Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 05:04 AM EDT

PDB ID	:	3HFZ
Title	:	Crystal structure of Thermus thermophilus Phenylalanyl-tRNA synthetase complexed with m-tyrosine
Authors	:	Klipcan, L.; Moor, N.; Kessler, N.; Safro, M.G.
Deposited on	:	2009-05-13
Resolution	:	2.90 Å(reported)

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

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

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

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

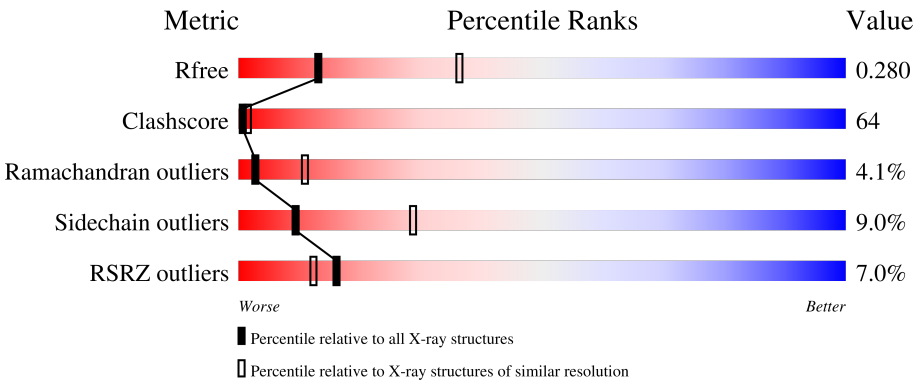
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	350	3%, 23%, 45%, 7%, 24%
2	B	785	8%, 37%, 55%, 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MTY	A	351	-	-	X	-
3	MTY	B	786	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8517 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.

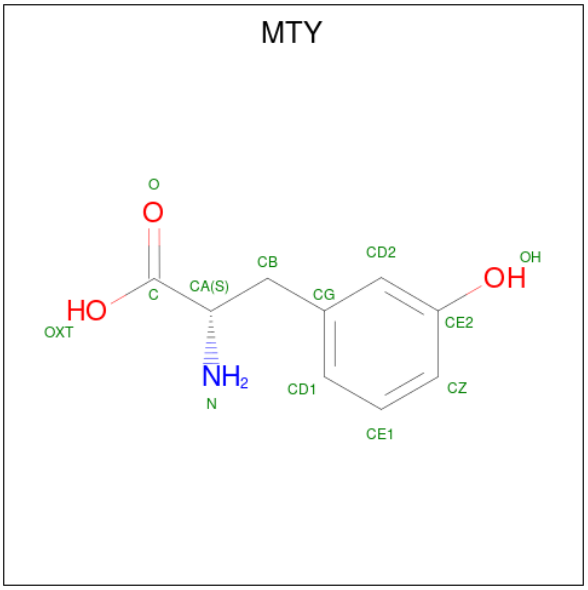
- Molecule 1 is a protein called Phenylalanyl-tRNA synthetase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2123	1388	363	365	7	11	0	0

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	785	6127	3925	1091	1101	10	46	0	0

- Molecule 3 is META-TYROSINE (three-letter code: MTY) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	13	9	1	3	0	0
3	B	1	13	9	1	3	0	0

- Molecule 4 is water.

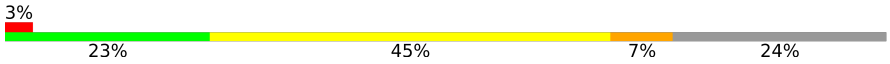
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	64	64	64	0	0
			Total	O		
4	B	177	177	177	0	0

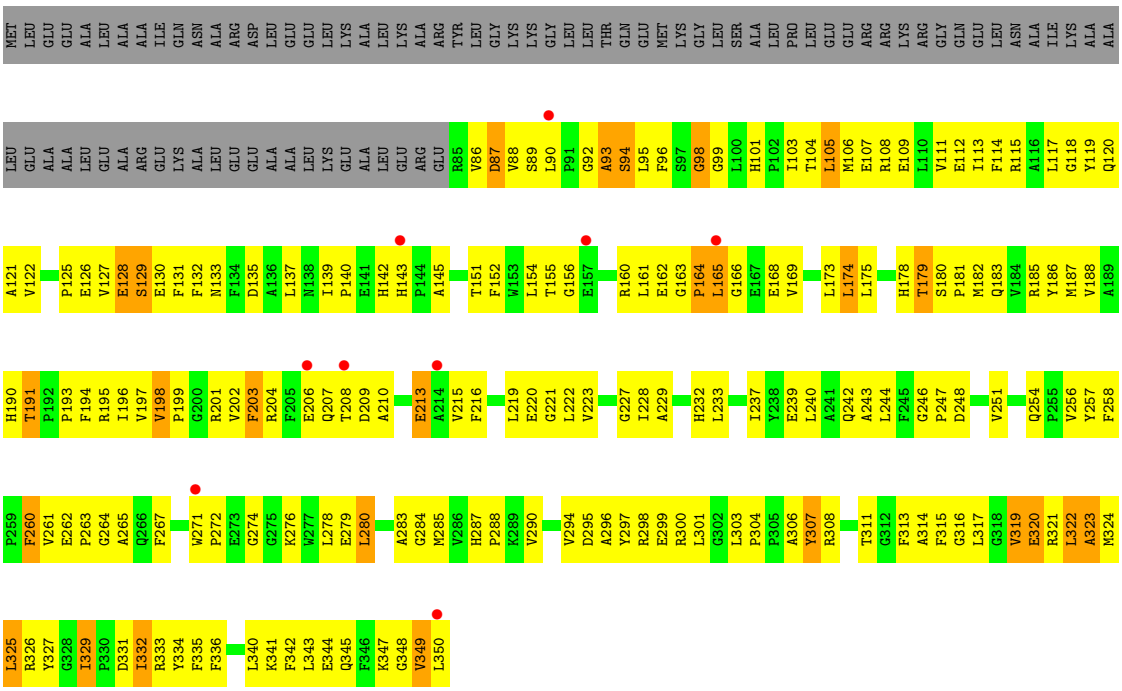
3 Residue-property plots (i)

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

• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

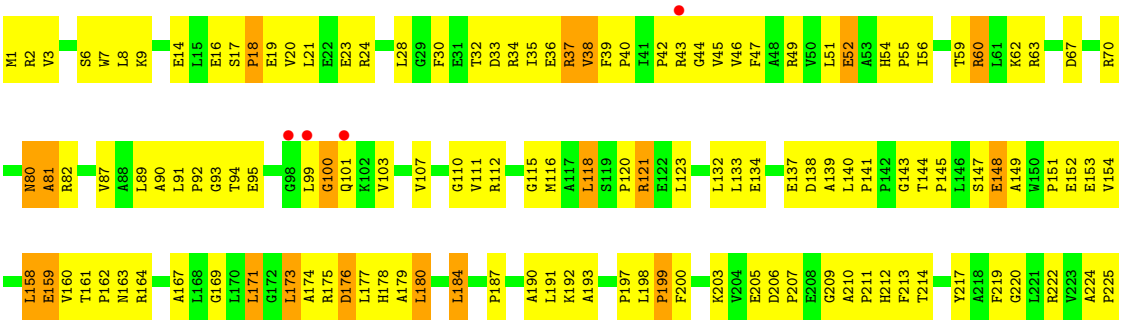
Chain A:

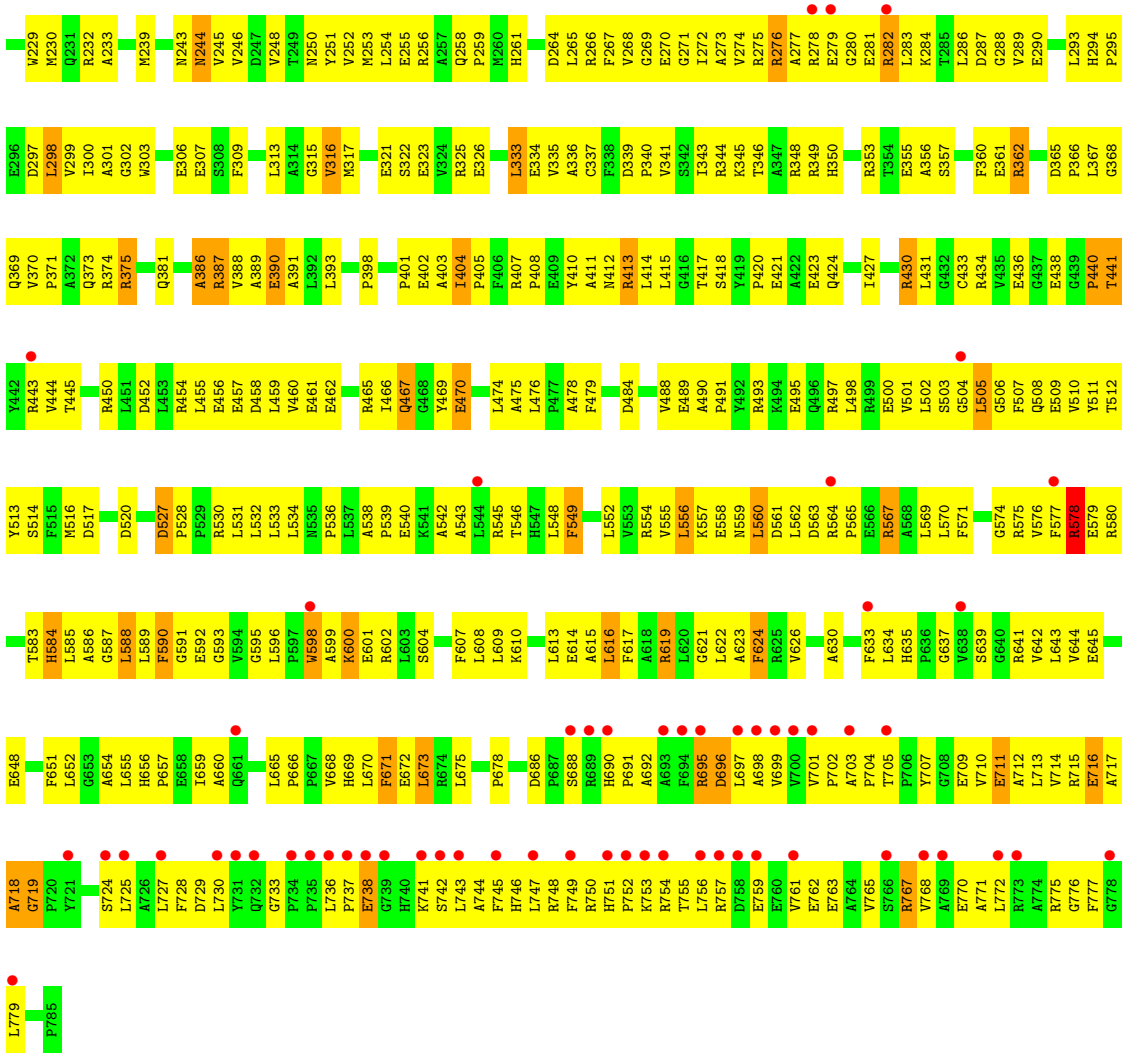




• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

Chain B:




W229 M230 Q231 R232 A233 M239 N243 N244 V245 V246 D247 V248 T249 N250 Y251 V252 M253 L254 E255 R256 A257 Q258 P259 M260 H261 D264 L265 R266 F267 V268 G269 E270 G271 I272 A273 V274 R275 R276 A277 R278 E279 G280 E281 R282 L283 K284 T285 L286 D287 G288 V289 E290 L293 H294 P295
E296 D297 L298 V299 I300 A301 G302 W303 E306 E307 S308 F309 L313 A314 G315 V316 M317 E321 S322 E323 V324 R325 E326 L333 E334 V335 A336 C337 F338 D339 P340 V341 S342 I343 R344 K345 T346 A347 R348 R349 H350 R353 T354 E355 A356 S357 F360 E361 R362 D365 P366 L367 G368
Q369 V370 P371 A372 Q373 R374 R375 Q381 A386 R387 V388 A389 E390 A391 L392 L393 P398 P401 E402 A403 I404 P405 F406 R407 P408 E409 Y410 A411 N412 R413 L414 L415 G416 T417 S418 Y419 P420 E421 A422 E423 Q424 I427 R430 L431 G432 C433 R434 V435 E436 G437 E438 G439 P440 T441
Y442 R443 V444 T445 R450 L451 D452 L453 R454 L455 E456 E457 D458 L459 V460 E461 E462 R465 I466 Q467 G468 Y469 E470 L474 A475 L476 P477 A478 F479 D484 V488 E489 A490 P491 Y492 R493 K494 E495 Q496 R497 L498 R499 E500 V501 L502 S503 G504 L505 G506 F507 Q508 E509 V510 Y511 T512
Y513 S514 F515 M516 D517 D520 D527 P528 P529 R530 L531 L532 L533 L534 N535 P536 L537 A538 P539 E540 K541 A542 A543 L544 R545 T546 H547 L548 F549 L552 V553 R554 V555 L556 K557 E558 N559 L560 D561 L562 D563 R564 P565 E566 R567 A568 L569 L570 F571 G574 R575 V576 F577 R578 E579 R580
T583 H584 L585 A586 G587 L588 L589 F590 G591 E592 G593 V594 G595 L596 P597 W598 A599 K600 E601 R602 L603 S604 F607 L608 L609 K610 L613 E614 A615 L616 F617 A618 R619 L620 G621 L622 A623 F624 R625 V626 A630 F633 L634 H635 P636 G637 V638 S639 G640 R641 V642 L643 V644 E645
E648 F651 L652 G653 A654 L655 H656 P657 E658 I659 A660 Q661 L665 P666 P667 V668 H669 L670 F671 E672 L673 R674 L675 P678 D686 P687 S688 R689 H690 P691 A692 A693 F694 R695 D696 L697 A698 V699 V700 V701 P702 A703 P704 T705 P706 Y707 G708 E709 V710 E711 A712 L713 V714 R715 E716 A717
A718 G719 P720 Y721 S724 L725 A726 L727 F728 D729 L730 Y731 G732 G733 P734 P735 L736 P737 E738 G739 H740 K741 S742 L743 A744 F745 H746 L747 R748 F749 R750 H751 P752 K753 R754 T755 L756 R757 D758 E759 E760 V761 E762 E763 A764 V765 S766 R767 V768 A769 E770 A771 L772 R773 A774 R775 G776 F777 G778
L779 P785

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.18Å 173.18Å 138.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.04 – 2.90 47.04 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.04-2.90) 99.2 (47.04-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.269 , 0.282 0.267 , 0.280	Depositor DCC
R_{free} test set	2688 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8517	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MTY

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	0.51	0/2191	0.70	0/2971
2	B	0.44	0/6280	0.71	3/8536 (0.0%)
All	All	0.46	0/8471	0.71	3/11507 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	387	ARG	N-CA-C	-5.86	95.18	111.00
2	B	38	VAL	N-CA-C	5.48	125.80	111.00
2	B	37	ARG	N-CA-C	-5.35	96.55	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2123	0	2075	299	0
2	B	6127	0	6180	766	1
3	A	13	0	9	8	0
3	B	13	0	9	11	0
4	A	64	0	0	120	0
4	B	177	0	0	254	1
All	All	8517	0	8273	1051	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (1051) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLY:HA3	4:A:391:HOH:O	1.16	1.31
4:A:408:HOH:O	2:B:579:GLU:HB3	1.18	1.31
2:B:9:LYS:HE2	4:B:951:HOH:O	1.22	1.29
2:B:33:ASP:HB3	4:B:843:HOH:O	1.18	1.27
1:A:112:GLU:HG2	4:A:377:HOH:O	1.15	1.26
2:B:532:LEU:HA	4:B:933:HOH:O	1.19	1.26
2:B:441:THR:HB	4:B:838:HOH:O	1.23	1.25
1:A:154:LEU:HB2	4:A:414:HOH:O	1.34	1.24
2:B:438:GLU:HB3	4:B:831:HOH:O	1.30	1.24
2:B:528:PRO:HD2	4:B:892:HOH:O	1.35	1.24
1:A:278:LEU:HB3	4:A:376:HOH:O	1.07	1.23
1:A:240:LEU:HA	4:A:402:HOH:O	1.36	1.23
2:B:388:VAL:HG12	4:B:954:HOH:O	1.39	1.22
2:B:478:ALA:HA	4:B:841:HOH:O	1.38	1.22
2:B:637:GLY:HA3	4:B:908:HOH:O	1.42	1.19
2:B:643:LEU:HD12	4:B:791:HOH:O	1.38	1.19
1:A:140:PRO:HD2	4:A:372:HOH:O	1.41	1.17
1:A:254:GLN:HG2	4:A:406:HOH:O	1.41	1.17
2:B:401:PRO:HA	4:B:803:HOH:O	1.45	1.16
2:B:779:LEU:HG	4:B:916:HOH:O	1.42	1.16
2:B:43:ARG:HD3	4:B:828:HOH:O	1.45	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PRO:HD2	4:A:366:HOH:O	1.44	1.15
2:B:407:ARG:CG	4:B:838:HOH:O	1.95	1.14
2:B:656:HIS:HB3	2:B:659:ILE:HD13	1.21	1.11
2:B:211:PRO:HD3	4:B:879:HOH:O	1.51	1.11
2:B:336:ALA:HB3	4:B:844:HOH:O	1.50	1.10
1:A:206:GLU:HB2	4:A:398:HOH:O	1.46	1.10
1:A:326:ARG:HD3	4:A:379:HOH:O	1.49	1.10
2:B:445:THR:HG23	4:B:894:HOH:O	1.50	1.10
2:B:635:HIS:HE1	4:B:908:HOH:O	1.34	1.10
2:B:543:ALA:HA	4:B:933:HOH:O	1.51	1.10
1:A:237:ILE:HG13	4:A:403:HOH:O	1.50	1.09
2:B:95:GLU:HB2	4:B:911:HOH:O	1.52	1.08
2:B:286:LEU:HD21	2:B:323:GLU:HG3	1.12	1.08
2:B:2:ARG:HD2	4:B:794:HOH:O	1.54	1.08
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.36	1.08
2:B:100:GLY:HA2	4:B:830:HOH:O	1.54	1.07
2:B:220:GLY:HA3	4:B:923:HOH:O	1.53	1.07
2:B:467:GLN:HE21	2:B:467:GLN:HA	1.20	1.06
2:B:303:TRP:HB3	4:B:922:HOH:O	1.56	1.06
2:B:427:ILE:HG13	4:B:952:HOH:O	1.53	1.06
2:B:736:LEU:HA	4:B:856:HOH:O	1.56	1.05
1:A:243:ALA:HB3	4:A:402:HOH:O	1.53	1.05
2:B:224:ALA:H	2:B:244:ASN:ND2	1.56	1.04
2:B:456:GLU:HA	4:B:837:HOH:O	1.55	1.04
1:A:237:ILE:HG23	4:A:403:HOH:O	1.57	1.04
1:A:135:ASP:HA	4:A:397:HOH:O	1.58	1.03
2:B:602:ARG:HH11	2:B:602:ARG:HB2	1.19	1.03
1:A:251:VAL:HG23	4:A:368:HOH:O	1.57	1.03
2:B:112:ARG:HG2	4:B:855:HOH:O	1.59	1.02
1:A:298:ARG:HG2	4:A:362:HOH:O	1.58	1.02
2:B:187:PRO:HG2	4:B:948:HOH:O	1.59	1.02
2:B:205:GLU:HG3	4:B:812:HOH:O	1.60	1.02
2:B:366:PRO:HD3	4:B:795:HOH:O	1.58	1.02
2:B:407:ARG:HG3	4:B:838:HOH:O	1.53	1.02
1:A:165:LEU:HD11	1:A:303:LEU:HD11	1.41	1.01
2:B:511:TYR:HE1	4:B:865:HOH:O	1.40	1.01
2:B:630:ALA:HB2	4:B:893:HOH:O	1.61	1.00
1:A:173:LEU:HB3	4:A:414:HOH:O	1.64	0.98
1:A:168:GLU:HG2	4:A:407:HOH:O	1.61	0.98
2:B:286:LEU:HD21	2:B:323:GLU:CG	1.94	0.98
1:A:190:HIS:HE1	4:A:355:HOH:O	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ARG:HD3	4:B:873:HOH:O	1.66	0.96
2:B:306:GLU:HG3	4:B:941:HOH:O	1.66	0.95
3:A:351:MTY:CB	4:A:381:HOH:O	2.13	0.95
2:B:776:GLY:HA3	4:B:959:HOH:O	1.65	0.95
2:B:532:LEU:HD23	4:B:933:HOH:O	1.66	0.94
1:A:299:GLU:HB3	4:A:385:HOH:O	1.66	0.94
2:B:56:ILE:CG1	4:B:842:HOH:O	2.16	0.94
2:B:557:LYS:HG2	2:B:665:LEU:HD21	1.50	0.94
2:B:199:PRO:HB2	4:B:924:HOH:O	1.68	0.93
2:B:759:GLU:HB2	4:B:801:HOH:O	1.68	0.93
2:B:775:ARG:HD2	4:B:874:HOH:O	1.67	0.93
1:A:248:ASP:CB	4:A:399:HOH:O	2.17	0.93
1:A:213:GLU:HG3	1:A:332:ILE:HD12	1.51	0.93
2:B:80:ASN:H	2:B:80:ASN:HD22	1.14	0.92
2:B:287:ASP:H	2:B:317:MET:HE2	1.29	0.92
2:B:24:ARG:HD3	4:B:942:HOH:O	1.69	0.92
2:B:589:LEU:HB2	2:B:609:LEU:HD12	1.50	0.92
2:B:717:ALA:HB3	4:B:925:HOH:O	1.68	0.91
1:A:279:GLU:CG	4:A:401:HOH:O	2.17	0.90
2:B:643:LEU:HB3	4:B:791:HOH:O	1.69	0.90
1:A:258:PHE:CE1	4:A:381:HOH:O	2.23	0.90
2:B:455:LEU:HD23	4:B:961:HOH:O	1.70	0.90
3:A:351:MTY:HD1	4:A:381:HOH:O	1.71	0.89
2:B:635:HIS:CE1	4:B:908:HOH:O	2.13	0.89
2:B:224:ALA:H	2:B:244:ASN:HD22	0.92	0.89
1:A:237:ILE:HA	4:A:403:HOH:O	1.71	0.88
3:A:351:MTY:HA	4:A:381:HOH:O	1.72	0.88
2:B:763:GLU:HG2	4:B:816:HOH:O	1.71	0.88
1:A:296:ALA:HA	4:A:405:HOH:O	1.74	0.88
2:B:211:PRO:CD	4:B:879:HOH:O	2.11	0.88
1:A:190:HIS:CE1	4:A:355:HOH:O	2.22	0.88
2:B:602:ARG:HB2	2:B:602:ARG:NH1	1.87	0.88
2:B:527:ASP:HB3	4:B:892:HOH:O	1.74	0.88
1:A:173:LEU:CB	4:A:414:HOH:O	2.19	0.87
1:A:271:TRP:HA	4:A:366:HOH:O	1.74	0.87
1:A:229:ALA:CB	4:B:869:HOH:O	2.23	0.87
1:A:229:ALA:HB2	4:B:869:HOH:O	1.74	0.87
1:A:98:GLY:HA2	4:B:958:HOH:O	1.73	0.87
1:A:160:ARG:CZ	4:A:408:HOH:O	2.21	0.87
1:A:155:THR:HB	2:B:534:LEU:HD21	1.56	0.86
2:B:350:HIS:HD2	4:B:891:HOH:O	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:CB	4:A:403:HOH:O	2.23	0.86
2:B:776:GLY:CA	4:B:959:HOH:O	2.19	0.86
1:A:272:PRO:CD	4:A:366:HOH:O	2.10	0.85
1:A:161:LEU:HD23	1:A:169:VAL:HG13	1.57	0.85
1:A:321:ARG:HG2	4:A:380:HOH:O	1.75	0.85
2:B:274:VAL:HG12	2:B:298:LEU:HD11	1.58	0.85
2:B:600:LYS:HE2	4:B:860:HOH:O	1.74	0.85
1:A:298:ARG:CG	4:A:362:HOH:O	2.19	0.85
1:A:142:HIS:HE1	4:A:361:HOH:O	1.60	0.85
3:A:351:MTY:CA	4:A:381:HOH:O	2.22	0.84
2:B:55:PRO:HG2	4:B:937:HOH:O	1.76	0.84
2:B:457:GLU:OE1	2:B:457:GLU:N	2.09	0.84
2:B:759:GLU:CB	4:B:801:HOH:O	2.22	0.84
2:B:707:TYR:OH	2:B:711:GLU:HG3	1.76	0.84
3:A:351:MTY:HB2	4:A:381:HOH:O	1.77	0.83
2:B:239:MET:HE1	2:B:355:GLU:HG3	1.58	0.83
2:B:222:ARG:HG3	4:B:962:HOH:O	1.76	0.83
2:B:578:ARG:HB3	4:B:870:HOH:O	1.76	0.83
1:A:121:ALA:N	4:A:378:HOH:O	2.11	0.83
2:B:1:MET:CE	4:B:834:HOH:O	2.25	0.82
2:B:193:ALA:HB2	4:B:957:HOH:O	1.78	0.82
1:A:261:VAL:HB	4:A:391:HOH:O	1.76	0.82
2:B:56:ILE:HG13	4:B:842:HOH:O	1.77	0.82
2:B:153:GLU:HB2	4:B:909:HOH:O	1.78	0.82
1:A:154:LEU:HD12	4:A:414:HOH:O	1.80	0.82
2:B:203:LYS:HG2	4:B:812:HOH:O	1.79	0.82
1:A:194:PHE:HB2	4:A:363:HOH:O	1.79	0.81
2:B:279:GLU:HB3	4:B:931:HOH:O	1.79	0.81
2:B:666:PRO:HD3	4:B:935:HOH:O	1.79	0.81
2:B:325:ARG:HH11	2:B:325:ARG:HB2	1.45	0.81
2:B:62:LYS:HD3	4:B:857:HOH:O	1.78	0.81
1:A:279:GLU:HG3	4:A:401:HOH:O	1.78	0.81
2:B:642:VAL:C	2:B:643:LEU:HD22	2.01	0.81
2:B:265:LEU:HD23	2:B:268:VAL:HG21	1.63	0.81
2:B:224:ALA:N	2:B:244:ASN:ND2	2.29	0.81
2:B:727:LEU:HB3	4:B:905:HOH:O	1.81	0.81
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.63	0.80
2:B:101:GLN:HB3	4:B:929:HOH:O	1.81	0.80
2:B:695:ARG:HB3	2:B:747:LEU:HB2	1.64	0.80
1:A:94:SER:CA	4:A:404:HOH:O	2.30	0.80
1:A:324:MET:HA	1:A:329:ILE:HG13	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:511:TYR:CE1	4:B:865:HOH:O	2.24	0.79
2:B:193:ALA:CB	4:B:957:HOH:O	2.30	0.79
2:B:718:ALA:HA	2:B:768:VAL:HG21	1.65	0.79
3:B:786:MTY:CD2	4:B:876:HOH:O	2.29	0.79
1:A:331:ASP:HB3	1:A:334:TYR:CE2	2.16	0.79
2:B:224:ALA:N	2:B:244:ASN:HD22	1.76	0.78
2:B:323:GLU:HG3	4:B:792:HOH:O	1.82	0.78
3:A:351:MTY:CD1	4:A:381:HOH:O	2.30	0.78
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.46	0.78
2:B:737:PRO:HD3	4:B:856:HOH:O	1.83	0.78
1:A:349:VAL:HG12	1:A:350:LEU:HD23	1.67	0.77
2:B:691:PRO:HA	4:B:913:HOH:O	1.84	0.77
1:A:86:VAL:CG1	4:A:384:HOH:O	2.32	0.77
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.67	0.77
2:B:600:LYS:CE	4:B:860:HOH:O	2.32	0.77
2:B:350:HIS:CD2	4:B:891:HOH:O	2.34	0.77
2:B:306:GLU:CB	4:B:941:HOH:O	2.32	0.77
2:B:567:ARG:HA	2:B:591:GLY:HA3	1.67	0.77
1:A:237:ILE:CG2	4:A:403:HOH:O	2.20	0.76
2:B:190:ALA:CB	4:B:852:HOH:O	2.33	0.76
1:A:264:GLY:HA2	4:A:391:HOH:O	1.84	0.76
2:B:666:PRO:HG3	4:B:935:HOH:O	1.84	0.76
2:B:80:ASN:HD22	2:B:80:ASN:N	1.84	0.76
1:A:119:TYR:CE1	4:A:373:HOH:O	2.38	0.76
2:B:54:HIS:CD2	4:B:817:HOH:O	2.37	0.76
2:B:656:HIS:CB	2:B:659:ILE:HD13	2.10	0.75
1:A:115:ARG:HG2	1:A:115:ARG:HH11	1.50	0.75
1:A:290:VAL:O	1:A:294:VAL:HG23	1.85	0.75
2:B:287:ASP:N	2:B:317:MET:HE2	2.01	0.75
2:B:457:GLU:O	2:B:460:VAL:HG22	1.86	0.75
2:B:516:MET:HE1	2:B:546:THR:H	1.51	0.75
2:B:775:ARG:HA	4:B:874:HOH:O	1.86	0.75
1:A:349:VAL:CG1	4:A:409:HOH:O	2.35	0.75
2:B:666:PRO:CG	4:B:935:HOH:O	2.34	0.75
2:B:746:HIS:HE1	4:B:900:HOH:O	1.69	0.75
2:B:158:LEU:HD22	2:B:159:GLU:H	1.52	0.74
2:B:567:ARG:HD2	4:B:940:HOH:O	1.86	0.74
2:B:55:PRO:CG	4:B:937:HOH:O	2.30	0.74
2:B:317:MET:HA	3:B:786:MTY:N	2.02	0.74
2:B:497:ARG:O	2:B:501:VAL:HG23	1.88	0.74
2:B:516:MET:CE	4:B:912:HOH:O	2.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG12	4:A:384:HOH:O	1.87	0.74
2:B:99:LEU:HD12	2:B:101:GLN:H	1.52	0.74
2:B:178:HIS:HE1	4:B:895:HOH:O	1.71	0.74
2:B:729:ASP:H	2:B:744:ALA:HB3	1.50	0.74
1:A:267:PHE:CE1	1:A:280:LEU:HB3	2.23	0.74
2:B:70:ARG:HD2	4:B:943:HOH:O	1.87	0.74
2:B:467:GLN:HA	2:B:467:GLN:NE2	2.01	0.74
1:A:195:ARG:HG2	1:A:223:VAL:HG13	1.70	0.73
2:B:265:LEU:HA	2:B:268:VAL:HG23	1.68	0.73
2:B:709:GLU:HA	4:B:956:HOH:O	1.87	0.73
2:B:205:GLU:CG	4:B:812:HOH:O	2.24	0.73
2:B:341:VAL:HG13	4:B:862:HOH:O	1.86	0.73
2:B:307:GLU:HG2	4:B:938:HOH:O	1.89	0.73
2:B:552:LEU:O	2:B:555:VAL:HG22	1.88	0.73
2:B:730:LEU:HD13	2:B:743:LEU:CD2	2.18	0.73
1:A:350:LEU:CD2	4:A:409:HOH:O	2.35	0.73
2:B:261:HIS:HD2	3:B:786:MTY:HA	1.54	0.73
2:B:282:ARG:HH12	2:B:290:GLU:HG3	1.53	0.72
2:B:62:LYS:CD	4:B:857:HOH:O	2.35	0.72
2:B:757:ARG:CG	4:B:848:HOH:O	2.36	0.72
1:A:301:LEU:HB3	4:A:411:HOH:O	1.88	0.72
2:B:193:ALA:HA	4:B:957:HOH:O	1.89	0.72
1:A:279:GLU:HG2	4:A:401:HOH:O	1.86	0.72
4:A:408:HOH:O	2:B:579:GLU:CB	1.94	0.72
2:B:401:PRO:CA	4:B:803:HOH:O	2.16	0.72
2:B:695:ARG:HH11	2:B:761:VAL:HG11	1.53	0.72
2:B:159:GLU:HB3	4:B:811:HOH:O	1.88	0.72
2:B:516:MET:HE3	4:B:912:HOH:O	1.86	0.72
1:A:239:GLU:O	4:A:402:HOH:O	2.07	0.72
2:B:282:ARG:HB3	2:B:282:ARG:NH1	2.04	0.72
1:A:265:ALA:HB2	2:B:469:TYR:HE2	1.55	0.72
2:B:589:LEU:HG	2:B:590:PHE:H	1.54	0.72
2:B:604:SER:HA	2:B:608:LEU:HD22	1.72	0.72
1:A:142:HIS:CE1	4:A:361:HOH:O	2.37	0.71
1:A:242:GLN:OE1	1:A:247:PRO:HA	1.90	0.71
2:B:698:ALA:HA	2:B:743:LEU:O	1.89	0.71
2:B:389:ALA:C	4:B:954:HOH:O	2.28	0.71
2:B:578:ARG:CB	4:B:870:HOH:O	2.35	0.71
2:B:699:VAL:HG13	2:B:772:LEU:HD21	1.71	0.71
1:A:128:GLU:OE2	1:A:132:PHE:HB2	1.89	0.71
2:B:730:LEU:HD13	2:B:743:LEU:HD23	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLY:HA3	2:B:94:THR:OG1	1.91	0.70
2:B:176:ASP:OD2	2:B:465:ARG:NH2	2.24	0.70
2:B:190:ALA:HB2	4:B:852:HOH:O	1.91	0.70
1:A:334:TYR:HA	4:A:364:HOH:O	1.90	0.70
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.72	0.70
2:B:757:ARG:HG3	4:B:848:HOH:O	1.89	0.70
2:B:757:ARG:HD2	4:B:827:HOH:O	1.90	0.70
2:B:193:ALA:CA	4:B:957:HOH:O	2.38	0.70
2:B:38:VAL:O	2:B:40:PRO:HD2	1.91	0.70
2:B:564:ARG:HD2	2:B:564:ARG:N	2.06	0.70
2:B:701:VAL:CG1	2:B:705:THR:HB	2.21	0.70
2:B:70:ARG:CD	4:B:943:HOH:O	2.40	0.70
2:B:696:ASP:OD1	2:B:746:HIS:HD2	1.75	0.70
1:A:261:VAL:CG2	4:A:391:HOH:O	2.38	0.69
2:B:90:ALA:HB2	2:B:118:LEU:HD11	1.72	0.69
2:B:737:PRO:CD	4:B:856:HOH:O	2.40	0.69
2:B:336:ALA:CB	4:B:844:HOH:O	2.22	0.69
2:B:542:ALA:O	4:B:933:HOH:O	2.09	0.69
1:A:237:ILE:CA	4:A:403:HOH:O	2.31	0.69
2:B:770:GLU:HB3	4:B:822:HOH:O	1.92	0.69
1:A:198:VAL:HG13	1:A:220:GLU:HB2	1.74	0.69
1:A:287:HIS:ND1	1:A:288:PRO:HD2	2.08	0.69
1:A:326:ARG:CD	4:A:379:HOH:O	2.20	0.69
2:B:761:VAL:O	2:B:765:VAL:HG13	1.92	0.69
2:B:279:GLU:CB	4:B:931:HOH:O	2.40	0.68
1:A:340:LEU:HD21	2:B:570:LEU:HD21	1.75	0.68
2:B:210:ALA:N	4:B:879:HOH:O	2.26	0.68
2:B:718:ALA:HA	2:B:768:VAL:CG2	2.22	0.68
1:A:254:GLN:O	1:A:265:ALA:HB1	1.93	0.68
2:B:725:LEU:HD21	2:B:745:PHE:HE1	1.57	0.68
1:A:94:SER:HA	4:A:404:HOH:O	1.90	0.68
1:A:165:LEU:CD1	1:A:303:LEU:HD11	2.21	0.68
2:B:512:THR:CG2	4:B:820:HOH:O	2.41	0.68
2:B:514:SER:HA	2:B:545:ARG:HD3	1.73	0.68
2:B:695:ARG:HH11	2:B:761:VAL:CG1	2.05	0.68
3:B:786:MTY:CG	4:B:876:HOH:O	2.41	0.68
2:B:666:PRO:CD	4:B:935:HOH:O	2.36	0.68
2:B:408:PRO:HD2	4:B:901:HOH:O	1.93	0.68
1:A:254:GLN:CG	4:A:406:HOH:O	2.14	0.67
2:B:33:ASP:O	2:B:34:ARG:HB3	1.94	0.67
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:GLU:HG3	4:B:799:HOH:O	1.94	0.67
2:B:279:GLU:CA	4:B:931:HOH:O	2.42	0.67
2:B:341:VAL:HG12	2:B:345:LYS:HE3	1.75	0.67
2:B:52:GLU:HG3	2:B:54:HIS:CE1	2.29	0.67
1:A:120:GLN:HG2	2:B:489:GLU:HB3	1.74	0.67
2:B:153:GLU:CG	4:B:909:HOH:O	2.41	0.67
2:B:407:ARG:HG2	4:B:838:HOH:O	1.73	0.67
1:A:263:PRO:HG3	2:B:461:GLU:HB2	1.76	0.67
1:A:332:ILE:HD13	1:A:335:PHE:HD2	1.58	0.67
1:A:204:ARG:NH2	4:A:394:HOH:O	2.21	0.67
1:A:260:PHE:N	1:A:260:PHE:CD1	2.63	0.67
1:A:320:GLU:HG2	1:A:332:ILE:HD11	1.76	0.67
2:B:239:MET:CE	2:B:355:GLU:HG3	2.24	0.67
2:B:607:PHE:HA	2:B:610:LYS:HB3	1.76	0.67
1:A:161:LEU:CD2	1:A:169:VAL:HG13	2.25	0.66
1:A:99:GLY:HA3	4:B:829:HOH:O	1.93	0.66
2:B:701:VAL:HG22	2:B:777:PHE:CD1	2.30	0.66
2:B:198:LEU:HD12	2:B:393:LEU:CD1	2.22	0.66
1:A:180:SER:O	1:A:183:GLN:HB3	1.95	0.66
2:B:751:HIS:HB3	2:B:754:ARG:O	1.94	0.66
2:B:62:LYS:CE	4:B:857:HOH:O	2.42	0.66
2:B:713:LEU:HD23	4:B:836:HOH:O	1.95	0.66
1:A:307:TYR:CD1	1:A:307:TYR:N	2.63	0.66
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.78	0.66
2:B:701:VAL:HG22	2:B:777:PHE:CE1	2.31	0.65
2:B:299:VAL:HG12	2:B:300:ILE:N	2.10	0.65
2:B:389:ALA:O	4:B:954:HOH:O	2.15	0.65
2:B:589:LEU:CG	2:B:590:PHE:H	2.07	0.65
1:A:251:VAL:CG2	4:A:368:HOH:O	2.30	0.65
2:B:80:ASN:H	2:B:80:ASN:ND2	1.91	0.65
2:B:176:ASP:CG	2:B:465:ARG:HH22	1.98	0.65
2:B:712:ALA:O	2:B:716:GLU:HB2	1.96	0.65
2:B:37:ARG:HH11	2:B:37:ARG:HB3	1.61	0.65
2:B:610:LYS:O	2:B:614:GLU:HG3	1.97	0.65
2:B:643:LEU:CB	4:B:791:HOH:O	2.36	0.65
2:B:749:PHE:CE2	4:B:906:HOH:O	2.49	0.65
1:A:229:ALA:N	1:A:232:HIS:HD2	1.95	0.65
2:B:203:LYS:HE3	4:B:812:HOH:O	1.96	0.65
2:B:220:GLY:CA	4:B:923:HOH:O	2.25	0.65
2:B:467:GLN:HG2	4:B:952:HOH:O	1.96	0.65
2:B:570:LEU:HD12	2:B:588:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:SER:HB2	2:B:752:PRO:HA	1.78	0.65
2:B:771:ALA:CB	4:B:839:HOH:O	2.44	0.65
2:B:141:PRO:HD2	2:B:144:THR:HG21	1.79	0.65
1:A:128:GLU:O	1:A:174:LEU:HD12	1.97	0.65
1:A:258:PHE:CZ	4:A:381:HOH:O	2.48	0.65
2:B:14:GLU:HB2	4:B:789:HOH:O	1.95	0.65
1:A:164:PRO:HG2	1:A:188:VAL:HG21	1.78	0.65
1:A:334:TYR:HD1	4:A:364:HOH:O	1.80	0.64
2:B:434:ARG:HH12	2:B:436:GLU:CD	2.01	0.64
2:B:341:VAL:CG1	2:B:345:LYS:HE3	2.26	0.64
2:B:283:LEU:HD23	2:B:284:LYS:N	2.12	0.64
1:A:267:PHE:HE1	1:A:280:LEU:HB3	1.63	0.64
2:B:37:ARG:HB3	2:B:37:ARG:NH1	2.13	0.64
2:B:222:ARG:CG	4:B:962:HOH:O	2.38	0.64
2:B:341:VAL:CG1	4:B:862:HOH:O	2.41	0.64
1:A:155:THR:HG23	1:A:155:THR:O	1.98	0.64
1:A:319:VAL:O	1:A:321:ARG:N	2.30	0.64
1:A:350:LEU:HD23	4:A:409:HOH:O	1.94	0.64
2:B:727:LEU:HA	2:B:744:ALA:O	1.98	0.64
1:A:209:ASP:O	1:A:333:ARG:HG3	1.97	0.64
2:B:333:LEU:CD2	4:B:915:HOH:O	2.45	0.64
2:B:210:ALA:CA	4:B:879:HOH:O	2.46	0.64
2:B:210:ALA:HA	4:B:879:HOH:O	1.96	0.64
2:B:585:LEU:O	2:B:673:LEU:HD12	1.98	0.64
2:B:643:LEU:CD1	4:B:791:HOH:O	2.14	0.64
1:A:119:TYR:HE1	4:A:373:HOH:O	1.77	0.63
2:B:95:GLU:N	4:B:911:HOH:O	2.28	0.63
2:B:669:HIS:HD2	4:B:823:HOH:O	1.81	0.63
2:B:717:ALA:CB	4:B:925:HOH:O	2.38	0.63
1:A:165:LEU:HD11	1:A:303:LEU:CD1	2.22	0.63
2:B:256:ARG:NH2	4:B:948:HOH:O	2.31	0.63
1:A:220:GLU:OE2	3:A:351:MTY:HD2	1.98	0.63
2:B:153:GLU:CD	4:B:909:HOH:O	2.36	0.63
2:B:256:ARG:NH2	2:B:375:ARG:HG3	2.12	0.63
2:B:686:ASP:CB	4:B:953:HOH:O	2.45	0.63
2:B:713:LEU:O	4:B:925:HOH:O	2.15	0.63
2:B:754:ARG:NH2	4:B:854:HOH:O	2.29	0.63
1:A:98:GLY:HA3	2:B:503:SER:O	1.98	0.63
1:A:155:THR:CB	2:B:534:LEU:HD21	2.29	0.63
2:B:49:ARG:HH21	2:B:51:LEU:CD2	2.10	0.63
2:B:666:PRO:O	2:B:668:VAL:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ILE:N	2:B:35:ILE:HD12	2.13	0.63
2:B:548:LEU:HD22	2:B:584:HIS:HB3	1.79	0.63
2:B:595:GLY:HA3	4:B:904:HOH:O	1.99	0.63
2:B:209:GLY:C	4:B:879:HOH:O	2.37	0.63
2:B:771:ALA:N	4:B:822:HOH:O	2.31	0.63
1:A:87:ASP:OD1	1:A:88:VAL:N	2.32	0.63
1:A:327:TYR:HE1	4:A:379:HOH:O	1.81	0.63
2:B:36:GLU:O	2:B:154:VAL:HA	1.97	0.63
2:B:82:ARG:HH22	2:B:134:GLU:CD	2.03	0.63
2:B:207:PRO:HD2	4:B:853:HOH:O	1.98	0.63
2:B:297:ASP:OD2	2:B:350:HIS:HE1	1.82	0.63
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.81	0.63
2:B:121:ARG:HG3	2:B:121:ARG:HH11	1.62	0.62
2:B:160:VAL:CG1	2:B:167:ALA:HB3	2.29	0.62
2:B:434:ARG:HH12	2:B:436:GLU:CG	2.12	0.62
2:B:635:HIS:O	2:B:639:SER:HB2	1.99	0.62
1:A:161:LEU:HD23	1:A:169:VAL:CG1	2.29	0.62
1:A:161:LEU:HD23	1:A:161:LEU:O	1.99	0.62
2:B:729:ASP:N	2:B:744:ALA:HB3	2.13	0.62
1:A:229:ALA:H	1:A:232:HIS:HD2	1.47	0.62
2:B:747:LEU:O	2:B:748:ARG:HG3	1.99	0.62
1:A:202:VAL:HG22	1:A:216:PHE:O	1.99	0.62
2:B:512:THR:HG21	4:B:820:HOH:O	1.98	0.62
2:B:751:HIS:HB2	2:B:756:LEU:HD21	1.80	0.62
2:B:325:ARG:HB2	2:B:325:ARG:NH1	2.14	0.62
2:B:589:LEU:HD22	2:B:609:LEU:HB2	1.80	0.62
2:B:701:VAL:HG11	2:B:705:THR:HB	1.82	0.62
2:B:336:ALA:HA	2:B:369:GLN:HG2	1.81	0.62
2:B:507:PHE:CD2	2:B:569:LEU:HG	2.34	0.61
2:B:248:VAL:O	2:B:252:VAL:HG23	2.00	0.61
2:B:346:THR:O	2:B:349:ARG:HB3	2.00	0.61
1:A:246:GLY:HA3	4:A:353:HOH:O	2.00	0.61
2:B:306:GLU:CG	4:B:941:HOH:O	2.30	0.61
1:A:340:LEU:C	1:A:342:PHE:H	2.03	0.61
2:B:158:LEU:CD2	2:B:159:GLU:H	2.14	0.61
2:B:198:LEU:CD1	2:B:393:LEU:HD13	2.24	0.61
2:B:374:ARG:NE	4:B:851:HOH:O	2.29	0.61
1:A:240:LEU:CA	4:A:402:HOH:O	2.15	0.61
1:A:343:LEU:HD13	2:B:509:GLU:O	2.00	0.61
2:B:255:GLU:OE2	2:B:375:ARG:HD2	2.01	0.60
2:B:617:PHE:HD1	2:B:622:LEU:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:ASP:C	2:B:565:PRO:HD3	2.20	0.60
1:A:139:ILE:HA	4:A:372:HOH:O	2.01	0.60
2:B:118:LEU:O	2:B:133:LEU:HD23	1.99	0.60
1:A:278:LEU:HD11	1:A:325:LEU:HD13	1.84	0.60
2:B:267:PHE:CE1	2:B:321:GLU:HG2	2.36	0.60
2:B:287:ASP:H	2:B:317:MET:CE	2.08	0.60
2:B:602:ARG:HH11	2:B:602:ARG:CB	2.04	0.60
2:B:578:ARG:O	2:B:579:GLU:HB2	2.01	0.60
2:B:297:ASP:O	2:B:299:VAL:HG23	2.02	0.60
2:B:370:VAL:HB	2:B:371:PRO:HD3	1.84	0.60
2:B:539:PRO:HG2	2:B:540:GLU:OE2	2.02	0.60
1:A:257:TYR:CD1	2:B:163:ASN:HB3	2.36	0.60
1:A:332:ILE:HD13	1:A:332:ILE:O	2.00	0.60
2:B:510:VAL:O	2:B:511:TYR:HD1	1.84	0.60
2:B:749:PHE:CD2	4:B:906:HOH:O	2.55	0.60
1:A:107:GLU:O	1:A:111:VAL:HG23	2.01	0.60
2:B:455:LEU:HA	4:B:961:HOH:O	2.00	0.60
2:B:609:LEU:HD23	2:B:609:LEU:O	2.02	0.60
1:A:86:VAL:C	4:A:384:HOH:O	2.40	0.59
2:B:333:LEU:HD23	4:B:915:HOH:O	2.02	0.59
2:B:334:GLU:OE1	3:B:786:MTY:HZ	2.02	0.59
1:A:297:TYR:O	1:A:297:TYR:CD1	2.55	0.59
2:B:287:ASP:N	2:B:317:MET:CE	2.65	0.59
2:B:549:PHE:CD1	2:B:549:PHE:C	2.75	0.59
2:B:52:GLU:CG	2:B:54:HIS:CE1	2.85	0.59
2:B:52:GLU:CG	2:B:54:HIS:HE1	2.15	0.59
2:B:56:ILE:HG12	4:B:842:HOH:O	1.87	0.59
2:B:549:PHE:HB3	2:B:672:GLU:OE1	2.03	0.59
1:A:168:GLU:CA	4:A:407:HOH:O	2.49	0.59
2:B:388:VAL:HB	4:B:957:HOH:O	2.01	0.59
1:A:151:THR:HG22	1:A:152:PHE:N	2.18	0.59
2:B:229:TRP:HD1	4:B:883:HOH:O	1.83	0.59
2:B:333:LEU:HD22	2:B:335:VAL:HG23	1.83	0.59
2:B:443:ARG:HD2	4:B:833:HOH:O	2.02	0.59
1:A:331:ASP:HB3	1:A:334:TYR:CD2	2.37	0.59
2:B:596:LEU:HD13	2:B:598:TRP:CH2	2.37	0.59
1:A:128:GLU:OE1	1:A:185:ARG:NH1	2.36	0.59
2:B:178:HIS:CD2	2:B:184:LEU:HB2	2.37	0.59
2:B:121:ARG:HG3	2:B:121:ARG:NH1	2.18	0.58
2:B:323:GLU:CG	4:B:792:HOH:O	2.47	0.58
2:B:659:ILE:N	2:B:659:ILE:HD12	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LEU:HD13	2:B:101:GLN:HB2	1.84	0.58
2:B:556:LEU:HD12	2:B:556:LEU:O	2.04	0.58
1:A:128:GLU:OE2	1:A:132:PHE:CB	2.51	0.58
2:B:210:ALA:N	2:B:211:PRO:HD3	2.19	0.58
2:B:418:SER:N	4:B:861:HOH:O	2.35	0.58
2:B:763:GLU:CG	4:B:816:HOH:O	2.39	0.58
2:B:212:HIS:ND1	2:B:398:PRO:HD3	2.19	0.58
2:B:403:ALA:HB2	2:B:445:THR:HG22	1.84	0.58
2:B:95:GLU:CB	4:B:911:HOH:O	2.25	0.58
2:B:445:THR:CG2	4:B:894:HOH:O	2.28	0.58
2:B:725:LEU:HD21	2:B:745:PHE:CE1	2.37	0.58
2:B:768:VAL:O	2:B:772:LEU:HB2	2.04	0.58
1:A:182:MET:HE3	1:A:182:MET:O	2.04	0.58
2:B:733:GLY:O	2:B:736:LEU:HB2	2.04	0.58
2:B:776:GLY:C	4:B:959:HOH:O	2.39	0.58
1:A:296:ALA:CA	4:A:405:HOH:O	2.43	0.58
2:B:243:ASN:OD1	2:B:246:VAL:HG23	2.03	0.58
1:A:140:PRO:HG2	1:A:143:HIS:HB2	1.84	0.57
1:A:297:TYR:O	1:A:301:LEU:HD13	2.04	0.57
2:B:505:LEU:O	2:B:505:LEU:HD23	2.03	0.57
2:B:589:LEU:O	2:B:590:PHE:HB3	2.03	0.57
1:A:163:GLY:HA2	1:A:185:ARG:HH21	1.69	0.57
2:B:265:LEU:HA	2:B:268:VAL:CG2	2.34	0.57
2:B:715:ARG:NH1	2:B:725:LEU:HD13	2.18	0.57
2:B:323:GLU:CB	4:B:792:HOH:O	2.52	0.57
1:A:94:SER:HB3	4:A:404:HOH:O	2.03	0.57
2:B:589:LEU:O	2:B:590:PHE:CB	2.53	0.57
2:B:633:PHE:CD1	2:B:634:LEU:HG	2.40	0.57
1:A:203:PHE:CD1	1:A:203:PHE:N	2.71	0.57
1:A:142:HIS:CD2	4:A:382:HOH:O	2.58	0.57
2:B:532:LEU:CA	4:B:933:HOH:O	2.03	0.57
2:B:253:MET:HE3	2:B:259:PRO:HG3	1.87	0.57
2:B:258:GLN:NE2	4:B:797:HOH:O	2.37	0.57
2:B:771:ALA:HB2	4:B:839:HOH:O	2.03	0.57
2:B:158:LEU:HD12	2:B:173:LEU:HD21	1.87	0.57
2:B:335:VAL:HB	2:B:373:GLN:NE2	2.20	0.57
2:B:345:LYS:HE3	4:B:862:HOH:O	2.05	0.57
2:B:413:ARG:O	4:B:869:HOH:O	2.17	0.57
2:B:609:LEU:HD22	2:B:652:LEU:HD11	1.87	0.57
1:A:94:SER:N	4:A:404:HOH:O	2.38	0.57
2:B:403:ALA:CB	2:B:445:THR:HG22	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.87	0.57
2:B:62:LYS:HE2	4:B:857:HOH:O	2.05	0.56
2:B:699:VAL:CG1	2:B:772:LEU:HD21	2.35	0.56
2:B:357:SER:O	2:B:361:GLU:HG3	2.05	0.56
2:B:557:LYS:CG	2:B:665:LEU:HD21	2.32	0.56
2:B:727:LEU:HD23	4:B:905:HOH:O	2.05	0.56
2:B:6:SER:OG	2:B:153:GLU:OE2	2.16	0.56
2:B:713:LEU:HA	4:B:836:HOH:O	2.05	0.56
2:B:517:ASP:HB3	2:B:520:ASP:OD2	2.05	0.56
1:A:92:GLY:O	4:A:404:HOH:O	2.17	0.56
2:B:590:PHE:CG	2:B:591:GLY:N	2.74	0.56
2:B:692:ALA:HB2	2:B:750:ARG:HD2	1.88	0.56
2:B:333:LEU:HG	4:B:915:HOH:O	2.04	0.56
2:B:440:PRO:HG2	2:B:441:THR:H	1.70	0.56
2:B:532:LEU:CD2	4:B:933:HOH:O	2.35	0.56
1:A:163:GLY:HA2	1:A:185:ARG:NH2	2.21	0.56
1:A:165:LEU:HD12	1:A:301:LEU:HD23	1.88	0.56
1:A:319:VAL:HG12	1:A:320:GLU:N	2.21	0.56
2:B:8:LEU:O	2:B:8:LEU:HD12	2.05	0.56
1:A:115:ARG:HG2	1:A:115:ARG:NH1	2.16	0.56
2:B:538:ALA:HB1	2:B:539:PRO:HD2	1.87	0.56
1:A:109:GLU:HG3	4:A:400:HOH:O	2.06	0.55
2:B:479:PHE:N	4:B:841:HOH:O	2.24	0.55
2:B:600:LYS:CD	4:B:860:HOH:O	2.54	0.55
1:A:283:ALA:HB2	1:A:315:PHE:CB	2.37	0.55
2:B:160:VAL:HG13	2:B:167:ALA:HB3	1.88	0.55
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.71	0.55
1:A:300:ARG:CZ	4:A:389:HOH:O	2.54	0.55
2:B:600:LYS:H	2:B:600:LYS:HD3	1.70	0.55
1:A:106:MET:HG2	1:A:323:ALA:HB2	1.88	0.55
2:B:554:ARG:O	2:B:558:GLU:HG3	2.06	0.55
2:B:604:SER:HA	2:B:608:LEU:CD2	2.37	0.55
1:A:233:LEU:O	1:A:237:ILE:HD13	2.07	0.55
2:B:467:GLN:HE21	2:B:467:GLN:CA	2.06	0.55
2:B:697:LEU:O	2:B:697:LEU:HD12	2.06	0.55
2:B:427:ILE:HD12	2:B:466:ILE:CG2	2.37	0.55
2:B:753:LYS:HB2	4:B:890:HOH:O	2.05	0.55
2:B:176:ASP:CG	2:B:465:ARG:NH2	2.59	0.55
2:B:634:LEU:HD11	2:B:651:PHE:CD1	2.42	0.55
1:A:96:PHE:CZ	4:B:940:HOH:O	2.53	0.54
1:A:320:GLU:O	1:A:324:MET:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ASN:O	2:B:244:ASN:C	2.46	0.54
1:A:197:VAL:HA	1:A:220:GLU:O	2.07	0.54
1:A:350:LEU:HD21	4:A:409:HOH:O	2.05	0.54
2:B:179:ALA:HB1	2:B:466:ILE:HD13	1.88	0.54
2:B:302:GLY:C	4:B:922:HOH:O	2.45	0.54
2:B:1:MET:O	2:B:2:ARG:C	2.45	0.54
2:B:55:PRO:HD2	4:B:937:HOH:O	2.07	0.54
2:B:390:GLU:O	2:B:390:GLU:HG2	2.08	0.54
2:B:557:LYS:HG2	2:B:665:LEU:CD2	2.32	0.54
1:A:165:LEU:HD12	4:A:411:HOH:O	2.08	0.54
2:B:623:ALA:HB3	2:B:645:GLU:HA	1.88	0.54
1:A:127:VAL:HG23	2:B:577:PHE:CE2	2.43	0.54
2:B:28:LEU:HD11	2:B:177:LEU:HD23	1.89	0.54
2:B:702:PRO:C	2:B:704:PRO:HD2	2.28	0.54
1:A:248:ASP:CG	4:A:399:HOH:O	2.43	0.54
2:B:299:VAL:CG1	2:B:300:ILE:N	2.71	0.54
2:B:701:VAL:HG21	2:B:710:VAL:HG22	1.90	0.54
1:A:96:PHE:HZ	4:B:940:HOH:O	1.90	0.54
2:B:600:LYS:HD3	2:B:600:LYS:N	2.23	0.54
1:A:164:PRO:HG3	1:A:185:ARG:HA	1.90	0.54
2:B:389:ALA:O	2:B:391:ALA:N	2.41	0.54
2:B:567:ARG:CD	4:B:886:HOH:O	2.55	0.54
1:A:201:ARG:NH1	1:A:336:PHE:CE1	2.76	0.54
1:A:221:GLY:HA3	1:A:315:PHE:CZ	2.43	0.54
1:A:321:ARG:O	1:A:324:MET:HB2	2.08	0.54
2:B:239:MET:HE3	2:B:254:LEU:HD21	1.88	0.54
2:B:412:ASN:O	2:B:414:LEU:N	2.41	0.54
2:B:644:VAL:O	2:B:645:GLU:HB2	2.07	0.54
1:A:182:MET:HE3	1:A:185:ARG:HB2	1.88	0.53
2:B:763:GLU:O	2:B:767:ARG:HG2	2.08	0.53
1:A:137:LEU:O	1:A:139:ILE:HG13	2.07	0.53
1:A:199:PRO:HB3	1:A:219:LEU:HD12	1.90	0.53
2:B:427:ILE:HG23	2:B:466:ILE:HD12	1.89	0.53
2:B:701:VAL:HG13	2:B:705:THR:HB	1.91	0.53
1:A:322:LEU:O	1:A:324:MET:N	2.41	0.53
2:B:724:SER:O	2:B:747:LEU:HA	2.09	0.53
1:A:194:PHE:CA	4:A:363:HOH:O	2.55	0.53
1:A:229:ALA:HB1	4:B:869:HOH:O	1.97	0.53
2:B:370:VAL:O	2:B:373:GLN:HB2	2.08	0.53
2:B:513:TYR:CE1	4:B:796:HOH:O	2.54	0.53
2:B:590:PHE:CD1	2:B:591:GLY:N	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:607:PHE:N	4:B:934:HOH:O	2.41	0.53
2:B:767:ARG:HE	2:B:767:ARG:N	2.06	0.53
2:B:55:PRO:CD	4:B:937:HOH:O	2.57	0.53
2:B:120:PRO:HG3	2:B:133:LEU:CD1	2.38	0.53
2:B:532:LEU:CB	4:B:933:HOH:O	2.49	0.53
2:B:619:ARG:HD2	2:B:619:ARG:O	2.08	0.53
2:B:755:THR:HG22	2:B:756:LEU:N	2.24	0.53
2:B:530:ARG:HG3	2:B:530:ARG:HH11	1.73	0.53
1:A:164:PRO:HB3	1:A:188:VAL:HG23	1.91	0.53
1:A:129:SER:O	1:A:131:PHE:N	2.41	0.53
1:A:160:ARG:NH2	4:A:408:HOH:O	2.37	0.53
2:B:140:LEU:HD21	2:B:149:ALA:HB2	1.91	0.53
2:B:258:GLN:HE22	2:B:369:GLN:NE2	2.07	0.53
1:A:298:ARG:NH1	1:A:304:PRO:O	2.41	0.53
2:B:30:PHE:HB3	2:B:158:LEU:CD2	2.39	0.52
2:B:206:ASP:OD2	2:B:276:ARG:HD3	2.09	0.52
2:B:502:LEU:HD13	2:B:571:PHE:CE2	2.44	0.52
2:B:588:LEU:HD23	2:B:588:LEU:O	2.08	0.52
2:B:699:VAL:HG22	2:B:772:LEU:HD21	1.91	0.52
2:B:163:ASN:O	2:B:452:ASP:HB3	2.08	0.52
2:B:258:GLN:HE22	2:B:369:GLN:HE21	1.57	0.52
2:B:404:ILE:HD12	2:B:454:ARG:O	2.09	0.52
2:B:770:GLU:CB	4:B:822:HOH:O	2.56	0.52
1:A:103:ILE:HG23	1:A:319:VAL:HG11	1.92	0.52
2:B:46:VAL:HB	2:B:143:GLY:O	2.08	0.52
2:B:567:ARG:CA	2:B:591:GLY:HA3	2.39	0.52
2:B:715:ARG:NH1	2:B:715:ARG:HB2	2.24	0.52
1:A:143:HIS:HA	4:A:383:HOH:O	2.10	0.52
2:B:637:GLY:CA	4:B:908:HOH:O	2.22	0.52
2:B:62:LYS:HB2	2:B:62:LYS:NZ	2.25	0.52
2:B:275:ARG:HG3	2:B:275:ARG:HH11	1.74	0.52
1:A:349:VAL:O	1:A:350:LEU:HB2	2.10	0.52
4:A:408:HOH:O	2:B:579:GLU:CA	2.40	0.52
2:B:270:GLU:CG	4:B:799:HOH:O	2.57	0.52
1:A:87:ASP:OD1	1:A:89:SER:N	2.39	0.52
1:A:340:LEU:C	1:A:342:PHE:N	2.62	0.52
2:B:450:ARG:NH2	2:B:452:ASP:OD2	2.41	0.52
2:B:517:ASP:OD1	2:B:540:GLU:HA	2.10	0.52
2:B:729:ASP:HB3	2:B:744:ALA:HB2	1.92	0.52
2:B:348:ARG:NH1	2:B:361:GLU:OE1	2.44	0.51
1:A:101:HIS:CB	2:B:509:GLU:OE1	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:LYS:HD3	4:B:860:HOH:O	2.10	0.51
1:A:283:ALA:HB2	1:A:315:PHE:HA	1.91	0.51
2:B:151:PRO:HG2	2:B:232:ARG:NH2	2.24	0.51
1:A:168:GLU:N	4:A:407:HOH:O	2.44	0.51
1:A:332:ILE:HD13	1:A:335:PHE:CD2	2.43	0.51
2:B:600:LYS:O	2:B:601:GLU:C	2.48	0.51
2:B:652:LEU:HD13	2:B:671:PHE:HB3	1.92	0.51
2:B:710:VAL:HG11	2:B:743:LEU:HD12	1.93	0.51
2:B:728:PHE:CZ	2:B:744:ALA:HB1	2.44	0.51
2:B:746:HIS:CE1	4:B:900:HOH:O	2.53	0.51
1:A:114:PHE:HA	1:A:117:LEU:HD12	1.92	0.51
1:A:115:ARG:CZ	2:B:493:ARG:HH21	2.23	0.51
1:A:182:MET:HG2	1:A:198:VAL:HG21	1.92	0.51
2:B:530:ARG:NH1	4:B:870:HOH:O	2.43	0.51
2:B:3:VAL:CG2	2:B:158:LEU:HB2	2.41	0.51
2:B:141:PRO:O	2:B:144:THR:HG23	2.10	0.51
2:B:261:HIS:CD2	3:B:786:MTY:HA	2.41	0.51
2:B:374:ARG:CD	4:B:851:HOH:O	2.59	0.51
1:A:201:ARG:NH1	1:A:336:PHE:HE1	2.08	0.51
2:B:9:LYS:HE3	4:B:947:HOH:O	2.11	0.51
2:B:222:ARG:HG3	2:B:222:ARG:O	2.11	0.51
2:B:250:ASN:O	2:B:253:MET:HB3	2.11	0.51
2:B:779:LEU:C	4:B:916:HOH:O	2.48	0.51
1:A:197:VAL:HG21	1:A:219:LEU:HD21	1.93	0.51
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.41	0.51
2:B:40:PRO:HG2	4:B:896:HOH:O	2.10	0.51
2:B:567:ARG:HB3	2:B:591:GLY:HA3	1.93	0.51
2:B:592:GLU:HG3	2:B:593:GLY:H	1.76	0.51
2:B:697:LEU:HD12	2:B:697:LEU:C	2.31	0.51
1:A:175:LEU:HB3	1:A:203:PHE:CD1	2.46	0.51
2:B:7:TRP:CE3	2:B:233:ALA:HB1	2.46	0.51
2:B:407:ARG:HD3	2:B:456:GLU:OE2	2.10	0.51
2:B:220:GLY:C	4:B:923:HOH:O	2.48	0.50
2:B:578:ARG:O	2:B:579:GLU:CB	2.59	0.50
2:B:613:LEU:HD21	2:B:671:PHE:CE2	2.45	0.50
2:B:686:ASP:HB2	4:B:953:HOH:O	2.10	0.50
1:A:168:GLU:HA	4:A:407:HOH:O	2.11	0.50
2:B:316:VAL:N	4:B:876:HOH:O	2.44	0.50
2:B:757:ARG:HG2	2:B:757:ARG:HH11	1.76	0.50
1:A:248:ASP:HB3	4:A:399:HOH:O	1.92	0.50
1:A:271:TRP:CA	4:A:366:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:O	1:A:342:PHE:N	2.45	0.50
2:B:360:PHE:HA	4:B:897:HOH:O	2.10	0.50
2:B:548:LEU:HD22	2:B:584:HIS:CB	2.40	0.50
2:B:408:PRO:HB3	2:B:424:GLN:NE2	2.27	0.50
2:B:644:VAL:HG11	2:B:678:PRO:HD2	1.94	0.50
2:B:713:LEU:HD13	2:B:772:LEU:HD12	1.94	0.50
2:B:710:VAL:O	2:B:714:VAL:HG23	2.11	0.50
2:B:267:PHE:CD1	2:B:321:GLU:HG2	2.47	0.50
2:B:403:ALA:HA	2:B:445:THR:HG22	1.92	0.50
2:B:659:ILE:HD12	2:B:659:ILE:H	1.76	0.50
2:B:584:HIS:HD2	2:B:672:GLU:OE2	1.94	0.50
2:B:753:LYS:N	4:B:890:HOH:O	2.45	0.50
1:A:264:GLY:O	1:A:265:ALA:HB2	2.11	0.50
2:B:527:ASP:CB	4:B:892:HOH:O	2.47	0.50
2:B:549:PHE:N	2:B:672:GLU:OE1	2.40	0.50
1:A:261:VAL:CB	4:A:391:HOH:O	2.40	0.49
2:B:145:PRO:HB3	4:B:826:HOH:O	2.11	0.49
2:B:564:ARG:N	2:B:564:ARG:CD	2.75	0.49
1:A:327:TYR:CE1	4:A:379:HOH:O	2.55	0.49
2:B:224:ALA:HB3	2:B:244:ASN:HD21	1.77	0.49
2:B:414:LEU:HD23	2:B:460:VAL:HG21	1.93	0.49
1:A:98:GLY:O	1:A:347:LYS:HE3	2.13	0.49
1:A:210:ALA:HA	1:A:331:ASP:OD1	2.12	0.49
2:B:402:GLU:N	4:B:803:HOH:O	2.38	0.49
2:B:17:SER:OG	2:B:20:VAL:HG23	2.12	0.49
2:B:206:ASP:CG	2:B:276:ARG:HH11	2.15	0.49
2:B:294:HIS:CE1	2:B:295:PRO:HG2	2.47	0.49
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.43	0.49
1:A:326:ARG:HG3	4:A:410:HOH:O	2.12	0.49
2:B:461:GLU:O	2:B:465:ARG:HG2	2.12	0.49
2:B:70:ARG:CB	4:B:943:HOH:O	2.60	0.49
2:B:715:ARG:HB2	2:B:715:ARG:HH11	1.75	0.49
1:A:94:SER:CB	4:A:404:HOH:O	2.56	0.49
1:A:287:HIS:CE1	1:A:288:PRO:HD2	2.48	0.49
2:B:586:ALA:HB2	2:B:672:GLU:HA	1.95	0.49
2:B:701:VAL:O	2:B:741:LYS:HG2	2.12	0.49
1:A:307:TYR:N	1:A:307:TYR:HD1	2.06	0.49
2:B:403:ALA:CA	2:B:445:THR:HG22	2.43	0.49
2:B:335:VAL:HB	2:B:373:GLN:HE21	1.78	0.49
2:B:500:GLU:HA	2:B:503:SER:OG	2.13	0.49
2:B:297:ASP:OD2	2:B:350:HIS:CE1	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:VAL:O	2:B:345:LYS:HG3	2.12	0.49
2:B:548:LEU:HD21	2:B:574:GLY:H	1.78	0.49
1:A:194:PHE:CB	4:A:363:HOH:O	2.47	0.48
2:B:51:LEU:HD11	2:B:67:ASP:HB2	1.93	0.48
2:B:192:LYS:H	2:B:381:GLN:HE22	1.58	0.48
1:A:183:GLN:O	1:A:187:MET:HG3	2.14	0.48
2:B:592:GLU:HG3	2:B:593:GLY:N	2.27	0.48
1:A:115:ARG:NE	2:B:493:ARG:HH21	2.11	0.48
2:B:91:LEU:HB3	2:B:92:PRO:HD2	1.95	0.48
2:B:214:THR:HA	2:B:393:LEU:O	2.14	0.48
2:B:253:MET:HE1	2:B:356:ALA:N	2.28	0.48
1:A:113:ILE:O	1:A:117:LEU:HD12	2.14	0.48
2:B:586:ALA:HB1	2:B:671:PHE:O	2.12	0.48
2:B:754:ARG:NH1	2:B:756:LEU:HD23	2.29	0.48
1:A:262:GLU:OE2	2:B:461:GLU:OE1	2.32	0.48
1:A:280:LEU:CD1	1:A:317:LEU:HD22	2.43	0.48
2:B:18:PRO:O	2:B:21:LEU:HB3	2.14	0.48
2:B:527:ASP:CA	4:B:892:HOH:O	2.61	0.48
2:B:316:VAL:HG22	2:B:357:SER:HB3	1.96	0.48
2:B:703:ALA:N	2:B:704:PRO:HD2	2.28	0.48
2:B:717:ALA:N	4:B:925:HOH:O	2.26	0.48
1:A:101:HIS:CE1	1:A:103:ILE:HG12	2.48	0.48
2:B:19:GLU:H	2:B:19:GLU:CD	2.17	0.48
2:B:213:PHE:HA	2:B:336:ALA:HB2	1.95	0.48
2:B:243:ASN:O	2:B:244:ASN:O	2.30	0.48
2:B:717:ALA:CB	4:B:839:HOH:O	2.62	0.48
2:B:38:VAL:HG22	2:B:153:GLU:O	2.13	0.48
2:B:336:ALA:HA	2:B:369:GLN:CG	2.44	0.48
1:A:118:GLY:C	4:A:392:HOH:O	2.51	0.48
2:B:99:LEU:O	2:B:101:GLN:HG2	2.14	0.48
2:B:729:ASP:HB3	2:B:744:ALA:CB	2.44	0.48
2:B:16:GLU:OE2	2:B:20:VAL:HG11	2.13	0.48
2:B:530:ARG:HG3	2:B:530:ARG:NH1	2.29	0.48
2:B:717:ALA:CA	4:B:925:HOH:O	2.62	0.48
1:A:93:ALA:O	1:A:95:LEU:N	2.47	0.47
2:B:39:PHE:HB2	2:B:152:GLU:HA	1.95	0.47
2:B:635:HIS:ND1	2:B:637:GLY:N	2.62	0.47
2:B:655:LEU:HG	2:B:656:HIS:N	2.29	0.47
2:B:747:LEU:N	2:B:747:LEU:HD12	2.29	0.47
1:A:114:PHE:HA	1:A:117:LEU:CD1	2.44	0.47
1:A:219:LEU:O	1:A:316:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HG3	1:A:326:ARG:NH1	2.29	0.47
2:B:643:LEU:HD13	2:B:648:GLU:HA	1.95	0.47
2:B:730:LEU:HD13	2:B:743:LEU:HD21	1.93	0.47
2:B:753:LYS:CA	4:B:890:HOH:O	2.61	0.47
1:A:240:LEU:O	1:A:244:LEU:HB2	2.14	0.47
1:A:285:MET:SD	1:A:313:PHE:HB3	2.54	0.47
2:B:277:ALA:O	2:B:295:PRO:HA	2.14	0.47
2:B:389:ALA:C	2:B:391:ALA:H	2.17	0.47
2:B:509:GLU:HA	2:B:571:PHE:CE1	2.50	0.47
1:A:180:SER:O	1:A:181:PRO:C	2.52	0.47
2:B:190:ALA:HB3	4:B:852:HOH:O	2.07	0.47
2:B:253:MET:HG3	2:B:259:PRO:HA	1.95	0.47
2:B:495:GLU:O	2:B:498:LEU:HB3	2.15	0.47
2:B:508:GLN:OE1	2:B:508:GLN:HA	2.14	0.47
2:B:589:LEU:CD2	2:B:609:LEU:HB2	2.45	0.47
2:B:688:SER:CB	2:B:752:PRO:HA	2.42	0.47
1:A:229:ALA:H	1:A:232:HIS:CD2	2.29	0.47
2:B:30:PHE:HB3	2:B:158:LEU:HD21	1.97	0.47
2:B:309:PHE:N	2:B:309:PHE:CD1	2.82	0.47
2:B:387:ARG:HA	4:B:825:HOH:O	2.14	0.47
2:B:516:MET:HG2	2:B:517:ASP:N	2.29	0.47
1:A:86:VAL:CA	4:A:384:HOH:O	2.63	0.47
1:A:210:ALA:CB	4:A:387:HOH:O	2.61	0.47
2:B:3:VAL:HG23	2:B:158:LEU:HB2	1.96	0.47
2:B:51:LEU:O	2:B:52:GLU:HB2	2.14	0.47
2:B:161:THR:HB	2:B:162:PRO:HD2	1.96	0.47
2:B:279:GLU:HA	4:B:931:HOH:O	2.08	0.47
2:B:317:MET:HA	3:B:786:MTY:H2	1.77	0.47
2:B:555:VAL:HG23	2:B:556:LEU:N	2.29	0.47
2:B:657:PRO:O	2:B:660:ALA:HB3	2.14	0.47
3:B:786:MTY:CE2	4:B:876:HOH:O	2.57	0.47
1:A:114:PHE:CE2	1:A:240:LEU:HD13	2.49	0.47
1:A:278:LEU:HD11	1:A:325:LEU:CD1	2.44	0.47
1:A:152:PHE:CD1	2:B:533:LEU:HD23	2.50	0.47
1:A:194:PHE:HA	4:A:363:HOH:O	2.13	0.47
2:B:253:MET:HE2	2:B:355:GLU:HB3	1.97	0.47
2:B:368:GLY:O	2:B:371:PRO:HD2	2.15	0.47
2:B:630:ALA:CB	4:B:893:HOH:O	2.41	0.47
1:A:125:PRO:HG3	1:A:185:ARG:NH1	2.30	0.46
1:A:208:THR:O	1:A:208:THR:HG22	2.16	0.46
2:B:171:LEU:O	2:B:171:LEU:CD2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:HIS:ND1	2:B:398:PRO:CD	2.78	0.46
2:B:580:ARG:HG2	2:B:580:ARG:HH11	1.78	0.46
2:B:633:PHE:CE1	2:B:634:LEU:HG	2.50	0.46
1:A:108:ARG:O	4:A:377:HOH:O	2.20	0.46
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.51	0.46
1:A:288:PRO:CG	2:B:457:GLU:HG2	2.45	0.46
2:B:699:VAL:O	2:B:742:SER:HA	2.15	0.46
2:B:28:LEU:CD1	2:B:177:LEU:HD23	2.45	0.46
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.51	0.46
1:A:301:LEU:HD23	4:A:411:HOH:O	2.14	0.46
2:B:230:MET:HE2	2:B:251:TYR:CD1	2.50	0.46
2:B:248:VAL:O	2:B:248:VAL:HG12	2.16	0.46
2:B:626:VAL:HG13	2:B:641:ARG:O	2.15	0.46
2:B:772:LEU:HG	2:B:777:PHE:HB2	1.97	0.46
1:A:164:PRO:CB	1:A:188:VAL:CG2	2.94	0.46
2:B:307:GLU:CG	4:B:938:HOH:O	2.58	0.46
2:B:635:HIS:CE1	2:B:637:GLY:H	2.33	0.46
2:B:517:ASP:HA	2:B:540:GLU:O	2.16	0.46
2:B:587:GLY:N	2:B:671:PHE:CE1	2.84	0.46
2:B:601:GLU:CD	2:B:601:GLU:H	2.19	0.46
2:B:759:GLU:HB3	4:B:801:HOH:O	2.02	0.46
1:A:228:ILE:HG22	1:A:229:ALA:N	2.31	0.46
2:B:211:PRO:HD2	4:B:879:HOH:O	1.98	0.46
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.80	0.46
2:B:420:PRO:HG2	2:B:423:GLU:HB2	1.97	0.46
2:B:556:LEU:HD12	2:B:556:LEU:C	2.37	0.46
2:B:602:ARG:NH1	4:B:904:HOH:O	2.48	0.46
2:B:609:LEU:HD22	2:B:652:LEU:CD1	2.46	0.46
2:B:624:PHE:C	2:B:624:PHE:CD2	2.88	0.46
2:B:20:VAL:O	2:B:23:GLU:HB3	2.15	0.46
2:B:178:HIS:CE1	4:B:895:HOH:O	2.54	0.46
2:B:222:ARG:CG	2:B:222:ARG:O	2.64	0.46
2:B:256:ARG:CZ	2:B:375:ARG:HG3	2.46	0.46
2:B:353:ARG:C	2:B:353:ARG:HD3	2.36	0.46
2:B:701:VAL:HG12	2:B:702:PRO:O	2.16	0.46
1:A:261:VAL:HG21	4:A:391:HOH:O	2.09	0.45
2:B:212:HIS:O	2:B:336:ALA:HB1	2.15	0.45
1:A:344:GLU:O	1:A:347:LYS:HG3	2.17	0.45
2:B:107:VAL:HG22	2:B:112:ARG:HB3	1.98	0.45
2:B:404:ILE:HG12	2:B:444:VAL:O	2.16	0.45
2:B:507:PHE:CE2	2:B:569:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASP:O	1:A:334:TYR:CD2	2.69	0.45
2:B:43:ARG:HG3	2:B:43:ARG:HH11	1.80	0.45
2:B:176:ASP:N	4:B:871:HOH:O	2.50	0.45
2:B:642:VAL:O	2:B:643:LEU:HD22	2.16	0.45
2:B:14:GLU:CB	4:B:789:HOH:O	2.60	0.45
2:B:461:GLU:O	2:B:461:GLU:HG2	2.16	0.45
2:B:545:ARG:NH2	2:B:548:LEU:HD11	2.31	0.45
2:B:80:ASN:HB2	2:B:82:ARG:HH12	1.81	0.45
2:B:264:ASP:OD2	2:B:266:ARG:HD3	2.17	0.45
2:B:459:LEU:O	2:B:462:GLU:HB2	2.17	0.45
2:B:660:ALA:HB1	2:B:665:LEU:O	2.16	0.45
1:A:283:ALA:HB1	1:A:314:ALA:O	2.17	0.45
2:B:47:PHE:CE1	2:B:139:ALA:HB3	2.52	0.45
2:B:669:HIS:CD2	4:B:823:HOH:O	2.63	0.45
1:A:179:THR:OG1	1:A:220:GLU:CG	2.65	0.45
1:A:179:THR:OG1	1:A:220:GLU:HG2	2.16	0.45
1:A:180:SER:O	1:A:183:GLN:N	2.36	0.45
1:A:260:PHE:HD2	4:A:356:HOH:O	2.00	0.45
2:B:60:ARG:C	2:B:60:ARG:HD3	2.37	0.45
2:B:365:ASP:HA	2:B:366:PRO:HD2	1.74	0.45
2:B:512:THR:HG22	4:B:820:HOH:O	2.09	0.45
2:B:557:LYS:HD3	2:B:561:ASP:OD2	2.16	0.45
1:A:187:MET:SD	1:A:307:TYR:CE2	3.10	0.45
2:B:277:ALA:HB2	2:B:299:VAL:HG21	1.98	0.45
2:B:559:ASN:O	2:B:561:ASP:N	2.50	0.45
2:B:563:ASP:C	2:B:564:ARG:HD2	2.35	0.45
2:B:707:TYR:CZ	4:B:905:HOH:O	2.56	0.45
1:A:280:LEU:HD11	1:A:322:LEU:HD21	1.99	0.45
2:B:567:ARG:HA	2:B:591:GLY:CA	2.42	0.45
2:B:593:GLY:CA	2:B:604:SER:HB3	2.47	0.45
2:B:615:ALA:O	2:B:617:PHE:N	2.50	0.45
2:B:43:ARG:HG3	2:B:43:ARG:NH1	2.32	0.44
2:B:70:ARG:NE	4:B:943:HOH:O	2.47	0.44
2:B:191:LEU:HD23	2:B:381:GLN:OE1	2.17	0.44
2:B:265:LEU:HD23	2:B:268:VAL:CG2	2.39	0.44
2:B:655:LEU:HG	2:B:656:HIS:H	1.82	0.44
2:B:659:ILE:H	2:B:659:ILE:CD1	2.30	0.44
2:B:707:TYR:CE1	4:B:905:HOH:O	2.70	0.44
2:B:754:ARG:HH11	2:B:756:LEU:HD23	1.82	0.44
1:A:109:GLU:O	1:A:113:ILE:HG13	2.17	0.44
1:A:299:GLU:CB	4:A:385:HOH:O	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:PRO:CD	4:B:853:HOH:O	2.59	0.44
2:B:267:PHE:N	2:B:267:PHE:CD2	2.85	0.44
2:B:589:LEU:CB	2:B:609:LEU:HD12	2.35	0.44
1:A:101:HIS:HB2	2:B:509:GLU:OE1	2.18	0.44
1:A:193:PRO:HB2	2:B:479:PHE:CD1	2.52	0.44
1:A:295:ASP:HA	1:A:298:ARG:HB2	1.99	0.44
1:A:306:ALA:HB3	1:A:307:TYR:CE1	2.53	0.44
1:A:319:VAL:O	1:A:320:GLU:C	2.55	0.44
2:B:153:GLU:OE1	2:B:154:VAL:N	2.46	0.44
2:B:701:VAL:HG13	2:B:702:PRO:HD2	1.99	0.44
1:A:155:THR:O	1:A:155:THR:CG2	2.66	0.44
1:A:156:GLY:HA3	2:B:531:LEU:HD23	2.00	0.44
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.17	0.44
1:A:297:TYR:O	1:A:297:TYR:HD1	1.98	0.44
2:B:253:MET:HE1	2:B:355:GLU:C	2.38	0.44
2:B:489:GLU:O	2:B:490:ALA:C	2.55	0.44
2:B:588:LEU:CB	2:B:670:LEU:HB3	2.47	0.44
1:A:86:VAL:HG13	4:A:384:HOH:O	2.11	0.44
1:A:182:MET:CE	1:A:185:ARG:HB2	2.47	0.44
2:B:333:LEU:CG	4:B:915:HOH:O	2.63	0.44
2:B:586:ALA:HB2	2:B:672:GLU:HG3	1.99	0.44
1:A:296:ALA:C	1:A:298:ARG:N	2.69	0.44
2:B:34:ARG:C	2:B:35:ILE:HD12	2.37	0.44
2:B:47:PHE:HB2	2:B:140:LEU:HD12	2.00	0.44
1:A:283:ALA:HA	3:A:351:MTY:CE1	2.47	0.44
1:A:322:LEU:O	1:A:323:ALA:C	2.56	0.44
2:B:158:LEU:HD22	2:B:159:GLU:N	2.27	0.44
2:B:198:LEU:O	2:B:200:PHE:N	2.44	0.44
2:B:441:THR:CB	4:B:838:HOH:O	2.10	0.44
2:B:587:GLY:O	2:B:671:PHE:CD1	2.71	0.44
2:B:616:LEU:HD12	2:B:616:LEU:O	2.18	0.44
2:B:381:GLN:HG3	2:B:386:ALA:O	2.18	0.44
3:B:786:MTY:HA	3:B:786:MTY:HD2	1.67	0.44
1:A:348:GLY:O	1:A:349:VAL:C	2.56	0.44
2:B:54:HIS:CD2	2:B:63:ARG:NH2	2.86	0.44
2:B:198:LEU:HA	2:B:199:PRO:HD2	1.87	0.44
2:B:280:GLY:N	4:B:931:HOH:O	2.50	0.44
2:B:315:GLY:H	3:B:786:MTY:HZ	1.82	0.44
2:B:602:ARG:CZ	4:B:904:HOH:O	2.66	0.44
2:B:759:GLU:O	2:B:763:GLU:HB3	2.18	0.44
1:A:228:ILE:CG2	1:A:229:ALA:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:ALA:HB2	2:B:299:VAL:CG2	2.47	0.43
2:B:286:LEU:C	2:B:288:GLY:H	2.21	0.43
1:A:185:ARG:C	4:A:386:HOH:O	2.56	0.43
1:A:185:ARG:O	1:A:188:VAL:HG22	2.18	0.43
2:B:276:ARG:HG3	2:B:295:PRO:O	2.18	0.43
2:B:427:ILE:HD12	2:B:466:ILE:HG21	1.99	0.43
2:B:711:GLU:HG2	2:B:725:LEU:HD21	2.00	0.43
1:A:164:PRO:HB3	1:A:188:VAL:CG2	2.48	0.43
2:B:52:GLU:HG2	2:B:54:HIS:HE1	1.82	0.43
2:B:115:GLY:O	2:B:116:MET:HB3	2.18	0.43
2:B:539:PRO:HG2	2:B:540:GLU:CD	2.38	0.43
2:B:715:ARG:O	2:B:718:ALA:N	2.50	0.43
1:A:117:LEU:HD21	1:A:239:GLU:HB3	1.99	0.43
2:B:138:ASP:O	2:B:139:ALA:C	2.56	0.43
2:B:164:ARG:O	2:B:167:ALA:HB3	2.19	0.43
2:B:206:ASP:OD2	2:B:276:ARG:NH1	2.38	0.43
2:B:273:ALA:N	2:B:301:ALA:O	2.43	0.43
2:B:563:ASP:O	2:B:565:PRO:HD3	2.18	0.43
1:A:115:ARG:NH2	2:B:493:ARG:HH21	2.17	0.43
1:A:162:GLU:O	1:A:185:ARG:NH2	2.52	0.43
1:A:349:VAL:HG13	4:A:409:HOH:O	2.11	0.43
2:B:197:PRO:HA	4:B:887:HOH:O	2.18	0.43
2:B:294:HIS:CG	2:B:295:PRO:HD2	2.53	0.43
2:B:556:LEU:O	2:B:560:LEU:HG	2.18	0.43
1:A:154:LEU:CD1	4:A:414:HOH:O	2.47	0.43
1:A:340:LEU:HB3	4:A:365:HOH:O	2.18	0.43
2:B:45:VAL:HG11	2:B:123:LEU:HD11	2.01	0.43
2:B:279:GLU:HG3	4:B:920:HOH:O	2.17	0.43
2:B:287:ASP:OD1	2:B:289:VAL:HB	2.19	0.43
2:B:497:ARG:HH22	2:B:619:ARG:HH12	1.66	0.43
2:B:651:PHE:CE2	2:B:672:GLU:HB3	2.54	0.43
2:B:652:LEU:HD12	2:B:670:LEU:O	2.19	0.43
2:B:710:VAL:O	2:B:713:LEU:HB3	2.18	0.43
1:A:331:ASP:O	1:A:334:TYR:HD2	2.02	0.43
2:B:326:GLU:CD	2:B:326:GLU:H	2.22	0.43
2:B:366:PRO:O	2:B:367:LEU:HD23	2.17	0.43
2:B:408:PRO:HG2	2:B:421:GLU:HG2	1.99	0.43
2:B:502:LEU:HD13	2:B:571:PHE:CD2	2.54	0.43
2:B:613:LEU:CD1	2:B:652:LEU:HD22	2.48	0.43
2:B:695:ARG:O	2:B:696:ASP:OD1	2.37	0.43
1:A:127:VAL:HG22	1:A:154:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:H	1:A:162:GLU:HG2	1.70	0.43
1:A:325:LEU:HD12	1:A:325:LEU:O	2.19	0.43
2:B:49:ARG:HG2	2:B:137:GLU:HG3	2.01	0.43
2:B:278:ARG:O	2:B:281:GLU:HB2	2.18	0.43
2:B:286:LEU:HB2	2:B:317:MET:HE3	2.00	0.43
2:B:690:HIS:CD2	2:B:754:ARG:HA	2.54	0.43
1:A:283:ALA:CB	1:A:315:PHE:HA	2.49	0.43
2:B:434:ARG:NH1	2:B:436:GLU:HG3	2.34	0.43
2:B:49:ARG:HH21	2:B:51:LEU:HD21	1.82	0.43
2:B:344:ARG:O	2:B:348:ARG:HD3	2.19	0.43
2:B:365:ASP:HB3	4:B:797:HOH:O	2.19	0.43
2:B:697:LEU:HB2	2:B:779:LEU:HD11	2.01	0.43
2:B:701:VAL:HG21	2:B:710:VAL:CG2	2.48	0.43
2:B:528:PRO:CD	4:B:892:HOH:O	2.20	0.42
1:A:122:VAL:O	1:A:122:VAL:HG23	2.19	0.42
1:A:140:PRO:HG2	1:A:143:HIS:CD2	2.53	0.42
2:B:737:PRO:O	2:B:738:GLU:O	2.37	0.42
2:B:62:LYS:NZ	2:B:81:ALA:HB3	2.34	0.42
2:B:516:MET:HE1	2:B:546:THR:N	2.27	0.42
1:A:142:HIS:NE2	4:A:382:HOH:O	2.36	0.42
1:A:271:TRP:HZ3	1:A:276:LYS:HE2	1.84	0.42
2:B:145:PRO:HD2	2:B:148:GLU:OE2	2.19	0.42
2:B:532:LEU:C	2:B:533:LEU:HD12	2.40	0.42
2:B:588:LEU:HD12	2:B:668:VAL:HG11	2.02	0.42
1:A:191:THR:CG2	2:B:484:ASP:OD2	2.68	0.42
2:B:213:PHE:HA	2:B:336:ALA:CB	2.49	0.42
2:B:588:LEU:HB2	2:B:670:LEU:HB3	2.02	0.42
2:B:637:GLY:N	4:B:908:HOH:O	2.48	0.42
1:A:164:PRO:CG	1:A:188:VAL:HG21	2.46	0.42
1:A:183:GLN:HG3	1:A:222:LEU:HD22	2.02	0.42
1:A:287:HIS:ND1	1:A:288:PRO:CD	2.81	0.42
1:A:306:ALA:HB3	1:A:307:TYR:CD1	2.55	0.42
2:B:659:ILE:N	2:B:659:ILE:CD1	2.83	0.42
1:A:280:LEU:HD12	1:A:317:LEU:HD22	2.00	0.42
2:B:410:TYR:O	2:B:411:ALA:C	2.55	0.42
2:B:755:THR:HG22	2:B:756:LEU:H	1.85	0.42
1:A:108:ARG:O	1:A:109:GLU:C	2.57	0.42
2:B:203:LYS:O	2:B:273:ALA:HA	2.19	0.42
2:B:642:VAL:O	2:B:648:GLU:HA	2.19	0.42
2:B:749:PHE:N	2:B:749:PHE:CD1	2.88	0.42
1:A:151:THR:CG2	1:A:152:PHE:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:HG23	2:B:484:ASP:OD2	2.20	0.42
2:B:707:TYR:CZ	2:B:711:GLU:HG3	2.54	0.42
1:A:164:PRO:C	1:A:166:GLY:H	2.23	0.42
1:A:180:SER:N	1:A:181:PRO:HD2	2.35	0.42
1:A:271:TRP:C	4:A:366:HOH:O	2.58	0.42
2:B:265:LEU:HD23	2:B:265:LEU:HA	1.93	0.42
2:B:415:LEU:HB3	2:B:417:THR:HG23	2.01	0.42
2:B:431:LEU:HD13	2:B:462:GLU:OE1	2.19	0.42
2:B:456:GLU:CB	4:B:837:HOH:O	2.67	0.42
2:B:630:ALA:CA	4:B:893:HOH:O	2.68	0.42
2:B:634:LEU:HD11	2:B:651:PHE:HD1	1.84	0.42
2:B:762:GLU:O	2:B:765:VAL:HG22	2.20	0.42
2:B:177:LEU:O	2:B:180:LEU:HB2	2.20	0.41
2:B:369:GLN:CD	2:B:369:GLN:H	2.24	0.41
2:B:564:ARG:O	2:B:565:PRO:C	2.59	0.41
2:B:643:LEU:HD22	2:B:643:LEU:N	2.33	0.41
2:B:743:LEU:O	2:B:745:PHE:HD2	2.03	0.41
2:B:751:HIS:CD2	2:B:754:ARG:CZ	3.03	0.41
1:A:210:ALA:HB3	4:A:387:HOH:O	2.20	0.41
2:B:224:ALA:O	2:B:244:ASN:ND2	2.53	0.41
2:B:717:ALA:O	2:B:719:GLY:N	2.44	0.41
2:B:173:LEU:O	2:B:175:ARG:N	2.53	0.41
2:B:187:PRO:CG	4:B:948:HOH:O	2.38	0.41
2:B:585:LEU:HB2	2:B:675:LEU:HD11	2.02	0.41
1:A:127:VAL:HG22	1:A:154:LEU:HD11	2.03	0.41
1:A:349:VAL:CG1	1:A:350:LEU:HD23	2.44	0.41
2:B:217:TYR:CE2	2:B:219:PHE:CD1	3.09	0.41
2:B:779:LEU:CG	4:B:916:HOH:O	2.24	0.41
2:B:99:LEU:O	2:B:101:GLN:N	2.54	0.41
2:B:178:HIS:O	2:B:430:ARG:NH1	2.43	0.41
2:B:282:ARG:HH11	2:B:282:ARG:CB	2.25	0.41
2:B:362:ARG:HG2	2:B:362:ARG:NH1	2.34	0.41
2:B:404:ILE:HG22	2:B:405:PRO:HD2	2.02	0.41
2:B:500:GLU:O	2:B:501:VAL:C	2.57	0.41
2:B:702:PRO:HD2	2:B:777:PHE:HE1	1.85	0.41
2:B:120:PRO:HD3	2:B:133:LEU:HD22	2.01	0.41
2:B:271:GLY:O	2:B:302:GLY:HA2	2.20	0.41
2:B:315:GLY:O	2:B:316:VAL:HG23	2.21	0.41
2:B:387:ARG:CA	4:B:825:HOH:O	2.69	0.41
2:B:434:ARG:NH1	2:B:436:GLU:CG	2.82	0.41
2:B:690:HIS:HB3	2:B:691:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HG21	2:B:513:TYR:CD1	2.56	0.41
2:B:101:GLN:HA	2:B:101:GLN:NE2	2.35	0.41
2:B:243:ASN:ND2	4:B:880:HOH:O	2.18	0.41
2:B:475:ALA:O	2:B:476:LEU:HD23	2.20	0.41
2:B:504:GLY:O	2:B:506:GLY:N	2.54	0.41
2:B:548:LEU:HD21	2:B:574:GLY:N	2.35	0.41
2:B:699:VAL:CG2	2:B:772:LEU:HD21	2.50	0.41
2:B:470:GLU:H	2:B:470:GLU:HG3	1.60	0.41
2:B:587:GLY:O	2:B:671:PHE:HD1	2.02	0.41
2:B:589:LEU:CG	2:B:590:PHE:N	2.79	0.41
1:A:115:ARG:HH21	2:B:493:ARG:HE	1.69	0.41
1:A:140:PRO:CG	1:A:143:HIS:CD2	3.04	0.41
1:A:143:HIS:CE1	1:A:145:ALA:HB2	2.56	0.41
2:B:232:ARG:CZ	4:B:909:HOH:O	2.69	0.41
2:B:339:ASP:O	2:B:343:ILE:HG12	2.20	0.41
2:B:533:LEU:HD12	2:B:533:LEU:N	2.35	0.41
2:B:613:LEU:HD12	2:B:652:LEU:HD22	2.03	0.41
2:B:654:ALA:HA	2:B:669:HIS:HA	2.02	0.41
2:B:770:GLU:CG	4:B:822:HOH:O	2.69	0.41
2:B:93:GLY:N	2:B:103:VAL:O	2.32	0.41
2:B:243:ASN:HB3	4:B:880:HOH:O	2.20	0.41
2:B:589:LEU:HB3	2:B:669:HIS:HB2	2.02	0.41
2:B:617:PHE:O	2:B:621:GLY:N	2.53	0.41
2:B:736:LEU:O	2:B:738:GLU:N	2.54	0.41
1:A:142:HIS:N	4:A:370:HOH:O	2.38	0.40
1:A:202:VAL:CG2	1:A:216:PHE:O	2.69	0.40
2:B:169:GLY:HA2	2:B:254:LEU:O	2.22	0.40
2:B:268:VAL:HG13	2:B:272:ILE:CD1	2.51	0.40
2:B:315:GLY:H	3:B:786:MTY:CZ	2.34	0.40
1:A:298:ARG:HG3	4:A:362:HOH:O	2.03	0.40
2:B:160:VAL:HG13	2:B:167:ALA:CB	2.51	0.40
2:B:269:GLY:HA2	4:B:885:HOH:O	2.21	0.40
2:B:474:LEU:N	2:B:474:LEU:HD12	2.35	0.40
1:A:201:ARG:HD2	1:A:215:VAL:CG1	2.52	0.40
2:B:691:PRO:CA	4:B:913:HOH:O	2.58	0.40
2:B:709:GLU:CA	4:B:956:HOH:O	2.59	0.40
2:B:715:ARG:O	2:B:716:GLU:C	2.58	0.40
1:A:173:LEU:HB2	4:A:414:HOH:O	2.01	0.40
2:B:297:ASP:O	2:B:298:LEU:C	2.60	0.40
2:B:589:LEU:HG	4:B:823:HOH:O	2.21	0.40
2:B:656:HIS:HA	2:B:657:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:LEU:O	2:B:714:VAL:C	2.59	0.40
1:A:197:VAL:CG2	1:A:219:LEU:HD21	2.51	0.40
2:B:56:ILE:HB	2:B:59:THR:OG1	2.21	0.40
2:B:192:LYS:N	2:B:381:GLN:HE22	2.19	0.40
2:B:458:ASP:O	2:B:462:GLU:HG2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:GLY:O	4:B:808:HOH:O[5_565]	2.13	0.07

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	264/350 (75%)	223 (84%)	25 (10%)	16 (6%)	1 4
2	B	783/785 (100%)	654 (84%)	102 (13%)	27 (3%)	3 15
All	All	1047/1135 (92%)	877 (84%)	127 (12%)	43 (4%)	3 11

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ALA
1	A	94	SER
1	A	319	VAL
1	A	320	GLU
1	A	349	VAL
2	B	244	ASN
2	B	390	GLU
2	B	590	PHE

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Mol	Chain	Res	Type
2	B	738	GLU
1	A	87	ASP
1	A	130	GLU
1	A	164	PRO
1	A	227	GLY
1	A	323	ALA
2	B	100	GLY
2	B	174	ALA
2	B	293	LEU
2	B	316	VAL
2	B	413	ARG
2	B	505	LEU
2	B	560	LEU
2	B	578	ARG
2	B	718	ALA
2	B	719	GLY
1	A	165	LEU
1	A	322	LEU
2	B	488	VAL
2	B	616	LEU
1	A	105	LEU
1	A	341	LYS
2	B	81	ALA
2	B	132	LEU
2	B	440	PRO
2	B	716	GLU
2	B	42	PRO
2	B	148	GLU
2	B	386	ALA
2	B	433	CYS
1	A	345	GLN
2	B	52	GLU
1	A	98	GLY
2	B	199	PRO
2	B	245	VAL

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	214/277 (77%)	190 (89%)	24 (11%)	6 18
2	B	630/630 (100%)	578 (92%)	52 (8%)	11 32
All	All	844/907 (93%)	768 (91%)	76 (9%)	9 29

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	104	THR
1	A	105	LEU
1	A	126	GLU
1	A	128	GLU
1	A	129	SER
1	A	133	ASN
1	A	174	LEU
1	A	178	HIS
1	A	179	THR
1	A	191	THR
1	A	196	ILE
1	A	198	VAL
1	A	203	PHE
1	A	213	GLU
1	A	256	VAL
1	A	260	PHE
1	A	280	LEU
1	A	307	TYR
1	A	308	ARG
1	A	311	THR
1	A	325	LEU
1	A	329	ILE
1	A	332	ILE
2	B	18	PRO
2	B	32	THR
2	B	60	ARG
2	B	80	ASN
2	B	87	VAL
2	B	89	LEU
2	B	111	VAL
2	B	118	LEU
2	B	121	ARG
2	B	147	SER

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Mol	Chain	Res	Type
2	B	158	LEU
2	B	159	GLU
2	B	171	LEU
2	B	173	LEU
2	B	176	ASP
2	B	180	LEU
2	B	184	LEU
2	B	276	ARG
2	B	282	ARG
2	B	298	LEU
2	B	313	LEU
2	B	322	SER
2	B	333	LEU
2	B	337	CYS
2	B	340	PRO
2	B	362	ARG
2	B	375	ARG
2	B	404	ILE
2	B	430	ARG
2	B	441	THR
2	B	467	GLN
2	B	470	GLU
2	B	527	ASP
2	B	549	PHE
2	B	556	LEU
2	B	562	LEU
2	B	567	ARG
2	B	575	ARG
2	B	576	VAL
2	B	578	ARG
2	B	584	HIS
2	B	588	LEU
2	B	598	TRP
2	B	600	LYS
2	B	619	ARG
2	B	624	PHE
2	B	671	PHE
2	B	673	LEU
2	B	695	ARG
2	B	696	ASP
2	B	711	GLU
2	B	767	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	HIS
1	A	183	GLN
1	A	190	HIS
1	A	218	GLN
1	A	232	HIS
2	B	54	HIS
2	B	80	ASN
2	B	101	GLN
2	B	178	HIS
2	B	231	GLN
2	B	244	ASN
2	B	258	GLN
2	B	261	HIS
2	B	350	HIS
2	B	467	GLN
2	B	584	HIS
2	B	669	HIS
2	B	732	GLN
2	B	746	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MTY	B	786	-	12,13,13	0.60	0	16,17,17	0.89	1 (6%)
3	MTY	A	351	-	12,13,13	0.44	0	16,17,17	0.97	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MTY	B	786	-	-	6/8/8/8	0/1/1/1
3	MTY	A	351	-	-	0/8/8/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	786	MTY	CG-CB-CA	-2.52	108.89	114.13
3	A	351	MTY	CG-CB-CA	-2.22	109.51	114.13

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	786	MTY	CA-CB-CG-CD2
3	B	786	MTY	CA-CB-CG-CD1
3	B	786	MTY	N-CA-CB-CG
3	B	786	MTY	OXT-C-CA-CB
3	B	786	MTY	C-CA-CB-CG
3	B	786	MTY	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	786	MTY	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	MTY	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	265/350 (75%)	0.32	9 (3%) 45 40	29, 61, 94, 104	0
2	B	779/785 (99%)	0.48	64 (8%) 11 9	35, 66, 119, 120	0
All	All	1044/1135 (91%)	0.44	73 (6%) 16 12	29, 65, 115, 120	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	98	GLY	6.0
2	B	761	VAL	5.8
2	B	756	LEU	5.8
2	B	99	LEU	5.3
2	B	731	TYR	4.9
2	B	768	VAL	4.8
2	B	735	PRO	4.6
2	B	736	LEU	4.6
2	B	779	LEU	4.6
2	B	749	PHE	4.4
2	B	739	GLY	4.4
2	B	689	ARG	4.0
2	B	778	GLY	3.9
2	B	701	VAL	3.9
2	B	698	ALA	3.9
2	B	732	GLN	3.7
2	B	743	LEU	3.7
2	B	738	GLU	3.7
2	B	745	PHE	3.7
2	B	752	PRO	3.7
2	B	697	LEU	3.6
2	B	721	TYR	3.6
2	B	747	LEU	3.6
2	B	759	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	350	LEU	3.5
2	B	742	SER	3.3
2	B	757	ARG	3.3
2	B	699	VAL	3.2
2	B	638	VAL	3.2
2	B	101	GLN	3.2
2	B	694	PHE	3.2
2	B	705	THR	3.1
2	B	693	ALA	3.0
2	B	773	ARG	2.9
2	B	730	LEU	2.9
2	B	766	SER	2.8
1	A	157	GLU	2.8
2	B	737	PRO	2.8
2	B	564	ARG	2.8
2	B	751	HIS	2.7
2	B	688	SER	2.7
2	B	633	PHE	2.7
2	B	695	ARG	2.7
2	B	753	LYS	2.6
2	B	443	ARG	2.6
2	B	734	PRO	2.6
2	B	690	HIS	2.5
2	B	278	ARG	2.5
2	B	772	LEU	2.5
1	A	214	ALA	2.5
2	B	741	LYS	2.5
2	B	577	PHE	2.5
2	B	504	GLY	2.4
1	A	143	HIS	2.4
2	B	279	GLU	2.4
1	A	165	LEU	2.3
1	A	271	TRP	2.3
2	B	661	GLN	2.3
2	B	598	TRP	2.2
2	B	725	LEU	2.2
2	B	703	ALA	2.2
2	B	727	LEU	2.2
1	A	90	LEU	2.1
2	B	282	ARG	2.1
2	B	724	SER	2.1
2	B	700	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	544	LEU	2.1
1	A	208	THR	2.1
2	B	754	ARG	2.0
2	B	769	ALA	2.0
2	B	758	ASP	2.0
1	A	206	GLU	2.0
2	B	43	ARG	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MTY	B	786	13/13	0.90	0.42	20,20,20,20	0
3	MTY	A	351	13/13	0.96	0.20	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.