Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:46 AM GMT

PDB ID	:	3PXI
Title	:	Structure of MecA108:ClpC
Authors	:	Wang, F.; Mei, Z.Q.; Wang, J.W.; Shi, Y.G.
Deposited on	:	2010-12-09
Resolution	:	6.93 Å(reported)

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

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

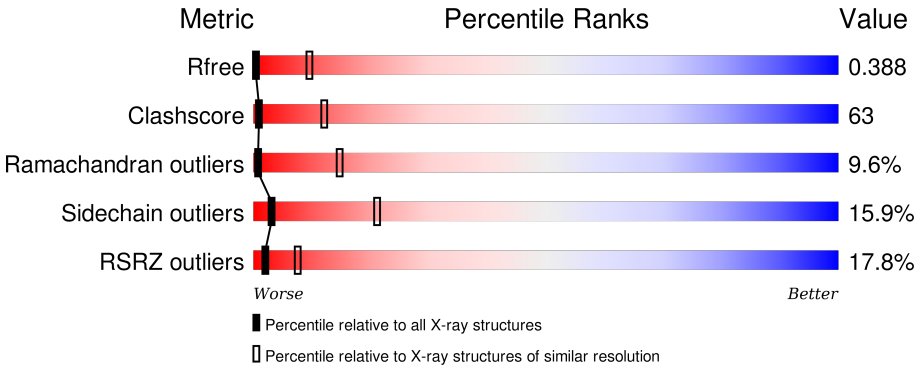
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.93 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	111	9% 61% 23% • 15%
1	b	111	35% 67% 18% 15%
1	c	111	22% 67% 18% 15%
2	A	758	15% 35% 44% 13% • 7%
2	B	758	17% 32% 44% 15% • 7%

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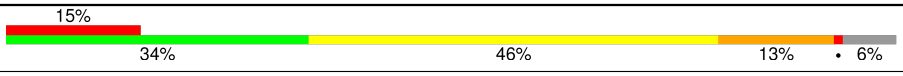
Mol	Chain	Length	Quality of chain
2	C	758	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18645 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 Adapter protein mecA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	94	Total	C	N	O	S	0	0	0
			755	486	118	149	2			
1	b	94	Total	C	N	O	S	0	0	0
			756	485	120	149	2			
1	c	94	Total	C	N	O	S	0	0	0
			763	491	120	150	2			

- Molecule 2 is a protein called Negative regulator of genetic competence ClpC/MecB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	708	Total	C	N	O	S	0	0	0
			5455	3394	993	1055	13			
2	B	704	Total	C	N	O	S	0	0	0
			5437	3385	985	1054	13			
2	C	711	Total	C	N	O	S	0	0	0
			5479	3410	993	1063	13			

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	ALA	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	THR	DELETION	UNP P37571
A	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	HIS	DELETION	UNP P37571
A	?	-	THR	DELETION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	ILE	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	ALA	DELETION	UNP P37571
A	?	-	GLU	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	ARG	DELETION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	SER	DELETION	UNP P37571
A	?	-	PRO	DELETION	UNP P37571
A	?	-	PRO	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	TYR	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	TYR	DELETION	UNP P37571
A	?	-	ASP	DELETION	UNP P37571
A	?	-	GLU	DELETION	UNP P37571
A	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	LYS	DELETION	UNP P37571
A	?	-	ARG	DELETION	UNP P37571
A	?	-	ASN	DELETION	UNP P37571
A	?	-	LYS	DELETION	UNP P37571
A	?	-	TYR	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	PHE	DELETION	UNP P37571
A	?	-	ASN	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	GLN	DELETION	UNP P37571
A	?	-	ASP	DELETION	UNP P37571
A	?	-	GLU	DELETION	UNP P37571
A	?	-	THR	DELETION	UNP P37571
A	?	-	GLN	DELETION	UNP P37571
A	?	-	ASN	DELETION	UNP P37571
A	?	-	HIS	DELETION	UNP P37571
A	?	-	LYS	DELETION	UNP P37571
A	?	-	ASP	DELETION	UNP P37571
A	?	-	MET	DELETION	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	ALA	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	THR	DELETION	UNP P37571
B	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	HIS	DELETION	UNP P37571
B	?	-	THR	DELETION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	ILE	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	ALA	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	ALA	DELETION	UNP P37571
B	?	-	GLU	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	ARG	DELETION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	SER	DELETION	UNP P37571
B	?	-	PRO	DELETION	UNP P37571
B	?	-	PRO	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	TYR	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	TYR	DELETION	UNP P37571
B	?	-	ASP	DELETION	UNP P37571
B	?	-	GLU	DELETION	UNP P37571
B	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	LYS	DELETION	UNP P37571
B	?	-	ARG	DELETION	UNP P37571
B	?	-	ASN	DELETION	UNP P37571
B	?	-	LYS	DELETION	UNP P37571
B	?	-	TYR	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	PHE	DELETION	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	GLN	DELETION	UNP P37571
B	?	-	ASP	DELETION	UNP P37571
B	?	-	GLU	DELETION	UNP P37571
B	?	-	THR	DELETION	UNP P37571
B	?	-	GLN	DELETION	UNP P37571
B	?	-	ASN	DELETION	UNP P37571
B	?	-	HIS	DELETION	UNP P37571
B	?	-	LYS	DELETION	UNP P37571
B	?	-	ASP	DELETION	UNP P37571
B	?	-	MET	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	ALA	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	THR	DELETION	UNP P37571
C	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	HIS	DELETION	UNP P37571
C	?	-	THR	DELETION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	ILE	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	ALA	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	ALA	DELETION	UNP P37571
C	?	-	GLU	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	ARG	DELETION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	SER	DELETION	UNP P37571
C	?	-	PRO	DELETION	UNP P37571
C	?	-	PRO	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	TYR	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	TYR	DELETION	UNP P37571

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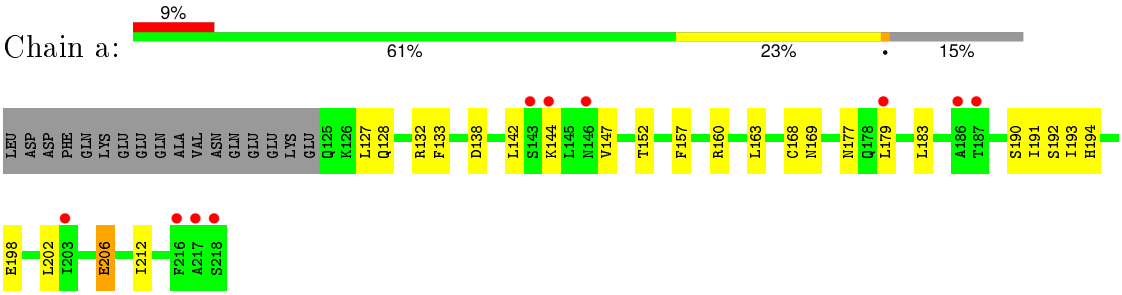
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	DELETION	UNP P37571
C	?	-	GLU	DELETION	UNP P37571
C	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	LYS	DELETION	UNP P37571
C	?	-	ARG	DELETION	UNP P37571
C	?	-	ASN	DELETION	UNP P37571
C	?	-	LYS	DELETION	UNP P37571
C	?	-	TYR	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	PHE	DELETION	UNP P37571
C	?	-	ASN	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	GLN	DELETION	UNP P37571
C	?	-	ASP	DELETION	UNP P37571
C	?	-	GLU	DELETION	UNP P37571
C	?	-	THR	DELETION	UNP P37571
C	?	-	GLN	DELETION	UNP P37571
C	?	-	ASN	DELETION	UNP P37571
C	?	-	HIS	DELETION	UNP P37571
C	?	-	LYS	DELETION	UNP P37571
C	?	-	ASP	DELETION	UNP P37571
C	?	-	MET	DELETION	UNP P37571

3 Residue-property plots (i)

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

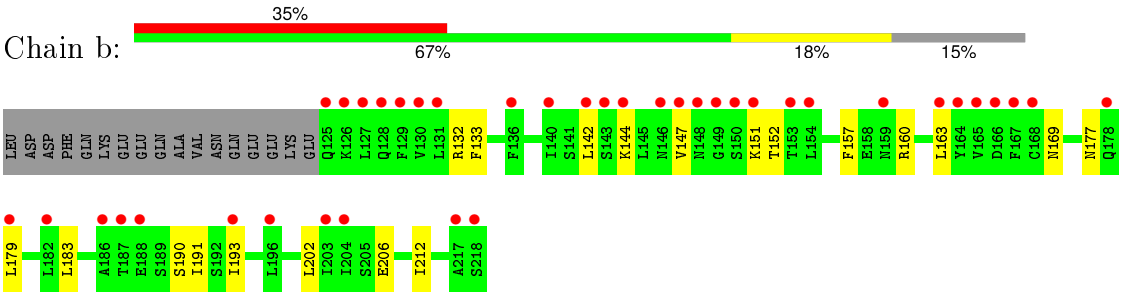
- Molecule 1: Adapter protein mecA 1

Chain a:



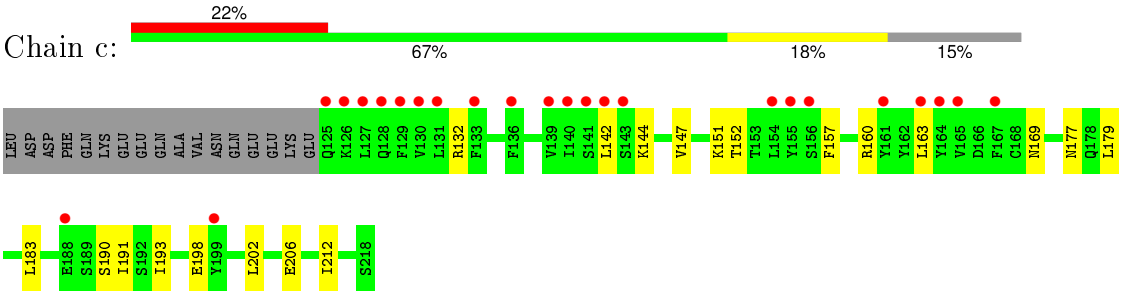
- Molecule 1: Adapter protein mecA 1

Chain b:



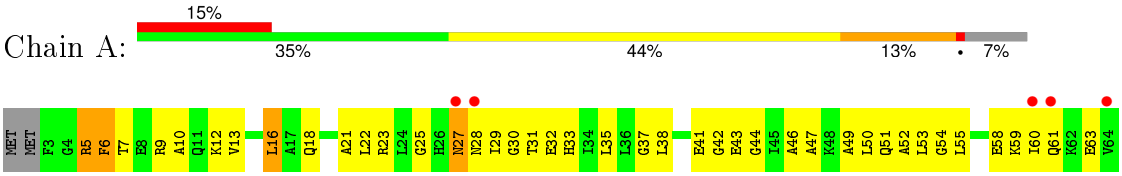
- Molecule 1: Adapter protein mecA 1

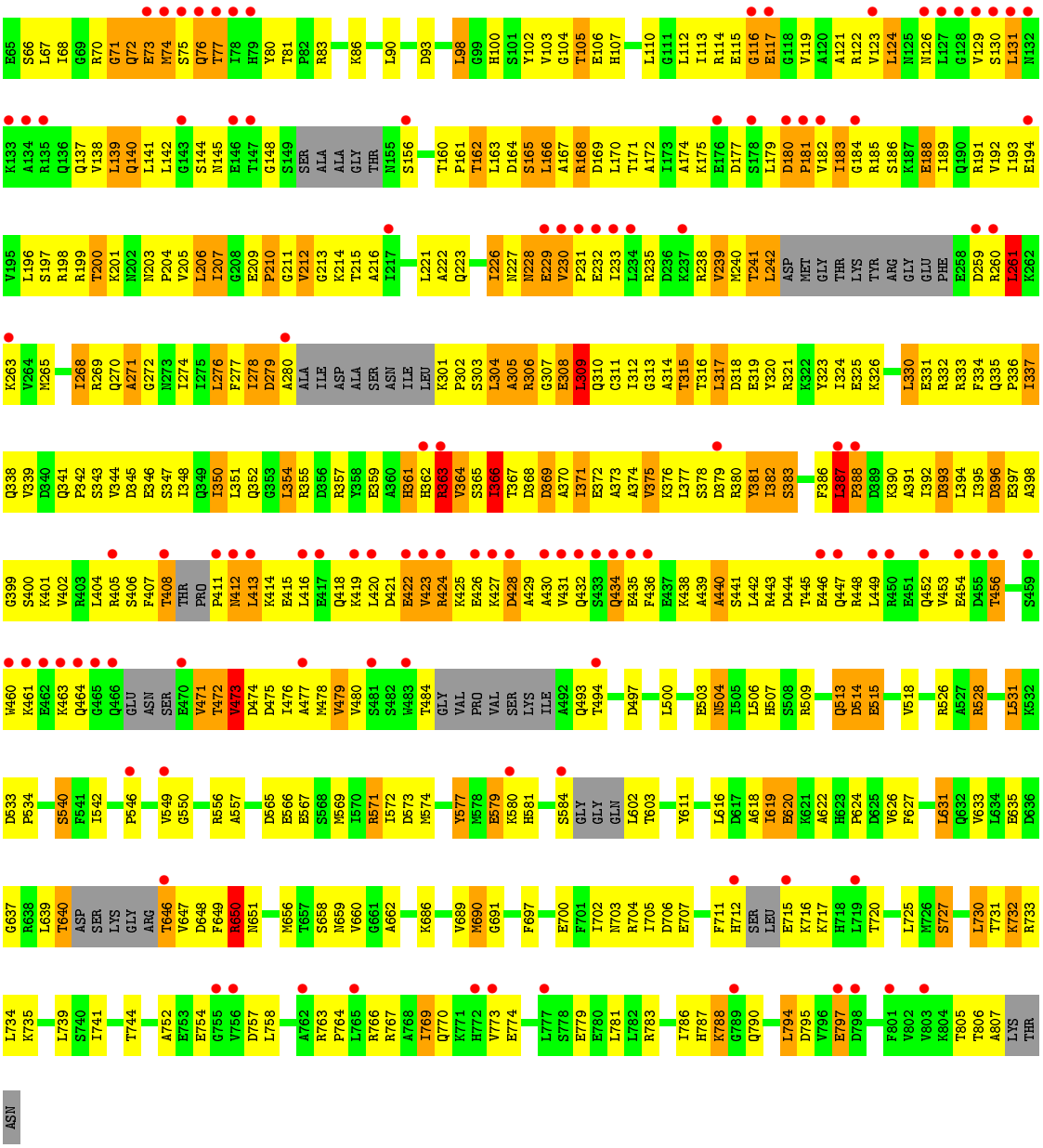
Chain c:



- Molecule 2: Negative regulator of genetic competence ClpC/MecB

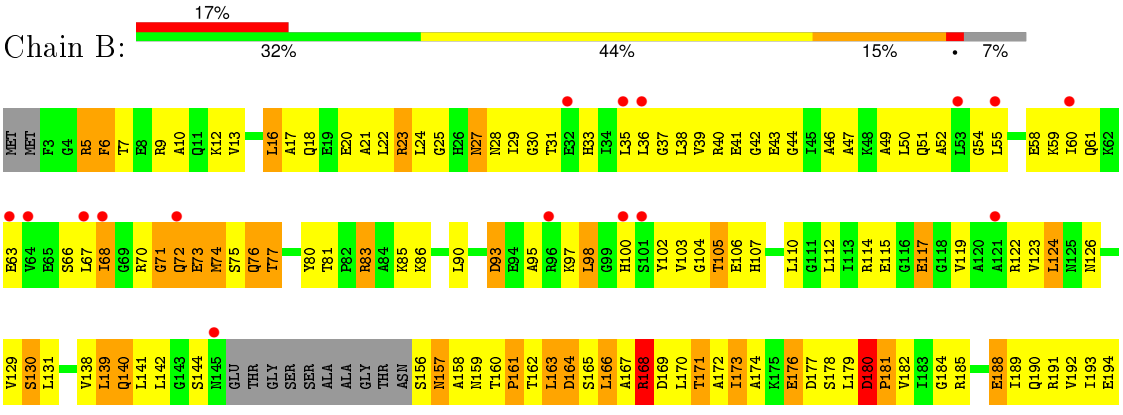
Chain A:

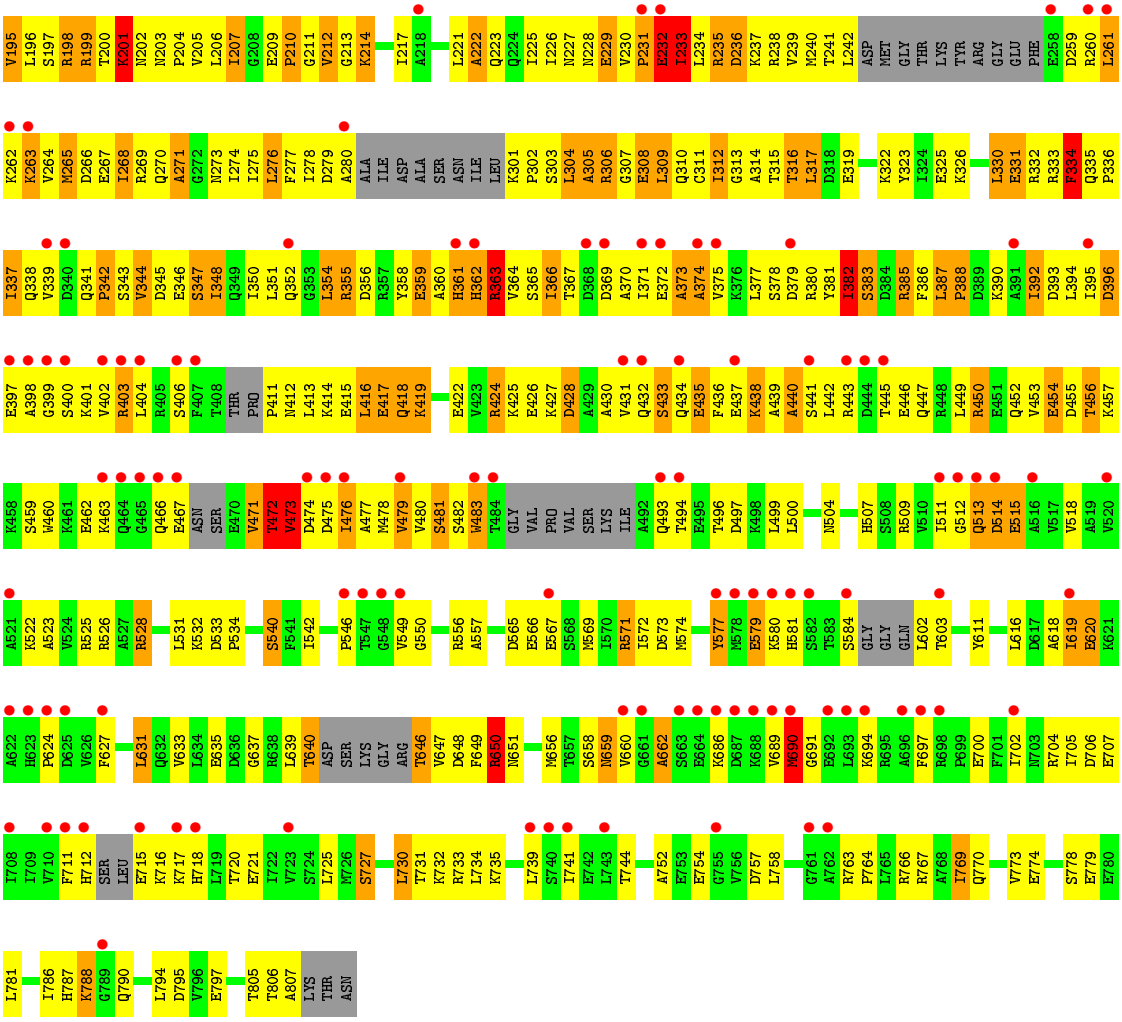




• Molecule 2: Negative regulator of genetic competence ClpC/MecB

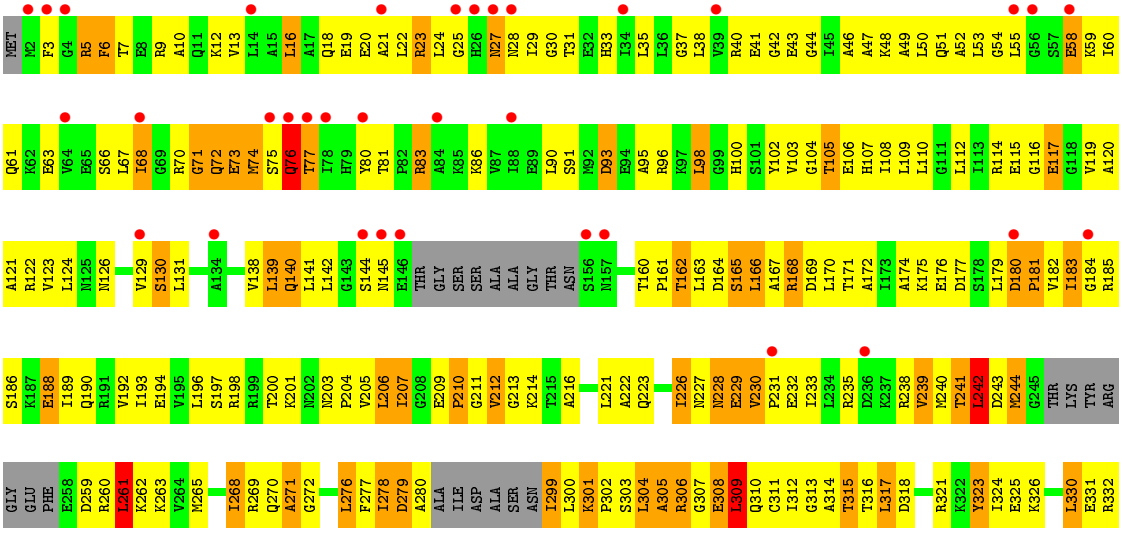
Chain B:

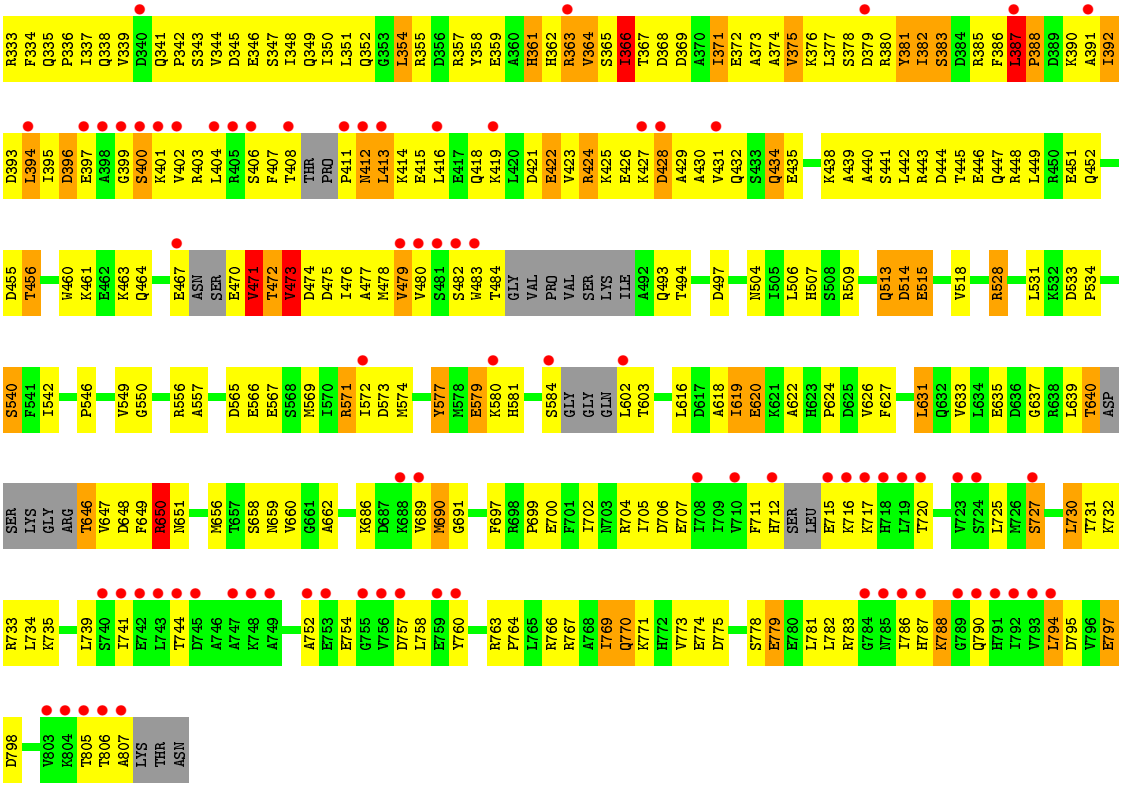




• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain C:




R333 F334 Q335 P336 I337 Q338 V339 D340 Q341 P342 S343 V344 D345 E346 S347 I348 Q349 I350 L351 Q352 G353 L354 R355 D356 R357 Y358 E359 A360 H361 H362 R363 V364 S365 I366 T367 D368 D369 A370 I371 E372 A373 A374 V375 K376 L377 S378 D379 R380 Y381 I382 S383 D384 R385 F386 L387 P388 D389 K390 A391 I392
D393 L394 I395 D396 E397 A398 G399 S400 K401 V402 R403 L404 R405 S406 F407 T408 THR PRO P411 N412 L413 K414 E415 L416 E417 Q418 K419 L420 D421 E422 V423 R424 K425 E426 K427 D428 A429 A430 V431 Q432 S433 Q434 E435 K438 A439 A440 S441 L442 R443 D444 T445 E446 Q447 R448 L449 R450 E451 Q452
D455 T456 W460 K461 E462 K463 Q464 E467 ASN SER E470 V471 T472 V473 D474 D475 I476 A477 M478 V479 V480 S481 S482 W483 T484 GLY VAL PRO VAL SER LYS ILE A492 Q493 T494 D497 N504 I505 L506 H507 S508 R509 Q513 D514 E515 V518 R528 L531 K532 D533 P534
S540 F541 I542 P546 V549 G550 R556 A557 D565 E566 E567 S568 M569 I570 R571 I572 D573 M574 Y577 M578 E579 K580 H581 S584 GLY GLY GLN L602 T603 L616 D617 A618 I619 E620 K621 A622 H623 P624 D625 V626 F627 L631 D632 V633 L634 E635 D636 G637 R638 L639 T640 ASP
SER LYS GLY ARG T646 V647 D648 F649 R650 N651 M656 T657 S658 N659 V660 G661 A662 K686 D687 K688 V689 M690 G691 F697 R698 P699 E700 F701 I702 N703 R704 I705 D706 E707 I708 I709 V710 F711 H712 SER LEU E715 K716 K717 H718 L719 T720 V723 S724 L725 M726 S727 L730 T731 K732
R733 L734 K735 L739 S740 I741 E742 L743 T744 D745 A746 A747 K748 A749 A752 E753 E754 G755 V756 D757 L758 E759 Y760 R763 P764 L765 R766 R767 A768 I769 Q770 K771 H772 V773 E774 D775 S778 E779 E780 L781 L782 R783 G784 N785 I786 H787 K788 G789 Q790 H791 I792 V793 L794 D795 V796 E797
D798 V803 K804 T805 T806 A807 LYS THR ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	141.81Å 141.81Å 656.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.15 – 6.93 49.15 – 6.93	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.15-6.93) 99.6 (49.15-6.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.07 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_596)	Depositor
R, R_{free}	0.407 , 0.422 0.363 , 0.388	Depositor DCC
R_{free} test set	332 reflections (4.74%)	DCC
Wilson B-factor (Å^2)	181.7	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 752.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.27$, $< L^2 > = 0.11$	Xtriage
Outliers	0 of 7006 reflections	Xtriage
F_o,F_c correlation	0.67	EDS
Total number of atoms	18645	wwPDB-VP
Average B, all atoms (Å^2)	642.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	a	0.48	0/768	0.66	1/1035 (0.1%)
1	b	0.56	0/768	0.67	0/1035
1	c	0.64	0/776	0.68	0/1046
2	A	0.52	1/5498 (0.0%)	0.70	2/7386 (0.0%)
2	B	0.58	2/5483 (0.0%)	0.80	2/7369 (0.0%)
2	C	0.53	1/5526 (0.0%)	0.72	2/7431 (0.0%)
All	All	0.55	4/18819 (0.0%)	0.73	7/25302 (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
2	A	0	1
2	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	515	GLU	CG-CD	5.50	1.60	1.51
2	A	515	GLU	CG-CD	5.49	1.60	1.51
2	C	515	GLU	CG-CD	5.42	1.60	1.51
2	B	334	PHE	CA-CB	5.26	1.65	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	161	PRO	N-CA-CB	6.09	110.61	103.30
2	C	161	PRO	N-CA-CB	5.88	110.35	103.30
2	B	161	PRO	N-CA-CB	5.25	109.60	103.30
1	a	138	ASP	CB-CG-OD1	5.23	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	515	GLU	OE1-CD-OE2	-5.15	117.12	123.30
2	B	515	GLU	OE1-CD-OE2	-5.11	117.17	123.30
2	A	515	GLU	OE1-CD-OE2	-5.09	117.19	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	210	PRO	Peptide
2	C	210	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	755	0	728	0	17
1	b	756	0	736	0	0
1	c	763	0	743	0	0
2	A	5455	0	5489	600	34
2	B	5437	0	5491	871	1
2	C	5479	0	5524	731	24
All	All	18645	0	18711	1994	41

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 63.

All (1994) 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)
2:B:694:LYS:HG3	2:C:760:TYR:CE2	1.20	1.59
2:B:694:LYS:CG	2:C:760:TYR:CE2	1.79	1.58
2:B:694:LYS:CD	2:C:760:TYR:HD2	1.05	1.57
2:B:694:LYS:CD	2:C:760:TYR:CD2	1.90	1.55
2:B:694:LYS:HD2	2:C:760:TYR:CD2	1.41	1.53
2:B:500:LEU:CD2	2:C:783:ARG:HG3	1.33	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:374:ALA:CB	2:A:476:ILE:HD13	1.29	1.52
2:A:374:ALA:CA	2:A:476:ILE:HG21	1.31	1.52
2:A:374:ALA:CA	2:A:476:ILE:CG2	1.86	1.49
2:B:394:LEU:HD23	2:B:483:TRP:CZ3	1.48	1.49
2:B:306:ARG:NH2	2:C:242:LEU:CD2	1.75	1.47
2:B:306:ARG:NH2	2:C:242:LEU:CD1	1.76	1.47
2:B:500:LEU:HD22	2:C:783:ARG:CG	1.43	1.47
2:B:306:ARG:CD	2:C:168:ARG:HH22	1.29	1.45
2:C:377:LEU:CD1	2:C:476:ILE:CG2	1.94	1.44
2:B:511:ILE:CD1	2:B:721:GLU:OE1	1.67	1.43
2:B:694:LYS:CG	2:C:760:TYR:CD2	2.01	1.42
2:B:306:ARG:HD3	2:C:168:ARG:NH2	1.29	1.41
2:A:374:ALA:HB2	2:A:476:ILE:CD1	1.48	1.41
2:B:511:ILE:HG22	2:B:718:HIS:ND1	1.28	1.41
2:C:377:LEU:HD12	2:C:476:ILE:CG2	1.50	1.39
2:A:374:ALA:N	2:A:476:ILE:HG21	1.15	1.38
2:B:306:ARG:CZ	2:C:242:LEU:CD2	2.01	1.37
2:B:306:ARG:CZ	2:C:242:LEU:HD21	1.56	1.35
2:B:511:ILE:CG2	2:B:718:HIS:ND1	1.89	1.35
2:B:690:MET:C	2:C:760:TYR:HH	1.30	1.34
2:B:367:THR:CG2	2:B:472:THR:HA	1.56	1.33
2:B:522:LYS:O	2:C:775:ASP:CB	1.75	1.33
2:A:374:ALA:HA	2:A:476:ILE:CG2	1.52	1.33
2:B:306:ARG:HH22	2:C:242:LEU:CG	1.41	1.32
2:B:306:ARG:NH1	2:C:242:LEU:HD22	1.39	1.32
2:B:367:THR:OG1	2:B:472:THR:HA	1.30	1.31
2:A:199:ARG:CD	2:B:358:TYR:OH	1.79	1.30
2:B:199:ARG:HH22	2:C:357:ARG:NH2	1.29	1.29
2:B:394:LEU:CD2	2:B:483:TRP:CZ3	2.15	1.29
2:B:367:THR:CB	2:B:472:THR:HA	1.62	1.29
2:B:306:ARG:HH22	2:C:242:LEU:CD1	1.34	1.29
2:B:522:LYS:O	2:C:775:ASP:CG	1.73	1.27
2:B:511:ILE:HD11	2:B:721:GLU:OE1	1.08	1.25
2:A:373:ALA:HB2	2:A:473:VAL:CG1	1.66	1.25
2:B:690:MET:C	2:C:760:TYR:OH	1.73	1.23
2:C:374:ALA:N	2:C:476:ILE:CD1	2.00	1.23
2:B:199:ARG:NH2	2:C:357:ARG:NH2	1.85	1.22
2:A:380:ARG:O	2:A:611:TYR:OH	1.53	1.21
2:A:181:PRO:HB2	2:A:182:VAL:HA	1.24	1.20
2:B:367:THR:CG2	2:B:472:THR:CA	2.19	1.20
2:A:233:ILE:CG2	2:B:361:HIS:HE2	1.52	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:373:ALA:CB	2:A:473:VAL:HG12	1.71	1.20
2:B:230:VAL:HG12	2:B:231:PRO:CD	1.71	1.18
2:C:377:LEU:CD1	2:C:476:ILE:HG22	1.60	1.18
2:B:522:LYS:O	2:C:775:ASP:HB3	1.29	1.18
2:B:306:ARG:HH22	2:C:242:LEU:CD2	1.43	1.18
2:B:199:ARG:NH2	2:C:357:ARG:HH21	1.39	1.17
2:B:304:LEU:HD22	2:B:305:ALA:N	1.58	1.17
2:B:694:LYS:HG2	2:C:760:TYR:CE2	1.76	1.17
2:B:181:PRO:HB2	2:B:182:VAL:HA	1.18	1.17
2:B:690:MET:O	2:C:760:TYR:OH	1.61	1.17
2:B:367:THR:HG21	2:B:472:THR:CB	1.75	1.17
2:B:363:ARG:O	2:B:471:VAL:HB	1.43	1.17
2:B:394:LEU:CD2	2:B:483:TRP:CE3	2.27	1.16
2:B:169:ASP:O	2:B:173:ILE:HB	1.44	1.16
2:B:306:ARG:NH1	2:C:242:LEU:CD2	2.01	1.16
2:B:515:GLU:OE1	2:B:712:HIS:NE2	1.78	1.16
2:A:374:ALA:N	2:A:476:ILE:CG2	1.96	1.16
2:A:199:ARG:NE	2:B:358:TYR:OH	1.78	1.16
2:B:306:ARG:NH2	2:C:242:LEU:HD21	1.48	1.15
2:C:515:GLU:OE1	2:C:712:HIS:NE2	1.78	1.15
2:A:394:LEU:HG	2:A:480:VAL:HG23	1.16	1.15
2:B:511:ILE:CD1	2:B:721:GLU:CD	2.14	1.15
2:A:515:GLU:OE1	2:A:712:HIS:NE2	1.78	1.15
2:A:408:THR:C	2:A:414:LYS:CE	2.16	1.14
2:B:694:LYS:HG3	2:C:760:TYR:CD2	1.73	1.14
2:B:13:VAL:HG21	2:B:38:LEU:HD23	1.22	1.14
2:B:511:ILE:HG22	2:B:718:HIS:CG	1.80	1.14
2:B:439:ALA:O	2:B:442:LEU:N	1.79	1.14
2:A:394:LEU:HG	2:A:480:VAL:CG2	1.78	1.13
2:B:531:LEU:O	2:C:733:ARG:NH2	1.80	1.13
2:C:13:VAL:HG21	2:C:38:LEU:HD23	1.23	1.13
2:B:363:ARG:HH12	2:B:476:ILE:N	1.45	1.13
2:B:694:LYS:CG	2:C:760:TYR:HE2	1.32	1.13
2:A:374:ALA:HA	2:A:476:ILE:HG23	1.17	1.12
2:B:180:ASP:HB2	2:B:181:PRO:HD2	1.31	1.12
2:B:526:ARG:HH21	2:C:771:LYS:HG3	1.07	1.11
2:A:373:ALA:HB2	2:A:473:VAL:HG12	1.19	1.11
2:B:231:PRO:HG2	2:B:232:GLU:HG2	1.22	1.11
2:C:374:ALA:N	2:C:476:ILE:HD13	1.65	1.11
2:B:369:ASP:HB3	2:B:473:VAL:CG2	1.81	1.10
2:A:13:VAL:HG21	2:A:38:LEU:HD23	1.25	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:394:LEU:HD13	2:C:479:VAL:HG11	1.11	1.09
2:B:525:ARG:O	2:C:778:SER:HB2	1.49	1.09
2:C:181:PRO:HB2	2:C:182:VAL:HA	1.21	1.08
2:C:394:LEU:HD13	2:C:479:VAL:CG1	1.82	1.08
2:A:394:LEU:CG	2:A:480:VAL:HG23	1.82	1.08
2:C:377:LEU:HD12	2:C:476:ILE:HG21	1.11	1.08
2:A:382:ILE:HA	2:A:383:SER:HB3	1.32	1.07
2:C:382:ILE:HA	2:C:383:SER:HB3	1.33	1.07
2:B:500:LEU:CD1	2:C:783:ARG:HG2	1.84	1.07
2:B:200:THR:CG2	2:C:392:ILE:HG22	1.85	1.07
2:B:500:LEU:HD11	2:C:783:ARG:HA	1.32	1.07
2:A:233:ILE:HG23	2:B:361:HIS:NE2	1.31	1.07
2:A:408:THR:O	2:A:414:LYS:HE3	1.52	1.07
2:C:242:LEU:HB3	2:C:243:ASP:HA	1.28	1.07
2:B:500:LEU:HD13	2:C:783:ARG:CG	1.85	1.06
2:B:367:THR:OG1	2:B:472:THR:CA	2.02	1.06
2:B:363:ARG:NH1	2:B:476:ILE:HD12	1.69	1.06
2:A:526:ARG:HG2	2:B:778:SER:HB3	1.30	1.06
2:A:374:ALA:CB	2:A:476:ILE:HG21	1.84	1.06
2:B:305:ALA:HA	2:B:309:LEU:HD21	1.30	1.06
2:B:526:ARG:NH2	2:C:771:LYS:HG3	1.65	1.06
2:B:370:ALA:HB1	2:B:476:ILE:HD13	1.37	1.05
2:B:200:THR:HG21	2:C:392:ILE:CG2	1.86	1.05
2:B:511:ILE:HD12	2:B:721:GLU:CD	1.76	1.05
2:A:199:ARG:HD3	2:B:358:TYR:OH	1.55	1.05
2:A:374:ALA:HB3	2:A:476:ILE:HD13	1.39	1.05
2:B:525:ARG:O	2:C:778:SER:CB	2.03	1.04
2:B:200:THR:HG21	2:C:392:ILE:HG22	1.05	1.04
2:A:373:ALA:CB	2:A:473:VAL:CG1	2.31	1.04
2:B:526:ARG:N	2:C:775:ASP:HA	1.38	1.03
2:B:306:ARG:NH2	2:C:242:LEU:HD11	1.50	1.03
2:B:500:LEU:HD13	2:C:783:ARG:HG2	1.06	1.03
2:A:408:THR:C	2:A:414:LYS:NZ	2.12	1.03
2:C:373:ALA:HB3	2:C:476:ILE:HD12	1.41	1.03
2:B:512:GLY:H	2:B:718:HIS:CE1	1.76	1.03
2:B:306:ARG:NH2	2:C:242:LEU:CG	2.10	1.02
2:A:374:ALA:CB	2:A:476:ILE:CG2	2.36	1.02
2:A:171:THR:HG22	2:A:175:LYS:HE3	1.41	1.01
2:A:233:ILE:CG2	2:B:361:HIS:NE2	2.10	1.00
2:A:367:THR:CB	2:A:472:THR:HG23	1.92	1.00
2:B:230:VAL:CG1	2:B:231:PRO:HD3	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ALA:HA	2:B:309:LEU:CD2	1.91	1.00
2:C:171:THR:HG22	2:C:175:LYS:HE3	1.44	1.00
2:B:441:SER:O	2:B:445:THR:HG23	1.62	1.00
2:B:526:ARG:NH2	2:C:771:LYS:CG	2.05	1.00
2:C:366:ILE:HG22	2:C:367:THR:HA	1.44	0.99
2:B:512:GLY:HA2	2:B:718:HIS:NE2	1.78	0.99
2:B:363:ARG:HH11	2:B:476:ILE:HD12	1.23	0.99
2:B:402:VAL:HG13	2:B:467:GLU:OE2	1.61	0.99
2:B:306:ARG:CZ	2:C:242:LEU:HD22	1.75	0.99
2:A:439:ALA:HA	2:A:442:LEU:HB2	1.44	0.99
2:B:230:VAL:HG12	2:B:231:PRO:HD3	1.02	0.99
2:B:379:ASP:HA	2:B:387:LEU:HD21	1.45	0.99
2:B:476:ILE:O	2:B:479:VAL:HB	1.61	0.99
2:B:439:ALA:HA	2:B:442:LEU:HD12	1.44	0.99
2:B:500:LEU:CD1	2:C:783:ARG:HA	1.90	0.98
2:C:377:LEU:CD1	2:C:476:ILE:HG21	1.73	0.98
2:B:512:GLY:CA	2:B:718:HIS:NE2	2.27	0.98
2:C:367:THR:OG1	2:C:471:VAL:CG1	2.11	0.98
2:B:185:ARG:HG2	2:B:188:GLU:HG2	1.46	0.98
2:C:439:ALA:HA	2:C:442:LEU:HB2	1.44	0.98
2:B:306:ARG:NH2	2:C:242:LEU:HD13	1.78	0.98
2:A:397:GLU:CB	2:A:479:VAL:HG13	1.93	0.98
2:C:367:THR:OG1	2:C:471:VAL:HG11	1.63	0.98
2:A:397:GLU:HB2	2:A:479:VAL:HG13	0.98	0.97
2:B:394:LEU:HD22	2:B:483:TRP:CE3	1.98	0.97
2:B:200:THR:CG2	2:C:392:ILE:CG2	2.41	0.97
2:B:240:MET:HG3	2:B:274:ILE:HD11	1.43	0.97
2:C:377:LEU:HD11	2:C:476:ILE:HG22	1.43	0.96
2:B:185:ARG:HH11	2:B:185:ARG:HB2	1.31	0.96
2:B:306:ARG:HH21	2:C:242:LEU:HD11	1.02	0.95
2:A:700:GLU:OE1	2:B:763:ARG:NH1	1.99	0.95
2:A:366:ILE:HG22	2:A:367:THR:HA	1.44	0.95
2:B:512:GLY:N	2:B:718:HIS:CE1	2.33	0.95
2:A:397:GLU:HB2	2:A:479:VAL:CG1	1.94	0.95
2:C:377:LEU:HD11	2:C:476:ILE:CG2	1.93	0.95
2:B:190:GLN:OE1	2:C:404:LEU:HD21	1.67	0.94
2:B:367:THR:HG23	2:B:472:THR:CA	1.95	0.94
2:A:371:ILE:HA	2:A:476:ILE:HD12	1.46	0.94
2:B:359:GLU:HG2	2:B:365:SER:N	1.81	0.94
2:B:276:LEU:N	2:B:310:GLN:O	2.00	0.94
2:B:694:LYS:HG2	2:C:760:TYR:HE2	1.13	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:394:LEU:CG	2:A:480:VAL:CG2	2.45	0.93
2:B:394:LEU:HA	2:B:483:TRP:CH2	2.03	0.93
2:A:363:ARG:HH12	2:A:475:ASP:CB	1.82	0.93
2:C:379:ASP:HA	2:C:387:LEU:HD21	1.50	0.93
2:C:98:LEU:HB3	2:C:100:HIS:HD2	1.33	0.93
2:B:367:THR:HG23	2:B:472:THR:N	1.82	0.93
2:A:374:ALA:HB2	2:A:476:ILE:CG1	1.99	0.93
2:A:374:ALA:CB	2:A:476:ILE:CD1	2.24	0.93
2:B:367:THR:HG21	2:B:472:THR:CG2	1.97	0.93
2:B:306:ARG:HH12	2:C:242:LEU:CD2	1.74	0.93
2:B:168:ARG:NH1	2:B:242:LEU:HB2	1.82	0.92
2:A:408:THR:O	2:A:414:LYS:CE	2.17	0.92
2:B:359:GLU:HA	2:B:364:VAL:O	1.70	0.92
2:B:526:ARG:NE	2:C:775:ASP:HB2	1.85	0.91
2:A:374:ALA:H	2:A:476:ILE:HG21	1.13	0.91
2:B:370:ALA:HB1	2:B:476:ILE:CD1	1.99	0.91
2:B:194:GLU:HA	2:C:400:SER:OG	1.70	0.91
2:B:185:ARG:NH1	2:B:185:ARG:HB2	1.86	0.91
2:C:402:VAL:CG1	2:C:467:GLU:OE1	2.19	0.91
2:B:306:ARG:HH12	2:C:242:LEU:HD22	0.93	0.91
2:C:181:PRO:HB2	2:C:182:VAL:CA	2.01	0.91
2:C:439:ALA:O	2:C:442:LEU:N	2.04	0.91
2:B:382:ILE:HA	2:B:383:SER:HB3	1.53	0.91
2:A:394:LEU:CD1	2:A:480:VAL:HG23	2.01	0.90
2:A:500:LEU:CD1	2:A:500:LEU:CB	2.49	0.90
2:A:394:LEU:HD21	2:A:480:VAL:HA	1.53	0.90
2:A:379:ASP:HA	2:A:387:LEU:HD21	1.51	0.90
2:B:378:SER:HB3	2:B:390:LYS:HE2	1.52	0.90
2:A:500:LEU:CD1	2:A:500:LEU:CD2	2.49	0.90
2:B:98:LEU:HB3	2:B:100:HIS:HD2	1.37	0.90
2:B:265:MET:CE	2:B:269:ARG:HH21	1.85	0.90
2:B:511:ILE:HG21	2:B:718:HIS:HA	1.53	0.89
2:A:370:ALA:CB	2:A:471:VAL:O	2.20	0.89
2:C:374:ALA:CA	2:C:476:ILE:HD13	2.02	0.89
2:B:434:GLN:HG2	2:B:434:GLN:O	1.72	0.89
2:C:556:ARG:HG2	2:C:569:MET:HE1	1.55	0.89
2:A:98:LEU:HB3	2:A:100:HIS:HD2	1.37	0.89
2:A:556:ARG:HG2	2:A:569:MET:HE1	1.54	0.89
2:A:181:PRO:HB2	2:A:182:VAL:CA	2.01	0.88
2:B:556:ARG:HG2	2:B:569:MET:HE1	1.54	0.88
2:B:367:THR:HG23	2:B:472:THR:HA	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:382:ILE:HG13	2:C:484:THR:HG23	1.52	0.88
2:A:371:ILE:HA	2:A:476:ILE:CD1	2.04	0.88
2:B:370:ALA:O	2:B:476:ILE:HG21	1.74	0.87
2:B:369:ASP:HB3	2:B:473:VAL:HG21	1.54	0.87
2:A:500:LEU:CB	2:A:500:LEU:CD2	2.52	0.87
2:B:180:ASP:CB	2:B:181:PRO:HD2	2.04	0.86
2:A:374:ALA:CA	2:A:476:ILE:HG23	1.83	0.86
2:B:428:ASP:O	2:B:431:VAL:HG12	1.75	0.86
2:B:367:THR:HG21	2:B:472:THR:HG23	1.56	0.86
2:B:523:ALA:O	2:C:775:ASP:OD1	1.93	0.86
2:B:233:ILE:HD13	2:B:233:ILE:O	1.76	0.86
2:B:198:ARG:HB3	2:C:396:ASP:OD2	1.75	0.85
2:C:206:LEU:HD12	2:C:313:GLY:O	1.76	0.85
2:B:180:ASP:HB2	2:B:181:PRO:CD	2.00	0.85
2:C:374:ALA:H	2:C:476:ILE:CD1	1.90	0.85
2:B:370:ALA:CB	2:B:476:ILE:HD13	2.06	0.85
2:A:165:SER:N	2:A:166:LEU:O	2.09	0.85
2:C:373:ALA:CB	2:C:476:ILE:HD12	2.06	0.85
2:C:321:ARG:O	2:C:325:GLU:HB2	1.75	0.85
2:B:369:ASP:C	2:B:473:VAL:HG22	1.96	0.85
2:B:402:VAL:HG13	2:B:467:GLU:CD	1.95	0.85
2:B:500:LEU:HD11	2:C:783:ARG:CA	2.07	0.85
2:C:165:SER:N	2:C:166:LEU:O	2.10	0.85
2:B:306:ARG:HH22	2:C:242:LEU:HD13	1.35	0.84
2:B:522:LYS:HA	2:C:779:GLU:OE2	1.77	0.84
2:B:181:PRO:CB	2:B:182:VAL:HA	2.05	0.84
2:A:374:ALA:HB2	2:A:476:ILE:CG2	2.03	0.84
2:C:377:LEU:HD13	2:C:476:ILE:HG22	1.59	0.84
2:B:456:THR:HA	2:B:459:SER:HB3	1.60	0.84
2:B:365:SER:O	2:B:366:ILE:HG12	1.78	0.84
2:C:185:ARG:HH21	2:C:342:PRO:HG3	1.42	0.83
2:B:367:THR:HG21	2:B:472:THR:OG1	1.78	0.83
2:C:201:LYS:HE2	2:C:432:GLN:HE21	84.71	0.83
2:B:512:GLY:HA2	2:B:718:HIS:HE2	1.41	0.83
2:A:526:ARG:CG	2:B:778:SER:HB3	2.07	0.83
2:A:321:ARG:O	2:A:325:GLU:HB2	1.76	0.83
2:B:365:SER:O	2:B:471:VAL:HG21	1.78	0.83
2:B:532:LYS:C	2:C:733:ARG:NH2	2.32	0.83
2:C:382:ILE:HG13	2:C:484:THR:CG2	2.08	0.83
2:B:367:THR:HG21	2:B:472:THR:CA	1.97	0.82
2:B:335:GLN:HG2	2:B:336:PRO:HD3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:300:LEU:CB	2:C:302:PRO:HD3	2.09	0.82
2:B:500:LEU:CD1	2:C:783:ARG:CG	2.50	0.82
2:C:444:ASP:O	2:C:448:ARG:HG3	1.79	0.82
2:A:603:THR:HB	2:A:647:VAL:HG21	1.61	0.82
2:B:366:ILE:HB	2:B:367:THR:HA	1.60	0.82
2:C:374:ALA:CA	2:C:476:ILE:CD1	2.57	0.82
2:A:272:GLY:HA2	2:A:308:GLU:HG3	1.62	0.82
2:C:706:ASP:O	2:C:707:GLU:HG2	1.80	0.82
2:B:526:ARG:N	2:C:775:ASP:CA	2.24	0.82
2:C:9:ARG:HD2	2:C:41:GLU:OE2	1.79	0.82
2:B:706:ASP:O	2:B:707:GLU:HG2	1.80	0.81
2:A:408:THR:C	2:A:414:LYS:HE3	1.93	0.81
2:B:363:ARG:NH1	2:B:476:ILE:N	2.28	0.81
2:A:341:GLN:HG3	2:A:387:LEU:H	1.45	0.81
2:B:306:ARG:NH2	2:C:242:LEU:HD22	1.77	0.81
2:A:526:ARG:HD3	2:B:778:SER:CB	2.10	0.81
2:A:366:ILE:CG2	2:A:367:THR:HA	2.09	0.81
2:A:439:ALA:O	2:A:442:LEU:N	2.13	0.81
2:C:366:ILE:CG2	2:C:367:THR:HA	2.10	0.81
2:A:434:GLN:O	2:A:434:GLN:HG2	1.77	0.81
2:B:496:THR:CG2	2:C:782:LEU:HD22	2.10	0.81
2:A:382:ILE:CA	2:A:383:SER:HB3	2.10	0.81
2:B:304:LEU:HD22	2:B:305:ALA:H	1.41	0.81
2:B:603:THR:HB	2:B:647:VAL:HG21	1.61	0.81
2:A:323:TYR:O	2:A:326:LYS:HB2	1.79	0.81
2:B:167:ALA:HB1	2:B:241:THR:O	1.81	0.81
2:C:427:LYS:O	2:C:431:VAL:HG23	1.81	0.81
2:A:394:LEU:HD12	2:A:476:ILE:O	1.79	0.81
2:A:185:ARG:HH21	2:A:342:PRO:HG3	1.43	0.81
2:B:240:MET:CG	2:B:274:ILE:HD11	2.11	0.81
2:B:308:GLU:O	2:B:309:LEU:HG	1.81	0.81
2:B:367:THR:OG1	2:B:472:THR:C	2.18	0.81
2:A:394:LEU:CD1	2:A:480:VAL:CG2	2.54	0.80
2:B:370:ALA:HB1	2:B:476:ILE:CG1	2.09	0.80
2:A:444:ASP:O	2:A:448:ARG:HG3	1.81	0.80
2:A:427:LYS:O	2:A:431:VAL:HG23	1.81	0.80
2:C:603:THR:HB	2:C:647:VAL:HG21	1.61	0.80
2:B:511:ILE:HD12	2:B:721:GLU:OE2	1.80	0.80
2:A:394:LEU:CD2	2:A:480:VAL:HA	2.10	0.80
2:C:272:GLY:HA2	2:C:308:GLU:HG3	1.62	0.80
2:C:242:LEU:CB	2:C:243:ASP:HA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:GLU:O	2:B:350:ILE:HG13	1.81	0.80
2:A:706:ASP:O	2:A:707:GLU:HG2	1.80	0.80
2:B:690:MET:O	2:C:760:TYR:CZ	2.35	0.80
2:B:359:GLU:HG2	2:B:365:SER:H	1.44	0.80
2:B:262:LYS:NZ	2:C:260:ARG:HH22	1.79	0.80
2:A:199:ARG:HD3	2:B:358:TYR:HH	1.46	0.80
2:A:21:ALA:HB3	2:A:22:LEU:HD22	1.64	0.80
2:B:500:LEU:CG	2:C:783:ARG:HG3	2.12	0.79
2:A:363:ARG:HH12	2:A:475:ASP:HB3	1.45	0.79
2:A:74:MET:HB3	2:A:76:GLN:NE2	1.97	0.79
2:C:203:ASN:O	2:C:334:PHE:HA	1.81	0.79
2:B:511:ILE:HG23	2:B:718:HIS:ND1	1.95	0.79
2:B:496:THR:HB	2:C:782:LEU:HB3	1.65	0.79
2:A:411:PRO:HB2	2:A:413:LEU:HG	1.64	0.79
2:C:227:ASN:HA	2:C:228:ASN:HB2	1.64	0.79
2:B:90:LEU:HD22	2:B:114:ARG:HD3	1.65	0.79
2:B:394:LEU:HD23	2:B:483:TRP:HZ3	1.39	0.79
2:B:367:THR:OG1	2:B:473:VAL:N	2.15	0.79
2:C:434:GLN:HG2	2:C:434:GLN:O	1.80	0.79
2:B:363:ARG:O	2:B:471:VAL:CB	2.29	0.79
2:B:305:ALA:CA	2:B:309:LEU:HD21	2.13	0.79
2:B:191:ARG:HG2	2:B:337:ILE:HG21	1.64	0.79
2:C:402:VAL:HG12	2:C:467:GLU:OE1	1.83	0.79
2:B:584:SER:HB3	2:B:602:LEU:HB3	1.63	0.79
2:C:74:MET:HB3	2:C:76:GLN:NE2	1.97	0.79
2:B:522:LYS:O	2:C:775:ASP:OD2	2.01	0.79
2:A:584:SER:HB3	2:A:602:LEU:HB3	1.63	0.79
2:C:13:VAL:HG23	2:C:37:GLY:O	1.83	0.79
2:C:584:SER:HB3	2:C:602:LEU:HB3	1.63	0.79
2:B:185:ARG:HG2	2:B:188:GLU:CG	2.12	0.78
2:A:227:ASN:HA	2:A:228:ASN:HB2	1.64	0.78
2:B:200:THR:HG23	2:C:358:TYR:OH	1.83	0.78
2:A:199:ARG:CZ	2:B:358:TYR:OH	2.31	0.78
2:B:74:MET:HB3	2:B:76:GLN:NE2	1.99	0.78
2:B:430:ALA:HB1	2:B:435:GLU:HG2	1.64	0.78
2:A:83:ARG:HD2	2:A:115:GLU:HG2	1.66	0.78
2:B:511:ILE:HD12	2:B:721:GLU:OE1	1.66	0.78
2:A:369:ASP:HB2	2:A:472:THR:HG22	1.64	0.78
2:C:181:PRO:CB	2:C:182:VAL:HA	2.07	0.78
2:C:394:LEU:CD1	2:C:479:VAL:HG11	2.06	0.78
2:A:526:ARG:HD3	2:B:778:SER:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ALA:HB3	2:B:22:LEU:HD22	1.65	0.77
2:B:690:MET:HB3	2:C:760:TYR:OH	1.84	0.77
2:C:402:VAL:HG13	2:C:467:GLU:OE1	1.84	0.77
2:C:35:LEU:HD21	2:C:60:ILE:HD13	1.67	0.77
2:A:183:ILE:HD12	2:A:350:ILE:HG12	1.65	0.77
2:B:129:VAL:O	2:B:129:VAL:HG12	1.83	0.77
2:B:355:ARG:HB3	2:B:355:ARG:HH11	1.47	0.77
2:A:546:PRO:HG2	2:A:549:VAL:HG21	1.67	0.77
2:B:546:PRO:HG2	2:B:549:VAL:HG21	1.67	0.77
2:C:423:VAL:O	2:C:424:ARG:C	2.21	0.77
2:C:374:ALA:N	2:C:476:ILE:HD11	1.99	0.77
2:B:345:ASP:HA	2:B:348:ILE:HD11	1.66	0.77
2:A:763:ARG:HB2	2:A:764:PRO:HD3	1.67	0.77
2:B:500:LEU:CG	2:C:783:ARG:CG	2.62	0.76
2:C:204:PRO:HG2	2:C:312:ILE:HG12	1.65	0.76
2:A:90:LEU:HD22	2:A:114:ARG:HD3	1.66	0.76
2:A:31:THR:HB	2:A:112:LEU:HD21	1.67	0.76
2:B:140:GLN:O	2:B:141:LEU:HD23	1.85	0.76
2:A:140:GLN:O	2:A:141:LEU:HD23	1.84	0.76
2:A:374:ALA:HB2	2:A:476:ILE:HD13	0.76	0.76
2:A:443:ARG:O	2:A:446:GLU:HB3	1.86	0.76
2:B:159:ASN:O	2:B:163:LEU:CB	2.34	0.76
2:C:341:GLN:HG3	2:C:387:LEU:H	1.50	0.76
2:A:371:ILE:CA	2:A:476:ILE:HD12	2.16	0.76
2:B:763:ARG:HB2	2:B:764:PRO:HD3	1.67	0.76
2:A:185:ARG:HG2	2:A:188:GLU:HG2	1.68	0.76
2:C:394:LEU:CD1	2:C:479:VAL:CG1	2.63	0.76
2:C:367:THR:H	2:C:471:VAL:HG21	1.51	0.76
2:B:379:ASP:HB2	2:B:387:LEU:HD11	1.68	0.75
2:C:230:VAL:HG13	2:C:231:PRO:HD2	1.67	0.75
2:C:546:PRO:HG2	2:C:549:VAL:HG21	1.67	0.75
2:B:5:ARG:NH1	2:B:5:ARG:H	1.84	0.75
2:C:411:PRO:HB2	2:C:413:LEU:HG	1.67	0.75
2:C:201:LYS:HE2	2:C:432:GLN:NE2	83.90	0.75
2:C:382:ILE:CD1	2:C:484:THR:HG21	2.17	0.75
2:B:31:THR:HB	2:B:112:LEU:HD21	1.67	0.75
2:A:206:LEU:HD12	2:A:313:GLY:O	1.87	0.75
2:B:276:LEU:O	2:B:311:CYS:HA	1.86	0.75
2:C:323:TYR:O	2:C:326:LYS:HB2	1.86	0.75
2:B:122:ARG:HD3	2:B:176:GLU:OE1	45.38	0.75
2:B:198:ARG:O	2:B:199:ARG:HB2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:ILE:O	2:B:399:GLY:N	2.19	0.75
2:C:183:ILE:HD12	2:C:350:ILE:HG12	1.69	0.75
2:C:300:LEU:C	2:C:302:PRO:HD3	2.07	0.75
2:A:441:SER:O	2:A:445:THR:HG23	1.87	0.75
2:C:5:ARG:H	2:C:5:ARG:NH1	1.85	0.75
2:A:181:PRO:CB	2:A:182:VAL:HA	2.10	0.75
2:C:377:LEU:HD12	2:C:476:ILE:HG23	1.67	0.75
2:C:382:ILE:CA	2:C:383:SER:HB3	2.13	0.74
2:B:364:VAL:HG22	2:B:366:ILE:O	1.87	0.74
2:B:184:GLY:HA3	2:B:185:ARG:C	2.08	0.74
2:A:13:VAL:HG23	2:A:37:GLY:O	1.87	0.74
2:B:232:GLU:O	2:B:233:ILE:HD13	1.86	0.74
2:B:369:ASP:HB3	2:B:473:VAL:HG22	1.66	0.74
2:B:363:ARG:HH12	2:B:476:ILE:H	1.34	0.74
2:B:402:VAL:CG1	2:B:467:GLU:OE2	2.34	0.74
2:A:203:ASN:O	2:A:334:PHE:HA	1.88	0.73
2:A:9:ARG:HD2	2:A:41:GLU:OE2	1.86	0.73
2:B:179:LEU:HB3	2:B:223:GLN:NE2	2.03	0.73
2:A:6:PHE:HB2	2:A:10:ALA:HB3	1.70	0.73
2:B:241:THR:HG22	2:B:277:PHE:HD1	1.53	0.73
2:A:703:ASN:HB3	2:B:767:ARG:CB	2.18	0.73
2:B:181:PRO:HB2	2:B:182:VAL:CA	2.09	0.73
2:B:200:THR:O	2:B:202:ASN:N	2.21	0.73
2:C:140:GLN:O	2:C:141:LEU:HD23	1.88	0.73
2:C:242:LEU:HB3	2:C:243:ASP:CA	2.15	0.73
2:C:441:SER:O	2:C:445:THR:HG23	1.88	0.73
2:B:358:TYR:C	2:B:360:ALA:H	1.91	0.73
2:C:60:ILE:HG22	2:C:61:GLN:N	2.03	0.73
2:B:361:HIS:O	2:B:362:HIS:HB2	1.88	0.73
2:B:500:LEU:HD21	2:C:783:ARG:N	2.03	0.73
2:A:355:ARG:NE	2:A:366:ILE:H	1.87	0.73
2:A:204:PRO:HG2	2:A:312:ILE:HG12	1.71	0.73
2:C:129:VAL:O	2:C:129:VAL:HG12	1.87	0.72
2:B:483:TRP:HD1	2:B:483:TRP:H	1.37	0.72
2:A:166:LEU:CB	2:A:167:ALA:HB2	2.20	0.72
2:C:103:VAL:HG12	2:C:104:GLY:N	2.04	0.72
2:C:373:ALA:C	2:C:476:ILE:HD13	2.09	0.72
2:C:21:ALA:HB3	2:C:22:LEU:HD22	1.70	0.72
2:C:6:PHE:HB2	2:C:10:ALA:HB3	1.71	0.72
2:C:166:LEU:CB	2:C:167:ALA:HB2	2.19	0.72
2:A:366:ILE:CB	2:A:367:THR:HA	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:THR:O	2:B:370:ALA:HB3	1.90	0.72
2:B:260:ARG:HA	2:B:263:LYS:HD3	1.71	0.72
2:B:214:LYS:NZ	2:B:314:ALA:HA	2.04	0.72
2:A:423:VAL:O	2:A:424:ARG:C	2.28	0.72
2:A:367:THR:CB	2:A:472:THR:CG2	2.66	0.72
2:A:129:VAL:O	2:A:129:VAL:HG12	1.88	0.72
2:A:21:ALA:HB2	2:A:29:ILE:CG2	2.19	0.72
2:A:373:ALA:HB3	2:A:473:VAL:CG1	2.20	0.72
2:B:189:ILE:HG22	2:B:190:GLN:N	2.05	0.71
2:B:377:LEU:CD2	2:B:480:VAL:HG21	2.20	0.71
2:B:6:PHE:HB2	2:B:10:ALA:HB3	1.72	0.71
2:A:5:ARG:NH1	2:A:5:ARG:H	1.88	0.71
2:A:355:ARG:HD3	2:A:365:SER:HB2	1.72	0.71
2:C:13:VAL:HG23	2:C:37:GLY:C	2.11	0.71
2:C:382:ILE:HD11	2:C:484:THR:HG21	1.70	0.71
2:B:21:ALA:HB2	2:B:29:ILE:CG2	2.20	0.71
2:C:185:ARG:HG2	2:C:188:GLU:HG2	1.73	0.71
2:B:269:ARG:HH12	2:B:306:ARG:HB3	1.54	0.71
2:B:694:LYS:HD2	2:C:760:TYR:HD2	0.54	0.71
2:B:500:LEU:CD1	2:C:783:ARG:CA	2.66	0.71
2:B:479:VAL:HG12	2:B:480:VAL:N	2.05	0.71
2:B:190:GLN:OE1	2:C:404:LEU:CD2	2.38	0.71
2:B:397:GLU:O	2:B:401:LYS:HB2	1.90	0.71
2:A:526:ARG:HG2	2:B:778:SER:CB	2.14	0.71
2:B:542:ILE:HG13	2:B:705:ILE:HD13	1.71	0.71
2:B:526:ARG:H	2:C:775:ASP:CG	1.91	0.71
2:B:214:LYS:HZ3	2:B:314:ALA:HA	1.55	0.71
2:A:378:SER:HB3	2:A:390:LYS:HD3	1.73	0.71
2:A:373:ALA:HB3	2:A:473:VAL:HG12	1.68	0.70
2:B:185:ARG:HH11	2:B:185:ARG:CB	2.04	0.70
2:B:411:PRO:C	2:B:413:LEU:H	1.94	0.70
2:A:542:ILE:HG13	2:A:705:ILE:HD13	1.71	0.70
2:A:627:PHE:O	2:A:631:LEU:HB2	1.92	0.70
2:A:408:THR:C	2:A:414:LYS:HZ1	1.92	0.70
2:C:374:ALA:HA	2:C:476:ILE:HD13	1.72	0.70
2:A:341:GLN:HG2	2:A:387:LEU:HB2	1.74	0.70
2:C:648:ASP:OD1	2:C:650:ARG:HG2	1.91	0.70
2:C:54:GLY:O	2:C:55:LEU:HD23	1.91	0.70
2:B:648:ASP:OD1	2:B:650:ARG:HG2	1.91	0.70
2:C:627:PHE:O	2:C:631:LEU:HB2	1.92	0.70
2:C:542:ILE:HG13	2:C:705:ILE:HD13	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ILE:O	2:B:338:GLN:HA	1.92	0.70
2:C:90:LEU:HD22	2:C:114:ARG:HD3	1.73	0.70
2:A:648:ASP:OD1	2:A:650:ARG:HG2	1.91	0.70
2:B:499:LEU:HD13	2:C:782:LEU:CD1	2.22	0.70
2:A:367:THR:H	2:A:471:VAL:CA	2.05	0.69
2:B:9:ARG:HD2	2:B:41:GLU:OE2	1.92	0.69
2:A:359:GLU:HG2	2:A:364:VAL:CG1	2.23	0.69
2:B:265:MET:HE1	2:B:269:ARG:HH21	1.56	0.69
2:C:341:GLN:HG2	2:C:387:LEU:HB2	1.75	0.69
2:C:355:ARG:HD3	2:C:365:SER:HB2	1.74	0.69
2:C:31:THR:HB	2:C:112:LEU:HD21	1.73	0.69
2:C:66:SER:O	2:C:67:LEU:HD23	1.92	0.69
2:A:107:HIS:HA	2:A:110:LEU:HD12	1.74	0.69
2:B:400:SER:OG	2:B:401:LYS:N	2.25	0.69
2:C:366:ILE:CB	2:C:367:THR:HA	2.23	0.69
2:B:306:ARG:HD3	2:C:168:ARG:HH22	0.56	0.69
2:C:443:ARG:O	2:C:446:GLU:HB3	1.92	0.69
2:A:382:ILE:HG13	2:A:484:THR:HB	1.73	0.69
2:B:206:LEU:HB2	2:B:313:GLY:O	1.93	0.69
2:B:482:SER:HG	2:B:483:TRP:HD1	1.39	0.69
2:A:212:VAL:HG13	2:A:342:PRO:HD3	1.75	0.69
2:B:191:ARG:HD2	2:B:337:ILE:HG22	1.75	0.69
2:C:359:GLU:HG2	2:C:364:VAL:CG1	2.22	0.69
2:B:627:PHE:O	2:B:631:LEU:HB2	1.91	0.69
2:A:341:GLN:CG	2:A:387:LEU:H	2.05	0.69
2:B:315:THR:OG1	2:B:319:GLU:HB3	1.92	0.69
2:A:624:PRO:HA	2:A:627:PHE:HD2	1.57	0.69
2:C:46:ALA:O	2:C:50:LEU:HD12	1.92	0.69
2:B:358:TYR:C	2:B:360:ALA:N	2.41	0.69
2:C:624:PRO:HA	2:C:627:PHE:HD2	1.58	0.69
2:A:10:ALA:HB2	2:A:104:GLY:HA2	1.73	0.68
2:C:21:ALA:HB2	2:C:29:ILE:CG2	2.23	0.68
2:A:494:THR:HA	2:A:497:ASP:HB2	1.75	0.68
2:A:373:ALA:CB	2:A:473:VAL:HG13	2.19	0.68
2:C:212:VAL:HG13	2:C:342:PRO:HD3	1.76	0.68
2:C:415:GLU:HA	2:C:418:GLN:CD	2.13	0.68
2:C:364:VAL:HG13	2:C:365:SER:HA	1.75	0.68
2:B:330:LEU:O	2:B:332:ARG:N	2.26	0.68
2:B:197:SER:HB3	2:C:361:HIS:CD2	2.28	0.68
2:B:233:ILE:CD1	2:B:233:ILE:O	2.40	0.68
2:B:449:LEU:O	2:B:452:GLN:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:371:ILE:HG22	2:C:372:GLU:N	2.08	0.68
2:B:168:ARG:HH12	2:B:242:LEU:HD13	1.57	0.68
2:B:335:GLN:HG2	2:B:336:PRO:CD	2.23	0.68
2:A:199:ARG:CD	2:B:358:TYR:CZ	2.77	0.68
2:B:439:ALA:O	2:B:442:LEU:CA	2.41	0.68
2:B:222:ALA:O	2:B:226:ILE:HG13	1.94	0.68
2:B:200:THR:CG2	2:C:392:ILE:HG21	2.22	0.68
2:B:382:ILE:CA	2:B:383:SER:HB3	2.24	0.68
2:B:624:PRO:HA	2:B:627:PHE:HD2	1.58	0.68
2:B:46:ALA:O	2:B:50:LEU:HD12	1.94	0.68
2:A:13:VAL:HG23	2:A:37:GLY:C	2.14	0.68
2:B:306:ARG:HD3	2:C:168:ARG:CZ	2.18	0.68
2:C:5:ARG:HE	2:C:102:TYR:HE1	1.42	0.68
2:A:364:VAL:HG13	2:A:365:SER:HA	1.76	0.67
2:C:183:ILE:HG22	2:C:184:GLY:N	2.09	0.67
2:A:342:PRO:HD2	2:A:388:PRO:HD3	1.74	0.67
2:C:301:LYS:N	2:C:302:PRO:HD3	2.09	0.67
2:B:204:PRO:HG2	2:B:312:ILE:HG13	1.75	0.67
2:B:194:GLU:CA	2:C:400:SER:OG	2.42	0.67
2:B:369:ASP:CB	2:B:473:VAL:CG2	2.67	0.67
2:A:233:ILE:HD11	2:B:399:GLY:O	1.94	0.67
2:A:445:THR:HG22	2:A:448:ARG:NH1	2.09	0.67
2:A:382:ILE:HA	2:A:383:SER:CB	2.13	0.67
2:A:6:PHE:N	2:A:6:PHE:CD2	2.62	0.67
2:A:377:LEU:HD11	2:A:477:ALA:HB2	1.77	0.67
2:B:365:SER:C	2:B:471:VAL:HG21	2.13	0.67
2:B:167:ALA:O	2:B:168:ARG:O	2.12	0.67
2:A:233:ILE:CD1	2:B:399:GLY:O	2.43	0.67
2:B:301:LYS:N	2:B:302:PRO:CD	2.58	0.67
2:A:103:VAL:HG12	2:A:104:GLY:N	2.10	0.66
2:A:231:PRO:HD3	2:B:404:LEU:HD13	1.75	0.66
2:B:169:ASP:N	2:B:173:ILE:HD12	2.10	0.66
2:A:354:LEU:HB3	2:A:357:ARG:NH1	2.09	0.66
2:A:66:SER:O	2:A:67:LEU:HD23	1.95	0.66
2:B:494:THR:HA	2:B:497:ASP:HB2	1.75	0.66
2:C:355:ARG:NE	2:C:366:ILE:H	1.92	0.66
2:B:355:ARG:HD2	2:B:365:SER:HA	1.78	0.66
2:A:197:SER:OG	2:B:400:SER:HB3	1.95	0.66
2:B:229:GLU:O	2:B:230:VAL:HG22	1.95	0.66
2:B:13:VAL:CG2	2:B:38:LEU:HD23	2.14	0.66
2:A:565:ASP:O	2:A:567:GLU:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:445:THR:HG22	2:C:448:ARG:NH1	2.10	0.66
2:B:437:GLU:C	2:B:439:ALA:H	1.96	0.66
2:B:437:GLU:O	2:B:439:ALA:N	2.27	0.66
2:C:509:ARG:HD3	2:C:557:ALA:HB2	1.77	0.66
2:B:620:GLU:HG3	2:B:658:SER:OG	1.96	0.66
2:B:13:VAL:HG23	2:B:37:GLY:C	2.15	0.66
2:C:10:ALA:HB2	2:C:104:GLY:HA2	1.76	0.66
2:C:515:GLU:OE1	2:C:712:HIS:CD2	2.49	0.66
2:B:499:LEU:HD12	2:C:782:LEU:HD13	1.77	0.66
2:B:262:LYS:NZ	2:C:260:ARG:NH2	2.42	0.66
2:C:494:THR:HA	2:C:497:ASP:HB2	1.75	0.66
2:B:500:LEU:CD2	2:C:783:ARG:CG	2.22	0.66
2:B:707:GLU:OE2	2:C:771:LYS:HD2	1.96	0.66
2:B:367:THR:CG2	2:B:472:THR:CB	2.55	0.66
2:C:10:ALA:O	2:C:13:VAL:HG12	1.96	0.66
2:B:565:ASP:O	2:B:567:GLU:N	2.27	0.66
2:A:371:ILE:HG22	2:A:372:GLU:N	2.11	0.66
2:A:201:LYS:HE2	2:A:432:GLN:NE2	84.32	0.66
2:C:354:LEU:HB3	2:C:357:ARG:NH1	2.10	0.66
2:C:373:ALA:C	2:C:476:ILE:CD1	2.64	0.66
2:B:499:LEU:CD1	2:C:782:LEU:CD1	2.74	0.66
2:B:766:ARG:HG3	2:B:766:ARG:HH11	1.61	0.66
2:B:162:THR:HA	2:B:264:VAL:HG11	1.78	0.65
2:B:171:THR:OG1	2:B:238:ARG:HA	1.95	0.65
2:C:359:GLU:HG2	2:C:364:VAL:HG12	1.76	0.65
2:B:262:LYS:HZ2	2:C:260:ARG:HH22	1.45	0.65
2:B:509:ARG:HD3	2:B:557:ALA:HB2	1.77	0.65
2:A:515:GLU:OE1	2:A:712:HIS:CD2	2.49	0.65
2:C:351:LEU:HD11	2:C:375:VAL:HG23	1.77	0.65
2:A:766:ARG:HH11	2:A:766:ARG:HG3	1.62	0.65
2:A:355:ARG:HE	2:A:366:ILE:H	1.44	0.65
2:A:110:LEU:HD21	2:A:138:VAL:HG11	1.78	0.65
2:A:5:ARG:HE	2:A:102:TYR:HE1	1.44	0.65
2:A:394:LEU:HG	2:A:480:VAL:HG22	1.75	0.65
2:B:394:LEU:HD21	2:B:483:TRP:CE3	2.29	0.65
2:B:174:ALA:CB	2:B:179:LEU:HD22	2.26	0.65
2:A:411:PRO:C	2:A:413:LEU:H	1.99	0.65
2:B:345:ASP:HA	2:B:348:ILE:CD1	2.26	0.65
2:C:565:ASP:C	2:C:567:GLU:H	2.00	0.65
2:B:306:ARG:CD	2:C:168:ARG:NH2	2.14	0.65
2:B:66:SER:O	2:B:67:LEU:HD23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:PRO:HA	2:C:335:GLN:O	1.96	0.65
2:C:343:SER:HB2	2:C:346:GLU:HG3	1.78	0.65
2:A:509:ARG:HD3	2:A:557:ALA:HB2	1.77	0.65
2:B:402:VAL:CG1	2:B:467:GLU:CD	2.63	0.65
2:A:172:ALA:HA	2:A:175:LYS:HD2	1.78	0.65
2:A:620:GLU:HG3	2:A:658:SER:OG	1.96	0.65
2:C:620:GLU:HG3	2:C:658:SER:OG	1.96	0.65
2:C:46:ALA:HB2	2:C:105:THR:O	1.96	0.65
2:B:565:ASP:C	2:B:567:GLU:H	2.00	0.65
2:A:46:ALA:O	2:A:50:LEU:HD12	1.96	0.65
2:A:54:GLY:O	2:A:55:LEU:HD23	1.97	0.65
2:B:54:GLY:O	2:B:55:LEU:HD23	1.97	0.65
2:A:363:ARG:NH1	2:A:475:ASP:CB	2.59	0.65
2:B:512:GLY:CA	2:B:718:HIS:CD2	2.80	0.65
2:A:565:ASP:C	2:A:567:GLU:H	2.00	0.65
2:B:727:SER:O	2:B:731:THR:HG23	1.98	0.64
2:B:500:LEU:CG	2:C:783:ARG:HG2	2.27	0.64
2:B:367:THR:CG2	2:B:472:THR:HG23	2.27	0.64
2:B:5:ARG:HE	2:B:102:TYR:HE1	1.44	0.64
2:C:727:SER:O	2:C:731:THR:HG23	1.98	0.64
2:B:364:VAL:HA	2:B:365:SER:C	2.17	0.64
2:B:620:GLU:CG	2:B:658:SER:OG	2.46	0.64
2:A:727:SER:O	2:A:731:THR:HG23	1.98	0.64
2:B:203:ASN:O	2:B:334:PHE:HA	1.98	0.64
2:C:6:PHE:CD2	2:C:6:PHE:N	2.66	0.64
2:B:445:THR:O	2:B:449:LEU:HD12	1.97	0.64
2:B:176:GLU:C	2:B:178:SER:H	2.00	0.64
2:B:515:GLU:OE1	2:B:712:HIS:CD2	2.49	0.64
2:A:370:ALA:O	2:A:473:VAL:HA	1.91	0.64
2:B:363:ARG:HG3	2:B:471:VAL:HA	1.79	0.64
2:B:361:HIS:O	2:B:362:HIS:CB	2.45	0.64
2:C:122:ARG:O	2:C:126:ASN:HB2	1.98	0.64
2:A:620:GLU:CG	2:A:658:SER:OG	2.46	0.64
2:A:359:GLU:HG2	2:A:364:VAL:HG12	1.79	0.64
2:B:164:ASP:CB	2:B:166:LEU:O	2.44	0.64
2:A:171:THR:CG2	2:A:175:LYS:HE3	2.24	0.64
2:B:231:PRO:O	2:B:233:ILE:N	2.31	0.64
2:A:221:LEU:O	2:A:222:ALA:C	2.36	0.63
2:A:230:VAL:HG13	2:A:231:PRO:HD2	1.79	0.63
2:A:415:GLU:O	2:A:419:LYS:HG3	1.98	0.63
2:A:29:ILE:HA	2:A:33:HIS:ND1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:620:GLU:CG	2:C:658:SER:OG	2.46	0.63
2:C:30:GLY:HA2	2:C:81:THR:OG1	1.98	0.63
2:B:13:VAL:HG23	2:B:37:GLY:O	1.97	0.63
2:C:172:ALA:HA	2:C:175:LYS:HD2	1.80	0.63
2:A:41:GLU:O	2:A:43:GLU:N	2.30	0.63
2:B:201:LYS:NZ	2:B:335:GLN:HG3	2.13	0.63
2:C:411:PRO:C	2:C:413:LEU:H	2.01	0.63
2:A:60:ILE:HG22	2:A:61:GLN:N	2.12	0.63
2:A:415:GLU:HA	2:A:418:GLN:CD	2.18	0.63
2:B:170:LEU:HB2	2:B:239:VAL:HB	1.81	0.63
2:B:46:ALA:HB2	2:B:105:THR:O	1.99	0.63
2:C:565:ASP:O	2:C:567:GLU:N	2.28	0.63
2:C:766:ARG:HH11	2:C:766:ARG:HG3	1.62	0.63
2:B:394:LEU:HD23	2:B:483:TRP:CH2	2.27	0.63
2:A:122:ARG:O	2:A:126:ASN:HB2	1.98	0.63
2:A:343:SER:HB2	2:A:346:GLU:HG3	1.79	0.63
2:B:122:ARG:O	2:B:126:ASN:HB2	1.97	0.63
2:B:232:GLU:HA	2:C:362:HIS:CD2	2.34	0.63
2:A:374:ALA:CB	2:A:476:ILE:HG23	2.18	0.63
2:B:10:ALA:HB2	2:B:104:GLY:HA2	1.80	0.63
2:C:374:ALA:N	2:C:476:ILE:HD12	2.09	0.63
2:A:318:ASP:O	2:A:321:ARG:N	2.31	0.63
2:C:74:MET:HB3	2:C:76:GLN:HE22	1.62	0.63
2:B:694:LYS:HD3	2:C:760:TYR:CD2	2.24	0.63
2:A:351:LEU:HD11	2:A:375:VAL:HG23	1.81	0.63
2:B:276:LEU:HD13	2:B:277:PHE:N	2.14	0.63
2:B:306:ARG:HH22	2:C:242:LEU:HD22	1.44	0.63
2:B:41:GLU:O	2:B:43:GLU:N	2.32	0.63
2:C:276:LEU:HD13	2:C:277:PHE:H	1.63	0.62
2:C:307:GLY:H	2:C:309:LEU:HD21	1.64	0.62
2:C:239:VAL:O	2:C:240:MET:HG2	1.99	0.62
2:C:12:LYS:O	2:C:16:LEU:HB2	1.98	0.62
2:B:690:MET:O	2:C:760:TYR:CE2	2.51	0.62
2:B:369:ASP:CB	2:B:473:VAL:HG22	2.29	0.62
2:B:191:ARG:O	2:B:195:VAL:HG22	1.99	0.62
2:B:330:LEU:C	2:B:332:ARG:H	2.02	0.62
2:B:499:LEU:HD13	2:C:782:LEU:HD11	1.81	0.62
2:C:41:GLU:O	2:C:43:GLU:N	2.32	0.62
2:C:171:THR:CG2	2:C:175:LYS:HE3	2.26	0.62
2:C:241:THR:HG22	2:C:277:PHE:HB3	1.81	0.62
2:A:307:GLY:H	2:A:309:LEU:HD21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:ARG:HD2	2:B:201:LYS:O	1.99	0.62
2:B:167:ALA:HB1	2:B:241:THR:C	2.19	0.62
2:C:452:GLN:O	2:C:456:THR:HG23	2.00	0.62
2:A:74:MET:HB3	2:A:76:GLN:HE22	1.62	0.62
2:B:107:HIS:HA	2:B:110:LEU:HD12	1.81	0.62
2:C:426:GLU:O	2:C:430:ALA:CB	2.48	0.62
2:A:35:LEU:HD21	2:A:60:ILE:HD13	1.80	0.62
2:A:352:GLN:O	2:A:355:ARG:HB3	1.99	0.62
2:A:408:THR:C	2:A:414:LYS:HE2	2.17	0.62
2:B:236:ASP:O	2:B:273:ASN:HB2	1.99	0.62
2:B:424:ARG:O	2:B:427:LYS:HB3	2.00	0.62
2:B:500:LEU:HD21	2:C:783:ARG:H	1.62	0.62
2:B:500:LEU:HD13	2:C:783:ARG:HA	1.81	0.62
2:A:382:ILE:HG13	2:A:484:THR:CB	2.30	0.62
2:C:300:LEU:CB	2:C:323:TYR:HE2	2.13	0.62
2:B:174:ALA:HB2	2:B:179:LEU:HD22	1.81	0.61
2:B:363:ARG:NH2	2:B:402:VAL:HG21	2.16	0.61
2:B:512:GLY:CA	2:B:718:HIS:CE1	2.82	0.61
2:A:355:ARG:HD3	2:A:365:SER:CB	2.31	0.61
2:B:204:PRO:HA	2:B:335:GLN:O	2.00	0.61
2:B:396:ASP:O	2:B:397:GLU:C	2.37	0.61
2:B:439:ALA:HA	2:B:442:LEU:CD1	2.26	0.61
2:B:706:ASP:CG	2:C:770:GLN:OE1	2.38	0.61
2:B:129:VAL:O	2:B:130:SER:O	2.18	0.61
2:A:197:SER:OG	2:B:400:SER:CB	2.48	0.61
2:B:351:LEU:HD21	2:B:392:ILE:HD13	1.83	0.61
2:B:366:ILE:CB	2:B:367:THR:HA	2.23	0.61
2:B:201:LYS:HA	2:B:332:ARG:O	2.00	0.61
2:B:6:PHE:N	2:B:6:PHE:CD2	2.66	0.61
2:C:341:GLN:CG	2:C:387:LEU:H	2.12	0.61
2:B:162:THR:HA	2:B:264:VAL:CG1	2.30	0.61
2:B:233:ILE:CG1	2:B:233:ILE:O	2.48	0.61
2:B:241:THR:HG22	2:B:277:PHE:CD1	2.35	0.61
2:A:199:ARG:HD2	2:B:358:TYR:OH	1.94	0.61
2:A:452:GLN:O	2:A:456:THR:HG23	1.99	0.61
2:B:119:VAL:O	2:B:123:VAL:HG23	2.01	0.61
2:B:342:PRO:HG2	2:B:388:PRO:HG3	1.82	0.61
2:A:10:ALA:O	2:A:13:VAL:HG12	2.01	0.61
2:B:74:MET:HB3	2:B:76:GLN:HE22	1.64	0.61
2:B:511:ILE:CG1	2:B:721:GLU:CD	2.69	0.61
2:A:697:PHE:HB2	2:A:702:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:ARG:HE	2:C:775:ASP:HB2	1.63	0.61
2:B:271:ALA:HB1	2:C:96:ARG:NH1	2.15	0.60
2:B:522:LYS:C	2:C:775:ASP:CG	2.57	0.60
2:B:304:LEU:HD13	2:B:306:ARG:N	2.15	0.60
2:C:377:LEU:HB3	2:C:480:VAL:HG21	1.83	0.60
2:C:22:LEU:O	2:C:25:GLY:N	2.33	0.60
2:B:193:ILE:HD12	2:B:193:ILE:O	6.03	0.60
2:B:356:ASP:HA	2:B:359:GLU:OE1	2.00	0.60
2:B:195:VAL:HA	2:B:198:ARG:HE	1.66	0.60
2:B:201:LYS:HB3	2:B:335:GLN:HG3	1.82	0.60
2:B:342:PRO:HD2	2:B:388:PRO:HD3	1.82	0.60
2:C:351:LEU:HD11	2:C:375:VAL:CG2	2.32	0.60
2:B:305:ALA:C	2:B:307:GLY:H	2.04	0.60
2:B:305:ALA:HB2	2:B:309:LEU:HD11	1.82	0.60
2:A:374:ALA:N	2:A:476:ILE:HG22	2.10	0.60
2:B:482:SER:OG	2:B:483:TRP:HD1	1.84	0.60
2:C:299:ILE:C	2:C:323:TYR:OH	2.39	0.60
2:B:466:GLN:O	2:B:467:GLU:HG3	2.02	0.60
2:A:119:VAL:O	2:A:123:VAL:HG23	2.01	0.60
2:B:198:ARG:HH11	2:C:396:ASP:HB3	1.66	0.60
2:C:449:LEU:O	2:C:452:GLN:HB3	2.01	0.60
2:C:382:ILE:HA	2:C:383:SER:CB	2.13	0.60
2:A:577:TYR:HE1	2:A:584:SER:HG	1.50	0.60
2:C:697:PHE:HB2	2:C:702:ILE:HD11	1.83	0.60
2:B:359:GLU:CG	2:B:365:SER:H	2.13	0.60
2:A:162:THR:O	2:A:164:ASP:N	2.35	0.60
2:B:194:GLU:HA	2:C:400:SER:CB	2.31	0.60
2:B:225:ILE:HD11	2:B:237:LYS:O	2.01	0.60
2:A:430:ALA:HB1	2:A:435:GLU:HG2	1.83	0.60
2:A:377:LEU:HD11	2:A:477:ALA:CB	2.32	0.60
2:A:199:ARG:HD3	2:B:358:TYR:CZ	2.36	0.60
2:B:766:ARG:HG3	2:B:766:ARG:NH1	2.17	0.60
2:B:472:THR:HG22	2:B:473:VAL:HG23	1.84	0.60
2:A:12:LYS:O	2:A:16:LEU:HB2	2.00	0.60
2:C:164:ASP:C	2:C:166:LEU:O	2.41	0.60
2:C:201:LYS:HD2	2:C:335:GLN:HG3	1.83	0.60
2:C:395:ILE:O	2:C:399:GLY:N	2.35	0.60
2:B:304:LEU:CD2	2:B:305:ALA:N	2.50	0.59
2:A:304:LEU:O	2:A:306:ARG:N	2.35	0.59
2:A:445:THR:HA	2:A:448:ARG:HD2	1.83	0.59
2:C:228:ASN:HD21	2:C:235:ARG:HH21	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:PRO:C	2:C:233:ILE:H	2.06	0.59
2:A:382:ILE:CA	2:A:383:SER:CB	2.76	0.59
2:B:396:ASP:O	2:B:399:GLY:N	2.34	0.59
2:A:306:ARG:N	2:A:309:LEU:HD11	2.17	0.59
2:B:525:ARG:CB	2:C:779:GLU:OE2	2.50	0.59
2:B:168:ARG:HH12	2:B:242:LEU:HB2	1.64	0.59
2:B:306:ARG:HH21	2:C:242:LEU:CD1	1.72	0.59
2:C:13:VAL:CG2	2:C:38:LEU:HD23	2.15	0.59
2:C:445:THR:HA	2:C:448:ARG:HD2	1.83	0.59
2:C:318:ASP:O	2:C:321:ARG:N	2.35	0.59
2:C:766:ARG:NH1	2:C:766:ARG:HG3	2.17	0.59
2:B:192:VAL:HG12	2:B:221:LEU:HD21	1.83	0.59
2:C:90:LEU:HD11	2:C:115:GLU:HB2	1.83	0.59
2:A:165:SER:CB	2:A:166:LEU:CB	2.81	0.59
2:A:183:ILE:HG22	2:A:184:GLY:N	2.17	0.59
2:B:166:LEU:HA	2:B:167:ALA:HB2	1.85	0.59
2:B:203:ASN:HD21	2:B:310:GLN:HA	1.68	0.59
2:C:86:LYS:HG2	2:C:115:GLU:CD	2.23	0.59
2:A:228:ASN:HD21	2:A:235:ARG:HH21	1.50	0.59
2:B:697:PHE:HB2	2:B:702:ILE:HD11	1.83	0.59
2:B:179:LEU:HB3	2:B:223:GLN:HE22	1.67	0.59
2:B:306:ARG:HA	2:C:168:ARG:NH2	2.16	0.59
2:A:169:ASP:O	2:A:172:ALA:HB3	2.02	0.59
2:B:231:PRO:HB2	2:C:403:ARG:HE	1.68	0.59
2:C:380:ARG:HG3	2:C:381:TYR:CD2	2.36	0.59
2:A:199:ARG:CD	2:B:358:TYR:HH	2.00	0.59
2:A:232:GLU:HA	2:A:235:ARG:HG3	1.84	0.59
2:B:706:ASP:O	2:C:767:ARG:CB	2.50	0.59
2:A:363:ARG:NH1	2:A:475:ASP:CG	2.56	0.59
2:B:185:ARG:HD3	2:B:339:VAL:HG13	1.85	0.59
2:C:367:THR:OG1	2:C:471:VAL:HG12	2.01	0.59
2:B:382:ILE:HA	2:B:383:SER:CB	2.22	0.59
2:B:496:THR:HG22	2:C:782:LEU:HD22	1.85	0.59
2:B:525:ARG:C	2:C:775:ASP:HA	2.19	0.58
2:A:241:THR:HG22	2:A:277:PHE:HB3	1.84	0.58
2:A:424:ARG:HG2	2:A:446:GLU:OE2	2.03	0.58
2:B:370:ALA:HA	2:B:473:VAL:HG13	1.85	0.58
2:B:347:SER:HB3	2:B:375:VAL:HG11	1.84	0.58
2:B:241:THR:HG22	2:B:277:PHE:HB3	1.85	0.58
2:C:439:ALA:CA	2:C:442:LEU:HB2	2.26	0.58
2:A:268:ILE:HD13	2:A:269:ARG:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:415:GLU:O	2:C:419:LYS:HG3	2.02	0.58
2:A:639:LEU:O	2:A:646:THR:HA	2.03	0.58
2:A:394:LEU:CD1	2:A:479:VAL:HB	2.34	0.58
2:B:211:GLY:HA2	2:B:212:VAL:HG22	1.86	0.58
2:B:232:GLU:OE2	2:C:361:HIS:HB3	2.04	0.58
2:C:179:LEU:HD12	2:C:180:ASP:N	2.19	0.58
2:C:169:ASP:O	2:C:172:ALA:HB3	2.03	0.58
2:B:12:LYS:O	2:B:16:LEU:HB2	2.04	0.58
2:B:83:ARG:HD2	2:B:115:GLU:HG2	1.86	0.58
2:B:268:ILE:C	2:B:270:GLN:H	2.06	0.58
2:C:446:GLU:O	2:C:449:LEU:HB2	2.03	0.58
2:C:306:ARG:N	2:C:309:LEU:HD11	2.19	0.58
2:C:639:LEU:O	2:C:646:THR:HA	2.03	0.58
2:C:203:ASN:OD1	2:C:310:GLN:HG3	2.03	0.58
2:C:201:LYS:CD	2:C:335:GLN:HG3	2.34	0.58
2:A:526:ARG:CD	2:B:778:SER:CB	2.82	0.58
2:A:200:THR:CB	2:B:393:ASP:CB	2.81	0.58
2:A:164:ASP:C	2:A:166:LEU:O	2.42	0.58
2:A:231:PRO:C	2:A:233:ILE:H	2.05	0.58
2:B:225:ILE:HA	2:B:230:VAL:HG21	1.85	0.58
2:C:232:GLU:HA	2:C:235:ARG:HG3	1.85	0.58
2:A:446:GLU:O	2:A:449:LEU:HB2	2.04	0.57
2:C:201:LYS:CE	2:C:432:GLN:HE21	83.80	0.57
2:C:355:ARG:HE	2:C:366:ILE:H	1.51	0.57
2:B:214:LYS:NZ	2:B:315:THR:H	2.02	0.57
2:B:60:ILE:HG22	2:B:61:GLN:N	2.18	0.57
2:B:355:ARG:CD	2:B:366:ILE:H	2.17	0.57
2:B:330:LEU:C	2:B:332:ARG:N	2.54	0.57
2:A:47:ALA:O	2:A:51:GLN:HG2	2.05	0.57
2:C:342:PRO:HD2	2:C:388:PRO:HD3	1.85	0.57
2:C:394:LEU:HD13	2:C:479:VAL:CB	2.34	0.57
2:B:639:LEU:O	2:B:646:THR:HA	2.03	0.57
2:A:6:PHE:CB	2:A:10:ALA:HB3	2.33	0.57
2:B:171:THR:OG1	2:B:239:VAL:N	2.35	0.57
2:A:426:GLU:O	2:A:430:ALA:CB	2.52	0.57
2:A:204:PRO:HA	2:A:335:GLN:O	2.04	0.57
2:C:404:LEU:O	2:C:407:PHE:N	2.38	0.57
2:A:280:ALA:C	2:A:301:LYS:HE2	2.25	0.57
2:B:29:ILE:HA	2:B:33:HIS:ND1	2.19	0.57
2:C:29:ILE:HA	2:C:33:HIS:ND1	2.19	0.57
2:A:380:ARG:HG3	2:A:381:TYR:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:439:ALA:O	2:A:440:ALA:C	2.43	0.57
2:B:240:MET:HB2	2:B:276:LEU:CD2	2.35	0.57
2:A:377:LEU:CD1	2:A:477:ALA:CB	2.82	0.57
2:B:138:VAL:O	2:B:142:LEU:HD12	2.05	0.57
2:B:207:ILE:HG13	2:B:207:ILE:O	2.05	0.57
2:A:198:ARG:HA	2:B:396:ASP:HB3	1.86	0.57
2:B:511:ILE:CG2	2:B:718:HIS:CE1	2.83	0.57
2:A:330:LEU:O	2:A:332:ARG:N	2.38	0.57
2:B:304:LEU:CD1	2:B:306:ARG:HG2	2.35	0.57
2:B:201:LYS:HD2	2:B:331:GLU:O	2.05	0.57
2:C:374:ALA:CA	2:C:476:ILE:HD11	2.32	0.57
2:B:103:VAL:HG12	2:B:104:GLY:N	2.19	0.57
2:A:233:ILE:HG23	2:B:361:HIS:HE2	0.58	0.57
2:C:6:PHE:CB	2:C:10:ALA:HB3	2.34	0.57
2:C:268:ILE:HD13	2:C:269:ARG:N	2.20	0.57
2:B:6:PHE:CB	2:B:10:ALA:HB3	2.34	0.57
2:B:198:ARG:O	2:B:199:ARG:CB	2.53	0.57
2:C:347:SER:O	2:C:350:ILE:HG13	2.05	0.57
2:B:358:TYR:O	2:B:360:ALA:N	2.37	0.57
2:C:781:LEU:HD23	2:C:786:ILE:HG13	1.87	0.57
2:B:525:ARG:HB3	2:C:779:GLU:OE2	2.05	0.56
2:A:364:VAL:HA	2:A:365:SER:O	2.05	0.56
2:B:344:VAL:O	2:B:347:SER:HB2	2.05	0.56
2:A:201:LYS:HD2	2:A:335:GLN:HG3	1.86	0.56
2:A:259:ASP:O	2:A:261:LEU:HG	2.05	0.56
2:B:480:VAL:O	2:B:482:SER:N	2.39	0.56
2:B:265:MET:CE	2:B:269:ARG:NH2	2.64	0.56
2:B:270:GLN:O	2:B:271:ALA:CB	2.53	0.56
2:C:301:LYS:N	2:C:302:PRO:CD	2.68	0.56
2:C:424:ARG:HG2	2:C:446:GLU:OE2	2.04	0.56
2:B:781:LEU:HD23	2:B:786:ILE:HG13	1.86	0.56
2:A:781:LEU:HD23	2:A:786:ILE:HG13	1.86	0.56
2:B:364:VAL:HG13	2:B:365:SER:HA	1.86	0.56
2:C:317:LEU:HD23	2:C:317:LEU:H	1.69	0.56
2:A:185:ARG:HG2	2:A:188:GLU:CG	2.36	0.56
2:B:124:LEU:N	2:B:124:LEU:HD23	2.19	0.56
2:B:434:GLN:N	2:B:435:GLU:HB3	2.20	0.56
2:C:72:GLN:C	2:C:74:MET:H	2.08	0.56
2:C:22:LEU:O	2:C:24:LEU:N	2.39	0.56
2:B:690:MET:CB	2:C:760:TYR:OH	2.52	0.56
2:B:525:ARG:O	2:C:778:SER:OG	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ARG:HH11	2:B:476:ILE:CD1	2.09	0.56
2:B:476:ILE:HG22	2:B:477:ALA:N	2.21	0.56
2:C:364:VAL:HA	2:C:365:SER:O	2.06	0.56
2:B:227:ASN:OD1	2:B:227:ASN:O	2.24	0.56
2:B:352:GLN:HA	2:B:355:ARG:HB2	1.87	0.56
2:B:385:ARG:HB2	2:B:390:LYS:HG2	1.87	0.56
2:C:382:ILE:CG1	2:C:484:THR:CG2	2.82	0.56
2:C:355:ARG:HD3	2:C:365:SER:CB	2.35	0.56
2:C:98:LEU:HB3	2:C:100:HIS:CD2	2.26	0.56
2:A:6:PHE:CB	2:A:10:ALA:CB	2.84	0.56
2:A:212:VAL:O	2:A:213:GLY:C	2.44	0.56
2:B:192:VAL:O	2:B:192:VAL:HG12	2.05	0.56
2:C:162:THR:O	2:C:164:ASP:N	2.38	0.56
2:B:511:ILE:HG13	2:B:721:GLU:CG	2.36	0.56
2:A:766:ARG:NH1	2:A:766:ARG:HG3	2.17	0.56
2:B:169:ASP:O	2:B:173:ILE:CB	2.37	0.56
2:C:83:ARG:HD2	2:C:115:GLU:HG2	1.87	0.56
2:B:531:LEU:C	2:C:733:ARG:NH2	2.57	0.56
2:B:54:GLY:O	2:B:59:LYS:HD3	2.06	0.56
2:B:373:ALA:C	2:B:377:LEU:HD13	2.26	0.56
2:A:241:THR:O	2:A:242:LEU:HB2	2.04	0.56
2:B:86:LYS:HG2	2:B:115:GLU:CD	2.26	0.56
2:A:203:ASN:OD1	2:A:310:GLN:HG3	2.06	0.56
2:B:169:ASP:H	2:B:173:ILE:HD12	1.68	0.56
2:B:169:ASP:OD1	2:B:238:ARG:HB3	2.06	0.56
2:C:103:VAL:CG1	2:C:104:GLY:N	2.68	0.56
2:B:438:LYS:O	2:B:442:LEU:HD12	2.06	0.56
2:A:201:LYS:CD	2:A:335:GLN:HG3	2.36	0.56
2:C:209:GLU:OE2	2:C:209:GLU:HA	2.06	0.56
2:C:9:ARG:HG3	2:C:9:ARG:HH11	1.70	0.56
2:B:382:ILE:CA	2:B:383:SER:CB	2.84	0.56
2:B:379:ASP:CB	2:B:387:LEU:HD11	2.36	0.55
2:C:124:LEU:HD23	2:C:124:LEU:N	2.19	0.55
2:C:138:VAL:O	2:C:142:LEU:HD12	2.06	0.55
2:B:526:ARG:HH11	2:C:770:GLN:HG2	1.71	0.55
2:B:526:ARG:HH11	2:C:770:GLN:CG	2.18	0.55
2:B:367:THR:HG1	2:B:473:VAL:N	2.04	0.55
2:B:483:TRP:CD1	2:B:483:TRP:N	2.73	0.55
2:C:212:VAL:HG12	2:C:212:VAL:O	2.07	0.55
2:C:382:ILE:CD1	2:C:484:THR:CG2	2.85	0.55
2:B:640:THR:HA	2:B:646:THR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:229:GLU:O	2:A:230:VAL:HG23	2.06	0.55
2:C:374:ALA:H	2:C:476:ILE:HD11	1.65	0.55
2:C:221:LEU:O	2:C:222:ALA:C	2.45	0.55
2:B:211:GLY:HA3	2:B:212:VAL:O	2.05	0.55
2:B:269:ARG:HH22	2:B:306:ARG:HB2	1.72	0.55
2:C:445:THR:HA	2:C:448:ARG:CD	2.37	0.55
2:A:54:GLY:O	2:A:59:LYS:HD3	2.06	0.55
2:A:171:THR:OG1	2:A:238:ARG:HA	2.06	0.55
2:B:47:ALA:O	2:B:51:GLN:HG2	2.06	0.55
2:B:402:VAL:HG13	2:B:467:GLU:OE1	2.05	0.55
2:B:197:SER:CB	2:C:361:HIS:CD2	2.89	0.55
2:B:198:ARG:CB	2:C:396:ASP:OD2	2.53	0.55
2:B:511:ILE:HG22	2:B:718:HIS:CE1	2.26	0.55
2:A:411:PRO:C	2:A:413:LEU:N	2.60	0.55
2:A:640:THR:HA	2:A:646:THR:HA	1.88	0.55
2:A:363:ARG:NH2	2:A:402:VAL:HG21	2.21	0.55
2:B:499:LEU:CD1	2:C:782:LEU:HD13	2.35	0.55
2:B:35:LEU:HD21	2:B:60:ILE:HD13	1.88	0.55
2:B:367:THR:CG2	2:B:472:THR:OG1	2.52	0.55
2:A:162:THR:C	2:A:164:ASP:N	2.60	0.55
2:A:185:ARG:O	2:A:189:ILE:HG13	2.07	0.55
2:B:166:LEU:HA	2:B:167:ALA:CB	2.36	0.55
2:C:165:SER:CB	2:C:166:LEU:CB	2.85	0.55
2:A:98:LEU:HB3	2:A:100:HIS:CD2	2.29	0.55
2:A:449:LEU:O	2:A:452:GLN:HB3	2.07	0.55
2:C:304:LEU:O	2:C:306:ARG:N	2.38	0.55
2:A:193:ILE:O	2:A:193:ILE:HD12	5.87	0.55
2:B:72:GLN:C	2:B:74:MET:H	2.10	0.55
2:C:426:GLU:O	2:C:430:ALA:HB2	2.07	0.55
2:C:171:THR:OG1	2:C:238:ARG:HA	2.07	0.55
2:C:72:GLN:CD	2:C:72:GLN:H	2.09	0.55
2:C:396:ASP:O	2:C:397:GLU:C	2.44	0.54
2:A:72:GLN:H	2:A:72:GLN:CD	2.11	0.54
2:B:260:ARG:O	2:B:263:LYS:HB2	2.07	0.54
2:C:348:ILE:HA	2:C:351:LEU:HD12	1.89	0.54
2:A:731:THR:HG22	2:A:741:ILE:HG13	1.89	0.54
2:A:424:ARG:O	2:A:428:ASP:N	2.26	0.54
2:C:179:LEU:HD12	2:C:180:ASP:H	1.72	0.54
2:A:445:THR:HA	2:A:448:ARG:CD	2.37	0.54
2:B:731:THR:HG22	2:B:741:ILE:HG13	1.89	0.54
2:B:460:TRP:CZ3	2:B:463:LYS:HG2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:276:LEU:HD13	2:A:277:PHE:H	1.72	0.54
2:A:207:ILE:HG13	2:A:317:LEU:HA	1.90	0.54
2:C:107:HIS:HA	2:C:110:LEU:HD12	1.89	0.54
2:C:439:ALA:O	2:C:440:ALA:C	2.46	0.54
2:B:5:ARG:CZ	2:B:5:ARG:H	2.21	0.54
2:C:139:LEU:C	2:C:141:LEU:H	2.11	0.54
2:C:640:THR:HA	2:C:646:THR:HA	1.88	0.54
2:A:168:ARG:HD2	2:A:168:ARG:N	2.22	0.54
2:A:402:VAL:C	2:A:404:LEU:H	2.11	0.54
2:B:378:SER:HB3	2:B:390:LYS:CE	2.31	0.54
2:B:571:ARG:HH21	2:B:573:ASP:HB2	1.72	0.54
2:A:381:TYR:HD2	2:A:381:TYR:N	2.06	0.54
2:B:72:GLN:H	2:B:72:GLN:CD	2.09	0.54
2:C:129:VAL:CG1	2:C:129:VAL:O	2.56	0.54
2:C:210:PRO:N	2:C:211:GLY:HA3	2.23	0.54
2:C:241:THR:O	2:C:242:LEU:HB2	2.07	0.54
2:B:382:ILE:HD13	2:B:611:TYR:OH	2.07	0.54
2:A:304:LEU:C	2:A:306:ARG:H	2.09	0.54
2:A:348:ILE:HD13	2:A:372:GLU:HG2	1.89	0.54
2:B:184:GLY:HA3	2:B:185:ARG:O	2.08	0.54
2:C:174:ALA:CB	2:C:222:ALA:HB1	2.38	0.54
2:B:624:PRO:HA	2:B:627:PHE:CD2	2.41	0.54
2:C:185:ARG:O	2:C:189:ILE:HG13	2.07	0.54
2:C:352:GLN:O	2:C:355:ARG:HB3	2.08	0.54
2:C:787:HIS:O	2:C:790:GLN:HG2	2.08	0.54
2:A:6:PHE:HB2	2:A:10:ALA:CB	2.38	0.54
2:A:624:PRO:HA	2:A:627:PHE:CD2	2.41	0.54
2:C:758:LEU:HD22	2:C:758:LEU:H	1.73	0.54
2:C:572:ILE:HG22	2:C:573:ASP:N	2.23	0.54
2:A:374:ALA:HB2	2:A:476:ILE:CB	2.37	0.54
2:B:30:GLY:HA2	2:B:81:THR:OG1	2.07	0.54
2:C:119:VAL:O	2:C:123:VAL:HG23	2.07	0.54
2:B:532:LYS:O	2:C:733:ARG:NH2	2.40	0.54
2:A:46:ALA:HB2	2:A:105:THR:O	2.08	0.54
2:B:526:ARG:NE	2:C:775:ASP:CB	2.65	0.54
2:A:398:ALA:H	2:A:479:VAL:HG22	1.73	0.54
2:B:365:SER:O	2:B:471:VAL:CG2	2.54	0.54
2:A:6:PHE:N	2:A:6:PHE:HD2	2.06	0.54
2:B:10:ALA:O	2:B:13:VAL:HG12	2.08	0.54
2:B:176:GLU:C	2:B:178:SER:N	2.61	0.54
2:B:9:ARG:O	2:B:13:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:421:ASP:O	2:C:423:VAL:N	2.40	0.54
2:C:445:THR:HG22	2:C:448:ARG:CZ	2.38	0.54
2:A:572:ILE:HG22	2:A:573:ASP:N	2.23	0.54
2:B:787:HIS:O	2:B:790:GLN:HG2	2.08	0.54
2:A:162:THR:C	2:A:164:ASP:H	2.10	0.53
2:C:381:TYR:HD2	2:C:381:TYR:N	2.06	0.53
2:C:47:ALA:O	2:C:51:GLN:HG2	2.08	0.53
2:A:124:LEU:N	2:A:124:LEU:HD23	2.23	0.53
2:A:171:THR:O	2:A:175:LYS:HG3	2.07	0.53
2:A:341:GLN:HE21	2:A:386:PHE:HA	1.73	0.53
2:B:103:VAL:HG13	2:B:107:HIS:HB2	1.90	0.53
2:C:168:ARG:N	2:C:168:ARG:HD2	2.23	0.53
2:C:348:ILE:HD13	2:C:372:GLU:HG2	1.91	0.53
2:B:571:ARG:O	2:B:571:ARG:HG3	2.08	0.53
2:C:571:ARG:HH21	2:C:573:ASP:HB2	1.72	0.53
2:A:787:HIS:O	2:A:790:GLN:HG2	2.08	0.53
2:B:525:ARG:NE	2:C:779:GLU:OE2	2.21	0.53
2:B:371:ILE:O	2:B:372:GLU:C	2.47	0.53
2:C:103:VAL:HG12	2:C:104:GLY:H	1.73	0.53
2:C:6:PHE:CB	2:C:10:ALA:CB	2.87	0.53
2:A:758:LEU:HD22	2:A:758:LEU:H	1.73	0.53
2:A:174:ALA:CB	2:A:222:ALA:HB1	2.37	0.53
2:B:305:ALA:C	2:B:307:GLY:N	2.62	0.53
2:C:304:LEU:C	2:C:306:ARG:H	2.12	0.53
2:B:512:GLY:HA3	2:B:718:HIS:CD2	2.43	0.53
2:C:5:ARG:CZ	2:C:5:ARG:H	2.21	0.53
2:A:571:ARG:HH21	2:A:573:ASP:HB2	1.72	0.53
2:A:533:ASP:HB2	2:B:733:ARG:CZ	2.39	0.53
2:B:526:ARG:N	2:C:775:ASP:CB	2.71	0.53
2:A:167:ALA:C	2:A:168:ARG:HD2	2.29	0.53
2:A:231:PRO:C	2:A:233:ILE:N	2.62	0.53
2:B:231:PRO:CG	2:B:232:GLU:HG2	2.16	0.53
2:C:103:VAL:HG13	2:C:107:HIS:HB2	1.91	0.53
2:C:415:GLU:O	2:C:418:GLN:HB2	2.08	0.53
2:C:377:LEU:O	2:C:381:TYR:HB2	2.07	0.53
2:A:235:ARG:CZ	2:A:235:ARG:HB3	2.38	0.53
2:A:381:TYR:CD2	2:A:381:TYR:N	2.77	0.53
2:B:316:THR:O	2:B:317:LEU:C	2.47	0.53
2:B:572:ILE:HG22	2:B:573:ASP:N	2.23	0.53
2:B:203:ASN:HD22	2:B:311:CYS:H	1.55	0.53
2:C:110:LEU:HD21	2:C:138:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:394:LEU:CD1	2:C:479:VAL:HB	2.39	0.53
2:A:445:THR:HG22	2:A:448:ARG:CZ	2.38	0.53
2:A:72:GLN:C	2:A:74:MET:H	2.10	0.53
2:C:235:ARG:HB3	2:C:235:ARG:CZ	2.38	0.53
2:C:731:THR:HG22	2:C:741:ILE:HG13	1.89	0.53
2:B:229:GLU:O	2:B:230:VAL:CG2	2.56	0.53
2:C:167:ALA:C	2:C:168:ARG:HD2	2.30	0.53
2:B:278:ILE:O	2:B:314:ALA:HB2	2.08	0.53
2:B:301:LYS:N	2:B:302:PRO:HD2	2.23	0.53
2:B:380:ARG:C	2:B:380:ARG:HD2	2.29	0.53
2:B:194:GLU:CB	2:C:400:SER:OG	2.57	0.53
2:C:382:ILE:CG1	2:C:484:THR:HG21	2.39	0.53
2:C:411:PRO:C	2:C:413:LEU:N	2.61	0.53
2:C:624:PRO:HA	2:C:627:PHE:CD2	2.41	0.53
2:A:571:ARG:HG3	2:A:571:ARG:O	2.08	0.53
2:C:635:GLU:HG2	2:C:704:ARG:HD3	1.90	0.53
2:C:162:THR:C	2:C:164:ASP:N	2.62	0.53
2:A:86:LYS:HG2	2:A:115:GLU:CD	2.29	0.53
2:C:700:GLU:O	2:C:704:ARG:NH1	2.42	0.53
2:B:635:GLU:HG2	2:B:704:ARG:HD3	1.90	0.53
2:C:259:ASP:O	2:C:261:LEU:HG	2.08	0.53
2:B:758:LEU:HD22	2:B:758:LEU:H	1.73	0.53
2:A:373:ALA:O	2:A:374:ALA:C	2.48	0.52
2:C:363:ARG:NH2	2:C:402:VAL:HG21	2.23	0.52
2:A:395:ILE:O	2:A:399:GLY:N	2.42	0.52
2:A:13:VAL:CG2	2:A:38:LEU:HD23	2.18	0.52
2:B:171:THR:CB	2:B:238:ARG:HA	2.38	0.52
2:B:6:PHE:CB	2:B:10:ALA:CB	2.88	0.52
2:C:381:TYR:CD2	2:C:381:TYR:N	2.77	0.52
2:A:635:GLU:HG2	2:A:704:ARG:HD3	1.90	0.52
2:A:63:GLU:O	2:A:67:LEU:HG	2.09	0.52
2:B:572:ILE:HD12	2:B:572:ILE:N	2.24	0.52
2:A:317:LEU:H	2:A:317:LEU:HD23	1.74	0.52
2:C:430:ALA:HB1	2:C:435:GLU:HG2	1.91	0.52
2:A:90:LEU:CD1	2:A:115:GLU:HB2	2.39	0.52
2:A:370:ALA:HB2	2:A:471:VAL:O	2.08	0.52
2:A:138:VAL:O	2:A:142:LEU:HD12	2.09	0.52
2:A:475:ASP:O	2:A:478:MET:HB2	2.09	0.52
2:B:305:ALA:HA	2:B:309:LEU:CD1	2.39	0.52
2:B:341:GLN:HB3	2:B:387:LEU:H	1.75	0.52
2:A:303:SER:O	2:A:306:ARG:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:VAL:HG13	2:C:231:PRO:CD	2.36	0.52
2:A:572:ILE:HD12	2:A:572:ILE:N	2.24	0.52
2:B:700:GLU:O	2:B:704:ARG:NH1	2.42	0.52
2:A:103:VAL:CG1	2:A:104:GLY:N	2.73	0.52
2:B:201:LYS:NZ	2:B:335:GLN:CG	2.72	0.52
2:C:300:LEU:C	2:C:302:PRO:CD	2.77	0.52
2:C:378:SER:HB3	2:C:390:LYS:HD3	1.92	0.52
2:A:29:ILE:HG13	2:A:80:TYR:CD1	2.44	0.52
2:C:572:ILE:HD12	2:C:572:ILE:N	2.24	0.52
2:B:526:ARG:N	2:C:775:ASP:CG	2.56	0.52
2:B:180:ASP:CB	2:B:181:PRO:CD	2.76	0.52
2:B:268:ILE:CG2	2:B:269:ARG:N	2.73	0.52
2:C:212:VAL:O	2:C:213:GLY:C	2.47	0.52
2:C:387:LEU:N	2:C:388:PRO:CD	2.72	0.52
2:C:404:LEU:C	2:C:406:SER:N	2.63	0.52
2:A:359:GLU:HG2	2:A:364:VAL:HG13	1.90	0.52
2:A:344:VAL:O	2:A:347:SER:HB2	2.10	0.52
2:C:303:SER:O	2:C:306:ARG:HB2	2.10	0.52
2:B:411:PRO:C	2:B:413:LEU:N	2.62	0.52
2:C:54:GLY:O	2:C:59:LYS:HD3	2.10	0.52
2:C:571:ARG:HG3	2:C:571:ARG:O	2.08	0.52
2:B:446:GLU:HG3	2:B:447:GLN:N	2.24	0.52
2:B:185:ARG:HB3	2:B:188:GLU:HB2	1.92	0.52
2:B:418:GLN:HG3	2:B:419:LYS:N	2.23	0.52
2:C:171:THR:O	2:C:175:LYS:HG3	2.10	0.52
2:B:29:ILE:HG13	2:B:80:TYR:CD1	2.45	0.52
2:A:139:LEU:C	2:A:141:LEU:H	2.13	0.52
2:C:442:LEU:O	2:C:445:THR:OG1	2.22	0.52
2:A:700:GLU:O	2:A:704:ARG:NH1	2.41	0.52
2:B:413:LEU:HD11	2:B:456:THR:HG21	1.92	0.52
2:A:398:ALA:HB2	2:A:479:VAL:CG2	2.40	0.51
2:B:511:ILE:HG13	2:B:721:GLU:CD	2.31	0.51
2:B:416:LEU:HD23	2:B:416:LEU:O	2.10	0.51
2:B:459:SER:O	2:B:462:GLU:HB2	2.10	0.51
2:A:531:LEU:HD21	2:B:781:LEU:CD1	2.40	0.51
2:C:482:SER:O	2:C:483:TRP:HD1	1.93	0.51
2:B:523:ALA:C	2:C:775:ASP:OD1	2.47	0.51
2:A:402:VAL:C	2:A:404:LEU:N	2.61	0.51
2:B:139:LEU:C	2:B:141:LEU:H	2.13	0.51
2:C:90:LEU:CD1	2:C:115:GLU:HB2	2.40	0.51
2:A:580:LYS:HG2	2:A:580:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:689:VAL:C	2:A:691:GLY:N	2.63	0.51
2:B:192:VAL:CG1	2:B:192:VAL:O	2.58	0.51
2:B:225:ILE:CD1	2:B:237:LYS:O	2.57	0.51
2:B:304:LEU:HD12	2:B:306:ARG:HG2	1.93	0.51
2:A:276:LEU:O	2:A:312:ILE:N	2.38	0.51
2:A:439:ALA:CA	2:A:442:LEU:HB2	2.29	0.51
2:B:268:ILE:HD11	2:B:274:ILE:CG2	2.40	0.51
2:C:183:ILE:CG2	2:C:184:GLY:N	2.71	0.51
2:C:414:LYS:O	2:C:418:GLN:HG3	2.10	0.51
2:C:359:GLU:HG2	2:C:364:VAL:HG13	1.92	0.51
2:C:231:PRO:C	2:C:233:ILE:N	2.62	0.51
2:C:580:LYS:HG2	2:C:580:LYS:O	2.11	0.51
2:B:356:ASP:HA	2:B:359:GLU:HG3	1.93	0.51
2:B:370:ALA:HB1	2:B:476:ILE:HG12	1.92	0.51
2:B:466:GLN:O	2:B:467:GLU:CG	2.58	0.51
2:A:363:ARG:NH1	2:A:475:ASP:HB3	2.18	0.51
2:C:382:ILE:CA	2:C:383:SER:CB	2.79	0.51
2:B:513:GLN:OE1	2:B:513:GLN:N	2.44	0.51
2:A:472:THR:O	2:A:474:ASP:N	2.43	0.51
2:A:381:TYR:HA	2:A:611:TYR:OH	2.11	0.51
2:B:203:ASN:ND2	2:B:310:GLN:HA	2.24	0.51
2:C:13:VAL:HG21	2:C:38:LEU:HA	1.92	0.51
2:C:185:ARG:HG2	2:C:188:GLU:CG	2.39	0.51
2:B:262:LYS:HZ3	2:C:260:ARG:NH2	2.08	0.51
2:B:649:PHE:O	2:B:651:ASN:N	2.44	0.51
2:B:336:PRO:O	2:B:337:ILE:HG23	2.11	0.51
2:C:162:THR:C	2:C:164:ASP:H	2.14	0.51
2:C:205:VAL:O	2:C:336:PRO:HA	2.11	0.51
2:B:22:LEU:O	2:B:24:LEU:N	2.44	0.51
2:B:689:VAL:C	2:B:691:GLY:N	2.63	0.51
2:B:304:LEU:HD22	2:B:305:ALA:CA	2.36	0.51
2:C:380:ARG:HG3	2:C:381:TYR:HD2	1.76	0.51
2:A:460:TRP:CZ3	2:A:463:LYS:HG2	2.46	0.51
2:C:193:ILE:O	2:C:193:ILE:HD12	5.85	0.51
2:B:228:ASN:HD21	2:B:235:ARG:HE	1.59	0.51
2:B:690:MET:CA	2:C:760:TYR:OH	2.58	0.51
2:B:763:ARG:N	2:B:764:PRO:CD	2.74	0.51
2:A:30:GLY:HA2	2:A:81:THR:OG1	2.10	0.51
2:C:330:LEU:O	2:C:332:ARG:N	2.44	0.51
2:A:649:PHE:O	2:A:651:ASN:N	2.44	0.51
2:A:209:GLU:OE2	2:A:209:GLU:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:387:LEU:N	2:A:388:PRO:CD	2.74	0.51
2:B:232:GLU:O	2:B:233:ILE:O	2.29	0.51
2:B:305:ALA:CA	2:B:309:LEU:HD11	2.40	0.51
2:C:124:LEU:C	2:C:126:ASN:H	2.13	0.51
2:B:509:ARG:HD3	2:B:557:ALA:CB	2.41	0.51
2:C:649:PHE:O	2:C:651:ASN:N	2.44	0.51
2:A:13:VAL:HG21	2:A:38:LEU:HA	1.92	0.50
2:A:404:LEU:O	2:A:407:PHE:N	2.40	0.50
2:A:421:ASP:O	2:A:423:VAL:N	2.44	0.50
2:C:74:MET:HB3	2:C:76:GLN:CD	2.32	0.50
2:C:689:VAL:C	2:C:691:GLY:N	2.63	0.50
2:B:690:MET:HB3	2:C:760:TYR:CZ	2.46	0.50
2:B:526:ARG:CZ	2:C:775:ASP:OD2	2.59	0.50
2:A:346:GLU:O	2:A:350:ILE:HG13	2.11	0.50
2:B:270:GLN:O	2:B:271:ALA:HB2	2.12	0.50
2:B:305:ALA:CB	2:B:309:LEU:HD11	2.40	0.50
2:C:167:ALA:HB1	2:C:241:THR:O	2.12	0.50
2:C:207:ILE:HG13	2:C:317:LEU:HA	1.93	0.50
2:C:470:GLU:O	2:C:471:VAL:HG23	2.11	0.50
2:A:411:PRO:O	2:A:413:LEU:N	2.45	0.50
2:A:763:ARG:N	2:A:764:PRO:CD	2.74	0.50
2:A:509:ARG:HD3	2:A:557:ALA:CB	2.41	0.50
2:A:513:GLN:N	2:A:513:GLN:OE1	2.44	0.50
2:B:689:VAL:O	2:B:691:GLY:N	2.44	0.50
2:A:370:ALA:HB3	2:A:471:VAL:O	2.07	0.50
2:B:90:LEU:CD1	2:B:115:GLU:HB2	2.42	0.50
2:A:179:LEU:HD12	2:A:180:ASP:N	2.27	0.50
2:A:210:PRO:N	2:A:211:GLY:HA3	2.26	0.50
2:A:428:ASP:O	2:A:431:VAL:N	2.44	0.50
2:B:169:ASP:OD2	2:B:172:ALA:HB3	2.11	0.50
2:B:341:GLN:HB3	2:B:387:LEU:HB2	1.93	0.50
2:C:428:ASP:O	2:C:431:VAL:N	2.45	0.50
2:B:511:ILE:CG2	2:B:718:HIS:HA	2.33	0.50
2:C:513:GLN:N	2:C:513:GLN:OE1	2.44	0.50
2:A:574:MET:HE3	2:A:616:LEU:HB3	1.93	0.50
2:B:694:LYS:HD2	2:C:760:TYR:CG	2.30	0.50
2:B:402:VAL:HG21	2:B:475:ASP:HB3	1.93	0.50
2:A:414:LYS:O	2:A:418:GLN:HG3	2.10	0.50
2:B:308:GLU:OE1	2:B:309:LEU:N	2.44	0.50
2:B:378:SER:O	2:B:390:LYS:NZ	2.39	0.50
2:B:98:LEU:HB3	2:B:100:HIS:CD2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:574:MET:CE	2:C:616:LEU:HB3	2.42	0.50
2:B:472:THR:HG22	2:B:473:VAL:H	1.76	0.50
2:B:268:ILE:C	2:B:270:GLN:N	2.65	0.50
2:C:184:GLY:CA	2:C:185:ARG:C	2.80	0.50
2:C:9:ARG:HG3	2:C:9:ARG:NH1	2.25	0.50
2:B:214:LYS:HZ1	2:B:315:THR:H	1.59	0.50
2:A:689:VAL:O	2:A:691:GLY:N	2.45	0.50
2:A:194:GLU:C	2:A:196:LEU:H	2.15	0.50
2:B:201:LYS:HZ1	2:B:335:GLN:CG	2.25	0.50
2:B:201:LYS:CB	2:B:335:GLN:HG3	2.41	0.50
2:B:361:HIS:C	2:B:362:HIS:CD2	2.84	0.50
2:C:425:LYS:O	2:C:429:ALA:N	2.45	0.50
2:C:475:ASP:O	2:C:478:MET:HB2	2.12	0.50
2:C:72:GLN:O	2:C:74:MET:N	2.45	0.50
2:A:226:ILE:HG22	2:A:227:ASN:N	2.26	0.50
2:C:689:VAL:O	2:C:691:GLY:N	2.44	0.50
2:B:580:LYS:HG2	2:B:580:LYS:O	2.11	0.50
2:A:205:VAL:O	2:A:336:PRO:HA	2.11	0.50
2:B:240:MET:HB2	2:B:276:LEU:HD21	1.94	0.50
2:B:577:TYR:HE1	2:B:584:SER:HG	1.59	0.50
2:C:73:GLU:O	2:C:74:MET:C	2.50	0.50
2:C:29:ILE:HG13	2:C:80:TYR:CD1	2.47	0.50
2:A:689:VAL:C	2:A:691:GLY:H	2.15	0.50
2:A:806:THR:O	2:A:807:ALA:C	2.50	0.50
2:B:806:THR:O	2:B:807:ALA:C	2.50	0.50
2:B:769:ILE:O	2:B:773:VAL:HB	2.12	0.50
2:A:184:GLY:CA	2:A:185:ARG:C	2.80	0.50
2:A:347:SER:O	2:A:350:ILE:HG13	2.10	0.50
2:C:269:ARG:HA	2:C:308:GLU:OE1	2.11	0.50
2:C:54:GLY:C	2:C:55:LEU:HD23	2.32	0.50
2:C:509:ARG:HD3	2:C:557:ALA:CB	2.41	0.50
2:A:572:ILE:CG2	2:A:573:ASP:N	2.75	0.50
2:B:689:VAL:C	2:B:691:GLY:H	2.15	0.50
2:A:415:GLU:O	2:A:418:GLN:HB2	2.11	0.50
2:C:307:GLY:C	2:C:309:LEU:H	2.14	0.50
2:C:377:LEU:HD13	2:C:476:ILE:CG2	2.19	0.50
2:C:689:VAL:C	2:C:691:GLY:H	2.15	0.50
2:A:364:VAL:HG23	2:A:366:ILE:O	2.12	0.49
2:A:366:ILE:HG22	2:A:367:THR:CA	2.30	0.49
2:A:351:LEU:HD11	2:A:375:VAL:CG2	2.42	0.49
2:A:90:LEU:HD11	2:A:115:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:269:ARG:HA	2:A:308:GLU:OE1	2.11	0.49
2:A:574:MET:CE	2:A:616:LEU:HB3	2.41	0.49
2:C:574:MET:HE3	2:C:616:LEU:HD13	1.94	0.49
2:B:574:MET:CE	2:B:616:LEU:HB3	2.41	0.49
2:B:574:MET:HE3	2:B:616:LEU:HD13	1.93	0.49
2:B:619:ILE:HG21	2:B:656:MET:CE	2.42	0.49
2:B:176:GLU:O	2:B:177:ASP:HB3	2.12	0.49
2:B:304:LEU:HD22	2:B:304:LEU:C	2.28	0.49
2:C:6:PHE:HB2	2:C:10:ALA:CB	2.42	0.49
2:C:364:VAL:HG22	2:C:365:SER:HA	1.93	0.49
2:C:472:THR:O	2:C:474:ASP:N	2.45	0.49
2:B:382:ILE:HD13	2:B:611:TYR:CE2	2.46	0.49
2:B:22:LEU:O	2:B:25:GLY:N	2.44	0.49
2:C:769:ILE:O	2:C:773:VAL:HB	2.12	0.49
2:B:454:GLU:O	2:B:457:LYS:N	2.39	0.49
2:B:70:ARG:HB3	2:B:71:GLY:HA3	1.94	0.49
2:A:619:ILE:HG21	2:A:656:MET:CE	2.42	0.49
2:B:500:LEU:HD13	2:C:783:ARG:CB	2.42	0.49
2:A:364:VAL:HG22	2:A:365:SER:C	2.33	0.49
2:A:265:MET:HA	2:A:268:ILE:CG2	2.42	0.49
2:A:29:ILE:HG13	2:A:80:TYR:HD1	1.78	0.49
2:B:572:ILE:CG2	2:B:573:ASP:N	2.75	0.49
2:B:355:ARG:HB3	2:B:355:ARG:NH1	2.22	0.49
2:B:129:VAL:O	2:B:130:SER:C	2.51	0.49
2:B:265:MET:O	2:B:268:ILE:HG22	2.13	0.49
2:C:300:LEU:CB	2:C:323:TYR:CE2	2.96	0.49
2:C:394:LEU:CD1	2:C:479:VAL:CB	2.90	0.49
2:C:35:LEU:HD21	2:C:60:ILE:CD1	2.41	0.49
2:C:806:THR:O	2:C:807:ALA:C	2.50	0.49
2:C:27:ASN:OD1	2:C:27:ASN:N	2.43	0.49
2:C:314:ALA:O	2:C:315:THR:HG23	2.13	0.49
2:A:140:GLN:O	2:A:140:GLN:HG3	2.11	0.49
2:A:769:ILE:O	2:A:773:VAL:HB	2.12	0.49
2:C:763:ARG:N	2:C:764:PRO:CD	2.74	0.49
2:A:373:ALA:H	2:A:473:VAL:HG13	1.76	0.49
2:B:74:MET:HB3	2:B:76:GLN:CD	2.32	0.49
2:C:366:ILE:HG22	2:C:368:ASP:H	1.77	0.49
2:B:343:SER:HB2	2:B:346:GLU:CG	2.42	0.49
2:C:577:TYR:HE1	2:C:584:SER:HG	1.60	0.49
2:A:565:ASP:C	2:A:567:GLU:N	2.66	0.49
2:B:398:ALA:C	2:B:400:SER:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ARG:HH11	2:B:9:ARG:HG3	1.78	0.49
2:C:122:ARG:HG3	2:C:126:ASN:HD22	1.78	0.49
2:B:382:ILE:CD1	2:B:611:TYR:HE2	2.25	0.49
2:B:351:LEU:CD2	2:B:392:ILE:HD13	2.42	0.49
2:A:184:GLY:HA3	2:A:185:ARG:C	2.33	0.49
2:A:194:GLU:O	2:A:198:ARG:HG3	2.13	0.49
2:A:363:ARG:HH12	2:A:475:ASP:CG	2.16	0.49
2:C:355:ARG:HH21	2:C:366:ILE:HA	1.78	0.49
2:A:49:ALA:O	2:A:52:ALA:HB3	2.13	0.49
2:A:103:VAL:HG13	2:A:107:HIS:HB2	1.94	0.49
2:B:73:GLU:O	2:B:74:MET:C	2.51	0.49
2:C:124:LEU:C	2:C:126:ASN:N	2.65	0.49
2:C:402:VAL:C	2:C:404:LEU:N	2.66	0.49
2:C:565:ASP:C	2:C:567:GLU:N	2.66	0.49
2:B:279:ASP:O	2:B:280:ALA:HB2	2.13	0.49
2:C:265:MET:HA	2:C:268:ILE:CG2	2.43	0.49
2:C:38:LEU:HD11	2:C:108:ILE:HG22	1.94	0.49
2:C:443:ARG:O	2:C:446:GLU:N	2.45	0.49
2:C:6:PHE:HD2	2:C:6:PHE:N	2.09	0.49
2:A:140:GLN:C	2:A:141:LEU:HD23	2.33	0.49
2:A:212:VAL:O	2:A:212:VAL:HG12	2.12	0.48
2:A:9:ARG:HG3	2:A:9:ARG:HH11	1.77	0.48
2:C:276:LEU:O	2:C:312:ILE:N	2.43	0.48
2:C:72:GLN:CB	2:C:74:MET:HG3	2.43	0.48
2:C:72:GLN:C	2:C:74:MET:N	2.67	0.48
2:C:411:PRO:O	2:C:413:LEU:N	2.46	0.48
2:A:5:ARG:CZ	2:A:5:ARG:H	2.26	0.48
2:A:366:ILE:HG22	2:A:368:ASP:H	1.78	0.48
2:B:266:ASP:C	2:B:268:ILE:H	2.16	0.48
2:C:206:LEU:N	2:C:313:GLY:O	2.42	0.48
2:C:229:GLU:O	2:C:230:VAL:HG23	2.13	0.48
2:C:44:GLY:HA3	2:C:105:THR:HG21	1.95	0.48
2:C:619:ILE:HG21	2:C:656:MET:CE	2.42	0.48
2:A:194:GLU:OE2	2:B:401:LYS:HE3	2.13	0.48
2:A:308:GLU:CD	2:A:308:GLU:C	2.72	0.48
2:B:650:ARG:HG3	2:B:650:ARG:HH11	1.78	0.48
2:C:243:ASP:O	2:C:244:MET:CB	2.60	0.48
2:B:436:PHE:O	2:B:439:ALA:HB3	2.13	0.48
2:B:496:THR:HG21	2:C:782:LEU:HD22	1.93	0.48
2:A:74:MET:HB3	2:A:76:GLN:CD	2.33	0.48
2:B:158:ALA:HB1	2:B:267:GLU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LEU:HD11	2:B:115:GLU:HB2	1.94	0.48
2:A:129:VAL:CG1	2:A:129:VAL:O	2.60	0.48
2:A:165:SER:CA	2:A:166:LEU:O	2.61	0.48
2:C:129:VAL:O	2:C:130:SER:O	2.30	0.48
2:C:265:MET:HA	2:C:268:ILE:HG22	1.94	0.48
2:B:416:LEU:HD21	2:B:449:LEU:HB3	1.96	0.48
2:B:532:LYS:C	2:C:733:ARG:HH22	2.09	0.48
2:C:365:SER:C	2:C:366:ILE:CG1	2.82	0.48
2:C:35:LEU:CD2	2:C:60:ILE:HD13	2.41	0.48
2:B:185:ARG:CB	2:B:188:GLU:HB2	2.43	0.48
2:C:9:ARG:O	2:C:13:VAL:HG12	2.13	0.48
2:B:577:TYR:CD2	2:B:577:TYR:N	2.82	0.48
2:C:572:ILE:CG2	2:C:573:ASP:N	2.75	0.48
2:A:348:ILE:CD1	2:A:372:GLU:HG2	2.42	0.48
2:B:13:VAL:HG21	2:B:38:LEU:CD2	2.16	0.48
2:B:140:GLN:C	2:B:141:LEU:HD23	2.33	0.48
2:C:421:ASP:O	2:C:422:GLU:C	2.51	0.48
2:B:156:SER:O	2:B:157:ASN:O	2.31	0.48
2:A:359:GLU:HA	2:A:364:VAL:HG12	1.95	0.48
2:B:305:ALA:HA	2:B:309:LEU:HD11	1.95	0.48
2:A:199:ARG:NE	2:B:358:TYR:HH	2.00	0.48
2:A:647:VAL:HG12	2:A:648:ASP:N	2.29	0.48
2:A:265:MET:HA	2:A:268:ILE:HG22	1.94	0.48
2:A:307:GLY:C	2:A:309:LEU:H	2.17	0.48
2:C:650:ARG:HG3	2:C:650:ARG:HH11	1.78	0.48
2:A:577:TYR:CD2	2:A:577:TYR:N	2.82	0.48
2:B:29:ILE:HG13	2:B:80:TYR:HD1	1.79	0.48
2:C:140:GLN:HG3	2:C:140:GLN:O	2.13	0.48
2:A:574:MET:HE3	2:A:616:LEU:HD13	1.95	0.48
2:A:396:ASP:O	2:A:397:GLU:C	2.51	0.48
2:B:351:LEU:CB	2:B:371:ILE:HD13	2.44	0.48
2:C:385:ARG:HB2	2:C:390:LYS:CG	2.44	0.48
2:C:385:ARG:HB2	2:C:390:LYS:HG3	1.95	0.48
2:C:577:TYR:CD2	2:C:577:TYR:N	2.82	0.48
2:B:415:GLU:O	2:B:418:GLN:HG3	2.14	0.48
2:C:70:ARG:HB3	2:C:71:GLY:HA3	1.96	0.48
2:A:196:LEU:HD12	2:A:310:GLN:NE2	2.29	0.48
2:C:122:ARG:HG3	2:C:126:ASN:ND2	2.29	0.48
2:C:196:LEU:HD13	2:C:204:PRO:HD3	1.95	0.48
2:C:242:LEU:HD12	2:C:243:ASP:O	2.14	0.48
2:C:268:ILE:HD11	2:C:308:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:437:GLU:C	2:B:439:ALA:N	2.66	0.48
2:A:83:ARG:O	2:A:86:LYS:HB3	2.14	0.48
2:B:647:VAL:HG12	2:B:648:ASP:N	2.29	0.48
2:A:73:GLU:O	2:A:74:MET:C	2.52	0.48
2:C:28:ASN:HD22	2:C:28:ASN:N	2.12	0.48
2:A:16:LEU:HD13	2:A:41:GLU:HB2	1.96	0.47
2:A:179:LEU:HB3	2:A:223:GLN:NE2	2.29	0.47
2:A:201:LYS:HE2	2:B:385:ARG:HH12	1.79	0.47
2:A:239:VAL:O	2:A:240:MET:HG2	2.13	0.47
2:A:6:PHE:HB3	2:A:10:ALA:CB	2.43	0.47
2:B:214:LYS:HZ3	2:B:314:ALA:CA	2.26	0.47
2:B:278:ILE:O	2:B:314:ALA:CB	2.62	0.47
2:A:355:ARG:HH21	2:A:366:ILE:HA	1.78	0.47
2:A:364:VAL:HG22	2:A:365:SER:HA	1.95	0.47
2:A:367:THR:H	2:A:471:VAL:C	2.18	0.47
2:A:367:THR:N	2:A:471:VAL:CA	2.76	0.47
2:B:618:ALA:HA	2:B:620:GLU:OE2	2.14	0.47
2:A:348:ILE:HA	2:A:351:LEU:HD12	1.96	0.47
2:A:184:GLY:HA2	2:A:185:ARG:HB2	1.95	0.47
2:A:230:VAL:HG13	2:A:231:PRO:CD	2.44	0.47
2:A:405:ARG:NH2	2:A:478:MET:CE	2.78	0.47
2:B:221:LEU:O	2:B:222:ALA:C	2.52	0.47
2:B:72:GLN:O	2:B:74:MET:N	2.47	0.47
2:C:473:VAL:O	2:C:476:ILE:N	2.47	0.47
2:B:5:ARG:NH1	2:B:5:ARG:N	2.59	0.47
2:A:618:ALA:HA	2:A:620:GLU:OE2	2.14	0.47
2:C:618:ALA:HA	2:C:620:GLU:OE2	2.14	0.47
2:A:44:GLY:HA3	2:A:105:THR:HG21	1.95	0.47
2:A:348:ILE:HG23	2:A:371:ILE:HG21	1.96	0.47
2:A:398:ALA:N	2:A:479:VAL:HG22	2.28	0.47
2:B:364:VAL:HA	2:B:365:SER:O	2.14	0.47
2:A:412:ASN:C	2:A:414:LYS:H	2.17	0.47
2:A:201:LYS:CE	2:A:432:GLN:NE2	83.40	0.47
2:B:268:ILE:HD11	2:B:274:ILE:HG23	1.96	0.47
2:C:341:GLN:HE21	2:C:386:PHE:HA	1.78	0.47
2:C:18:GLN:O	2:C:21:ALA:N	2.48	0.47
2:A:439:ALA:O	2:A:443:ARG:N	2.44	0.47
2:C:261:LEU:HG	2:C:261:LEU:H	1.52	0.47
2:A:214:LYS:O	2:A:216:ALA:N	2.47	0.47
2:B:184:GLY:CA	2:B:185:ARG:C	2.81	0.47
2:B:201:LYS:HB3	2:B:335:GLN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:GLU:H	2:B:229:GLU:HG3	1.39	0.47
2:B:233:ILE:O	2:B:234:LEU:HG	2.15	0.47
2:C:123:VAL:HB	2:C:124:LEU:HD23	1.96	0.47
2:A:425:LYS:O	2:A:429:ALA:N	2.47	0.47
2:C:647:VAL:HG12	2:C:648:ASP:N	2.29	0.47
2:C:226:ILE:HG22	2:C:227:ASN:N	2.29	0.47
2:B:565:ASP:C	2:B:567:GLU:N	2.66	0.47
2:A:380:ARG:HG3	2:A:381:TYR:HD2	1.79	0.47
2:B:356:ASP:CA	2:B:359:GLU:HG3	2.45	0.47
2:A:124:LEU:C	2:A:126:ASN:N	2.68	0.47
2:B:129:VAL:CG1	2:B:129:VAL:O	2.54	0.47
2:B:201:LYS:HZ1	2:B:335:GLN:HG2	1.80	0.47
2:B:30:GLY:HA2	2:B:81:THR:CG2	2.43	0.47
2:C:179:LEU:HB3	2:C:223:GLN:NE2	2.30	0.47
2:C:425:LYS:O	2:C:426:GLU:C	2.53	0.47
2:A:405:ARG:O	2:A:408:THR:HG22	2.14	0.47
2:B:13:VAL:HG21	2:B:38:LEU:HA	1.97	0.47
2:C:204:PRO:HD2	2:C:311:CYS:O	2.15	0.47
2:C:364:VAL:HG22	2:C:365:SER:C	2.35	0.47
2:C:574:MET:HE3	2:C:616:LEU:HB3	1.96	0.47
2:C:752:ALA:C	2:C:754:GLU:H	2.18	0.47
2:C:633:VAL:O	2:C:637:GLY:N	2.47	0.47
2:A:408:THR:C	2:A:414:LYS:HZ3	2.10	0.47
2:B:6:PHE:HB2	2:B:10:ALA:CB	2.43	0.47
2:C:38:LEU:HD13	2:C:109:LEU:HB2	1.96	0.47
2:C:86:LYS:HG2	2:C:115:GLU:OE2	2.15	0.47
2:A:650:ARG:HH11	2:A:650:ARG:HG3	1.79	0.47
2:A:378:SER:HB3	2:A:390:LYS:CD	2.43	0.47
2:B:739:LEU:HG	2:B:788:LYS:HE2	1.97	0.47
2:A:179:LEU:HD12	2:A:180:ASP:H	1.80	0.47
2:B:176:GLU:O	2:B:178:SER:N	2.48	0.47
2:C:374:ALA:HA	2:C:476:ILE:CD1	2.35	0.47
2:B:22:LEU:N	2:B:22:LEU:HD22	2.29	0.47
2:C:22:LEU:N	2:C:22:LEU:HD22	2.30	0.47
2:A:330:LEU:C	2:A:332:ARG:N	2.66	0.47
2:B:633:VAL:O	2:B:637:GLY:N	2.47	0.47
2:A:365:SER:O	2:A:366:ILE:HG13	2.15	0.47
2:B:367:THR:OG1	2:B:370:ALA:HB2	2.15	0.47
2:C:270:GLN:O	2:C:271:ALA:HB2	2.15	0.47
2:C:421:ASP:C	2:C:423:VAL:N	2.67	0.47
2:C:435:GLU:HG3	2:C:438:LYS:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:LEU:HA	2:C:442:LEU:HD23	1.51	0.47
2:A:301:LYS:N	2:A:302:PRO:CD	2.77	0.47
2:A:633:VAL:O	2:A:637:GLY:N	2.47	0.47
2:A:370:ALA:O	2:A:476:ILE:HD12	2.15	0.46
2:B:10:ALA:HA	2:B:13:VAL:HG12	1.98	0.46
2:B:191:ARG:HG2	2:B:337:ILE:CG2	2.41	0.46
2:B:192:VAL:CG1	2:B:221:LEU:HD21	2.44	0.46
2:C:402:VAL:C	2:C:404:LEU:H	2.18	0.46
2:C:359:GLU:HA	2:C:364:VAL:HG12	1.97	0.46
2:A:619:ILE:HG12	2:A:656:MET:HB3	1.97	0.46
2:A:739:LEU:HG	2:A:788:LYS:HE2	1.97	0.46
2:A:335:GLN:HG2	2:A:336:PRO:HD2	1.97	0.46
2:B:27:ASN:OD1	2:B:27:ASN:N	2.47	0.46
2:B:203:ASN:ND2	2:B:311:CYS:H	2.13	0.46
2:C:165:SER:CA	2:C:166:LEU:O	2.62	0.46
2:B:271:ALA:CB	2:C:96:ARG:NH1	2.78	0.46
2:B:356:ASP:O	2:B:359:GLU:HG3	2.15	0.46
2:B:124:LEU:C	2:B:126:ASN:N	2.68	0.46
2:B:124:LEU:C	2:B:126:ASN:H	2.17	0.46
2:A:320:TYR:O	2:A:321:ARG:C	2.54	0.46
2:B:262:LYS:HZ2	2:C:260:ARG:NH2	2.08	0.46
2:C:18:GLN:HA	2:C:21:ALA:HB2	1.98	0.46
2:C:67:LEU:C	2:C:68:ILE:HG13	2.35	0.46
2:A:731:THR:HG22	2:A:741:ILE:CG1	2.45	0.46
2:B:373:ALA:O	2:B:377:LEU:HD13	2.14	0.46
2:A:203:ASN:O	2:A:335:GLN:N	2.49	0.46
2:C:103:VAL:CG1	2:C:104:GLY:H	2.27	0.46
2:C:203:ASN:O	2:C:335:GLN:N	2.48	0.46
2:B:435:GLU:HG3	2:B:438:LYS:CB	2.46	0.46
2:A:269:ARG:HG2	2:A:307:GLY:HA3	1.97	0.46
2:A:435:GLU:HG3	2:A:438:LYS:CB	2.46	0.46
2:A:22:LEU:O	2:A:25:GLY:N	2.47	0.46
2:A:278:ILE:HG13	2:A:313:GLY:HA2	1.98	0.46
2:B:54:GLY:C	2:B:55:LEU:HD23	2.36	0.46
2:B:640:THR:HG22	2:B:646:THR:HB	1.98	0.46
2:A:377:LEU:O	2:A:381:TYR:HB2	2.16	0.46
2:A:377:LEU:CD1	2:A:477:ALA:HA	2.46	0.46
2:B:386:PHE:C	2:B:388:PRO:HD2	2.36	0.46
2:B:72:GLN:C	2:B:74:MET:N	2.69	0.46
2:C:731:THR:HG22	2:C:741:ILE:CG1	2.45	0.46
2:C:763:ARG:CB	2:C:764:PRO:HD3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:461:LYS:O	2:A:464:GLN:HB2	2.16	0.46
2:A:70:ARG:HB3	2:A:71:GLY:HA3	1.98	0.46
2:A:351:LEU:O	2:A:355:ARG:N	2.48	0.46
2:A:374:ALA:H	2:A:476:ILE:CG2	1.95	0.46
2:B:171:THR:CG2	2:B:226:ILE:HD11	2.46	0.46
2:C:412:ASN:C	2:C:414:LYS:H	2.18	0.46
2:C:365:SER:O	2:C:366:ILE:HG13	2.16	0.46
2:C:278:ILE:HG13	2:C:313:GLY:HA2	1.98	0.46
2:C:640:THR:HG22	2:C:646:THR:HB	1.98	0.46
2:B:752:ALA:C	2:B:754:GLU:H	2.18	0.46
2:B:480:VAL:O	2:B:481:SER:C	2.54	0.46
2:B:190:GLN:HB3	2:C:404:LEU:HD21	1.98	0.46
2:B:230:VAL:O	2:C:407:PHE:CZ	2.69	0.46
2:C:377:LEU:O	2:C:381:TYR:N	2.42	0.46
2:C:365:SER:C	2:C:366:ILE:HG13	2.36	0.46
2:A:72:GLN:O	2:A:74:MET:N	2.49	0.46
2:B:46:ALA:HB2	2:B:105:THR:C	2.36	0.46
2:C:460:TRP:CZ3	2:C:463:LYS:HG2	2.50	0.46
2:B:170:LEU:N	2:B:239:VAL:O	2.49	0.46
2:C:6:PHE:HB3	2:C:10:ALA:CB	2.45	0.46
2:A:526:ARG:CG	2:B:778:SER:CB	2.83	0.46
2:A:268:ILE:C	2:A:268:ILE:HD13	2.35	0.46
2:A:270:GLN:O	2:A:271:ALA:HB2	2.15	0.46
2:B:70:ARG:CB	2:B:71:GLY:HA3	2.45	0.46
2:B:422:GLU:O	2:B:426:GLU:N	2.38	0.46
2:A:394:LEU:CG	2:A:480:VAL:HG22	2.41	0.46
2:B:369:ASP:O	2:B:473:VAL:HG13	2.16	0.46
2:A:404:LEU:C	2:A:406:SER:N	2.69	0.46
2:B:6:PHE:HD2	2:B:6:PHE:N	2.11	0.46
2:C:194:GLU:C	2:C:196:LEU:H	2.19	0.46
2:B:731:THR:HG22	2:B:741:ILE:CG1	2.45	0.46
2:B:279:ASP:O	2:B:280:ALA:CB	2.64	0.46
2:A:365:SER:C	2:A:366:ILE:CG1	2.84	0.46
2:A:421:ASP:O	2:A:422:GLU:C	2.54	0.46
2:B:106:GLU:CD	2:B:106:GLU:H	2.19	0.46
2:B:199:ARG:HH22	2:C:357:ARG:HH21	0.58	0.46
2:B:212:VAL:HA	2:B:213:GLY:C	2.35	0.46
2:B:185:ARG:NH2	2:B:342:PRO:HG3	2.31	0.46
2:A:305:ALA:C	2:A:309:LEU:HD11	2.36	0.46
2:A:72:GLN:C	2:A:74:MET:N	2.69	0.46
2:B:619:ILE:HG12	2:B:656:MET:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:739:LEU:HG	2:C:788:LYS:HE2	1.97	0.46
2:B:39:VAL:O	2:B:39:VAL:HG22	2.15	0.46
2:A:53:LEU:HD22	2:A:53:LEU:N	2.31	0.46
2:B:500:LEU:HD11	2:C:783:ARG:N	2.31	0.45
2:A:375:VAL:HG12	2:A:376:LYS:N	2.30	0.45
2:B:275:ILE:HA	2:B:310:GLN:O	2.15	0.45
2:C:305:ALA:C	2:C:309:LEU:HD11	2.37	0.45
2:A:640:THR:HG22	2:A:646:THR:HB	1.98	0.45
2:C:619:ILE:HG12	2:C:656:MET:HB3	1.97	0.45
2:A:752:ALA:C	2:A:754:GLU:H	2.18	0.45
2:A:186:SER:HA	2:A:189:ILE:HD12	1.97	0.45
2:A:405:ARG:HH22	2:A:478:MET:CE	2.29	0.45
2:B:189:ILE:O	2:B:192:VAL:HB	2.16	0.45
2:B:233:ILE:HG12	2:B:233:ILE:O	2.16	0.45
2:B:269:ARG:HH12	2:B:306:ARG:CB	2.27	0.45
2:C:184:GLY:HA3	2:C:185:ARG:C	2.36	0.45
2:C:90:LEU:O	2:C:93:ASP:N	2.47	0.45
2:A:74:MET:HE2	2:A:76:GLN:HE22	1.81	0.45
2:C:461:LYS:O	2:C:464:GLN:HB2	2.16	0.45
2:B:526:ARG:HD2	2:C:770:GLN:HG3	1.98	0.45
2:A:473:VAL:O	2:A:476:ILE:N	2.49	0.45
2:A:170:LEU:HB2	2:A:239:VAL:HB	1.98	0.45
2:B:396:ASP:C	2:B:399:GLY:H	2.18	0.45
2:A:110:LEU:HD21	2:A:138:VAL:CG1	2.47	0.45
2:A:424:ARG:O	2:A:427:LYS:HB3	2.16	0.45
2:B:191:ARG:O	2:B:195:VAL:CG2	2.65	0.45
2:B:211:GLY:HA3	2:B:212:VAL:C	2.36	0.45
2:B:306:ARG:CA	2:C:168:ARG:NH2	2.79	0.45
2:A:72:GLN:CB	2:A:74:MET:HG3	2.46	0.45
2:C:227:ASN:HA	2:C:228:ASN:CB	2.36	0.45
2:C:348:ILE:HG23	2:C:371:ILE:HG21	1.99	0.45
2:C:330:LEU:C	2:C:332:ARG:N	2.70	0.45
2:C:344:VAL:O	2:C:347:SER:HB2	2.17	0.45
2:B:117:GLU:OE1	2:B:117:GLU:HA	2.15	0.45
2:B:234:LEU:HD23	2:B:237:LYS:HD2	1.98	0.45
2:C:117:GLU:HA	2:C:117:GLU:OE1	2.15	0.45
2:C:396:ASP:O	2:C:399:GLY:N	2.50	0.45
2:C:175:LYS:C	2:C:177:ASP:H	2.20	0.45
2:C:620:GLU:OE2	2:C:658:SER:HA	2.17	0.45
2:A:646:THR:OG1	2:A:646:THR:O	2.35	0.45
2:A:649:PHE:C	2:A:651:ASN:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:649:PHE:C	2:C:651:ASN:H	2.20	0.45
2:B:730:LEU:HD22	2:B:734:LEU:HG	1.99	0.45
2:C:476:ILE:O	2:C:479:VAL:N	2.50	0.45
2:B:442:LEU:HA	2:B:445:THR:OG1	2.17	0.45
2:B:499:LEU:CD1	2:C:782:LEU:HD11	2.46	0.45
2:B:214:LYS:NZ	2:B:315:THR:N	2.64	0.45
2:A:113:ILE:HG13	2:A:131:LEU:HD13	1.98	0.45
2:A:9:ARG:O	2:A:13:VAL:HG12	2.17	0.45
2:B:110:LEU:HD21	2:B:138:VAL:HG11	1.99	0.45
2:B:140:GLN:O	2:B:140:GLN:HG3	2.15	0.45
2:B:174:ALA:HB1	2:B:179:LEU:HD22	1.98	0.45
2:B:179:LEU:HD12	2:B:179:LEU:HA	1.46	0.45
2:B:342:PRO:HG2	2:B:388:PRO:HB3	1.98	0.45
2:A:426:GLU:O	2:A:430:ALA:HB2	2.17	0.45
2:C:228:ASN:O	2:C:228:ASN:OD1	2.34	0.45
2:C:5:ARG:NH1	2:C:5:ARG:N	2.61	0.45
2:A:739:LEU:HA	2:A:739:LEU:HD23	1.61	0.45
2:A:507:HIS:NE2	2:A:514:ASP:OD1	2.48	0.45
2:C:192:VAL:O	2:C:196:LEU:HB2	2.17	0.45
2:C:268:ILE:C	2:C:270:GLN:N	2.69	0.45
2:B:436:PHE:O	2:B:437:GLU:C	2.53	0.45
2:B:439:ALA:O	2:B:440:ALA:C	2.55	0.45
2:A:425:LYS:O	2:A:426:GLU:C	2.54	0.45
2:C:507:HIS:NE2	2:C:514:ASP:OD1	2.48	0.45
2:C:49:ALA:O	2:C:52:ALA:HB3	2.16	0.45
2:B:351:LEU:O	2:B:354:LEU:N	2.49	0.45
2:B:473:VAL:O	2:B:474:ASP:C	2.56	0.45
2:B:162:THR:O	2:B:164:ASP:N	2.49	0.45
2:B:72:GLN:CB	2:B:74:MET:HG3	2.47	0.45
2:C:385:ARG:HB3	2:C:386:PHE:H	1.53	0.45
2:C:416:LEU:O	2:C:419:LYS:N	2.50	0.45
2:A:18:GLN:O	2:A:21:ALA:HB3	2.17	0.45
2:B:18:GLN:O	2:B:21:ALA:HB3	2.17	0.45
2:A:730:LEU:HD22	2:A:734:LEU:HG	1.99	0.45
2:A:394:LEU:HD13	2:A:479:VAL:CB	2.28	0.44
2:B:351:LEU:HB2	2:B:371:ILE:HD13	1.99	0.44
2:B:363:ARG:HH12	2:B:475:ASP:C	2.15	0.44
2:B:129:VAL:C	2:B:130:SER:O	2.55	0.44
2:B:231:PRO:CG	2:B:232:GLU:N	2.78	0.44
2:B:266:ASP:OD1	2:B:269:ARG:HD2	2.17	0.44
2:B:28:ASN:HD22	2:B:28:ASN:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:SER:HB3	2:C:108:ILE:HA	1.98	0.44
2:C:194:GLU:O	2:C:198:ARG:HG3	2.16	0.44
2:C:424:ARG:O	2:C:427:LYS:HB3	2.17	0.44
2:B:438:LYS:O	2:B:442:LEU:CD1	2.65	0.44
2:B:411:PRO:O	2:B:413:LEU:N	2.50	0.44
2:A:314:ALA:O	2:A:315:THR:HG23	2.16	0.44
2:A:10:ALA:HA	2:A:13:VAL:HG12	2.00	0.44
2:B:342:PRO:HG2	2:B:388:PRO:CG	2.47	0.44
2:A:620:GLU:OE2	2:A:658:SER:HA	2.16	0.44
2:B:477:ALA:O	2:B:480:VAL:N	2.50	0.44
2:A:179:LEU:HD23	2:A:223:GLN:HE21	1.83	0.44
2:A:9:ARG:NH1	2:A:9:ARG:HG3	2.32	0.44
2:B:304:LEU:CD2	2:B:305:ALA:H	2.22	0.44
2:C:439:ALA:O	2:C:442:LEU:CA	2.65	0.44
2:C:373:ALA:O	2:C:374:ALA:C	2.55	0.44
2:A:23:ARG:NH1	2:A:61:GLN:HE22	2.14	0.44
2:C:646:THR:OG1	2:C:646:THR:O	2.34	0.44
2:B:23:ARG:NH1	2:B:61:GLN:HE22	2.14	0.44
2:B:691:GLY:N	2:C:760:TYR:OH	2.42	0.44
2:B:351:LEU:HG	2:B:392:ILE:CD1	2.48	0.44
2:B:373:ALA:O	2:B:374:ALA:C	2.55	0.44
2:A:210:PRO:HA	2:A:214:LYS:HE3	1.99	0.44
2:B:63:GLU:O	2:B:67:LEU:HG	2.17	0.44
2:C:196:LEU:HD12	2:C:310:GLN:NE2	2.32	0.44
2:A:265:MET:O	2:A:268:ILE:CG2	2.66	0.44
2:A:22:LEU:N	2:A:22:LEU:HD22	2.31	0.44
2:C:140:GLN:C	2:C:141:LEU:HD23	2.36	0.44
2:A:365:SER:C	2:A:366:ILE:HG13	2.37	0.44
2:C:182:VAL:HG12	2:C:183:ILE:N	2.32	0.44
2:C:308:GLU:O	2:C:310:GLN:N	2.51	0.44
2:C:204:PRO:CG	2:C:312:ILE:HG12	2.43	0.44
2:C:335:GLN:HG2	2:C:336:PRO:HD2	1.99	0.44
2:C:13:VAL:CG2	2:C:37:GLY:C	2.82	0.44
2:C:363:ARG:HH21	2:C:402:VAL:HG21	1.82	0.44
2:A:434:GLN:HA	2:A:435:GLU:C	2.37	0.44
2:C:259:ASP:C	2:C:261:LEU:H	2.21	0.44
2:A:398:ALA:CB	2:A:479:VAL:CG2	2.95	0.44
2:B:363:ARG:CG	2:B:471:VAL:HA	2.47	0.44
2:A:405:ARG:NH2	2:A:478:MET:HE3	2.33	0.44
2:B:103:VAL:CG1	2:B:104:GLY:N	2.80	0.44
2:B:276:LEU:O	2:B:311:CYS:CA	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:PHE:HB3	2:B:10:ALA:CB	2.46	0.44
2:B:439:ALA:C	2:B:441:SER:N	2.69	0.44
2:C:382:ILE:HG13	2:C:484:THR:HG21	1.91	0.44
2:B:496:THR:CB	2:C:782:LEU:HD22	2.47	0.44
2:C:29:ILE:HG13	2:C:80:TYR:HD1	1.82	0.44
2:A:398:ALA:HA	2:A:401:LYS:HB3	2.00	0.44
2:B:86:LYS:HG2	2:B:115:GLU:OE2	2.18	0.44
2:B:180:ASP:N	2:B:180:ASP:OD1	2.46	0.44
2:C:424:ARG:O	2:C:425:LYS:C	2.56	0.44
2:C:170:LEU:HB2	2:C:239:VAL:HB	2.00	0.44
2:C:364:VAL:HG13	2:C:365:SER:CA	2.47	0.44
2:A:261:LEU:H	2:A:261:LEU:HG	1.48	0.44
2:B:85:LYS:HE3	2:B:85:LYS:HB2	1.76	0.44
2:B:93:ASP:C	2:B:95:ALA:H	2.21	0.44
2:A:352:GLN:HA	2:A:355:ARG:CB	2.48	0.44
2:A:367:THR:CB	2:A:472:THR:HA	2.47	0.44
2:A:167:ALA:HB1	2:A:241:THR:O	2.18	0.44
2:C:166:LEU:HA	2:C:167:ALA:HA	1.78	0.44
2:C:386:PHE:C	2:C:388:PRO:HD2	2.38	0.44
2:C:341:GLN:CG	2:C:387:LEU:HB2	2.46	0.44
2:C:364:VAL:HG23	2:C:366:ILE:O	2.17	0.44
2:A:18:GLN:HA	2:A:21:ALA:HB2	2.00	0.44
2:B:22:LEU:C	2:B:24:LEU:N	2.72	0.44
2:B:620:GLU:OE2	2:B:658:SER:HA	2.16	0.44
2:B:633:VAL:O	2:B:637:GLY:HA2	2.18	0.44
2:B:209:GLU:HA	2:B:210:PRO:HD3	1.81	0.44
2:C:300:LEU:N	2:C:323:TYR:OH	2.51	0.44
2:C:302:PRO:HB2	2:C:304:LEU:HG	1.98	0.44
2:C:308:GLU:C	2:C:308:GLU:CD	2.76	0.44
2:C:403:ARG:O	2:C:406:SER:HB3	2.17	0.44
2:C:201:LYS:CE	2:C:432:GLN:NE2	83.00	0.44
2:A:265:MET:O	2:A:268:ILE:HG23	2.18	0.44
2:A:633:VAL:O	2:A:637:GLY:HA2	2.18	0.44
2:A:351:LEU:HD22	2:A:395:ILE:CD1	2.48	0.43
2:C:22:LEU:C	2:C:24:LEU:N	2.70	0.43
2:B:319:GLU:O	2:B:322:LYS:HB2	2.17	0.43
2:A:5:ARG:NH1	2:A:5:ARG:N	2.63	0.43
2:B:514:ASP:O	2:B:518:VAL:HG23	2.18	0.43
2:A:233:ILE:HD11	2:B:361:HIS:HB3	1.99	0.43
2:C:169:ASP:HA	2:C:240:MET:HE2	2.00	0.43
2:C:206:LEU:H	2:C:206:LEU:HD12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:GLN:HB3	2:C:74:MET:HG3	1.99	0.43
2:B:649:PHE:C	2:B:651:ASN:H	2.20	0.43
2:A:514:ASP:O	2:A:518:VAL:HG23	2.18	0.43
2:A:377:LEU:HD12	2:A:477:ALA:HA	2.00	0.43
2:A:175:LYS:C	2:A:177:ASP:H	2.20	0.43
2:A:182:VAL:HG12	2:A:183:ILE:N	2.33	0.43
2:B:168:ARG:HH12	2:B:242:LEU:CD1	2.28	0.43
2:B:191:ARG:HD2	2:B:337:ILE:CG2	2.47	0.43
2:B:232:GLU:OE1	2:C:400:SER:HB2	2.18	0.43
2:C:201:LYS:CE	2:C:335:GLN:HG3	2.49	0.43
2:C:386:PHE:CB	2:C:388:PRO:HD2	2.48	0.43
2:A:199:ARG:HD2	2:B:358:TYR:CZ	2.53	0.43
2:B:18:GLN:HA	2:B:21:ALA:HB2	2.00	0.43
2:A:546:PRO:HG2	2:A:549:VAL:CG2	2.44	0.43
2:B:646:THR:OG1	2:B:646:THR:O	2.34	0.43
2:C:324:ILE:HA	2:C:330:LEU:CB	2.48	0.43
2:A:52:ALA:HB3	2:A:137:GLN:HG2	1.99	0.43
2:C:633:VAL:O	2:C:637:GLY:HA2	2.18	0.43
2:C:730:LEU:HD22	2:C:734:LEU:HG	1.99	0.43
2:C:182:VAL:HG12	2:C:183:ILE:H	1.83	0.43
2:B:194:GLU:CD	2:C:401:LYS:HB2	2.38	0.43
2:C:12:LYS:HG2	2:C:16:LEU:HD12	2.01	0.43
2:B:574:MET:HE3	2:B:616:LEU:HB3	1.99	0.43
2:A:53:LEU:HD22	2:A:53:LEU:H	1.84	0.43
2:B:507:HIS:NE2	2:B:514:ASP:OD1	2.48	0.43
2:A:302:PRO:HB2	2:A:304:LEU:HG	2.01	0.43
2:A:426:GLU:O	2:A:430:ALA:HB3	2.18	0.43
2:B:193:ILE:CD1	2:B:193:ILE:O	5.81	0.43
2:C:70:ARG:CB	2:C:71:GLY:HA3	2.47	0.43
2:C:514:ASP:O	2:C:518:VAL:HG23	2.19	0.43
2:A:339:VAL:O	2:A:339:VAL:HG12	2.18	0.43
2:C:186:SER:HA	2:C:189:ILE:HD12	2.00	0.43
2:C:210:PRO:HA	2:C:214:LYS:HE3	2.00	0.43
2:C:269:ARG:HG2	2:C:307:GLY:HA3	2.00	0.43
2:B:382:ILE:HG22	2:B:382:ILE:O	2.19	0.43
2:A:268:ILE:C	2:A:270:GLN:N	2.69	0.43
2:A:116:GLY:O	2:A:121:ALA:CB	2.66	0.43
2:A:191:ARG:HG2	2:A:337:ILE:HG21	2.01	0.43
2:B:339:VAL:HG12	2:B:339:VAL:O	2.18	0.43
2:C:346:GLU:O	2:C:350:ILE:HG13	2.19	0.43
2:C:412:ASN:C	2:C:414:LYS:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:ILE:CD1	2:B:611:TYR:CE2	3.00	0.43
2:A:261:LEU:C	2:A:263:LYS:H	2.22	0.43
2:A:204:PRO:HD2	2:A:311:CYS:O	2.18	0.43
2:B:188:GLU:HB3	2:B:217:ILE:CD1	2.49	0.43
2:B:335:GLN:CG	2:B:336:PRO:CD	2.93	0.43
2:C:268:ILE:HD13	2:C:268:ILE:C	2.39	0.43
2:C:98:LEU:C	2:C:100:HIS:H	2.22	0.43
2:A:321:ARG:HD2	2:A:325:GLU:OE1	2.18	0.43
2:B:766:ARG:CG	2:B:766:ARG:HH11	2.31	0.43
2:A:70:ARG:CB	2:A:71:GLY:HA3	2.48	0.43
2:C:739:LEU:HA	2:C:739:LEU:HD23	1.61	0.43
2:A:32:GLU:HB3	2:A:119:VAL:CG1	2.49	0.43
2:B:198:ARG:NH1	2:C:396:ASP:HB3	2.33	0.43
2:C:424:ARG:O	2:C:428:ASP:N	2.30	0.43
2:C:93:ASP:C	2:C:95:ALA:H	2.21	0.43
2:C:67:LEU:O	2:C:68:ILE:CG1	2.67	0.43
2:A:54:GLY:C	2:A:55:LEU:HD23	2.39	0.43
2:A:324:ILE:HA	2:A:330:LEU:CB	2.48	0.43
2:C:735:LYS:HE3	2:C:735:LYS:HB2	1.88	0.43
2:A:279:ASP:OD2	2:A:279:ASP:N	2.51	0.43
2:A:359:GLU:CA	2:A:364:VAL:HG12	2.49	0.43
2:B:370:ALA:HB1	2:B:476:ILE:CB	2.49	0.43
2:A:211:GLY:C	2:A:213:GLY:H	2.22	0.43
2:A:478:MET:HB3	2:A:478:MET:HE2	1.60	0.43
2:B:67:LEU:C	2:B:68:ILE:HG13	2.39	0.43
2:C:183:ILE:CD1	2:C:349:GLN:HB2	2.49	0.43
2:B:345:ASP:O	2:B:348:ILE:HG13	2.19	0.43
2:A:259:ASP:C	2:A:261:LEU:H	2.22	0.43
2:B:528:ARG:O	2:B:528:ARG:HG3	2.19	0.43
2:A:192:VAL:O	2:A:196:LEU:HB2	2.19	0.42
2:C:471:VAL:HG12	2:C:472:THR:N	2.33	0.42
2:A:540:SER:HB2	2:A:706:ASP:H	1.85	0.42
2:C:23:ARG:NH1	2:C:61:GLN:HE22	2.16	0.42
2:A:117:GLU:HA	2:A:117:GLU:OE1	2.16	0.42
2:B:359:GLU:HG2	2:B:364:VAL:C	2.36	0.42
2:A:103:VAL:HG12	2:A:104:GLY:H	1.82	0.42
2:B:203:ASN:O	2:B:335:GLN:N	2.51	0.42
2:C:129:VAL:O	2:C:130:SER:C	2.57	0.42
2:A:364:VAL:HG13	2:A:365:SER:CA	2.48	0.42
2:A:416:LEU:HD21	2:A:452:GLN:HE22	1.84	0.42
2:B:308:GLU:O	2:B:309:LEU:CG	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ARG:HH21	2:C:357:ARG:NH2	2.00	0.42
2:C:139:LEU:O	2:C:141:LEU:N	2.52	0.42
2:C:22:LEU:C	2:C:24:LEU:H	2.22	0.42
2:B:533:ASP:OD1	2:B:534:PRO:HD2	2.20	0.42
2:A:393:ASP:O	2:A:479:VAL:CG1	2.68	0.42
2:B:480:VAL:C	2:B:482:SER:N	2.72	0.42
2:A:124:LEU:C	2:A:126:ASN:H	2.21	0.42
2:A:169:ASP:HA	2:A:240:MET:HE2	2.01	0.42
2:A:32:GLU:N	2:A:32:GLU:OE2	2.53	0.42
2:A:416:LEU:O	2:A:419:LYS:N	2.52	0.42
2:B:9:ARG:NH1	2:B:9:ARG:HG3	2.33	0.42
2:C:540:SER:HB2	2:C:706:ASP:H	1.85	0.42
2:B:20:GLU:O	2:B:21:ALA:C	2.55	0.42
2:C:18:GLN:O	2:C:19:GLU:C	2.58	0.42
2:C:279:ASP:N	2:C:279:ASP:OD2	2.53	0.42
2:A:335:GLN:HG2	2:A:336:PRO:CD	2.50	0.42
2:B:341:GLN:OE1	2:B:387:LEU:HD23	2.20	0.42
2:C:396:ASP:C	2:C:399:GLY:H	2.21	0.42
2:B:343:SER:O	2:B:346:GLU:N	2.53	0.42
2:A:72:GLN:HB3	2:A:74:MET:HG3	2.01	0.42
2:B:20:GLU:CD	2:B:40:ARG:NH1	2.72	0.42
2:C:67:LEU:O	2:C:68:ILE:HG12	2.19	0.42
2:A:732:LYS:HE3	2:A:732:LYS:HB2	1.85	0.42
2:B:500:LEU:CD2	2:C:779:GLU:O	2.67	0.42
2:A:377:LEU:O	2:A:381:TYR:N	2.47	0.42
2:A:362:HIS:O	2:A:363:ARG:HB2	2.18	0.42
2:A:420:LEU:HA	2:A:449:LEU:HD13	2.01	0.42
2:B:511:ILE:CG2	2:B:718:HIS:CG	2.67	0.42
2:B:511:ILE:HG13	2:B:721:GLU:HB3	2.02	0.42
2:B:261:LEU:HB3	2:B:262:LYS:H	1.29	0.42
2:C:18:GLN:O	2:C:21:ALA:HB3	2.19	0.42
2:B:44:GLY:HA3	2:B:105:THR:HG21	2.01	0.42
2:C:616:LEU:HD23	2:C:616:LEU:N	2.35	0.42
2:C:528:ARG:O	2:C:528:ARG:HG3	2.19	0.42
2:B:75:SER:O	2:B:77:THR:N	2.52	0.42
2:B:540:SER:HB2	2:B:706:ASP:H	1.84	0.42
2:B:325:GLU:OE1	2:B:325:GLU:HA	2.19	0.42
2:A:395:ILE:HG13	2:A:476:ILE:HG12	2.02	0.42
2:B:363:ARG:HH11	2:B:363:ARG:HD3	1.67	0.42
2:B:367:THR:CB	2:B:472:THR:HG23	2.49	0.42
2:A:177:ASP:C	2:A:179:LEU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:ARG:CZ	2:B:342:PRO:HG3	2.49	0.42
2:B:201:LYS:HZ2	2:B:335:GLN:HG3	1.83	0.42
2:B:200:THR:HG23	2:C:392:ILE:CG2	2.42	0.42
2:C:439:ALA:O	2:C:443:ARG:N	2.47	0.42
2:B:206:LEU:HB3	2:B:214:LYS:HE3	2.02	0.42
2:B:422:GLU:HA	2:B:425:LYS:HB2	2.01	0.42
2:B:49:ALA:O	2:B:52:ALA:HB3	2.20	0.42
2:B:414:LYS:O	2:B:417:GLU:HB2	2.20	0.42
2:B:525:ARG:HB3	2:C:779:GLU:CD	2.41	0.42
2:C:242:LEU:HD12	2:C:243:ASP:CA	2.50	0.42
2:C:335:GLN:HG2	2:C:336:PRO:CD	2.49	0.42
2:A:528:ARG:O	2:A:528:ARG:HG3	2.19	0.42
2:B:500:LEU:HB3	2:C:783:ARG:CG	2.50	0.42
2:B:90:LEU:HD13	2:B:114:ARG:HB3	2.02	0.42
2:B:351:LEU:O	2:B:352:GLN:C	2.57	0.42
2:A:13:VAL:CG2	2:A:38:LEU:HA	2.50	0.42
2:B:205:VAL:O	2:B:336:PRO:HA	2.20	0.42
2:B:194:GLU:OE1	2:C:397:GLU:O	2.38	0.42
2:C:41:GLU:O	2:C:41:GLU:HG2	2.20	0.42
2:C:434:GLN:HA	2:C:435:GLU:C	2.40	0.42
2:C:83:ARG:O	2:C:86:LYS:HB3	2.20	0.42
2:B:496:THR:HB	2:C:782:LEU:HD22	2.00	0.42
2:B:17:ALA:O	2:B:21:ALA:N	2.52	0.42
2:A:531:LEU:HD21	2:B:781:LEU:HD13	2.00	0.42
2:A:616:LEU:HD23	2:A:616:LEU:N	2.35	0.42
2:C:797:GLU:HB3	2:C:798:ASP:H	1.67	0.42
2:C:53:LEU:HD22	2:C:53:LEU:N	2.35	0.42
2:B:112:LEU:HA	2:B:112:LEU:HD23	1.79	0.41
2:B:202:ASN:C	2:B:202:ASN:OD1	2.57	0.41
2:B:274:ILE:O	2:B:274:ILE:HG23	2.20	0.41
2:B:72:GLN:HB3	2:B:74:MET:HG3	2.02	0.41
2:C:335:GLN:CD	2:C:336:PRO:HD2	2.41	0.41
2:C:366:ILE:HG22	2:C:367:THR:CA	2.31	0.41
2:B:472:THR:O	2:B:473:VAL:C	2.58	0.41
2:A:412:ASN:C	2:A:414:LYS:N	2.73	0.41
2:B:103:VAL:HA	2:B:107:HIS:ND1	2.34	0.41
2:B:198:ARG:HH12	2:C:397:GLU:N	2.17	0.41
2:C:416:LEU:HD21	2:C:452:GLN:HE22	1.84	0.41
2:C:9:ARG:HD3	2:C:9:ARG:HA	1.79	0.41
2:A:513:GLN:HG3	2:A:711:PHE:CD1	2.56	0.41
2:A:579:GLU:HB3	2:A:581:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:506:LEU:HD23	2:C:506:LEU:HA	1.87	0.41
2:B:472:THR:O	2:B:474:ASP:N	2.53	0.41
2:B:647:VAL:HG12	2:B:648:ASP:H	1.85	0.41
2:C:139:LEU:C	2:C:141:LEU:N	2.73	0.41
2:B:616:LEU:HD23	2:B:616:LEU:N	2.35	0.41
2:C:752:ALA:C	2:C:754:GLU:N	2.73	0.41
2:C:533:ASP:OD1	2:C:534:PRO:HD2	2.19	0.41
2:A:370:ALA:HB1	2:A:471:VAL:O	2.11	0.41
2:A:214:LYS:C	2:A:216:ALA:N	2.74	0.41
2:B:195:VAL:HA	2:B:198:ARG:NE	2.31	0.41
2:B:225:ILE:HA	2:B:230:VAL:CG2	2.51	0.41
2:C:211:GLY:C	2:C:213:GLY:H	2.24	0.41
2:C:374:ALA:HB2	2:C:476:ILE:HD11	2.01	0.41
2:B:450:ARG:C	2:B:452:GLN:N	2.74	0.41
2:B:763:ARG:N	2:B:764:PRO:HD2	2.36	0.41
2:A:434:GLN:HB2	2:A:436:PHE:CD1	2.55	0.41
2:C:112:LEU:HA	2:C:112:LEU:HD23	1.77	0.41
2:A:766:ARG:HH11	2:A:766:ARG:CG	2.32	0.41
2:A:758:LEU:CD2	2:A:758:LEU:H	2.33	0.41
2:A:715:GLU:O	2:A:716:LYS:C	2.58	0.41
2:C:116:GLY:O	2:C:121:ALA:CB	2.68	0.41
2:B:526:ARG:HG3	2:C:775:ASP:HB2	0.85	0.41
2:A:166:LEU:HA	2:A:167:ALA:HA	1.77	0.41
2:C:355:ARG:NH2	2:C:366:ILE:HA	2.36	0.41
2:A:139:LEU:C	2:A:141:LEU:N	2.74	0.41
2:A:28:ASN:N	2:A:28:ASN:HD22	2.18	0.41
2:C:546:PRO:HG2	2:C:549:VAL:CG2	2.44	0.41
2:C:339:VAL:O	2:C:339:VAL:HG12	2.20	0.41
2:A:238:ARG:HB2	2:A:274:ILE:HD12	2.03	0.41
2:A:423:VAL:HG21	2:A:449:LEU:CD1	2.50	0.41
2:A:446:GLU:HG2	2:A:447:GLN:N	2.36	0.41
2:B:201:LYS:HZ3	2:B:331:GLU:HA	1.85	0.41
2:C:183:ILE:CG2	2:C:184:GLY:H	2.33	0.41
2:B:232:GLU:HB3	2:C:361:HIS:HA	2.03	0.41
2:C:647:VAL:HG12	2:C:648:ASP:H	1.86	0.41
2:A:533:ASP:OD1	2:A:534:PRO:HD2	2.19	0.41
2:B:758:LEU:CD2	2:B:758:LEU:H	2.33	0.41
2:C:513:GLN:HG3	2:C:711:PHE:CD1	2.55	0.41
2:A:622:ALA:HB1	2:A:626:VAL:HG21	2.03	0.41
2:C:20:GLU:CD	2:C:40:ARG:NH1	2.74	0.41
2:A:106:GLU:CD	2:A:106:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:123:VAL:HB	2:A:124:LEU:HD23	2.03	0.41
2:A:174:ALA:HB3	2:A:222:ALA:HB1	2.01	0.41
2:B:241:THR:HB	2:B:242:LEU:H	1.57	0.41
2:B:196:LEU:HD21	2:B:275:ILE:HD12	2.03	0.41
2:C:10:ALA:HA	2:C:13:VAL:HG12	2.03	0.41
2:C:375:VAL:HG12	2:C:376:LYS:N	2.36	0.41
2:A:531:LEU:HD21	2:B:781:LEU:HD12	2.03	0.41
2:B:513:GLN:HG3	2:B:711:PHE:CD1	2.56	0.41
2:C:622:ALA:HB1	2:C:626:VAL:HG21	2.03	0.41
2:A:194:GLU:C	2:A:196:LEU:N	2.74	0.41
2:A:421:ASP:C	2:A:423:VAL:N	2.70	0.41
2:C:419:LYS:O	2:C:421:ASP:N	2.54	0.41
2:C:426:GLU:O	2:C:430:ALA:HB3	2.20	0.41
2:B:97:LYS:O	2:B:98:LEU:HG	2.20	0.41
2:C:639:LEU:HA	2:C:639:LEU:HD23	1.92	0.41
2:B:715:GLU:O	2:B:716:LYS:C	2.58	0.41
2:B:735:LYS:HB2	2:B:735:LYS:HE3	1.88	0.41
2:C:75:SER:O	2:C:77:THR:N	2.53	0.41
2:B:471:VAL:O	2:B:472:THR:O	2.39	0.41
2:A:122:ARG:HG3	2:A:126:ASN:HD22	1.85	0.41
2:B:207:ILE:O	2:B:207:ILE:CG1	2.66	0.41
2:B:304:LEU:HD13	2:B:306:ARG:HG2	2.03	0.41
2:C:214:LYS:O	2:C:216:ALA:N	2.53	0.41
2:C:13:VAL:CG2	2:C:38:LEU:HA	2.51	0.41
2:B:192:VAL:HG21	2:B:217:ILE:CG2	2.50	0.41
2:B:385:ARG:CB	2:B:390:LYS:HG2	2.49	0.41
2:C:447:GLN:O	2:C:448:ARG:C	2.57	0.41
2:B:511:ILE:HG22	2:B:718:HIS:CB	2.42	0.41
2:C:321:ARG:HD2	2:C:325:GLU:OE1	2.21	0.41
2:A:269:ARG:NH2	2:A:306:ARG:HB3	2.36	0.41
2:A:763:ARG:N	2:A:764:PRO:HD2	2.36	0.41
2:B:316:THR:H	2:B:319:GLU:HB3	1.86	0.41
2:A:27:ASN:OD1	2:A:27:ASN:N	2.54	0.41
2:A:330:LEU:C	2:A:332:ARG:H	2.24	0.41
2:B:752:ALA:C	2:B:754:GLU:N	2.73	0.41
2:A:453:VAL:HG12	2:A:454:GLU:N	2.35	0.41
2:C:106:GLU:H	2:C:106:GLU:CD	2.22	0.41
2:A:506:LEU:HA	2:A:506:LEU:HD23	1.87	0.41
2:A:735:LYS:HE3	2:A:735:LYS:HB2	1.88	0.41
2:B:744:THR:HG21	2:B:795:ASP:CG	2.42	0.41
2:A:381:TYR:O	2:A:382:ILE:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:386:PHE:C	2:A:388:PRO:HD2	2.41	0.41
2:B:205:VAL:HG23	2:B:335:GLN:N	2.36	0.41
2:B:232:GLU:HA	2:C:362:HIS:NE2	2.36	0.41
2:C:476:ILE:HG22	2:C:477:ALA:N	2.36	0.41
2:C:577:TYR:HD2	2:C:577:TYR:N	2.19	0.41
2:B:259:ASP:C	2:B:260:ARG:HG3	2.41	0.41
2:B:193:ILE:CG1	2:B:193:ILE:O	4.54	0.41
2:A:649:PHE:C	2:A:651:ASN:N	2.74	0.41
2:C:744:THR:HG21	2:C:795:ASP:CG	2.42	0.41
2:A:75:SER:O	2:A:77:THR:N	2.54	0.41
2:A:476:ILE:HG22	2:A:477:ALA:N	2.36	0.40
2:C:184:GLY:HA2	2:C:185:ARG:HB2	2.03	0.40
2:C:201:LYS:HB3	2:C:335:GLN:HB2	2.03	0.40
2:C:209:GLU:HA	2:C:210:PRO:HD3	1.86	0.40
2:C:404:LEU:C	2:C:406:SER:H	2.24	0.40
2:C:83:ARG:HD3	2:C:83:ARG:HA	1.92	0.40
2:C:475:ASP:O	2:C:479:VAL:HG23	2.20	0.40
2:A:577:TYR:HD2	2:A:577:TYR:N	2.19	0.40
2:A:773:VAL:HG22	2:A:794:LEU:HD12	2.03	0.40
2:C:715:GLU:O	2:C:716:LYS:C	2.58	0.40
2:B:526:ARG:NH1	2:C:770:GLN:HG2	2.36	0.40
2:A:122:ARG:HG3	2:A:126:ASN:ND2	2.37	0.40
2:B:387:LEU:N	2:B:388:PRO:CD	2.84	0.40
2:B:395:ILE:HD12	2:B:395:ILE:H	1.86	0.40
2:C:120:ALA:O	2:C:123:VAL:N	2.54	0.40
2:C:377:LEU:HD11	2:C:476:ILE:HG21	1.73	0.40
2:B:434:GLN:O	2:B:434:GLN:CG	2.51	0.40
2:B:36:LEU:O	2:B:40:ARG:HB2	2.21	0.40
2:A:112:LEU:HA	2:A:112:LEU:HD23	1.83	0.40
2:A:620:GLU:HG2	2:A:658:SER:OG	2.21	0.40
2:C:649:PHE:C	2:C:651:ASN:N	2.74	0.40
2:C:451:GLU:O	2:C:455:ASP:HB2	2.21	0.40
2:C:579:GLU:HB3	2:C:581:HIS:CE1	2.56	0.40
2:B:403:ARG:O	2:B:406:SER:HB3	2.20	0.40
2:B:500:LEU:HD13	2:C:783:ARG:CA	2.47	0.40
2:B:373:ALA:O	2:B:375:VAL:N	2.54	0.40
2:A:209:GLU:HA	2:A:210:PRO:HD3	1.81	0.40
2:B:197:SER:OG	2:B:232:GLU:HG3	2.21	0.40
2:B:188:GLU:HB3	2:B:217:ILE:HD11	2.04	0.40
2:C:67:LEU:C	2:C:68:ILE:CG1	2.89	0.40
2:C:348:ILE:CD1	2:C:372:GLU:HG2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:579:GLU:HB3	2:B:581:HIS:CE1	2.56	0.40
2:A:476:ILE:O	2:A:479:VAL:N	2.54	0.40
2:A:12:LYS:HG2	2:A:16:LEU:HD12	2.03	0.40
2:B:229:GLU:CB	2:C:407:PHE:CD1	3.05	0.40
2:C:265:MET:O	2:C:268:ILE:HG23	2.22	0.40
2:C:354:LEU:H	2:C:354:LEU:HG	1.74	0.40
2:B:439:ALA:CA	2:B:442:LEU:HD12	2.31	0.40
2:B:531:LEU:C	2:C:733:ARG:HH22	2.24	0.40
2:C:239:VAL:C	2:C:240:MET:HG2	2.41	0.40
2:A:318:ASP:O	2:A:319:GLU:C	2.59	0.40
2:C:773:VAL:HG22	2:C:794:LEU:HD12	2.03	0.40
2:A:181:PRO:CB	2:A:182:VAL:CA	2.82	0.40
2:A:207:ILE:HD12	2:A:317:LEU:O	2.21	0.40
2:A:204:PRO:CG	2:A:312:ILE:HG12	2.47	0.40
2:B:161:PRO:O	2:B:162:THR:C	2.60	0.40
2:C:63:GLU:O	2:C:67:LEU:HG	2.21	0.40
2:C:766:ARG:CG	2:C:766:ARG:HH11	2.32	0.40
2:C:261:LEU:C	2:C:263:LYS:H	2.24	0.40
2:A:744:THR:HG21	2:A:795:ASP:CG	2.42	0.40
2:B:659:ASN:O	2:B:662:ALA:HB3	2.22	0.40

All (41) 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:a:194:HIS:CD2	2:C:48:LYS:NZ[10_445]	1.03	1.17
2:A:500:LEU:CB	2:A:500:LEU:CB[8_555]	1.04	1.16
1:a:128:GLN:NE2	2:A:787:HIS:NE2[8_545]	1.09	1.11
1:a:128:GLN:NE2	2:A:787:HIS:CD2[8_545]	1.25	0.95
1:a:128:GLN:CD	2:A:787:HIS:NE2[8_545]	1.38	0.82
2:A:797:GLU:OE2	2:C:58:GLU:OE2[6_454]	1.42	0.78
2:A:500:LEU:CA	2:A:500:LEU:CB[8_555]	1.44	0.76
1:a:128:GLN:CG	2:A:787:HIS:CE1[8_545]	1.50	0.70
2:A:797:GLU:CD	2:C:58:GLU:OE2[6_454]	1.51	0.69
2:A:361:HIS:NE2	2:C:197:SER:O[10_445]	1.51	0.69
2:A:404:LEU:CD2	2:C:190:GLN:NE2[10_445]	1.51	0.69
1:a:192:SER:OG	2:C:141:LEU:O[10_445]	1.53	0.67
2:A:763:ARG:NH2	2:C:699:PRO:CG[10_445]	1.54	0.66
1:a:194:HIS:CD2	2:C:48:LYS:CE[10_445]	1.55	0.65
1:a:194:HIS:CG	2:C:48:LYS:NZ[10_445]	1.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:194:HIS:NE2	2:C:48:LYS:CD[10_445]	1.63	0.57
2:A:503:GLU:OE2	2:A:504:ASN:OD1[8_555]	1.65	0.55
1:a:128:GLN:CG	2:A:787:HIS:NE2[8_545]	1.66	0.54
2:A:361:HIS:CD2	2:C:197:SER:O[10_445]	1.66	0.54
2:A:500:LEU:CD1	2:A:500:LEU:CD2[8_555]	1.71	0.49
1:a:168:CYS:SG	2:A:781:LEU:O[8_545]	1.75	0.45
1:a:194:HIS:CD2	2:C:48:LYS:CD[10_445]	1.78	0.42
2:A:500:LEU:CB	2:A:500:LEU:CD2[8_555]	1.83	0.37
2:A:797:GLU:OE1	2:C:58:GLU:OE2[6_454]	1.87	0.33
2:A:763:ARG:NH1	2:C:699:PRO:CB[10_445]	1.91	0.29
2:A:404:LEU:CD2	2:C:190:GLN:CD[10_445]	1.98	0.22
2:A:733:ARG:CZ	2:C:533:ASP:CB[10_445]	1.99	0.21
2:A:763:ARG:CZ	2:C:699:PRO:CB[10_445]	1.99	0.21
2:A:404:LEU:CD2	2:C:190:GLN:CG[10_445]	2.02	0.18
1:a:206:GLU:OE2	2:A:783:ARG:CG[8_545]	2.02	0.18
2:A:763:ARG:CZ	2:C:699:PRO:CG[10_445]	2.03	0.17
1:a:127:LEU:O	2:A:787:HIS:ND1[8_545]	2.04	0.16
2:A:494:THR:CG2	2:B:781:LEU:O[8_555]	2.07	0.13
1:a:192:SER:CB	2:C:141:LEU:O[10_445]	2.08	0.12
2:A:797:GLU:OE2	2:C:58:GLU:CD[6_454]	2.09	0.11
2:A:733:ARG:NH2	2:C:533:ASP:N[10_445]	2.09	0.11
2:A:242:LEU:CD2	2:C:306:ARG:NH2[10_445]	2.09	0.11
2:A:500:LEU:CA	2:A:500:LEU:CA[8_555]	2.09	0.11
1:a:127:LEU:CD1	2:A:787:HIS:CB[8_545]	2.14	0.06
2:A:260:ARG:NH2	2:C:262:LYS:NZ[10_445]	2.15	0.05
1:a:128:GLN:CD	2:A:787:HIS:CE1[8_545]	2.17	0.03

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	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	3 34
1	b	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	3 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	c	92/111 (83%)	75 (82%)	13 (14%)	4 (4%)	3 34
2	A	686/758 (90%)	493 (72%)	127 (18%)	66 (10%)	1 15
2	B	682/758 (90%)	491 (72%)	115 (17%)	76 (11%)	0 11
2	C	691/758 (91%)	492 (71%)	130 (19%)	69 (10%)	1 14
All	All	2335/2607 (90%)	1703 (73%)	409 (18%)	223 (10%)	1 15

All (223) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	169	ASN
2	A	42	GLY
2	A	98	LEU
2	A	144	SER
2	A	183	ILE
2	A	261	LEU
2	A	271	ALA
2	A	306	ARG
2	A	309	LEU
2	A	333	ARG
2	A	363	ARG
2	A	366	ILE
2	A	382	ILE
2	A	471	VAL
2	A	473	VAL
2	A	566	GLU
2	B	42	GLY
2	B	98	LEU
2	B	130	SER
2	B	144	SER
2	B	157	ASN
2	B	164	ASP
2	B	168	ARG
2	B	180	ASP
2	B	181	PRO
2	B	198	ARG
2	B	201	LYS
2	B	210	PRO
2	B	214	LYS
2	B	231	PRO
2	B	232	GLU
2	B	233	ILE

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Mol	Chain	Res	Type
2	B	261	LEU
2	B	271	ALA
2	B	305	ALA
2	B	308	GLU
2	B	333	ARG
2	B	363	ARG
2	B	366	ILE
2	B	373	ALA
2	B	382	ILE
2	B	412	ASN
2	B	438	LYS
2	B	472	THR
2	B	566	GLU
1	c	169	ASN
2	C	42	GLY
2	C	98	LEU
2	C	130	SER
2	C	144	SER
2	C	183	ILE
2	C	242	LEU
2	C	244	MET
2	C	261	LEU
2	C	271	ALA
2	C	299	ILE
2	C	306	ARG
2	C	309	LEU
2	C	333	ARG
2	C	363	ARG
2	C	366	ILE
2	C	382	ILE
2	C	391	ALA
2	C	392	ILE
2	C	471	VAL
2	C	473	VAL
2	C	566	GLU
1	a	144	LYS
1	a	177	ASN
2	A	156	SER
2	A	163	LEU
2	A	165	SER
2	A	166	LEU
2	A	229	GLU

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Mol	Chain	Res	Type
2	A	383	SER
2	A	391	ALA
2	A	493	GLN
2	A	662	ALA
2	A	690	MET
1	b	169	ASN
2	B	166	LEU
2	B	171	THR
2	B	199	ARG
2	B	331	GLU
2	B	362	HIS
2	B	433	SER
2	B	440	ALA
2	B	455	ASP
2	B	493	GLN
2	B	662	ALA
2	B	690	MET
1	c	144	LYS
1	c	206	GLU
2	C	3	PHE
2	C	77	THR
2	C	163	LEU
2	C	165	SER
2	C	166	LEU
2	C	280	ALA
2	C	331	GLU
2	C	383	SER
2	C	493	GLN
2	C	662	ALA
2	C	690	MET
2	A	73	GLU
2	A	77	THR
2	A	130	SER
2	A	162	THR
2	A	168	ARG
2	A	181	PRO
2	A	200	THR
2	A	228	ASN
2	A	305	ALA
2	A	330	LEU
2	A	331	GLU
2	A	375	VAL

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Mol	Chain	Res	Type
2	A	388	PRO
2	A	412	ASN
2	A	413	LEU
2	A	788	LYS
1	b	144	LYS
1	b	206	GLU
2	B	77	THR
2	B	263	LYS
2	B	334	PHE
2	B	388	PRO
2	B	481	SER
2	B	788	LYS
1	c	177	ASN
2	C	23	ARG
2	C	68	ILE
2	C	73	GLU
2	C	140	GLN
2	C	145	ASN
2	C	162	THR
2	C	168	ARG
2	C	181	PRO
2	C	228	ASN
2	C	229	GLU
2	C	330	LEU
2	C	375	VAL
2	C	388	PRO
2	C	412	ASN
2	C	413	LEU
2	C	788	LYS
2	A	71	GLY
2	A	74	MET
2	A	145	ASN
2	A	148	GLY
2	A	212	VAL
2	A	215	THR
2	A	226	ILE
2	A	316	THR
2	A	400	SER
2	A	422	GLU
2	A	434	GLN
2	A	650	ARG
2	A	757	ASP

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Mol	Chain	Res	Type
2	A	779	GLU
1	b	177	ASN
2	B	68	ILE
2	B	71	GLY
2	B	73	GLU
2	B	74	MET
2	B	140	GLN
2	B	163	LEU
2	B	165	SER
2	B	176	GLU
2	B	212	VAL
2	B	330	LEU
2	B	344	VAL
2	B	359	GLU
2	B	374	ALA
2	B	385	ARG
2	B	450	ARG
2	B	650	ARG
2	B	757	ASP
2	B	779	GLU
2	C	71	GLY
2	C	74	MET
2	C	200	THR
2	C	212	VAL
2	C	226	ILE
2	C	301	LYS
2	C	305	ALA
2	C	316	THR
2	C	422	GLU
2	C	434	GLN
2	C	650	ARG
2	C	757	ASP
2	C	779	GLU
1	a	206	GLU
2	A	68	ILE
2	A	140	GLN
2	A	774	GLU
2	B	23	ARG
2	B	160	THR
2	B	306	ARG
2	B	342	PRO
2	B	774	GLU

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Mol	Chain	Res	Type
2	C	400	SER
2	C	774	GLU
2	A	440	ALA
2	B	222	ALA
2	B	383	SER
2	C	76	GLN
2	C	323	TYR
2	A	116	GLY
2	A	479	VAL
2	B	473	VAL
2	A	160	THR
2	B	471	VAL
2	B	476	ILE
2	A	392	ILE
2	A	423	VAL
2	C	160	THR
2	C	387	LEU
2	A	387	LEU
2	B	392	ILE
2	A	550	GLY
2	B	550	GLY
2	C	479	VAL
2	C	550	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	83/104 (80%)	67 (81%)	16 (19%)	2 13
1	b	84/104 (81%)	68 (81%)	16 (19%)	2 13
1	c	85/104 (82%)	69 (81%)	16 (19%)	2 13
2	A	571/645 (88%)	487 (85%)	84 (15%)	4 24
2	B	573/645 (89%)	476 (83%)	97 (17%)	2 18
2	C	576/645 (89%)	492 (85%)	84 (15%)	4 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1972/2247 (88%)	1659 (84%)	313 (16%)	3 21

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	132	ARG
1	a	133	PHE
1	a	142	LEU
1	a	147	VAL
1	a	152	THR
1	a	157	PHE
1	a	160	ARG
1	a	163	LEU
1	a	179	LEU
1	a	183	LEU
1	a	190	SER
1	a	191	ILE
1	a	193	ILE
1	a	198	GLU
1	a	202	LEU
1	a	212	ILE
2	A	5	ARG
2	A	6	PHE
2	A	7	THR
2	A	16	LEU
2	A	27	ASN
2	A	58	GLU
2	A	72	GLN
2	A	76	GLN
2	A	93	ASP
2	A	105	THR
2	A	117	GLU
2	A	124	LEU
2	A	131	LEU
2	A	139	LEU
2	A	180	ASP
2	A	188	GLU
2	A	206	LEU
2	A	207	ILE
2	A	230	VAL
2	A	239	VAL
2	A	241	THR

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Mol	Chain	Res	Type
2	A	242	LEU
2	A	261	LEU
2	A	268	ILE
2	A	276	LEU
2	A	278	ILE
2	A	279	ASP
2	A	304	LEU
2	A	308	GLU
2	A	309	LEU
2	A	315	THR
2	A	317	LEU
2	A	337	ILE
2	A	338	GLN
2	A	345	ASP
2	A	350	ILE
2	A	354	LEU
2	A	361	HIS
2	A	363	ARG
2	A	364	VAL
2	A	366	ILE
2	A	369	ASP
2	A	371	ILE
2	A	381	TYR
2	A	387	LEU
2	A	393	ASP
2	A	396	ASP
2	A	408	THR
2	A	424	ARG
2	A	428	ASP
2	A	456	THR
2	A	472	THR
2	A	473	VAL
2	A	504	ASN
2	A	513	GLN
2	A	514	ASP
2	A	528	ARG
2	A	531	LEU
2	A	540	SER
2	A	571	ARG
2	A	577	TYR
2	A	579	GLU
2	A	619	ILE

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Mol	Chain	Res	Type
2	A	620	GLU
2	A	631	LEU
2	A	640	THR
2	A	646	THR
2	A	650	ARG
2	A	659	ASN
2	A	660	VAL
2	A	686	LYS
2	A	690	MET
2	A	717	LYS
2	A	720	THR
2	A	725	LEU
2	A	727	SER
2	A	730	LEU
2	A	732	LYS
2	A	767	ARG
2	A	769	ILE
2	A	770	GLN
2	A	794	LEU
2	A	797	GLU
2	A	805	THR
1	b	132	ARG
1	b	133	PHE
1	b	142	LEU
1	b	147	VAL
1	b	151	LYS
1	b	152	THR
1	b	157	PHE
1	b	160	ARG
1	b	163	LEU
1	b	179	LEU
1	b	183	LEU
1	b	190	SER
1	b	191	ILE
1	b	193	ILE
1	b	202	LEU
1	b	212	ILE
2	B	5	ARG
2	B	6	PHE
2	B	7	THR
2	B	16	LEU
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	58	GLU
2	B	72	GLN
2	B	76	GLN
2	B	83	ARG
2	B	93	ASP
2	B	105	THR
2	B	117	GLU
2	B	124	LEU
2	B	131	LEU
2	B	139	LEU
2	B	168	ARG
2	B	173	ILE
2	B	180	ASP
2	B	188	GLU
2	B	195	VAL
2	B	201	LYS
2	B	207	ILE
2	B	229	GLU
2	B	232	GLU
2	B	233	ILE
2	B	235	ARG
2	B	236	ASP
2	B	265	MET
2	B	268	ILE
2	B	276	LEU
2	B	303	SER
2	B	304	LEU
2	B	309	LEU
2	B	312	ILE
2	B	316	THR
2	B	317	LEU
2	B	323	TYR
2	B	326	LYS
2	B	337	ILE
2	B	347	SER
2	B	348	ILE
2	B	354	LEU
2	B	355	ARG
2	B	361	HIS
2	B	363	ARG
2	B	381	TYR
2	B	382	ILE

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Mol	Chain	Res	Type
2	B	387	LEU
2	B	396	ASP
2	B	403	ARG
2	B	416	LEU
2	B	417	GLU
2	B	418	GLN
2	B	419	LYS
2	B	424	ARG
2	B	428	ASP
2	B	432	GLN
2	B	433	SER
2	B	435	GLU
2	B	443	ARG
2	B	453	VAL
2	B	454	GLU
2	B	456	THR
2	B	472	THR
2	B	473	VAL
2	B	478	MET
2	B	479	VAL
2	B	483	TRP
2	B	504	ASN
2	B	513	GLN
2	B	514	ASP
2	B	528	ARG
2	B	540	SER
2	B	571	ARG
2	B	577	TYR
2	B	579	GLU
2	B	619	ILE
2	B	620	GLU
2	B	631	LEU
2	B	640	THR
2	B	646	THR
2	B	650	ARG
2	B	659	ASN
2	B	660	VAL
2	B	686	LYS
2	B	690	MET
2	B	717	LYS
2	B	720	THR
2	B	725	LEU

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Mol	Chain	Res	Type
2	B	727	SER
2	B	730	LEU
2	B	732	LYS
2	B	769	ILE
2	B	770	GLN
2	B	794	LEU
2	B	797	GLU
2	B	805	THR
1	c	132	ARG
1	c	142	LEU
1	c	147	VAL
1	c	151	LYS
1	c	152	THR
1	c	157	PHE
1	c	160	ARG
1	c	163	LEU
1	c	179	LEU
1	c	183	LEU
1	c	190	SER
1	c	191	ILE
1	c	193	ILE
1	c	198	GLU
1	c	202	LEU
1	c	212	ILE
2	C	5	ARG
2	C	6	PHE
2	C	7	THR
2	C	16	LEU
2	C	27	ASN
2	C	58	GLU
2	C	72	GLN
2	C	76	GLN
2	C	83	ARG
2	C	93	ASP
2	C	105	THR
2	C	117	GLU
2	C	131	LEU
2	C	139	LEU
2	C	176	GLU
2	C	180	ASP
2	C	188	GLU
2	C	206	LEU

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Mol	Chain	Res	Type
2	C	207	ILE
2	C	230	VAL
2	C	239	VAL
2	C	241	THR
2	C	242	LEU
2	C	261	LEU
2	C	268	ILE
2	C	276	LEU
2	C	278	ILE
2	C	279	ASP
2	C	304	LEU
2	C	308	GLU
2	C	309	LEU
2	C	315	THR
2	C	317	LEU
2	C	337	ILE
2	C	338	GLN
2	C	345	ASP
2	C	354	LEU
2	C	361	HIS
2	C	364	VAL
2	C	366	ILE
2	C	369	ASP
2	C	371	ILE
2	C	381	TYR
2	C	387	LEU
2	C	393	ASP
2	C	394	LEU
2	C	396	ASP
2	C	408	THR
2	C	424	ARG
2	C	428	ASP
2	C	456	THR
2	C	471	VAL
2	C	472	THR
2	C	473	VAL
2	C	504	ASN
2	C	513	GLN
2	C	514	ASP
2	C	528	ARG
2	C	531	LEU
2	C	540	SER

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Mol	Chain	Res	Type
2	C	571	ARG
2	C	577	TYR
2	C	579	GLU
2	C	619	ILE
2	C	620	GLU
2	C	631	LEU
2	C	640	THR
2	C	646	THR
2	C	650	ARG
2	C	659	ASN
2	C	660	VAL
2	C	686	LYS
2	C	690	MET
2	C	717	LYS
2	C	720	THR
2	C	725	LEU
2	C	727	SER
2	C	730	LEU
2	C	732	LYS
2	C	769	ILE
2	C	770	GLN
2	C	794	LEU
2	C	797	GLU
2	C	805	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	159	ASN
1	a	207	HIS
2	A	51	GLN
2	A	61	GLN
2	A	72	GLN
2	A	76	GLN
2	A	100	HIS
2	A	126	ASN
2	A	137	GLN
2	A	223	GLN
2	A	228	ASN
2	A	310	GLN
2	A	338	GLN
2	A	341	GLN

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Mol	Chain	Res	Type
2	A	362	HIS
2	A	432	GLN
2	A	623	HIS
2	A	659	ASN
2	A	770	GLN
2	A	785	ASN
1	b	159	ASN
1	b	207	HIS
2	B	51	GLN
2	B	61	GLN
2	B	72	GLN
2	B	76	GLN
2	B	100	HIS
2	B	126	ASN
2	B	137	GLN
2	B	202	ASN
2	B	203	ASN
2	B	223	GLN
2	B	227	ASN
2	B	228	ASN
2	B	310	GLN
2	B	361	HIS
2	B	362	HIS
2	B	623	HIS
2	B	659	ASN
2	B	770	GLN
2	B	785	ASN
1	c	159	ASN
1	c	194	HIS
1	c	207	HIS
2	C	28	ASN
2	C	51	GLN
2	C	61	GLN
2	C	72	GLN
2	C	76	GLN
2	C	100	HIS
2	C	126	ASN
2	C	137	GLN
2	C	223	GLN
2	C	228	ASN
2	C	338	GLN
2	C	341	GLN

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Mol	Chain	Res	Type
2	C	362	HIS
2	C	432	GLN
2	C	623	HIS
2	C	659	ASN
2	C	785	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	94/111 (84%)	0.88	10 (10%)	8	13	583, 624, 738, 792	0
1	b	94/111 (84%)	1.74	39 (41%)	0	4	543, 603, 730, 756	0
1	c	94/111 (84%)	1.25	24 (25%)	1	5	523, 590, 707, 731	0
2	A	708/758 (93%)	1.08	116 (16%)	2	8	508, 632, 810, 849	0
2	B	704/758 (92%)	1.03	127 (18%)	2	7	523, 661, 747, 823	0
2	C	711/758 (93%)	0.98	113 (15%)	3	8	426, 601, 842, 889	0
All	All	2405/2607 (92%)	1.06	429 (17%)	2	7	426, 636, 815, 889	0

All (429) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	411	PRO	7.8
2	A	465	GLY	7.5
2	A	231	PRO	7.4
2	A	466	GLN	7.1
2	C	720	THR	6.6
2	C	807	ALA	6.5
2	C	806	THR	6.3
2	C	741	ILE	6.3
2	B	664	GLU	6.2
2	A	230	VAL	6.0
2	C	481	SER	5.9
2	B	444	ASP	5.6
2	A	76	GLN	5.6
2	C	27	ASN	5.5
2	C	748	LYS	5.4
2	B	689	VAL	5.4
2	B	688	LYS	5.3
2	C	756	VAL	5.3
2	A	412	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	464	GLN	5.3
2	A	427	LYS	5.3
2	C	467	GLU	5.2
2	B	687	ASP	5.2
2	C	483	TRP	5.0
2	A	798	ASP	5.0
1	b	218	SER	5.0
2	C	719	LEU	5.0
2	A	27	ASN	5.0
2	C	26	HIS	4.9
2	B	584	SER	4.8
2	A	413	LEU	4.8
2	A	75	SER	4.8
2	B	262	LYS	4.8
2	B	547	THR	4.8
2	B	374	ALA	4.8
2	C	727	SER	4.6
2	C	743	LEU	4.6
2	C	752	ALA	4.6
2	A	130	SER	4.5
2	B	740	SER	4.5
2	C	28	ASN	4.5
1	b	146	ASN	4.4
2	C	716	LYS	4.4
2	A	431	VAL	4.3
2	B	403	ARG	4.3
2	C	723	VAL	4.3
2	A	176	GLU	4.3
2	C	145	ASN	4.3
2	A	28	ASN	4.3
2	C	787	HIS	4.3
2	B	761	GLY	4.2
2	A	129	VAL	4.2
2	A	77	THR	4.2
2	A	147	THR	4.1
2	B	693	LEU	4.1
2	A	78	ILE	4.0
1	b	149	GLY	4.0
2	C	405	ARG	4.0
1	b	217	ALA	4.0
2	B	513	GLN	4.0
2	A	797	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	441	SER	4.0
2	C	755	GLY	4.0
2	B	512	GLY	4.0
1	b	150	SER	4.0
1	b	164	TYR	4.0
2	B	690	MET	3.9
2	B	549	VAL	3.9
2	A	424	ARG	3.9
2	B	261	LEU	3.8
1	b	165	VAL	3.8
2	B	362	HIS	3.8
2	A	646	THR	3.8
2	C	77	THR	3.7
2	A	74	MET	3.7
2	B	398	ALA	3.7
2	B	697	PHE	3.7
2	C	791	HIS	3.7
1	b	166	ASP	3.7
2	A	755	GLY	3.7
2	C	724	SER	3.7
2	A	462	GLU	3.7
1	b	167	PHE	3.6
2	B	580	LYS	3.6
2	C	715	GLU	3.6
2	B	361	HIS	3.6
2	A	464	GLN	3.6
2	B	53	LEU	3.6
2	B	352	GLN	3.5
2	C	78	ILE	3.5
2	C	397	GLU	3.5
2	C	742	GLU	3.5
2	A	259	ASP	3.5
2	A	260	ARG	3.5
2	C	146	GLU	3.5
2	A	463	LYS	3.5
2	B	511	ILE	3.5
2	B	443	ARG	3.5
2	C	401	LYS	3.5
2	A	135	ARG	3.5
1	c	161	TYR	3.5
2	A	455	ASP	3.5
2	B	445	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	c	129	PHE	3.5
1	a	217	ALA	3.5
2	C	2	MET	3.5
2	A	426	GLU	3.5
2	A	432	GLN	3.4
1	c	127	LEU	3.4
2	C	398	ALA	3.4
2	C	792	ILE	3.4
2	B	465	GLY	3.4
2	C	402	VAL	3.4
2	C	803	VAL	3.4
2	A	232	GLU	3.4
2	B	369	ASP	3.4
2	B	710	VAL	3.4
1	b	129	PHE	3.4
2	B	60	ILE	3.4
2	A	801	PHE	3.4
1	c	188	GLU	3.4
2	A	446	GLU	3.3
1	b	188	GLU	3.3
2	A	133	LYS	3.3
2	A	419	LYS	3.3
2	A	229	GLU	3.3
2	C	412	ASN	3.3
2	C	805	THR	3.3
2	B	258	GLU	3.3
2	B	431	VAL	3.3
1	c	142	LEU	3.2
2	B	68	ILE	3.2
2	C	231	PRO	3.2
2	C	793	VAL	3.2
2	A	61	GLN	3.2
2	A	772	HIS	3.2
2	A	379	ASP	3.2
2	A	233	ILE	3.2
2	A	481	SER	3.2
2	B	368	ASP	3.2
2	B	712	HIS	3.2
2	A	430	ALA	3.2
2	C	790	GLN	3.2
2	A	182	VAL	3.2
2	A	756	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	A	79	HIS	3.1
2	C	480	VAL	3.1
2	B	402	VAL	3.1
2	B	391	ALA	3.1
1	a	218	SER	3.1
1	a	216	PHE	3.1
1	b	130	VAL	3.0
1	b	203	ILE	3.0
2	C	794	LEU	3.0
1	c	126	LYS	3.0
2	C	757	ASP	3.0
1	b	154	LEU	3.0
2	B	516	ALA	3.0
2	B	567	GLU	3.0
2	B	741	ILE	3.0
2	B	121	ALA	3.0
2	A	362	HIS	3.0
2	B	434	GLN	3.0
2	A	146	GLU	3.0
2	B	762	ALA	2.9
2	A	178	SER	2.9
2	B	627	PHE	2.9
2	B	582	SER	2.9
2	A	460	TRP	2.9
1	b	163	LEU	2.9
2	A	131	LEU	2.9
2	B	546	PRO	2.9
2	C	745	ASP	2.9
2	C	688	LYS	2.9
2	B	603	THR	2.9
2	C	408	THR	2.9
2	C	718	HIS	2.9
2	A	156	SER	2.9
2	B	692	GLU	2.9
2	A	127	LEU	2.9
2	B	755	GLY	2.9
2	C	55	LEU	2.9
2	A	237	LYS	2.8
1	b	179	LEU	2.8
2	B	474	ASP	2.8
2	C	64	VAL	2.8
2	C	411	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	434	GLN	2.8
2	B	686	LYS	2.8
2	A	549	VAL	2.8
2	A	387	LEU	2.8
1	c	164	TYR	2.8
2	B	579	GLU	2.8
2	B	467	GLU	2.8
2	A	789	GLY	2.8
1	c	143	SER	2.8
2	B	696	ALA	2.8
1	b	153	THR	2.8
2	A	447	GLN	2.8
2	C	749	ALA	2.8
2	C	740	SER	2.8
1	b	178	GLN	2.8
2	B	578	MET	2.7
1	b	126	LYS	2.7
2	A	580	LYS	2.7
2	A	417	GLU	2.7
2	B	437	GLU	2.7
2	B	715	GLU	2.7
2	A	423	VAL	2.7
1	b	128	GLN	2.7
2	A	762	ALA	2.7
2	A	470	GLU	2.7
2	A	420	LEU	2.7
2	C	789	GLY	2.7
1	b	159	ASN	2.7
2	A	132	ASN	2.7
2	B	375	VAL	2.7
1	b	186	ALA	2.7
1	a	186	ALA	2.7
1	c	133	PHE	2.7
2	B	432	GLN	2.7
2	B	718	HIS	2.7
2	A	436	PHE	2.7
2	B	232	GLU	2.7
1	a	179	LEU	2.6
1	b	148	ASN	2.6
2	C	406	SER	2.6
2	C	785	ASN	2.6
2	A	143	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	663	SER	2.6
2	C	753	GLU	2.6
2	C	584	SER	2.6
2	C	68	ILE	2.6
2	C	710	VAL	2.6
2	A	134	ALA	2.6
2	C	379	ASP	2.6
2	B	548	GLY	2.6
2	A	452	GLN	2.6
2	A	584	SER	2.6
2	B	35	LEU	2.6
2	B	371	ILE	2.6
2	C	144	SER	2.6
1	b	127	LEU	2.6
2	B	406	SER	2.6
2	B	577	TYR	2.6
2	A	765	LEU	2.6
2	B	625	ASP	2.6
2	B	483	TRP	2.5
2	A	712	HIS	2.5
2	C	482	SER	2.5
2	A	456	THR	2.5
2	C	236	ASP	2.5
2	A	450	ARG	2.5
2	C	25	GLY	2.5
2	A	180	ASP	2.5
2	A	217	ILE	2.5
2	A	803	VAL	2.5
2	A	715	GLU	2.5
2	B	407	PHE	2.5
2	B	743	LEU	2.5
2	A	116	GLY	2.5
2	B	280	ALA	2.5
2	B	661	GLY	2.5
2	C	184	GLY	2.5
1	b	147	VAL	2.5
2	B	263	LYS	2.5
2	B	723	VAL	2.5
2	C	784	GLY	2.5
2	B	55	LEU	2.5
2	A	428	ASP	2.5
2	B	67	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	363	ARG	2.5
2	B	520	VAL	2.5
2	A	435	GLU	2.5
1	b	151	LYS	2.5
1	c	156	SER	2.5
2	A	60	ILE	2.5
2	B	708	ILE	2.5
2	A	388	PRO	2.5
1	c	140	ILE	2.5
2	C	419	LYS	2.5
2	C	760	TYR	2.5
2	A	128	GLY	2.5
2	B	395	ILE	2.4
2	A	454	GLU	2.4
2	B	400	SER	2.4
2	A	477	ALA	2.4
2	A	181	PRO	2.4
2	A	459	SER	2.4
1	b	143	SER	2.4
2	B	63	GLU	2.4
2	B	698	ARG	2.4
1	b	196	LEU	2.4
1	c	155	TYR	2.4
2	C	340	ASP	2.4
1	b	144	LYS	2.4
2	C	804	LYS	2.4
2	A	64	VAL	2.4
1	a	144	LYS	2.4
1	c	154	LEU	2.4
2	B	484	THR	2.4
2	C	708	ILE	2.4
1	b	136	PHE	2.4
1	c	167	PHE	2.4
2	C	427	LYS	2.4
2	B	339	VAL	2.4
2	C	156	SER	2.4
2	C	413	LEU	2.4
2	A	194	GLU	2.4
2	C	56	GLY	2.4
2	C	34	ILE	2.4
2	B	145	ASN	2.4
2	C	400	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	21	ALA	2.4
1	a	203	ILE	2.3
2	B	72	GLN	2.3
1	b	193	ILE	2.3
1	c	141	SER	2.3
2	B	476	ILE	2.3
2	B	622	ALA	2.3
2	B	479	VAL	2.3
2	C	399	GLY	2.3
2	B	475	ASP	2.3
1	b	131	LEU	2.3
2	C	416	LEU	2.3
2	C	689	VAL	2.3
2	C	747	ALA	2.3
2	B	404	LEU	2.3
2	B	711	PHE	2.3
2	C	129	VAL	2.3
2	B	101	SER	2.3
2	A	73	GLU	2.3
1	b	142	LEU	2.3
1	c	130	VAL	2.3
2	B	231	PRO	2.3
2	B	624	PRO	2.3
1	a	187	THR	2.3
2	C	180	ASP	2.3
1	c	165	VAL	2.3
2	A	483	TRP	2.3
2	C	786	ILE	2.3
2	B	514	ASP	2.3
2	B	581	HIS	2.3
2	C	744	THR	2.3
1	b	168	CYS	2.3
2	A	123	VAL	2.3
2	B	372	GLU	2.3
2	A	449	LEU	2.2
2	C	572	ILE	2.2
2	A	546	PRO	2.2
2	B	463	LYS	2.2
2	B	623	HIS	2.2
2	B	660	VAL	2.2
2	C	428	ASP	2.2
2	C	84	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	c	139	VAL	2.2
2	C	14	LEU	2.2
1	b	125	GLN	2.2
2	C	4	GLY	2.2
2	B	32	GLU	2.2
2	C	58	GLU	2.2
1	c	125	GLN	2.2
2	A	363	ARG	2.2
2	B	100	HIS	2.2
2	C	404	LEU	2.2
1	c	128	GLN	2.2
2	C	479	VAL	2.2
1	b	140	ILE	2.2
2	A	433	SER	2.2
1	a	143	SER	2.2
2	B	466	GLN	2.2
1	c	136	PHE	2.2
2	C	3	PHE	2.2
2	A	494	THR	2.2
1	c	131	LEU	2.1
2	A	126	ASN	2.1
2	C	134	ALA	2.1
2	C	39	VAL	2.1
2	C	431	VAL	2.1
2	B	340	ASP	2.1
2	C	580	LYS	2.1
1	b	182	LEU	2.1
2	A	263	LYS	2.1
2	A	280	ALA	2.1
2	A	405	ARG	2.1
1	a	146	ASN	2.1
2	A	719	LEU	2.1
2	A	408	THR	2.1
2	B	494	THR	2.1
2	B	218	ALA	2.1
2	B	96	ARG	2.1
2	A	773	VAL	2.1
2	B	64	VAL	2.1
2	C	80	TYR	2.1
1	c	163	LEU	2.1
2	B	521	ALA	2.1
2	C	712	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	789	GLY	2.1
2	B	397	GLU	2.1
2	A	777	LEU	2.1
2	B	399	GLY	2.1
1	b	204	ILE	2.1
2	B	379	ASP	2.1
2	B	717	LYS	2.1
2	C	88	ILE	2.1
2	B	260	ARG	2.1
2	C	394	LEU	2.1
2	A	422	GLU	2.1
2	B	694	LYS	2.1
1	b	187	THR	2.1
2	B	739	LEU	2.1
2	A	117	GLU	2.0
2	B	702	ILE	2.0
1	c	199	TYR	2.0
2	A	416	LEU	2.0
2	C	75	SER	2.0
2	C	157	ASN	2.0
2	C	387	LEU	2.0
2	C	391	ALA	2.0
2	C	759	GLU	2.0
2	C	76	GLN	2.0
2	C	717	LYS	2.0
2	B	36	LEU	2.0
2	A	184	GLY	2.0
2	A	461	LYS	2.0
2	A	234	LEU	2.0
2	B	493	GLN	2.0
2	B	619	ILE	2.0
2	C	602	LEU	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.