:H:433:ILE:HG21	2.19	0.42
1:H:186:ALA:HB2	1:H:210:THR:HG22	2.02	0.42
1:I:338:PHE:CD1	1:J:340:VAL:HG13	2.54	0.42
1:L:146:TYR:HD2	1:L:161:TYR:HE2	1.67	0.42
1:A:270:GLU:O	1:A:273:LEU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASP:HB2	1:A:352:LEU:HD21	2.01	0.42
1:B:330:LEU:HA	1:B:330:LEU:HD23	1.85	0.42
1:B:334:LYS:O	1:B:334:LYS:HG3	2.19	0.42
1:C:430:LEU:HD12	1:C:430:LEU:HA	1.83	0.42
1:D:144:LEU:HD12	1:D:144:LEU:C	2.40	0.42
1:D:398:LEU:N	1:D:399:PRO:CD	2.83	0.42
1:E:457:ASP:O	1:E:459:PRO:HD3	2.20	0.42
1:G:187:PHE:HA	1:G:190:LEU:HG	2.00	0.42
1:G:287:VAL:O	1:G:290:SER:OG	2.33	0.42
1:H:113:VAL:O	1:H:117:ILE:HG12	2.20	0.42
1:H:159:LYS:HE3	1:H:161:TYR:CE1	2.55	0.42
1:H:181:THR:HG23	1:H:215:THR:HB	2.01	0.42
1:I:146:TYR:HD2	1:I:161:TYR:HE2	1.67	0.42
1:I:229:TYR:HE2	1:I:231:GLU:HB2	1.85	0.42
1:J:159:LYS:HE3	1:J:161:TYR:CE1	2.55	0.42
1:C:38:THR:OG1	1:C:39:ILE:N	2.48	0.42
1:C:81:GLN:OE1	1:C:433:ILE:CG2	2.68	0.42
1:C:89:SER:HB2	1:C:92:GLU:HG2	2.02	0.42
1:D:354:PHE:CD2	1:D:361:ALA:HB1	2.55	0.42
1:D:393:SER:CB	1:D:397:GLN:NE2	2.82	0.42
1:E:324:PRO:HD3	1:F:328:SER:HB2	2.01	0.42
1:G:77:LEU:CD2	1:G:389:TYR:CD1	3.03	0.42
1:G:294:SER:HA	1:H:289:MET:HE1	2.01	0.42
1:H:354:PHE:CE2	1:H:361:ALA:HB1	2.54	0.42
1:H:392:LEU:HD23	1:H:392:LEU:HA	1.85	0.42
1:J:180:VAL:HA	1:J:215:THR:O	2.20	0.42
1:L:96:LEU:HD11	1:L:420:GLU:HG2	2.01	0.42
1:C:254:ILE:CD1	1:C:254:ILE:C	2.88	0.42
1:F:85:ARG:HG3	1:F:114:GLU:OE2	2.20	0.42
1:H:96:LEU:HD11	1:H:420:GLU:HG2	2.00	0.42
1:H:260:ASP:OD1	1:H:261:GLY:N	2.52	0.42
1:H:458:ASP:HB3	1:H:463:LEU:HD21	2.01	0.42
1:K:293:SER:HB3	1:L:337:ASP:HB3	2.02	0.42
1:K:463:LEU:N	1:K:463:LEU:HD23	2.34	0.42
1:A:324:PRO:HD3	1:B:328:SER:HB2	2.01	0.42
1:A:374:ILE:HD13	1:B:372:GLU:HB2	2.02	0.42
1:C:467:LYS:NZ	1:D:461:ILE:HD11	2.35	0.42
1:D:301:ASN:HD21	1:D:303:ALA:HB3	1.85	0.42
1:D:394:GLN:C	1:D:398:LEU:HD23	2.41	0.42
1:E:159:LYS:HE3	1:E:161:TYR:CE1	2.55	0.42
1:E:404:LEU:HD23	1:E:404:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:ASN:HD21	1:F:255:ARG:HG3	1.85	0.42
1:F:185:ILE:O	1:F:186:ALA:HB3	2.19	0.42
1:G:363:GLN:HB3	1:H:373:GLU:OE1	2.19	0.42
1:H:398:LEU:N	1:H:399:PRO:CD	2.82	0.42
1:I:81:GLN:OE1	1:I:433:ILE:HG21	2.20	0.42
1:K:220:ASP:OD2	1:K:223:SER:HB2	2.20	0.42
1:K:226:TYR:HB2	1:K:244:TYR:HB2	2.02	0.42
1:B:104:ALA:O	1:B:108:GLU:HG3	2.20	0.42
1:B:187:PHE:HA	1:B:190:LEU:HG	2.00	0.42
1:D:159:LYS:HE3	1:D:161:TYR:CE1	2.54	0.42
1:E:270:GLU:O	1:E:273:LEU:HB3	2.20	0.42
1:G:77:LEU:HD23	1:G:389:TYR:CD1	2.53	0.42
1:G:275:ASP:HB2	1:G:352:LEU:HD21	2.02	0.42
1:H:144:LEU:HD23	1:H:166:TYR:CE1	2.54	0.42
1:H:414:ILE:CG2	1:H:417:LEU:HD11	2.50	0.42
1:H:458:ASP:OD2	1:H:461:ILE:O	2.38	0.42
1:I:144:LEU:HB2	1:I:252:ILE:O	2.20	0.42
1:J:357:MET:HE1	1:J:384:THR:OG1	2.20	0.42
1:L:458:ASP:HB3	1:L:463:LEU:HD21	2.02	0.42
1:A:237:VAL:HG11	1:A:240:SER:HB3	2.02	0.41
1:B:81:GLN:OE1	1:B:433:ILE:HG21	2.20	0.41
1:C:250:PRO:HB3	1:C:407:GLN:HE21	1.85	0.41
1:E:81:GLN:OE1	1:E:433:ILE:CG2	2.68	0.41
1:F:187:PHE:CD2	1:F:205:LYS:CB	3.03	0.41
1:G:16:VAL:O	1:G:20:LEU:HG	2.20	0.41
1:H:142:ASN:OD1	1:H:265:GLY:N	2.48	0.41
1:J:392:LEU:HD23	1:J:392:LEU:HA	1.86	0.41
1:K:104:ALA:O	1:K:108:GLU:HG3	2.20	0.41
1:L:330:LEU:HD23	1:L:330:LEU:HA	1.84	0.41
1:L:372:GLU:C	1:L:374:ILE:H	2.22	0.41
1:D:187:PHE:HA	1:D:190:LEU:HG	2.01	0.41
1:E:294:SER:O	1:F:289:MET:HE2	2.19	0.41
1:F:59:GLN:C	1:F:59:GLN:OE1	2.58	0.41
1:F:131:PHE:CD1	1:G:391:ILE:HD11	2.54	0.41
1:G:458:ASP:HB3	1:G:463:LEU:HD21	2.02	0.41
1:H:159:LYS:NZ	1:I:260:ASP:O	2.54	0.41
1:H:358:LEU:HD23	1:H:358:LEU:HA	1.91	0.41
1:H:488:LYS:HG3	1:I:460:ASP:HB3	2.02	0.41
1:I:137:LEU:HD13	1:I:254:ILE:HD13	2.01	0.41
1:K:301:ASN:ND2	1:K:303:ALA:HB3	2.34	0.41
1:L:216:HIS:HB3	1:L:229:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:237:VAL:HG11	1:L:240:SER:HB3	2.03	0.41
1:B:254:ILE:C	1:B:254:ILE:CD1	2.88	0.41
1:E:136:GLN:O	1:E:140:ALA:HB3	2.20	0.41
1:E:144:LEU:HD23	1:E:166:TYR:CE1	2.56	0.41
1:F:254:ILE:CD1	1:F:254:ILE:C	2.88	0.41
1:G:145:LEU:HB3	1:G:158:MET:HE3	2.01	0.41
1:G:369:VAL:HG13	1:G:373:GLU:OE1	2.20	0.41
1:G:438:ASP:OD1	1:G:438:ASP:N	2.54	0.41
1:H:254:ILE:CD1	1:H:254:ILE:C	2.89	0.41
1:H:354:PHE:CD2	1:H:361:ALA:HB1	2.54	0.41
1:H:359:ASN:ND2	1:I:376:TYR:CE2	2.88	0.41
1:I:27:TYR:OH	1:I:262:GLU:HG3	2.20	0.41
1:J:34:CYS:SG	1:J:269:ILE:O	2.73	0.41
1:K:230:GLU:CB	1:K:237:VAL:HG21	2.43	0.41
1:L:354:PHE:CE2	1:L:361:ALA:HB1	2.56	0.41
1:C:385:LEU:O	1:C:388:VAL:HG13	2.20	0.41
1:D:181:THR:CG2	1:D:215:THR:HB	2.50	0.41
1:D:357:MET:SD	1:D:385:LEU:HB2	2.60	0.41
1:E:145:LEU:HD13	1:E:158:MET:HE1	2.02	0.41
1:E:181:THR:CG2	1:E:215:THR:HB	2.50	0.41
1:F:430:LEU:HG	1:F:435:ARG:O	2.19	0.41
1:G:374:ILE:HD13	1:H:373:GLU:N	2.34	0.41
1:H:315:GLN:N	1:H:318:ASP:OD2	2.53	0.41
1:H:404:LEU:HD23	1:H:404:LEU:HA	1.85	0.41
1:J:185:ILE:O	1:J:186:ALA:HB3	2.20	0.41
1:J:393:SER:CB	1:J:397:GLN:NE2	2.83	0.41
1:K:142:ASN:C	1:K:143:VAL:HG23	2.41	0.41
1:K:144:LEU:HB2	1:K:252:ILE:O	2.20	0.41
1:K:338:PHE:CD1	1:L:340:VAL:HG13	2.56	0.41
1:A:101:ASP:OD1	1:A:101:ASP:N	2.53	0.41
1:A:289:MET:CE	1:L:294:SER:HA	2.50	0.41
1:B:144:LEU:C	1:B:144:LEU:HD12	2.41	0.41
1:C:39:ILE:HG13	1:D:271:GLU:HB3	2.03	0.41
1:C:250:PRO:HB3	1:C:407:GLN:NE2	2.36	0.41
1:C:372:GLU:C	1:C:374:ILE:H	2.22	0.41
1:E:75:LEU:HD11	1:F:387:GLY:N	2.35	0.41
1:E:83:TRP:CE3	1:E:84:MET:HE3	2.55	0.41
1:F:142:ASN:C	1:F:143:VAL:HG23	2.41	0.41
1:F:344:VAL:O	1:F:348:ILE:HD12	2.20	0.41
1:H:58:TRP:CD1	1:H:284:GLU:HB2	2.55	0.41
1:H:229:TYR:HE2	1:H:231:GLU:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:ILE:HG13	1:K:271:GLU:HB3	2.03	0.41
1:J:108:GLU:OE2	1:K:479:SER:HA	2.19	0.41
1:J:332:LEU:CD1	1:J:332:LEU:C	2.83	0.41
1:K:254:ILE:HD12	1:K:254:ILE:C	2.40	0.41
1:K:270:GLU:O	1:K:273:LEU:HB3	2.20	0.41
1:L:91:TYR:O	1:L:95:GLN:HG2	2.21	0.41
1:L:137:LEU:HD13	1:L:254:ILE:HD13	2.02	0.41
1:A:96:LEU:HD11	1:A:420:GLU:HG2	2.01	0.41
1:B:78:PHE:CE2	1:B:130:LEU:HD23	2.55	0.41
1:C:136:GLN:O	1:C:140:ALA:HB3	2.20	0.41
1:D:77:LEU:HD23	1:D:389:TYR:CD1	2.53	0.41
1:D:185:ILE:O	1:D:186:ALA:HB3	2.20	0.41
1:D:270:GLU:O	1:D:273:LEU:HB3	2.21	0.41
1:D:354:PHE:CE2	1:D:361:ALA:HB1	2.56	0.41
1:D:445:CYS:HB3	1:D:476:ILE:HD11	2.02	0.41
1:J:226:TYR:HB2	1:J:244:TYR:HB2	2.03	0.41
1:J:359:ASN:ND2	1:K:376:TYR:CE2	2.88	0.41
1:K:151:GLU:O	1:K:153:SER:N	2.54	0.41
1:L:136:GLN:O	1:L:140:ALA:HB3	2.21	0.41
1:G:115:ARG:NH2	1:H:90:GLU:OE1	2.53	0.41
1:G:181:THR:CG2	1:G:215:THR:HB	2.50	0.41
1:G:230:GLU:CB	1:G:237:VAL:HG21	2.43	0.41
1:H:127:ARG:HH12	1:I:394:GLN:HB2	1.85	0.41
1:I:59:GLN:HG3	1:I:280:GLU:OE1	2.20	0.41
1:J:358:LEU:HD23	1:J:358:LEU:HA	1.88	0.41
1:L:145:LEU:HD13	1:L:158:MET:CE	2.50	0.41
1:L:159:LYS:HE3	1:L:161:TYR:CE1	2.55	0.41
1:L:287:VAL:O	1:L:290:SER:OG	2.32	0.41
1:A:110:LEU:O	1:A:113:VAL:HB	2.21	0.41
1:A:334:LYS:HG3	1:A:334:LYS:O	2.20	0.41
1:A:394:GLN:OE1	1:L:127:ARG:NH1	2.54	0.41
1:C:81:GLN:OE1	1:C:433:ILE:HG21	2.21	0.41
1:C:187:PHE:HA	1:C:190:LEU:HG	2.01	0.41
1:F:209:GLU:O	1:F:210:THR:OG1	2.32	0.41
1:G:430:LEU:HD12	1:G:430:LEU:HA	1.87	0.41
1:H:170:ARG:CZ	1:H:255:ARG:HD2	2.51	0.41
1:I:138:VAL:CG1	1:I:269:ILE:HD11	2.51	0.41
1:J:229:TYR:HE2	1:J:231:GLU:HB2	1.85	0.41
1:K:259:LEU:HD23	1:K:259:LEU:HA	1.91	0.41
1:L:398:LEU:N	1:L:399:PRO:CD	2.83	0.41
1:A:11:ASP:N	1:A:11:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:NE2	1:A:162:ARG:HD2	2.36	0.41
1:B:216:HIS:HB3	1:B:229:TYR:CE1	2.55	0.41
1:B:414:ILE:CG2	1:B:417:LEU:HD11	2.51	0.41
1:C:8:LEU:HD12	1:C:218:TYR:HB3	2.03	0.41
1:E:59:GLN:C	1:E:59:GLN:OE1	2.59	0.41
1:E:220:ASP:OD2	1:E:223:SER:HB2	2.20	0.41
1:E:275:ASP:HB2	1:E:352:LEU:HD21	2.03	0.41
1:E:357:MET:HE1	1:E:384:THR:OG1	2.21	0.41
1:E:430:LEU:HG	1:E:435:ARG:O	2.20	0.41
1:E:458:ASP:HB3	1:E:463:LEU:HD21	2.03	0.41
1:F:144:LEU:HB2	1:F:252:ILE:O	2.21	0.41
1:F:273:LEU:HA	1:F:276:LEU:HB3	2.02	0.41
1:F:453:ALA:N	1:F:454:PRO:CD	2.84	0.41
1:G:354:PHE:CE2	1:G:361:ALA:HB1	2.56	0.41
1:H:138:VAL:HG13	1:H:269:ILE:HG13	2.03	0.41
1:H:332:LEU:CD1	1:H:332:LEU:C	2.83	0.41
1:I:125:SER:CA	1:J:394:GLN:NE2	2.58	0.41
1:I:146:TYR:CE1	1:I:148:PRO:HB3	2.56	0.41
1:I:301:ASN:HD21	1:I:303:ALA:HB3	1.85	0.41
1:J:334:LYS:HG3	1:J:334:LYS:O	2.21	0.41
1:J:401:VAL:CG1	1:J:426:ILE:HG21	2.43	0.41
1:J:458:ASP:HB3	1:J:463:LEU:HD21	2.02	0.41
1:K:137:LEU:HD13	1:K:254:ILE:HD13	2.02	0.41
1:K:170:ARG:CZ	1:K:255:ARG:HD2	2.51	0.41
1:K:467:LYS:CE	1:L:461:ILE:HD11	2.50	0.41
1:A:138:VAL:HG13	1:A:269:ILE:HG13	2.02	0.41
1:B:145:LEU:HD13	1:B:158:MET:CE	2.51	0.41
1:B:275:ASP:N	1:B:275:ASP:OD1	2.53	0.41
1:C:309:ARG:HG3	1:C:310:ARG:N	2.36	0.41
1:D:131:PHE:HB2	1:E:391:ILE:HD11	2.01	0.41
1:F:414:ILE:CG2	1:F:417:LEU:HD11	2.51	0.41
1:F:414:ILE:HG22	1:F:417:LEU:HD11	2.03	0.41
1:F:430:LEU:HD12	1:F:430:LEU:HA	1.87	0.41
1:G:91:TYR:O	1:G:95:GLN:HG2	2.20	0.41
1:H:104:ALA:O	1:H:108:GLU:HG3	2.21	0.41
1:H:275:ASP:N	1:H:275:ASP:OD1	2.54	0.41
1:I:315:GLN:N	1:I:318:ASP:OD2	2.54	0.41
1:J:354:PHE:CE2	1:J:361:ALA:HB1	2.56	0.41
1:J:372:GLU:C	1:J:374:ILE:H	2.23	0.41
1:L:230:GLU:CB	1:L:237:VAL:HG21	2.44	0.41
1:A:217:ILE:HA	1:A:227:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASN:C	1:B:143:VAL:HG23	2.42	0.40
1:C:237:VAL:HG11	1:C:240:SER:HB3	2.02	0.40
1:D:294:SER:O	1:E:289:MET:HE2	2.21	0.40
1:D:332:LEU:O	1:D:333:GLU:HG2	2.20	0.40
1:D:401:VAL:CG1	1:D:426:ILE:HG21	2.40	0.40
1:G:137:LEU:HD13	1:G:254:ILE:HD13	2.03	0.40
1:G:151:GLU:HA	1:G:151:GLU:OE2	2.21	0.40
1:H:146:TYR:HD2	1:H:161:TYR:HE2	1.69	0.40
1:H:220:ASP:OD2	1:H:223:SER:HB2	2.21	0.40
1:I:145:LEU:HD13	1:I:158:MET:HE1	2.03	0.40
1:K:159:LYS:HE3	1:K:161:TYR:CE1	2.55	0.40
1:L:226:TYR:HB2	1:L:244:TYR:HB2	2.03	0.40
1:L:385:LEU:HD23	1:L:385:LEU:O	2.21	0.40
1:B:250:PRO:HB3	1:B:407:GLN:HE21	1.87	0.40
1:B:287:VAL:O	1:B:290:SER:OG	2.34	0.40
1:B:354:PHE:CE2	1:B:361:ALA:HB1	2.56	0.40
1:B:401:VAL:CG1	1:B:426:ILE:HG21	2.43	0.40
1:C:186:ALA:HB2	1:C:210:THR:HG22	2.03	0.40
1:D:142:ASN:C	1:D:143:VAL:HG23	2.41	0.40
1:D:144:LEU:HD23	1:D:166:TYR:CE1	2.56	0.40
1:E:77:LEU:CD2	1:E:389:TYR:CD1	3.04	0.40
1:E:79:PRO:HD2	1:E:83:TRP:CD1	2.57	0.40
1:G:259:LEU:HD23	1:G:259:LEU:HA	1.93	0.40
1:G:357:MET:SD	1:G:385:LEU:HB2	2.62	0.40
1:I:58:TRP:CD2	1:I:284:GLU:HB2	2.56	0.40
1:I:194:ILE:O	1:I:198:VAL:N	2.54	0.40
1:J:146:TYR:HD2	1:J:161:TYR:HE2	1.69	0.40
1:K:254:ILE:HD12	1:K:254:ILE:O	2.21	0.40
1:K:389:TYR:OH	1:K:429:GLY:HA2	2.20	0.40
1:B:142:ASN:O	1:B:143:VAL:CG2	2.70	0.40
1:C:138:VAL:HG12	1:C:269:ILE:CD1	2.43	0.40
1:D:27:TYR:OH	1:D:262:GLU:HG3	2.22	0.40
1:D:260:ASP:OD1	1:D:261:GLY:N	2.54	0.40
1:D:404:LEU:HD23	1:D:404:LEU:HA	1.86	0.40
1:F:58:TRP:NE1	1:F:284:GLU:OE1	2.54	0.40
1:F:159:LYS:CD	1:G:172:ALA:O	2.64	0.40
1:F:250:PRO:HB3	1:F:407:GLN:HE21	1.86	0.40
1:G:81:GLN:OE1	1:G:433:ILE:CG2	2.69	0.40
1:G:110:LEU:O	1:G:113:VAL:HB	2.22	0.40
1:G:160:LEU:O	1:H:260:ASP:HB2	2.22	0.40
1:G:398:LEU:N	1:G:399:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:414:ILE:HG22	1:H:417:LEU:HD11	2.02	0.40
1:I:142:ASN:C	1:I:143:VAL:HG23	2.42	0.40
1:I:159:LYS:HE3	1:I:161:TYR:CE1	2.57	0.40
1:J:354:PHE:CD2	1:J:361:ALA:HB1	2.57	0.40
1:K:27:TYR:OH	1:K:262:GLU:HG3	2.21	0.40
1:L:85:ARG:HG3	1:L:114:GLU:OE2	2.21	0.40
1:A:332:LEU:CD1	1:A:332:LEU:C	2.86	0.40
1:A:376:TYR:CE2	1:L:359:ASN:ND2	2.89	0.40
1:C:181:THR:CG2	1:C:215:THR:HB	2.51	0.40
1:C:212:ASP:OD1	1:C:212:ASP:N	2.54	0.40
1:C:393:SER:CB	1:C:397:GLN:NE2	2.85	0.40
1:C:401:VAL:CG1	1:C:426:ILE:HG21	2.42	0.40
1:C:414:ILE:CG2	1:C:417:LEU:HD11	2.51	0.40
1:E:237:VAL:HG11	1:E:240:SER:HB3	2.04	0.40
1:F:113:VAL:O	1:F:117:ILE:HG12	2.22	0.40
1:F:354:PHE:CD2	1:F:361:ALA:HB1	2.57	0.40
1:G:354:PHE:CD2	1:G:361:ALA:HB1	2.56	0.40
1:G:458:ASP:OD2	1:G:461:ILE:O	2.39	0.40
1:J:11:ASP:N	1:J:11:ASP:OD1	2.55	0.40
1:J:184:GLN:HA	1:J:211:ILE:O	2.21	0.40
1:J:445:CYS:SG	1:J:449:TRP:CE2	3.14	0.40
1:J:456:ARG:HA	1:J:463:LEU:HD11	2.03	0.40
1:K:59:GLN:C	1:K:59:GLN:OE1	2.59	0.40
1:K:217:ILE:HA	1:K:227:LEU:O	2.21	0.40
1:K:401:VAL:CG1	1:K:426:ILE:HG21	2.39	0.40
1:K:430:LEU:HD12	1:K:430:LEU:HA	1.86	0.40
1:L:142:ASN:ND2	1:L:255:ARG:HG3	2.36	0.40
1:L:186:ALA:HB2	1:L:210:THR:HG22	2.02	0.40
1:L:357:MET:SD	1:L:385:LEU:HB2	2.61	0.40
1:B:27:TYR:CE2	1:B:264:TYR:HB2	2.57	0.40
1:C:144:LEU:HD23	1:C:166:TYR:CE1	2.57	0.40
1:E:146:TYR:HD2	1:E:161:TYR:HE2	1.70	0.40
1:E:374:ILE:HD13	1:F:372:GLU:HB2	2.03	0.40
1:F:18:GLU:OE1	1:F:18:GLU:HA	2.20	0.40
1:G:113:VAL:O	1:G:117:ILE:HG12	2.21	0.40
1:K:187:PHE:CD2	1:K:205:LYS:CB	3.05	0.40
1:K:254:ILE:CD1	1:K:254:ILE:C	2.89	0.40
1:K:488:LYS:HG3	1:L:460:ASP:HB3	2.03	0.40

All (13) 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:321:THR:CG2	1:G:91:TYR:CE2[3_445]	1.14	1.06
1:D:18:GLU:OE1	1:H:222:ASP:OD1[3_445]	1.32	0.88
1:B:321:THR:CG2	1:G:91:TYR:CZ[3_445]	1.46	0.74
1:C:423:GLU:OE1	1:H:206:LYS:NZ[2_454]	1.47	0.73
1:B:321:THR:CG2	1:G:91:TYR:OH[3_445]	1.78	0.42
1:A:196:LYS:NZ	1:C:192:GLU:OE1[4_545]	1.87	0.33
1:C:423:GLU:CD	1:H:206:LYS:NZ[2_454]	1.88	0.32
1:C:423:GLU:OE2	1:H:206:LYS:NZ[2_454]	1.96	0.24
1:A:234:GLY:O	1:I:238:GLN:NE2[3_545]	1.97	0.23
1:D:11:ASP:OD2	1:H:6:THR:CG2[3_445]	1.97	0.23
1:D:18:GLU:CD	1:H:222:ASP:OD1[3_445]	2.03	0.17
1:B:309:ARG:NH2	1:G:423:GLU:OE2[3_445]	2.06	0.14
1:B:321:THR:CB	1:G:91:TYR:CE2[3_445]	2.07	0.13

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	475/490 (97%)	410 (86%)	54 (11%)	11 (2%)	6 38
1	B	475/490 (97%)	404 (85%)	59 (12%)	12 (2%)	5 36
1	C	475/490 (97%)	414 (87%)	50 (10%)	11 (2%)	6 38
1	D	475/490 (97%)	407 (86%)	56 (12%)	12 (2%)	5 36
1	E	475/490 (97%)	407 (86%)	55 (12%)	13 (3%)	5 35
1	F	475/490 (97%)	409 (86%)	53 (11%)	13 (3%)	5 35
1	G	475/490 (97%)	412 (87%)	51 (11%)	12 (2%)	5 36
1	H	475/490 (97%)	408 (86%)	55 (12%)	12 (2%)	5 36
1	I	475/490 (97%)	410 (86%)	53 (11%)	12 (2%)	5 36
1	J	475/490 (97%)	406 (86%)	56 (12%)	13 (3%)	5 35
1	K	475/490 (97%)	408 (86%)	55 (12%)	12 (2%)	5 36
1	L	475/490 (97%)	408 (86%)	56 (12%)	11 (2%)	6 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5700/5880 (97%)	4903 (86%)	653 (12%)	144 (2%)	5 36

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	VAL
1	A	210	THR
1	B	143	VAL
1	B	210	THR
1	C	143	VAL
1	C	210	THR
1	D	143	VAL
1	D	210	THR
1	E	143	VAL
1	E	210	THR
1	F	143	VAL
1	F	210	THR
1	G	143	VAL
1	G	210	THR
1	H	143	VAL
1	H	210	THR
1	I	143	VAL
1	I	210	THR
1	J	210	THR
1	K	143	VAL
1	K	210	THR
1	L	143	VAL
1	L	210	THR
1	A	152	GLY
1	A	224	GLY
1	B	152	GLY
1	B	224	GLY
1	C	224	GLY
1	C	369	VAL
1	D	152	GLY
1	D	224	GLY
1	D	233	GLU
1	E	152	GLY
1	E	224	GLY
1	F	224	GLY
1	G	152	GLY
1	G	224	GLY

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Mol	Chain	Res	Type
1	G	233	GLU
1	G	369	VAL
1	H	152	GLY
1	H	224	GLY
1	H	369	VAL
1	I	152	GLY
1	I	224	GLY
1	I	233	GLU
1	J	143	VAL
1	J	152	GLY
1	J	224	GLY
1	J	233	GLU
1	K	152	GLY
1	K	224	GLY
1	L	152	GLY
1	L	224	GLY
1	L	369	VAL
1	A	233	GLU
1	A	369	VAL
1	B	155	TYR
1	B	233	GLU
1	B	369	VAL
1	C	152	GLY
1	C	233	GLU
1	D	369	VAL
1	E	233	GLU
1	E	369	VAL
1	F	152	GLY
1	F	233	GLU
1	F	369	VAL
1	G	186	ALA
1	H	233	GLU
1	I	369	VAL
1	J	369	VAL
1	K	233	GLU
1	K	369	VAL
1	L	233	GLU
1	A	186	ALA
1	B	186	ALA
1	E	186	ALA
1	H	186	ALA
1	I	186	ALA

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Mol	Chain	Res	Type
1	J	186	ALA
1	K	186	ALA
1	L	186	ALA
1	A	253	PRO
1	C	186	ALA
1	C	253	PRO
1	C	263	SER
1	D	186	ALA
1	D	222	ASP
1	F	186	ALA
1	F	253	PRO
1	G	263	SER
1	H	222	ASP
1	H	253	PRO
1	I	222	ASP
1	I	253	PRO
1	I	263	SER
1	J	222	ASP
1	J	253	PRO
1	J	263	SER
1	A	257	VAL
1	A	263	SER
1	B	253	PRO
1	B	257	VAL
1	B	263	SER
1	C	257	VAL
1	D	257	VAL
1	E	222	ASP
1	E	253	PRO
1	E	257	VAL
1	E	269	ILE
1	F	222	ASP
1	F	257	VAL
1	F	263	SER
1	G	222	ASP
1	G	257	VAL
1	H	257	VAL
1	H	263	SER
1	I	257	VAL
1	J	257	VAL
1	K	253	PRO
1	K	257	VAL

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Mol	Chain	Res	Type
1	K	373	GLU
1	L	257	VAL
1	L	269	ILE
1	A	269	ILE
1	D	253	PRO
1	D	274	GLY
1	F	269	ILE
1	G	253	PRO
1	G	269	ILE
1	H	269	ILE
1	I	269	ILE
1	K	274	GLY
1	L	253	PRO
1	C	269	ILE
1	D	269	ILE
1	E	274	GLY
1	J	269	ILE
1	J	274	GLY
1	K	269	ILE
1	B	269	ILE
1	E	454	PRO
1	F	274	GLY
1	L	274	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	405/415 (98%)	373 (92%)	32 (8%)	12 44
1	B	405/415 (98%)	369 (91%)	36 (9%)	9 40
1	C	405/415 (98%)	370 (91%)	35 (9%)	10 41
1	D	405/415 (98%)	369 (91%)	36 (9%)	9 40
1	E	405/415 (98%)	368 (91%)	37 (9%)	9 39
1	F	405/415 (98%)	370 (91%)	35 (9%)	10 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	405/415 (98%)	367 (91%)	38 (9%)	8	38
1	H	405/415 (98%)	370 (91%)	35 (9%)	10	41
1	I	405/415 (98%)	369 (91%)	36 (9%)	9	40
1	J	405/415 (98%)	370 (91%)	35 (9%)	10	41
1	K	405/415 (98%)	370 (91%)	35 (9%)	10	41
1	L	405/415 (98%)	367 (91%)	38 (9%)	8	38
All	All	4860/4980 (98%)	4432 (91%)	428 (9%)	10	40

All (428) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	69	LEU
1	A	89	SER
1	A	91	TYR
1	A	146	TYR
1	A	147	LEU
1	A	154	ASN
1	A	155	TYR
1	A	183	ASP
1	A	185	ILE
1	A	228	ARG
1	A	235	MET
1	A	254	ILE
1	A	255	ARG
1	A	273	LEU
1	A	275	ASP
1	A	277	ARG
1	A	289	MET
1	A	306	THR
1	A	330	LEU
1	A	370	THR
1	A	381	LEU
1	A	388	VAL
1	A	390	SER
1	A	392	LEU
1	A	397	GLN
1	A	400	LEU
1	A	405	LEU
1	A	468	LEU

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Mol	Chain	Res	Type
1	A	479	SER
1	A	489	GLN
1	A	490	GLN
1	B	18	GLU
1	B	59	GLN
1	B	69	LEU
1	B	89	SER
1	B	91	TYR
1	B	146	TYR
1	B	147	LEU
1	B	153	SER
1	B	154	ASN
1	B	155	TYR
1	B	179	MET
1	B	183	ASP
1	B	185	ILE
1	B	228	ARG
1	B	235	MET
1	B	254	ILE
1	B	255	ARG
1	B	260	ASP
1	B	273	LEU
1	B	275	ASP
1	B	277	ARG
1	B	289	MET
1	B	306	THR
1	B	330	LEU
1	B	370	THR
1	B	381	LEU
1	B	388	VAL
1	B	390	SER
1	B	392	LEU
1	B	397	GLN
1	B	400	LEU
1	B	405	LEU
1	B	438	ASP
1	B	468	LEU
1	B	479	SER
1	B	490	GLN
1	C	18	GLU
1	C	59	GLN
1	C	69	LEU

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Mol	Chain	Res	Type
1	C	89	SER
1	C	91	TYR
1	C	146	TYR
1	C	147	LEU
1	C	154	ASN
1	C	155	TYR
1	C	183	ASP
1	C	185	ILE
1	C	204	GLU
1	C	228	ARG
1	C	235	MET
1	C	243	THR
1	C	254	ILE
1	C	255	ARG
1	C	273	LEU
1	C	275	ASP
1	C	277	ARG
1	C	289	MET
1	C	330	LEU
1	C	370	THR
1	C	381	LEU
1	C	388	VAL
1	C	390	SER
1	C	392	LEU
1	C	397	GLN
1	C	400	LEU
1	C	405	LEU
1	C	438	ASP
1	C	468	LEU
1	C	479	SER
1	C	489	GLN
1	C	490	GLN
1	D	11	ASP
1	D	18	GLU
1	D	59	GLN
1	D	69	LEU
1	D	89	SER
1	D	91	TYR
1	D	146	TYR
1	D	147	LEU
1	D	154	ASN
1	D	155	TYR

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Mol	Chain	Res	Type
1	D	179	MET
1	D	183	ASP
1	D	185	ILE
1	D	204	GLU
1	D	228	ARG
1	D	235	MET
1	D	254	ILE
1	D	255	ARG
1	D	273	LEU
1	D	275	ASP
1	D	277	ARG
1	D	289	MET
1	D	306	THR
1	D	330	LEU
1	D	370	THR
1	D	381	LEU
1	D	388	VAL
1	D	390	SER
1	D	392	LEU
1	D	397	GLN
1	D	400	LEU
1	D	405	LEU
1	D	438	ASP
1	D	468	LEU
1	D	479	SER
1	D	490	GLN
1	E	18	GLU
1	E	59	GLN
1	E	69	LEU
1	E	89	SER
1	E	91	TYR
1	E	146	TYR
1	E	147	LEU
1	E	154	ASN
1	E	155	TYR
1	E	179	MET
1	E	183	ASP
1	E	185	ILE
1	E	228	ARG
1	E	235	MET
1	E	243	THR
1	E	254	ILE

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Mol	Chain	Res	Type
1	E	255	ARG
1	E	260	ASP
1	E	273	LEU
1	E	275	ASP
1	E	277	ARG
1	E	289	MET
1	E	306	THR
1	E	330	LEU
1	E	370	THR
1	E	381	LEU
1	E	388	VAL
1	E	390	SER
1	E	392	LEU
1	E	397	GLN
1	E	400	LEU
1	E	405	LEU
1	E	438	ASP
1	E	468	LEU
1	E	479	SER
1	E	489	GLN
1	E	490	GLN
1	F	18	GLU
1	F	69	LEU
1	F	89	SER
1	F	91	TYR
1	F	146	TYR
1	F	147	LEU
1	F	154	ASN
1	F	155	TYR
1	F	179	MET
1	F	183	ASP
1	F	185	ILE
1	F	228	ARG
1	F	235	MET
1	F	243	THR
1	F	254	ILE
1	F	255	ARG
1	F	273	LEU
1	F	275	ASP
1	F	277	ARG
1	F	289	MET
1	F	306	THR

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Mol	Chain	Res	Type
1	F	330	LEU
1	F	370	THR
1	F	381	LEU
1	F	388	VAL
1	F	390	SER
1	F	392	LEU
1	F	397	GLN
1	F	400	LEU
1	F	405	LEU
1	F	438	ASP
1	F	468	LEU
1	F	479	SER
1	F	489	GLN
1	F	490	GLN
1	G	18	GLU
1	G	59	GLN
1	G	69	LEU
1	G	89	SER
1	G	91	TYR
1	G	146	TYR
1	G	147	LEU
1	G	154	ASN
1	G	155	TYR
1	G	183	ASP
1	G	185	ILE
1	G	218	TYR
1	G	228	ARG
1	G	235	MET
1	G	243	THR
1	G	254	ILE
1	G	255	ARG
1	G	260	ASP
1	G	273	LEU
1	G	277	ARG
1	G	289	MET
1	G	306	THR
1	G	328	SER
1	G	330	LEU
1	G	357	MET
1	G	370	THR
1	G	381	LEU
1	G	388	VAL

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Mol	Chain	Res	Type
1	G	390	SER
1	G	392	LEU
1	G	397	GLN
1	G	400	LEU
1	G	405	LEU
1	G	411	THR
1	G	468	LEU
1	G	479	SER
1	G	489	GLN
1	G	490	GLN
1	H	18	GLU
1	H	69	LEU
1	H	89	SER
1	H	91	TYR
1	H	146	TYR
1	H	147	LEU
1	H	154	ASN
1	H	155	TYR
1	H	179	MET
1	H	183	ASP
1	H	185	ILE
1	H	228	ARG
1	H	235	MET
1	H	243	THR
1	H	254	ILE
1	H	255	ARG
1	H	273	LEU
1	H	275	ASP
1	H	277	ARG
1	H	289	MET
1	H	306	THR
1	H	330	LEU
1	H	357	MET
1	H	370	THR
1	H	381	LEU
1	H	388	VAL
1	H	390	SER
1	H	392	LEU
1	H	397	GLN
1	H	400	LEU
1	H	405	LEU
1	H	411	THR

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Mol	Chain	Res	Type
1	H	468	LEU
1	H	479	SER
1	H	490	GLN
1	I	18	GLU
1	I	69	LEU
1	I	89	SER
1	I	91	TYR
1	I	146	TYR
1	I	147	LEU
1	I	154	ASN
1	I	155	TYR
1	I	183	ASP
1	I	185	ILE
1	I	201	GLN
1	I	228	ARG
1	I	235	MET
1	I	243	THR
1	I	254	ILE
1	I	255	ARG
1	I	273	LEU
1	I	275	ASP
1	I	277	ARG
1	I	289	MET
1	I	306	THR
1	I	328	SER
1	I	330	LEU
1	I	357	MET
1	I	370	THR
1	I	381	LEU
1	I	388	VAL
1	I	390	SER
1	I	392	LEU
1	I	397	GLN
1	I	400	LEU
1	I	405	LEU
1	I	468	LEU
1	I	479	SER
1	I	489	GLN
1	I	490	GLN
1	J	18	GLU
1	J	69	LEU
1	J	89	SER

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Mol	Chain	Res	Type
1	J	91	TYR
1	J	146	TYR
1	J	147	LEU
1	J	154	ASN
1	J	155	TYR
1	J	179	MET
1	J	183	ASP
1	J	185	ILE
1	J	228	ARG
1	J	235	MET
1	J	243	THR
1	J	254	ILE
1	J	255	ARG
1	J	273	LEU
1	J	275	ASP
1	J	277	ARG
1	J	289	MET
1	J	306	THR
1	J	330	LEU
1	J	357	MET
1	J	370	THR
1	J	381	LEU
1	J	388	VAL
1	J	390	SER
1	J	392	LEU
1	J	397	GLN
1	J	400	LEU
1	J	405	LEU
1	J	411	THR
1	J	468	LEU
1	J	479	SER
1	J	490	GLN
1	K	18	GLU
1	K	59	GLN
1	K	69	LEU
1	K	89	SER
1	K	91	TYR
1	K	146	TYR
1	K	147	LEU
1	K	154	ASN
1	K	155	TYR
1	K	179	MET

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Mol	Chain	Res	Type
1	K	183	ASP
1	K	185	ILE
1	K	218	TYR
1	K	228	ARG
1	K	235	MET
1	K	254	ILE
1	K	255	ARG
1	K	273	LEU
1	K	275	ASP
1	K	277	ARG
1	K	289	MET
1	K	306	THR
1	K	330	LEU
1	K	357	MET
1	K	370	THR
1	K	381	LEU
1	K	388	VAL
1	K	390	SER
1	K	392	LEU
1	K	397	GLN
1	K	400	LEU
1	K	405	LEU
1	K	468	LEU
1	K	479	SER
1	K	490	GLN
1	L	18	GLU
1	L	59	GLN
1	L	69	LEU
1	L	89	SER
1	L	91	TYR
1	L	146	TYR
1	L	147	LEU
1	L	154	ASN
1	L	155	TYR
1	L	179	MET
1	L	183	ASP
1	L	185	ILE
1	L	228	ARG
1	L	235	MET
1	L	243	THR
1	L	254	ILE
1	L	255	ARG

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Mol	Chain	Res	Type
1	L	260	ASP
1	L	273	LEU
1	L	275	ASP
1	L	277	ARG
1	L	289	MET
1	L	306	THR
1	L	330	LEU
1	L	357	MET
1	L	370	THR
1	L	381	LEU
1	L	388	VAL
1	L	390	SER
1	L	392	LEU
1	L	397	GLN
1	L	400	LEU
1	L	405	LEU
1	L	438	ASP
1	L	468	LEU
1	L	479	SER
1	L	489	GLN
1	L	490	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	178	GLN
1	A	216	HIS
1	A	238	GLN
1	A	397	GLN
1	B	156	ASN
1	B	178	GLN
1	B	216	HIS
1	B	238	GLN
1	B	397	GLN
1	C	156	ASN
1	C	178	GLN
1	C	216	HIS
1	C	238	GLN
1	C	283	GLN
1	C	397	GLN
1	D	67	ASN

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Mol	Chain	Res	Type
1	D	156	ASN
1	D	178	GLN
1	D	216	HIS
1	D	238	GLN
1	D	397	GLN
1	E	156	ASN
1	E	178	GLN
1	E	201	GLN
1	E	216	HIS
1	E	397	GLN
1	F	156	ASN
1	F	178	GLN
1	F	216	HIS
1	F	238	GLN
1	F	397	GLN
1	G	156	ASN
1	G	178	GLN
1	G	216	HIS
1	G	238	GLN
1	G	397	GLN
1	H	156	ASN
1	H	178	GLN
1	H	216	HIS
1	H	238	GLN
1	H	397	GLN
1	I	156	ASN
1	I	178	GLN
1	I	397	GLN
1	J	124	ASN
1	J	156	ASN
1	J	178	GLN
1	J	201	GLN
1	J	216	HIS
1	J	238	GLN
1	J	397	GLN
1	J	407	GLN
1	K	156	ASN
1	K	178	GLN
1	K	216	HIS
1	K	238	GLN
1	K	397	GLN
1	L	156	ASN

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Mol	Chain	Res	Type
1	L	178	GLN
1	L	216	HIS
1	L	238	GLN
1	L	397	GLN

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	479/490 (97%)	0.19	26 (5%)	25	16	117, 182, 267, 312	1 (0%)
1	B	479/490 (97%)	0.22	30 (6%)	20	11	104, 183, 282, 332	1 (0%)
1	C	479/490 (97%)	0.25	32 (6%)	17	10	108, 189, 279, 347	1 (0%)
1	D	479/490 (97%)	0.17	32 (6%)	17	10	120, 190, 267, 313	1 (0%)
1	E	479/490 (97%)	0.25	33 (6%)	16	10	126, 190, 273, 329	1 (0%)
1	F	479/490 (97%)	0.14	20 (4%)	36	23	127, 197, 280, 328	1 (0%)
1	G	479/490 (97%)	0.40	50 (10%)	6	3	128, 199, 288, 343	1 (0%)
1	H	479/490 (97%)	0.25	38 (7%)	12	7	131, 194, 271, 290	1 (0%)
1	I	479/490 (97%)	0.27	36 (7%)	14	8	121, 197, 276, 331	1 (0%)
1	J	479/490 (97%)	0.23	34 (7%)	16	9	112, 188, 281, 339	1 (0%)
1	K	479/490 (97%)	0.07	14 (2%)	51	35	95, 187, 268, 313	1 (0%)
1	L	479/490 (97%)	0.23	42 (8%)	10	6	105, 183, 269, 323	1 (0%)
All	All	5748/5880 (97%)	0.22	387 (6%)	17	10	95, 190, 274, 347	12 (0%)

All (387) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	422	VAL	9.2
1	A	369	VAL	7.5
1	D	365	THR	7.4
1	E	150	PRO	6.8
1	A	367	GLU	6.8
1	J	189	ALA	6.7
1	C	421	ALA	6.6
1	G	368	ARG	6.6
1	C	492	MET	6.1
1	C	422	VAL	6.1
1	H	319	PHE	6.1

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Mol	Chain	Res	Type	RSRZ
1	J	493	ALA	6.0
1	B	366	GLY	5.9
1	H	365	THR	5.7
1	C	222	ASP	5.6
1	G	363	GLN	5.5
1	I	204	GLU	5.4
1	G	415	PRO	5.3
1	F	460	ASP	5.2
1	H	368	ARG	5.1
1	G	413	GLN	5.1
1	L	493	ALA	5.1
1	K	422	VAL	4.9
1	G	371	ALA	4.8
1	I	178	GLN	4.8
1	G	414	ILE	4.8
1	A	187	PHE	4.5
1	G	189	ALA	4.5
1	G	209	GLU	4.5
1	C	493	ALA	4.5
1	I	216	HIS	4.5
1	J	368	ARG	4.5
1	D	202	GLY	4.5
1	H	19	ARG	4.4
1	L	12	GLY	4.4
1	L	363	GLN	4.4
1	G	191	PRO	4.4
1	B	368	ARG	4.4
1	J	149	GLU	4.3
1	J	205	LYS	4.3
1	B	189	ALA	4.3
1	G	192	GLU	4.3
1	C	192	GLU	4.2
1	F	492	MET	4.2
1	L	415	PRO	4.2
1	B	208	ASP	4.2
1	G	490	GLN	4.2
1	G	367	GLU	4.1
1	B	362	VAL	4.1
1	H	373	GLU	4.1
1	J	367	GLU	4.1
1	I	205	LYS	4.0
1	I	494	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	417	LEU	3.9
1	I	208	ASP	3.9
1	G	416	GLU	3.9
1	E	172	ALA	3.8
1	D	420	GLU	3.8
1	E	492	MET	3.8
1	A	216	HIS	3.8
1	H	493	ALA	3.8
1	G	370	THR	3.8
1	I	301	ASN	3.8
1	L	373	GLU	3.8
1	L	370	THR	3.7
1	E	320	VAL	3.7
1	K	204	GLU	3.7
1	G	204	GLU	3.6
1	C	172	ALA	3.6
1	H	369	VAL	3.6
1	J	193	ASP	3.6
1	J	231	GLU	3.6
1	C	367	GLU	3.6
1	D	231	GLU	3.6
1	I	419	LYS	3.6
1	D	189	ALA	3.5
1	J	366	GLY	3.5
1	F	208	ASP	3.5
1	G	219	LEU	3.4
1	L	306	THR	3.4
1	H	251	TYR	3.4
1	G	5	ARG	3.4
1	L	178	GLN	3.4
1	K	415	PRO	3.4
1	K	414	ILE	3.4
1	F	362	VAL	3.4
1	D	204	GLU	3.4
1	E	91	TYR	3.4
1	L	231	GLU	3.4
1	A	76	ALA	3.4
1	G	178	GLN	3.4
1	K	421	ALA	3.4
1	D	369	VAL	3.4
1	C	419	LYS	3.3
1	C	198	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	193	ASP	3.3
1	F	178	GLN	3.3
1	J	188	GLY	3.3
1	D	195	ARG	3.3
1	H	187	PHE	3.3
1	H	367	GLU	3.3
1	B	417	LEU	3.3
1	L	179	MET	3.3
1	H	10	GLU	3.3
1	E	419	LYS	3.3
1	D	198	VAL	3.3
1	I	232	VAL	3.3
1	B	190	LEU	3.2
1	D	421	ALA	3.2
1	A	421	ALA	3.2
1	E	368	ARG	3.2
1	J	414	ILE	3.2
1	C	214	TYR	3.2
1	I	187	PHE	3.2
1	J	178	GLN	3.2
1	B	421	ALA	3.2
1	J	204	GLU	3.2
1	A	368	ARG	3.1
1	J	235	MET	3.1
1	J	420	GLU	3.1
1	G	22	ASN	3.1
1	C	178	GLN	3.1
1	I	455	MET	3.1
1	A	233	GLU	3.1
1	H	215	THR	3.1
1	J	237	VAL	3.1
1	D	458	ASP	3.1
1	J	421	ALA	3.1
1	I	462	ASN	3.1
1	K	189	ALA	3.0
1	L	204	GLU	3.0
1	I	368	ARG	3.0
1	J	238	GLN	3.0
1	G	10	GLU	3.0
1	K	177	LEU	3.0
1	B	110	LEU	3.0
1	G	199	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	458	ASP	3.0
1	H	168	VAL	3.0
1	L	307	GLN	3.0
1	J	419	LYS	3.0
1	C	103	LEU	3.0
1	K	188	GLY	3.0
1	J	365	THR	3.0
1	I	249	CYS	3.0
1	C	374	ILE	3.0
1	H	247	GLU	3.0
1	I	231	GLU	3.0
1	D	457	ASP	3.0
1	A	251	TYR	3.0
1	C	482	LEU	3.0
1	G	188	GLY	3.0
1	H	248	ALA	3.0
1	G	208	ASP	3.0
1	G	374	ILE	2.9
1	J	206	LYS	2.9
1	L	492	MET	2.9
1	E	202	GLY	2.9
1	G	231	GLU	2.9
1	L	251	TYR	2.9
1	D	5	ARG	2.9
1	G	454	PRO	2.9
1	A	363	GLN	2.9
1	G	232	VAL	2.9
1	C	369	VAL	2.8
1	G	216	HIS	2.8
1	E	17	TYR	2.8
1	G	185	ILE	2.8
1	L	194	ILE	2.8
1	C	231	GLU	2.8
1	E	198	VAL	2.8
1	G	200	GLY	2.8
1	B	461	ILE	2.8
1	B	212	ASP	2.8
1	B	251	TYR	2.8
1	K	302	PRO	2.8
1	A	238	GLN	2.8
1	I	263	SER	2.8
1	F	373	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	181	THR	2.8
1	J	489	GLN	2.8
1	C	221	GLU	2.7
1	H	218	TYR	2.7
1	J	229	TYR	2.7
1	B	233	GLU	2.7
1	I	490	GLN	2.7
1	C	212	ASP	2.7
1	D	452	LEU	2.7
1	I	214	TYR	2.7
1	G	372	GLU	2.7
1	C	456	ARG	2.7
1	B	365	THR	2.7
1	F	17	TYR	2.7
1	G	492	MET	2.7
1	J	306	THR	2.7
1	L	366	GLY	2.7
1	G	297	ILE	2.7
1	G	366	GLY	2.7
1	H	419	LYS	2.6
1	G	198	VAL	2.6
1	E	311	LEU	2.6
1	F	461	ILE	2.6
1	G	319	PHE	2.6
1	C	239	GLY	2.6
1	E	421	ALA	2.6
1	C	423	GLU	2.6
1	A	372	GLU	2.6
1	L	247	GLU	2.6
1	A	371	ALA	2.6
1	E	246	LYS	2.6
1	E	369	VAL	2.6
1	J	185	ILE	2.6
1	A	419	LYS	2.6
1	A	260	ASP	2.6
1	D	485	GLU	2.6
1	L	238	GLN	2.6
1	I	296	VAL	2.6
1	F	23	ASP	2.6
1	J	215	THR	2.6
1	L	205	LYS	2.6
1	A	373	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	8	LEU	2.5
1	G	180	VAL	2.5
1	L	454	PRO	2.5
1	L	489	GLN	2.5
1	H	320	VAL	2.5
1	L	237	VAL	2.5
1	L	367	GLU	2.5
1	B	178	GLN	2.5
1	H	189	ALA	2.5
1	B	330	LEU	2.5
1	H	305	ILE	2.5
1	D	367	GLU	2.5
1	F	483	LEU	2.5
1	G	311	LEU	2.5
1	B	209	GLU	2.5
1	I	179	MET	2.5
1	C	373	GLU	2.5
1	H	492	MET	2.5
1	G	302	PRO	2.5
1	J	490	GLN	2.5
1	G	184	GLN	2.5
1	A	177	LEU	2.5
1	J	494	GLN	2.5
1	B	420	GLU	2.5
1	F	232	VAL	2.5
1	G	320	VAL	2.5
1	H	234	GLY	2.5
1	F	368	ARG	2.4
1	D	460	ASP	2.4
1	L	371	ALA	2.4
1	E	201	GLN	2.4
1	I	371	ALA	2.4
1	A	206	LYS	2.4
1	E	482	LEU	2.4
1	L	369	VAL	2.4
1	G	461	ILE	2.4
1	I	43	PHE	2.4
1	I	323	ARG	2.4
1	I	209	GLU	2.4
1	K	232	VAL	2.4
1	E	483	LEU	2.4
1	L	11	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	423	GLU	2.4
1	C	179	MET	2.4
1	G	187	PHE	2.4
1	H	416	GLU	2.4
1	B	13	ALA	2.4
1	I	370	THR	2.4
1	H	371	ALA	2.4
1	K	20	LEU	2.4
1	L	17	TYR	2.4
1	L	217	ILE	2.4
1	L	213	VAL	2.4
1	H	420	GLU	2.3
1	L	422	VAL	2.3
1	G	251	TYR	2.3
1	I	215	THR	2.3
1	D	177	LEU	2.3
1	D	366	GLY	2.3
1	K	369	VAL	2.3
1	G	194	ILE	2.3
1	D	99	ASP	2.3
1	H	221	GLU	2.3
1	E	178	GLN	2.3
1	L	421	ALA	2.3
1	D	319	PHE	2.3
1	J	422	VAL	2.3
1	D	419	LYS	2.3
1	D	187	PHE	2.3
1	J	364	ARG	2.3
1	K	184	GLN	2.3
1	H	214	TYR	2.3
1	I	225	GLU	2.3
1	E	493	ALA	2.3
1	H	90	GLU	2.3
1	I	21	LYS	2.3
1	H	364	ARG	2.3
1	H	231	GLU	2.3
1	A	178	GLN	2.3
1	L	223	SER	2.3
1	H	330	LEU	2.3
1	I	237	VAL	2.3
1	C	420	GLU	2.3
1	B	99	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	193	ASP	2.3
1	D	178	GLN	2.3
1	A	149	GLU	2.3
1	I	22	ASN	2.3
1	F	319	PHE	2.3
1	H	370	THR	2.3
1	A	494	GLN	2.3
1	B	364	ARG	2.3
1	F	367	GLU	2.3
1	F	306	THR	2.3
1	I	207	ALA	2.3
1	F	330	LEU	2.3
1	E	216	HIS	2.3
1	L	236	GLU	2.3
1	F	192	GLU	2.2
1	J	169	GLN	2.2
1	D	12	GLY	2.2
1	B	416	GLU	2.2
1	D	422	VAL	2.2
1	C	193	ASP	2.2
1	L	416	GLU	2.2
1	J	415	PRO	2.2
1	B	483	LEU	2.2
1	B	216	HIS	2.2
1	G	362	VAL	2.2
1	H	414	ILE	2.2
1	J	187	PHE	2.2
1	E	367	GLU	2.2
1	C	248	ALA	2.2
1	D	194	ILE	2.2
1	C	326	ASP	2.2
1	E	319	PHE	2.2
1	G	21	LYS	2.2
1	H	329	PHE	2.2
1	C	232	VAL	2.2
1	A	201	GLN	2.2
1	B	192	GLU	2.2
1	I	251	TYR	2.2
1	B	369	VAL	2.2
1	C	368	ARG	2.2
1	D	13	ALA	2.2
1	E	321	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	251	TYR	2.1
1	F	366	GLY	2.1
1	L	300	VAL	2.1
1	H	169	GLN	2.1
1	J	202	GLY	2.1
1	E	456	ARG	2.1
1	E	460	ASP	2.1
1	A	420	GLU	2.1
1	B	361	ALA	2.1
1	G	158	MET	2.1
1	L	80	MET	2.1
1	H	229	TYR	2.1
1	H	424	PRO	2.1
1	L	319	PHE	2.1
1	C	229	TYR	2.1
1	C	5	ARG	2.1
1	A	460	ASP	2.1
1	D	227	LEU	2.1
1	D	196	LYS	2.1
1	E	197	ALA	2.1
1	L	452	LEU	2.1
1	I	454	PRO	2.0
1	I	297	ILE	2.0
1	B	235	MET	2.0
1	B	456	ARG	2.0
1	L	374	ILE	2.0
1	E	365	THR	2.0
1	A	298	GLY	2.0
1	B	169	GLN	2.0
1	E	161	TYR	2.0
1	I	99	ASP	2.0
1	A	299	LEU	2.0
1	D	98	SER	2.0
1	L	372	GLU	2.0
1	F	331	GLN	2.0
1	E	185	ILE	2.0
1	G	306	THR	2.0
1	D	148	PRO	2.0
1	E	223	SER	2.0
1	E	247	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.