Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 – 10:43 PM EDT

PDB ID	:	3DPN
Title	:	Crystal Structure of cpaf s499a mutant
Authors	:	Chai, J.; Huang, Z.
Deposited on	:	2008-07-09
Resolution	:	3.30 Å(reported)

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

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

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

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

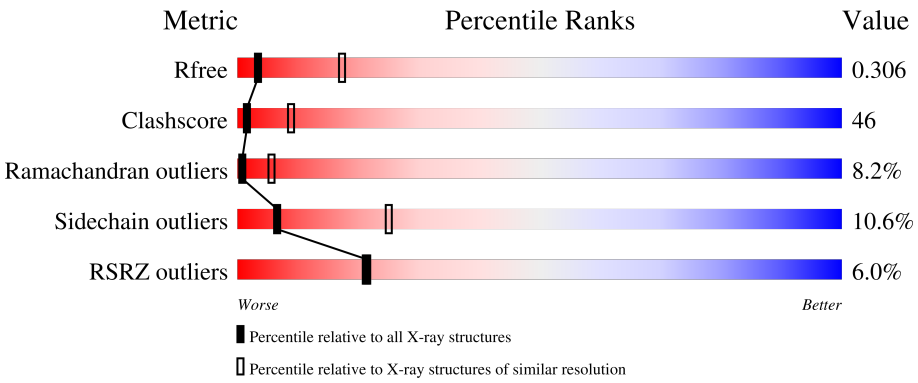
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	583	8%; 36%; 45%; 9%; • ; 8%
1	B	583	3%; 36%; 45%; 9%; • ; 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8476 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 Protein CT_858.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	4238	2719	709	796	14	0	0	0
1	B	537	4238	2719	709	796	14	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

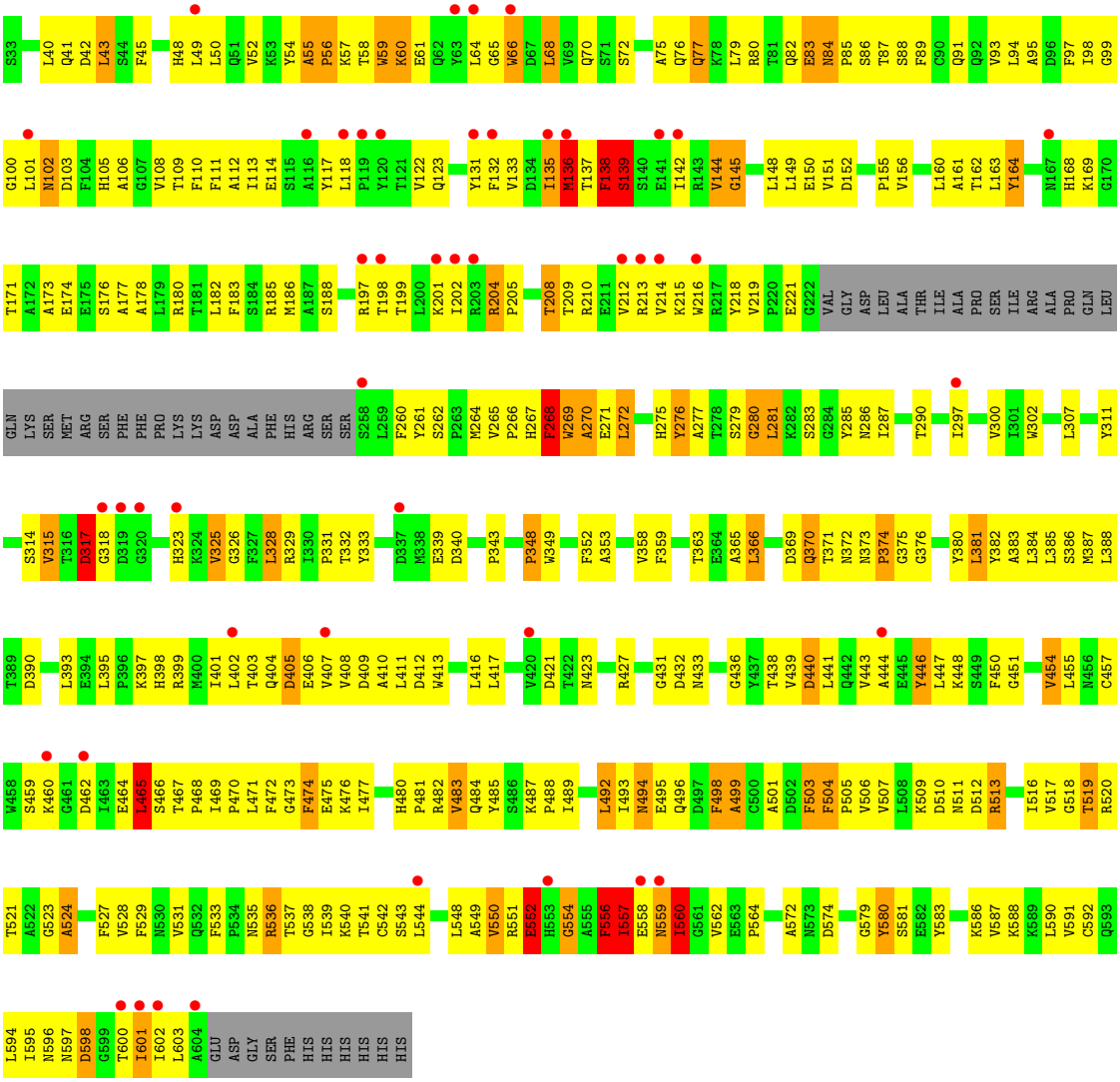
Chain	Residue	Modelled	Actual	Comment	Reference
A	499	ALA	SER	engineered mutation	UNP O84866
A	610	HIS	-	expression tag	UNP O84866
A	611	HIS	-	expression tag	UNP O84866
A	612	HIS	-	expression tag	UNP O84866
A	613	HIS	-	expression tag	UNP O84866
A	614	HIS	-	expression tag	UNP O84866
A	615	HIS	-	expression tag	UNP O84866
B	499	ALA	SER	engineered mutation	UNP O84866
B	610	HIS	-	expression tag	UNP O84866
B	611	HIS	-	expression tag	UNP O84866
B	612	HIS	-	expression tag	UNP O84866
B	613	HIS	-	expression tag	UNP O84866
B	614	HIS	-	expression tag	UNP O84866
B	615	HIS	-	expression tag	UNP O84866

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.

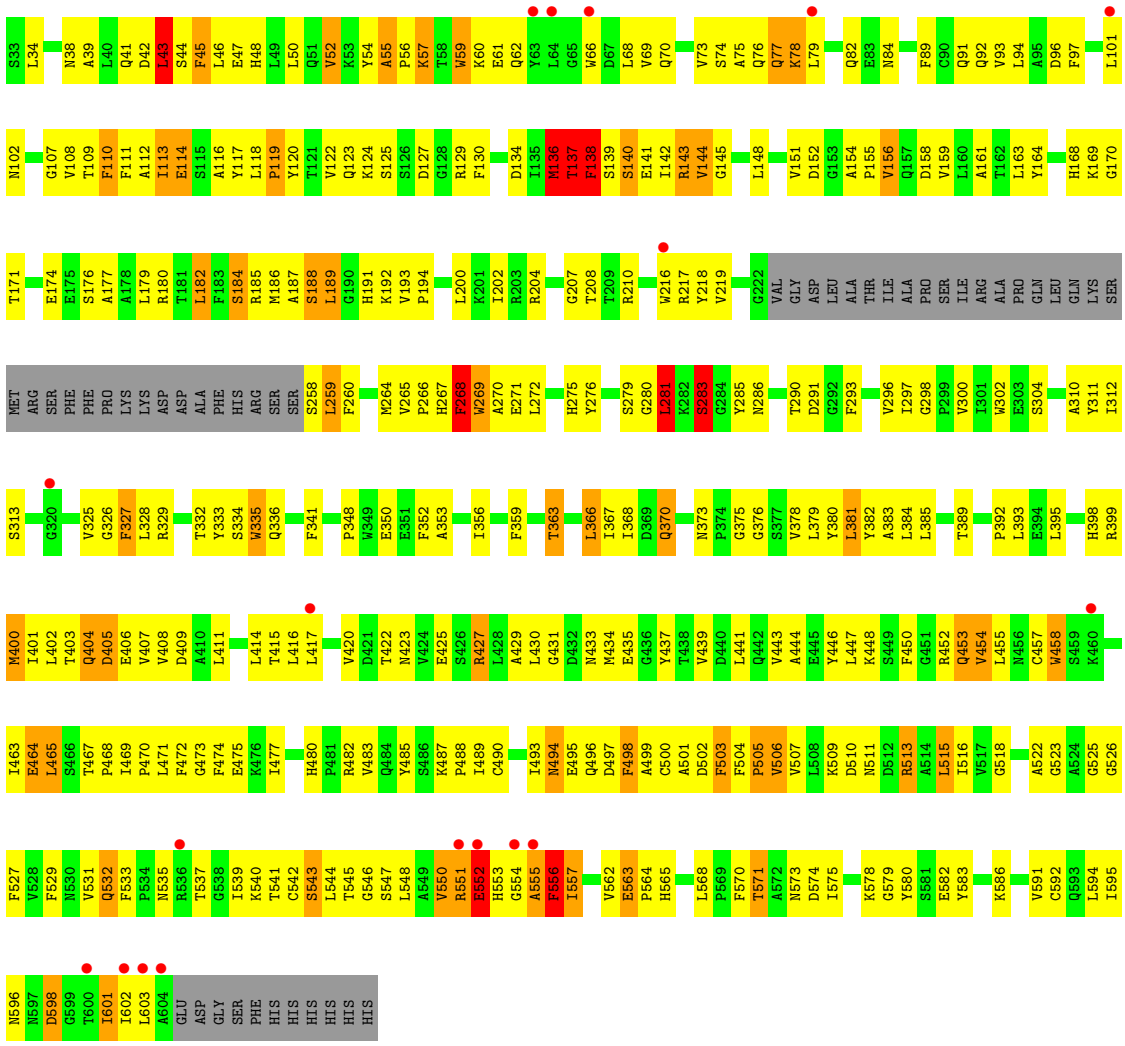
• Molecule 1: Protein CT_858

Chain A: 8% 36% 45% 9% • 8%



• Molecule 1: Protein CT_858

Chain B: 3% 36% 45% 9% • 8%


S33 L34 N38 A39 L40 Q41 D42 L43 S44 F45 L46 E47 H48 L49 L50 Q51 V52 K53 Y54 A55 P56 K57 T58 W59 K60 E61 Q62 Y63 L64 G65 W66 D67 L68 V69 Q70 V73 S74 A75 Q76 Q77 K78 L79 Q82 E83 N84 F89 C90 Q91 Q92 V93 L94 A95 D96 F97 L101
N102 G107 V108 T109 F110 F111 A112 I113 E114 S115 A116 Y117 L118 P119 Y120 T121 V122 Q123 K124 S125 S126 D127 G128 R129 F130 D134 I135 M136 T137 F138 S139 S140 E141 I142 R143 V144 G145 L148 V151 D152 G153 A154 P155 V156 Q157 D158 V159 L160 A161 T162 L163 Y164 H168 K169 G170
T171 E174 E175 S176 A177 A178 L179 R180 T181 L182 F183 S184 R185 M186 A187 S188 L189 G190 H191 K192 V193 P194 L200 K201 I202 R203 R204 G207 T208 T209 R210 W216 R217 Y218 V219 G222 VAL GLY ASP LEU ALA THR ILE ALA PRO SER ILE ARG ALA PRO GLN LEU GLN LYS SER
MET ARG SER PHE PHE PRO LYS LYS ASP ASP ALA PHE HIS ARG SER SER S258 L259 F260 M264 V265 P266 H267 F268 W269 A270 E271 L272 H275 Y276 S279 G280 L281 K282 S283 G284 Y285 N286 T290 D291 G292 F293 V296 I297 G298 P299 V300 I301 W302 E303 S304 A310 Y311 I312
S313 G320 V325 G326 F327 L328 R329 T332 Y333 S334 W335 Q336 F341 P348 W349 E350 E351 F352 A353 I356 F359 T363 L366 I367 I368 D369 Q370 N373 P374 G375 G376 S377 V378 L379 Y380 L381 Y382 A383 L384 L385 T389 P392 L393 E394 L395 H398 R399
M400 I401 L402 T403 Q404 D405 E406 V407 V408 D409 A410 L411 L414 T415 L416 L417 V420 D421 T422 N423 V424 E425 S426 R427 L428 A429 L430 G431 D432 N433 M434 E435 G436 Y437 T438 V439 D440 L441 Q442 V443 A444 E445 Y446 L447 K448 S449 F450 G451 R452 Q453 V454 L455 N456 C457 W458 S459 K460
I463 E464 L465 S466 T467 P468 I469 P470 L471 F472 G473 F474 E475 K476 I477 H480 P481 R482 V483 Q484 Y485 S486 K487 P488 I489 C490 I493 N494 E495 Q496 D497 F498 A499 C500 A501 D502 F503 F504 P505 V506 V507 L508 K509 D510 N511 D512 R513 A514 L515 I516 V517 G518 A522 G523 A524 G525 G526
F527 V528 F529 N530 V531 Q532 F533 P534 N535 R536 T537 G538 I539 K540 T541 C542 S543 L544 T545 G546 S547 L548 A549 V550 R551 E552 H553 G554 A555 F556 I557 V562 E563 P564 H565 L568 P569 F570 T571 A572 N573 D574 I575 K578 G579 Y580 S581 E582 Y583 K586 V591 C592 Q593 L594 I595
N596 N597 D598 G599 T600 I601 I602 L603 A604 GLU ASP GLY SER PHE HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	192.67Å 192.67Å 338.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30 49.90 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.30) 98.7 (49.90-3.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.305 0.261 , 0.306	Depositor DCC
R_{free} test set	1814 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å^2)	100.6	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 132.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8476	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.47	0/4344	0.76	4/5905 (0.1%)
1	B	0.48	0/4344	0.79	6/5905 (0.1%)
All	All	0.47	0/8688	0.78	10/11810 (0.1%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	PHE	N-CA-C	11.85	143.00	111.00
1	B	556	PHE	N-CA-C	7.79	132.03	111.00
1	A	554	GLY	N-CA-C	6.73	129.92	113.10
1	B	281	LEU	N-CA-C	-6.38	93.78	111.00
1	B	137	THR	C-N-CA	-5.65	107.58	121.70
1	A	560	ILE	CB-CA-C	-5.50	100.59	111.60
1	B	136	MET	N-CA-C	5.49	125.81	111.00
1	B	598	ASP	N-CA-C	5.26	125.20	111.00
1	A	557	ILE	N-CA-C	5.19	125.02	111.00
1	A	135	ILE	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	PHE	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	4238	0	4157	386	0
1	B	4238	0	4157	384	0
All	All	8476	0	8314	768	0

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 46.

All (768) 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:550:VAL:HG12	1:A:554:GLY:HA2	1.29	1.12
1:B:54:TYR:CZ	1:B:56:PRO:HG2	1.90	1.05
1:A:557:ILE:HG22	1:A:558:GLU:N	1.71	1.04
1:B:47:GLU:HG3	1:B:68:LEU:HD11	1.39	1.04
1:A:398:HIS:HD2	1:A:471:LEU:HD21	1.22	1.01
1:A:54:TYR:CZ	1:A:56:PRO:HG2	1.97	1.00
1:A:408:VAL:HA	1:A:411:LEU:HD12	1.43	0.99
1:A:398:HIS:CD2	1:A:471:LEU:HD21	1.99	0.96
1:A:487:LYS:HB3	1:A:488:PRO:HD2	1.48	0.95
1:A:523:GLY:HA2	1:A:560:ILE:HG22	1.47	0.95
1:A:359:PHE:O	1:A:363:THR:HG22	1.65	0.94
1:A:427:ARG:HA	1:A:439:VAL:HG11	1.50	0.92
1:B:516:ILE:H	1:B:565:HIS:CD2	1.90	0.90
1:A:601:ILE:HG22	1:A:602:ILE:HG13	1.54	0.89
1:B:119:PRO:HG3	1:B:137:THR:HB	1.53	0.87
1:B:118:LEU:HG	1:B:216:TRP:CE3	2.10	0.87
1:A:457:CYS:SG	1:A:467:THR:HG22	2.14	0.87
1:A:557:ILE:HG22	1:A:558:GLU:H	1.37	0.87
1:B:136:MET:HE3	1:B:283:SER:HB3	1.56	0.86
1:A:427:ARG:HG2	1:A:439:VAL:HB	1.57	0.86
1:A:144:VAL:HG12	1:A:145:GLY:H	1.39	0.86
1:A:333:TYR:CE2	1:A:381:LEU:HD23	2.11	0.86
1:A:180:ARG:HD2	1:A:496:GLN:HE21	1.41	0.85
1:B:515:LEU:HD23	1:B:565:HIS:HD2	1.40	0.84
1:B:119:PRO:HB2	1:B:137:THR:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ARG:HB3	1:B:555:ALA:HB3	1.58	0.84
1:B:367:ILE:HD11	1:B:591:VAL:HG21	1.61	0.83
1:B:366:LEU:HD13	1:B:368:ILE:HD11	1.61	0.82
1:A:451:GLY:O	1:A:454:VAL:HG23	1.80	0.82
1:A:431:GLY:O	1:A:439:VAL:HG21	1.80	0.81
1:A:523:GLY:CA	1:A:560:ILE:HG22	2.10	0.81
1:B:515:LEU:HD23	1:B:565:HIS:CD2	2.17	0.80
1:B:395:LEU:HD11	1:B:477:ILE:HG13	1.64	0.80
1:B:161:ALA:HA	1:B:164:TYR:CD2	2.17	0.79
1:B:457:CYS:SG	1:B:467:THR:HG22	2.22	0.79
1:B:554:GLY:O	1:B:556:PHE:N	2.15	0.79
1:A:177:ALA:HA	1:A:180:ARG:HD3	1.62	0.79
1:A:468:PRO:HB3	1:A:550:VAL:HG21	1.65	0.79
1:A:556:PHE:O	1:A:557:ILE:HG12	1.83	0.78
1:A:402:LEU:CD2	1:A:454:VAL:HG12	2.14	0.78
1:A:135:ILE:HD11	1:A:142:ILE:HG22	1.65	0.78
1:B:571:THR:HG23	1:B:574:ASP:OD2	1.84	0.78
1:A:176:SER:OG	1:A:495:GLU:HG3	1.83	0.78
1:A:506:VAL:HG13	1:A:507:VAL:N	1.99	0.77
1:A:455:LEU:N	1:A:455:LEU:HD23	1.99	0.76
1:B:592:CYS:HA	1:B:595:ILE:HD12	1.66	0.76
1:B:66:TRP:CH2	1:B:68:LEU:HB2	2.21	0.76
1:B:177:ALA:HA	1:B:180:ARG:HD3	1.67	0.75
1:B:264:MET:CE	1:B:526:GLY:H	1.97	0.75
1:A:43:LEU:HD11	1:A:75:ALA:CB	2.17	0.75
1:B:264:MET:HE3	1:B:526:GLY:H	1.50	0.75
1:B:335:TRP:HB2	1:B:348:PRO:HG3	1.66	0.75
1:A:180:ARG:HB2	1:A:180:ARG:HH11	1.52	0.74
1:B:452:ARG:O	1:B:454:VAL:N	2.19	0.74
1:B:112:ALA:O	1:B:188:SER:HB3	1.88	0.73
1:B:326:GLY:O	1:B:366:LEU:HD23	1.88	0.73
1:B:367:ILE:HD11	1:B:591:VAL:CG2	2.18	0.73
1:A:133:VAL:HB	1:A:285:TYR:CE1	2.23	0.73
1:B:350:GLU:O	1:B:353:ALA:HB3	1.87	0.73
1:B:184:SER:O	1:B:185:ARG:HD3	1.89	0.73
1:B:82:GLN:HG3	1:B:89:PHE:CE2	2.23	0.72
1:B:389:THR:HG21	1:B:393:LEU:HD11	1.70	0.72
1:A:43:LEU:HD11	1:A:75:ALA:HB1	1.71	0.72
1:A:144:VAL:HG12	1:A:145:GLY:N	2.04	0.72
1:B:543:SER:C	1:B:544:LEU:HD23	2.10	0.72
1:B:379:LEU:O	1:B:382:TYR:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:VAL:CG1	1:A:554:GLY:HA2	2.15	0.71
1:B:55:ALA:HB2	1:B:546:GLY:O	1.90	0.71
1:B:557:ILE:HG22	1:B:557:ILE:O	1.90	0.71
1:B:144:VAL:HG12	1:B:145:GLY:N	2.06	0.71
1:A:506:VAL:HB	1:A:562:VAL:HG21	1.73	0.70
1:A:267:HIS:CG	1:A:268:PHE:H	2.08	0.70
1:B:119:PRO:CG	1:B:137:THR:HB	2.21	0.70
1:A:529:PHE:O	1:A:543:SER:HA	1.90	0.70
1:B:537:THR:O	1:B:537:THR:HG22	1.90	0.70
1:B:258:SER:O	1:B:260:PHE:N	2.21	0.70
1:A:516:ILE:H	1:A:516:ILE:HD12	1.56	0.70
1:A:559:ASN:O	1:A:560:ILE:HB	1.91	0.70
1:B:136:MET:HE3	1:B:283:SER:H	1.56	0.70
1:A:446:TYR:O	1:A:473:GLY:HA3	1.92	0.69
1:A:402:LEU:N	1:A:402:LEU:HD12	2.08	0.69
1:B:54:TYR:CZ	1:B:56:PRO:CG	2.74	0.69
1:B:502:ASP:OD2	1:B:562:VAL:HG23	1.93	0.69
1:A:111:PHE:CE1	1:A:540:LYS:HA	2.27	0.69
1:A:352:PHE:HD2	1:A:387:MET:CE	2.06	0.69
1:B:171:THR:OG1	1:B:174:GLU:HG3	1.92	0.68
1:A:54:TYR:CZ	1:A:101:LEU:HD13	2.29	0.68
1:A:504:PHE:HB3	1:A:505:PRO:CD	2.24	0.68
1:B:433:ASN:HA	1:B:439:VAL:HG23	1.75	0.68
1:A:54:TYR:CE1	1:A:56:PRO:HG2	2.29	0.68
1:A:402:LEU:HD23	1:A:454:VAL:HG12	1.74	0.68
1:A:557:ILE:CG2	1:A:558:GLU:H	1.97	0.68
1:A:352:PHE:CD2	1:A:387:MET:CE	2.76	0.67
1:A:556:PHE:C	1:A:557:ILE:HG12	2.13	0.67
1:B:537:THR:O	1:B:537:THR:CG2	2.42	0.67
1:A:180:ARG:NH1	1:A:180:ARG:CB	2.57	0.67
1:A:557:ILE:CG2	1:A:558:GLU:N	2.42	0.67
1:B:398:HIS:HB3	1:B:547:SER:HB2	1.76	0.67
1:A:276:TYR:CE1	1:A:286:ASN:HB3	2.30	0.67
1:A:383:ALA:O	1:A:386:SER:HB3	1.94	0.67
1:B:516:ILE:H	1:B:565:HIS:HD2	1.42	0.67
1:B:552:GLU:OE2	1:B:555:ALA:HB2	1.95	0.67
1:A:587:VAL:O	1:A:591:VAL:HG23	1.95	0.67
1:A:516:ILE:HD12	1:A:516:ILE:N	2.09	0.67
1:B:471:LEU:HD22	1:B:527:PHE:CE1	2.30	0.67
1:A:118:LEU:HD12	1:A:183:PHE:CD2	2.31	0.66
1:A:559:ASN:O	1:A:560:ILE:CB	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:THR:OG1	1:B:468:PRO:HD2	1.96	0.66
1:A:506:VAL:CG1	1:A:507:VAL:N	2.58	0.66
1:A:518:GLY:O	1:A:564:PRO:HG3	1.95	0.66
1:A:177:ALA:O	1:A:180:ARG:HB2	1.95	0.66
1:B:464:GLU:O	1:B:465:LEU:HB2	1.95	0.66
1:B:136:MET:HE2	1:B:281:LEU:HA	1.77	0.66
1:A:536:ARG:HH11	1:A:536:ARG:HB3	1.61	0.66
1:A:535:ASN:ND2	1:A:539:ILE:HB	2.11	0.66
1:B:108:VAL:HG12	1:B:109:THR:N	2.11	0.65
1:B:168:HIS:CE1	1:B:170:GLY:HA2	2.31	0.65
1:B:543:SER:O	1:B:544:LEU:HD23	1.96	0.65
1:B:414:LEU:C	1:B:416:LEU:H	1.99	0.65
1:A:40:LEU:CD2	1:A:76:GLN:HG2	2.27	0.65
1:B:143:ARG:HH21	1:B:204:ARG:NH1	1.95	0.65
1:B:489:ILE:HD12	1:B:513:ARG:HH11	1.62	0.65
1:A:328:LEU:HD11	1:A:352:PHE:HE1	1.62	0.65
1:B:136:MET:CE	1:B:283:SER:HB3	2.27	0.65
1:B:502:ASP:O	1:B:506:VAL:HG12	1.96	0.65
1:B:591:VAL:O	1:B:594:LEU:HB2	1.97	0.65
1:A:352:PHE:CD2	1:A:387:MET:HE2	2.32	0.65
1:B:359:PHE:O	1:B:363:THR:HB	1.96	0.65
1:B:368:ILE:HD13	1:B:489:ILE:HG23	1.78	0.65
1:B:192:LYS:O	1:B:194:PRO:HD3	1.97	0.65
1:B:54:TYR:CE2	1:B:56:PRO:HG2	2.31	0.64
1:B:143:ARG:NH2	1:B:204:ARG:HD2	2.12	0.64
1:B:601:ILE:HG22	1:B:602:ILE:HG13	1.79	0.64
1:B:161:ALA:HA	1:B:164:TYR:HD2	1.60	0.64
1:A:122:VAL:HG12	1:A:123:GLN:N	2.13	0.64
1:A:602:ILE:HG22	1:A:603:LEU:N	2.11	0.64
1:B:179:LEU:HD23	1:B:182:LEU:HD12	1.79	0.64
1:B:186:MET:H	1:B:191:HIS:CD2	2.16	0.64
1:A:440:ASP:O	1:A:443:VAL:N	2.29	0.64
1:A:494:ASN:N	1:A:494:ASN:HD22	1.93	0.64
1:A:401:ILE:C	1:A:402:LEU:HD12	2.18	0.64
1:B:169:LYS:HA	1:B:169:LYS:HE2	1.80	0.64
1:A:180:ARG:CZ	1:A:268:PHE:CZ	2.81	0.64
1:A:369:ASP:HA	1:A:492:LEU:HB2	1.80	0.64
1:B:180:ARG:NH1	1:B:180:ARG:HB2	2.12	0.64
1:A:592:CYS:HA	1:A:595:ILE:HG12	1.80	0.63
1:A:103:ASP:OD1	1:A:105:HIS:HB2	1.99	0.63
1:A:180:ARG:HH11	1:A:180:ARG:CB	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HB3	1:A:511:ASN:ND2	2.11	0.63
1:B:487:LYS:HB3	1:B:488:PRO:HD2	1.81	0.63
1:A:114:GLU:HB2	1:A:221:GLU:HB2	1.80	0.63
1:A:489:ILE:HG13	1:A:513:ARG:NH2	2.14	0.63
1:B:74:SER:O	1:B:77:GLN:HB2	1.98	0.63
1:B:400:MET:HB2	1:B:402:LEU:HD21	1.80	0.63
1:A:297:ILE:HG23	1:A:311:TYR:OH	1.99	0.63
1:A:79:LEU:HD21	1:A:93:VAL:HG11	1.80	0.62
1:A:105:HIS:HD2	1:A:528:VAL:HG12	1.64	0.62
1:B:180:ARG:HD2	1:B:496:GLN:NE2	2.14	0.62
1:A:48:HIS:CE1	1:A:52:VAL:HG21	2.33	0.62
1:B:143:ARG:HE	1:B:204:ARG:NH1	1.96	0.62
1:B:125:SER:HA	1:B:575:ILE:CD1	2.30	0.62
1:A:315:VAL:CG1	1:A:588:LYS:HD2	2.29	0.62
1:A:328:LEU:HD22	1:A:329:ARG:N	2.14	0.62
1:B:108:VAL:HG12	1:B:109:THR:H	1.65	0.62
1:A:59:TRP:CH2	1:A:557:ILE:HB	2.35	0.62
1:A:387:MET:HG2	1:A:480:HIS:HD2	1.64	0.62
1:A:520:ARG:HD3	1:A:559:ASN:OD1	1.99	0.62
1:B:552:GLU:OE2	1:B:555:ALA:CB	2.48	0.62
1:A:204:ARG:HB3	1:A:205:PRO:HD2	1.81	0.62
1:A:326:GLY:O	1:A:366:LEU:HD23	1.99	0.62
1:B:341:PHE:CE1	1:B:348:PRO:HD3	2.35	0.62
1:B:381:LEU:HD13	1:B:381:LEU:C	2.19	0.62
1:A:59:TRP:CZ2	1:A:557:ILE:HB	2.35	0.61
1:A:506:VAL:CG1	1:A:507:VAL:H	2.13	0.61
1:B:54:TYR:CE1	1:B:56:PRO:HG2	2.35	0.61
1:B:352:PHE:CE2	1:B:356:ILE:HD11	2.35	0.61
1:B:471:LEU:HD22	1:B:527:PHE:HE1	1.65	0.61
1:B:591:VAL:O	1:B:595:ILE:HG13	2.00	0.61
1:A:592:CYS:HA	1:A:595:ILE:CG1	2.29	0.61
1:B:398:HIS:HA	1:B:548:LEU:O	2.00	0.61
1:B:122:VAL:HG12	1:B:123:GLN:N	2.15	0.61
1:A:106:ALA:HA	1:A:543:SER:O	1.99	0.61
1:A:137:THR:HG22	1:A:137:THR:O	2.01	0.61
1:A:409:ASP:HA	1:A:412:ASP:OD2	2.01	0.61
1:B:498:PHE:CD1	1:B:498:PHE:N	2.69	0.61
1:A:267:HIS:CG	1:A:268:PHE:N	2.69	0.61
1:A:583:TYR:O	1:A:587:VAL:HG23	2.00	0.61
1:A:122:VAL:HG13	1:A:131:TYR:O	2.00	0.61
1:A:365:ALA:HB2	1:A:595:ILE:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:HB2	1:B:208:THR:HG23	1.82	0.61
1:A:173:ALA:HA	1:A:495:GLU:HB2	1.83	0.61
1:A:332:THR:HA	1:A:374:PRO:HD2	1.83	0.61
1:A:464:GLU:O	1:A:465:LEU:HB2	2.01	0.60
1:B:138:PHE:HD2	1:B:140:SER:HB2	1.65	0.60
1:A:446:TYR:C	1:A:473:GLY:HA3	2.20	0.60
1:A:493:ILE:HG13	1:A:519:THR:O	2.01	0.60
1:A:66:TRP:CH2	1:A:68:LEU:HB2	2.37	0.60
1:B:55:ALA:HB3	1:B:56:PRO:CD	2.30	0.60
1:B:136:MET:HE2	1:B:281:LEU:CA	2.31	0.60
1:A:160:LEU:HD21	1:A:182:LEU:HD12	1.83	0.60
1:A:365:ALA:HB2	1:A:595:ILE:CD1	2.31	0.60
1:B:89:PHE:O	1:B:93:VAL:HG23	2.01	0.60
1:A:399:ARG:HG3	1:A:399:ARG:HH11	1.67	0.60
1:B:116:ALA:HB3	1:B:185:ARG:HB2	1.83	0.60
1:A:180:ARG:NH1	1:A:180:ARG:HB3	2.15	0.59
1:A:556:PHE:C	1:A:556:PHE:CD2	2.75	0.59
1:A:591:VAL:HA	1:A:594:LEU:HD12	1.84	0.59
1:B:542:CYS:SG	1:B:544:LEU:HD21	2.42	0.59
1:A:60:LYS:HD2	1:A:64:LEU:HD12	1.82	0.59
1:B:264:MET:HG2	1:B:526:GLY:O	2.02	0.59
1:B:535:ASN:ND2	1:B:539:ILE:HB	2.18	0.59
1:B:158:ASP:O	1:B:161:ALA:HB3	2.03	0.59
1:B:494:ASN:ND2	1:B:496:GLN:H	1.99	0.59
1:B:136:MET:CE	1:B:281:LEU:HD23	2.31	0.59
1:A:59:TRP:CE2	1:A:557:ILE:HG13	2.38	0.59
1:A:590:LEU:HD23	1:A:600:THR:HG21	1.83	0.59
1:B:45:PHE:O	1:B:48:HIS:HB3	2.02	0.59
1:B:497:ASP:O	1:B:522:ALA:HB3	2.03	0.59
1:A:397:LYS:O	1:A:550:VAL:HG23	2.02	0.59
1:A:269:TRP:O	1:A:272:LEU:N	2.35	0.59
1:B:601:ILE:HD12	1:B:601:ILE:N	2.18	0.59
1:B:503:PHE:HA	1:B:506:VAL:CG1	2.33	0.58
1:B:111:PHE:CD2	1:B:540:LYS:HB2	2.37	0.58
1:A:182:LEU:HD23	1:A:182:LEU:C	2.24	0.58
1:A:297:ILE:HD11	1:A:325:VAL:CG1	2.33	0.58
1:A:551:ARG:HD2	1:A:552:GLU:HG3	1.84	0.58
1:A:506:VAL:HG22	1:A:510:ASP:OD2	2.04	0.58
1:A:556:PHE:O	1:A:557:ILE:CG1	2.50	0.58
1:A:602:ILE:CG2	1:A:603:LEU:N	2.67	0.58
1:B:111:PHE:CE2	1:B:540:LYS:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LEU:HD13	1:B:444:ALA:HB1	1.85	0.58
1:B:136:MET:SD	1:B:281:LEU:HD23	2.43	0.58
1:B:571:THR:O	1:B:575:ILE:HG13	2.03	0.58
1:A:50:LEU:HD12	1:A:68:LEU:HD12	1.85	0.58
1:B:502:ASP:O	1:B:505:PRO:HG2	2.04	0.58
1:A:517:VAL:HG12	1:A:518:GLY:N	2.19	0.58
1:A:474:PHE:CD1	1:A:474:PHE:N	2.72	0.58
1:B:110:PHE:N	1:B:110:PHE:CD1	2.71	0.58
1:B:151:VAL:O	1:B:152:ASP:HB2	2.03	0.58
1:B:202:ILE:HG12	1:B:210:ARG:O	2.04	0.58
1:A:72:SER:O	1:A:75:ALA:HB3	2.04	0.57
1:A:59:TRP:O	1:A:61:GLU:N	2.37	0.57
1:A:411:LEU:HD13	1:B:411:LEU:HD11	1.85	0.57
1:A:180:ARG:NH1	1:A:268:PHE:CZ	2.72	0.57
1:B:50:LEU:O	1:B:54:TYR:HB3	2.04	0.57
1:A:118:LEU:HD12	1:A:183:PHE:HD2	1.68	0.57
1:B:119:PRO:CB	1:B:137:THR:HB	2.35	0.57
1:A:135:ILE:O	1:A:136:MET:O	2.22	0.57
1:A:474:PHE:N	1:A:474:PHE:HD1	2.02	0.57
1:A:509:LYS:HB2	1:A:516:ILE:CD1	2.34	0.57
1:B:94:LEU:O	1:B:97:PHE:HB3	2.04	0.57
1:B:407:VAL:O	1:B:411:LEU:HG	2.05	0.57
1:A:541:THR:HG22	1:A:542:CYS:N	2.20	0.57
1:A:352:PHE:HD2	1:A:387:MET:HE1	1.69	0.57
1:A:405:ASP:HA	1:A:408:VAL:HG23	1.86	0.56
1:A:307:LEU:CD2	1:A:348:PRO:HB3	2.35	0.56
1:A:591:VAL:O	1:A:594:LEU:HB2	2.05	0.56
1:B:38:ASN:O	1:B:39:ALA:C	2.43	0.56
1:B:122:VAL:HG11	1:B:130:PHE:HB3	1.87	0.56
1:B:311:TYR:OH	1:B:327:PHE:CD1	2.56	0.56
1:B:180:ARG:HD2	1:B:496:GLN:HE21	1.70	0.56
1:A:469:ILE:HG23	1:A:470:PRO:HD2	1.88	0.56
1:A:474:PHE:HD1	1:A:474:PHE:H	1.53	0.56
1:B:427:ARG:HA	1:B:431:GLY:O	2.04	0.56
1:A:118:LEU:HG	1:A:216:TRP:CE3	2.41	0.56
1:B:265:VAL:HG13	1:B:266:PRO:HD2	1.87	0.56
1:B:138:PHE:CD2	1:B:140:SER:HB2	2.41	0.56
1:B:467:THR:O	1:B:469:ILE:HG13	2.06	0.56
1:B:56:PRO:O	1:B:57:LYS:C	2.44	0.56
1:B:117:TYR:CD2	1:B:217:ARG:HB2	2.41	0.56
1:B:161:ALA:HA	1:B:164:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ASP:C	1:A:439:VAL:HG23	2.26	0.55
1:A:269:TRP:O	1:A:270:ALA:C	2.45	0.55
1:A:471:LEU:HD22	1:A:527:PHE:HE1	1.71	0.55
1:B:144:VAL:HG12	1:B:145:GLY:H	1.71	0.55
1:B:399:ARG:NH2	1:B:465:LEU:HD23	2.20	0.55
1:A:105:HIS:CD2	1:A:528:VAL:HG12	2.42	0.55
1:A:517:VAL:HG12	1:A:518:GLY:H	1.71	0.55
1:B:176:SER:OG	1:B:495:GLU:HG3	2.05	0.55
1:A:387:MET:HG2	1:A:480:HIS:CD2	2.41	0.55
1:A:398:HIS:HD2	1:A:471:LEU:CD2	2.08	0.55
1:B:125:SER:HA	1:B:575:ILE:HD11	1.88	0.55
1:A:509:LYS:HB2	1:A:516:ILE:HD13	1.88	0.55
1:B:54:TYR:HD1	1:B:544:LEU:HB3	1.72	0.55
1:B:427:ARG:HG2	1:B:439:VAL:HB	1.89	0.55
1:B:398:HIS:HD2	1:B:471:LEU:HG	1.72	0.55
1:A:89:PHE:O	1:A:93:VAL:HG23	2.06	0.55
1:A:412:ASP:O	1:A:416:LEU:HB2	2.06	0.55
1:B:114:GLU:HA	1:B:219:VAL:O	2.06	0.55
1:B:573:ASN:HB2	1:B:582:GLU:OE2	2.07	0.55
1:A:79:LEU:CD2	1:A:93:VAL:HG11	2.36	0.55
1:A:405:ASP:HA	1:A:408:VAL:CG2	2.37	0.55
1:B:310:ALA:HA	1:B:327:PHE:O	2.07	0.55
1:B:411:LEU:CD2	1:B:455:LEU:HD11	2.36	0.55
1:B:550:VAL:HG21	1:B:554:GLY:HA2	1.89	0.55
1:A:433:ASN:N	1:A:439:VAL:HG23	2.22	0.54
1:B:335:TRP:HB2	1:B:348:PRO:CG	2.35	0.54
1:B:532:GLN:O	1:B:533:PHE:HB3	2.07	0.54
1:B:498:PHE:N	1:B:498:PHE:HD1	2.05	0.54
1:B:499:ALA:O	1:B:502:ASP:N	2.32	0.54
1:B:363:THR:HG21	1:B:485:TYR:CE1	2.43	0.54
1:A:307:LEU:HD21	1:A:348:PRO:HB3	1.90	0.54
1:A:387:MET:HB3	1:A:483:VAL:HG22	1.90	0.54
1:B:333:TYR:C	1:B:376:GLY:HA3	2.27	0.54
1:B:450:PHE:O	1:B:454:VAL:HG23	2.08	0.54
1:B:378:VAL:O	1:B:381:LEU:HB3	2.07	0.54
1:B:116:ALA:HB2	1:B:194:PRO:HD2	1.89	0.54
1:B:107:GLY:HA3	1:B:267:HIS:CD2	2.43	0.54
1:A:317:ASP:OD2	1:A:317:ASP:N	2.40	0.53
1:A:557:ILE:HG22	1:A:559:ASN:H	1.73	0.53
1:B:50:LEU:HD23	1:B:544:LEU:HD13	1.90	0.53
1:B:363:THR:HG21	1:B:485:TYR:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ARG:C	1:B:454:VAL:N	2.61	0.53
1:B:541:THR:HG22	1:B:542:CYS:N	2.24	0.53
1:A:352:PHE:CD2	1:A:387:MET:HE1	2.43	0.53
1:A:549:ALA:O	1:A:556:PHE:HB3	2.08	0.53
1:B:187:ALA:C	1:B:189:LEU:H	2.12	0.53
1:B:297:ILE:CD1	1:B:313:SER:HB2	2.39	0.53
1:A:110:PHE:HA	1:A:538:GLY:O	2.09	0.53
1:A:551:ARG:O	1:A:552:GLU:C	2.47	0.53
1:B:56:PRO:O	1:B:59:TRP:N	2.42	0.53
1:B:77:GLN:O	1:B:79:LEU:N	2.41	0.53
1:A:150:GLU:HG2	1:A:155:PRO:HA	1.90	0.53
1:A:395:LEU:HD21	1:A:477:ILE:HD11	1.90	0.53
1:A:450:PHE:O	1:A:454:VAL:HG22	2.09	0.53
1:A:537:THR:HG22	1:A:537:THR:O	2.08	0.53
1:B:204:ARG:HB2	1:B:208:THR:CG2	2.38	0.53
1:B:333:TYR:N	1:B:375:GLY:O	2.38	0.53
1:B:389:THR:HG21	1:B:393:LEU:CD1	2.39	0.53
1:B:427:ARG:NH1	1:B:427:ARG:HB2	2.24	0.53
1:A:265:VAL:HG13	1:A:266:PRO:HD2	1.90	0.53
1:B:443:VAL:O	1:B:446:TYR:HB2	2.08	0.53
1:B:463:ILE:O	1:B:465:LEU:N	2.42	0.53
1:A:182:LEU:HD22	1:A:183:PHE:CD1	2.44	0.52
1:A:416:LEU:O	1:A:416:LEU:HD23	2.09	0.52
1:A:487:LYS:CB	1:A:488:PRO:HD2	2.32	0.52
1:B:120:TYR:CD1	1:B:120:TYR:N	2.77	0.52
1:B:179:LEU:O	1:B:182:LEU:N	2.37	0.52
1:B:414:LEU:O	1:B:416:LEU:N	2.43	0.52
1:B:433:ASN:CA	1:B:439:VAL:HG23	2.39	0.52
1:A:480:HIS:HB3	1:A:483:VAL:O	2.09	0.52
1:A:506:VAL:HG13	1:A:507:VAL:H	1.69	0.52
1:B:54:TYR:CD1	1:B:544:LEU:HB3	2.44	0.52
1:B:494:ASN:C	1:B:494:ASN:HD22	2.12	0.52
1:A:180:ARG:CZ	1:A:180:ARG:HB3	2.40	0.52
1:A:541:THR:CG2	1:A:542:CYS:N	2.72	0.52
1:B:119:PRO:CB	1:B:137:THR:H	2.16	0.52
1:A:108:VAL:HG12	1:A:109:THR:N	2.24	0.52
1:A:144:VAL:CG1	1:A:145:GLY:H	2.15	0.52
1:A:161:ALA:HA	1:A:164:TYR:CE2	2.45	0.52
1:A:399:ARG:HG3	1:A:399:ARG:NH1	2.25	0.52
1:B:156:VAL:O	1:B:159:VAL:N	2.43	0.52
1:B:327:PHE:HD2	1:B:327:PHE:C	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LEU:O	1:B:382:TYR:HB2	2.09	0.52
1:B:265:VAL:CG1	1:B:266:PRO:HD2	2.39	0.52
1:B:276:TYR:HE1	1:B:286:ASN:HB3	1.74	0.52
1:B:505:PRO:HG2	1:B:506:VAL:H	1.75	0.52
1:A:50:LEU:HD12	1:A:68:LEU:CD1	2.40	0.52
1:B:39:ALA:HB1	1:B:79:LEU:HD22	1.92	0.52
1:B:180:ARG:HB2	1:B:180:ARG:HH11	1.72	0.52
1:B:403:THR:O	1:B:405:ASP:N	2.43	0.52
1:A:297:ILE:CD1	1:A:325:VAL:HG11	2.40	0.51
1:A:509:LYS:HG2	1:A:509:LYS:O	2.10	0.51
1:B:43:LEU:O	1:B:46:LEU:N	2.39	0.51
1:B:56:PRO:CD	1:B:545:THR:HB	2.40	0.51
1:B:148:LEU:HD11	1:B:200:LEU:HD22	1.91	0.51
1:B:272:LEU:O	1:B:275:HIS:N	2.39	0.51
1:B:379:LEU:O	1:B:380:TYR:C	2.49	0.51
1:B:601:ILE:HG22	1:B:602:ILE:N	2.25	0.51
1:A:439:VAL:HG12	1:A:440:ASP:N	2.26	0.51
1:B:327:PHE:C	1:B:327:PHE:CD2	2.83	0.51
1:A:597:ASN:O	1:A:598:ASP:HB2	2.10	0.51
1:B:502:ASP:OD2	1:B:523:GLY:O	2.29	0.51
1:A:451:GLY:O	1:A:454:VAL:CG2	2.57	0.51
1:B:334:SER:HB3	1:B:376:GLY:HA2	1.93	0.51
1:B:541:THR:CG2	1:B:542:CYS:N	2.72	0.51
1:B:279:SER:O	1:B:280:GLY:C	2.48	0.51
1:B:516:ILE:N	1:B:565:HIS:HD2	2.08	0.51
1:A:59:TRP:CZ2	1:A:557:ILE:CB	2.94	0.50
1:A:402:LEU:HD21	1:A:454:VAL:HG12	1.92	0.50
1:A:406:GLU:N	1:A:406:GLU:OE2	2.44	0.50
1:B:50:LEU:HD13	1:B:66:TRP:HH2	1.76	0.50
1:B:264:MET:HE2	1:B:526:GLY:H	1.75	0.50
1:B:381:LEU:HD13	1:B:385:LEU:HD12	1.92	0.50
1:B:311:TYR:OH	1:B:327:PHE:HD1	1.92	0.50
1:B:470:PRO:HG2	1:B:473:GLY:HA2	1.93	0.50
1:A:132:PHE:HE1	1:A:148:LEU:HB2	1.76	0.50
1:A:297:ILE:HD11	1:A:325:VAL:HG12	1.92	0.50
1:A:494:ASN:HD22	1:A:494:ASN:H	1.57	0.50
1:B:56:PRO:HB2	1:B:60:LYS:HG2	1.94	0.50
1:A:98:ILE:C	1:A:100:GLY:H	2.15	0.50
1:B:398:HIS:HE2	1:B:503:PHE:HZ	1.59	0.50
1:B:450:PHE:C	1:B:452:ARG:N	2.64	0.50
1:A:333:TYR:C	1:A:376:GLY:HA3	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:HIS:CE1	1:A:549:ALA:HB2	2.47	0.50
1:A:113:ILE:O	1:A:114:GLU:C	2.50	0.50
1:B:328:LEU:HD22	1:B:329:ARG:N	2.27	0.50
1:A:417:LEU:HD12	1:A:417:LEU:O	2.12	0.50
1:A:516:ILE:H	1:A:516:ILE:CD1	2.23	0.50
1:B:143:ARG:NE	1:B:204:ARG:HH11	2.10	0.50
1:B:176:SER:O	1:B:179:LEU:HB2	2.12	0.50
1:B:311:TYR:C	1:B:311:TYR:CD1	2.85	0.50
1:A:427:ARG:O	1:A:431:GLY:O	2.29	0.49
1:B:144:VAL:CG1	1:B:145:GLY:N	2.74	0.49
1:B:161:ALA:C	1:B:163:LEU:H	2.16	0.49
1:B:186:MET:H	1:B:191:HIS:HD2	1.58	0.49
1:A:40:LEU:HD21	1:A:76:GLN:HG2	1.94	0.49
1:A:218:TYR:CG	1:A:219:VAL:N	2.80	0.49
1:A:366:LEU:HB2	1:A:485:TYR:CZ	2.47	0.49
1:A:441:LEU:HD13	1:A:441:LEU:C	2.33	0.49
1:A:444:ALA:O	1:A:448:LYS:HG3	2.13	0.49
1:A:265:VAL:CG1	1:A:266:PRO:HD2	2.42	0.49
1:A:390:ASP:HA	1:A:484:GLN:OE1	2.13	0.49
1:B:333:TYR:OH	1:B:504:PHE:CG	2.65	0.49
1:B:450:PHE:O	1:B:452:ARG:N	2.45	0.49
1:A:185:ARG:HG3	1:A:185:ARG:HH11	1.78	0.49
1:A:185:ARG:HG3	1:A:185:ARG:NH1	2.27	0.49
1:A:504:PHE:HB3	1:A:505:PRO:HD3	1.94	0.49
1:A:339:GLU:O	1:A:340:ASP:HB2	2.12	0.49
1:B:551:ARG:CB	1:B:555:ALA:HB3	2.37	0.49
1:B:42:ASP:O	1:B:43:LEU:O	2.30	0.49
1:B:50:LEU:HD13	1:B:66:TRP:CH2	2.48	0.49
1:B:118:LEU:HD21	1:B:216:TRP:HA	1.95	0.49
1:B:82:GLN:HG3	1:B:89:PHE:HE2	1.71	0.49
1:B:293:PHE:HZ	1:B:570:PHE:CE1	2.30	0.49
1:B:366:LEU:HD22	1:B:368:ILE:HD12	1.94	0.49
1:B:494:ASN:ND2	1:B:494:ASN:C	2.64	0.49
1:A:64:LEU:HD23	1:A:169:LYS:HD2	1.95	0.49
1:A:470:PRO:O	1:A:472:PHE:O	2.31	0.48
1:B:414:LEU:C	1:B:416:LEU:N	2.65	0.48
1:A:76:GLN:O	1:A:77:GLN:C	2.52	0.48
1:A:439:VAL:O	1:A:440:ASP:HB2	2.12	0.48
1:A:498:PHE:CD1	1:A:498:PHE:N	2.81	0.48
1:B:463:ILE:HG13	1:B:464:GLU:N	2.27	0.48
1:B:571:THR:O	1:B:574:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:TRP:O	1:B:270:ALA:C	2.50	0.48
1:B:367:ILE:C	1:B:368:ILE:HD12	2.33	0.48
1:A:43:LEU:HD11	1:A:75:ALA:HB3	1.96	0.48
1:A:118:LEU:HG	1:A:216:TRP:CZ3	2.48	0.48
1:A:373:ASN:OD1	1:A:374:PRO:HD2	2.13	0.48
1:A:440:ASP:O	1:A:441:LEU:C	2.52	0.48
1:B:76:GLN:O	1:B:77:GLN:O	2.32	0.48
1:B:403:THR:O	1:B:407:VAL:HG23	2.12	0.48
1:B:463:ILE:C	1:B:465:LEU:N	2.67	0.48
1:B:328:LEU:O	1:B:368:ILE:HA	2.13	0.48
1:B:568:LEU:HD22	1:B:583:TYR:HD1	1.77	0.48
1:A:556:PHE:C	1:A:556:PHE:HD2	2.16	0.48
1:B:114:GLU:O	1:B:193:VAL:HG21	2.13	0.48
1:B:179:LEU:O	1:B:180:ARG:C	2.51	0.48
1:B:352:PHE:CG	1:B:384:LEU:HD22	2.48	0.48
1:B:463:ILE:C	1:B:465:LEU:H	2.16	0.48
1:B:276:TYR:CE1	1:B:286:ASN:HB3	2.48	0.48
1:B:509:LYS:C	1:B:511:ASN:H	2.16	0.48
1:B:434:MET:O	1:B:435:GLU:C	2.52	0.48
1:A:280:GLY:O	1:A:281:LEU:C	2.52	0.48
1:B:143:ARG:NH2	1:B:204:ARG:NH1	2.62	0.48
1:A:352:PHE:HD2	1:A:387:MET:HE2	1.69	0.48
1:B:430:LEU:HB2	1:B:439:VAL:HG11	1.96	0.48
1:B:499:ALA:HA	1:B:525:GLY:HA2	1.95	0.48
1:B:89:PHE:O	1:B:92:GLN:HB2	2.14	0.47
1:B:327:PHE:HD2	1:B:328:LEU:N	2.11	0.47
1:A:387:MET:SD	1:A:480:HIS:HD2	2.37	0.47
1:A:487:LYS:HB3	1:A:488:PRO:CD	2.32	0.47
1:B:164:TYR:CE1	1:B:168:HIS:NE2	2.82	0.47
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.79	0.47
1:B:264:MET:SD	1:B:378:VAL:HG22	2.54	0.47
1:B:535:ASN:HD21	1:B:539:ILE:HB	1.78	0.47
1:A:372:ASN:H	1:A:494:ASN:HD21	1.62	0.47
1:A:457:CYS:SG	1:A:466:SER:HB2	2.54	0.47
1:A:493:ILE:HD13	1:A:516:ILE:CG2	2.45	0.47
1:B:122:VAL:HG12	1:B:123:GLN:H	1.79	0.47
1:B:368:ILE:CD1	1:B:489:ILE:HG23	2.44	0.47
1:A:586:LYS:O	1:A:590:LEU:HD12	2.14	0.47
1:A:601:ILE:HG22	1:A:602:ILE:N	2.29	0.47
1:B:114:GLU:HG2	1:B:193:VAL:CB	2.44	0.47
1:B:259:LEU:O	1:B:527:PHE:CD2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:THR:HA	1:B:373:ASN:OD1	2.13	0.47
1:A:122:VAL:HG12	1:A:123:GLN:H	1.79	0.47
1:A:161:ALA:HA	1:A:164:TYR:CD2	2.49	0.47
1:A:202:ILE:HG13	1:A:202:ILE:O	2.15	0.47
1:A:276:TYR:O	1:A:277:ALA:C	2.51	0.47
1:A:381:LEU:C	1:A:381:LEU:HD13	2.35	0.47
1:B:114:GLU:HG2	1:B:193:VAL:HG21	1.97	0.47
1:B:164:TYR:CD1	1:B:168:HIS:CD2	3.03	0.47
1:B:503:PHE:O	1:B:506:VAL:HG13	2.14	0.47
1:A:441:LEU:HD13	1:A:441:LEU:O	2.15	0.47
1:A:558:GLU:O	1:A:559:ASN:HB2	2.14	0.47
1:B:140:SER:OG	1:B:141:GLU:N	2.47	0.47
1:B:312:ILE:HG23	1:B:325:VAL:O	2.15	0.47
1:A:136:MET:SD	1:A:136:MET:N	2.88	0.47
1:A:144:VAL:CG1	1:A:145:GLY:N	2.74	0.47
1:A:267:HIS:O	1:A:268:PHE:C	2.53	0.47
1:A:381:LEU:HD13	1:A:382:TYR:N	2.30	0.47
1:A:433:ASN:HD22	1:A:436:GLY:H	1.61	0.47
1:A:503:PHE:O	1:A:507:VAL:HG23	2.15	0.47
1:B:143:ARG:HE	1:B:204:ARG:HH11	1.62	0.47
1:B:437:TYR:CE2	1:B:474:PHE:HE2	2.33	0.47
1:B:503:PHE:O	1:B:506:VAL:CG1	2.62	0.47
1:B:505:PRO:O	1:B:506:VAL:C	2.53	0.47
1:A:42:ASP:CG	1:A:535:ASN:HB2	2.35	0.46
1:A:176:SER:O	1:A:177:ALA:C	2.53	0.46
1:A:214:VAL:HG12	1:A:215:LYS:N	2.31	0.46
1:B:302:TRP:O	1:B:311:TYR:HB2	2.15	0.46
1:B:446:TYR:CE2	1:B:475:GLU:N	2.78	0.46
1:B:452:ARG:C	1:B:454:VAL:H	2.19	0.46
1:A:182:LEU:HD22	1:A:183:PHE:CE1	2.49	0.46
1:A:260:PHE:HA	1:A:527:PHE:CD2	2.50	0.46
1:A:302:TRP:CZ2	1:A:358:VAL:HG11	2.50	0.46
1:B:401:ILE:HG22	1:B:401:ILE:O	2.15	0.46
1:B:441:LEU:HD23	1:B:441:LEU:C	2.35	0.46
1:B:444:ALA:O	1:B:448:LYS:HG3	2.15	0.46
1:A:287:ILE:N	1:A:287:ILE:HD12	2.31	0.46
1:B:483:VAL:HG23	1:B:483:VAL:O	2.15	0.46
1:A:373:ASN:HB3	1:A:501:ALA:HB2	1.96	0.46
1:A:550:VAL:HG12	1:A:554:GLY:CA	2.22	0.46
1:B:60:LYS:HG3	1:B:101:LEU:HD22	1.98	0.46
1:A:54:TYR:O	1:A:55:ALA:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:CYS:CB	1:A:466:SER:HB2	2.45	0.46
1:A:602:ILE:CG2	1:A:603:LEU:H	2.29	0.46
1:B:264:MET:HE2	1:B:526:GLY:N	2.31	0.46
1:B:570:PHE:HE2	1:B:583:TYR:CD2	2.33	0.46
1:B:368:ILE:HD12	1:B:368:ILE:N	2.30	0.46
1:B:382:TYR:O	1:B:385:LEU:HB2	2.16	0.46
1:A:94:LEU:O	1:A:95:ALA:C	2.54	0.46
1:A:317:ASP:HB2	1:A:318:GLY:H	1.58	0.46
1:A:402:LEU:N	1:A:402:LEU:CD1	2.79	0.46
1:A:427:ARG:HA	1:A:439:VAL:CG1	2.35	0.46
1:B:55:ALA:CB	1:B:56:PRO:CD	2.94	0.46
1:B:204:ARG:CG	1:B:208:THR:HG23	2.46	0.46
1:B:503:PHE:O	1:B:504:PHE:C	2.53	0.46
1:B:137:THR:O	1:B:137:THR:CG2	2.64	0.45
1:B:506:VAL:HG13	1:B:507:VAL:H	1.82	0.45
1:B:601:ILE:HD12	1:B:601:ILE:H	1.82	0.45
1:A:333:TYR:CE1	1:A:373:ASN:ND2	2.84	0.45
1:A:387:MET:CG	1:A:480:HIS:HD2	2.27	0.45
1:A:467:THR:OG1	1:A:468:PRO:HD2	2.17	0.45
1:B:91:GLN:HA	1:B:110:PHE:CE2	2.51	0.45
1:B:117:TYR:CD2	1:B:217:ARG:CB	2.99	0.45
1:A:100:GLY:C	1:A:102:ASN:N	2.69	0.45
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.77	0.45
1:B:389:THR:CG2	1:B:393:LEU:HD11	2.43	0.45
1:A:54:TYR:O	1:A:54:TYR:CG	2.69	0.45
1:A:423:ASN:HA	1:A:441:LEU:HB2	1.98	0.45
1:B:118:LEU:HG	1:B:216:TRP:CZ3	2.51	0.45
1:B:143:ARG:NE	1:B:204:ARG:NH1	2.64	0.45
1:B:293:PHE:HZ	1:B:570:PHE:HE1	1.64	0.45
1:B:446:TYR:CD2	1:B:474:PHE:HA	2.52	0.45
1:A:83:GLU:O	1:A:84:ASN:C	2.54	0.45
1:A:102:ASN:HD22	1:A:102:ASN:HA	1.57	0.45
1:A:407:VAL:HG12	1:A:411:LEU:HD11	1.98	0.45
1:B:59:TRP:C	1:B:61:GLU:N	2.69	0.45
1:B:76:GLN:O	1:B:77:GLN:C	2.54	0.45
1:B:82:GLN:CG	1:B:89:PHE:HE2	2.28	0.45
1:B:506:VAL:HG13	1:B:507:VAL:N	2.32	0.45
1:A:118:LEU:CD2	1:A:216:TRP:HA	2.47	0.45
1:A:132:PHE:CE2	1:A:142:ILE:HG21	2.51	0.45
1:A:135:ILE:CD1	1:A:142:ILE:O	2.64	0.45
1:A:403:THR:O	1:A:406:GLU:OE2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ALA:HB3	1:B:56:PRO:HD3	1.97	0.45
1:B:180:ARG:NH1	1:B:268:PHE:CZ	2.85	0.45
1:B:516:ILE:N	1:B:516:ILE:HD12	2.31	0.45
1:A:197:ARG:HB3	1:A:213:ARG:HE	1.81	0.45
1:A:395:LEU:HB2	1:A:475:GLU:O	2.17	0.45
1:A:443:VAL:O	1:A:446:TYR:HB2	2.17	0.45
1:A:506:VAL:HB	1:A:562:VAL:CG2	2.43	0.45
1:A:82:GLN:C	1:A:83:GLU:O	2.55	0.45
1:A:136:MET:CE	1:A:281:LEU:HA	2.47	0.45
1:A:410:ALA:HB2	1:A:454:VAL:HG21	1.98	0.45
1:B:602:ILE:CG2	1:B:603:LEU:N	2.80	0.45
1:A:410:ALA:CB	1:A:454:VAL:HG21	2.47	0.44
1:A:413:TRP:CE3	1:A:413:TRP:HA	2.53	0.44
1:A:556:PHE:O	1:A:556:PHE:CD2	2.70	0.44
1:B:134:ASP:OD2	1:B:283:SER:HB2	2.18	0.44
1:B:185:ARG:HG3	1:B:185:ARG:NH1	2.32	0.44
1:B:366:LEU:HD22	1:B:368:ILE:CD1	2.47	0.44
1:A:135:ILE:HD11	1:A:142:ILE:CG2	2.43	0.44
1:A:427:ARG:CA	1:A:439:VAL:HG11	2.36	0.44
1:B:493:ILE:O	1:B:518:GLY:HA3	2.18	0.44
1:A:88:SER:O	1:A:91:GLN:HB2	2.17	0.44
1:A:333:TYR:HB2	1:A:375:GLY:O	2.17	0.44
1:A:370:GLN:HE21	1:A:370:GLN:HB3	1.63	0.44
1:B:143:ARG:NH2	1:B:204:ARG:HH11	2.15	0.44
1:A:539:ILE:H	1:A:539:ILE:HD12	1.82	0.44
1:B:117:TYR:HD2	1:B:217:ARG:CB	2.31	0.44
1:B:152:ASP:O	1:B:154:ALA:N	2.50	0.44
1:B:176:SER:O	1:B:179:LEU:N	2.50	0.44
1:B:186:MET:O	1:B:191:HIS:HB2	2.17	0.44
1:B:302:TRP:CH2	1:B:304:SER:HB2	2.53	0.44
1:A:603:LEU:HD23	1:A:603:LEU:O	2.17	0.44
1:B:568:LEU:HD22	1:B:583:TYR:CD1	2.52	0.44
1:A:151:VAL:HG12	1:A:152:ASP:OD2	2.18	0.44
1:A:297:ILE:HD11	1:A:325:VAL:HG11	1.97	0.44
1:A:498:PHE:O	1:A:501:ALA:HB3	2.17	0.44
1:B:550:VAL:HG23	1:B:551:ARG:N	2.30	0.44
1:A:539:ILE:HD12	1:A:539:ILE:N	2.32	0.44
1:B:108:VAL:CG1	1:B:109:THR:N	2.80	0.44
1:B:127:ASP:OD1	1:B:129:ARG:NH2	2.46	0.44
1:A:49:LEU:HD11	1:A:531:VAL:HG11	2.00	0.44
1:A:133:VAL:HB	1:A:285:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:TYR:CZ	1:A:286:ASN:HB3	2.53	0.44
1:A:358:VAL:O	1:A:358:VAL:CG1	2.66	0.44
1:A:574:ASP:HB3	1:A:580:TYR:HA	2.00	0.44
1:B:563:GLU:O	1:B:563:GLU:HG2	2.17	0.44
1:A:373:ASN:HB3	1:A:501:ALA:CB	2.48	0.43
1:A:533:PHE:CD1	1:A:533:PHE:C	2.91	0.43
1:B:60:LYS:HA	1:B:60:LYS:HD3	1.82	0.43
1:B:94:LEU:CD1	1:B:537:THR:HG21	2.48	0.43
1:B:107:GLY:HA3	1:B:267:HIS:NE2	2.33	0.43
1:B:118:LEU:HA	1:B:119:PRO:HD2	1.76	0.43
1:B:267:HIS:O	1:B:268:PHE:C	2.56	0.43
1:A:50:LEU:HD21	1:A:98:ILE:CD1	2.48	0.43
1:A:503:PHE:C	1:A:506:VAL:HG12	2.39	0.43
1:B:42:ASP:O	1:B:43:LEU:C	2.55	0.43
1:B:77:GLN:O	1:B:78:LYS:C	2.57	0.43
1:B:111:PHE:CE2	1:B:540:LYS:CB	3.00	0.43
1:B:168:HIS:NE2	1:B:170:GLY:HA2	2.33	0.43
1:B:531:VAL:O	1:B:531:VAL:HG12	2.18	0.43
1:A:122:VAL:CG1	1:A:123:GLN:N	2.78	0.43
1:A:164:TYR:HB3	1:A:168:HIS:CD2	2.54	0.43
1:A:511:ASN:O	1:A:512:ASP:HB2	2.19	0.43
1:A:591:VAL:O	1:A:595:ILE:HG12	2.17	0.43
1:B:138:PHE:HB3	1:B:139:SER:H	1.16	0.43
1:B:392:PRO:HA	1:B:477:ILE:O	2.18	0.43
1:B:411:LEU:HD21	1:B:455:LEU:HD11	2.00	0.43
1:A:138:PHE:O	1:A:139:SER:O	2.36	0.43
1:A:443:VAL:O	1:A:446:TYR:N	2.46	0.43
1:A:498:PHE:O	1:A:501:ALA:N	2.51	0.43
1:B:116:ALA:CB	1:B:194:PRO:HD2	2.48	0.43
1:B:136:MET:HE2	1:B:281:LEU:C	2.39	0.43
1:B:334:SER:O	1:B:336:GLN:N	2.52	0.43
1:A:152:ASP:H	1:A:199:THR:HB	1.83	0.43
1:A:209:THR:O	1:A:210:ARG:HD3	2.17	0.43
1:A:416:LEU:HD23	1:A:416:LEU:C	2.39	0.43
1:A:471:LEU:HD22	1:A:527:PHE:CE1	2.53	0.43
1:A:480:HIS:O	1:A:482:ARG:N	2.52	0.43
1:B:113:ILE:O	1:B:114:GLU:C	2.56	0.43
1:B:420:VAL:HG13	1:B:425:GLU:HB3	2.00	0.43
1:B:579:GLY:O	1:B:580:TYR:C	2.57	0.43
1:A:279:SER:O	1:A:280:GLY:C	2.57	0.43
1:A:314:SER:HA	1:A:323:HIS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:GLN:HE21	1:B:370:GLN:HB3	1.52	0.43
1:B:422:THR:O	1:B:423:ASN:C	2.57	0.43
1:B:504:PHE:HB3	1:B:505:PRO:CD	2.49	0.43
1:B:516:ILE:HG22	1:B:564:PRO:HA	2.00	0.43
1:A:160:LEU:O	1:A:163:LEU:N	2.50	0.43
1:A:352:PHE:CD2	1:A:384:LEU:HD22	2.54	0.43
1:B:380:TYR:O	1:B:383:ALA:HB3	2.19	0.43
1:B:416:LEU:O	1:B:417:LEU:HD23	2.19	0.43
1:A:155:PRO:O	1:A:156:VAL:C	2.57	0.43
1:A:260:PHE:HA	1:A:527:PHE:CE2	2.54	0.43
1:A:495:GLU:HG2	1:A:496:GLN:HG3	2.00	0.43
1:B:352:PHE:O	1:B:356:ILE:HG12	2.19	0.43
1:A:94:LEU:O	1:A:97:PHE:HB3	2.18	0.43
1:A:180:ARG:CD	1:A:496:GLN:HE21	2.23	0.43
1:A:395:LEU:HG	1:A:476:LYS:HA	2.01	0.43
1:A:411:LEU:HD13	1:B:411:LEU:CD1	2.49	0.43
1:A:592:CYS:HA	1:A:595:ILE:HG13	2.00	0.43
1:B:296:VAL:HA	1:B:311:TYR:OH	2.19	0.43
1:A:198:THR:O	1:A:213:ARG:HA	2.19	0.42
1:A:328:LEU:HD22	1:A:328:LEU:C	2.38	0.42
1:A:371:THR:O	1:A:372:ASN:HB2	2.19	0.42
1:B:108:VAL:CG1	1:B:109:THR:H	2.32	0.42
1:A:87:THR:O	1:A:88:SER:C	2.57	0.42
1:A:403:THR:N	1:A:406:GLU:OE2	2.47	0.42
1:A:492:LEU:N	1:A:492:LEU:CD2	2.82	0.42
1:A:315:VAL:HG11	1:A:588:LYS:HD2	2.01	0.42
1:A:492:LEU:N	1:A:492:LEU:HD23	2.34	0.42
1:B:48:HIS:CE1	1:B:52:VAL:HG21	2.55	0.42
1:B:272:LEU:HA	1:B:272:LEU:HD23	1.59	0.42
1:A:398:HIS:ND1	1:A:549:ALA:HA	2.35	0.42
1:A:467:THR:O	1:A:469:ILE:HG13	2.18	0.42
1:A:171:THR:OG1	1:A:174:GLU:HG3	2.19	0.42
1:A:399:ARG:NH2	1:A:465:LEU:HD23	2.34	0.42
1:B:155:PRO:O	1:B:156:VAL:C	2.58	0.42
1:A:65:GLY:O	1:A:66:TRP:C	2.58	0.42
1:B:124:LYS:HG2	1:B:125:SER:O	2.19	0.42
1:A:264:MET:HB2	1:A:264:MET:HE2	1.80	0.42
1:A:212:VAL:HG12	1:A:213:ARG:N	2.35	0.42
1:A:466:SER:O	1:A:467:THR:C	2.58	0.42
1:A:523:GLY:O	1:A:524:ALA:O	2.37	0.42
1:B:73:VAL:O	1:B:76:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:TRP:O	1:B:458:TRP:CG	2.73	0.42
1:B:471:LEU:O	1:B:472:PHE:HB2	2.20	0.42
1:B:551:ARG:HD2	1:B:552:GLU:HG3	2.01	0.42
1:A:76:GLN:OE1	1:A:80:ARG:NH1	2.53	0.42
1:A:385:LEU:HD21	1:A:504:PHE:CD1	2.54	0.42
1:A:601:ILE:N	1:A:601:ILE:HD12	2.35	0.42
1:B:601:ILE:H	1:B:601:ILE:CD1	2.32	0.42
1:A:136:MET:HG2	1:A:281:LEU:HD23	2.01	0.41
1:A:349:TRP:HB3	1:A:380:TYR:HE1	1.84	0.41
1:A:403:THR:O	1:A:407:VAL:HG23	2.19	0.41
1:A:493:ILE:HD13	1:A:516:ILE:HG21	2.01	0.41
1:B:122:VAL:CG1	1:B:123:GLN:N	2.82	0.41
1:B:186:MET:CE	1:B:275:HIS:HB2	2.50	0.41
1:B:399:ARG:NE	1:B:465:LEU:HG	2.35	0.41
1:B:489:ILE:HG22	1:B:490:CYS:N	2.34	0.41
1:B:601:ILE:N	1:B:601:ILE:CD1	2.81	0.41
1:A:579:GLY:O	1:A:581:SER:N	2.53	0.41
1:B:75:ALA:O	1:B:79:LEU:HD12	2.20	0.41
1:B:427:ARG:HG3	1:B:439:VAL:O	2.20	0.41
1:A:138:PHE:O	1:A:139:SER:C	2.58	0.41
1:A:462:ASP:C	1:A:464:GLU:N	2.73	0.41
1:A:533:PHE:CD1	1:A:533:PHE:O	2.74	0.41
1:A:55:ALA:HB3	1:A:56:PRO:HD3	2.03	0.41
1:A:197:ARG:HD3	1:A:213:ARG:HG2	2.02	0.41
1:A:358:VAL:O	1:A:358:VAL:HG12	2.20	0.41
1:A:446:TYR:HB3	1:A:473:GLY:HA3	2.02	0.41
1:B:382:TYR:O	1:B:383:ALA:C	2.59	0.41
1:B:416:LEU:HD21	1:B:429:ALA:HB1	2.02	0.41
1:B:515:LEU:HA	1:B:565:HIS:CD2	2.56	0.41
1:A:83:GLU:O	1:A:85:PRO:N	2.53	0.41
1:A:464:GLU:O	1:A:465:LEU:CB	2.68	0.41
1:B:452:ARG:O	1:B:453:GLN:C	2.57	0.41
1:B:489:ILE:CG2	1:B:490:CYS:N	2.83	0.41
1:B:568:LEU:CD2	1:B:583:TYR:HD1	2.33	0.41
1:A:54:TYR:CE1	1:A:56:PRO:CG	3.03	0.41
1:A:529:PHE:HB2	1:A:544:LEU:O	2.20	0.41
1:B:73:VAL:O	1:B:74:SER:C	2.59	0.41
1:B:499:ALA:O	1:B:500:CYS:C	2.59	0.41
1:A:204:ARG:HB2	1:A:208:THR:HG23	2.02	0.41
1:A:353:ALA:HA	1:A:387:MET:HE3	2.03	0.41
1:A:399:ARG:HB3	1:A:465:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:PHE:C	1:B:45:PHE:CD2	2.94	0.41
1:B:94:LEU:HD12	1:B:537:THR:HG21	2.03	0.41
1:B:152:ASP:C	1:B:154:ALA:N	2.73	0.41
1:B:450:PHE:C	1:B:452:ARG:H	2.23	0.41
1:B:516:ILE:N	1:B:565:HIS:CD2	2.72	0.41
1:A:307:LEU:HD23	1:A:348:PRO:HB3	2.02	0.41
1:A:498:PHE:O	1:A:499:ALA:C	2.59	0.41
1:A:57:LYS:O	1:A:58:THR:C	2.58	0.41
1:A:177:ALA:O	1:A:178:ALA:C	2.58	0.41
1:A:260:PHE:O	1:A:262:SER:N	2.49	0.41
1:B:59:TRP:CH2	1:B:557:ILE:O	2.73	0.41
1:B:139:SER:O	1:B:140:SER:O	2.39	0.41
1:B:163:LEU:HA	1:B:163:LEU:HD23	1.78	0.41
1:B:218:TYR:CG	1:B:219:VAL:N	2.89	0.41
1:B:297:ILE:HD12	1:B:298:GLY:N	2.36	0.41
1:B:516:ILE:HG22	1:B:564:PRO:CB	2.50	0.41
1:B:571:THR:HG21	1:B:582:GLU:OE1	2.21	0.41
1:A:149:LEU:HB2	1:A:201:LYS:O	2.21	0.41
1:A:269:TRP:O	1:A:271:GLU:N	2.53	0.41
1:A:395:LEU:HD21	1:A:477:ILE:CD1	2.50	0.41
1:A:447:LEU:O	1:A:450:PHE:HB3	2.21	0.41
1:B:94:LEU:HD23	1:B:94:LEU:HA	1.88	0.41
1:B:136:MET:HE1	1:B:281:LEU:HD23	2.01	0.41
1:B:204:ARG:CB	1:B:208:THR:HG23	2.50	0.41
1:B:271:GLU:O	1:B:272:LEU:C	2.59	0.41
1:A:454:VAL:C	1:A:455:LEU:HD23	2.42	0.40
1:A:523:GLY:CA	1:A:560:ILE:CG2	2.92	0.40
1:B:123:GLN:NE2	1:B:285:TYR:HE2	2.19	0.40
1:B:417:LEU:HB3	1:B:448:LYS:HD2	2.02	0.40
1:A:112:ALA:O	1:A:113:ILE:HD13	2.20	0.40
1:A:188:SER:HB3	1:A:271:GLU:OE2	2.21	0.40
1:A:417:LEU:CD1	1:A:448:LYS:HG2	2.52	0.40
1:A:54:TYR:CE2	1:A:101:LEU:HD13	2.56	0.40
1:B:114:GLU:HG2	1:B:193:VAL:HB	2.04	0.40
1:A:55:ALA:O	1:A:57:LYS:N	2.55	0.40
1:A:180:ARG:CB	1:A:180:ARG:CZ	2.99	0.40
1:A:265:VAL:HG12	1:A:266:PRO:N	2.37	0.40
1:A:439:VAL:HG12	1:A:440:ASP:H	1.86	0.40
1:B:39:ALA:CB	1:B:79:LEU:HD22	2.51	0.40
1:B:136:MET:CE	1:B:283:SER:H	2.27	0.40
1:B:480:HIS:CE1	1:B:482:ARG:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:ALA:O	1:B:505:PRO:CD	2.68	0.40
1:A:98:ILE:C	1:A:100:GLY:N	2.75	0.40
1:A:186:MET:CE	1:A:275:HIS:HB2	2.51	0.40
1:A:333:TYR:CD2	1:A:381:LEU:HB2	2.56	0.40
1:B:54:TYR:CE1	1:B:56:PRO:CG	3.02	0.40

There are no symmetry-related clashes.

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	533/583 (91%)	397 (74%)	90 (17%)	46 (9%)	1 5
1	B	533/583 (91%)	404 (76%)	88 (16%)	41 (8%)	1 6
All	All	1066/1166 (91%)	801 (75%)	178 (17%)	87 (8%)	1 5

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	136	MET
1	A	139	SER
1	A	261	TYR
1	A	268	PHE
1	A	283	SER
1	A	317	ASP
1	A	524	ALA
1	A	552	GLU
1	A	559	ASN
1	B	43	LEU
1	B	44	SER
1	B	57	LYS

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Mol	Chain	Res	Type
1	B	77	GLN
1	B	114	GLU
1	B	140	SER
1	B	259	LEU
1	B	268	PHE
1	B	335	TRP
1	B	453	GLN
1	B	465	LEU
1	B	552	GLU
1	B	555	ALA
1	B	556	PHE
1	B	557	ILE
1	B	596	ASN
1	B	598	ASP
1	B	601	ILE
1	A	59	TRP
1	A	66	TRP
1	A	83	GLU
1	A	276	TYR
1	A	280	GLY
1	A	281	LEU
1	A	331	PRO
1	A	404	GLN
1	A	465	LEU
1	A	521	THR
1	A	557	ILE
1	A	580	TYR
1	A	596	ASN
1	A	598	ASP
1	B	62	GLN
1	B	78	LYS
1	B	156	VAL
1	B	281	LEU
1	B	404	GLN
1	B	415	THR
1	B	578	LYS
1	A	144	VAL
1	A	270	ALA
1	A	343	PRO
1	A	405	ASP
1	A	440	ASP
1	A	556	PHE

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Mol	Chain	Res	Type
1	A	560	ILE
1	B	34	LEU
1	B	119	PRO
1	B	188	SER
1	B	283	SER
1	B	464	GLU
1	A	99	GLY
1	A	145	GLY
1	B	207	GLY
1	B	510	ASP
1	A	55	ALA
1	A	204	ARG
1	A	460	LYS
1	A	499	ALA
1	A	572	ALA
1	A	601	ILE
1	B	52	VAL
1	B	55	ALA
1	B	144	VAL
1	B	427	ARG
1	B	505	PRO
1	A	77	GLN
1	A	164	TYR
1	A	504	PHE
1	A	56	PRO
1	A	481	PRO
1	B	69	VAL
1	B	454	VAL
1	B	506	VAL
1	B	408	VAL
1	A	348	PRO
1	A	374	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	463/505 (92%)	418 (90%)	45 (10%)	8 29
1	B	463/505 (92%)	410 (89%)	53 (11%)	5 22
All	All	926/1010 (92%)	828 (89%)	98 (11%)	6 25

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	43	LEU
1	A	45	PHE
1	A	68	LEU
1	A	70	GLN
1	A	84	ASN
1	A	86	SER
1	A	102	ASN
1	A	117	TYR
1	A	136	MET
1	A	138	PHE
1	A	139	SER
1	A	162	THR
1	A	208	THR
1	A	268	PHE
1	A	269	TRP
1	A	272	LEU
1	A	290	THR
1	A	300	VAL
1	A	315	VAL
1	A	317	ASP
1	A	325	VAL
1	A	328	LEU
1	A	366	LEU
1	A	370	GLN
1	A	381	LEU
1	A	421	ASP
1	A	438	THR
1	A	446	TYR
1	A	454	VAL
1	A	459	SER
1	A	465	LEU
1	A	474	PHE
1	A	483	VAL
1	A	492	LEU

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Mol	Chain	Res	Type
1	A	494	ASN
1	A	498	PHE
1	A	503	PHE
1	A	513	ARG
1	A	519	THR
1	A	536	ARG
1	A	548	LEU
1	A	550	VAL
1	A	552	GLU
1	A	556	PHE
1	B	41	GLN
1	B	43	LEU
1	B	45	PHE
1	B	59	TRP
1	B	70	GLN
1	B	84	ASN
1	B	96	ASP
1	B	102	ASN
1	B	110	PHE
1	B	113	ILE
1	B	136	MET
1	B	137	THR
1	B	138	PHE
1	B	142	ILE
1	B	143	ARG
1	B	182	LEU
1	B	184	SER
1	B	189	LEU
1	B	268	PHE
1	B	269	TRP
1	B	281	LEU
1	B	283	SER
1	B	290	THR
1	B	291	ASP
1	B	300	VAL
1	B	327	PHE
1	B	363	THR
1	B	366	LEU
1	B	370	GLN
1	B	381	LEU
1	B	400	MET
1	B	404	GLN

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Mol	Chain	Res	Type
1	B	405	ASP
1	B	406	GLU
1	B	409	ASP
1	B	447	LEU
1	B	458	TRP
1	B	494	ASN
1	B	498	PHE
1	B	503	PHE
1	B	513	ARG
1	B	515	LEU
1	B	529	PHE
1	B	532	GLN
1	B	543	SER
1	B	550	VAL
1	B	551	ARG
1	B	552	GLU
1	B	553	HIS
1	B	556	PHE
1	B	563	GLU
1	B	571	THR
1	B	586	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	102	ASN
1	A	105	HIS
1	A	123	GLN
1	A	286	ASN
1	A	370	GLN
1	A	433	ASN
1	A	442	GLN
1	A	480	HIS
1	A	494	ASN
1	A	496	GLN
1	A	532	GLN
1	A	565	HIS
1	A	596	ASN
1	B	84	ASN
1	B	102	ASN
1	B	105	HIS

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Mol	Chain	Res	Type
1	B	123	GLN
1	B	191	HIS
1	B	274	ASN
1	B	275	HIS
1	B	362	ASN
1	B	419	ASN
1	B	494	ASN
1	B	496	GLN
1	B	530	ASN
1	B	565	HIS
1	B	596	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	537/583 (92%)	0.34	46 (8%)	10	10	54, 107, 187, 198	0
1	B	537/583 (92%)	0.18	18 (3%)	45	43	43, 90, 169, 198	0
All	All	1074/1166 (92%)	0.26	64 (5%)	21	21	43, 98, 181, 198	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	600	THR	6.2
1	B	554	GLY	5.4
1	A	66	TRP	5.1
1	B	600	THR	4.8
1	A	604	ALA	4.7
1	A	320	GLY	4.2
1	B	604	ALA	3.5
1	A	101	LEU	3.4
1	A	601	ILE	3.4
1	B	63	TYR	3.4
1	B	64	LEU	3.3
1	A	136	MET	3.1
1	A	214	VAL	3.1
1	B	460	LYS	3.1
1	A	116	ALA	3.1
1	A	142	ILE	3.1
1	B	555	ALA	3.1
1	A	420	VAL	3.1
1	B	417	LEU	3.0
1	B	551	ARG	3.0
1	A	120	TYR	3.0
1	B	603	LEU	3.0
1	A	212	VAL	2.9
1	A	141	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	66	TRP	2.8
1	A	197	ARG	2.7
1	A	558	GLU	2.7
1	A	135	ILE	2.7
1	A	216	TRP	2.7
1	A	64	LEU	2.6
1	B	536	ARG	2.6
1	A	213	ARG	2.6
1	A	63	TYR	2.5
1	A	202	ILE	2.5
1	A	318	GLY	2.5
1	A	198	THR	2.5
1	A	553	HIS	2.4
1	B	216	TRP	2.4
1	A	319	ASP	2.3
1	A	201	LYS	2.3
1	A	462	ASP	2.3
1	A	602	ILE	2.3
1	A	203	ARG	2.3
1	A	407	VAL	2.3
1	A	337	ASP	2.3
1	A	444	ALA	2.3
1	A	460	LYS	2.2
1	A	49	LEU	2.2
1	A	258	SER	2.2
1	A	402	LEU	2.2
1	A	132	PHE	2.2
1	B	79	LEU	2.2
1	B	602	ILE	2.2
1	B	101	LEU	2.2
1	B	552	GLU	2.1
1	A	131	TYR	2.1
1	A	559	ASN	2.1
1	A	544	LEU	2.1
1	A	119	PRO	2.1
1	A	323	HIS	2.1
1	A	297	ILE	2.1
1	B	320	GLY	2.0
1	A	167	ASN	2.0
1	A	118	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.