Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 04:22 PM JST

PDB ID	:	7DRS
Title	:	Structure of SspE_40224
Authors	:	Haiyan, G.; Jinchuan, Z.; Chen, S.; Wang, L.; Wu, G.
Deposited on	:	2020-12-29
Resolution	:	3.42 Å(reported)

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

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

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

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

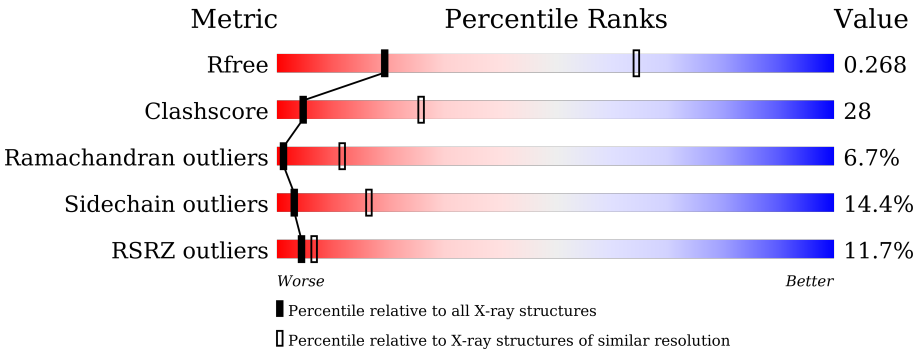
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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

Mol	Chain	Length	Quality of chain
1	A	771	7% 46% 43% 10% ·
1	B	771	23% 48% 39% 11% ·
1	C	771	7% 45% 41% 12% ·
1	D	771	9% 45% 42% 11% ·

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 24548 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 SspE protein.

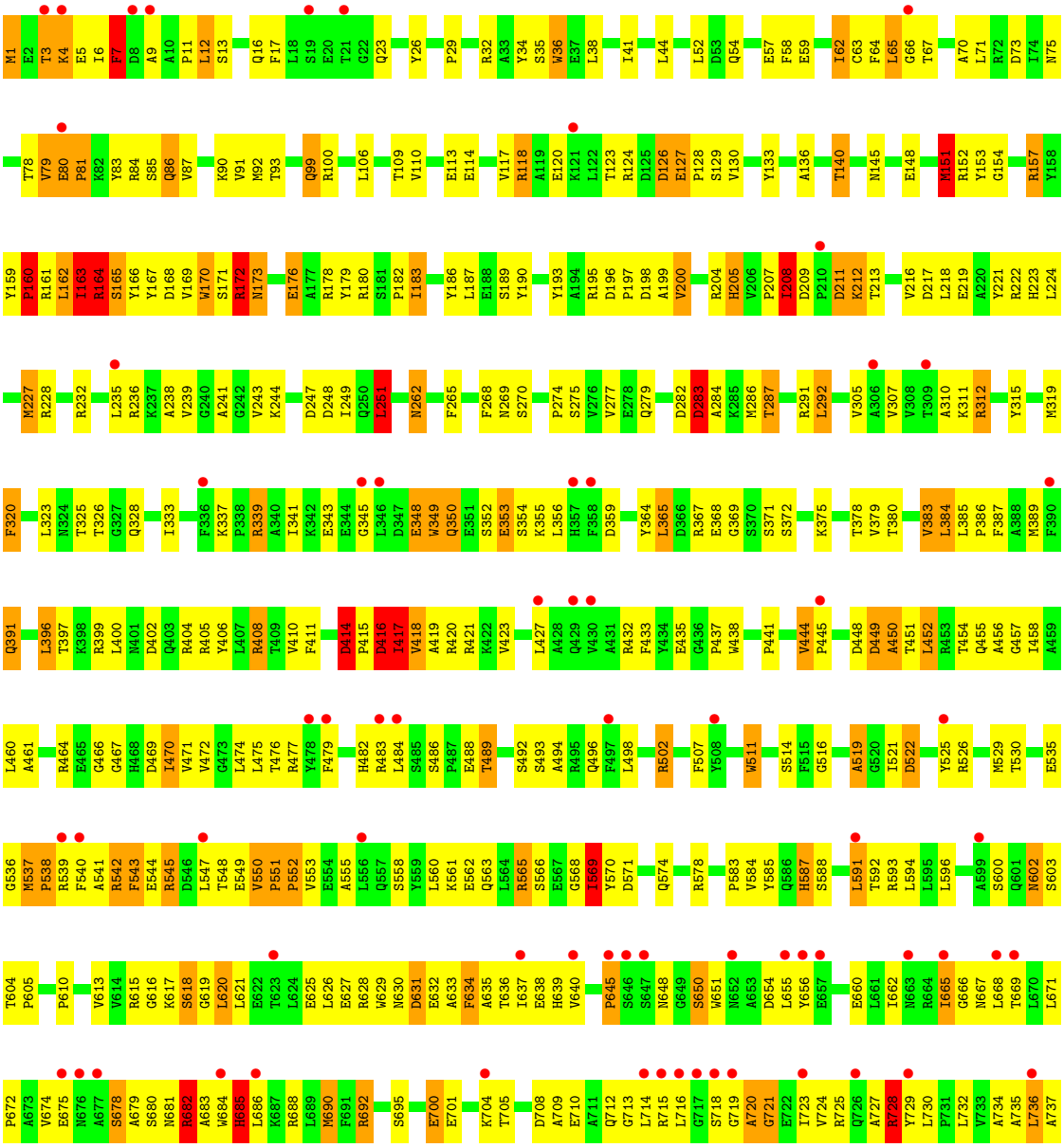
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	771	Total	C	N	O	S	0	0	0
			6137	3872	1079	1166	20			
1	A	771	Total	C	N	O	S	0	0	0
			6137	3872	1079	1166	20			
1	B	771	Total	C	N	O	S	0	0	0
			6137	3872	1079	1166	20			
1	C	771	Total	C	N	O	S	0	0	0
			6137	3872	1079	1166	20			

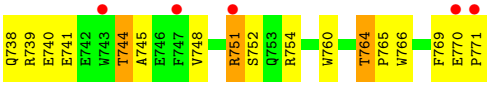
3 Residue-property plots (i)

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

- Molecule 1: SspE protein

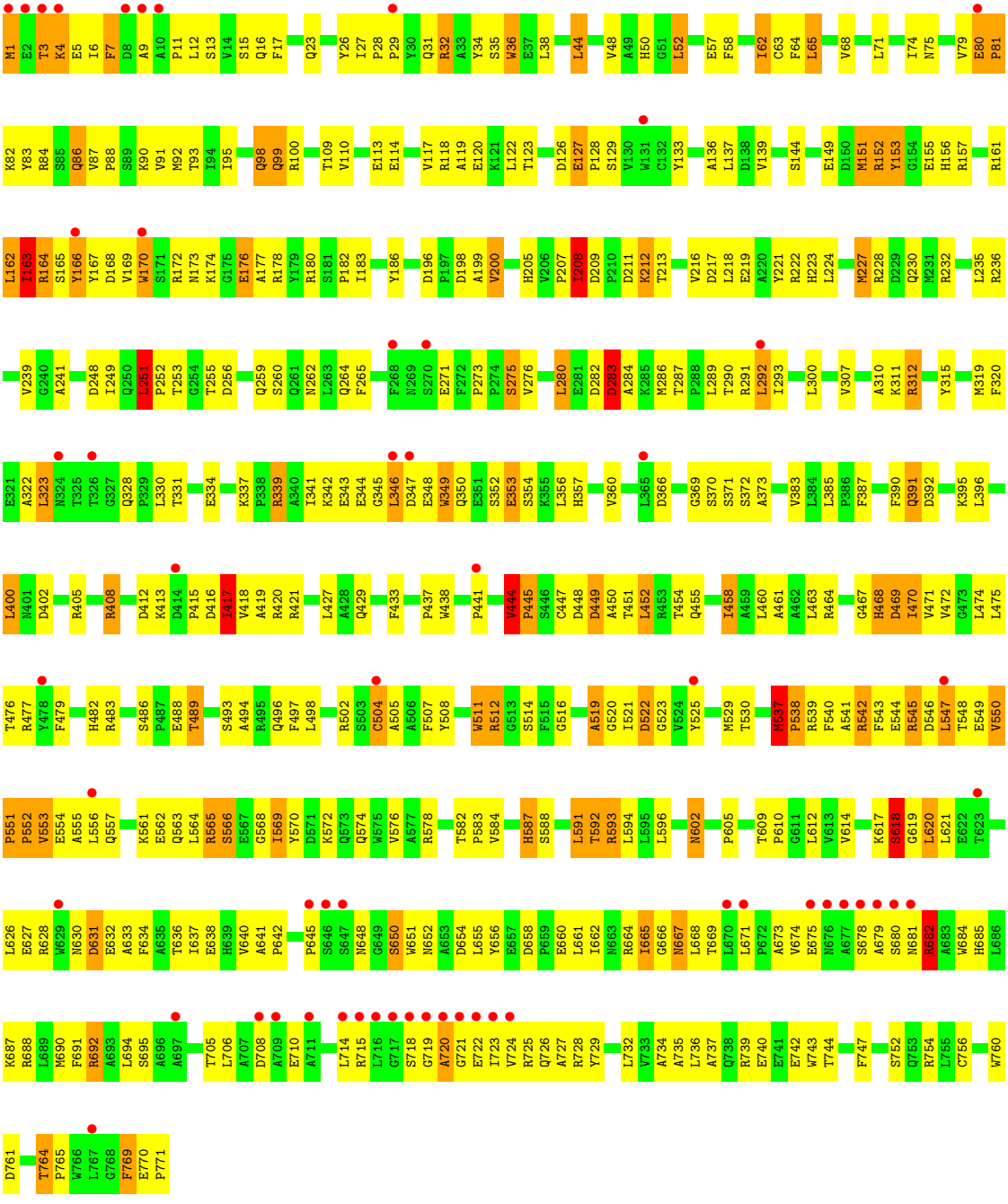
Chain D:





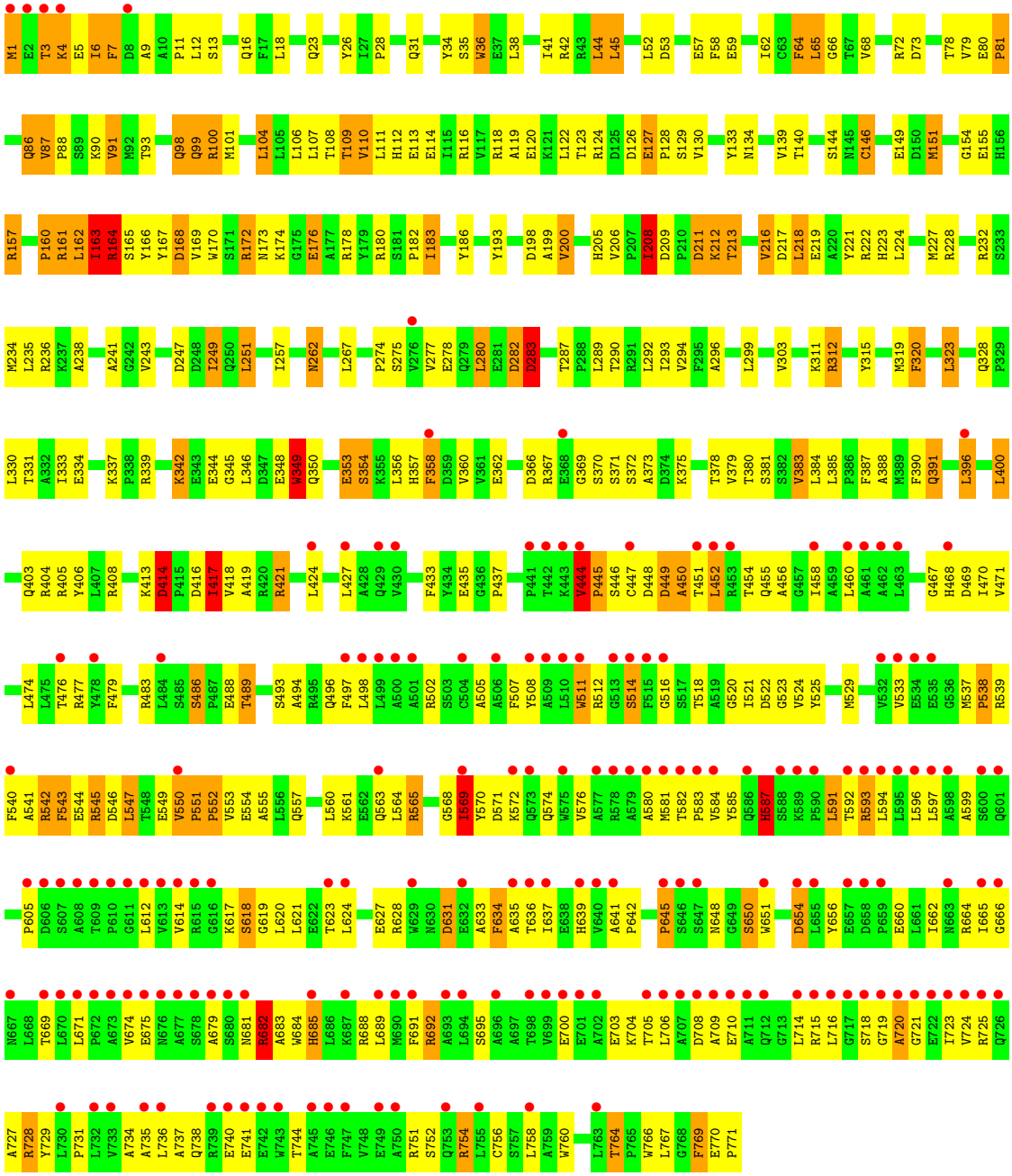
• Molecule 1: SspE protein

Chain A:



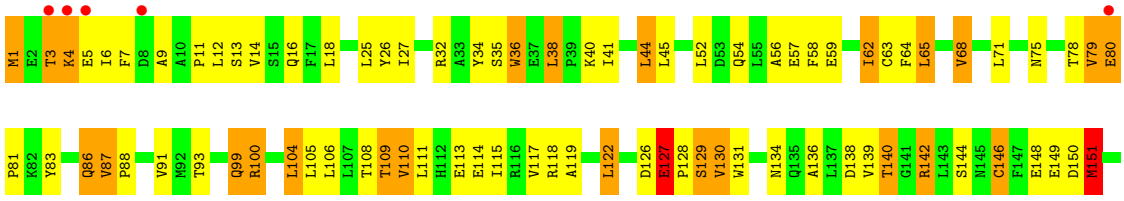
• Molecule 1: SspE protein

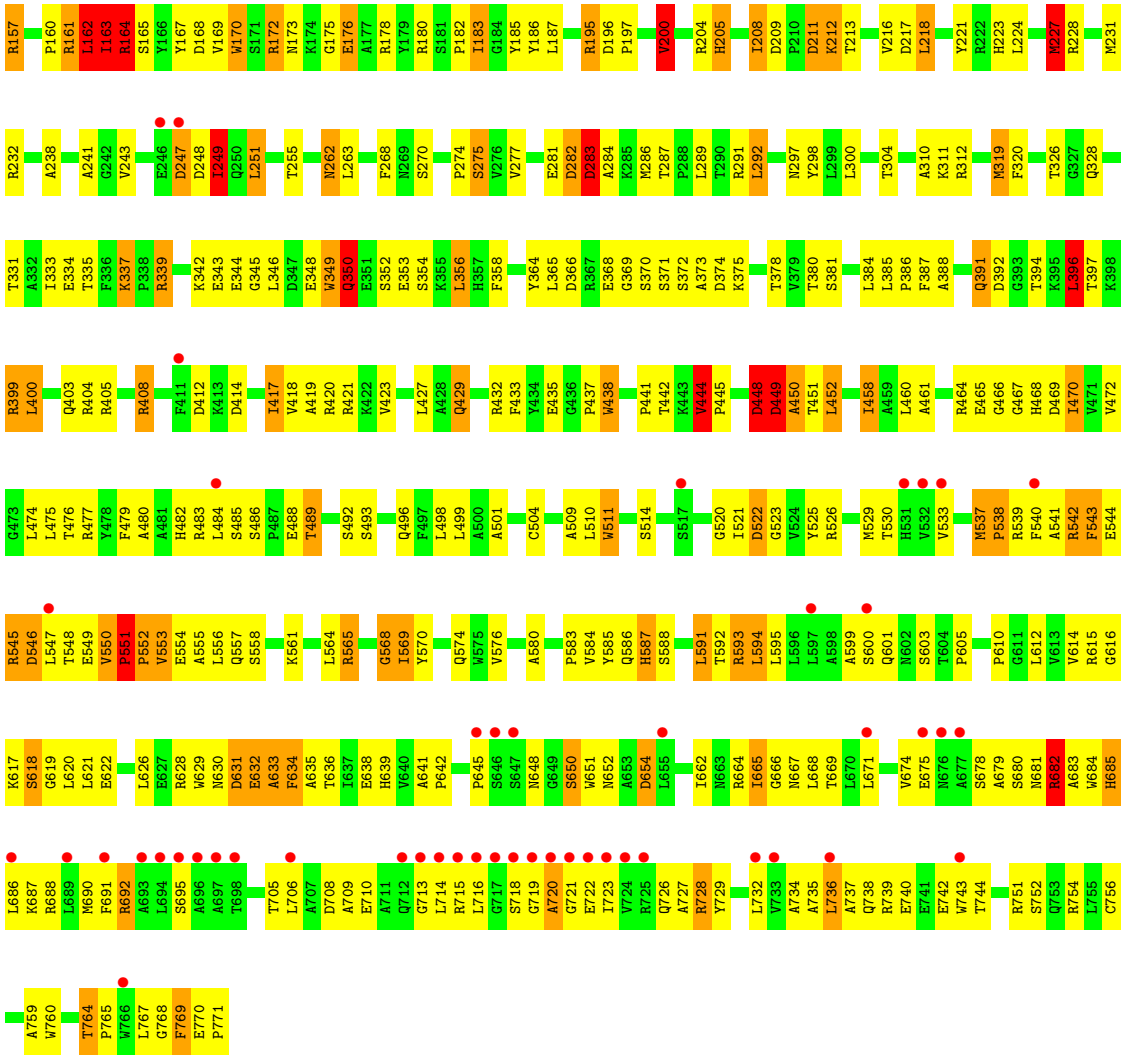
Chain B:



• Molecule 1: SspE protein

Chain C:




R157 P160 R161 L162 I163 R164 S165 Y166 Y167 D168 V169 W170 S171 R172 N173 K174 G175 E176 A177 R178 Y179 R180 S181 P182 I183 G184 Y185 Y186 L187 R195 D196 P197 V200 R204 H205 I208 D209 P210 D211 K212 T213 V216 D217 L218 Y221 R222 H223 L224 M227 R228 M231
R232 A238 A241 G242 V243 E246 D247 D248 I249 Q250 L251 T255 N262 L263 F268 N269 S270 P274 S275 V276 V277 E281 D282 D283 A284 K285 M286 T287 P288 L289 T290 R291 L292 N297 Y298 L299 L300 T304 A310 K311 R312 M319 F320 T326 G327 Q328
T331 A332 I333 E334 T335 F336 K337 P338 R339 K342 E343 E344 G345 L346 D347 E348 W349 Q350 E351 S352 E353 S354 K355 L356 H357 F358 Y364 L365 D366 R367 E368 G369 S370 S371 S372 A373 D374 K375 T378 V379 T380 S381 L384 L385 P386 F387 A388 Q391 D392 G393 T394 K395 L396 T397 K398
R399 L400 Q403 R404 R405 R408 F411 D412 K413 D414 I417 V418 A419 R420 R421 K422 V423 L427 A428 Q429 R432 F433 Y434 E435 G436 P437 W438 P441 T442 K443 V444 P445 D448 D449 A450 T451 L452 I458 A459 L460 A461 R464 E465 G466 G467 H468 D469 I470 V471 V472
G473 L474 L475 T476 R477 Y478 F479 A480 A481 H482 R483 L484 S485 S486 P487 E488 T489 S492 S493 Q496 F497 L498 L499 A500 A501 C504 A509 L510 W511 S514 S517 G520 I521 D522 G523 V524 Y525 R526 M529 T530 H531 V532 V533 M537 P538 R539 F540 A541 R542 F543 E544
R545 D546 L547 T548 E549 V550 P551 P552 V553 E554 A555 L556 Q557 S558 K561 L564 R565 G568 I569 Y570 Q574 W575 V576 A580 P583 V584 Y585 Q586 H587 S588 L591 T592 R593 L594 L595 L596 L597 A598 A599 S600 Q601 N602 S603 T604 P605 P610 G611 L612 V613 V614 R615 G616
K617 S618 G619 L620 L621 E622 L626 E627 R628 W629 N630 D631 E632 A633 F634 A635 T636 I637 E638 H639 V640 A641 P642 P645 S646 S647 N648 G649 S650 W651 N652 A653 D654 L655 I662 N663 R664 I665 G666 N667 L668 T669 L670 L671 V674 E675 N676 A677 S678 A679 S680 N681 R682 A683 W684 H685
L686 K687 R688 L689 M690 F691 R692 A693 L694 S695 A696 A697 T698 T705 L706 A707 D708 A709 E710 A711 Q712 G713 L714 R715 L716 G717 S718 G719 A720 G721 E722 I723 V724 R725 Q726 A727 R728 Y729 L732 V733 A734 A735 L736 A737 Q738 R739 E740 E741 E742 W743 T744 R751 S752 Q753 R754 L755 C756
A759 W760 T764 P765 W766 L767 G768 F769 E770 P771

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.08Å 138.15Å 293.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.14 – 3.42 51.95 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.14-3.42) 99.7 (51.95-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.212 , 0.264 0.221 , 0.268	Depositor DCC
R_{free} test set	3031 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	121.6	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 100.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24548	wwPDB-VP
Average B, all atoms (Å^2)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.63	2/6272 (0.0%)	0.85	8/8515 (0.1%)
1	B	0.60	3/6272 (0.0%)	0.83	11/8515 (0.1%)
1	C	0.79	9/6272 (0.1%)	0.98	24/8515 (0.3%)
1	D	0.70	5/6272 (0.1%)	0.91	13/8515 (0.2%)
All	All	0.69	19/25088 (0.1%)	0.90	56/34060 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	5
1	D	0	3
All	All	0	11

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	80	GLU	CB-CG	7.56	1.66	1.52
1	C	146	CYS	CB-SG	-6.49	1.71	1.82
1	C	185	TYR	CG-CD1	-6.38	1.30	1.39
1	C	63	CYS	CB-SG	-6.34	1.71	1.82
1	B	349	TRP	CB-CG	6.06	1.61	1.50
1	C	161	ARG	CB-CG	-5.96	1.36	1.52
1	C	68	VAL	CB-CG1	-5.94	1.40	1.52
1	D	80	GLU	CG-CD	5.86	1.60	1.51
1	C	80	GLU	CB-CG	5.79	1.63	1.52
1	A	504	CYS	CB-SG	-5.77	1.72	1.81
1	C	151	MET	CG-SD	-5.66	1.66	1.81
1	B	146	CYS	CB-SG	-5.54	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	700	GLU	CG-CD	-5.39	1.43	1.51
1	D	170	TRP	CG-CD2	-5.36	1.34	1.43
1	C	170	TRP	CG-CD2	-5.25	1.34	1.43
1	A	80	GLU	CB-CG	5.19	1.62	1.52
1	C	40	LYS	CD-CE	5.19	1.64	1.51
1	B	80	GLU	CB-CG	5.11	1.61	1.52
1	D	728	ARG	CG-CD	5.10	1.64	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	251	LEU	CA-CB-CG	10.36	139.12	115.30
1	B	346	LEU	CA-CB-CG	9.05	136.11	115.30
1	C	251	LEU	CA-CB-CG	8.93	135.85	115.30
1	D	251	LEU	CA-CB-CG	8.93	135.83	115.30
1	A	346	LEU	CA-CB-CG	8.91	135.79	115.30
1	C	345	GLY	N-CA-C	-8.23	92.53	113.10
1	C	291	ARG	NE-CZ-NH1	-8.01	116.29	120.30
1	C	142	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	B	345	GLY	N-CA-C	-7.43	94.52	113.10
1	C	249	ILE	CG1-CB-CG2	-7.43	95.05	111.40
1	C	346	LEU	CA-CB-CG	7.23	131.94	115.30
1	B	172	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	C	200	VAL	C-N-CA	7.04	139.30	121.70
1	C	227	MET	CG-SD-CE	-7.03	88.95	100.20
1	A	556	LEU	CA-CB-CG	6.56	130.40	115.30
1	C	111	LEU	CB-CG-CD2	-6.56	99.85	111.00
1	D	345	GLY	N-CA-C	-6.46	96.94	113.10
1	A	345	GLY	N-CA-C	-6.42	97.04	113.10
1	C	170	TRP	CA-CB-CG	6.42	125.90	113.70
1	C	162	LEU	CB-CG-CD1	-6.24	100.39	111.00
1	D	152	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	100	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	218	LEU	CA-CB-CG	6.12	129.37	115.30
1	C	195	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	D	145	ASN	CA-C-O	5.99	132.69	120.10
1	A	170	TRP	CA-CB-CG	5.90	124.92	113.70
1	D	172	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	D	178	ARG	CB-CG-CD	-5.75	96.64	111.60
1	C	356	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	417	ILE	N-CA-C	-5.66	95.72	111.00
1	B	100	ARG	CG-CD-NE	-5.65	99.93	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	178	ARG	CA-CB-CG	5.51	125.53	113.40
1	B	161	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	104	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	D	172	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	D	417	ILE	N-CA-C	-5.39	96.45	111.00
1	C	556	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	151	MET	CG-SD-CE	5.36	108.77	100.20
1	D	7	PHE	CB-CG-CD2	5.33	124.53	120.80
1	B	218	LEU	CA-CB-CG	5.25	127.39	115.30
1	B	178	ARG	CB-CG-CD	-5.23	98.00	111.60
1	D	690	MET	CA-CB-CG	5.19	122.13	113.30
1	B	178	ARG	CA-CB-CG	5.18	124.81	113.40
1	C	396	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	A	537	MET	CB-CG-SD	-5.16	96.92	112.40
1	D	118	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	C	178	ARG	CB-CG-CD	-5.14	98.24	111.60
1	C	151	MET	C-N-CA	-5.13	108.86	121.70
1	D	404	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	C	438	TRP	CA-CB-CG	-5.12	103.98	113.70
1	B	417	ILE	N-CA-C	-5.07	97.31	111.00
1	C	319	MET	CB-CG-SD	-5.06	97.21	112.40
1	A	251	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	122	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	C	263	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	A	152	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	PRO	Peptide
1	A	553	VAL	Peptide
1	B	160	PRO	Peptide
1	C	151	MET	Peptide
1	C	160	PRO	Peptide
1	C	551	PRO	Peptide
1	C	553	VAL	Peptide
1	C	79	VAL	Peptide
1	D	160	PRO	Peptide
1	D	173	ASN	Peptide
1	D	79	VAL	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	6137	0	6046	338	1
1	B	6137	0	6046	345	1
1	C	6137	0	6045	353	2
1	D	6137	0	6046	351	2
All	All	24548	0	24183	1365	3

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 28.

All (1365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:628:ARG:HA	1:C:631:ASP:HB2	1.44	0.99
1:A:418:VAL:H	1:A:421:ARG:HD2	1.25	0.98
1:B:126:ASP:HB3	1:B:129:SER:HB3	1.45	0.98
1:A:126:ASP:HB3	1:A:129:SER:HB3	1.44	0.96
1:D:126:ASP:HB3	1:D:129:SER:HB3	1.47	0.95
1:C:114:GLU:OE1	1:C:118:ARG:NH1	2.00	0.95
1:C:173:ASN:HB2	1:C:176:GLU:OE2	1.67	0.95
1:A:553:VAL:HB	1:A:554:GLU:HG3	1.51	0.93
1:D:692:ARG:HG3	1:D:737:ALA:HB1	1.50	0.92
1:A:584:VAL:HG12	1:A:592:THR:HG22	1.49	0.92
1:D:628:ARG:HA	1:D:631:ASP:HB2	1.49	0.92
1:D:1:MET:HA	1:D:4:LYS:HB2	1.51	0.92
1:A:496:GLN:HA	1:A:553:VAL:HG13	1.53	0.90
1:B:703:GLU:OE2	1:B:725:ARG:NE	2.05	0.89
1:B:477:ARG:HD3	1:B:542:ARG:H	1.37	0.89
1:A:688:ARG:NH1	1:A:740:GLU:OE2	2.05	0.89
1:D:474:LEU:O	1:D:477:ARG:HB3	1.75	0.87
1:B:628:ARG:HA	1:B:631:ASP:HB2	1.57	0.86
1:D:724:VAL:HG12	1:D:725:ARG:HG3	1.58	0.85
1:A:391:GLN:O	1:A:391:GLN:NE2	2.08	0.85
1:C:126:ASP:HB3	1:C:129:SER:HB3	1.57	0.85
1:B:593:ARG:HH21	1:B:635:ALA:HB1	1.42	0.84
1:B:183:ILE:HD12	1:B:183:ILE:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:PHE:O	1:D:545:ARG:NH2	2.11	0.83
1:C:208:ILE:HG13	1:C:209:ASP:H	1.43	0.83
1:A:208:ILE:HD13	1:A:209:ASP:H	1.43	0.83
1:A:593:ARG:HG3	1:A:637:ILE:HD11	1.61	0.83
1:B:612:LEU:HB3	1:B:754:ARG:HD3	1.61	0.83
1:C:496:GLN:HA	1:C:553:VAL:HG13	1.62	0.82
1:A:641:ALA:H	1:A:667:ASN:HD21	1.25	0.82
1:D:385:LEU:HD22	1:D:396:LEU:HB3	1.62	0.81
1:A:433:PHE:CG	1:A:476:THR:HG22	2.14	0.81
1:D:552:PRO:HG2	1:D:555:ALA:H	1.46	0.81
1:D:182:PRO:HD3	1:D:221:TYR:HE1	1.45	0.81
1:A:692:ARG:HG3	1:A:737:ALA:HB1	1.63	0.81
1:A:114:GLU:OE1	1:A:118:ARG:NH1	2.14	0.80
1:C:183:ILE:H	1:C:183:ILE:HD12	1.46	0.80
1:A:612:LEU:HB3	1:A:754:ARG:HD3	1.61	0.80
1:C:692:ARG:HG3	1:C:737:ALA:HB1	1.64	0.80
1:B:208:ILE:HD13	1:B:209:ASP:H	1.47	0.80
1:D:173:ASN:HB2	1:D:176:GLU:OE2	1.83	0.79
1:A:182:PRO:HB2	1:A:224:LEU:HD13	1.63	0.79
1:A:391:GLN:OE1	1:A:542:ARG:NH1	2.14	0.79
1:B:682:ARG:HH21	1:B:716:LEU:HD13	1.46	0.79
1:C:1:MET:HA	1:C:4:LYS:HB2	1.62	0.79
1:B:36:TRP:CD1	1:B:99:GLN:HG2	2.18	0.78
1:C:474:LEU:O	1:C:477:ARG:HB3	1.83	0.78
1:D:114:GLU:OE1	1:D:118:ARG:NH1	2.16	0.78
1:B:565:ARG:HG2	1:B:570:TYR:CE2	2.18	0.78
1:C:36:TRP:CD1	1:C:99:GLN:HG2	2.19	0.78
1:B:571:ASP:OD2	1:B:574:GLN:NE2	2.16	0.77
1:B:38:LEU:N	1:B:227:MET:HE1	1.98	0.77
1:D:496:GLN:HA	1:D:553:VAL:HG13	1.66	0.77
1:B:710:GLU:HA	1:B:714:LEU:H	1.50	0.77
1:C:612:LEU:HB3	1:C:754:ARG:HD3	1.66	0.77
1:D:124:ARG:HD3	1:D:133:TYR:CD2	2.19	0.77
1:A:1:MET:HA	1:A:4:LYS:HB2	1.66	0.77
1:A:565:ARG:HG2	1:A:570:TYR:CE2	2.20	0.77
1:A:715:ARG:HB3	1:A:719:GLY:HA2	1.67	0.77
1:C:391:GLN:O	1:C:391:GLN:NE2	2.17	0.77
1:D:720:ALA:HB1	1:D:723:ILE:HD12	1.64	0.77
1:D:469:ASP:O	1:D:472:VAL:HG23	1.85	0.77
1:D:680:SER:O	1:D:682:ARG:NH2	2.17	0.76
1:A:196:ASP:HB3	1:A:199:ALA:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ASP:OD1	1:A:420:ARG:NH2	2.19	0.76
1:C:433:PHE:CG	1:C:476:THR:HG22	2.20	0.76
1:B:525:TYR:O	1:B:529:MET:HG2	1.86	0.76
1:C:484:LEU:HB3	1:C:548:THR:HG22	1.67	0.76
1:A:173:ASN:HB2	1:A:176:GLU:OE2	1.85	0.75
1:A:479:PHE:CE1	1:A:483:ARG:HD2	2.20	0.75
1:D:12:LEU:HB3	1:D:16:GLN:HG3	1.67	0.75
1:C:388:ALA:HB2	1:C:396:LEU:HD23	1.68	0.75
1:C:715:ARG:HB3	1:C:719:GLY:HA2	1.69	0.75
1:D:367:ARG:NH1	1:D:435:GLU:OE2	2.20	0.74
1:A:477:ARG:HD3	1:A:542:ARG:H	1.51	0.74
1:B:110:VAL:HA	1:B:228:ARG:HH11	1.52	0.74
1:D:168:ASP:OD1	1:D:180:ARG:N	2.19	0.74
1:A:552:PRO:HG2	1:A:555:ALA:H	1.52	0.74
1:A:617:LYS:O	1:A:619:GLY:N	2.21	0.74
1:A:525:TYR:O	1:A:529:MET:HG2	1.87	0.74
1:C:5:GLU:O	1:C:7:PHE:N	2.19	0.74
1:C:161:ARG:O	1:C:162:LEU:HB2	1.87	0.74
1:A:128:PRO:HG3	1:A:275:SER:HB2	1.70	0.73
1:C:614:VAL:HG12	1:C:754:ARG:HH11	1.52	0.73
1:B:34:TYR:HD2	1:B:224:LEU:HD12	1.51	0.73
1:C:4:LYS:O	1:C:5:GLU:HG3	1.89	0.73
1:C:35:SER:O	1:C:223:HIS:NE2	2.22	0.73
1:D:183:ILE:HD12	1:D:183:ILE:H	1.53	0.73
1:A:565:ARG:HH21	1:A:771:PRO:HB3	1.53	0.72
1:C:470:ILE:HD12	1:C:522:ASP:OD2	1.88	0.72
1:B:280:LEU:HD21	1:B:290:THR:HG21	1.70	0.72
1:D:525:TYR:O	1:D:529:MET:HG2	1.89	0.72
1:C:544:GLU:HB2	1:C:545:ARG:NH2	2.05	0.72
1:C:684:TRP:HD1	1:C:742:GLU:OE2	1.72	0.72
1:D:584:VAL:HG12	1:D:592:THR:HG22	1.72	0.72
1:D:454:THR:HG21	1:D:627:GLU:OE2	1.89	0.72
1:A:339:ARG:HG2	1:A:408:ARG:NH2	2.04	0.72
1:D:208:ILE:HG21	1:D:221:TYR:CD2	2.25	0.71
1:A:36:TRP:CD1	1:A:99:GLN:HG2	2.25	0.71
1:A:208:ILE:HG21	1:A:221:TYR:CD2	2.26	0.71
1:A:666:GLY:H	1:A:752:SER:HB3	1.55	0.71
1:B:9:ALA:HB3	1:C:9:ALA:HB3	1.71	0.71
1:D:617:LYS:O	1:D:619:GLY:N	2.23	0.71
1:A:52:LEU:HD13	1:A:252:PRO:HD2	1.71	0.71
1:A:628:ARG:HA	1:A:631:ASP:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ARG:HB3	1:B:719:GLY:HA2	1.72	0.71
1:A:470:ILE:HG21	1:A:522:ASP:HA	1.72	0.71
1:B:3:THR:O	1:B:5:GLU:N	2.23	0.71
1:C:638:GLU:OE2	1:C:687:LYS:NZ	2.18	0.71
1:C:705:THR:HA	1:C:708:ASP:HB2	1.73	0.71
1:D:391:GLN:O	1:D:391:GLN:NE2	2.24	0.71
1:B:1:MET:HA	1:B:4:LYS:HB2	1.73	0.71
1:D:312:ARG:HD3	1:D:315:TYR:CE2	2.26	0.71
1:D:470:ILE:HG21	1:D:522:ASP:HA	1.73	0.71
1:C:441:PRO:HG2	1:C:461:ALA:HB2	1.73	0.71
1:D:283:ASP:HA	1:D:287:THR:HB	1.72	0.71
1:B:614:VAL:HG12	1:B:754:ARG:HH11	1.55	0.70
1:A:127:GLU:OE2	1:A:128:PRO:HD3	1.90	0.70
1:A:280:LEU:HD21	1:A:290:THR:HG21	1.73	0.70
1:B:505:ALA:O	1:B:508:TYR:HB3	1.91	0.70
1:C:651:TRP:CZ3	1:C:684:TRP:HB2	2.26	0.70
1:C:688:ARG:NH1	1:C:740:GLU:OE2	2.24	0.70
1:B:120:GLU:HG2	1:B:200:VAL:HG11	1.73	0.70
1:C:617:LYS:O	1:C:619:GLY:N	2.24	0.70
1:B:86:GLN:NE2	1:B:172:ARG:HG2	2.07	0.70
1:B:564:LEU:HB3	1:B:570:TYR:HB3	1.74	0.70
1:C:622:GLU:O	1:C:628:ARG:NH1	2.24	0.70
1:D:477:ARG:HD3	1:D:542:ARG:H	1.57	0.70
1:D:617:LYS:HB3	1:D:620:LEU:HB2	1.73	0.70
1:B:396:LEU:HD11	1:B:403:GLN:HG2	1.74	0.69
1:D:9:ALA:HB3	1:A:9:ALA:HB3	1.75	0.69
1:A:605:PRO:HB3	1:A:735:ALA:HB2	1.74	0.69
1:C:538:PRO:HB2	1:C:550:VAL:HG13	1.73	0.69
1:A:50:HIS:NE2	1:A:402:ASP:OD1	2.25	0.69
1:D:529:MET:SD	1:D:541:ALA:HB2	2.33	0.69
1:A:13:SER:H	1:A:16:GLN:HE21	1.38	0.69
1:C:385:LEU:HD22	1:C:396:LEU:HB3	1.75	0.69
1:A:27:ILE:HB	1:A:164:ARG:HA	1.75	0.69
1:C:3:THR:O	1:C:5:GLU:N	2.26	0.69
1:A:474:LEU:HG	1:A:529:MET:HE2	1.74	0.69
1:C:3:THR:O	1:C:3:THR:OG1	2.10	0.68
1:D:438:TRP:CE3	1:D:464:ARG:HG3	2.29	0.68
1:D:634:PHE:HD1	1:D:634:PHE:H	1.38	0.68
1:B:3:THR:O	1:B:3:THR:OG1	2.11	0.68
1:D:760:TRP:O	1:D:764:THR:OG1	2.11	0.68
1:D:715:ARG:HB3	1:D:719:GLY:HA2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ARG:NH1	1:B:435:GLU:OE2	2.26	0.68
1:C:418:VAL:H	1:C:421:ARG:HD2	1.59	0.68
1:C:545:ARG:NH2	1:C:545:ARG:H	1.92	0.68
1:B:380:THR:O	1:B:384:LEU:HB2	1.94	0.68
1:C:545:ARG:H	1:C:545:ARG:HH21	1.42	0.68
1:D:113:GLU:OE2	1:D:232:ARG:NH2	2.27	0.67
1:A:11:PRO:O	1:A:12:LEU:HD23	1.94	0.67
1:A:385:LEU:HD22	1:A:396:LEU:HB3	1.76	0.67
1:B:4:LYS:O	1:B:5:GLU:HG3	1.95	0.67
1:B:110:VAL:HG12	1:B:228:ARG:HE	1.59	0.67
1:B:651:TRP:CZ3	1:B:684:TRP:HB2	2.29	0.67
1:B:584:VAL:HG13	1:B:591:LEU:HD13	1.77	0.67
1:A:612:LEU:HD13	1:A:754:ARG:HD2	1.77	0.67
1:C:544:GLU:HB2	1:C:545:ARG:HH22	1.58	0.67
1:B:418:VAL:H	1:B:421:ARG:HD2	1.59	0.67
1:A:418:VAL:N	1:A:421:ARG:HD2	2.06	0.67
1:D:36:TRP:CD1	1:D:99:GLN:HG2	2.30	0.67
1:C:542:ARG:NH1	1:C:544:GLU:O	2.28	0.67
1:D:418:VAL:H	1:D:421:ARG:HD2	1.59	0.67
1:C:636:THR:HG23	1:C:675:GLU:HG2	1.77	0.67
1:D:551:PRO:HB2	1:D:552:PRO:HD3	1.76	0.66
1:B:710:GLU:HG2	1:B:715:ARG:HG3	1.77	0.66
1:C:553:VAL:HB	1:C:554:GLU:HG3	1.77	0.66
1:C:642:PRO:HD3	1:C:651:TRP:CZ2	2.29	0.66
1:D:364:TYR:CE1	1:D:368:GLU:HG3	2.31	0.66
1:A:3:THR:O	1:A:5:GLU:N	2.27	0.66
1:B:474:LEU:HG	1:B:529:MET:SD	2.35	0.66
1:B:58:PHE:CE2	1:B:405:ARG:HD3	2.29	0.66
1:B:561:LYS:HE3	1:B:769:PHE:HA	1.77	0.66
1:C:584:VAL:HG12	1:C:592:THR:HG22	1.78	0.66
1:A:724:VAL:HG12	1:A:725:ARG:HG3	1.78	0.66
1:B:486:SER:HB3	1:B:488:GLU:OE2	1.95	0.66
1:C:180:ARG:HH12	1:C:212:LYS:HE2	1.61	0.66
1:C:605:PRO:HB3	1:C:735:ALA:HB2	1.78	0.66
1:A:651:TRP:CZ3	1:A:684:TRP:HB2	2.32	0.65
1:C:182:PRO:HD3	1:C:221:TYR:HE1	1.61	0.65
1:C:344:GLU:OE1	1:C:421:ARG:NH2	2.28	0.65
1:D:565:ARG:HG2	1:D:570:TYR:CE2	2.30	0.65
1:B:283:ASP:OD2	1:B:283:ASP:N	2.29	0.65
1:A:127:GLU:HB3	1:A:128:PRO:HD2	1.77	0.65
1:C:400:LEU:HD12	1:C:404:ARG:HH21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ARG:HD3	1:B:542:ARG:N	2.10	0.65
1:B:689:LEU:HB3	1:B:709:ALA:HB2	1.77	0.65
1:D:127:GLU:OE2	1:D:128:PRO:HD3	1.97	0.65
1:A:705:THR:HA	1:A:708:ASP:HB2	1.78	0.65
1:B:34:TYR:CD2	1:B:224:LEU:HD12	2.31	0.65
1:B:538:PRO:HB2	1:B:550:VAL:HG13	1.78	0.65
1:B:605:PRO:HG3	1:B:734:ALA:HB3	1.78	0.65
1:C:343:GLU:OE2	1:C:420:ARG:CZ	2.45	0.65
1:D:489:THR:O	1:D:489:THR:OG1	2.15	0.65
1:C:113:GLU:O	1:C:117:VAL:HG12	1.97	0.65
1:C:543:PHE:O	1:C:545:ARG:NH2	2.28	0.65
1:C:128:PRO:HD3	1:C:275:SER:HB2	1.78	0.65
1:C:213:THR:O	1:C:213:THR:OG1	2.14	0.65
1:A:472:VAL:O	1:A:476:THR:HG23	1.97	0.64
1:A:542:ARG:HD3	1:A:547:LEU:H	1.61	0.64
1:B:692:ARG:NH2	1:B:740:GLU:OE1	2.30	0.64
1:C:183:ILE:H	1:C:183:ILE:CD1	2.10	0.64
1:A:544:GLU:HB2	1:A:545:ARG:NH2	2.13	0.64
1:B:87:VAL:HG22	1:B:88:PRO:HD2	1.78	0.64
1:B:666:GLY:H	1:B:752:SER:HB3	1.63	0.64
1:D:538:PRO:HB3	1:D:550:VAL:HG22	1.80	0.64
1:B:12:LEU:HB3	1:B:16:GLN:HG3	1.80	0.64
1:C:634:PHE:HD1	1:C:634:PHE:H	1.43	0.64
1:A:441:PRO:HG2	1:A:461:ALA:HB2	1.79	0.64
1:A:449:ASP:O	1:A:451:THR:N	2.30	0.64
1:B:206:VAL:O	1:B:208:ILE:N	2.28	0.64
1:B:650:SER:OG	1:B:683:ALA:HB1	1.98	0.64
1:C:477:ARG:HD3	1:C:542:ARG:H	1.63	0.64
1:D:458:ILE:HG13	1:D:629:TRP:HB2	1.79	0.64
1:A:529:MET:SD	1:A:541:ALA:HB2	2.38	0.64
1:B:127:GLU:HB3	1:B:128:PRO:HD2	1.80	0.64
1:B:238:ALA:HB2	1:B:249:ILE:HD13	1.79	0.64
1:D:4:LYS:O	1:D:5:GLU:HG3	1.98	0.63
1:D:199:ALA:O	1:D:200:VAL:HB	1.98	0.63
1:A:564:LEU:O	1:A:569:ILE:N	2.31	0.63
1:C:561:LYS:NZ	1:C:768:GLY:O	2.25	0.63
1:B:565:ARG:HH21	1:B:771:PRO:HB3	1.64	0.63
1:A:12:LEU:HB3	1:A:16:GLN:HG3	1.80	0.63
1:A:674:VAL:HG11	1:A:679:ALA:H	1.64	0.63
1:B:98:GLN:OE1	1:B:99:GLN:N	2.30	0.63
1:B:706:LEU:HD12	1:B:714:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ILE:HG21	1:D:221:TYR:HD2	1.62	0.63
1:D:449:ASP:O	1:D:451:THR:N	2.32	0.63
1:C:369:GLY:O	1:C:371:SER:N	2.31	0.63
1:C:680:SER:O	1:C:682:ARG:NH2	2.31	0.63
1:A:542:ARG:HD2	1:A:544:GLU:O	1.99	0.63
1:A:710:GLU:HG2	1:A:715:ARG:HG3	1.81	0.63
1:B:104:LEU:HD21	1:B:299:LEU:HD11	1.79	0.63
1:C:651:TRP:NE1	1:C:683:ALA:HA	2.14	0.63
1:D:441:PRO:HG2	1:D:461:ALA:HB2	1.81	0.63
1:D:665:ILE:HD13	1:D:665:ILE:H	1.63	0.63
1:B:127:GLU:HB3	1:B:128:PRO:CD	2.29	0.63
1:B:180:ARG:HH12	1:B:212:LYS:HE2	1.63	0.63
1:B:636:THR:HB	1:B:671:LEU:O	1.99	0.63
1:C:127:GLU:HB3	1:C:128:PRO:CD	2.29	0.63
1:C:485:SER:OG	1:C:489:THR:OG1	2.17	0.63
1:B:86:GLN:HE21	1:B:172:ARG:HG2	1.64	0.62
1:C:59:GLU:HG2	1:C:262:ASN:HB3	1.81	0.62
1:A:681:ASN:OD1	1:A:682:ARG:N	2.32	0.62
1:B:489:THR:O	1:B:489:THR:OG1	2.17	0.62
1:A:417:ILE:O	1:A:419:ALA:N	2.31	0.62
1:D:163:ILE:HD13	1:D:168:ASP:HB3	1.82	0.62
1:A:27:ILE:HD13	1:A:98:GLN:NE2	2.15	0.62
1:A:511:TRP:CH2	1:A:519:ALA:HB3	2.35	0.62
1:C:138:ASP:CG	1:C:142:ARG:HH12	2.03	0.62
1:A:153:TYR:CD1	1:B:134:ASN:HB3	2.35	0.62
1:B:576:VAL:HG13	1:B:756:CYS:HB2	1.81	0.62
1:B:312:ARG:HD3	1:B:315:TYR:CE2	2.35	0.62
1:B:369:GLY:O	1:B:371:SER:N	2.33	0.62
1:C:477:ARG:CZ	1:C:542:ARG:HB3	2.29	0.62
1:D:569:ILE:HG23	1:D:574:GLN:HB3	1.82	0.62
1:D:542:ARG:HD2	1:D:544:GLU:O	2.00	0.62
1:A:463:LEU:HD21	1:A:505:ALA:HA	1.82	0.62
1:D:492:SER:O	1:D:496:GLN:HG3	2.00	0.61
1:D:182:PRO:HD3	1:D:221:TYR:CE1	2.32	0.61
1:A:642:PRO:O	1:A:656:TYR:OH	2.18	0.61
1:A:760:TRP:O	1:A:764:THR:OG1	2.18	0.61
1:C:228:ARG:HA	1:C:231:MET:HE3	1.81	0.61
1:D:274:PRO:HA	1:D:277:VAL:HG22	1.80	0.61
1:D:325:THR:HB	1:A:100:ARG:HH22	1.65	0.61
1:D:681:ASN:OD1	1:D:682:ARG:N	2.33	0.61
1:B:44:LEU:HD21	1:B:65:LEU:HD21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:O	1:B:477:ARG:HB3	2.01	0.61
1:C:136:ALA:O	1:C:140:THR:HB	2.01	0.61
1:C:612:LEU:HD13	1:C:754:ARG:HD2	1.82	0.61
1:D:701:GLU:O	1:D:705:THR:OG1	2.19	0.61
1:B:518:THR:HG22	1:B:521:ILE:HD12	1.82	0.61
1:C:38:LEU:N	1:C:227:MET:HE3	2.16	0.61
1:C:54:GLN:OE1	1:C:405:ARG:NH1	2.33	0.61
1:D:163:ILE:O	1:D:168:ASP:OD2	2.19	0.61
1:A:12:LEU:HA	1:A:16:GLN:HE21	1.65	0.61
1:B:551:PRO:HB2	1:B:552:PRO:HD3	1.83	0.61
1:B:636:THR:HG21	1:B:675:GLU:HG2	1.83	0.61
1:C:452:LEU:HD11	1:C:499:LEU:HD23	1.82	0.61
1:A:23:GLN:O	1:A:161:ARG:NH1	2.34	0.61
1:A:32:ARG:O	1:A:164:ARG:NH2	2.34	0.61
1:B:354:SER:HB3	1:B:424:LEU:HD12	1.83	0.61
1:B:57:GLU:HG2	1:B:58:PHE:CE2	2.36	0.60
1:C:352:SER:O	1:C:354:SER:N	2.34	0.60
1:C:387:PHE:CE2	1:C:427:LEU:HG	2.36	0.60
1:C:520:GLY:O	1:C:523:GLY:N	2.35	0.60
1:C:83:TYR:CD1	1:C:169:VAL:HG11	2.37	0.60
1:C:539:ARG:O	1:C:550:VAL:HG11	2.00	0.60
1:D:71:LEU:HD12	1:D:310:ALA:O	2.01	0.60
1:D:600:SER:HB3	1:D:732:LEU:HD21	1.82	0.60
1:A:163:ILE:O	1:A:164:ARG:HB2	2.02	0.60
1:A:341:ILE:HG12	1:A:349:TRP:CZ2	2.37	0.60
1:A:477:ARG:CZ	1:A:542:ARG:HB3	2.32	0.60
1:B:539:ARG:O	1:B:550:VAL:HG11	2.02	0.60
1:C:552:PRO:HG2	1:C:555:ALA:H	1.66	0.60
1:A:283:ASP:OD2	1:A:283:ASP:N	2.32	0.60
1:A:602:ASN:HB2	1:A:620:LEU:HB3	1.84	0.60
1:A:588:SER:OG	1:A:591:LEU:HB2	2.02	0.60
1:C:710:GLU:HG2	1:C:715:ARG:HG3	1.84	0.60
1:D:411:PHE:O	1:D:420:ARG:HG2	2.02	0.59
1:B:163:ILE:O	1:B:168:ASP:OD2	2.20	0.59
1:B:533:VAL:O	1:B:538:PRO:HD2	2.01	0.59
1:B:715:ARG:HG2	1:B:720:ALA:HB2	1.84	0.59
1:A:217:ASP:C	1:A:219:GLU:H	2.06	0.59
1:D:636:THR:HB	1:D:671:LEU:O	2.02	0.59
1:A:128:PRO:HB3	1:A:276:VAL:HG22	1.83	0.59
1:B:474:LEU:HG	1:B:529:MET:HE1	1.84	0.59
1:D:414:ASP:HB3	1:D:419:ALA:HB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ILE:HD12	1:B:170:TRP:CE2	2.37	0.59
1:C:223:HIS:HE1	1:C:227:MET:HE2	1.66	0.59
1:C:438:TRP:CE3	1:C:464:ARG:HG3	2.38	0.59
1:A:551:PRO:HB2	1:A:552:PRO:HD3	1.85	0.59
1:A:570:TYR:HB2	1:A:769:PHE:HZ	1.67	0.59
1:D:26:TYR:HD2	1:D:93:THR:HG22	1.66	0.59
1:D:764:THR:N	1:D:765:PRO:HD2	2.18	0.59
1:A:474:LEU:O	1:A:477:ARG:HB3	2.02	0.59
1:B:5:GLU:OE2	1:B:311:LYS:HB2	2.03	0.59
1:C:223:HIS:HE1	1:C:227:MET:CE	2.16	0.59
1:A:83:TYR:CZ	1:A:176:GLU:HB2	2.38	0.59
1:A:417:ILE:C	1:A:419:ALA:H	2.06	0.59
1:A:38:LEU:N	1:A:227:MET:HE3	2.18	0.58
1:A:449:ASP:O	1:A:452:LEU:N	2.32	0.58
1:D:127:GLU:HB3	1:D:128:PRO:HD2	1.85	0.58
1:D:216:VAL:HG12	1:D:217:ASP:H	1.68	0.58
1:D:437:PRO:HB2	1:D:460:LEU:HD13	1.85	0.58
1:A:127:GLU:HB3	1:A:128:PRO:CD	2.32	0.58
1:C:57:GLU:HG2	1:C:58:PHE:CE2	2.38	0.58
1:C:545:ARG:HH21	1:C:545:ARG:N	2.01	0.58
1:C:667:ASN:ND2	1:C:743:TRP:HE1	2.01	0.58
1:D:223:HIS:HE1	1:D:227:MET:CE	2.16	0.58
1:D:432:ARG:NH2	1:D:435:GLU:OE1	2.36	0.58
1:B:692:ARG:HG3	1:B:737:ALA:HB1	1.85	0.58
1:D:565:ARG:HG2	1:D:570:TYR:HE2	1.69	0.58
1:A:13:SER:H	1:A:16:GLN:NE2	2.01	0.58
1:C:525:TYR:O	1:C:529:MET:HG2	2.02	0.58
1:B:16:GLN:HE22	1:C:3:THR:HG22	1.69	0.58
1:B:208:ILE:HG21	1:B:221:TYR:CD2	2.39	0.58
1:B:449:ASP:O	1:B:451:THR:N	2.37	0.58
1:C:449:ASP:O	1:C:451:THR:N	2.36	0.58
1:A:4:LYS:O	1:A:5:GLU:HG3	2.04	0.58
1:A:232:ARG:HD3	1:A:236:ARG:CZ	2.33	0.58
1:D:705:THR:HA	1:D:708:ASP:HB2	1.86	0.58
1:A:57:GLU:HG2	1:A:58:PHE:CE2	2.38	0.58
1:C:208:ILE:HG21	1:C:221:TYR:CD2	2.38	0.58
1:D:209:ASP:OD1	1:D:212:LYS:N	2.36	0.58
1:D:484:LEU:HB3	1:D:548:THR:HG22	1.86	0.58
1:B:391:GLN:O	1:B:391:GLN:NE2	2.37	0.58
1:D:484:LEU:HD22	1:D:547:LEU:HD23	1.84	0.58
1:D:538:PRO:HB2	1:D:550:VAL:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:THR:O	1:D:5:GLU:N	2.36	0.58
1:D:472:VAL:O	1:D:476:THR:HG23	2.04	0.58
1:A:417:ILE:HG13	1:A:421:ARG:NH1	2.19	0.57
1:B:64:PHE:CE2	1:C:319:MET:HG2	2.39	0.57
1:A:29:PRO:HB3	1:A:165:SER:HB2	1.85	0.57
1:A:520:GLY:O	1:A:523:GLY:N	2.38	0.57
1:C:223:HIS:CE1	1:C:227:MET:HE2	2.39	0.57
1:C:26:TYR:CE2	1:C:79:VAL:HA	2.39	0.57
1:C:34:TYR:CD2	1:C:224:LEU:HD12	2.39	0.57
1:D:219:GLU:HA	1:D:222:ARG:HD2	1.85	0.57
1:B:114:GLU:OE1	1:B:118:ARG:NH1	2.37	0.57
1:B:208:ILE:HG21	1:B:221:TYR:HD2	1.68	0.57
1:B:257:ILE:HD13	1:B:294:VAL:HG21	1.87	0.57
1:C:148:GLU:OE2	1:C:195:ARG:NH1	2.37	0.57
1:C:417:ILE:O	1:C:419:ALA:N	2.31	0.57
1:D:397:THR:OG1	1:D:402:ASP:OD2	2.20	0.57
1:D:605:PRO:HB3	1:D:735:ALA:HB2	1.86	0.57
1:A:449:ASP:HB3	1:A:452:LEU:HB2	1.84	0.57
1:D:38:LEU:N	1:D:227:MET:HE3	2.19	0.57
1:A:417:ILE:C	1:A:419:ALA:N	2.57	0.57
1:A:562:GLU:HG2	1:A:565:ARG:NH1	2.20	0.57
1:A:722:GLU:O	1:A:726:GLN:NE2	2.37	0.57
1:C:475:LEU:HD21	1:C:504:CYS:SG	2.44	0.57
1:D:127:GLU:HB3	1:D:128:PRO:CD	2.34	0.57
1:A:496:GLN:CA	1:A:553:VAL:HG13	2.32	0.57
1:A:486:SER:O	1:A:488:GLU:N	2.38	0.57
1:B:57:GLU:HG2	1:B:58:PHE:CD2	2.39	0.57
1:C:682:ARG:HE	1:C:716:LEU:HD13	1.69	0.57
1:D:544:GLU:HB2	1:D:545:ARG:NH2	2.20	0.57
1:A:516:GLY:O	1:A:587:HIS:NE2	2.37	0.57
1:C:283:ASP:OD2	1:C:283:ASP:N	2.37	0.57
1:D:474:LEU:HG	1:D:529:MET:HE1	1.86	0.56
1:B:471:VAL:HG22	1:B:525:TYR:CZ	2.40	0.56
1:C:13:SER:OG	1:C:16:GLN:HG2	2.05	0.56
1:D:549:GLU:HG3	1:D:550:VAL:HG23	1.86	0.56
1:D:688:ARG:NH1	1:D:740:GLU:OE2	2.38	0.56
1:A:572:LYS:HE2	1:A:760:TRP:CZ3	2.39	0.56
1:A:706:LEU:HD12	1:A:714:LEU:HD23	1.86	0.56
1:B:128:PRO:HD3	1:B:275:SER:HB2	1.86	0.56
1:B:650:SER:OG	1:B:651:TRP:N	2.39	0.56
1:C:26:TYR:CD1	1:C:163:ILE:HG22	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:TYR:CE2	1:C:176:GLU:HB2	2.39	0.56
1:C:186:TYR:CE2	1:C:205:HIS:CD2	2.93	0.56
1:C:666:GLY:H	1:C:752:SER:HB3	1.69	0.56
1:D:682:ARG:HH21	1:D:716:LEU:HD13	1.71	0.56
1:A:161:ARG:O	1:A:162:LEU:HB2	2.05	0.56
1:B:219:GLU:HA	1:B:222:ARG:HD2	1.87	0.56
1:B:372:SER:OG	1:B:373:ALA:N	2.37	0.56
1:D:7:PHE:C	1:D:7:PHE:CD2	2.79	0.56
1:D:680:SER:HA	1:D:690:MET:HE1	1.88	0.56
1:B:349:TRP:CD1	1:B:349:TRP:C	2.79	0.56
1:A:13:SER:OG	1:A:16:GLN:HG2	2.05	0.56
1:A:208:ILE:HD12	1:A:221:TYR:CE2	2.41	0.56
1:B:385:LEU:HD22	1:B:396:LEU:HB3	1.86	0.56
1:B:581:MET:SD	1:B:664:ARG:NH1	2.79	0.56
1:B:669:THR:CG2	1:B:751:ARG:HH22	2.18	0.56
1:C:510:LEU:HD13	1:C:564:LEU:HD21	1.88	0.56
1:A:155:GLU:HB2	1:A:174:LYS:HG2	1.88	0.56
1:C:87:VAL:HG13	1:C:88:PRO:O	2.06	0.56
1:C:168:ASP:OD1	1:C:180:ARG:N	2.38	0.56
1:C:720:ALA:HB1	1:C:723:ILE:HB	1.88	0.56
1:A:228:ARG:HD3	1:A:228:ARG:C	2.26	0.56
1:B:706:LEU:HD13	1:B:723:ILE:HG22	1.87	0.56
1:C:100:ARG:HG3	1:C:100:ARG:HH11	1.71	0.56
1:D:343:GLU:OE2	1:D:420:ARG:CZ	2.53	0.56
1:D:387:PHE:CE2	1:D:427:LEU:HG	2.40	0.56
1:A:488:GLU:HG2	1:A:489:THR:N	2.19	0.56
1:B:705:THR:HA	1:B:708:ASP:HB2	1.88	0.56
1:C:163:ILE:O	1:C:164:ARG:HB2	2.04	0.56
1:A:720:ALA:HB1	1:A:723:ILE:HD12	1.87	0.55
1:B:113:GLU:OE2	1:B:232:ARG:NH2	2.39	0.55
1:B:617:LYS:O	1:B:619:GLY:N	2.39	0.55
1:C:59:GLU:HG2	1:C:262:ASN:CB	2.36	0.55
1:D:537:MET:CB	1:D:538:PRO:HD3	2.37	0.55
1:D:588:SER:OG	1:D:591:LEU:HB2	2.06	0.55
1:A:496:GLN:CD	1:A:553:VAL:HG22	2.26	0.55
1:A:578:ARG:O	1:A:582:THR:HG23	2.06	0.55
1:B:333:ILE:HD12	1:B:380:THR:HG23	1.87	0.55
1:B:682:ARG:NH2	1:B:716:LEU:HD13	2.19	0.55
1:C:538:PRO:HB3	1:C:550:VAL:HG22	1.88	0.55
1:C:688:ARG:HD3	1:C:692:ARG:HH12	1.72	0.55
1:D:86:GLN:OE1	1:D:171:SER:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:PRO:HG3	1:D:734:ALA:HB3	1.88	0.55
1:A:477:ARG:NH2	1:A:547:LEU:O	2.39	0.55
1:B:760:TRP:O	1:B:764:THR:OG1	2.25	0.55
1:C:130:VAL:O	1:C:134:ASN:ND2	2.39	0.55
1:C:621:LEU:HD12	1:C:729:TYR:HD2	1.72	0.55
1:C:722:GLU:O	1:C:726:GLN:NE2	2.39	0.55
1:D:232:ARG:HD3	1:D:236:ARG:CZ	2.36	0.55
1:B:149:GLU:HB2	1:B:161:ARG:NH2	2.21	0.55
1:B:168:ASP:OD1	1:B:180:ARG:N	2.33	0.55
1:B:455:GLN:O	1:B:458:ILE:HG22	2.07	0.55
1:C:364:TYR:CE1	1:C:368:GLU:HG3	2.41	0.55
1:D:496:GLN:HG2	1:D:553:VAL:HG22	1.87	0.55
1:A:493:SER:OG	1:A:494:ALA:N	2.39	0.55
1:A:621:LEU:HD12	1:A:729:TYR:HD2	1.71	0.55
1:B:34:TYR:CE1	1:B:36:TRP:HB2	2.42	0.55
1:B:86:GLN:HB3	1:B:172:ARG:HH21	1.71	0.55
1:B:414:ASP:HB3	1:B:419:ALA:CB	2.37	0.55
1:D:26:TYR:CE2	1:D:79:VAL:HA	2.42	0.55
1:A:438:TRP:CE3	1:A:464:ARG:HG3	2.42	0.55
1:B:583:PRO:HG3	1:B:660:GLU:HG2	1.87	0.55
1:C:630:ASN:O	1:C:632:GLU:HG3	2.05	0.55
1:D:284:ALA:O	1:D:286:MET:N	2.34	0.55
1:D:551:PRO:HB2	1:D:552:PRO:CD	2.36	0.55
1:D:628:ARG:HA	1:D:631:ASP:CB	2.30	0.55
1:C:127:GLU:HB3	1:C:128:PRO:HD2	1.88	0.55
1:C:565:ARG:HH21	1:C:771:PRO:HB3	1.72	0.55
1:A:605:PRO:HA	1:A:735:ALA:HB2	1.88	0.55
1:A:674:VAL:HG13	1:A:678:SER:HB3	1.89	0.55
1:B:593:ARG:NH2	1:B:635:ALA:HB1	2.18	0.55
1:B:634:PHE:HD1	1:B:634:PHE:H	1.54	0.55
1:D:516:GLY:O	1:D:587:HIS:NE2	2.39	0.55
1:C:57:GLU:HG2	1:C:58:PHE:CD2	2.42	0.55
1:C:408:ARG:HD3	1:C:412:ASP:OD2	2.07	0.55
1:A:113:GLU:O	1:A:117:VAL:HG12	2.06	0.55
1:A:180:ARG:NH1	1:A:213:THR:HG22	2.21	0.55
1:A:489:THR:O	1:A:489:THR:OG1	2.25	0.55
1:C:119:ALA:O	1:C:122:LEU:HB2	2.07	0.55
1:D:372:SER:OG	1:D:375:LYS:HB3	2.07	0.54
1:B:542:ARG:HE	1:B:547:LEU:HD12	1.72	0.54
1:C:374:ASP:OD1	1:C:374:ASP:N	2.39	0.54
1:D:120:GLU:HG2	1:D:200:VAL:HG11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:HG2	1:A:200:VAL:HG11	1.90	0.54
1:B:414:ASP:HB3	1:B:419:ALA:HB1	1.88	0.54
1:C:18:LEU:HB2	1:C:146:CYS:SG	2.47	0.54
1:C:496:GLN:CA	1:C:553:VAL:HG13	2.35	0.54
1:D:312:ARG:HD3	1:D:315:TYR:CD2	2.42	0.54
1:D:632:GLU:HA	1:D:635:ALA:HB3	1.88	0.54
1:A:26:TYR:HD2	1:A:93:THR:HG22	1.71	0.54
1:A:507:PHE:CZ	1:A:511:TRP:HD1	2.25	0.54
1:C:526:ARG:O	1:C:530:THR:HG23	2.07	0.54
1:C:636:THR:CG2	1:C:675:GLU:HG2	2.37	0.54
1:D:161:ARG:HA	1:D:170:TRP:HH2	1.73	0.54
1:D:630:ASN:O	1:D:632:GLU:N	2.40	0.54
1:A:569:ILE:HG23	1:A:574:GLN:HB3	1.90	0.54
1:C:437:PRO:HD3	1:C:479:PHE:CE2	2.42	0.54
1:C:565:ARG:O	1:C:568:GLY:N	2.41	0.54
1:C:605:PRO:HG3	1:C:734:ALA:HB3	1.89	0.54
1:C:674:VAL:HG11	1:C:679:ALA:H	1.72	0.54
1:B:186:TYR:OH	1:B:228:ARG:HD2	2.06	0.54
1:C:343:GLU:OE2	1:C:420:ARG:NH1	2.40	0.54
1:B:557:GLN:O	1:B:561:LYS:HD3	2.08	0.54
1:B:570:TYR:HD1	1:B:769:PHE:CZ	2.25	0.54
1:C:344:GLU:OE2	1:C:352:SER:HB2	2.08	0.54
1:C:561:LYS:HD2	1:C:767:LEU:HB3	1.89	0.54
1:D:621:LEU:HD12	1:D:729:TYR:CD2	2.42	0.54
1:D:688:ARG:HD3	1:D:692:ARG:HH12	1.73	0.54
1:A:437:PRO:HB2	1:A:460:LEU:HD13	1.89	0.54
1:B:724:VAL:HG12	1:B:725:ARG:HG3	1.90	0.54
1:D:70:ALA:HB3	1:D:92:MET:HE3	1.90	0.54
1:A:87:VAL:HG22	1:A:88:PRO:HD2	1.89	0.54
1:B:36:TRP:HE3	1:B:41:ILE:HD13	1.73	0.54
1:B:645:PRO:HB2	1:B:648:ASN:HA	1.90	0.54
1:C:104:LEU:O	1:C:108:THR:HG23	2.08	0.54
1:D:565:ARG:HH21	1:D:771:PRO:HB3	1.73	0.54
1:B:344:GLU:OE1	1:B:421:ARG:NH2	2.41	0.54
1:B:417:ILE:HG13	1:B:421:ARG:NH1	2.23	0.54
1:C:126:ASP:O	1:C:128:PRO:HD2	2.06	0.54
1:D:160:PRO:HG2	1:D:179:TYR:CD1	2.42	0.53
1:A:260:SER:O	1:A:264:GLN:HG3	2.08	0.53
1:A:284:ALA:O	1:A:286:MET:N	2.36	0.53
1:B:549:GLU:HG3	1:B:550:VAL:HG23	1.89	0.53
1:D:349:TRP:CD1	1:D:349:TRP:C	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:ARG:CZ	1:A:740:GLU:OE2	2.56	0.53
1:B:38:LEU:H	1:B:227:MET:HE1	1.71	0.53
1:D:651:TRP:CZ3	1:D:684:TRP:HB2	2.44	0.53
1:A:118:ARG:HB2	1:A:289:LEU:HD13	1.90	0.53
1:C:163:ILE:O	1:C:168:ASP:OD2	2.26	0.53
1:A:416:ASP:HB2	1:A:419:ALA:HB3	1.90	0.53
1:A:662:ILE:HD12	1:A:662:ILE:H	1.73	0.53
1:B:612:LEU:HD13	1:B:754:ARG:HD2	1.89	0.53
1:C:88:PRO:HG2	1:C:91:VAL:HG12	1.90	0.53
1:D:415:PRO:O	1:D:420:ARG:NH1	2.42	0.53
1:C:441:PRO:O	1:C:444:VAL:HG22	2.09	0.53
1:D:674:VAL:HG11	1:D:679:ALA:H	1.72	0.53
1:A:680:SER:HA	1:A:690:MET:HE1	1.89	0.53
1:B:542:ARG:HG3	1:B:542:ARG:HH11	1.74	0.53
1:D:35:SER:O	1:D:223:HIS:NE2	2.36	0.53
1:A:511:TRP:CD2	1:A:521:ILE:HG12	2.44	0.53
1:D:86:GLN:CB	1:D:172:ARG:HE	2.21	0.53
1:A:315:TYR:O	1:A:319:MET:HG3	2.09	0.53
1:B:486:SER:O	1:B:488:GLU:N	2.42	0.53
1:B:669:THR:HG23	1:B:751:ARG:HH12	1.73	0.53
1:C:509:ALA:HA	1:C:591:LEU:HD21	1.91	0.53
1:C:551:PRO:HB2	1:C:552:PRO:HD3	1.89	0.53
1:A:557:GLN:O	1:A:561:LYS:HD3	2.09	0.52
1:C:674:VAL:HG11	1:C:679:ALA:N	2.24	0.52
1:D:81:PRO:HD3	1:D:166:TYR:H	1.73	0.52
1:A:26:TYR:CE2	1:A:79:VAL:HA	2.45	0.52
1:A:479:PHE:HE1	1:A:483:ARG:HD2	1.69	0.52
1:B:5:GLU:O	1:B:7:PHE:N	2.40	0.52
1:B:729:TYR:CE2	1:B:731:PRO:HG3	2.44	0.52
1:C:337:LYS:HB2	1:C:337:LYS:HZ2	1.74	0.52
1:A:674:VAL:HG11	1:A:679:ALA:N	2.23	0.52
1:B:1:MET:SD	1:C:62:ILE:HD13	2.49	0.52
1:B:106:LEU:O	1:B:109:THR:HG22	2.09	0.52
1:B:163:ILE:O	1:B:164:ARG:HB2	2.09	0.52
1:B:163:ILE:HD12	1:B:170:TRP:CD2	2.44	0.52
1:D:715:ARG:HG2	1:D:720:ALA:HB2	1.91	0.52
1:A:454:THR:HG21	1:A:627:GLU:OE2	2.09	0.52
1:B:621:LEU:HD13	1:B:728:ARG:HH12	1.72	0.52
1:C:372:SER:OG	1:C:373:ALA:N	2.43	0.52
1:A:545:ARG:NH2	1:A:545:ARG:H	2.08	0.52
1:A:546:ASP:O	1:A:548:THR:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:HG22	1:B:7:PHE:HB3	1.92	0.52
1:B:537:MET:CB	1:B:538:PRO:HD3	2.40	0.52
1:C:180:ARG:HD3	1:C:213:THR:HG22	1.92	0.52
1:D:3:THR:O	1:D:3:THR:OG1	2.27	0.52
1:D:715:ARG:HG2	1:D:720:ALA:CB	2.40	0.52
1:A:79:VAL:HG23	1:A:82:LYS:HD3	1.91	0.52
1:A:81:PRO:O	1:A:169:VAL:HG13	2.10	0.52
1:B:375:LYS:HA	1:B:378:THR:HG22	1.91	0.52
1:C:83:TYR:HD1	1:C:169:VAL:HG11	1.74	0.52
1:C:537:MET:HB2	1:C:538:PRO:HD3	1.92	0.52
1:C:764:THR:O	1:C:769:PHE:HB2	2.10	0.52
1:D:84:ARG:HG3	1:D:84:ARG:O	2.08	0.52
1:D:471:VAL:HG12	1:D:475:LEU:HG	1.92	0.52
1:D:630:ASN:O	1:D:632:GLU:HG3	2.10	0.52
1:A:209:ASP:OD1	1:A:212:LYS:N	2.43	0.52
1:A:764:THR:N	1:A:765:PRO:HD2	2.25	0.52
1:C:115:ILE:HG23	1:C:289:LEU:HD11	1.92	0.52
1:C:569:ILE:HG23	1:C:574:GLN:HB3	1.92	0.52
1:A:27:ILE:HD13	1:A:98:GLN:HE21	1.73	0.52
1:A:282:ASP:N	1:A:282:ASP:OD1	2.42	0.52
1:D:7:PHE:HD1	1:D:319:MET:SD	2.33	0.52
1:A:605:PRO:CB	1:A:735:ALA:HB2	2.39	0.52
1:B:488:GLU:HG2	1:B:489:THR:N	2.24	0.52
1:B:496:GLN:HG2	1:B:553:VAL:HG13	1.92	0.52
1:C:433:PHE:CB	1:C:476:THR:HG22	2.39	0.52
1:C:537:MET:CB	1:C:538:PRO:HD3	2.40	0.52
1:D:32:ARG:O	1:D:164:ARG:NH2	2.43	0.51
1:D:161:ARG:O	1:D:162:LEU:HB2	2.09	0.51
1:D:186:TYR:OH	1:D:228:ARG:HD2	2.11	0.51
1:D:196:ASP:OD1	1:D:197:PRO:HD2	2.09	0.51
1:B:474:LEU:HG	1:B:529:MET:CE	2.40	0.51
1:B:584:VAL:HG12	1:B:592:THR:HG22	1.92	0.51
1:C:163:ILE:HD13	1:C:168:ASP:HB3	1.93	0.51
1:C:486:SER:O	1:C:488:GLU:N	2.43	0.51
1:C:615:ARG:HG2	1:C:616:GLY:H	1.75	0.51
1:D:375:LYS:O	1:D:378:THR:HG22	2.10	0.51
1:D:456:ALA:HB3	1:D:498:LEU:HD22	1.92	0.51
1:D:662:ILE:HD12	1:D:662:ILE:H	1.73	0.51
1:B:13:SER:OG	1:B:16:GLN:HG2	2.11	0.51
1:A:3:THR:O	1:A:3:THR:OG1	2.26	0.51
1:B:417:ILE:O	1:B:419:ALA:N	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:PHE:CG	1:B:476:THR:HG22	2.44	0.51
1:B:437:PRO:HG3	1:B:479:PHE:HE2	1.75	0.51
1:D:34:TYR:CD2	1:D:224:LEU:HD12	2.45	0.51
1:D:583:PRO:HG3	1:D:660:GLU:HG2	1.93	0.51
1:D:154:GLY:O	1:D:157:ARG:HB2	2.11	0.51
1:D:339:ARG:HG2	1:D:408:ARG:CZ	2.41	0.51
1:A:58:PHE:CE2	1:A:405:ARG:HD3	2.45	0.51
1:B:623:THR:HG22	1:B:634:PHE:HZ	1.75	0.51
1:D:458:ILE:HD11	1:D:629:TRP:HE3	1.75	0.51
1:D:602:ASN:HB2	1:D:620:LEU:HB3	1.91	0.51
1:D:603:SER:HB3	1:D:613:VAL:CG1	2.40	0.51
1:A:636:THR:OG1	1:A:675:GLU:HG2	2.11	0.51
1:B:414:ASP:OD1	1:B:544:GLU:OE2	2.29	0.51
1:D:452:LEU:HB3	1:D:498:LEU:HD13	1.92	0.51
1:A:161:ARG:HA	1:A:170:TRP:HH2	1.75	0.51
1:A:621:LEU:HD12	1:A:729:TYR:CD2	2.44	0.51
1:B:23:GLN:O	1:B:161:ARG:NH1	2.44	0.51
1:A:688:ARG:HB3	1:A:692:ARG:CZ	2.41	0.51
1:C:681:ASN:OD1	1:C:682:ARG:N	2.43	0.51
1:C:706:LEU:O	1:C:710:GLU:HG3	2.10	0.51
1:A:496:GLN:NE2	1:A:553:VAL:HG22	2.25	0.51
1:A:561:LYS:O	1:A:564:LEU:N	2.44	0.51
1:B:182:PRO:HD3	1:B:221:TYR:CE1	2.45	0.51
1:B:353:GLU:O	1:B:356:LEU:HB2	2.11	0.51
1:D:57:GLU:HG2	1:D:58:PHE:CD2	2.46	0.51
1:D:62:ILE:HG22	1:A:315:TYR:CE1	2.46	0.51
1:C:86:GLN:HE22	1:C:172:ARG:H	1.57	0.51
1:C:337:LYS:HB2	1:C:337:LYS:NZ	2.26	0.51
1:D:54:GLN:OE1	1:D:405:ARG:NH1	2.44	0.50
1:A:344:GLU:O	1:A:349:TRP:HB3	2.11	0.50
1:B:173:ASN:HB2	1:B:176:GLU:OE2	2.11	0.50
1:A:433:PHE:O	1:A:437:PRO:HD2	2.11	0.50
1:C:650:SER:OG	1:C:683:ALA:HB1	2.11	0.50
1:A:569:ILE:HD12	1:A:578:ARG:NH2	2.26	0.50
1:B:516:GLY:O	1:B:587:HIS:NE2	2.45	0.50
1:B:537:MET:HB2	1:B:538:PRO:HD3	1.93	0.50
1:C:56:ALA:O	1:C:262:ASN:ND2	2.44	0.50
1:C:274:PRO:HA	1:C:277:VAL:HG22	1.92	0.50
1:C:692:ARG:HG3	1:C:737:ALA:CB	2.38	0.50
1:D:486:SER:O	1:D:488:GLU:N	2.45	0.50
1:D:610:PRO:O	1:D:739:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ASP:OD1	1:B:282:ASP:N	2.44	0.50
1:B:11:PRO:O	1:B:12:LEU:HD23	2.11	0.50
1:B:418:VAL:N	1:B:421:ARG:HD2	2.27	0.50
1:C:45:LEU:N	1:C:45:LEU:HD23	2.26	0.50
1:A:35:SER:O	1:A:223:HIS:NE2	2.37	0.50
1:B:26:TYR:CZ	1:B:79:VAL:HA	2.47	0.50
1:D:385:LEU:HB2	1:D:386:PRO:HD3	1.94	0.50
1:A:576:VAL:HG13	1:A:756:CYS:HB2	1.94	0.50
1:C:472:VAL:O	1:C:476:THR:HG23	2.11	0.50
1:C:680:SER:HA	1:C:690:MET:CE	2.41	0.50
1:B:213:THR:O	1:B:213:THR:OG1	2.21	0.50
1:B:238:ALA:HB2	1:B:249:ILE:CD1	2.42	0.50
1:B:671:LEU:HD11	1:B:691:PHE:HE1	1.77	0.50
1:D:36:TRP:HE3	1:D:41:ILE:HD13	1.76	0.50
1:D:78:THR:O	1:D:80:GLU:HG2	2.12	0.50
1:B:585:TYR:HA	1:B:592:THR:HG21	1.94	0.50
1:C:448:ASP:O	1:C:450:ALA:N	2.45	0.50
1:D:83:TYR:HD1	1:D:169:VAL:HG11	1.77	0.49
1:D:217:ASP:C	1:D:219:GLU:H	2.16	0.49
1:D:511:TRP:HH2	1:D:519:ALA:HB3	1.76	0.49
1:A:569:ILE:CG2	1:A:574:GLN:HB3	2.42	0.49
1:A:634:PHE:HD1	1:A:634:PHE:H	1.60	0.49
1:B:477:ARG:CZ	1:B:542:ARG:HB3	2.42	0.49
1:C:149:GLU:HB2	1:C:161:ARG:NH2	2.27	0.49
1:A:265:PHE:CZ	1:A:271:GLU:HG3	2.47	0.49
1:C:86:GLN:NE2	1:C:172:ARG:H	2.09	0.49
1:D:207:PRO:O	1:D:208:ILE:HG22	2.13	0.49
1:D:511:TRP:CD2	1:D:521:ILE:HG12	2.48	0.49
1:D:744:THR:O	1:D:748:VAL:HG23	2.12	0.49
1:B:557:GLN:HB3	1:B:767:LEU:O	2.13	0.49
1:B:565:ARG:NH2	1:B:771:PRO:HB3	2.26	0.49
1:C:452:LEU:HB3	1:C:498:LEU:HD13	1.94	0.49
1:C:538:PRO:CB	1:C:550:VAL:HG22	2.42	0.49
1:A:496:GLN:HG2	1:A:553:VAL:HG22	1.93	0.49
1:B:180:ARG:HH22	1:B:212:LYS:NZ	2.10	0.49
1:B:444:VAL:HG12	1:B:445:PRO:HD3	1.94	0.49
1:D:479:PHE:HE1	1:D:483:ARG:NE	2.10	0.49
1:A:13:SER:N	1:A:16:GLN:HE21	2.08	0.49
1:A:565:ARG:HH21	1:A:771:PRO:CB	2.23	0.49
1:C:217:ASP:O	1:C:218:LEU:HB2	2.12	0.49
1:C:593:ARG:HH21	1:C:635:ALA:HB1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:ILE:HD12	1:C:662:ILE:H	1.78	0.49
1:D:239:VAL:HG11	1:D:292:LEU:HD13	1.94	0.49
1:D:326:THR:HG21	1:A:323:LEU:O	2.12	0.49
1:D:621:LEU:HD12	1:D:729:TYR:HD2	1.77	0.49
1:C:148:GLU:OE1	1:C:195:ARG:NH1	2.44	0.49
1:C:148:GLU:CD	1:C:195:ARG:NH1	2.66	0.49
1:C:509:ALA:HB2	1:C:594:LEU:HD12	1.93	0.49
1:C:570:TYR:N	1:C:570:TYR:CD2	2.80	0.49
1:C:709:ALA:HB1	1:C:714:LEU:HB2	1.94	0.49
1:D:38:LEU:CA	1:D:227:MET:HE3	2.42	0.49
1:A:113:GLU:OE2	1:A:232:ARG:NH2	2.46	0.49
1:A:126:ASP:OD1	1:A:126:ASP:O	2.31	0.49
1:A:239:VAL:HG11	1:A:292:LEU:HD13	1.93	0.49
1:A:458:ILE:N	1:A:626:LEU:HB2	2.28	0.49
1:B:570:TYR:HD1	1:B:769:PHE:HZ	1.59	0.49
1:B:642:PRO:HD3	1:B:651:TRP:CZ2	2.48	0.49
1:C:583:PRO:HB2	1:C:586:GLN:HG3	1.95	0.49
1:C:641:ALA:HA	1:C:651:TRP:CH2	2.47	0.49
1:B:86:GLN:NE2	1:B:172:ARG:H	2.10	0.49
1:B:569:ILE:HG12	1:B:574:GLN:HB3	1.95	0.49
1:C:282:ASP:OD1	1:C:282:ASP:N	2.46	0.49
1:C:546:ASP:O	1:C:548:THR:N	2.44	0.49
1:D:433:PHE:CG	1:D:476:THR:HG22	2.48	0.49
1:D:569:ILE:HD12	1:D:578:ARG:NH2	2.28	0.49
1:A:223:HIS:CE1	1:A:227:MET:HE2	2.47	0.49
1:D:151:MET:SD	1:D:151:MET:N	2.85	0.49
1:D:728:ARG:HD3	1:D:729:TYR:N	2.27	0.49
1:A:163:ILE:O	1:A:168:ASP:OD2	2.31	0.49
1:C:36:TRP:HE3	1:C:41:ILE:HD13	1.78	0.49
1:D:603:SER:HB3	1:D:613:VAL:HG11	1.95	0.48
1:A:544:GLU:HB2	1:A:545:ARG:HH22	1.77	0.48
1:B:155:GLU:H	1:B:174:LYS:HE2	1.77	0.48
1:B:681:ASN:O	1:B:682:ARG:HB2	2.13	0.48
1:B:110:VAL:CG2	1:B:235:LEU:HD12	2.43	0.48
1:B:654:ASP:OD1	1:B:654:ASP:N	2.47	0.48
1:A:706:LEU:HG	1:A:710:GLU:OE2	2.13	0.48
1:B:354:SER:HB3	1:B:424:LEU:CD1	2.42	0.48
1:C:449:ASP:O	1:C:452:LEU:N	2.41	0.48
1:C:529:MET:HB3	1:C:541:ALA:HB2	1.96	0.48
1:D:389:MET:CE	1:D:526:ARG:HH11	2.26	0.48
1:D:728:ARG:HD3	1:D:729:TYR:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HG3	1:A:80:GLU:HG3	1.93	0.48
1:C:52:LEU:HD23	1:C:298:TYR:CD1	2.49	0.48
1:C:106:LEU:O	1:C:110:VAL:HG12	2.13	0.48
1:C:636:THR:HB	1:C:671:LEU:O	2.13	0.48
1:D:562:GLU:HG2	1:D:565:ARG:NH1	2.28	0.48
1:A:665:ILE:CD1	1:A:665:ILE:H	2.27	0.48
1:B:445:PRO:HG3	1:B:497:PHE:HD1	1.79	0.48
1:B:514:SER:O	1:B:582:THR:HG21	2.14	0.48
1:B:572:LYS:HE2	1:B:760:TRP:CZ3	2.48	0.48
1:B:669:THR:HG21	1:B:751:ARG:HH22	1.78	0.48
1:C:588:SER:OG	1:C:591:LEU:HB2	2.14	0.48
1:D:365:LEU:HD12	1:D:379:VAL:HG12	1.95	0.48
1:A:516:GLY:O	1:A:587:HIS:CD2	2.66	0.48
1:B:123:THR:O	1:B:129:SER:OG	2.23	0.48
1:D:213:THR:O	1:D:213:THR:OG1	2.30	0.48
1:D:674:VAL:HG13	1:D:678:SER:H	1.78	0.48
1:A:57:GLU:HG2	1:A:58:PHE:CD2	2.49	0.48
1:B:26:TYR:CE2	1:B:79:VAL:HA	2.49	0.48
1:B:524:VAL:HG22	1:B:563:GLN:NE2	2.29	0.48
1:D:666:GLY:H	1:D:752:SER:HB3	1.79	0.48
1:B:161:ARG:O	1:B:162:LEU:HB2	2.13	0.48
1:B:496:GLN:NE2	1:B:553:VAL:HG22	2.29	0.48
1:C:371:SER:OG	1:C:375:LYS:HG2	2.14	0.48
1:C:469:ASP:O	1:C:472:VAL:HG23	2.14	0.48
1:A:400:LEU:HD13	1:A:400:LEU:HA	1.75	0.48
1:B:34:TYR:HD1	1:B:99:GLN:OE1	1.97	0.48
1:C:27:ILE:HB	1:C:164:ARG:HA	1.95	0.48
1:C:65:LEU:HD23	1:C:65:LEU:HA	1.61	0.48
1:C:555:ALA:HA	1:C:558:SER:OG	2.14	0.48
1:B:636:THR:CG2	1:B:675:GLU:HG2	2.43	0.48
1:B:709:ALA:HB3	1:B:714:LEU:HD22	1.95	0.48
1:B:720:ALA:HB1	1:B:723:ILE:HD12	1.95	0.48
1:C:470:ILE:HG21	1:C:522:ASP:HA	1.95	0.48
1:D:113:GLU:O	1:D:117:VAL:HG12	2.14	0.47
1:D:406:TYR:CZ	1:D:410:VAL:HG21	2.49	0.47
1:D:502:ARG:CZ	1:D:766:TRP:CD1	2.97	0.47
1:D:511:TRP:CH2	1:D:519:ALA:HB3	2.49	0.47
1:D:526:ARG:O	1:D:530:THR:HG23	2.14	0.47
1:A:369:GLY:O	1:A:371:SER:N	2.44	0.47
1:C:25:LEU:O	1:C:162:LEU:HA	2.14	0.47
1:C:554:GLU:HA	1:C:557:GLN:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:PRO:HD3	1:C:651:TRP:CE2	2.48	0.47
1:C:650:SER:OG	1:C:651:TRP:N	2.45	0.47
1:D:9:ALA:CB	1:A:9:ALA:HB3	2.42	0.47
1:D:315:TYR:HE1	1:A:62:ILE:HG22	1.79	0.47
1:D:432:ARG:HD3	1:D:483:ARG:HH12	1.79	0.47
1:A:610:PRO:HB2	1:A:739:ARG:HA	1.95	0.47
1:B:164:ARG:NH1	1:B:183:ILE:HD11	2.28	0.47
1:C:268:PHE:O	1:C:270:SER:HB3	2.13	0.47
1:C:474:LEU:HG	1:C:529:MET:HE1	1.97	0.47
1:D:5:GLU:O	1:D:7:PHE:N	2.48	0.47
1:A:331:THR:N	1:A:334:GLU:OE1	2.47	0.47
1:B:217:ASP:O	1:B:218:LEU:HB2	2.13	0.47
1:C:488:GLU:HG2	1:C:489:THR:HG22	1.94	0.47
1:D:34:TYR:HD2	1:D:224:LEU:HD12	1.80	0.47
1:D:136:ALA:O	1:D:140:THR:HB	2.14	0.47
1:D:596:LEU:HD21	1:D:665:ILE:HG22	1.96	0.47
1:A:357:HIS:O	1:A:360:VAL:HB	2.15	0.47
1:A:496:GLN:CG	1:A:553:VAL:HG22	2.45	0.47
1:A:605:PRO:CA	1:A:735:ALA:HB2	2.43	0.47
1:B:700:GLU:HG2	1:B:704:LYS:HE3	1.96	0.47
1:C:709:ALA:CB	1:C:714:LEU:HB2	2.44	0.47
1:B:454:THR:HG21	1:B:627:GLU:OE2	2.15	0.47
1:B:512:ARG:NE	1:B:518:THR:HG23	2.30	0.47
1:C:11:PRO:O	1:C:12:LEU:HD23	2.14	0.47
1:C:204:ARG:O	1:C:205:HIS:CB	2.63	0.47
1:C:247:ASP:N	1:C:247:ASP:OD1	2.46	0.47
1:C:484:LEU:CB	1:C:548:THR:HG22	2.40	0.47
1:D:26:TYR:CZ	1:D:79:VAL:HA	2.50	0.47
1:D:674:VAL:HG11	1:D:679:ALA:N	2.30	0.47
1:B:86:GLN:HE22	1:B:172:ARG:H	1.63	0.47
1:B:124:ARG:HD3	1:B:133:TYR:CD2	2.50	0.47
1:B:682:ARG:HE	1:B:716:LEU:HD13	1.78	0.47
1:C:228:ARG:HD3	1:C:228:ARG:C	2.35	0.47
1:C:706:LEU:HG	1:C:710:GLU:OE2	2.15	0.47
1:D:714:LEU:O	1:D:714:LEU:HG	2.13	0.47
1:A:469:ASP:O	1:A:471:VAL:N	2.47	0.47
1:A:512:ARG:NH1	1:A:588:SER:HB3	2.30	0.47
1:A:549:GLU:HG3	1:A:550:VAL:HG23	1.96	0.47
1:B:199:ALA:O	1:B:200:VAL:HB	2.15	0.47
1:B:507:PHE:CD1	1:B:560:LEU:HB3	2.50	0.47
1:B:544:GLU:HB2	1:B:545:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:PRO:O	1:B:656:TYR:OH	2.26	0.47
1:C:128:PRO:CD	1:C:275:SER:HB2	2.44	0.47
1:C:208:ILE:HG13	1:C:209:ASP:N	2.21	0.47
1:C:599:ALA:HB2	1:C:759:ALA:HB2	1.97	0.47
1:D:651:TRP:NE1	1:D:683:ALA:HA	2.29	0.47
1:A:186:TYR:OH	1:A:228:ARG:HD2	2.14	0.47
1:B:449:ASP:O	1:B:452:LEU:N	2.46	0.47
1:C:32:ARG:O	1:C:164:ARG:NH2	2.47	0.47
1:D:569:ILE:HD13	1:D:574:GLN:HB3	1.96	0.47
1:D:585:TYR:CD1	1:D:637:ILE:HG21	2.50	0.47
1:B:366:ASP:O	1:B:370:SER:HB2	2.15	0.47
1:B:580:ALA:O	1:B:664:ARG:HD3	2.15	0.47
1:C:580:ALA:O	1:C:664:ARG:HD3	2.15	0.47
1:D:678:SER:OG	1:D:721:GLY:HA3	2.15	0.47
1:A:339:ARG:HG2	1:A:408:ARG:HH22	1.77	0.47
1:A:658:ASP:OD2	1:A:664:ARG:NH2	2.48	0.47
1:B:11:PRO:HB3	1:C:7:PHE:CD2	2.51	0.47
1:B:26:TYR:CE2	1:B:165:SER:HB3	2.50	0.47
1:B:400:LEU:HD13	1:B:400:LEU:HA	1.70	0.47
1:B:552:PRO:HG2	1:B:555:ALA:H	1.80	0.47
1:C:26:TYR:CZ	1:C:79:VAL:HA	2.49	0.47
1:C:375:LYS:O	1:C:378:THR:HG22	2.15	0.47
1:C:458:ILE:HD11	1:C:629:TRP:HB2	1.97	0.47
1:D:239:VAL:HG12	1:D:251:LEU:HD21	1.97	0.46
1:D:283:ASP:HA	1:D:287:THR:CB	2.43	0.46
1:D:337:LYS:O	1:D:341:ILE:HG13	2.15	0.46
1:D:339:ARG:HG2	1:D:408:ARG:NH2	2.30	0.46
1:D:605:PRO:HA	1:D:613:VAL:HG22	1.97	0.46
1:A:537:MET:HB2	1:A:538:PRO:HD3	1.96	0.46
1:A:665:ILE:H	1:A:665:ILE:HD13	1.80	0.46
1:B:539:ARG:NH1	1:B:543:PHE:HD1	2.14	0.46
1:B:688:ARG:HD3	1:B:692:ARG:HH22	1.80	0.46
1:C:601:GLN:HG2	1:C:622:GLU:HG2	1.97	0.46
1:C:728:ARG:HD3	1:C:729:TYR:N	2.30	0.46
1:D:85:SER:C	1:D:86:GLN:HG3	2.35	0.46
1:D:380:THR:HG22	1:D:384:LEU:HD22	1.97	0.46
1:D:415:PRO:HA	1:D:420:ARG:CZ	2.45	0.46
1:A:339:ARG:CG	1:A:408:ARG:HH22	2.28	0.46
1:B:455:GLN:HG2	1:B:624:LEU:O	2.15	0.46
1:D:208:ILE:HG23	1:D:209:ASP:N	2.28	0.46
1:D:282:ASP:N	1:D:282:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LEU:CD1	1:B:294:VAL:HG13	2.46	0.46
1:B:388:ALA:HA	1:B:406:TYR:OH	2.15	0.46
1:C:284:ALA:O	1:C:286:MET:N	2.48	0.46
1:C:396:LEU:HD11	1:C:403:GLN:HA	1.97	0.46
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.50	0.46
1:D:538:PRO:CB	1:D:550:VAL:HG22	2.44	0.46
1:D:615:ARG:HG2	1:D:616:GLY:N	2.30	0.46
1:A:538:PRO:HB2	1:A:550:VAL:HG13	1.97	0.46
1:A:610:PRO:O	1:A:739:ARG:HB2	2.15	0.46
1:B:42:ARG:HA	1:B:234:MET:HE3	1.97	0.46
1:B:280:LEU:HD12	1:B:280:LEU:HA	1.77	0.46
1:B:507:PHE:CZ	1:B:511:TRP:HD1	2.33	0.46
1:B:542:ARG:HD2	1:B:544:GLU:O	2.15	0.46
1:C:442:THR:HG22	1:C:626:LEU:HD21	1.96	0.46
1:D:239:VAL:HA	1:D:291:ARG:NH1	2.30	0.46
1:B:161:ARG:HA	1:B:170:TRP:HH2	1.80	0.46
1:B:715:ARG:HG2	1:B:720:ALA:CB	2.44	0.46
1:D:212:LYS:HB3	1:D:213:THR:H	1.47	0.46
1:A:669:THR:HG22	1:A:732:LEU:HD13	1.98	0.46
1:B:337:LYS:HE2	1:B:358:PHE:CD1	2.51	0.46
1:C:665:ILE:HG12	1:C:752:SER:HB2	1.98	0.46
1:D:26:TYR:O	1:D:93:THR:HA	2.16	0.46
1:D:482:HIS:HA	1:D:493:SER:OG	2.16	0.46
1:B:337:LYS:HZ2	1:B:362:GLU:CD	2.19	0.46
1:C:452:LEU:HD11	1:C:499:LEU:CD2	2.46	0.46
1:C:522:ASP:OD1	1:C:522:ASP:N	2.47	0.46
1:C:585:TYR:HA	1:C:592:THR:HG21	1.98	0.46
1:C:669:THR:CG2	1:C:751:ARG:HH22	2.29	0.46
1:D:537:MET:HB2	1:D:538:PRO:HD3	1.98	0.46
1:D:636:THR:CG2	1:D:675:GLU:HG2	2.45	0.46
1:A:71:LEU:HD12	1:A:310:ALA:O	2.15	0.46
1:A:445:PRO:HD3	1:A:497:PHE:HE1	1.81	0.46
1:A:682:ARG:HA	1:A:682:ARG:HD3	1.52	0.46
1:D:448:ASP:OD2	1:D:449:ASP:N	2.49	0.46
1:D:544:GLU:HB2	1:D:545:ARG:HH22	1.81	0.46
1:A:5:GLU:OE2	1:A:311:LYS:HB2	2.15	0.46
1:A:110:VAL:CG2	1:A:235:LEU:HD12	2.45	0.46
1:A:441:PRO:O	1:A:444:VAL:HG22	2.15	0.46
1:A:537:MET:CB	1:A:538:PRO:HD3	2.46	0.46
1:B:688:ARG:NH1	1:B:740:GLU:OE2	2.49	0.46
1:C:164:ARG:HH11	1:C:164:ARG:HG3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:549:GLU:HG3	1:C:550:VAL:HG23	1.97	0.46
1:D:148:GLU:OE1	1:D:195:ARG:NH1	2.49	0.46
1:D:645:PRO:HG3	1:D:656:TYR:OH	2.15	0.46
1:A:612:LEU:HB3	1:A:754:ARG:CD	2.39	0.46
1:B:139:VAL:HG21	1:B:293:ILE:HG23	1.98	0.46
1:B:445:PRO:HG3	1:B:497:PHE:CD1	2.51	0.46
1:B:445:PRO:HB2	1:B:446:SER:H	1.62	0.46
1:B:538:PRO:HB3	1:B:550:VAL:HG22	1.98	0.46
1:C:691:PHE:HD2	1:C:736:LEU:HD22	1.79	0.46
1:D:84:ARG:O	1:D:85:SER:C	2.54	0.45
1:B:651:TRP:CH2	1:B:684:TRP:HB2	2.51	0.45
1:C:5:GLU:CD	1:C:311:LYS:HB2	2.36	0.45
1:C:349:TRP:O	1:C:350:GLN:HB2	2.16	0.45
1:A:208:ILE:HG23	1:A:209:ASP:N	2.31	0.45
1:A:474:LEU:HG	1:A:529:MET:CE	2.45	0.45
1:A:638:GLU:OE2	1:A:687:LYS:NZ	2.46	0.45
1:B:26:TYR:O	1:B:93:THR:HA	2.16	0.45
1:B:35:SER:O	1:B:223:HIS:CE1	2.69	0.45
1:D:247:ASP:OD1	1:D:247:ASP:N	2.48	0.45
1:D:634:PHE:HB3	1:D:730:LEU:HD22	1.99	0.45
1:B:576:VAL:HG13	1:B:756:CYS:CB	2.45	0.45
1:B:691:PHE:CE2	1:B:736:LEU:HD13	2.52	0.45
1:C:331:THR:N	1:C:334:GLU:OE1	2.45	0.45
1:C:333:ILE:HD12	1:C:380:THR:HG23	1.97	0.45
1:D:163:ILE:O	1:D:164:ARG:HB2	2.14	0.45
1:A:542:ARG:HE	1:A:547:LEU:HD12	1.80	0.45
1:B:417:ILE:HG13	1:B:421:ARG:CZ	2.47	0.45
1:C:612:LEU:HB3	1:C:754:ARG:CD	2.43	0.45
1:C:682:ARG:HB2	1:C:686:LEU:HB2	1.99	0.45
1:D:610:PRO:HB2	1:D:739:ARG:HA	1.98	0.45
1:D:685:HIS:O	1:D:688:ARG:HB2	2.17	0.45
1:B:5:GLU:CD	1:B:311:LYS:HB2	2.36	0.45
1:B:78:THR:OG1	1:B:93:THR:HG21	2.16	0.45
1:B:689:LEU:HD13	1:B:709:ALA:HA	1.99	0.45
1:D:682:ARG:NH2	1:D:716:LEU:HD13	2.31	0.45
1:D:682:ARG:HA	1:D:682:ARG:HD3	1.49	0.45
1:D:682:ARG:HB3	1:D:683:ALA:H	1.46	0.45
1:B:221:TYR:N	1:B:221:TYR:CD1	2.84	0.45
1:B:274:PRO:O	1:B:277:VAL:HG22	2.17	0.45
1:B:493:SER:OG	1:B:494:ALA:N	2.49	0.45
1:D:204:ARG:O	1:D:205:HIS:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:692:ARG:NE	1:D:737:ALA:O	2.49	0.45
1:A:15:SER:HB2	1:A:300:LEU:HD22	1.98	0.45
1:A:84:ARG:O	1:A:84:ARG:HG3	2.15	0.45
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.69	0.45
1:B:496:GLN:HA	1:B:553:VAL:HG13	1.97	0.45
1:C:228:ARG:HA	1:C:231:MET:CE	2.47	0.45
1:A:452:LEU:HD22	1:A:452:LEU:HA	1.78	0.45
1:A:538:PRO:HB3	1:A:550:VAL:HG22	1.98	0.45
1:B:208:ILE:HG23	1:B:209:ASP:N	2.31	0.45
1:C:397:THR:OG1	1:C:399:ARG:HG3	2.16	0.45
1:D:65:LEU:HA	1:D:65:LEU:HD23	1.58	0.45
1:A:208:ILE:HD13	1:A:209:ASP:N	2.23	0.45
1:A:469:ASP:N	1:A:469:ASP:OD1	2.48	0.45
1:A:618:SER:OG	1:A:619:GLY:N	2.49	0.45
1:C:100:ARG:HG3	1:C:100:ARG:NH1	2.31	0.45
1:D:7:PHE:HE2	1:A:11:PRO:HD3	1.81	0.45
1:A:163:ILE:HD12	1:A:170:TRP:CD2	2.51	0.45
1:A:251:LEU:O	1:A:291:ARG:NH2	2.40	0.45
1:A:413:LYS:O	1:A:415:PRO:HD3	2.17	0.45
1:B:118:ARG:HB2	1:B:289:LEU:HD13	1.98	0.45
1:B:356:LEU:HA	1:B:356:LEU:HD23	1.67	0.45
1:B:681:ASN:OD1	1:B:682:ARG:N	2.50	0.45
1:C:496:GLN:CD	1:C:553:VAL:HG22	2.38	0.45
1:C:728:ARG:HD3	1:C:729:TYR:H	1.82	0.45
1:A:136:ALA:HB2	1:A:293:ILE:HD11	1.99	0.44
1:A:312:ARG:HD3	1:A:315:TYR:CE2	2.52	0.44
1:B:110:VAL:HA	1:B:228:ARG:NH1	2.28	0.44
1:B:662:ILE:HD12	1:B:662:ILE:H	1.81	0.44
1:A:213:THR:O	1:A:213:THR:OG1	2.34	0.44
1:C:227:MET:O	1:C:231:MET:HE2	2.17	0.44
1:C:600:SER:HB3	1:C:732:LEU:HD21	1.99	0.44
1:D:59:GLU:HG2	1:D:262:ASN:HB3	2.00	0.44
1:D:369:GLY:O	1:D:371:SER:N	2.46	0.44
1:D:448:ASP:O	1:D:450:ALA:N	2.50	0.44
1:D:522:ASP:OD1	1:D:522:ASP:N	2.51	0.44
1:D:710:GLU:HG2	1:D:715:ARG:HG3	1.99	0.44
1:A:28:PRO:HG2	1:A:31:GLN:HG2	1.98	0.44
1:A:482:HIS:HA	1:A:493:SER:HB2	1.98	0.44
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.83	0.44
1:C:78:THR:OG1	1:C:93:THR:HG21	2.18	0.44
1:C:551:PRO:HB2	1:C:552:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:GLN:O	1:C:561:LYS:HD3	2.16	0.44
1:D:417:ILE:HD12	1:D:417:ILE:HA	1.73	0.44
1:D:417:ILE:O	1:D:419:ALA:N	2.46	0.44
1:D:700:GLU:HG2	1:D:704:LYS:HE3	1.98	0.44
1:B:104:LEU:O	1:B:108:THR:HG23	2.18	0.44
1:B:212:LYS:HB3	1:B:213:THR:H	1.45	0.44
1:B:320:PHE:HD1	1:B:320:PHE:O	2.00	0.44
1:B:396:LEU:CD1	1:B:403:GLN:HG2	2.45	0.44
1:B:413:LYS:HD3	1:B:544:GLU:OE1	2.16	0.44
1:B:452:LEU:HB3	1:B:498:LEU:HD13	2.00	0.44
1:C:113:GLU:OE2	1:C:232:ARG:NH2	2.50	0.44
1:C:452:LEU:HD22	1:C:452:LEU:HA	1.80	0.44
1:C:615:ARG:HG2	1:C:616:GLY:N	2.32	0.44
1:C:631:ASP:C	1:C:633:ALA:H	2.21	0.44
1:D:165:SER:O	1:D:166:TYR:HB2	2.17	0.44
1:D:337:LYS:HE3	1:D:337:LYS:HB2	1.57	0.44
1:D:530:THR:O	1:D:539:ARG:NH1	2.51	0.44
1:A:165:SER:O	1:A:166:TYR:HB2	2.17	0.44
1:A:530:THR:O	1:A:539:ARG:HD2	2.18	0.44
1:A:584:VAL:HG13	1:A:591:LEU:HD13	1.99	0.44
1:B:112:HIS:O	1:B:116:ARG:HB2	2.17	0.44
1:C:496:GLN:HG2	1:C:553:VAL:HG22	2.00	0.44
1:D:348:GLU:O	1:D:348:GLU:HG2	2.18	0.44
1:D:416:ASP:HB2	1:D:417:ILE:O	2.18	0.44
1:D:617:LYS:CB	1:D:620:LEU:HB2	2.44	0.44
1:A:273:PRO:HG2	1:A:276:VAL:CG2	2.48	0.44
1:A:710:GLU:HA	1:A:714:LEU:H	1.83	0.44
1:B:372:SER:OG	1:B:375:LYS:HB3	2.18	0.44
1:B:682:ARG:HB3	1:B:683:ALA:H	1.49	0.44
1:C:71:LEU:HD12	1:C:310:ALA:O	2.18	0.44
1:D:223:HIS:HE1	1:D:227:MET:HE2	1.82	0.44
1:D:333:ILE:HD12	1:D:380:THR:HG23	2.00	0.44
1:B:122:LEU:HD22	1:B:129:SER:OG	2.17	0.44
1:B:416:ASP:HB2	1:B:417:ILE:H	1.56	0.44
1:B:418:VAL:HA	1:B:421:ARG:CD	2.48	0.44
1:B:561:LYS:HG2	1:B:769:PHE:CE1	2.52	0.44
1:C:26:TYR:O	1:C:93:THR:HA	2.18	0.44
1:C:161:ARG:HA	1:C:170:TRP:HH2	1.81	0.44
1:A:5:GLU:O	1:A:7:PHE:N	2.51	0.44
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.59	0.44
1:A:650:SER:OG	1:A:651:TRP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ARG:HD3	1:B:236:ARG:CZ	2.47	0.44
1:B:605:PRO:HA	1:B:735:ALA:HB2	2.00	0.44
1:C:109:THR:HG22	1:C:228:ARG:HE	1.82	0.44
1:C:496:GLN:HA	1:C:553:VAL:CG1	2.42	0.44
1:D:5:GLU:CD	1:D:311:LYS:HB2	2.38	0.44
1:D:186:TYR:CZ	1:D:205:HIS:HD2	2.35	0.44
1:D:385:LEU:CD2	1:D:396:LEU:HB3	2.42	0.44
1:D:400:LEU:HD13	1:D:400:LEU:HA	1.62	0.44
1:A:387:PHE:CE2	1:A:427:LEU:HG	2.53	0.44
1:A:452:LEU:HB3	1:A:498:LEU:HD13	1.99	0.44
1:A:563:GLN:O	1:A:566:SER:OG	2.33	0.44
1:A:638:GLU:O	1:A:668:LEU:HA	2.18	0.44
1:B:7:PHE:CD1	1:B:319:MET:HE3	2.53	0.44
1:B:111:LEU:HD22	1:B:296:ALA:HB2	1.98	0.44
1:C:26:TYR:HD2	1:C:93:THR:HG22	1.83	0.44
1:C:44:LEU:HD21	1:C:65:LEU:HD21	1.98	0.44
1:D:57:GLU:HG2	1:D:58:PHE:CE2	2.53	0.43
1:D:163:ILE:HD11	1:D:179:TYR:CE1	2.53	0.43
1:D:482:HIS:CE1	1:D:494:ALA:HB2	2.53	0.43
1:D:561:LYS:HE2	1:D:771:PRO:HD2	2.00	0.43
1:A:168:ASP:HA	1:A:178:ARG:O	2.18	0.43
1:A:468:HIS:CE1	1:A:508:TYR:HB2	2.53	0.43
1:B:81:PRO:HG2	1:B:169:VAL:HG22	2.00	0.43
1:B:379:VAL:O	1:B:383:VAL:HG12	2.18	0.43
1:C:488:GLU:HG2	1:C:489:THR:N	2.33	0.43
1:D:187:LEU:HD23	1:D:187:LEU:HA	1.74	0.43
1:D:569:ILE:HB	1:D:578:ARG:NH1	2.33	0.43
1:D:569:ILE:CG2	1:D:574:GLN:HB3	2.47	0.43
1:D:625:GLU:OE1	1:D:628:ARG:NH1	2.52	0.43
1:D:679:ALA:HA	1:D:716:LEU:O	2.18	0.43
1:D:709:ALA:O	1:D:713:GLY:N	2.50	0.43
1:B:11:PRO:HB3	1:C:7:PHE:CE2	2.52	0.43
1:B:127:GLU:OE2	1:B:128:PRO:HD3	2.18	0.43
1:B:507:PHE:HB2	1:B:560:LEU:HD13	1.99	0.43
1:C:339:ARG:HG2	1:C:408:ARG:CZ	2.49	0.43
1:D:228:ARG:C	1:D:228:ARG:HD3	2.39	0.43
1:D:433:PHE:CB	1:D:476:THR:HG22	2.49	0.43
1:D:638:GLU:O	1:D:668:LEU:HA	2.19	0.43
1:A:353:GLU:HB2	1:A:421:ARG:HE	1.83	0.43
1:A:743:TRP:CZ3	1:A:747:PHE:HE2	2.36	0.43
1:C:149:GLU:HG2	1:C:150:ASP:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:ARG:O	1:C:542:ARG:HG3	2.15	0.43
1:C:610:PRO:O	1:C:739:ARG:HB2	2.18	0.43
1:C:669:THR:HG21	1:C:736:LEU:HD12	1.99	0.43
1:D:7:PHE:CE2	1:A:11:PRO:HD3	2.53	0.43
1:D:11:PRO:O	1:D:12:LEU:HD23	2.19	0.43
1:D:13:SER:OG	1:D:16:GLN:HG2	2.18	0.43
1:D:265:PHE:O	1:D:269:ASN:N	2.51	0.43
1:D:418:VAL:N	1:D:421:ARG:HD2	2.31	0.43
1:D:571:ASP:O	1:D:574:GLN:N	2.51	0.43
1:D:650:SER:OG	1:D:651:TRP:N	2.50	0.43
1:D:710:GLU:HA	1:D:714:LEU:H	1.84	0.43
1:A:352:SER:O	1:A:354:SER:N	2.52	0.43
1:A:614:VAL:HG12	1:A:754:ARG:HH11	1.83	0.43
1:C:331:THR:O	1:C:335:THR:HG23	2.18	0.43
1:C:433:PHE:CD1	1:C:476:THR:HG22	2.51	0.43
1:D:26:TYR:CD2	1:D:93:THR:HG22	2.50	0.43
1:D:29:PRO:HG3	1:D:80:GLU:HG3	2.00	0.43
1:D:78:THR:OG1	1:D:93:THR:HG21	2.18	0.43
1:D:190:TYR:CD1	1:D:190:TYR:C	2.92	0.43
1:D:352:SER:O	1:D:354:SER:N	2.52	0.43
1:A:23:GLN:OE1	1:A:92:MET:HG3	2.19	0.43
1:A:395:LYS:HG3	1:A:395:LYS:O	2.17	0.43
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.66	0.43
1:C:520:GLY:O	1:C:521:ILE:C	2.56	0.43
1:D:186:TYR:CZ	1:D:205:HIS:CD2	3.06	0.43
1:D:666:GLY:O	1:D:751:ARG:HD2	2.18	0.43
1:C:162:LEU:HA	1:C:162:LEU:HD23	1.84	0.43
1:C:666:GLY:N	1:C:752:SER:HB3	2.34	0.43
1:D:565:ARG:O	1:D:568:GLY:N	2.51	0.43
1:A:149:GLU:OE1	1:A:151:MET:SD	2.77	0.43
1:A:156:HIS:ND1	1:A:177:ALA:HB3	2.34	0.43
1:A:482:HIS:HA	1:A:493:SER:CB	2.49	0.43
1:C:44:LEU:CD2	1:C:65:LEU:HD21	2.48	0.43
1:C:110:VAL:HG21	1:C:232:ARG:HA	2.00	0.43
1:C:139:VAL:HG22	1:C:297:ASN:OD1	2.19	0.43
1:C:164:ARG:HH11	1:C:164:ARG:CG	2.31	0.43
1:C:533:VAL:O	1:C:538:PRO:HD2	2.19	0.43
1:C:654:ASP:OD1	1:C:654:ASP:N	2.49	0.43
1:D:59:GLU:HG2	1:D:262:ASN:CB	2.49	0.43
1:D:353:GLU:HB2	1:D:421:ARG:HE	1.83	0.43
1:D:433:PHE:CE2	1:D:438:TRP:CD1	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:GLN:O	1:A:458:ILE:HG22	2.19	0.43
1:A:469:ASP:O	1:A:472:VAL:HG23	2.19	0.43
1:C:417:ILE:C	1:C:419:ALA:N	2.72	0.43
1:D:339:ARG:HG2	1:D:408:ARG:NH1	2.33	0.43
1:A:113:GLU:OE1	1:A:232:ARG:NH2	2.52	0.43
1:A:511:TRP:CZ3	1:A:519:ALA:HB3	2.54	0.43
1:B:455:GLN:NE2	1:B:766:TRP:HZ2	2.17	0.43
1:C:465:GLU:CD	1:C:629:TRP:HE1	2.22	0.43
1:C:638:GLU:O	1:C:668:LEU:HA	2.19	0.43
1:A:551:PRO:HB2	1:A:552:PRO:CD	2.47	0.43
1:C:576:VAL:HG13	1:C:756:CYS:HB2	2.00	0.43
1:D:11:PRO:HB3	1:A:7:PHE:CE2	2.54	0.42
1:D:615:ARG:HG2	1:D:616:GLY:H	1.84	0.42
1:A:477:ARG:HD3	1:A:542:ARG:N	2.28	0.42
1:B:87:VAL:HG13	1:B:88:PRO:O	2.19	0.42
1:B:468:HIS:NE2	1:B:521:ILE:HG21	2.34	0.42
1:B:554:GLU:HA	1:B:557:GLN:HG3	2.01	0.42
1:C:385:LEU:N	1:C:386:PRO:CD	2.82	0.42
1:C:684:TRP:HE1	1:C:742:GLU:HA	1.83	0.42
1:D:172:ARG:H	1:D:172:ARG:HD3	1.84	0.42
1:D:268:PHE:O	1:D:270:SER:N	2.52	0.42
1:D:391:GLN:OE1	1:D:542:ARG:NH1	2.51	0.42
1:B:72:ARG:NH1	1:B:90:LYS:HA	2.34	0.42
1:B:470:ILE:H	1:B:470:ILE:HG12	1.57	0.42
1:B:522:ASP:OD1	1:B:522:ASP:N	2.52	0.42
1:C:760:TRP:CZ2	1:C:764:THR:HG21	2.54	0.42
1:D:123:THR:O	1:D:123:THR:OG1	2.33	0.42
1:D:235:LEU:O	1:D:238:ALA:N	2.49	0.42
1:D:604:THR:O	1:D:613:VAL:HG13	2.19	0.42
1:B:59:GLU:HG2	1:B:262:ASN:CB	2.49	0.42
1:B:447:CYS:HB2	1:B:494:ALA:HB1	2.01	0.42
1:B:520:GLY:O	1:B:523:GLY:N	2.53	0.42
1:B:709:ALA:CB	1:B:714:LEU:HB2	2.49	0.42
1:D:379:VAL:O	1:D:383:VAL:HG12	2.19	0.42
1:A:217:ASP:C	1:A:219:GLU:N	2.72	0.42
1:A:232:ARG:HD3	1:A:236:ARG:NH2	2.35	0.42
1:A:366:ASP:O	1:A:370:SER:HB2	2.19	0.42
1:A:640:VAL:HB	1:A:667:ASN:ND2	2.35	0.42
1:B:119:ALA:O	1:B:122:LEU:HB2	2.19	0.42
1:C:433:PHE:CE2	1:C:438:TRP:NE1	2.87	0.42
1:C:561:LYS:HE3	1:C:769:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:TYR:HB3	1:D:93:THR:HG22	2.02	0.42
1:D:59:GLU:H	1:D:59:GLU:HG3	1.46	0.42
1:D:244:LYS:HA	1:D:248:ASP:OD2	2.20	0.42
1:D:356:LEU:HD23	1:D:356:LEU:HA	1.88	0.42
1:A:114:GLU:HB3	1:A:292:LEU:HD23	2.01	0.42
1:A:139:VAL:HG21	1:A:293:ILE:HG23	2.00	0.42
1:A:337:LYS:O	1:A:341:ILE:HG13	2.20	0.42
1:A:469:ASP:C	1:A:471:VAL:N	2.72	0.42
1:A:542:ARG:O	1:A:542:ARG:HG3	2.12	0.42
1:B:740:GLU:HB3	1:B:741:GLU:H	1.66	0.42
1:C:105:LEU:HD13	1:C:105:LEU:HA	1.80	0.42
1:C:183:ILE:HD12	1:C:183:ILE:N	2.24	0.42
1:C:492:SER:O	1:C:496:GLN:HG3	2.19	0.42
1:D:11:PRO:HB3	1:A:7:PHE:CD2	2.54	0.42
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.65	0.42
1:C:128:PRO:O	1:C:131:TRP:HB3	2.19	0.42
1:C:437:PRO:HB2	1:C:460:LEU:CD1	2.50	0.42
1:D:386:PRO:O	1:D:389:MET:N	2.53	0.42
1:D:734:ALA:O	1:D:736:LEU:N	2.44	0.42
1:A:26:TYR:O	1:A:93:THR:HA	2.20	0.42
1:A:133:TYR:CZ	1:A:137:LEU:HD11	2.55	0.42
1:A:511:TRP:CE3	1:A:521:ILE:HD11	2.54	0.42
1:B:58:PHE:HE2	1:B:405:ARG:HD3	1.81	0.42
1:B:247:ASP:OD1	1:B:247:ASP:N	2.50	0.42
1:A:122:LEU:HD22	1:A:129:SER:OG	2.19	0.42
1:A:300:LEU:HA	1:A:300:LEU:HD23	1.63	0.42
1:A:341:ILE:HG12	1:A:349:TRP:CE2	2.55	0.42
1:A:372:SER:OG	1:A:373:ALA:N	2.50	0.42
1:A:433:PHE:CB	1:A:476:THR:HG22	2.48	0.42
1:B:28:PRO:HG2	1:B:31:GLN:HG2	2.01	0.42
1:B:45:LEU:HD21	1:B:107:LEU:HD13	2.02	0.42
1:B:623:THR:HG22	1:B:634:PHE:CZ	2.54	0.42
1:B:639:HIS:HB3	1:B:641:ALA:O	2.20	0.42
1:C:12:LEU:HB3	1:C:16:GLN:HG3	2.02	0.42
1:C:186:TYR:OH	1:C:228:ARG:HD2	2.19	0.42
1:C:460:LEU:HD21	1:C:501:ALA:HB1	2.02	0.42
1:C:496:GLN:CG	1:C:553:VAL:HG22	2.50	0.42
1:D:17:PHE:CD1	1:D:307:VAL:HG21	2.55	0.42
1:D:23:GLN:HG3	1:D:90:LYS:HD3	2.02	0.42
1:D:535:GLU:HG3	1:D:536:GLY:N	2.34	0.42
1:A:346:LEU:HB3	1:A:347:ASP:H	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PHE:CD2	1:A:476:THR:HG22	2.54	0.42
1:B:112:HIS:NE2	1:B:140:THR:HG23	2.35	0.42
1:B:216:VAL:HG12	1:B:217:ASP:H	1.85	0.42
1:B:315:TYR:O	1:B:319:MET:HG3	2.20	0.42
1:B:337:LYS:HE3	1:B:337:LYS:HB2	1.30	0.42
1:B:357:HIS:O	1:B:360:VAL:HB	2.20	0.42
1:B:674:VAL:HG11	1:B:679:ALA:H	1.85	0.42
1:C:196:ASP:OD1	1:C:197:PRO:HD2	2.20	0.42
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.68	0.42
1:C:610:PRO:HB2	1:C:738:GLN:O	2.19	0.42
1:C:628:ARG:CA	1:C:631:ASP:HB2	2.33	0.42
1:C:651:TRP:CH2	1:C:684:TRP:HB2	2.54	0.42
1:D:292:LEU:HD12	1:D:292:LEU:HA	1.87	0.42
1:D:639:HIS:HA	1:D:667:ASN:O	2.20	0.42
1:D:671:LEU:HD23	1:D:671:LEU:HA	1.67	0.42
1:A:445:PRO:HG3	1:A:497:PHE:HD1	1.84	0.42
1:A:655:LEU:HB2	1:A:656:TYR:CD1	2.54	0.42
1:B:221:TYR:N	1:B:221:TYR:HD1	2.17	0.42
1:C:764:THR:N	1:C:765:PRO:HD2	2.35	0.42
1:D:555:ALA:HA	1:D:558:SER:OG	2.20	0.41
1:D:569:ILE:HB	1:D:578:ARG:CZ	2.50	0.41
1:D:610:PRO:HB2	1:D:738:GLN:O	2.19	0.41
1:A:44:LEU:HA	1:A:44:LEU:HD22	1.80	0.41
1:A:123:THR:O	1:A:123:THR:OG1	2.32	0.41
1:A:152:ARG:HH21	1:A:152:ARG:HD3	1.64	0.41
1:A:445:PRO:HG3	1:A:497:PHE:CD1	2.55	0.41
1:A:630:ASN:O	1:A:632:GLU:N	2.53	0.41
1:A:665:ILE:HG12	1:A:752:SER:HB2	2.02	0.41
1:A:690:MET:O	1:A:694:LEU:HD12	2.20	0.41
1:B:342:LYS:HG3	1:C:80:GLU:OE1	2.18	0.41
1:C:420:ARG:O	1:C:423:VAL:HB	2.19	0.41
1:C:682:ARG:HD3	1:C:682:ARG:HA	1.57	0.41
1:D:218:LEU:O	1:D:222:ARG:HG3	2.20	0.41
1:D:239:VAL:HG21	1:D:292:LEU:HD22	2.02	0.41
1:D:679:ALA:HB2	1:D:720:ALA:HA	2.01	0.41
1:A:35:SER:N	1:A:99:GLN:OE1	2.35	0.41
1:A:155:GLU:HG3	1:A:174:LYS:HE2	2.02	0.41
1:B:128:PRO:HG3	1:B:275:SER:HB2	2.03	0.41
1:C:349:TRP:CD1	1:C:349:TRP:C	2.94	0.41
1:C:365:LEU:O	1:C:369:GLY:N	2.37	0.41
1:C:429:GLN:HG2	1:C:480:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:THR:O	1:D:455:GLN:HG3	2.20	0.41
1:D:488:GLU:HG2	1:D:489:THR:N	2.34	0.41
1:D:655:LEU:HD23	1:D:745:ALA:HA	2.01	0.41
1:D:679:ALA:CB	1:D:720:ALA:HA	2.50	0.41
1:A:34:TYR:CD2	1:A:224:LEU:HD12	2.55	0.41
1:A:38:LEU:HD13	1:A:230:GLN:OE1	2.19	0.41
1:A:742:GLU:HG3	1:A:743:TRP:H	1.85	0.41
1:B:23:GLN:HG3	1:B:90:LYS:HD3	2.03	0.41
1:B:299:LEU:HA	1:B:303:VAL:CG2	2.50	0.41
1:B:387:PHE:CD2	1:B:427:LEU:HG	2.56	0.41
1:B:448:ASP:O	1:B:450:ALA:N	2.54	0.41
1:C:432:ARG:HA	1:C:435:GLU:OE1	2.20	0.41
1:C:511:TRP:CD2	1:C:521:ILE:HG12	2.55	0.41
1:C:595:LEU:HD23	1:C:595:LEU:HA	1.73	0.41
1:D:159:TYR:OH	1:D:171:SER:HA	2.21	0.41
1:A:17:PHE:CE1	1:A:307:VAL:HG21	2.56	0.41
1:A:253:THR:O	1:A:256:ASP:HB2	2.20	0.41
1:A:542:ARG:HD3	1:A:547:LEU:N	2.32	0.41
1:B:381:SER:OG	1:B:403:GLN:OE1	2.36	0.41
1:B:455:GLN:CD	1:B:766:TRP:HZ2	2.24	0.41
1:B:682:ARG:HD3	1:B:682:ARG:HA	1.62	0.41
1:C:1:MET:HA	1:C:4:LYS:CB	2.41	0.41
1:D:67:THR:H	1:D:100:ARG:NH1	2.18	0.41
1:D:73:ASP:HB3	1:D:91:VAL:HG22	2.03	0.41
1:D:507:PHE:O	1:D:511:TRP:HB2	2.20	0.41
1:A:74:ILE:HD12	1:A:74:ILE:HA	1.78	0.41
1:A:153:TYR:CE1	1:B:134:ASN:HB3	2.55	0.41
1:A:583:PRO:HD3	1:A:660:GLU:OE1	2.21	0.41
1:A:617:LYS:HB3	1:A:620:LEU:HB2	2.02	0.41
1:B:151:MET:O	1:B:157:ARG:HD3	2.20	0.41
1:C:541:ALA:O	1:C:542:ARG:C	2.59	0.41
1:C:713:GLY:O	1:C:716:LEU:HG	2.20	0.41
1:D:12:LEU:HD12	1:D:17:PHE:HA	2.02	0.41
1:D:44:LEU:HD21	1:D:65:LEU:HD21	2.02	0.41
1:D:457:GLY:C	1:D:626:LEU:HB2	2.41	0.41
1:D:565:ARG:HH21	1:D:771:PRO:CB	2.33	0.41
1:B:41:ILE:H	1:B:41:ILE:HG12	1.66	0.41
1:B:66:GLY:HA3	1:B:100:ARG:NH1	2.35	0.41
1:B:183:ILE:H	1:B:183:ILE:CD1	2.14	0.41
1:B:469:ASP:C	1:B:471:VAL:N	2.74	0.41
1:B:477:ARG:HD3	1:B:541:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:PRO:HB2	1:B:552:PRO:CD	2.49	0.41
1:B:642:PRO:HD3	1:B:651:TRP:CH2	2.56	0.41
1:C:429:GLN:HG2	1:C:480:ALA:HB2	2.02	0.41
1:C:688:ARG:CZ	1:C:740:GLU:OE2	2.68	0.41
1:D:153:TYR:CD2	1:C:134:ASN:HB3	2.56	0.41
1:D:739:ARG:HG2	1:D:740:GLU:O	2.21	0.41
1:A:23:GLN:HA	1:A:90:LYS:O	2.21	0.41
1:A:86:GLN:HE21	1:A:173:ASN:ND2	2.18	0.41
1:A:255:THR:O	1:A:259:GLN:HG3	2.21	0.41
1:A:634:PHE:CD1	1:A:634:PHE:N	2.88	0.41
1:B:154:GLY:O	1:B:157:ARG:HB2	2.21	0.41
1:B:249:ILE:N	1:B:249:ILE:HD12	2.35	0.41
1:B:337:LYS:HE2	1:B:358:PHE:CE1	2.56	0.41
1:B:390:PHE:HD2	1:B:476:THR:OG1	2.02	0.41
1:B:599:ALA:O	1:B:758:LEU:HD23	2.21	0.41
1:C:86:GLN:CD	1:C:172:ARG:HD3	2.40	0.41
1:C:414:ASP:HB3	1:C:419:ALA:HB1	2.03	0.41
1:C:641:ALA:N	1:C:667:ASN:OD1	2.51	0.41
1:C:671:LEU:HD11	1:C:691:PHE:HE1	1.85	0.41
1:C:760:TRP:CE2	1:C:764:THR:HG21	2.56	0.41
1:A:87:VAL:CG2	1:A:88:PRO:HD2	2.49	0.41
1:A:87:VAL:HG13	1:A:88:PRO:O	2.21	0.41
1:A:119:ALA:O	1:A:122:LEU:HB2	2.20	0.41
1:A:416:ASP:HB2	1:A:417:ILE:H	1.44	0.41
1:A:605:PRO:HG3	1:A:734:ALA:HB3	2.03	0.41
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.61	0.41
1:B:312:ARG:HD3	1:B:315:TYR:CD2	2.55	0.41
1:B:596:LEU:HD13	1:B:669:THR:HA	2.02	0.41
1:B:628:ARG:HA	1:B:631:ASP:CB	2.41	0.41
1:C:172:ARG:HH11	1:C:172:ARG:HG3	1.84	0.41
1:D:66:GLY:HA2	1:A:322:ALA:HB1	2.03	0.41
1:D:355:LYS:HD2	1:D:359:ASP:OD2	2.21	0.41
1:D:391:GLN:HE21	1:D:391:GLN:HB3	1.62	0.41
1:D:482:HIS:ND1	1:D:494:ALA:HB2	2.36	0.41
1:D:740:GLU:HB3	1:D:741:GLU:H	1.68	0.41
1:A:17:PHE:CD1	1:A:307:VAL:HG21	2.56	0.41
1:A:330:LEU:HA	1:A:330:LEU:HD23	1.83	0.41
1:A:342:LYS:C	1:A:343:GLU:HG2	2.40	0.41
1:A:511:TRP:HH2	1:A:519:ALA:HB3	1.83	0.41
1:B:73:ASP:HB3	1:B:91:VAL:HG22	2.03	0.41
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:SER:OG	1:B:619:GLY:N	2.54	0.41
1:B:720:ALA:HB1	1:B:723:ILE:HB	2.03	0.41
1:C:18:LEU:HA	1:C:18:LEU:HD23	1.72	0.41
1:C:86:GLN:NE2	1:C:172:ARG:HD3	2.36	0.41
1:C:349:TRP:O	1:C:349:TRP:CD1	2.74	0.41
1:C:523:GLY:HA2	1:C:526:ARG:NH2	2.36	0.41
1:C:630:ASN:O	1:C:632:GLU:N	2.54	0.41
1:C:639:HIS:HB3	1:C:641:ALA:O	2.21	0.41
1:C:665:ILE:H	1:C:665:ILE:HD13	1.86	0.41
1:D:420:ARG:O	1:D:423:VAL:HB	2.20	0.41
1:D:563:GLN:O	1:D:566:SER:OG	2.39	0.41
1:A:31:GLN:NE2	1:A:95:ILE:O	2.54	0.41
1:A:168:ASP:OD1	1:A:180:ARG:N	2.38	0.41
1:B:44:LEU:HD22	1:B:44:LEU:HA	1.68	0.41
1:C:164:ARG:CG	1:C:164:ARG:NH1	2.83	0.41
1:C:600:SER:HA	1:C:603:SER:OG	2.21	0.41
1:C:678:SER:OG	1:C:679:ALA:N	2.51	0.41
1:D:67:THR:H	1:D:100:ARG:HH12	1.69	0.40
1:D:396:LEU:HD13	1:D:397:THR:N	2.36	0.40
1:D:416:ASP:HB2	1:D:417:ILE:H	1.25	0.40
1:A:642:PRO:HD3	1:A:651:TRP:CE2	2.56	0.40
1:A:742:GLU:HG3	1:A:743:TRP:N	2.36	0.40
1:B:18:LEU:HB2	1:B:146:CYS:SG	2.61	0.40
1:B:404:ARG:HH11	1:B:404:ARG:HD2	1.72	0.40
1:B:488:GLU:OE1	1:B:489:THR:HG22	2.21	0.40
1:C:173:ASN:O	1:C:175:GLY:O	2.39	0.40
1:C:238:ALA:HB2	1:C:249:ILE:HD13	2.02	0.40
1:C:691:PHE:CD2	1:C:736:LEU:HD22	2.56	0.40
1:D:507:PHE:CD1	1:D:560:LEU:HD22	2.56	0.40
1:A:596:LEU:HD21	1:A:665:ILE:HG22	2.03	0.40
1:B:26:TYR:HD2	1:B:93:THR:HG22	1.85	0.40
1:C:223:HIS:CE1	1:C:227:MET:CE	3.00	0.40
1:C:537:MET:HE2	1:C:537:MET:HB3	1.83	0.40
1:D:26:TYR:CD1	1:D:163:ILE:HG22	2.55	0.40
1:D:284:ALA:C	1:D:286:MET:H	2.22	0.40
1:D:437:PRO:HD3	1:D:479:PHE:CE2	2.57	0.40
1:D:496:GLN:CA	1:D:553:VAL:HG13	2.45	0.40
1:D:549:GLU:CG	1:D:550:VAL:HG23	2.49	0.40
1:D:596:LEU:HD13	1:D:669:THR:HA	2.03	0.40
1:A:475:LEU:HD21	1:A:504:CYS:SG	2.61	0.40
1:A:671:LEU:HD11	1:A:691:PHE:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:HH22	1:B:212:LYS:HZ3	1.68	0.40
1:B:585:TYR:CD1	1:B:637:ILE:HG21	2.56	0.40
1:B:728:ARG:NE	1:B:728:ARG:HA	2.36	0.40
1:C:208:ILE:HG12	1:C:221:TYR:CE2	2.56	0.40
1:C:283:ASP:HA	1:C:287:THR:OG1	2.21	0.40
1:C:292:LEU:HD12	1:C:292:LEU:HA	1.84	0.40
1:C:349:TRP:O	1:C:350:GLN:CB	2.69	0.40
1:D:320:PHE:HD1	1:D:320:PHE:O	2.05	0.40
1:D:584:VAL:HG13	1:D:591:LEU:HD13	2.04	0.40
1:A:549:GLU:O	1:A:550:VAL:HB	2.21	0.40
1:B:323:LEU:O	1:C:326:THR:HG21	2.22	0.40
1:B:331:THR:HG23	1:B:334:GLU:OE1	2.21	0.40
1:B:437:PRO:HG3	1:B:479:PHE:CE2	2.54	0.40
1:B:456:ALA:O	1:B:460:LEU:HG	2.21	0.40
1:B:734:ALA:O	1:B:738:GLN:HG3	2.22	0.40
1:C:151:MET:O	1:C:157:ARG:HG2	2.22	0.40
1:C:404:ARG:HH11	1:C:404:ARG:HD2	1.73	0.40
1:C:651:TRP:HE1	1:C:683:ALA:HA	1.83	0.40
1:C:706:LEU:HD12	1:C:714:LEU:HD23	2.04	0.40
1:D:161:ARG:O	1:D:162:LEU:O	2.40	0.40
1:D:686:LEU:HD21	1:D:712:GLN:HB3	2.04	0.40
1:A:65:LEU:HA	1:A:65:LEU:HD23	1.52	0.40
1:A:218:LEU:O	1:A:222:ARG:HG3	2.21	0.40
1:A:417:ILE:O	1:A:418:VAL:HB	2.22	0.40
1:A:447:CYS:HB2	1:A:494:ALA:HB1	2.03	0.40
1:A:760:TRP:HE3	1:A:761:ASP:OD1	2.03	0.40
1:B:507:PHE:CZ	1:B:511:TRP:CD1	3.09	0.40
1:B:597:LEU:HD22	1:B:623:THR:HB	2.04	0.40
1:C:366:ASP:O	1:C:370:SER:HB2	2.21	0.40
1:C:482:HIS:HA	1:C:493:SER:CB	2.52	0.40

All (3) 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:D:85:SER:N	1:C:211:ASP:OD2[4_457]	1.94	0.26
1:D:84:ARG:N	1:C:211:ASP:OD2[4_457]	2.13	0.07
1:A:236:ARG:NH1	1:B:278:GLU:OE1[4_447]	2.18	0.02

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	769/771 (100%)	613 (80%)	105 (14%)	51 (7%)	1	12
1	B	769/771 (100%)	605 (79%)	117 (15%)	47 (6%)	1	13
1	C	769/771 (100%)	612 (80%)	104 (14%)	53 (7%)	1	11
1	D	769/771 (100%)	609 (79%)	105 (14%)	55 (7%)	1	10
All	All	3076/3084 (100%)	2439 (79%)	431 (14%)	206 (7%)	1	12

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4	LYS
1	D	36	TRP
1	D	127	GLU
1	D	200	VAL
1	D	205	HIS
1	D	208	ILE
1	D	283	ASP
1	D	350	GLN
1	D	353	GLU
1	D	538	PRO
1	D	551	PRO
1	D	552	PRO
1	D	565	ARG
1	D	618	SER
1	D	633	ALA
1	D	645	PRO
1	D	650	SER
1	D	682	ARG
1	D	727	ALA
1	A	4	LYS
1	A	36	TRP
1	A	127	GLU

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Mol	Chain	Res	Type
1	A	200	VAL
1	A	205	HIS
1	A	208	ILE
1	A	241	ALA
1	A	283	ASP
1	A	350	GLN
1	A	353	GLU
1	A	444	VAL
1	A	551	PRO
1	A	552	PRO
1	A	565	ARG
1	A	618	SER
1	A	631	ASP
1	A	633	ALA
1	A	645	PRO
1	A	650	SER
1	A	682	ARG
1	A	721	GLY
1	A	727	ALA
1	A	770	GLU
1	B	4	LYS
1	B	6	ILE
1	B	127	GLU
1	B	205	HIS
1	B	208	ILE
1	B	241	ALA
1	B	283	ASP
1	B	353	GLU
1	B	551	PRO
1	B	552	PRO
1	B	618	SER
1	B	633	ALA
1	B	645	PRO
1	B	650	SER
1	B	682	ARG
1	B	770	GLU
1	C	4	LYS
1	C	6	ILE
1	C	36	TRP
1	C	127	GLU
1	C	205	HIS
1	C	208	ILE

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Mol	Chain	Res	Type
1	C	283	ASP
1	C	350	GLN
1	C	353	GLU
1	C	551	PRO
1	C	552	PRO
1	C	618	SER
1	C	631	ASP
1	C	633	ALA
1	C	645	PRO
1	C	650	SER
1	C	682	ARG
1	C	727	ALA
1	C	770	GLU
1	D	6	ILE
1	D	211	ASP
1	D	241	ALA
1	D	417	ILE
1	D	444	VAL
1	D	450	ALA
1	D	467	GLY
1	D	587	HIS
1	D	631	ASP
1	D	685	HIS
1	D	695	SER
1	D	720	ALA
1	D	721	GLY
1	A	6	ILE
1	A	163	ILE
1	A	211	ASP
1	A	417	ILE
1	A	450	ALA
1	A	467	GLY
1	A	569	ILE
1	A	685	HIS
1	A	695	SER
1	A	718	SER
1	A	720	ALA
1	B	36	TRP
1	B	81	PRO
1	B	162	LEU
1	B	200	VAL
1	B	211	ASP

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Mol	Chain	Res	Type
1	B	350	GLN
1	B	417	ILE
1	B	444	VAL
1	B	445	PRO
1	B	467	GLY
1	B	538	PRO
1	B	565	ARG
1	B	587	HIS
1	B	685	HIS
1	B	695	SER
1	B	721	GLY
1	C	81	PRO
1	C	211	ASP
1	C	241	ALA
1	C	417	ILE
1	C	444	VAL
1	C	445	PRO
1	C	450	ALA
1	C	467	GLY
1	C	565	ARG
1	C	587	HIS
1	C	685	HIS
1	C	721	GLY
1	D	162	LEU
1	D	164	ARG
1	D	416	ASP
1	D	445	PRO
1	D	569	ILE
1	D	718	SER
1	D	770	GLU
1	A	162	LEU
1	A	445	PRO
1	A	538	PRO
1	A	587	HIS
1	B	450	ALA
1	B	569	ILE
1	B	631	ASP
1	B	718	SER
1	B	720	ALA
1	C	200	VAL
1	C	248	ASP
1	C	449	ASP

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Mol	Chain	Res	Type
1	C	538	PRO
1	C	695	SER
1	C	720	ALA
1	D	81	PRO
1	D	620	LEU
1	A	81	PRO
1	A	566	SER
1	B	164	ARG
1	B	727	ALA
1	C	162	LEU
1	C	164	ARG
1	C	281	GLU
1	C	392	ASP
1	C	448	ASP
1	C	569	ILE
1	C	620	LEU
1	D	466	GLY
1	D	519	ALA
1	D	736	LEU
1	A	166	TYR
1	A	248	ASP
1	A	392	ASP
1	A	519	ALA
1	A	537	MET
1	A	550	VAL
1	A	648	ASN
1	A	673	ALA
1	B	620	LEU
1	C	537	MET
1	C	632	GLU
1	C	648	ASN
1	C	718	SER
1	D	126	ASP
1	D	414	ASP
1	D	550	VAL
1	D	648	ASN
1	D	728	ARG
1	A	620	LEU
1	A	736	LEU
1	B	163	ILE
1	B	166	TYR
1	B	168	ASP

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Mol	Chain	Res	Type
1	B	414	ASP
1	B	550	VAL
1	C	247	ASP
1	C	550	VAL
1	D	160	PRO
1	B	568	GLY
1	C	163	ILE
1	C	466	GLY
1	C	568	GLY
1	D	418	VAL
1	D	537	MET
1	D	163	ILE
1	A	568	GLY
1	D	640	VAL
1	D	672	PRO
1	B	160	PRO

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	651/651 (100%)	560 (86%)	91 (14%)	3	17
1	B	651/651 (100%)	558 (86%)	93 (14%)	3	17
1	C	651/651 (100%)	553 (85%)	98 (15%)	3	15
1	D	651/651 (100%)	558 (86%)	93 (14%)	3	17
All	All	2604/2604 (100%)	2229 (86%)	375 (14%)	3	16

All (375) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1	MET
1	D	3	THR
1	D	7	PHE
1	D	12	LEU
1	D	52	LEU

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Mol	Chain	Res	Type
1	D	62	ILE
1	D	63	CYS
1	D	64	PHE
1	D	65	LEU
1	D	75	ASN
1	D	86	GLN
1	D	87	VAL
1	D	99	GLN
1	D	106	LEU
1	D	109	THR
1	D	110	VAL
1	D	130	VAL
1	D	140	THR
1	D	151	MET
1	D	157	ARG
1	D	163	ILE
1	D	164	ARG
1	D	165	SER
1	D	167	TYR
1	D	172	ARG
1	D	176	GLU
1	D	183	ILE
1	D	189	SER
1	D	193	TYR
1	D	198	ASP
1	D	208	ILE
1	D	211	ASP
1	D	212	LYS
1	D	227	MET
1	D	243	VAL
1	D	249	ILE
1	D	251	LEU
1	D	262	ASN
1	D	275	SER
1	D	279	GLN
1	D	283	ASP
1	D	287	THR
1	D	292	LEU
1	D	305	VAL
1	D	312	ARG
1	D	320	PHE
1	D	323	LEU

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Mol	Chain	Res	Type
1	D	328	GLN
1	D	339	ARG
1	D	348	GLU
1	D	349	TRP
1	D	350	GLN
1	D	365	LEU
1	D	383	VAL
1	D	384	LEU
1	D	391	GLN
1	D	396	LEU
1	D	399	ARG
1	D	408	ARG
1	D	414	ASP
1	D	416	ASP
1	D	444	VAL
1	D	449	ASP
1	D	452	LEU
1	D	470	ILE
1	D	489	THR
1	D	502	ARG
1	D	511	TRP
1	D	514	SER
1	D	522	ASP
1	D	540	PHE
1	D	542	ARG
1	D	543	PHE
1	D	545	ARG
1	D	569	ILE
1	D	591	LEU
1	D	593	ARG
1	D	594	LEU
1	D	602	ASN
1	D	618	SER
1	D	634	PHE
1	D	654	ASP
1	D	665	ILE
1	D	678	SER
1	D	682	ARG
1	D	685	HIS
1	D	692	ARG
1	D	728	ARG
1	D	744	THR

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Mol	Chain	Res	Type
1	D	751	ARG
1	D	754	ARG
1	D	764	THR
1	D	769	PHE
1	A	1	MET
1	A	3	THR
1	A	7	PHE
1	A	32	ARG
1	A	44	LEU
1	A	48	VAL
1	A	52	LEU
1	A	62	ILE
1	A	63	CYS
1	A	64	PHE
1	A	65	LEU
1	A	68	VAL
1	A	75	ASN
1	A	86	GLN
1	A	91	VAL
1	A	98	GLN
1	A	99	GLN
1	A	109	THR
1	A	144	SER
1	A	151	MET
1	A	153	TYR
1	A	157	ARG
1	A	163	ILE
1	A	164	ARG
1	A	167	TYR
1	A	172	ARG
1	A	176	GLU
1	A	183	ILE
1	A	198	ASP
1	A	208	ILE
1	A	212	LYS
1	A	216	VAL
1	A	227	MET
1	A	249	ILE
1	A	251	LEU
1	A	262	ASN
1	A	275	SER
1	A	280	LEU

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Mol	Chain	Res	Type
1	A	283	ASP
1	A	287	THR
1	A	292	LEU
1	A	312	ARG
1	A	320	PHE
1	A	323	LEU
1	A	328	GLN
1	A	339	ARG
1	A	348	GLU
1	A	349	TRP
1	A	383	VAL
1	A	390	PHE
1	A	391	GLN
1	A	400	LEU
1	A	408	ARG
1	A	429	GLN
1	A	444	VAL
1	A	448	ASP
1	A	449	ASP
1	A	452	LEU
1	A	458	ILE
1	A	468	HIS
1	A	469	ASP
1	A	470	ILE
1	A	489	THR
1	A	502	ARG
1	A	511	TRP
1	A	512	ARG
1	A	514	SER
1	A	522	ASP
1	A	540	PHE
1	A	542	ARG
1	A	543	PHE
1	A	545	ARG
1	A	547	LEU
1	A	591	LEU
1	A	592	THR
1	A	593	ARG
1	A	594	LEU
1	A	602	ASN
1	A	609	THR
1	A	618	SER

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Mol	Chain	Res	Type
1	A	652	ASN
1	A	654	ASP
1	A	661	LEU
1	A	665	ILE
1	A	667	ASN
1	A	682	ARG
1	A	692	ARG
1	A	728	ARG
1	A	744	THR
1	A	764	THR
1	A	769	PHE
1	B	1	MET
1	B	3	THR
1	B	7	PHE
1	B	44	LEU
1	B	45	LEU
1	B	52	LEU
1	B	53	ASP
1	B	62	ILE
1	B	64	PHE
1	B	65	LEU
1	B	68	VAL
1	B	86	GLN
1	B	87	VAL
1	B	91	VAL
1	B	98	GLN
1	B	99	GLN
1	B	101	MET
1	B	104	LEU
1	B	109	THR
1	B	110	VAL
1	B	130	VAL
1	B	144	SER
1	B	151	MET
1	B	157	ARG
1	B	163	ILE
1	B	164	ARG
1	B	167	TYR
1	B	176	GLU
1	B	183	ILE
1	B	193	TYR
1	B	198	ASP

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Mol	Chain	Res	Type
1	B	208	ILE
1	B	211	ASP
1	B	212	LYS
1	B	213	THR
1	B	216	VAL
1	B	243	VAL
1	B	249	ILE
1	B	251	LEU
1	B	262	ASN
1	B	280	LEU
1	B	282	ASP
1	B	283	ASP
1	B	287	THR
1	B	292	LEU
1	B	312	ARG
1	B	320	PHE
1	B	323	LEU
1	B	328	GLN
1	B	339	ARG
1	B	342	LYS
1	B	348	GLU
1	B	349	TRP
1	B	354	SER
1	B	358	PHE
1	B	383	VAL
1	B	391	GLN
1	B	396	LEU
1	B	400	LEU
1	B	408	ARG
1	B	414	ASP
1	B	421	ARG
1	B	444	VAL
1	B	449	ASP
1	B	452	LEU
1	B	483	ARG
1	B	486	SER
1	B	489	THR
1	B	502	ARG
1	B	511	TRP
1	B	514	SER
1	B	540	PHE
1	B	542	ARG

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Mol	Chain	Res	Type
1	B	543	PHE
1	B	545	ARG
1	B	546	ASP
1	B	547	LEU
1	B	569	ILE
1	B	587	HIS
1	B	591	LEU
1	B	593	ARG
1	B	594	LEU
1	B	634	PHE
1	B	654	ASP
1	B	665	ILE
1	B	682	ARG
1	B	685	HIS
1	B	692	ARG
1	B	728	ARG
1	B	744	THR
1	B	754	ARG
1	B	764	THR
1	B	769	PHE
1	C	1	MET
1	C	3	THR
1	C	14	VAL
1	C	38	LEU
1	C	44	LEU
1	C	62	ILE
1	C	64	PHE
1	C	65	LEU
1	C	68	VAL
1	C	75	ASN
1	C	86	GLN
1	C	87	VAL
1	C	99	GLN
1	C	100	ARG
1	C	109	THR
1	C	110	VAL
1	C	127	GLU
1	C	129	SER
1	C	130	VAL
1	C	140	THR
1	C	144	SER
1	C	157	ARG

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Mol	Chain	Res	Type
1	C	163	ILE
1	C	164	ARG
1	C	165	SER
1	C	167	TYR
1	C	172	ARG
1	C	176	GLU
1	C	183	ILE
1	C	200	VAL
1	C	212	LYS
1	C	216	VAL
1	C	227	MET
1	C	243	VAL
1	C	249	ILE
1	C	251	LEU
1	C	255	THR
1	C	262	ASN
1	C	275	SER
1	C	282	ASP
1	C	283	ASP
1	C	292	LEU
1	C	304	THR
1	C	312	ARG
1	C	320	PHE
1	C	328	GLN
1	C	337	LYS
1	C	339	ARG
1	C	342	LYS
1	C	348	GLU
1	C	349	TRP
1	C	350	GLN
1	C	356	LEU
1	C	358	PHE
1	C	381	SER
1	C	384	LEU
1	C	391	GLN
1	C	394	THR
1	C	396	LEU
1	C	399	ARG
1	C	400	LEU
1	C	408	ARG
1	C	429	GLN
1	C	444	VAL

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Mol	Chain	Res	Type
1	C	448	ASP
1	C	449	ASP
1	C	452	LEU
1	C	458	ILE
1	C	468	HIS
1	C	470	ILE
1	C	483	ARG
1	C	489	THR
1	C	511	TRP
1	C	514	SER
1	C	522	ASP
1	C	540	PHE
1	C	542	ARG
1	C	543	PHE
1	C	545	ARG
1	C	546	ASP
1	C	547	LEU
1	C	587	HIS
1	C	591	LEU
1	C	593	ARG
1	C	594	LEU
1	C	618	SER
1	C	634	PHE
1	C	652	ASN
1	C	654	ASP
1	C	665	ILE
1	C	682	ARG
1	C	685	HIS
1	C	692	ARG
1	C	728	ARG
1	C	736	LEU
1	C	744	THR
1	C	764	THR
1	C	769	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	16	GLN
1	D	205	HIS
1	D	401	ASN
1	A	16	GLN

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Mol	Chain	Res	Type
1	A	98	GLN
1	A	173	ASN
1	A	328	GLN
1	A	401	ASN
1	A	667	ASN
1	B	16	GLN
1	B	401	ASN
1	C	223	HIS
1	C	269	ASN
1	C	391	GLN
1	C	455	GLN

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 monosaccharides 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	771/771 (100%)	0.52	57 (7%) 14 17	84, 138, 228, 331	0
1	B	771/771 (100%)	1.33	178 (23%) 0 1	74, 180, 334, 405	0
1	C	771/771 (100%)	0.56	54 (7%) 16 19	57, 129, 243, 347	0
1	D	771/771 (100%)	0.63	71 (9%) 9 11	67, 143, 228, 341	0
All	All	3084/3084 (100%)	0.76	360 (11%) 4 7	57, 142, 295, 405	0

All (360) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	722	GLU	30.8
1	B	637	ILE	16.5
1	D	718	SER	15.5
1	C	696	ALA	14.8
1	B	721	GLY	13.5
1	B	723	ILE	13.0
1	D	717	GLY	12.8
1	D	677	ALA	12.4
1	D	676	ASN	12.4
1	B	724	VAL	12.2
1	A	718	SER	12.0
1	C	697	ALA	10.4
1	B	711	ALA	10.3
1	C	718	SER	10.3
1	B	670	LEU	9.7
1	B	595	LEU	9.6
1	B	504	CYS	9.4
1	B	736	LEU	9.2
1	B	719	GLY	8.9
1	B	690	MET	8.7
1	B	640	VAL	8.6

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Mol	Chain	Res	Type	RSRZ
1	B	508	TYR	8.3
1	B	596	LEU	8.2
1	B	655	LEU	8.1
1	B	592	THR	7.9
1	B	708	ASP	7.8
1	C	719	GLY	7.7
1	A	719	GLY	7.6
1	B	594	LEU	7.6
1	C	714	LEU	7.5
1	B	641	ALA	7.4
1	C	716	LEU	7.4
1	A	675	GLU	7.4
1	B	636	THR	7.3
1	B	629	TRP	7.3
1	B	675	GLU	7.3
1	B	720	ALA	7.2
1	B	516	GLY	7.2
1	B	611	GLY	7.0
1	C	646	SER	6.9
1	A	676	ASN	6.8
1	B	707	ALA	6.8
1	B	715	ARG	6.8
1	D	675	GLU	6.8
1	B	732	LEU	6.8
1	C	676	ASN	6.7
1	B	702	ALA	6.6
1	A	677	ALA	6.5
1	B	718	SER	6.5
1	C	717	GLY	6.5
1	A	646	SER	6.5
1	B	710	GLU	6.5
1	B	709	ALA	6.3
1	B	696	ALA	6.2
1	C	694	LEU	6.1
1	B	533	VAL	5.9
1	A	717	GLY	5.9
1	B	691	PHE	5.8
1	B	458	ILE	5.8
1	B	647	SER	5.8
1	D	719	GLY	5.7
1	D	716	LEU	5.3
1	B	763	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	669	THR	5.3
1	C	725	ARG	5.1
1	B	441	PRO	5.0
1	B	671	LEU	5.0
1	B	579	ALA	5.0
1	C	686	LEU	5.0
1	B	506	ALA	5.0
1	B	442	THR	5.0
1	D	8	ASP	5.0
1	B	646	SER	5.0
1	B	462	ALA	4.9
1	A	715	ARG	4.9
1	D	743	TRP	4.8
1	C	715	ARG	4.8
1	C	677	ALA	4.8
1	B	484	LEU	4.7
1	C	675	GLU	4.7
1	B	509	ALA	4.7
1	D	714	LEU	4.7
1	B	635	ALA	4.7
1	B	706	LEU	4.7
1	D	668	LEU	4.6
1	C	743	TRP	4.6
1	B	453	ARG	4.6
1	A	8	ASP	4.6
1	B	741	GLU	4.5
1	B	747	PHE	4.5
1	C	647	SER	4.5
1	B	676	ASN	4.5
1	B	705	THR	4.5
1	B	447	CYS	4.5
1	D	623	THR	4.4
1	B	698	THR	4.4
1	A	716	LEU	4.3
1	A	714	LEU	4.3
1	D	547	LEU	4.2
1	D	771	PRO	4.2
1	B	651	TRP	4.2
1	B	500	ALA	4.2
1	B	3	THR	4.1
1	B	396	LEU	4.1
1	B	678	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	646	SER	4.1
1	B	535	GLU	4.1
1	B	685	HIS	4.1
1	B	460	LEU	4.1
1	B	639	HIS	4.0
1	B	658	ASP	4.0
1	B	679	ALA	4.0
1	B	513	GLY	4.0
1	B	597	LEU	3.9
1	D	497	PHE	3.9
1	B	733	VAL	3.9
1	B	735	ALA	3.9
1	B	725	ARG	3.9
1	B	510	LEU	3.9
1	B	755	LEU	3.9
1	D	655	LEU	3.8
1	A	80	GLU	3.8
1	B	689	LEU	3.8
1	D	715	ARG	3.8
1	B	743	TRP	3.7
1	B	739	ARG	3.7
1	A	645	PRO	3.7
1	B	712	GLN	3.7
1	B	677	ALA	3.6
1	B	693	ALA	3.6
1	C	533	VAL	3.6
1	A	4	LYS	3.6
1	B	750	ALA	3.6
1	B	742	GLU	3.6
1	B	673	ALA	3.6
1	B	583	PRO	3.6
1	C	720	ALA	3.6
1	B	575	TRP	3.6
1	B	569	ILE	3.6
1	B	610	PRO	3.6
1	B	674	VAL	3.6
1	B	501	ALA	3.6
1	B	451	THR	3.5
1	B	657	GLU	3.5
1	B	584	VAL	3.5
1	B	717	GLY	3.5
1	B	1	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	721	GLY	3.4
1	A	697	ALA	3.4
1	A	3	THR	3.4
1	B	701	GLU	3.4
1	B	532	VAL	3.4
1	D	684	TRP	3.3
1	B	429	GLN	3.3
1	C	689	LEU	3.3
1	D	686	LEU	3.3
1	A	1	MET	3.3
1	C	695	SER	3.3
1	C	723	ILE	3.3
1	C	713	GLY	3.2
1	C	736	LEU	3.2
1	B	590	PRO	3.2
1	C	484	LEU	3.2
1	D	484	LEU	3.2
1	B	606	ASP	3.2
1	B	615	ARG	3.2
1	A	671	LEU	3.2
1	C	8	ASP	3.2
1	B	607	SER	3.2
1	B	672	PRO	3.1
1	A	723	ILE	3.1
1	C	600	SER	3.1
1	C	724	VAL	3.1
1	D	723	ILE	3.1
1	B	499	LEU	3.1
1	C	547	LEU	3.1
1	B	687	LYS	3.1
1	B	667	ASN	3.1
1	B	600	SER	3.1
1	B	745	ALA	3.1
1	B	593	ARG	3.1
1	B	577	ALA	3.0
1	A	721	GLY	3.0
1	B	588	SER	3.0
1	C	691	PHE	3.0
1	B	443	LYS	3.0
1	C	732	LEU	3.0
1	A	414	ASP	3.0
1	B	654	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	463	LEU	3.0
1	B	699	VAL	3.0
1	D	669	THR	3.0
1	C	597	LEU	3.0
1	B	608	ALA	2.9
1	B	578	ARG	2.9
1	D	358	PHE	2.9
1	D	345	GLY	2.9
1	B	478	TYR	2.9
1	D	637	ILE	2.9
1	A	724	VAL	2.9
1	B	601	GLN	2.9
1	B	550	VAL	2.9
1	C	3	THR	2.8
1	B	730	LEU	2.8
1	D	729	TYR	2.8
1	C	698	THR	2.8
1	B	700	GLU	2.8
1	D	309	THR	2.8
1	D	747	PHE	2.8
1	A	670	LEU	2.8
1	B	613	VAL	2.8
1	B	645	PRO	2.8
1	D	736	LEU	2.7
1	B	582	THR	2.7
1	A	678	SER	2.7
1	D	665	ILE	2.7
1	B	746	GLU	2.7
1	B	452	LEU	2.7
1	B	612	LEU	2.7
1	A	681	ASN	2.7
1	D	429	GLN	2.7
1	B	586	GLN	2.7
1	B	514	SER	2.7
1	A	170	TRP	2.7
1	A	629	TRP	2.7
1	B	444	VAL	2.7
1	B	511	TRP	2.7
1	B	8	ASP	2.7
1	C	671	LEU	2.7
1	C	693	ALA	2.7
1	D	652	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	704	LYS	2.6
1	A	623	THR	2.6
1	B	609	THR	2.6
1	A	647	SER	2.6
1	C	733	VAL	2.6
1	D	663	ASN	2.6
1	B	598	ALA	2.6
1	B	632	GLU	2.6
1	D	656	TYR	2.6
1	A	720	ALA	2.6
1	B	659	PRO	2.6
1	B	714	LEU	2.6
1	B	573	GLN	2.6
1	D	390	PHE	2.6
1	A	680	SER	2.6
1	A	166	TYR	2.6
1	B	580	ALA	2.6
1	D	540	PHE	2.5
1	B	749	GLU	2.5
1	C	766	TRP	2.5
1	D	479	PHE	2.5
1	D	66	GLY	2.5
1	B	616	GLY	2.5
1	B	753	GLN	2.5
1	D	9	ALA	2.5
1	D	726	GLN	2.5
1	B	623	THR	2.5
1	B	726	GLN	2.5
1	D	640	VAL	2.5
1	C	706	LEU	2.5
1	B	663	ASN	2.5
1	D	525	TYR	2.5
1	B	740	GLU	2.5
1	A	346	LEU	2.4
1	A	268	PHE	2.4
1	A	711	ALA	2.4
1	B	540	PHE	2.4
1	A	679	ALA	2.4
1	B	358	PHE	2.4
1	D	3	THR	2.4
1	B	716	LEU	2.4
1	D	478	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	694	LEU	2.4
1	A	131	TRP	2.4
1	C	4	LYS	2.4
1	A	441	PRO	2.4
1	B	581	MET	2.4
1	B	614	VAL	2.4
1	C	540	PHE	2.4
1	A	547	LEU	2.4
1	A	556	LEU	2.4
1	A	365	LEU	2.4
1	A	478	TYR	2.3
1	B	4	LYS	2.3
1	B	572	LYS	2.3
1	D	346	LEU	2.3
1	B	497	PHE	2.3
1	D	770	GLU	2.3
1	D	306	ALA	2.3
1	B	534	GLU	2.3
1	C	645	PRO	2.3
1	B	430	VAL	2.3
1	C	531	HIS	2.3
1	D	235	LEU	2.2
1	A	9	ALA	2.2
1	B	498	LEU	2.2
1	D	21	THR	2.2
1	A	2	GLU	2.2
1	D	4	LYS	2.2
1	B	758	LEU	2.2
1	C	411	PHE	2.2
1	D	80	GLU	2.2
1	B	2	GLU	2.2
1	D	210	PRO	2.2
1	A	709	ALA	2.2
1	B	461	ALA	2.2
1	C	712	GLN	2.2
1	A	326	THR	2.2
1	B	681	ASN	2.2
1	D	591	LEU	2.2
1	C	655	LEU	2.2
1	D	121	LYS	2.2
1	D	657	GLU	2.2
1	C	80	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	270	SER	2.2
1	D	751	ARG	2.2
1	B	427	LEU	2.1
1	B	368	GLU	2.1
1	C	722	GLU	2.1
1	A	324	ASN	2.1
1	B	563	GLN	2.1
1	D	483	ARG	2.1
1	A	10	ALA	2.1
1	B	468	HIS	2.1
1	A	504	CYS	2.1
1	A	722	GLU	2.1
1	A	29	PRO	2.1
1	B	424	LEU	2.1
1	D	599	ALA	2.1
1	C	532	VAL	2.1
1	D	556	LEU	2.1
1	D	647	SER	2.1
1	B	589	LYS	2.1
1	C	247	ASP	2.1
1	A	292	LEU	2.1
1	D	645	PRO	2.1
1	B	476	THR	2.1
1	B	624	LEU	2.1
1	B	605	PRO	2.1
1	D	19	SER	2.1
1	C	5	GLU	2.1
1	A	708	ASP	2.1
1	D	427	LEU	2.1
1	A	767	LEU	2.1
1	D	445	PRO	2.1
1	C	246	GLU	2.1
1	D	430	VAL	2.1
1	A	347	ASP	2.1
1	D	539	ARG	2.1
1	D	508	TYR	2.0
1	A	525	TYR	2.0
1	B	665	ILE	2.0
1	D	336	PHE	2.0
1	C	517	SER	2.0
1	B	515	PHE	2.0
1	D	357	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	276	VAL	2.0
1	B	680	SER	2.0
1	B	666	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.