W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 11:12 PM GMT

PDB ID : 1J5O
Title : CRYSTAL STRUCTURE OF MET184ILE MUTANT OF HIV-1 REVERSE
TRANSCRIPTASE IN COMPLEX WITH DOUBLE STRANDED DNA
TEMPLATE-PRIMER
Authors : Sarafianos, S.G.; Das, K.; Arnold, E.
Deposited on : 2002-05-24
Resolution : 3.50 Å(reported)

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1 Overall quality at a glance ⓘ

The reported resolution of this entry is 3.50 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	Percentile Ranks	Value
Rfree		0.334
Clashscore		61
Ramachandran outliers		8.5%
Sidechain outliers		16.2%
RSRZ outliers		0.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
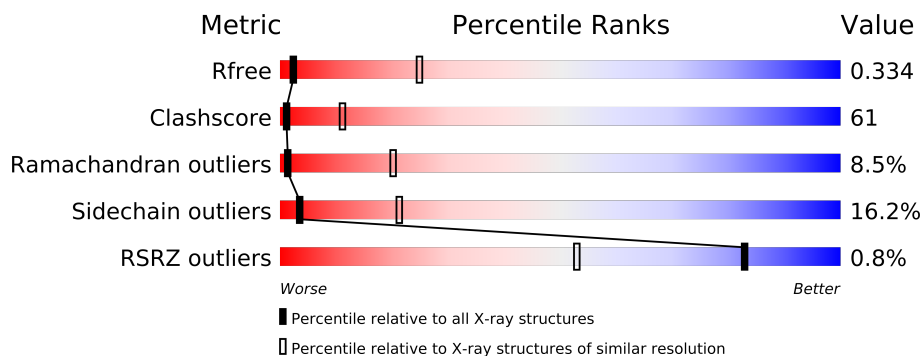
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	T	19	
2	P	18	
3	A	558	
4	B	430	
5	L	214	
6	H	220	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 11720 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA chain called 5'-D(*AP*TP*GP*GP*CP*GP*CP*CP*CP*GP*AP*A P*CP*AP*GP*GP*GP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	19	Total	C	N	O	P	0	0	0
			390	184	80	108	18			

- Molecule 2 is a DNA chain called 5'-D(*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*G P*GP*CP*GP*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	18	Total	C	N	O	P	0	0	0
			363	173	64	109	17			

- Molecule 3 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	558	Total	C	N	O	S	0	0	0
			4292	2778	713	795	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ILE	MET	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 4 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	430	Total	C	N	O	S	0	0	0
			3411	2217	568	620	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	ILE	MET	ENGINEERED	UNP P03366
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 5 is a protein called ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	214	Total 1616	C 1010	N 256	O 343	S 7	0	0	0

- Molecule 6 is a protein called ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	220	Total 1648	C 1037	N 270	O 333	S 8	0	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
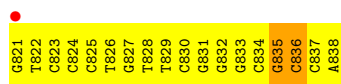
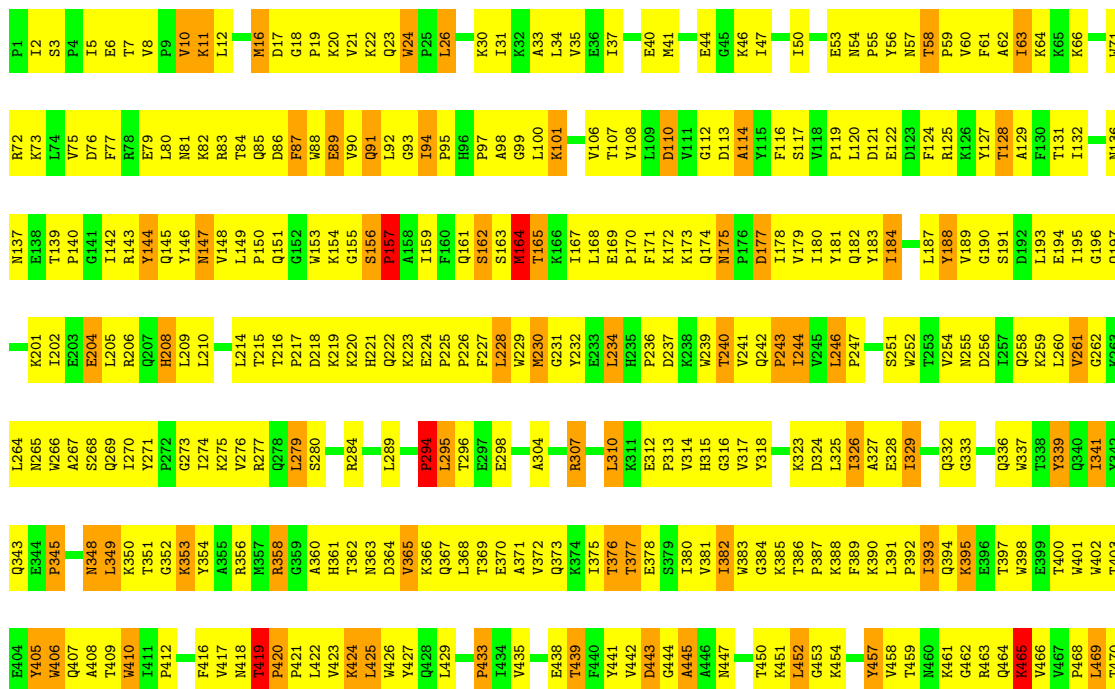• Molecule 1: 5'-D(*AP*TP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP* AP*C)-3'

Chain T:

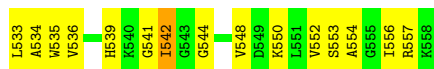• Molecule 2: 5'-D(*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*A)-3'
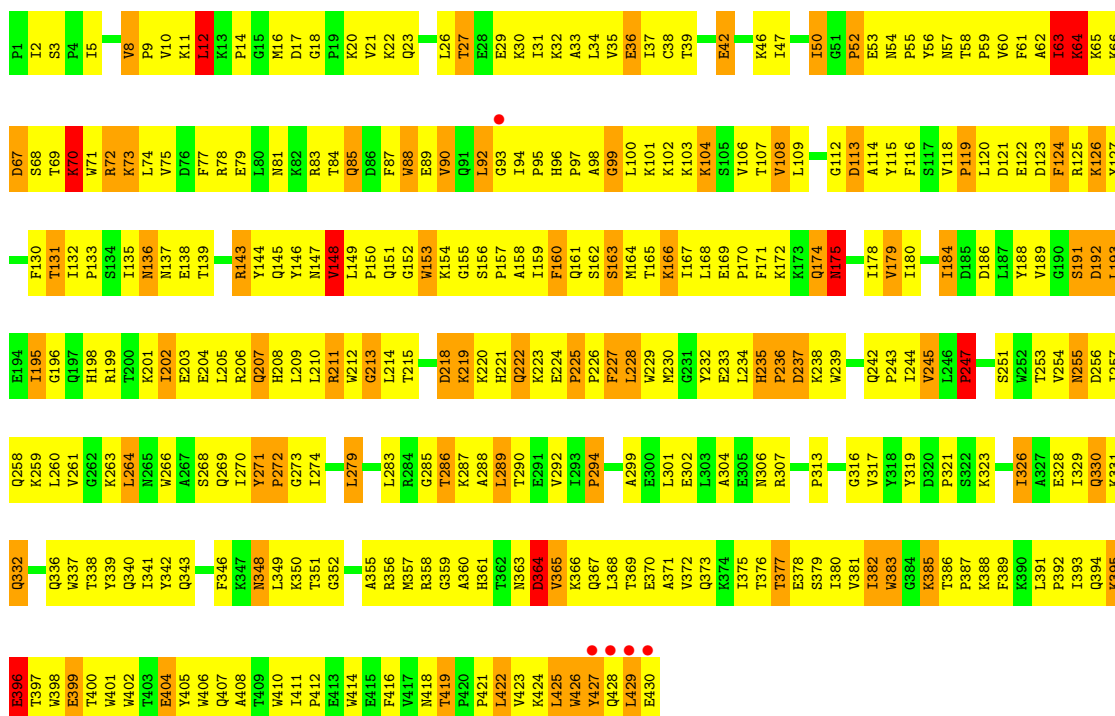
Chain P:

• Molecule 3: Reverse transcriptase

Chain A:

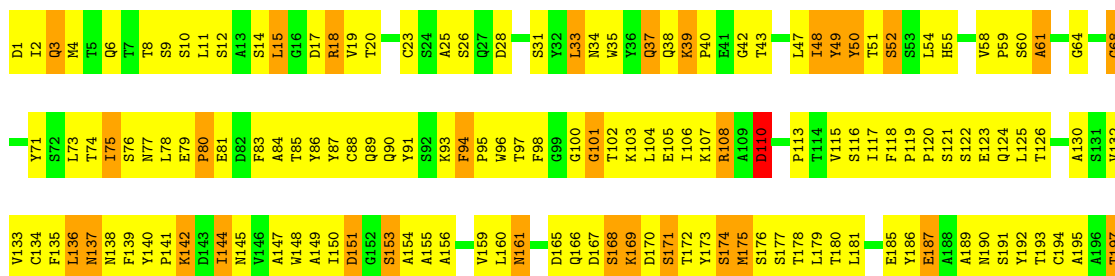N471 T472 T473 N474 Q475 K476 T477 E478 L479 Q480 A481 I482 Y483 L484 A485 L486 Q487 G490 L491 E492 V493 N494 T497 D498 S499 Q500 Y501 A502 L503 G504 I505 I506 Q507 A508 Q509 P510 D511 K512 S513 E514 S515 E516 L517 V518 N519 Q520 I521 E522 E523 Q524 L525 I526 K527 E528 E529 K530 V531 Y532

L533 A534 W535 V536 H539 K540 G541 I542 G543 G544 V548 D549 K550 L551 V552 S553 A554 G555 I556 R557 K558

• Molecule 4: Reverse transcriptase

Chain B:

P1 I2 S3 P4 I5 V8 P9 V10 K11 L2 K13 P14 G15 M16 D17 G18 P19 K20 V21 K22 Q23 L26 T27 E28 E29 K30 I31 K32 L34 V35 E36 I37 C38 T39 E42 K46 I47 I50 G51 P52 E53 N54 P55 Y56 N57 T58 P59 V60 F61 A62 I63 K64 K65 K66

D67 S68 T69 K70 W71 R72 K73 L74 V75 D76 F77 R78 E79 L80 N81 K82 R83 T84 Q85 D86 F87 W88 E89 V90 Q91 L92 G93 I94 P95 H96 P97 A98 G99 L100 K101 K102 K103 K104 S105 V106 T107 V108 L109 G112 D113 A114 Y115 F116 S117 V118 P119 L120 D121 E122 D123 F124 R125 K126 Y127

F130 T131 I132 P133 S134 I135 N136 N137 E138 T139 R143 Y144 Q145 Y146 N147 V148 L149 P150 Q151 G152 W153 K154 G155 S156 P157 A158 I159 F160 Q161 S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 K172 K173 Q174 N175 I178 V179 I180 I184 D185 D186 L187 Y188 V189 G190 S191 D192 L193

E194 I195 G196 Q197 H198 R199 T200 K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 R211 W212 G213 L214 T215 D218 K219 K220 H221 Q222 K223 E224 P225 P226 F227 I228 W229 M230 G231 Y232 E233 L234 H235 P236 D237 K238 W239 Q242 P243 I244 V245 L246 P247 S251 W252 T253 V254 N255 D256 I257

Q258 K259 L260 V261 G262 K263 L264 N265 W266 A267 S268 Q269 I270 Y271 P272 G273 I274 L279 L283 R284 G285 T286 K287 A288 L289 T290 E291 V292 I293 P294 A299 E300 L301 E302 L303 A304 E305 N306 R307 P313 G316 V317 Y318 Y319 D320 P321 S322 K323 I326 A327 E328 I329 Q330 K331

Q332 Q336 W337 T338 Y339 Q340 I341 Y342 Q343 F346 K347 N348 L349 K350 T351 G352 A355 R356 M357 R358 G359 A360 H361 T362 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377 E378 S379 I380 V381 I382 W383 G384 K385 T386 P387 K388 F389 K390 L391 P392 I393 Q394 K395

E396 T397 W398 E399 T400 W401 W402 T403 E404 Y405 W406 Q407 A408 T409 W410 I411 P412 E413 W414 E415 F416 V417 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427 Q428 L429 E430

• Molecule 5: ANTIBODY (LIGHT CHAIN)

Chain L:

D1 I2 Q3 M4 T5 Q6 T7 T8 S9 S10 L11 S12 A13 S14 L15 G16 D17 R18 V19 T20 C23 S24 A25 S26 Q27 D28 S31 Y32 L33 N34 W35 Y36 Q37 Q38 K39 P40 E41 G42 T43 L47 I48 Y49 Y50 T51 S52 S53 L54 H55 V58 P59 S60 A61 G64 G68

Y71 S72 L73 T74 I75 S76 N77 L78 E79 P80 E81 D82 F83 A84 T85 Y86 Y87 C88 Q89 Q90 Y91 S92 K93 F94 P95 W96 T97 F98 G99 G100 G101 T102 K103 L104 E105 I106 K107 R108 A109 D110 P113 T114 V115 S116 I117 F118 P119 P120 S121 S122 E123 Q124 L125 T126 A130 S131 V132

V133 C134 F135 L136 N137 N138 F139 Y140 P141 K142 D143 I144 N145 V146 A147 W148 A149 I150 D151 G152 S153 S154 A155 A156 V159 L160 N161 D165 Q166 D167 S168 K169 D170 S171 T172 Y173 S174 M175 S176 S177 T178 L179 T180 L181 E185 Y186 E187 A188 A189 N190 S191 Y192 T193 C194 A195 A196 T197

H198 K199 T200 S203 P204 I205 V206 K207 S208 F209 N210 A211 N212 E213 C214

• Molecule 6: ANTIBODY (HEAVY CHAIN)

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	169.18Å 169.18Å 221.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.50 39.97 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (10.00-3.50) 91.4 (39.97-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.262 , 0.338 0.281 , 0.334	Depositor DCC
R_{free} test set	1219 reflections (3.04%)	DCC
Wilson B-factor (Å^2)	98.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 72.4	EDS
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
L-test for twinning	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Outliers	0 of 42000 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	11720	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	T	0.55	0/439	0.76	0/676
2	P	0.56	1/405 (0.2%)	0.81	0/623
3	A	0.56	0/4404	0.78	2/6017 (0.0%)
4	B	0.63	0/3510	0.84	4/4784 (0.1%)
5	L	0.54	0/1654	0.85	0/2256
6	H	0.58	0/1691	0.85	0/2320
All	All	0.58	1/12103 (0.0%)	0.82	6/16676 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1
3	A	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	835	DG	O3'-P	-5.99	1.53	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	247	PRO	N-CA-CB	6.75	111.39	103.30
4	B	243	PRO	N-CA-CB	6.31	110.87	103.30
3	A	294	PRO	N-CA-CB	5.91	110.39	103.30
3	A	247	PRO	N-CA-CB	5.63	110.06	103.30
4	B	313	PRO	N-CA-CB	5.37	109.74	103.30
4	B	186	ASP	N-CA-C	5.08	124.72	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	144	TYR	Sidechain
2	P	836	DC	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	390	0	212	55	0
2	P	363	0	204	103	0
3	A	4292	0	4127	482	0
4	B	3411	0	3300	446	0
5	L	1616	0	1517	174	0
6	H	1648	0	1602	184	0
All	All	11720	0	10962	1380	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 61.

All (1380) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:822:DT:H2"	2:P:823:DC:C6	1.75	1.22
1:T:803:DG:H2"	1:T:804:DG:C5'	1.77	1.14
2:P:831:DG:H2"	2:P:832:DG:H5'	1.17	1.11
3:A:20:LYS:HA	3:A:57:ASN:H	1.15	1.10
3:A:333:GLY:H	3:A:336:GLN:HB2	0.99	1.09
6:H:61:TYR:HE2	6:H:70:THR:HA	1.17	1.08
2:P:823:DC:H2"	2:P:824:DC:C5'	1.84	1.07
2:P:823:DC:H2"	2:P:824:DC:H5"	1.07	1.07
4:B:103:LYS:HZ2	4:B:191:SER:HA	1.20	1.05
3:A:106:VAL:HB	3:A:227:PHE:HE2	1.17	1.05
2:P:823:DC:C2'	2:P:824:DC:H5"	1.85	1.04
2:P:825:DC:H2"	2:P:826:DT:H5'	1.04	1.03
2:P:825:DC:H2"	2:P:826:DT:C5'	1.87	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:803:DG:H2"	1:T:804:DG:H5'	1.38	1.03
3:A:20:LYS:HG2	3:A:56:TYR:HA	1.42	1.02
2:P:833:DG:H2"	2:P:834:DC:OP2	1.56	1.01
4:B:103:LYS:HZ3	4:B:192:ASP:H	1.04	1.00
5:L:33:LEU:HD21	5:L:88:CYS:SG	2.03	0.98
1:T:815:DG:H2"	1:T:816:DG:C8	1.99	0.97
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.46	0.96
2:P:825:DC:C2'	2:P:826:DT:H5'	1.96	0.95
3:A:333:GLY:N	3:A:336:GLN:HB2	1.80	0.95
5:L:137:ASN:HA	5:L:174:SER:HB3	1.49	0.95
1:T:817:DG:H2"	1:T:818:DA:H5'	1.49	0.94
3:A:279:LEU:HD12	3:A:279:LEU:H	1.31	0.94
6:H:61:TYR:CE2	6:H:70:THR:HA	2.01	0.94
4:B:50:ILE:HD12	4:B:145:GLN:HG3	1.47	0.94
2:P:821:DG:H2'	2:P:822:DT:H71	1.47	0.94
2:P:831:DG:C2'	2:P:832:DG:H5'	1.99	0.93
5:L:161:ASN:HB3	5:L:177:SER:HA	1.50	0.93
5:L:15:LEU:HD21	5:L:80:PRO:HD3	1.52	0.92
6:H:40:ARG:NH1	6:H:91:ASP:HA	1.83	0.91
3:A:101:LYS:HD2	3:A:101:LYS:H	1.33	0.91
2:P:822:DT:H2"	2:P:823:DC:H6	1.28	0.91
6:H:195:SER:O	6:H:199:PRO:HD2	1.71	0.91
1:T:801:DA:H2"	1:T:802:DT:C7	2.00	0.91
3:A:458:VAL:HG12	3:A:459:THR:H	1.33	0.90
5:L:144:ILE:HG12	5:L:145:ASN:H	1.35	0.90
4:B:342:TYR:HB3	4:B:348:ASN:HA	1.54	0.90
6:H:14:PRO:HG3	6:H:121:VAL:HG12	1.54	0.89
1:T:810:DG:H2"	1:T:811:DA:C8	2.07	0.89
6:H:163:THR:H	6:H:206:ASN:ND2	1.70	0.89
3:A:178:ILE:HA	3:A:191:SER:HB3	1.51	0.89
3:A:454:LYS:HA	3:A:468:PRO:HA	1.54	0.89
1:T:811:DA:H2"	1:T:812:DA:OP2	1.70	0.88
3:A:106:VAL:HB	3:A:227:PHE:CE2	2.09	0.88
3:A:62:ALA:HA	3:A:73:LYS:HA	1.54	0.88
1:T:812:DA:H2"	1:T:813:DC:OP2	1.72	0.88
4:B:268:SER:HA	4:B:274:ILE:HG13	1.53	0.88
2:P:828:DT:H4'	2:P:828:DT:OP1	1.72	0.87
2:P:837:DC:H2"	2:P:838:DA:O5'	1.74	0.87
2:P:822:DT:H2"	2:P:823:DC:C5	2.10	0.86
2:P:837:DC:H2"	2:P:838:DA:C5'	2.04	0.86
4:B:372:VAL:HG12	4:B:389:PHE:CD2	2.10	0.86
6:H:103:THR:HB	6:H:107:ASP:HB2	1.58	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:801:DA:H2"	1:T:802:DT:H71	1.56	0.86
5:L:110:ASP:HA	5:L:140:TYR:CB	2.06	0.86
1:T:810:DG:H2"	1:T:811:DA:H8	1.41	0.85
4:B:10:VAL:HG22	4:B:87:PHE:HZ	1.37	0.85
4:B:387:PRO:HG2	4:B:389:PHE:CE1	2.10	0.85
2:P:821:DG:H2'	2:P:822:DT:C7	2.06	0.85
4:B:55:PRO:HG2	4:B:56:TYR:CD2	2.12	0.85
3:A:450:THR:HB	3:A:452:LEU:HG	1.57	0.84
3:A:277:ARG:HH12	3:A:336:GLN:N	1.75	0.83
4:B:254:VAL:HB	4:B:289:LEU:HA	1.59	0.83
4:B:219:LYS:N	4:B:219:LYS:HZ2	1.77	0.83
2:P:830:DC:C2'	2:P:831:DG:C8	2.62	0.83
3:A:34:LEU:HA	3:A:37:ILE:HD12	1.60	0.82
5:L:47:LEU:HA	5:L:58:VAL:HG21	1.60	0.82
4:B:402:TRP:HH2	4:B:411:ILE:HD13	1.44	0.82
3:A:329:ILE:HG22	3:A:339:TYR:HB3	1.61	0.82
4:B:274:ILE:HA	4:B:306:ASN:HD21	1.45	0.82
4:B:219:LYS:HZ2	4:B:219:LYS:H	1.28	0.81
2:P:821:DG:C2'	2:P:822:DT:H71	2.10	0.81
6:H:62:ASN:HD22	6:H:65:LEU:HG	1.44	0.81
5:L:48:ILE:HG22	5:L:54:LEU:HA	1.60	0.81
3:A:458:VAL:HG22	3:A:464:GLN:HG2	1.63	0.81
2:P:833:DG:H1'	2:P:834:DC:H5'	1.63	0.81
3:A:294:PRO:C	3:A:296:THR:H	1.84	0.81
3:A:120:LEU:HD12	3:A:121:ASP:H	1.46	0.81
4:B:146:TYR:CE2	4:B:150:PRO:HA	2.15	0.80
5:L:205:ILE:H	5:L:205:ILE:HD12	1.44	0.80
4:B:292:VAL:C	4:B:294:PRO:HD3	2.02	0.80
3:A:483:TYR:HA	3:A:486:LEU:HD12	1.63	0.80
3:A:479:LEU:HD13	3:A:502:ALA:HB1	1.62	0.79
2:P:830:DC:H2'	2:P:831:DG:C8	2.17	0.79
4:B:153:TRP:O	4:B:157:PRO:HD2	1.82	0.79
3:A:327:ALA:HB2	3:A:341:ILE:HG23	1.62	0.79
3:A:122:GLU:HA	3:A:125:ARG:HD2	1.65	0.79
2:P:838:DA:H1'	3:A:184:ILE:HD12	1.62	0.79
2:P:827:DG:H2"	2:P:828:DT:O5'	1.83	0.79
6:H:40:ARG:HB2	6:H:50:LEU:HD11	1.63	0.79
2:P:829:DT:H2"	2:P:830:DC:C6	2.18	0.79
4:B:270:ILE:HB	4:B:271:TYR:HD1	1.48	0.79
4:B:292:VAL:O	4:B:294:PRO:HD3	1.82	0.79
6:H:156:PHE:HB3	6:H:157:PRO:HD3	1.64	0.79
6:H:62:ASN:HD21	6:H:64:SER:HB3	1.47	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:254:VAL:CB	4:B:289:LEU:HA	2.12	0.78
2:P:824:DC:H1'	3:A:475:GLN:HE22	1.47	0.78
3:A:457:TYR:CE2	3:A:465:LYS:HB3	2.19	0.78
3:A:501:TYR:CE1	3:A:505:ILE:HD11	2.19	0.78
4:B:10:VAL:HG22	4:B:87:PHE:CZ	2.18	0.78
4:B:31:ILE:O	4:B:35:VAL:HG23	1.84	0.78
1:T:803:DG:H2"	1:T:804:DG:H5"	1.64	0.78
3:A:501:TYR:CZ	3:A:505:ILE:HD11	2.18	0.78
3:A:261:VAL:HG13	3:A:276:VAL:HG11	1.67	0.77
6:H:92:THR:HB	6:H:121:VAL:HG23	1.66	0.77
3:A:542:ILE:HG22	4:B:283:LEU:HD23	1.66	0.77
4:B:103:LYS:NZ	4:B:191:SER:HA	1.99	0.77
4:B:270:ILE:HB	4:B:271:TYR:CD1	2.20	0.77
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.20	0.77
4:B:22:LYS:HZ3	4:B:23:GLN:N	1.83	0.77
3:A:518:VAL:O	3:A:522:ILE:HG13	1.85	0.77
4:B:373:GLN:HE22	4:B:406:TRP:HA	1.49	0.77
2:P:837:DC:H4'	3:A:230:MET:HE2	1.65	0.77
5:L:175:MET:HG3	5:L:176:SER:N	1.99	0.76
5:L:51:THR:HG21	5:L:71:TYR:HD2	1.49	0.76
4:B:209:LEU:HB3	4:B:215:THR:HB	1.66	0.76
6:H:187:LEU:HD23	6:H:188:SER:N	2.01	0.76
1:T:804:DG:H2"	1:T:805:DC:O5'	1.84	0.76
2:P:822:DT:C2'	2:P:823:DC:C5	2.68	0.76
3:A:20:LYS:HA	3:A:57:ASN:N	1.98	0.76
4:B:271:TYR:HB2	4:B:274:ILE:HD11	1.68	0.76
4:B:103:LYS:NZ	4:B:192:ASP:H	1.83	0.76
3:A:482:ILE:HG22	3:A:486:LEU:HD11	1.68	0.76
6:H:2:ILE:HG22	6:H:26:GLY:HA3	1.69	0.75
3:A:435:VAL:HA	4:B:290:THR:CG2	2.17	0.75
2:P:830:DC:H2"	2:P:831:DG:C8	2.21	0.75
4:B:67:ASP:HB2	4:B:220:LYS:HA	1.67	0.75
3:A:164:MET:O	3:A:168:LEU:HD23	1.87	0.75
1:T:812:DA:H1'	1:T:813:DC:O5'	1.86	0.74
4:B:47:ILE:HG23	4:B:145:GLN:O	1.86	0.74
4:B:88:TRP:NE1	4:B:92:LEU:HD22	2.01	0.74
3:A:206:ARG:HG2	3:A:216:THR:HG21	1.70	0.74
6:H:165:ASN:HB2	6:H:169:LEU:HD13	1.68	0.74
3:A:260:LEU:O	3:A:264:LEU:HG	1.87	0.74
5:L:37:GLN:HB3	5:L:47:LEU:HD11	1.70	0.74
4:B:138:GLU:HG2	4:B:139:THR:HG23	1.69	0.74
6:H:49:TRP:CZ2	6:H:51:ALA:HA	2.23	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:L:144:ILE:HG12	5:L:145:ASN:N	2.02	0.74
3:A:407:GLN:HE21	4:B:393:ILE:HA	1.53	0.74
3:A:447:ASN:HB3	3:A:450:THR:HG23	1.68	0.73
5:L:161:ASN:HB3	5:L:177:SER:CA	2.18	0.73
3:A:175:ASN:HB2	3:A:178:ILE:HD13	1.69	0.73
4:B:115:TYR:HB3	4:B:149:LEU:HB2	1.71	0.73
3:A:304:ALA:HA	3:A:307:ARG:HB2	1.69	0.73
4:B:68:SER:OG	4:B:219:LYS:HB2	1.89	0.73
6:H:182:SER:O	6:H:184:LEU:HD12	1.88	0.73
3:A:523:GLU:HA	3:A:526:ILE:HD12	1.71	0.73
3:A:153:TRP:CZ3	3:A:155:GLY:HA3	2.24	0.73
5:L:1:ASP:H3	5:L:93:LYS:HD2	1.54	0.73
3:A:224:GLU:HB3	3:A:225:PRO:HD3	1.70	0.72
4:B:225:PRO:HB2	4:B:226:PRO:CD	2.19	0.72
3:A:442:VAL:HG12	3:A:443:ASP:H	1.54	0.72
3:A:509:GLN:N	3:A:510:PRO:HD3	2.04	0.72
2:P:837:DC:H2"	2:P:838:DA:H5'	1.71	0.72
2:P:837:DC:H4'	3:A:230:MET:CE	2.18	0.72
3:A:407:GLN:NE2	4:B:393:ILE:HA	2.05	0.72
3:A:23:GLN:OE1	3:A:59:PRO:HA	1.89	0.72
4:B:385:LYS:HD2	4:B:385:LYS:N	2.04	0.72
3:A:542:ILE:H	3:A:542:ILE:HD12	1.53	0.71
3:A:479:LEU:HD13	3:A:502:ALA:CB	2.20	0.71
5:L:3:GLN:HA	5:L:3:GLN:HE21	1.54	0.71
4:B:161:GLN:O	4:B:165:THR:HG23	1.90	0.71
4:B:230:MET:CE	6:H:104:SER:HA	2.20	0.71
3:A:87:PHE:CE1	3:A:155:GLY:HA2	2.25	0.71
3:A:420:PRO:HB2	3:A:421:PRO:HD2	1.73	0.71
2:P:829:DT:H2"	2:P:830:DC:O4'	1.90	0.71
1:T:803:DG:H5'	1:T:803:DG:H8	1.55	0.71
4:B:239:TRP:CZ3	4:B:378:GLU:HG3	2.25	0.71
3:A:90:VAL:O	3:A:91:GLN:HG2	1.90	0.71
3:A:457:TYR:HE2	3:A:465:LYS:HB3	1.55	0.71
3:A:472:THR:HA	3:A:476:LYS:HD2	1.73	0.71
2:P:838:DA:H4'	3:A:183:TYR:CE2	2.26	0.71
4:B:368:LEU:O	4:B:371:ALA:HB3	1.91	0.71
5:L:51:THR:HG21	5:L:71:TYR:CD2	2.25	0.71
3:A:215:THR:O	3:A:217:PRO:HD3	1.91	0.71
2:P:826:DT:H2"	2:P:827:DG:C8	2.26	0.70
3:A:181:TYR:HE1	4:B:136:ASN:HD22	1.38	0.70
5:L:19:VAL:O	5:L:74:THR:HG23	1.91	0.70
3:A:458:VAL:HG12	3:A:459:THR:N	2.06	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:329:ILE:HA	4:B:338:THR:O	1.90	0.70
5:L:110:ASP:HA	5:L:140:TYR:HB2	1.73	0.70
3:A:450:THR:O	3:A:452:LEU:HD23	1.91	0.70
6:H:16:GLN:O	6:H:87:VAL:HG23	1.92	0.70
4:B:166:LYS:O	4:B:169:GLU:HB3	1.91	0.70
4:B:14:PRO:O	4:B:16:MET:HG2	1.92	0.70
4:B:366:LYS:O	4:B:370:GLU:HG3	1.92	0.70
4:B:421:PRO:O	4:B:425:LEU:HD13	1.91	0.70
2:P:830:DC:H2'	2:P:831:DG:N7	2.07	0.69
4:B:274:ILE:HA	4:B:306:ASN:ND2	2.06	0.69
6:H:178:ALA:HB2	6:H:187:LEU:HB2	1.73	0.69
6:H:92:THR:OG1	6:H:120:THR:HA	1.91	0.69
3:A:435:VAL:HG22	4:B:290:THR:HG23	1.75	0.69
2:P:833:DG:C2'	2:P:834:DC:OP2	2.39	0.69
5:L:198:HIS:HB3	5:L:200:THR:HG23	1.74	0.69
3:A:329:ILE:HD13	3:A:329:ILE:H	1.55	0.69
3:A:33:ALA:O	3:A:37:ILE:HG13	1.91	0.69
5:L:1:ASP:N	5:L:93:LYS:HD2	2.07	0.69
5:L:147:ALA:HB3	5:L:195:ALA:HB3	1.72	0.69
4:B:29:GLU:HG2	4:B:71:TRP:CH2	2.28	0.69
2:P:824:DC:C1'	3:A:475:GLN:HE22	2.05	0.69
1:T:801:DA:C2'	1:T:802:DT:H71	2.23	0.69
6:H:40:ARG:HH11	6:H:91:ASP:HA	1.56	0.69
3:A:438:GLU:HG2	3:A:461:LYS:HE3	1.75	0.69
4:B:365:VAL:O	4:B:369:THR:HG23	1.92	0.69
3:A:435:VAL:HA	4:B:290:THR:HG21	1.74	0.69
4:B:29:GLU:HG2	4:B:71:TRP:HH2	1.56	0.69
2:P:829:DT:C2'	2:P:830:DC:C6	2.76	0.69
3:A:501:TYR:O	3:A:505:ILE:HG13	1.93	0.69
3:A:79:GLU:O	3:A:83:ARG:HG3	1.93	0.69
5:L:12:SER:HB3	5:L:105:GLU:HG3	1.75	0.69
4:B:224:GLU:HA	4:B:227:PHE:CE2	2.27	0.69
3:A:120:LEU:HD12	3:A:121:ASP:N	2.07	0.69
6:H:147:THR:C	6:H:148:LEU:HD22	2.14	0.69
4:B:83:ARG:HH11	4:B:83:ARG:HG2	1.56	0.68
4:B:22:LYS:HZ3	4:B:23:GLN:H	1.38	0.68
5:L:136:LEU:HD12	5:L:175:MET:HG2	1.76	0.68
4:B:106:VAL:HG13	4:B:234:LEU:HB3	1.76	0.68
3:A:548:VAL:O	3:A:552:VAL:HG23	1.94	0.68
5:L:23:CYS:HB2	5:L:35:TRP:CH2	2.28	0.68
4:B:63:ILE:HG12	4:B:63:ILE:O	1.92	0.68
4:B:393:ILE:HD11	4:B:397:THR:HG21	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:L:83:PHE:HA	5:L:104:LEU:HG	1.76	0.68
1:T:818:DA:H2	2:P:822:DT:O2	1.75	0.68
4:B:257:ILE:HG13	4:B:258:GLN:N	2.09	0.68
6:H:31:THR:HB	6:H:34:ILE:HG13	1.75	0.68
4:B:331:LYS:O	4:B:331:LYS:HG2	1.93	0.68
1:T:803:DG:C5'	1:T:803:DG:H8	2.06	0.67
3:A:101:LYS:CD	3:A:101:LYS:H	2.04	0.67
6:H:1:GLN:HG2	6:H:2:ILE:HD13	1.76	0.67
1:T:815:DG:H2"	1:T:816:DG:H8	1.56	0.67
6:H:143:ASN:ND2	6:H:145:MET:HB2	2.09	0.67
3:A:307:ARG:HG3	3:A:307:ARG:HH11	1.58	0.67
4:B:125:ARG:HD3	4:B:147:ASN:HA	1.76	0.67
4:B:425:LEU:C	4:B:427:TYR:H	1.98	0.67
6:H:62:ASN:ND2	6:H:65:LEU:HG	2.09	0.67
6:H:162:VAL:HA	6:H:206:ASN:O	1.94	0.67
3:A:454:LYS:HG2	3:A:468:PRO:HB3	1.74	0.67
3:A:156:SER:HB2	3:A:157:PRO:HD3	1.75	0.67
3:A:500:GLN:O	3:A:503:LEU:HB3	1.95	0.67
6:H:212:SER:O	6:H:214:THR:HG23	1.96	0.67
3:A:473:THR:O	3:A:477:THR:HG23	1.95	0.66
4:B:244:ILE:CB	4:B:426:TRP:HE1	2.08	0.66
3:A:324:ASP:O	3:A:343:GLN:HG2	1.95	0.66
5:L:110:ASP:HA	5:L:140:TYR:HB3	1.77	0.66
5:L:140:TYR:HB3	5:L:141:PRO:HD3	1.78	0.66
6:H:89:THR:O	6:H:92:THR:HG22	1.94	0.66
2:P:830:DC:H4'	2:P:830:DC:OP1	1.95	0.66
2:P:824:DC:H1'	3:A:475:GLN:NE2	2.11	0.66
2:P:831:DG:C6	2:P:832:DG:C6	2.84	0.66
3:A:40:GLU:O	3:A:44:GLU:HG3	1.96	0.66
3:A:19:PRO:HG3	3:A:80:LEU:HD23	1.78	0.66
4:B:206:ARG:NH2	4:B:219:LYS:HG3	2.11	0.66
4:B:60:VAL:CG1	4:B:75:VAL:HG22	2.23	0.65
5:L:192:TYR:HB2	5:L:209:PHE:CE2	2.29	0.65
2:P:837:DC:C2'	2:P:838:DA:H5'	2.26	0.65
5:L:6:GLN:HE22	5:L:87:TYR:HA	1.61	0.65
4:B:424:LYS:C	4:B:426:TRP:H	2.00	0.65
5:L:120:PRO:HG3	5:L:132:VAL:HG22	1.78	0.65
4:B:319:TYR:CE2	4:B:321:PRO:HG3	2.31	0.65
3:A:92:LEU:HG	3:A:92:LEU:O	1.94	0.65
4:B:60:VAL:HA	4:B:74:LEU:O	1.95	0.65
6:H:163:THR:H	6:H:206:ASN:HD21	1.44	0.65
4:B:236:PRO:HG2	4:B:237:ASP:H	1.62	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:400:THR:HA	3:A:403:THR:OG1	1.96	0.65
4:B:103:LYS:HZ3	4:B:192:ASP:N	1.87	0.65
4:B:104:LYS:HB2	4:B:192:ASP:HA	1.79	0.65
4:B:55:PRO:HG2	4:B:56:TYR:HD2	1.59	0.65
4:B:47:ILE:CG2	4:B:144:TYR:HB3	2.27	0.65
3:A:155:GLY:C	3:A:159:ILE:HG12	2.18	0.65
2:P:825:DC:C6	2:P:826:DT:H72	2.32	0.64
5:L:33:LEU:HD11	5:L:88:CYS:SG	2.36	0.64
5:L:107:LYS:HD2	5:L:140:TYR:OH	1.97	0.64
3:A:337:TRP:NE1	3:A:367:GLN:HB3	2.12	0.64
4:B:164:MET:SD	4:B:168:LEU:HD11	2.37	0.64
6:H:198:TRP:HD1	6:H:203:VAL:HG23	1.62	0.64
4:B:423:VAL:HG12	4:B:428:GLN:HA	1.79	0.64
3:A:325:LEU:HB3	3:A:387:PRO:HB3	1.79	0.64
4:B:372:VAL:HG12	4:B:389:PHE:CE2	2.32	0.64
3:A:146:TYR:CD2	3:A:150:PRO:HB3	2.32	0.64
3:A:225:PRO:HB2	3:A:226:PRO:HD3	1.78	0.64
3:A:348:ASN:HD22	3:A:349:LEU:H	1.45	0.64
4:B:118:VAL:HG13	4:B:119:PRO:HD2	1.77	0.64
4:B:212:TRP:O	4:B:214:LEU:N	2.31	0.64
3:A:12:LEU:HD23	3:A:124:PHE:HE1	1.61	0.64
3:A:332:GLN:HB3	3:A:336:GLN:HB3	1.79	0.64
3:A:393:ILE:HG12	3:A:397:THR:OG1	1.98	0.64
3:A:5:ILE:HD12	3:A:6:GLU:H	1.62	0.64
4:B:195:ILE:HD11	4:B:199:ARG:HE	1.63	0.64
4:B:373:GLN:NE2	4:B:406:TRP:HA	2.12	0.64
4:B:180:ILE:HG12	4:B:189:VAL:HG22	1.80	0.64
3:A:154:LYS:O	3:A:157:PRO:HD2	1.98	0.64
3:A:26:LEU:HD11	3:A:61:PHE:HA	1.80	0.63
4:B:50:ILE:N	4:B:50:ILE:HD13	2.14	0.63
5:L:1:ASP:HA	5:L:95:PRO:HB2	1.80	0.63
3:A:459:THR:CG2	3:A:463:ARG:HB3	2.28	0.63
2:P:838:DA:H1'	3:A:184:ILE:CD1	2.28	0.63
5:L:48:ILE:HD11	5:L:73:LEU:HD13	1.80	0.63
4:B:218:ASP:C	4:B:219:LYS:HD3	2.19	0.63
5:L:130:ALA:HB3	5:L:181:LEU:O	1.99	0.63
3:A:94:ILE:HB	3:A:95:PRO:HD2	1.79	0.63
3:A:542:ILE:HD12	3:A:542:ILE:N	2.13	0.63
4:B:30:LYS:HZ3	4:B:61:PHE:HD1	1.45	0.63
4:B:258:GLN:O	4:B:261:VAL:HG12	1.98	0.63
4:B:195:ILE:HG23	4:B:196:GLY:H	1.62	0.63
3:A:150:PRO:HG2	3:A:153:TRP:HB3	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:34:LEU:O	4:B:38:CYS:HB2	1.98	0.63
2:P:822:DT:C2'	2:P:823:DC:C6	2.67	0.63
4:B:39:THR:O	4:B:42:GLU:HB3	1.98	0.63
4:B:195:ILE:O	4:B:199:ARG:HG3	1.98	0.63
3:A:254:VAL:HG22	3:A:289:LEU:O	1.98	0.63
3:A:132:ILE:HG23	3:A:142:ILE:HB	1.81	0.63
4:B:230:MET:HE2	6:H:104:SER:HA	1.80	0.62
3:A:326:ILE:HG23	3:A:388:LYS:HB2	1.80	0.62
1:T:803:DG:H5'	1:T:803:DG:C8	2.34	0.62
5:L:159:VAL:HG12	5:L:161:ASN:OD1	2.00	0.62
3:A:486:LEU:HB3	3:A:528:LYS:NZ	2.14	0.62
5:L:197:THR:HG23	5:L:204:PRO:HA	1.80	0.62
5:L:141:PRO:HD2	5:L:198:HIS:CE1	2.33	0.62
4:B:425:LEU:O	4:B:427:TYR:N	2.32	0.62
6:H:61:TYR:HE2	6:H:70:THR:CA	2.02	0.62
3:A:179:VAL:N	3:A:190:GLY:O	2.32	0.62
3:A:240:THR:HG23	3:A:315:HIS:HA	1.80	0.62
1:T:815:DG:C2'	1:T:816:DG:C8	2.81	0.62
6:H:49:TRP:CE2	6:H:51:ALA:HA	2.35	0.62
6:H:132:TYR:HB2	6:H:151:LEU:HB3	1.81	0.62
2:P:831:DG:C4	2:P:832:DG:N7	2.68	0.62
3:A:277:ARG:HH12	3:A:336:GLN:H	1.46	0.62
3:A:215:THR:C	3:A:217:PRO:HD3	2.19	0.62
4:B:174:GLN:O	4:B:175:ASN:HB3	1.99	0.62
4:B:395:LYS:HG3	4:B:416:PHE:CE1	2.34	0.62
3:A:129:ALA:HA	3:A:145:GLN:HA	1.82	0.62
3:A:31:ILE:O	3:A:35:VAL:HG23	1.99	0.62
4:B:402:TRP:CH2	4:B:411:ILE:HD13	2.30	0.62
6:H:165:ASN:HB2	6:H:169:LEU:CD1	2.29	0.62
3:A:461:LYS:O	3:A:463:ARG:N	2.30	0.62
2:P:838:DA:H4'	3:A:183:TYR:CD2	2.35	0.62
4:B:166:LYS:O	4:B:170:PRO:HD3	1.99	0.61
6:H:148:LEU:HB2	6:H:191:VAL:HG23	1.82	0.61
3:A:362:THR:HG22	3:A:366:LYS:NZ	2.15	0.61
6:H:37:THR:HG23	6:H:52:THR:OG1	2.00	0.61
1:T:801:DA:C2'	1:T:802:DT:C7	2.77	0.61
3:A:279:LEU:HD12	3:A:279:LEU:N	2.10	0.61
4:B:387:PRO:HG2	4:B:389:PHE:HE1	1.59	0.61
3:A:294:PRO:C	3:A:296:THR:N	2.53	0.61
4:B:96:HIS:NE2	4:B:100:LEU:HD23	2.15	0.61
4:B:328:GLU:HB2	4:B:340:GLN:NE2	2.16	0.61
4:B:422:LEU:O	4:B:425:LEU:HD22	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:106:VAL:HG12	4:B:234:LEU:O	2.00	0.61
6:H:130:SER:HB3	6:H:153:LYS:O	1.99	0.61
4:B:421:PRO:HA	4:B:424:LYS:CB	2.31	0.61
5:L:4:MET:SD	5:L:25:ALA:HA	2.40	0.61
3:A:12:LEU:HD11	3:A:127:TYR:CZ	2.35	0.61
3:A:155:GLY:O	3:A:159:ILE:HG12	2.01	0.61
3:A:21:VAL:N	3:A:57:ASN:O	2.33	0.61
6:H:40:ARG:HH12	6:H:91:ASP:HA	1.63	0.61
6:H:146:VAL:O	6:H:192:THR:HA	2.00	0.61
5:L:169:LYS:HZ2	5:L:169:LYS:N	1.97	0.61
5:L:6:GLN:NE2	5:L:88:CYS:H	1.99	0.61
3:A:165:THR:HG23	3:A:182:GLN:HE22	1.65	0.61
6:H:10:GLY:HA2	6:H:118:SER:O	2.00	0.61
5:L:10:SER:HB3	5:L:103:LYS:HB2	1.80	0.61
3:A:363:ASN:OD1	3:A:365:VAL:HG23	2.00	0.61
5:L:89:GLN:HG3	5:L:98:PHE:CE1	2.35	0.61
6:H:39:ILE:HG23	6:H:48:GLU:O	2.00	0.61
5:L:150:ILE:HG23	5:L:191:SER:O	2.00	0.61
5:L:148:TRP:CE3	5:L:179:LEU:HD22	2.35	0.61
3:A:242:GLN:N	3:A:243:PRO:HD2	2.14	0.61
3:A:377:THR:HG22	3:A:378:GLU:N	2.16	0.61
5:L:150:ILE:HG21	5:L:189:ALA:HB1	1.83	0.61
3:A:53:GLU:O	3:A:55:PRO:HD3	2.00	0.61
6:H:165:ASN:HD21	6:H:203:VAL:HA	1.64	0.61
4:B:135:ILE:O	4:B:135:ILE:HG13	2.00	0.61
4:B:191:SER:H	4:B:198:HIS:CE1	2.18	0.60
4:B:328:GLU:C	4:B:329:ILE:HD12	2.21	0.60
6:H:219:LYS:HD2	6:H:219:LYS:C	2.21	0.60
1:T:804:DG:H8	1:T:804:DG:H5'	1.65	0.60
5:L:52:SER:HA	5:L:64:GLY:HA3	1.82	0.60
6:H:62:ASN:HD22	6:H:65:LEU:CG	2.13	0.60
6:H:162:VAL:HB	6:H:207:VAL:HA	1.82	0.60
4:B:395:LYS:HG3	4:B:416:PHE:HE1	1.64	0.60
4:B:326:ILE:HG13	4:B:342:TYR:O	2.02	0.60
3:A:119:PRO:HA	3:A:148:VAL:HG12	1.81	0.60
3:A:64:LYS:HG2	3:A:72:ARG:H	1.65	0.60
5:L:14:SER:O	5:L:78:LEU:HD12	2.01	0.60
4:B:167:ILE:O	4:B:170:PRO:HD2	2.01	0.60
4:B:323:LYS:HB2	4:B:343:GLN:NE2	2.17	0.60
6:H:161:THR:OG1	6:H:208:ALA:HB3	2.01	0.60
5:L:94:PHE:O	5:L:96:TRP:N	2.33	0.60
3:A:509:GLN:H	3:A:510:PRO:HD3	1.66	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:245:VAL:CB	4:B:427:TYR:HE1	2.15	0.60
5:L:105:GLU:HB2	5:L:166:GLN:OE1	2.01	0.60
4:B:171:PHE:CD1	4:B:205:LEU:HG	2.37	0.60
4:B:47:ILE:HG21	4:B:144:TYR:HD2	1.67	0.60
3:A:372:VAL:HA	3:A:375:ILE:HD12	1.84	0.60
5:L:12:SER:HA	5:L:105:GLU:O	2.01	0.60
4:B:285:GLY:O	4:B:287:LYS:N	2.34	0.60
4:B:319:TYR:CZ	4:B:383:TRP:HB3	2.37	0.60
4:B:36:GLU:O	4:B:39:THR:HG22	2.02	0.60
4:B:255:ASN:HB2	4:B:289:LEU:HD13	1.83	0.60
4:B:375:ILE:O	4:B:378:GLU:HB3	2.01	0.60
4:B:260:LEU:O	4:B:263:LYS:HB3	2.02	0.60
3:A:80:LEU:O	3:A:83:ARG:N	2.35	0.59
3:A:261:VAL:HA	3:A:264:LEU:HD12	1.82	0.59
3:A:279:LEU:CD1	3:A:279:LEU:H	2.07	0.59
4:B:230:MET:HE1	6:H:104:SER:HA	1.83	0.59
6:H:2:ILE:HD11	6:H:112:HIS:CE1	2.36	0.59
6:H:143:ASN:HD21	6:H:145:MET:HB2	1.65	0.59
3:A:122:GLU:HA	3:A:125:ARG:CD	2.31	0.59
4:B:58:THR:HG23	4:B:59:PRO:HD2	1.83	0.59
4:B:89:GLU:HA	4:B:92:LEU:HD23	1.84	0.59
3:A:188:TYR:HE2	3:A:234:LEU:HD11	1.66	0.59
5:L:141:PRO:HD2	5:L:198:HIS:NE2	2.17	0.59
4:B:202:ILE:HG22	4:B:203:GLU:N	2.17	0.59
3:A:329:ILE:HD11	3:A:392:PRO:HD2	1.85	0.59
5:L:3:GLN:HB3	5:L:26:SER:OG	2.02	0.59
3:A:50:ILE:HG22	3:A:145:GLN:HG2	1.84	0.59
1:T:806:DG:H2"	1:T:807:DC:OP2	2.02	0.59
4:B:50:ILE:HG21	4:B:145:GLN:OE1	2.02	0.59
4:B:423:VAL:C	4:B:425:LEU:H	2.04	0.59
5:L:148:TRP:O	5:L:155:ALA:HA	2.02	0.59
6:H:161:THR:O	6:H:208:ALA:N	2.33	0.59
5:L:11:LEU:HD11	5:L:19:VAL:HG11	1.84	0.59
3:A:202:ILE:O	3:A:205:LEU:HB3	2.03	0.59
2:P:828:DT:H2"	2:P:829:DT:O5'	2.03	0.59
3:A:453:GLY:O	3:A:469:LEU:HD12	2.02	0.59
4:B:266:TRP:HA	4:B:269:GLN:NE2	2.17	0.59
5:L:31:SER:O	5:L:50:TYR:HD1	1.85	0.59
3:A:472:THR:CA	3:A:476:LYS:HD2	2.33	0.59
6:H:164:TRP:HA	6:H:204:THR:O	2.03	0.59
4:B:125:ARG:O	4:B:127:TYR:N	2.36	0.59
6:H:24:PHE:CZ	6:H:78:ASN:HA	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:474:ASN:H	3:A:474:ASN:HD22	1.50	0.59
4:B:342:TYR:HA	4:B:349:LEU:HD13	1.83	0.59
4:B:399:GLU:O	4:B:401:TRP:N	2.36	0.59
4:B:106:VAL:O	4:B:234:LEU:HB3	2.03	0.59
4:B:336:GLN:HA	4:B:355:ALA:HA	1.83	0.59
4:B:301:LEU:HG	4:B:302:GLU:OE2	2.03	0.59
2:P:833:DG:N2	2:P:834:DC:C2	2.70	0.59
5:L:37:GLN:O	5:L:37:GLN:HG3	2.01	0.59
3:A:121:ASP:O	3:A:125:ARG:HG3	2.03	0.58
3:A:427:TYR:OH	3:A:510:PRO:HD2	2.02	0.58
5:L:6:GLN:HB2	5:L:100:GLY:O	2.03	0.58
6:H:18:PHE:CD2	6:H:87:VAL:HG21	2.38	0.58
4:B:98:ALA:O	4:B:100:LEU:N	2.36	0.58
4:B:98:ALA:O	4:B:101:LYS:HG2	2.04	0.58
3:A:402:TRP:HE3	4:B:331:LYS:HZ1	1.51	0.58
4:B:103:LYS:HA	4:B:192:ASP:OD2	2.03	0.58
4:B:395:LYS:HA	4:B:416:PHE:CE1	2.39	0.58
5:L:39:LYS:HG3	5:L:40:PRO:HD2	1.86	0.58
5:L:35:TRP:HB2	5:L:48:ILE:CG1	2.33	0.58
3:A:234:LEU:HD23	3:A:318:TYR:OH	2.04	0.58
1:T:805:DC:H2"	1:T:806:DG:C8	2.39	0.58
4:B:22:LYS:NZ	4:B:23:GLN:H	2.00	0.58
3:A:201:LYS:O	3:A:204:GLU:HB3	2.02	0.58
3:A:277:ARG:HB3	3:A:336:GLN:NE2	2.19	0.58
3:A:373:GLN:OE1	4:B:397:THR:HA	2.02	0.58
4:B:73:LYS:CD	4:B:151:GLN:HE21	2.17	0.58
3:A:442:VAL:HG12	3:A:443:ASP:N	2.18	0.58
4:B:207:GLN:O	4:B:210:LEU:HB2	2.04	0.58
5:L:20:THR:HG23	5:L:74:THR:OG1	2.03	0.58
4:B:195:ILE:CD1	4:B:199:ARG:HE	2.16	0.58
3:A:270:ILE:HD12	3:A:314:VAL:HG23	1.85	0.58
3:A:398:TRP:HH2	3:A:409:THR:HG22	1.68	0.58
3:A:506:ILE:N	3:A:506:ILE:HD13	2.19	0.58
3:A:358:ARG:HH12	4:B:394:GLN:HG3	1.69	0.58
3:A:532:TYR:CD2	3:A:533:LEU:N	2.72	0.58
3:A:441:TYR:CE2	3:A:544:GLY:N	2.72	0.58
4:B:247:PRO:CB	4:B:307:ARG:HH22	2.17	0.58
1:T:815:DG:H2"	1:T:816:DG:N7	2.18	0.57
4:B:369:THR:OG1	4:B:370:GLU:N	2.37	0.57
3:A:168:LEU:O	3:A:172:LYS:HG3	2.05	0.57
6:H:72:SER:OG	6:H:81:PHE:HD1	1.87	0.57
5:L:3:GLN:NE2	5:L:3:GLN:HA	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:96:HIS:HE2	4:B:100:LEU:HD23	1.70	0.57
3:A:377:THR:O	3:A:381:VAL:HG23	2.04	0.57
3:A:210:LEU:HA	3:A:214:LEU:O	2.03	0.57
4:B:357:MET:HB3	4:B:361:HIS:HE1	1.69	0.57
2:P:836:DC:H2"	2:P:837:DC:O5'	2.04	0.57
3:A:339:TYR:CD2	3:A:375:ILE:HG12	2.40	0.57
3:A:486:LEU:HB3	3:A:528:LYS:HZ1	1.69	0.57
5:L:186:TYR:HA	5:L:192:TYR:OH	2.03	0.57
5:L:120:PRO:HB2	5:L:125:LEU:HD21	1.86	0.57
1:T:801:DA:H2"	1:T:802:DT:C5	2.39	0.57
4:B:429:LEU:HD12	4:B:429:LEU:H	1.70	0.57
4:B:64:LYS:HB3	4:B:64:LYS:NZ	2.20	0.57
2:P:825:DC:C2'	2:P:826:DT:C5'	2.71	0.57
4:B:118:VAL:CG1	4:B:119:PRO:HD2	2.33	0.57
4:B:266:TRP:HA	4:B:269:GLN:HE21	1.69	0.57
5:L:117:ILE:HD12	5:L:194:CYS:HB2	1.87	0.57
6:H:218:LYS:HE2	6:H:219:LYS:NZ	2.20	0.57
3:A:246:LEU:HD11	3:A:307:ARG:HE	1.70	0.57
4:B:98:ALA:C	4:B:100:LEU:N	2.57	0.57
3:A:98:ALA:HB1	3:A:383:TRP:HZ2	1.70	0.57
1:T:803:DG:C5'	1:T:803:DG:C8	2.88	0.57
4:B:191:SER:OG	4:B:193:LEU:HG	2.04	0.57
3:A:531:VAL:HG12	3:A:532:TYR:N	2.19	0.57
2:P:823:DC:C3'	2:P:824:DC:H5"	2.33	0.57
4:B:27:THR:HG23	4:B:30:LYS:HG3	1.87	0.57
3:A:62:ALA:CA	3:A:73:LYS:HA	2.30	0.57
6:H:17:PRO:HB3	6:H:85:MET:HG3	1.85	0.57
4:B:163:SER:O	4:B:167:ILE:HG13	2.05	0.56
4:B:34:LEU:HD23	4:B:132:ILE:HG12	1.86	0.56
3:A:516:GLU:O	3:A:520:GLN:HG3	2.05	0.56
2:P:823:DC:C2	2:P:824:DC:C6	2.93	0.56
5:L:137:ASN:CA	5:L:174:SER:HB3	2.29	0.56
5:L:15:LEU:HA	5:L:78:LEU:HB2	1.87	0.56
4:B:342:TYR:HA	4:B:349:LEU:CD1	2.35	0.56
4:B:254:VAL:CG2	4:B:289:LEU:HA	2.35	0.56
6:H:143:ASN:OD1	6:H:144:SER:N	2.38	0.56
6:H:95:TYR:N	6:H:95:TYR:CD1	2.70	0.56
4:B:329:ILE:N	4:B:329:ILE:HD12	2.20	0.56
4:B:180:ILE:HA	4:B:188:TYR:O	2.05	0.56
3:A:106:VAL:HG12	3:A:107:THR:N	2.21	0.56
4:B:47:ILE:CD1	4:B:146:TYR:HA	2.36	0.56
6:H:163:THR:N	6:H:206:ASN:HD21	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:406:TRP:CZ2	4:B:410:TRP:O	2.58	0.56
5:L:2:ILE:HD11	5:L:93:LYS:HB3	1.86	0.56
6:H:169:LEU:N	6:H:169:LEU:HD12	2.21	0.56
4:B:369:THR:HG22	4:B:398:TRP:CH2	2.40	0.56
4:B:212:TRP:CD1	4:B:213:GLY:N	2.73	0.56
3:A:46:LYS:HD3	3:A:116:PHE:HD2	1.69	0.56
3:A:519:ASN:HA	3:A:522:ILE:HD12	1.85	0.56
4:B:406:TRP:HZ2	4:B:410:TRP:O	1.88	0.56
4:B:393:ILE:HD11	4:B:397:THR:CG2	2.34	0.56
4:B:113:ASP:O	4:B:116:PHE:HB2	2.06	0.56
6:H:218:LYS:HE2	6:H:219:LYS:HZ1	1.71	0.56
6:H:27:PHE:CD2	6:H:34:ILE:HG21	2.41	0.56
3:A:425:LEU:HD12	3:A:425:LEU:H	1.71	0.56
4:B:30:LYS:NZ	4:B:61:PHE:HD1	2.04	0.56
3:A:444:GLY:O	3:A:445:ALA:HB2	2.06	0.56
4:B:402:TRP:HH2	4:B:411:ILE:CD1	2.16	0.56
3:A:110:ASP:O	3:A:217:PRO:HD2	2.06	0.56
6:H:33:GLY:O	6:H:101:ALA:HA	2.06	0.56
3:A:470:THR:HG22	3:A:471:ASN:N	2.21	0.56
1:T:802:DT:H2"	1:T:803:DG:OP2	2.05	0.56
4:B:75:VAL:HG11	4:B:77:PHE:CZ	2.41	0.56
3:A:394:GLN:HG2	3:A:416:PHE:CE1	2.40	0.56
4:B:101:LYS:HE3	4:B:102:LYS:HE3	1.88	0.56
3:A:363:ASN:HA	3:A:511:ASP:H	1.68	0.55
3:A:515:SER:O	3:A:519:ASN:HB2	2.06	0.55
4:B:163:SER:HA	4:B:166:LYS:HE2	1.88	0.55
3:A:363:ASN:HB3	3:A:509:GLN:O	2.06	0.55
4:B:393:ILE:HG13	4:B:394:GLN:N	2.21	0.55
3:A:94:ILE:HG13	3:A:95:PRO:O	2.06	0.55
4:B:146:TYR:CD2	4:B:150:PRO:HA	2.40	0.55
5:L:113:PRO:HB3	5:L:139:PHE:CD2	2.42	0.55
3:A:101:LYS:N	3:A:101:LYS:HD2	2.12	0.55
6:H:92:THR:O	6:H:92:THR:HG23	2.07	0.55
3:A:171:PHE:CZ	3:A:205:LEU:HB2	2.42	0.55
5:L:85:THR:HA	5:L:102:THR:O	2.05	0.55
5:L:23:CYS:HB2	5:L:35:TRP:HH2	1.71	0.55
5:L:34:ASN:N	5:L:89:GLN:O	2.38	0.55
4:B:115:TYR:OH	4:B:157:PRO:HB3	2.06	0.55
5:L:166:GLN:HE21	5:L:171:SER:HB3	1.71	0.55
3:A:441:TYR:HE2	3:A:544:GLY:N	2.05	0.55
3:A:491:LEU:HD23	3:A:491:LEU:H	1.72	0.55
3:A:255:ASN:HA	3:A:258:GLN:HE21	1.72	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:171:PHE:CZ	4:B:201:LYS:HD2	2.41	0.55
4:B:155:GLY:O	4:B:158:ALA:HB3	2.06	0.55
6:H:31:THR:HB	6:H:34:ILE:CG1	2.35	0.55
5:L:50:TYR:CE2	6:H:106:THR:HB	2.42	0.55
6:H:32:SER:O	6:H:55:TRP:CE2	2.60	0.55
4:B:191:SER:H	4:B:198:HIS:HE1	1.54	0.55
2:P:823:DC:C2	2:P:824:DC:C5	2.94	0.55
3:A:180:ILE:CG2	3:A:187:LEU:HD22	2.36	0.55
6:H:27:PHE:HD2	6:H:34:ILE:HG21	1.72	0.55
5:L:34:ASN:OD1	5:L:49:TYR:HA	2.07	0.55
3:A:469:LEU:N	3:A:469:LEU:HD12	2.22	0.55
4:B:81:ASN:O	4:B:154:LYS:HE3	2.07	0.55
5:L:75:ILE:HD12	5:L:75:ILE:N	2.21	0.55
3:A:458:VAL:CG1	3:A:459:THR:H	2.13	0.55
4:B:16:MET:O	4:B:18:GLY:N	2.36	0.55
5:L:135:PHE:CE2	6:H:190:SER:HB3	2.42	0.55
4:B:423:VAL:C	4:B:425:LEU:N	2.61	0.55
6:H:53:ILE:HD12	6:H:80:ALA:HB1	1.89	0.55
4:B:228:LEU:HD23	4:B:232:TYR:HE1	1.70	0.54
3:A:178:ILE:N	3:A:178:ILE:HD12	2.22	0.54
5:L:107:LYS:HA	5:L:140:TYR:OH	2.07	0.54
5:L:187:GLU:HA	5:L:212:ASN:HB3	1.88	0.54
3:A:261:VAL:HG13	3:A:276:VAL:CG1	2.35	0.54
4:B:130:PHE:CZ	4:B:144:TYR:HB2	2.42	0.54
1:T:810:DG:C6	1:T:811:DA:N6	2.75	0.54
5:L:51:THR:CG2	5:L:71:TYR:HD2	2.20	0.54
3:A:63:ILE:HG23	3:A:63:ILE:O	2.06	0.54
4:B:107:THR:HG22	4:B:108:VAL:H	1.72	0.54
5:L:35:TRP:CZ3	5:L:88:CYS:HB2	2.42	0.54
4:B:16:MET:HB3	4:B:83:ARG:HD2	1.89	0.54
3:A:450:THR:C	3:A:452:LEU:H	2.11	0.54
4:B:32:LYS:O	4:B:35:VAL:HB	2.08	0.54
4:B:393:ILE:HD12	4:B:394:GLN:OE1	2.08	0.54
5:L:2:ILE:N	5:L:2:ILE:HD12	2.22	0.54
6:H:132:TYR:HD2	6:H:151:LEU:HD23	1.73	0.54
4:B:330:GLN:HB2	4:B:338:THR:OG1	2.07	0.54
3:A:99:GLY:HA2	3:A:383:TRP:NE1	2.22	0.54
3:A:219:LYS:N	3:A:219:LYS:HD2	2.22	0.54
4:B:115:TYR:CD1	4:B:156:SER:HB3	2.43	0.54
4:B:195:ILE:HG23	4:B:196:GLY:N	2.23	0.54
4:B:304:ALA:HA	4:B:307:ARG:HG3	1.90	0.54
3:A:502:ALA:O	3:A:506:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:H:150:CYS:O	6:H:188:SER:HA	2.07	0.54
3:A:317:VAL:HG22	3:A:318:TYR:H	1.72	0.54
3:A:246:LEU:N	3:A:246:LEU:HD23	2.22	0.54
6:H:59:ASN:OD1	6:H:61:TYR:HE1	1.91	0.54
4:B:23:GLN:NE2	4:B:26:LEU:HD11	2.22	0.54
4:B:33:ALA:O	4:B:37:ILE:HG22	2.07	0.54
6:H:69:LEU:HD11	6:H:82:LEU:HD21	1.89	0.54
4:B:68:SER:OG	4:B:219:LYS:NZ	2.38	0.54
5:L:186:TYR:HE2	5:L:213:GLU:O	1.90	0.54
3:A:380:ILE:O	3:A:384:GLY:N	2.39	0.54
4:B:195:ILE:HD11	4:B:233:GLU:HG3	1.90	0.54
2:P:830:DC:C4	2:P:831:DG:O6	2.61	0.53
4:B:143:ARG:C	4:B:144:TYR:HD1	2.11	0.53
4:B:236:PRO:O	4:B:238:LYS:N	2.42	0.53
4:B:266:TRP:CD1	4:B:269:GLN:NE2	2.70	0.53
3:A:377:THR:O	3:A:380:ILE:HB	2.08	0.53
4:B:47:ILE:HG21	4:B:144:TYR:HB3	1.91	0.53
4:B:22:LYS:CD	4:B:23:GLN:H	2.21	0.53
3:A:225:PRO:HA	3:A:236:PRO:HD3	1.91	0.53
3:A:41:MET:HB2	3:A:47:ILE:HD11	1.90	0.53
5:L:75:ILE:HD12	5:L:75:ILE:H	1.74	0.53
5:L:149:ALA:HA	5:L:154:ALA:O	2.08	0.53
2:P:831:DG:C2'	2:P:832:DG:H8	2.20	0.53
4:B:21:VAL:HG12	4:B:22:LYS:N	2.23	0.53
4:B:394:GLN:O	4:B:397:THR:HB	2.08	0.53
6:H:34:ILE:HG22	6:H:35:GLY:N	2.24	0.53
3:A:24:TRP:NE1	3:A:61:PHE:CZ	2.76	0.53
4:B:376:THR:O	4:B:380:ILE:HG13	2.09	0.53
3:A:16:MET:CE	3:A:16:MET:H	2.21	0.53
3:A:10:VAL:HG21	3:A:153:TRP:CZ2	2.43	0.53
6:H:2:ILE:CG2	6:H:26:GLY:HA3	2.37	0.53
4:B:64:LYS:HG3	4:B:71:TRP:CE2	2.43	0.53
3:A:41:MET:O	3:A:44:GLU:HB2	2.08	0.53
3:A:97:PRO:HG3	3:A:232:TYR:CD2	2.43	0.53
6:H:94:ILE:HA	6:H:117:THR:O	2.07	0.53
4:B:271:TYR:N	4:B:271:TYR:CD1	2.76	0.53
3:A:169:GLU:O	3:A:172:LYS:HB2	2.09	0.53
6:H:17:PRO:HB2	6:H:85:MET:HE3	1.89	0.53
2:P:825:DC:C4	2:P:826:DT:C4	2.97	0.53
5:L:79:GLU:O	5:L:81:GLU:N	2.41	0.53
6:H:128:PRO:HA	6:H:212:SER:OG	2.09	0.53
3:A:171:PHE:CD2	3:A:205:LEU:HD13	2.43	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:271:TYR:CE2	3:A:310:LEU:HD23	2.44	0.53
6:H:125:ALA:O	6:H:127:THR:HG23	2.09	0.53
3:A:505:ILE:O	3:A:510:PRO:HG2	2.08	0.53
2:P:833:DG:C2	2:P:834:DC:C2	2.97	0.53
4:B:47:ILE:HD13	4:B:146:TYR:HA	1.90	0.53
4:B:92:LEU:O	4:B:95:PRO:HG3	2.09	0.53
3:A:50:ILE:HD12	3:A:54:ASN:HB2	1.91	0.53
6:H:42:PRO:HB2	6:H:45:LYS:HB2	1.90	0.53
4:B:357:MET:HB3	4:B:361:HIS:CE1	2.43	0.53
4:B:235:HIS:ND1	4:B:235:HIS:N	2.56	0.53
4:B:254:VAL:HB	4:B:289:LEU:CA	2.35	0.52
4:B:224:GLU:HA	4:B:227:PHE:HE2	1.73	0.52
3:A:254:VAL:HG21	3:A:289:LEU:HA	1.91	0.52
3:A:378:GLU:O	3:A:382:ILE:HG12	2.09	0.52
4:B:229:TRP:HA	4:B:232:TYR:CD1	2.44	0.52
4:B:418:ASN:CG	4:B:419:THR:N	2.63	0.52
2:P:824:DC:H2"	2:P:825:DC:O5'	2.09	0.52
4:B:254:VAL:O	4:B:258:GLN:HB2	2.08	0.52
3:A:153:TRP:CE3	3:A:155:GLY:HA3	2.45	0.52
4:B:328:GLU:HB2	4:B:340:GLN:HE21	1.73	0.52
6:H:148:LEU:N	6:H:191:VAL:O	2.37	0.52
5:L:39:LYS:HB3	5:L:43:THR:OG1	2.09	0.52
6:H:72:SER:OG	6:H:81:PHE:CD1	2.62	0.52
3:A:11:LYS:O	3:A:85:GLN:HG2	2.09	0.52
2:P:830:DC:C2'	2:P:831:DG:H8	2.17	0.52
3:A:107:THR:HG22	3:A:108:VAL:N	2.25	0.52
4:B:203:GLU:O	4:B:206:ARG:HB2	2.10	0.52
6:H:160:VAL:HG13	6:H:160:VAL:O	2.10	0.52
3:A:87:PHE:HE1	3:A:155:GLY:HA2	1.73	0.52
3:A:482:ILE:O	3:A:486:LEU:HG	2.10	0.52
5:L:15:LEU:HD23	5:L:78:LEU:O	2.10	0.52
5:L:37:GLN:HG2	5:L:47:LEU:HD21	1.92	0.52
3:A:329:ILE:HD11	3:A:391:LEU:HA	1.92	0.52
4:B:406:TRP:CZ2	4:B:408:ALA:HB3	2.44	0.52
5:L:193:THR:HG22	5:L:194:CYS:N	2.23	0.52
3:A:167:ILE:N	3:A:167:ILE:HD12	2.25	0.52
4:B:178:ILE:HG22	4:B:179:VAL:N	2.25	0.52
4:B:47:ILE:HG21	4:B:144:TYR:CD2	2.44	0.52
3:A:459:THR:HG21	3:A:463:ARG:HB3	1.91	0.52
6:H:104:SER:OG	6:H:105:VAL:N	2.41	0.52
3:A:435:VAL:HA	4:B:290:THR:HG23	1.90	0.52
6:H:156:PHE:CB	6:H:157:PRO:HD3	2.37	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:H:173:VAL:HG22	6:H:191:VAL:HG12	1.92	0.52
3:A:533:LEU:HD12	3:A:534:ALA:N	2.25	0.52
5:L:149:ALA:HB1	5:L:153:SER:HA	1.91	0.52
2:P:828:DT:C6	2:P:829:DT:H72	2.45	0.52
6:H:66:LYS:HD3	6:H:67:SER:N	2.24	0.52
4:B:73:LYS:HD3	4:B:146:TYR:OH	2.10	0.52
3:A:465:LYS:HZ2	3:A:465:LYS:HB2	1.75	0.52
3:A:307:ARG:HG3	3:A:307:ARG:NH1	2.25	0.52
4:B:96:HIS:NE2	4:B:382:ILE:O	2.43	0.52
4:B:195:ILE:CG1	4:B:199:ARG:HE	2.23	0.52
3:A:241:VAL:C	3:A:243:PRO:HD2	2.31	0.52
6:H:94:ILE:HG22	6:H:96:TYR:CE1	2.45	0.52
6:H:165:ASN:HD22	6:H:169:LEU:HD11	1.75	0.51
4:B:369:THR:HA	4:B:398:TRP:HH2	1.75	0.51
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.93	0.51
5:L:191:SER:HB2	5:L:210:ASN:OD1	2.11	0.51
3:A:554:ALA:C	3:A:556:ILE:H	2.14	0.51
3:A:86:ASP:O	4:B:55:PRO:HB3	2.10	0.51
3:A:337:TRP:HE1	3:A:367:GLN:HB3	1.75	0.51
3:A:153:TRP:CH2	3:A:155:GLY:HA3	2.45	0.51
6:H:2:ILE:HG22	6:H:26:GLY:CA	2.40	0.51
4:B:101:LYS:HG3	4:B:102:LYS:HG3	1.92	0.51
4:B:160:PHE:CD2	4:B:164:MET:HB2	2.45	0.51
3:A:332:GLN:HB3	3:A:336:GLN:CB	2.39	0.51
3:A:447:ASN:HB3	3:A:450:THR:CG2	2.36	0.51
5:L:39:LYS:CG	5:L:40:PRO:HD2	2.40	0.51
3:A:170:PRO:O	3:A:174:GLN:HG2	2.09	0.51
3:A:277:ARG:HB3	3:A:336:GLN:HE21	1.75	0.51
5:L:33:LEU:CD2	5:L:88:CYS:SG	2.89	0.51
6:H:160:VAL:HG23	6:H:208:ALA:O	2.10	0.51
4:B:16:MET:HE2	4:B:83:ARG:HA	1.92	0.51
5:L:116:SER:O	5:L:134:CYS:HA	2.10	0.51
3:A:317:VAL:HG22	3:A:318:TYR:N	2.25	0.51
4:B:93:GLY:HA3	4:B:161:GLN:HG3	1.92	0.51
4:B:163:SER:O	4:B:166:LYS:HG3	2.11	0.51
3:A:403:THR:O	3:A:406:TRP:HZ3	1.93	0.51
3:A:193:LEU:HD13	3:A:197:GLN:HG3	1.93	0.51
3:A:328:GLU:HB3	3:A:390:LYS:HB2	1.92	0.51
5:L:134:CYS:SG	5:L:136:LEU:HD21	2.50	0.51
3:A:556:ILE:HG12	3:A:557:ARG:N	2.26	0.51
3:A:523:GLU:HA	3:A:526:ILE:HB	1.91	0.51
3:A:438:GLU:OE1	3:A:463:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:287:LYS:HG3	4:B:288:ALA:H	1.75	0.51
3:A:155:GLY:C	3:A:157:PRO:HD2	2.32	0.51
6:H:1:GLN:HG2	6:H:2:ILE:CD1	2.40	0.51
3:A:408:ALA:HA	4:B:364:ASP:OD2	2.11	0.51
3:A:326:ILE:N	3:A:326:ILE:HD12	2.26	0.51
3:A:270:ILE:HA	3:A:351:THR:HG23	1.93	0.51
6:H:165:ASN:ND2	6:H:203:VAL:HA	2.25	0.51
2:P:829:DT:C2	2:P:830:DC:C2	2.99	0.51
2:P:829:DT:O2	2:P:830:DC:C2	2.64	0.51
3:A:459:THR:HG22	3:A:463:ARG:HB3	1.91	0.51
4:B:16:MET:CE	4:B:83:ARG:HA	2.41	0.51
3:A:395:LYS:HD2	3:A:395:LYS:N	2.26	0.51
3:A:113:ASP:OD1	3:A:116:PHE:HB2	2.11	0.51
4:B:279:LEU:HD23	4:B:299:ALA:HB1	1.93	0.51
2:P:830:DC:C2'	2:P:831:DG:N7	2.73	0.50
4:B:178:ILE:HG12	4:B:191:SER:HB2	1.93	0.50
3:A:453:GLY:O	3:A:468:PRO:HA	2.11	0.50
4:B:206:ARG:HH22	4:B:219:LYS:HG3	1.75	0.50
4:B:402:TRP:CE2	4:B:414:TRP:HH2	2.28	0.50
3:A:120:LEU:HD21	3:A:128:THR:HG21	1.92	0.50
3:A:128:THR:OG1	3:A:146:TYR:HB2	2.11	0.50
3:A:120:LEU:N	3:A:148:VAL:HA	2.26	0.50
3:A:473:THR:H	3:A:476:LYS:HB2	1.76	0.50
4:B:160:PHE:CD2	4:B:160:PHE:O	2.64	0.50
6:H:132:TYR:CD2	6:H:151:LEU:HD23	2.46	0.50
5:L:150:ILE:O	5:L:151:ASP:C	2.49	0.50
6:H:53:ILE:HG21	6:H:73:LYS:HG2	1.91	0.50
3:A:323:LYS:HB3	3:A:343:GLN:NE2	2.27	0.50
2:P:825:DC:N3	2:P:826:DT:C4	2.79	0.50
3:A:88:TRP:CZ3	4:B:57:ASN:HB3	2.47	0.50
3:A:532:TYR:C	3:A:532:TYR:CD2	2.84	0.50
1:T:812:DA:C4	1:T:813:DC:C5	2.99	0.50
6:H:207:VAL:HG12	6:H:208:ALA:N	2.25	0.50
3:A:337:TRP:CH2	3:A:368:LEU:HB2	2.46	0.50
3:A:480:GLN:HE22	3:A:483:TYR:HD2	1.59	0.50
4:B:23:GLN:OE1	4:B:59:PRO:HA	2.12	0.50
3:A:419:THR:OG1	3:A:420:PRO:HD3	2.11	0.50
4:B:328:GLU:OE2	4:B:430:GLU:HG2	2.11	0.50
3:A:47:ILE:HG22	3:A:145:GLN:O	2.11	0.50
2:P:834:DC:OP2	2:P:834:DC:H2'	2.12	0.50
1:T:818:DA:C2	2:P:822:DT:O2	2.60	0.50
1:T:809:DC:H2"	1:T:810:DG:O5'	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:H:206:ASN:O	6:H:206:ASN:ND2	2.45	0.50
5:L:198:HIS:C	5:L:200:THR:H	2.13	0.50
5:L:1:ASP:CA	5:L:95:PRO:HB2	2.42	0.50
4:B:332:GLN:OE1	4:B:424:LYS:HA	2.12	0.50
3:A:194:GLU:O	3:A:197:GLN:N	2.45	0.50
3:A:523:GLU:O	3:A:526:ILE:HB	2.11	0.50
2:P:831:DG:C4	2:P:832:DG:C8	3.00	0.50
4:B:30:LYS:HG2	4:B:62:ALA:HB3	1.93	0.50
3:A:354:TYR:CZ	3:A:356:ARG:HB3	2.46	0.50
4:B:223:LYS:HE2	6:H:60:ARG:HH22	1.76	0.50
4:B:127:TYR:N	4:B:127:TYR:CD2	2.75	0.50
5:L:133:VAL:HG11	6:H:134:LEU:HD13	1.93	0.50
6:H:22:CYS:HB2	6:H:38:TRP:CH2	2.46	0.50
3:A:242:GLN:C	3:A:244:ILE:H	2.15	0.50
4:B:104:LYS:HD3	4:B:192:ASP:OD1	2.12	0.50
3:A:438:GLU:HG2	3:A:461:LYS:CE	2.42	0.50
3:A:255:ASN:HA	3:A:258:GLN:NE2	2.26	0.50
6:H:175:THR:HG23	6:H:189:SER:HB2	1.94	0.50
4:B:67:ASP:HA	4:B:221:HIS:HB2	1.94	0.49
3:A:433:PRO:HB2	3:A:494:ASN:HD21	1.76	0.49
3:A:329:ILE:HG22	3:A:339:TYR:CB	2.37	0.49
3:A:182:GLN:HA	3:A:187:LEU:HD23	1.93	0.49
3:A:491:LEU:O	3:A:529:GLU:HB3	2.11	0.49
5:L:48:ILE:CG2	5:L:54:LEU:HA	2.37	0.49
6:H:198:TRP:HZ2	6:H:220:ILE:HG12	1.77	0.49
4:B:386:THR:CG2	4:B:412:PRO:HB3	2.42	0.49
6:H:94:ILE:HG22	6:H:116:GLY:HA3	1.93	0.49
3:A:170:PRO:O	3:A:173:LYS:HB2	2.12	0.49
1:T:805:DC:H2"	1:T:806:DG:H8	1.77	0.49
6:H:95:TYR:N	6:H:95:TYR:HD1	2.10	0.49
3:A:354:TYR:OH	3:A:370:GLU:HB3	2.12	0.49
3:A:480:GLN:NE2	3:A:483:TYR:HB3	2.27	0.49
4:B:90:VAL:O	4:B:94:ILE:N	2.45	0.49
3:A:139:THR:HB	3:A:140:PRO:HD3	1.95	0.49
1:T:802:DT:O5'	1:T:802:DT:H6	1.95	0.49
3:A:83:ARG:HH11	3:A:83:ARG:HG2	1.78	0.49
4:B:348:ASN:HD21	4:B:429:LEU:HB3	1.76	0.49
4:B:78:ARG:CZ	4:B:411:ILE:HG22	2.42	0.49
3:A:392:PRO:O	3:A:393:ILE:HB	2.13	0.49
4:B:115:TYR:CE1	4:B:156:SER:HB3	2.47	0.49
3:A:382:ILE:HB	3:A:383:TRP:CE3	2.47	0.49
3:A:171:PHE:CE2	3:A:205:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:L:9:SER:O	5:L:102:THR:HA	2.12	0.49
6:H:56:ASP:O	6:H:57:ASP:HB3	2.12	0.49
3:A:394:GLN:O	3:A:397:THR:OG1	2.30	0.49
4:B:153:TRP:CH2	4:B:155:GLY:HA3	2.48	0.49
6:H:147:THR:HA	6:H:191:VAL:O	2.12	0.49
5:L:190:ASN:HA	5:L:212:ASN:OD1	2.11	0.49
5:L:170:ASP:O	5:L:172:THR:HG23	2.12	0.49
4:B:225:PRO:HB2	4:B:226:PRO:HD2	1.94	0.49
4:B:266:TRP:CH2	4:B:423:VAL:HG22	2.47	0.49
6:H:148:LEU:HB2	6:H:191:VAL:CG2	2.43	0.49
1:T:815:DG:N2	1:T:816:DG:C2	2.81	0.49
3:A:348:ASN:HD22	3:A:349:LEU:N	2.10	0.49
3:A:269:GLN:O	3:A:350:LYS:HG2	2.11	0.49
2:P:833:DG:O5'	2:P:833:DG:H2'	2.12	0.49
2:P:832:DG:C2	2:P:833:DG:O6	2.65	0.49
6:H:49:TRP:HZ3	6:H:62:ASN:HA	1.78	0.49
5:L:35:TRP:HB2	5:L:48:ILE:HG13	1.94	0.49
1:T:810:DG:C2'	1:T:811:DA:C8	2.91	0.49
6:H:2:ILE:HD11	6:H:112:HIS:NE2	2.28	0.49
3:A:5:ILE:HD12	3:A:6:GLU:N	2.28	0.49
3:A:131:THR:HG23	3:A:143:ARG:HD2	1.93	0.49
3:A:329:ILE:CD1	3:A:391:LEU:HA	2.42	0.49
3:A:7:THR:HG21	3:A:121:ASP:HA	1.94	0.49
6:H:176:PHE:HD1	6:H:188:SER:O	1.95	0.49
4:B:112:GLY:O	4:B:114:ALA:N	2.46	0.49
4:B:3:SER:OG	4:B:5:ILE:HG13	2.13	0.49
3:A:277:ARG:HA	3:A:280:SER:HB2	1.94	0.49
4:B:201:LYS:O	4:B:204:GLU:HB2	2.13	0.49
4:B:58:THR:CG2	4:B:59:PRO:HD2	2.43	0.49
4:B:162:SER:OG	4:B:163:SER:N	2.45	0.49
4:B:164:MET:HA	4:B:167:ILE:HD12	1.94	0.49
6:H:146:VAL:C	6:H:192:THR:HG23	2.33	0.49
3:A:295:LEU:O	3:A:298:GLU:N	2.46	0.49
2:P:837:DC:C1'	2:P:838:DA:H5'	2.43	0.48
3:A:106:VAL:HG12	3:A:107:THR:H	1.76	0.48
3:A:442:VAL:HG12	3:A:481:ALA:HB1	1.95	0.48
3:A:420:PRO:O	3:A:422:LEU:N	2.46	0.48
6:H:73:LYS:HA	6:H:80:ALA:HA	1.95	0.48
4:B:178:ILE:CD1	4:B:201:LYS:HG2	2.44	0.48
3:A:408:ALA:O	4:B:393:ILE:HD12	2.12	0.48
6:H:27:PHE:HD1	6:H:27:PHE:H	1.60	0.48
3:A:46:LYS:HD3	3:A:116:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:522:ILE:O	3:A:526:ILE:HG13	2.14	0.48
2:P:831:DG:C2	2:P:832:DG:C4	3.01	0.48
2:P:831:DG:N1	2:P:832:DG:C6	2.80	0.48
4:B:368:LEU:HD11	4:B:391:LEU:CD2	2.43	0.48
3:A:484:LEU:O	3:A:487:GLN:N	2.46	0.48
5:L:49:TYR:CD2	5:L:49:TYR:N	2.82	0.48
4:B:62:ALA:C	4:B:63:ILE:HG22	2.34	0.48
4:B:83:ARG:NH1	4:B:83:ARG:HG2	2.26	0.48
5:L:133:VAL:HG22	5:L:134:CYS:N	2.28	0.48
2:P:837:DC:H1'	2:P:838:DA:H5'	1.96	0.48
4:B:254:VAL:HG21	4:B:289:LEU:HA	1.94	0.48
4:B:98:ALA:C	4:B:100:LEU:H	2.16	0.48
4:B:122:GLU:HA	4:B:125:ARG:HE	1.79	0.48
4:B:34:LEU:HG	4:B:132:ILE:HD11	1.95	0.48
5:L:118:PHE:HA	5:L:119:PRO:HD3	1.72	0.48
2:P:821:DG:C2'	2:P:822:DT:C7	2.81	0.48
2:P:831:DG:C2'	2:P:832:DG:C8	2.97	0.48
3:A:112:GLY:HA3	3:A:217:PRO:HG2	1.95	0.48
3:A:98:ALA:HB1	3:A:383:TRP:CZ2	2.47	0.48
6:H:72:SER:HG	6:H:81:PHE:HD1	1.61	0.48
2:P:831:DG:C2	2:P:832:DG:C5	3.01	0.48
5:L:167:ASP:C	5:L:169:LYS:H	2.17	0.48
5:L:6:GLN:OE1	5:L:101:GLY:HA2	2.14	0.48
3:A:146:TYR:CE2	3:A:150:PRO:HA	2.49	0.48
6:H:34:ILE:HG22	6:H:35:GLY:H	1.77	0.48
3:A:271:TYR:CE1	3:A:314:VAL:HG22	2.49	0.48
4:B:388:LYS:N	4:B:388:LYS:HD3	2.29	0.48
2:P:823:DC:C2'	2:P:824:DC:C5'	2.68	0.48
3:A:18:GLY:HA3	3:A:56:TYR:CD2	2.48	0.48
3:A:459:THR:HG21	3:A:463:ARG:HE	1.79	0.48
3:A:88:TRP:CH2	4:B:21:VAL:O	2.66	0.48
3:A:325:LEU:HB3	3:A:387:PRO:CB	2.43	0.48
3:A:242:GLN:O	3:A:244:ILE:N	2.47	0.48
5:L:115:VAL:HG13	5:L:136:LEU:CD2	2.44	0.48
5:L:124:GLN:HE21	6:H:153:LYS:NZ	2.11	0.48
6:H:37:THR:HG22	6:H:38:TRP:N	2.28	0.48
1:T:804:DG:H2"	1:T:805:DC:C5'	2.43	0.47
1:T:804:DG:C2	1:T:805:DC:N3	2.82	0.47
3:A:277:ARG:CZ	3:A:336:GLN:HG2	2.44	0.47
6:H:195:SER:O	6:H:196:SER:C	2.50	0.47
3:A:465:LYS:HG3	3:A:466:VAL:N	2.29	0.47
5:L:51:THR:O	5:L:51:THR:HG22	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:194:GLU:O	3:A:196:GLY:N	2.47	0.47
4:B:339:TYR:CZ	4:B:352:GLY:HA3	2.49	0.47
4:B:88:TRP:HE1	4:B:92:LEU:HD22	1.78	0.47
6:H:173:VAL:HG12	6:H:174:HIS:N	2.29	0.47
2:P:831:DG:C6	2:P:832:DG:O6	2.68	0.47
6:H:163:THR:CA	6:H:206:ASN:HD21	2.28	0.47
3:A:498:ASP:HA	3:A:536:VAL:O	2.14	0.47
3:A:229:TRP:CE3	3:A:234:LEU:HD12	2.48	0.47
3:A:304:ALA:O	3:A:307:ARG:HB2	2.15	0.47
4:B:223:LYS:HG2	4:B:224:GLU:H	1.79	0.47
4:B:120:LEU:HB3	4:B:147:ASN:O	2.14	0.47
3:A:24:TRP:CD1	3:A:24:TRP:N	2.81	0.47
3:A:366:LYS:O	3:A:369:THR:HB	2.14	0.47
4:B:68:SER:HG	4:B:219:LYS:HB2	1.80	0.47
4:B:402:TRP:CZ2	4:B:414:TRP:HH2	2.32	0.47
4:B:123:ASP:O	4:B:125:ARG:N	2.47	0.47
4:B:229:TRP:HA	4:B:232:TYR:CG	2.50	0.47
3:A:420:PRO:CB	3:A:421:PRO:HD2	2.42	0.47
6:H:131:VAL:HA	6:H:151:LEU:O	2.14	0.47
1:T:804:DG:C8	1:T:804:DG:H5'	2.48	0.47
3:A:20:LYS:CG	3:A:56:TYR:HD2	2.28	0.47
6:H:65:LEU:O	6:H:66:LYS:C	2.52	0.47
4:B:193:LEU:HD23	4:B:193:LEU:N	2.29	0.47
4:B:50:ILE:CD1	4:B:145:GLN:HG3	2.31	0.47
4:B:73:LYS:HD3	4:B:151:GLN:HE21	1.77	0.47
4:B:369:THR:O	4:B:372:VAL:CG2	2.62	0.47
5:L:198:HIS:O	5:L:200:THR:N	2.40	0.47
4:B:88:TRP:CD1	4:B:89:GLU:N	2.83	0.47
3:A:503:LEU:CD1	3:A:535:TRP:HB2	2.45	0.47
4:B:425:LEU:C	4:B:427:TYR:N	2.67	0.47
3:A:550:LYS:HA	3:A:553:SER:O	2.15	0.47
3:A:333:GLY:H	3:A:336:GLN:CB	1.94	0.47
3:A:536:VAL:HG12	3:A:542:ILE:HD13	1.97	0.47
3:A:354:TYR:OH	3:A:356:ARG:HB3	2.15	0.47
3:A:508:ALA:O	3:A:509:GLN:HB2	2.15	0.47
6:H:11:ILE:HG12	6:H:120:THR:OG1	2.15	0.47
3:A:122:GLU:O	3:A:125:ARG:HB2	2.15	0.47
4:B:22:LYS:HD2	4:B:23:GLN:H	1.80	0.47
4:B:169:GLU:O	4:B:172:LYS:HG3	2.15	0.47
6:H:155:TYR:CE1	6:H:185:TYR:HB2	2.49	0.47
4:B:365:VAL:O	4:B:368:LEU:N	2.48	0.47
5:L:116:SER:O	5:L:135:PHE:N	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:395:LYS:O	4:B:396:GLU:C	2.53	0.47
4:B:225:PRO:HB2	4:B:226:PRO:HD3	1.96	0.47
4:B:121:ASP:O	4:B:125:ARG:HG3	2.14	0.47
4:B:107:THR:HG22	4:B:108:VAL:N	2.29	0.47
6:H:96:TYR:N	6:H:96:TYR:CD1	2.84	0.47
2:P:823:DC:O2	2:P:824:DC:C6	2.67	0.46
2:P:826:DT:OP1	3:A:361:HIS:NE2	2.45	0.46
6:H:164:TRP:HB2	6:H:169:LEU:HB2	1.97	0.46
6:H:104:SER:HB3	6:H:107:ASP:OD2	2.16	0.46
4:B:115:TYR:HB3	4:B:149:LEU:CB	2.42	0.46
4:B:266:TRP:CZ2	4:B:423:VAL:HG22	2.51	0.46
6:H:148:LEU:HD22	6:H:148:LEU:N	2.30	0.46
5:L:98:PHE:CD2	6:H:47:LEU:HB3	2.51	0.46
3:A:88:TRP:HH2	4:B:21:VAL:O	1.99	0.46
3:A:408:ALA:HB2	4:B:337:TRP:CH2	2.50	0.46
3:A:410:TRP:CH2	3:A:412:PRO:HA	2.50	0.46
4:B:263:LYS:HE3	4:B:425:LEU:O	2.14	0.46
2:P:822:DT:C2'	2:P:823:DC:H5	2.27	0.46
4:B:391:LEU:HD23	4:B:392:PRO:HD2	1.97	0.46
4:B:254:VAL:HG22	4:B:294:PRO:HG2	1.97	0.46
3:A:294:PRO:O	3:A:296:THR:N	2.48	0.46
3:A:81:ASN:OD1	3:A:154:LYS:HG2	2.15	0.46
3:A:420:PRO:O	3:A:422:LEU:HD23	2.15	0.46
3:A:395:LYS:HE2	3:A:416:PHE:HB2	1.97	0.46
3:A:47:ILE:HD12	3:A:144:TYR:CD2	2.50	0.46
2:P:825:DC:C4	2:P:826:DT:O4	2.68	0.46
4:B:191:SER:CB	4:B:193:LEU:HG	2.45	0.46
4:B:131:THR:HG23	4:B:143:ARG:HG2	1.96	0.46
4:B:73:LYS:HZ2	4:B:146:TYR:HE1	1.62	0.46
6:H:92:THR:HG1	6:H:120:THR:HA	1.77	0.46
3:A:150:PRO:HG2	3:A:153:TRP:CB	2.46	0.46
4:B:106:VAL:N	4:B:234:LEU:O	2.45	0.46
3:A:171:PHE:HB2	3:A:208:HIS:HD2	1.80	0.46
1:T:803:DG:C2	1:T:804:DG:C5	3.04	0.46
4:B:23:GLN:HE21	4:B:26:LEU:HD11	1.81	0.46
3:A:420:PRO:HB2	3:A:421:PRO:CD	2.44	0.46
4:B:224:GLU:O	4:B:227:PHE:CE2	2.68	0.46
3:A:385:LYS:HG2	3:A:386:THR:N	2.31	0.46
4:B:404:GLU:HB2	4:B:405:TYR:CE2	2.50	0.46
2:P:833:DG:N3	2:P:834:DC:C6	2.83	0.46
3:A:261:VAL:HA	3:A:264:LEU:CD1	2.45	0.46
4:B:42:GLU:HA	4:B:47:ILE:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:L:195:ALA:HA	5:L:206:VAL:HG22	1.96	0.46
6:H:55:TRP:CG	6:H:56:ASP:N	2.84	0.46
2:P:835:DG:H2"	2:P:836:DC:O5'	2.16	0.46
3:A:276:VAL:HG12	3:A:280:SER:OG	2.16	0.46
4:B:367:GLN:O	4:B:371:ALA:N	2.44	0.46
3:A:439:THR:HA	3:A:494:ASN:HB2	1.98	0.46
5:L:120:PRO:CB	5:L:125:LEU:HD21	2.45	0.46
3:A:231:GLY:O	3:A:241:VAL:HG12	2.16	0.46
6:H:61:TYR:OH	6:H:71:VAL:HG22	2.16	0.46
3:A:8:VAL:O	3:A:121:ASP:HB2	2.16	0.46
4:B:160:PHE:HD2	4:B:164:MET:HB2	1.81	0.46
4:B:122:GLU:HA	4:B:125:ARG:NE	2.31	0.46
5:L:160:LEU:O	5:L:178:THR:N	2.46	0.46
4:B:118:VAL:O	4:B:148:VAL:HG12	2.15	0.46
6:H:37:THR:O	6:H:97:CYS:HA	2.15	0.46
4:B:69:THR:CG2	4:B:70:LYS:N	2.79	0.46
1:T:805:DC:H5"	3:A:93:GLY:HA2	1.98	0.45
4:B:272:PRO:HG2	4:B:273:GLY:H	1.80	0.45
3:A:439:THR:OG1	3:A:439:THR:O	2.31	0.45
5:L:193:THR:HG23	5:L:208:SER:OG	2.15	0.45
5:L:167:ASP:O	5:L:169:LYS:N	2.49	0.45
4:B:350:LYS:HG2	4:B:351:THR:N	2.31	0.45
3:A:427:TYR:HE1	3:A:522:ILE:HG23	1.81	0.45
3:A:542:ILE:CD1	3:A:542:ILE:N	2.77	0.45
3:A:483:TYR:O	3:A:486:LEU:HB2	2.17	0.45
5:L:12:SER:HB3	5:L:105:GLU:CG	2.44	0.45
5:L:10:SER:CB	5:L:103:LYS:HB2	2.44	0.45
5:L:31:SER:HB2	5:L:50:TYR:HE1	1.80	0.45
3:A:188:TYR:HE2	3:A:234:LEU:CD1	2.28	0.45
3:A:163:SER:O	3:A:167:ILE:HD13	2.16	0.45
3:A:390:LYS:HB3	3:A:417:VAL:HG21	1.98	0.45
5:L:98:PHE:HD2	6:H:47:LEU:O	2.00	0.45
3:A:101:LYS:NZ	3:A:181:TYR:OH	2.49	0.45
4:B:170:PRO:O	4:B:174:GLN:HB2	2.17	0.45
3:A:470:THR:O	3:A:471:ASN:HB2	2.15	0.45
4:B:404:GLU:HB2	4:B:405:TYR:CD2	2.52	0.45
4:B:52:PRO:O	4:B:54:ASN:N	2.50	0.45
5:L:28:ASP:HA	5:L:68:GLY:O	2.16	0.45
3:A:522:ILE:HG22	3:A:526:ILE:HD11	1.99	0.45
6:H:95:TYR:H	6:H:95:TYR:HD1	1.65	0.45
4:B:377:THR:O	4:B:381:VAL:HG23	2.17	0.45
3:A:266:TRP:O	3:A:269:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:274:ILE:CG2	3:A:275:LYS:N	2.79	0.45
1:T:815:DG:C2	1:T:816:DG:C6	3.05	0.45
5:L:33:LEU:HA	5:L:89:GLN:O	2.17	0.45
5:L:17:ASP:O	5:L:78:LEU:HG	2.16	0.45
4:B:29:GLU:CG	4:B:71:TRP:HH2	2.27	0.45
6:H:145:MET:SD	6:H:194:PRO:HA	2.56	0.45
4:B:208:HIS:ND1	4:B:208:HIS:C	2.69	0.45
3:A:107:THR:HG23	3:A:221:HIS:O	2.16	0.45
4:B:368:LEU:HD11	4:B:391:LEU:HD22	1.99	0.45
4:B:88:TRP:CD1	4:B:92:LEU:HD22	2.52	0.45
4:B:385:LYS:CD	4:B:385:LYS:N	2.76	0.45
3:A:361:HIS:CD2	3:A:505:ILE:HG23	2.52	0.45
3:A:354:TYR:CD1	3:A:371:ALA:HA	2.52	0.45
3:A:486:LEU:HD22	3:A:528:LYS:NZ	2.32	0.45
3:A:206:ARG:CG	3:A:216:THR:HG21	2.44	0.45
4:B:195:ILE:HG13	4:B:199:ARG:HE	1.81	0.45
3:A:267:ALA:HB1	3:A:271:TYR:HD2	1.81	0.45
2:P:833:DG:C4	2:P:834:DC:C5	3.05	0.45
5:L:139:PHE:CE2	5:L:174:SER:HA	2.52	0.45
4:B:113:ASP:O	4:B:116:PHE:N	2.47	0.45
6:H:6:GLU:CD	6:H:6:GLU:H	2.20	0.45
3:A:425:LEU:HD12	3:A:425:LEU:N	2.31	0.45
4:B:376:THR:O	4:B:379:SER:N	2.50	0.45
5:L:142:LYS:HE2	5:L:142:LYS:O	2.17	0.45
4:B:66:LYS:O	4:B:67:ASP:HB3	2.16	0.44
5:L:108:ARG:HB3	5:L:140:TYR:CD1	2.52	0.44
3:A:450:THR:C	3:A:452:LEU:N	2.71	0.44
4:B:378:GLU:O	4:B:382:ILE:HG12	2.17	0.44
2:P:825:DC:H2'	2:P:826:DT:C7	2.47	0.44
1:T:815:DG:N3	1:T:816:DG:C5	2.84	0.44
4:B:221:HIS:O	4:B:222:GLN:HG3	2.17	0.44
1:T:811:DA:H1'	1:T:812:DA:O5'	2.17	0.44
5:L:108:ARG:HB3	5:L:140:TYR:CE1	2.53	0.44
3:A:146:TYR:HE2	3:A:150:PRO:HA	1.81	0.44
4:B:88:TRP:HD1	4:B:89:GLU:HG3	1.83	0.44
4:B:224:GLU:O	4:B:227:PHE:CZ	2.70	0.44
3:A:116:PHE:HZ	3:A:151:GLN:OE1	1.99	0.44
6:H:69:LEU:HD12	6:H:83:ASN:O	2.17	0.44
1:T:818:DA:H1'	1:T:819:DC:C6	2.52	0.44
4:B:326:ILE:O	4:B:341:ILE:HA	2.16	0.44
4:B:369:THR:O	4:B:370:GLU:C	2.56	0.44
4:B:369:THR:O	4:B:372:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:88:TRP:CD1	3:A:89:GLU:O	2.70	0.44
5:L:84:ALA:O	5:L:86:TYR:CD1	2.70	0.44
3:A:533:LEU:HD12	3:A:534:ALA:H	1.83	0.44
4:B:279:LEU:CD2	4:B:299:ALA:HB1	2.47	0.44
4:B:286:THR:HG22	4:B:286:THR:O	2.17	0.44
6:H:155:TYR:CE2	6:H:160:VAL:HG11	2.53	0.44
4:B:271:TYR:H	4:B:271:TYR:HD1	1.65	0.44
3:A:470:THR:CG2	3:A:471:ASN:N	2.81	0.44
6:H:216:VAL:HG22	6:H:217:ASP:N	2.32	0.44
2:P:830:DC:H2"	2:P:831:DG:H8	1.76	0.44
6:H:121:VAL:O	6:H:122:SER:HB2	2.17	0.44
4:B:236:PRO:O	4:B:237:ASP:C	2.56	0.44
3:A:50:ILE:CG2	3:A:145:GLN:HG2	2.47	0.44
6:H:38:TRP:CZ3	6:H:97:CYS:HB3	2.52	0.44
3:A:492:GLU:O	3:A:493:VAL:HB	2.18	0.44
6:H:96:TYR:N	6:H:96:TYR:HD1	2.16	0.44
5:L:122:SER:O	5:L:126:THR:HG23	2.17	0.44
5:L:18:ARG:HA	5:L:76:SER:O	2.17	0.44
4:B:222:GLN:HA	4:B:229:TRP:CD1	2.52	0.44
4:B:74:LEU:HA	4:B:74:LEU:HD23	1.59	0.44
4:B:79:GLU:CD	4:B:83:ARG:HH12	2.21	0.44
3:A:10:VAL:HG21	3:A:153:TRP:HZ2	1.80	0.44
4:B:22:LYS:NZ	4:B:23:GLN:O	2.51	0.44
6:H:132:TYR:HE2	6:H:153:LYS:HD3	1.82	0.44
2:P:822:DT:H2'	2:P:823:DC:H5	1.83	0.44
1:T:814:DA:H2"	1:T:815:DG:C8	2.53	0.44
3:A:79:GLU:O	3:A:82:LYS:HB3	2.18	0.44
4:B:130:PHE:O	4:B:143:ARG:HB3	2.18	0.44
4:B:230:MET:HE1	6:H:103:THR:O	2.16	0.44
3:A:87:PHE:CZ	3:A:155:GLY:HA2	2.53	0.44
3:A:418:ASN:O	3:A:419:THR:HG23	2.18	0.44
6:H:27:PHE:CD1	6:H:27:PHE:N	2.80	0.44
5:L:169:LYS:HD3	5:L:169:LYS:HA	1.65	0.44
6:H:21:THR:HG23	6:H:81:PHE:CD2	2.53	0.44
6:H:115:GLN:HG2	6:H:115:GLN:O	2.17	0.44
2:P:838:DA:C1'	3:A:184:ILE:HD12	2.40	0.44
4:B:257:ILE:HG13	4:B:258:GLN:H	1.79	0.44
4:B:289:LEU:HD12	4:B:290:THR:N	2.32	0.44
3:A:154:LYS:C	3:A:157:PRO:HD2	2.38	0.44
4:B:406:TRP:CG	4:B:407:GLN:N	2.85	0.44
4:B:12:LEU:HA	4:B:85:GLN:H	1.83	0.44
2:P:838:DA:C4'	3:A:183:TYR:CE2	3.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:818:DA:H2"	1:T:819:DC:C5	2.53	0.44
3:A:463:ARG:O	3:A:464:GLN:HG3	2.18	0.44
4:B:22:LYS:HZ1	4:B:23:GLN:HB3	1.83	0.44
6:H:78:ASN:OD1	6:H:78:ASN:N	2.51	0.44
6:H:81:PHE:N	6:H:81:PHE:CD1	2.86	0.44
3:A:521:ILE:O	3:A:525:LEU:HD22	2.18	0.43
3:A:368:LEU:HD21	3:A:391:LEU:HB3	2.00	0.43
4:B:359:GLY:C	4:B:361:HIS:H	2.21	0.43
2:P:827:DG:C2'	2:P:828:DT:O5'	2.57	0.43
4:B:103:LYS:NZ	4:B:192:ASP:N	2.57	0.43
6:H:9:PRO:C	6:H:11:ILE:H	2.21	0.43
4:B:18:GLY:HA3	4:B:56:TYR:CE1	2.53	0.43
4:B:78:ARG:NH1	4:B:412:PRO:O	2.51	0.43
4:B:395:LYS:O	4:B:397:THR:N	2.51	0.43
3:A:406:TRP:HA	4:B:331:LYS:HD3	1.99	0.43
6:H:209:HIS:CE1	6:H:212:SER:H	2.36	0.43
5:L:10:SER:HB3	5:L:103:LYS:HD3	1.99	0.43
2:P:832:DG:C2	2:P:833:DG:C6	3.06	0.43
3:A:20:LYS:HG2	3:A:56:TYR:HD2	1.83	0.43
3:A:339:TYR:CE1	3:A:352:GLY:CA	3.01	0.43
4:B:58:THR:HG22	4:B:59:PRO:N	2.32	0.43
4:B:135:ILE:O	4:B:137:ASN:N	2.52	0.43
5:L:38:GLN:HG3	5:L:43:THR:O	2.18	0.43
6:H:114:GLY:O	6:H:115:GLN:C	2.57	0.43
4:B:152:GLY:HA2	4:B:184:ILE:HG22	1.99	0.43
3:A:2:ILE:CG2	3:A:3:SER:N	2.80	0.43
4:B:72:ARG:HG3	4:B:72:ARG:HH11	1.83	0.43
4:B:104:LYS:HB2	4:B:192:ASP:CA	2.48	0.43
3:A:453:GLY:O	3:A:469:LEU:N	2.42	0.43
3:A:348:ASN:ND2	3:A:349:LEU:H	2.15	0.43
6:H:6:GLU:HG3	6:H:97:CYS:SG	2.58	0.43
3:A:171:PHE:CE2	3:A:205:LEU:HB2	2.53	0.43
3:A:427:TYR:CE1	3:A:522:ILE:HG23	2.53	0.43
5:L:23:CYS:HB2	5:L:35:TRP:CZ2	2.54	0.43
6:H:91:ASP:O	6:H:95:TYR:OH	2.28	0.43
3:A:482:ILE:HG22	3:A:486:LEU:CD1	2.44	0.43
3:A:182:GLN:HG2	4:B:139:THR:HG22	1.99	0.43
3:A:225:PRO:HB2	3:A:226:PRO:CD	2.47	0.43
4:B:224:GLU:CD	5:L:96:TRP:HZ2	2.22	0.43
3:A:255:ASN:O	3:A:259:LYS:N	2.48	0.43
5:L:61:ALA:O	5:L:75:ILE:HA	2.17	0.43
3:A:262:GLY:HA2	3:A:265:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:463:ARG:CG	3:A:464:GLN:N	2.82	0.43
3:A:175:ASN:CB	3:A:178:ILE:HD13	2.46	0.43
3:A:408:ALA:HB2	4:B:337:TRP:HH2	1.82	0.43
4:B:260:LEU:HD21	4:B:264:LEU:HD23	2.00	0.43
4:B:126:LYS:HG3	4:B:127:TYR:CD2	2.54	0.43
3:A:239:TRP:CD1	3:A:316:GLY:O	2.71	0.43
3:A:427:TYR:CZ	3:A:525:LEU:HD23	2.53	0.43
4:B:65:LYS:HE3	4:B:220:LYS:HE3	2.01	0.43
5:L:160:LEU:O	5:L:177:SER:HA	2.19	0.43
6:H:89:THR:O	6:H:90:ALA:C	2.57	0.43
5:L:2:ILE:HD12	5:L:2:ILE:H	1.83	0.43
4:B:152:GLY:HA2	4:B:184:ILE:CG2	2.48	0.43
4:B:78:ARG:CZ	4:B:411:ILE:CG2	2.96	0.43
5:L:193:THR:CG2	5:L:206:VAL:HG13	2.49	0.43
3:A:402:TRP:HE3	4:B:331:LYS:NZ	2.15	0.43
2:P:837:DC:C4'	3:A:230:MET:CE	2.93	0.43
3:A:19:PRO:CG	3:A:80:LEU:HD23	2.48	0.43
4:B:130:PHE:N	4:B:130:PHE:CD1	2.87	0.43
4:B:326:ILE:HD12	4:B:342:TYR:CE1	2.54	0.43
6:H:158:GLU:HA	6:H:185:TYR:CD2	2.52	0.43
5:L:115:VAL:HG13	5:L:136:LEU:HD22	2.01	0.43
6:H:176:PHE:CD1	6:H:176:PHE:N	2.86	0.43
4:B:163:SER:HA	4:B:166:LYS:CE	2.49	0.43
3:A:500:GLN:OE1	4:B:421:PRO:HD2	2.19	0.43
4:B:125:ARG:C	4:B:127:TYR:N	2.72	0.43
5:L:211:ALA:HB1	5:L:213:GLU:OE1	2.18	0.43
6:H:146:VAL:O	6:H:192:THR:HG23	2.19	0.43
3:A:219:LYS:N	3:A:219:LYS:CD	2.82	0.43
6:H:29:LEU:HD23	6:H:29:LEU:HA	1.74	0.43
3:A:56:TYR:CE1	3:A:127:TYR:CE1	3.07	0.43
3:A:57:ASN:OD1	3:A:58:THR:N	2.51	0.43
4:B:229:TRP:HA	4:B:232:TYR:CE1	2.53	0.43
5:L:80:PRO:HG2	5:L:81:GLU:OE2	2.19	0.43
3:A:354:TYR:CE2	3:A:356:ARG:HB3	2.54	0.43
3:A:443:ASP:HB2	3:A:548:VAL:CG1	2.49	0.43
5:L:166:GLN:NE2	5:L:171:SER:HB3	2.32	0.43
4:B:376:THR:O	4:B:377:THR:C	2.56	0.43
3:A:512:LYS:O	3:A:513:SER:HB2	2.19	0.43
4:B:63:ILE:O	4:B:65:LYS:N	2.52	0.42
4:B:114:ALA:HB1	4:B:160:PHE:CZ	2.53	0.42
5:L:124:GLN:HG3	6:H:132:TYR:CZ	2.53	0.42
3:A:17:ASP:O	3:A:83:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:H:14:PRO:HG3	6:H:121:VAL:CG1	2.36	0.42
3:A:393:ILE:HG13	3:A:423:VAL:O	2.19	0.42
4:B:148:VAL:HB	4:B:149:LEU:H	1.52	0.42
3:A:443:ASP:HB2	3:A:548:VAL:HG11	2.01	0.42
3:A:353:LYS:HD3	3:A:353:LYS:C	2.40	0.42
6:H:210:PRO:HG2	6:H:211:ALA:H	1.83	0.42
3:A:161:GLN:O	3:A:162:SER:C	2.57	0.42
3:A:277:ARG:NH1	3:A:336:GLN:HG2	2.34	0.42
4:B:104:LYS:H	4:B:192:ASP:HA	1.84	0.42
3:A:458:VAL:HA	3:A:464:GLN:HA	2.00	0.42
4:B:21:VAL:CG1	4:B:22:LYS:N	2.81	0.42
3:A:410:TRP:CD2	4:B:363:ASN:ND2	2.87	0.42
3:A:380:ILE:HD13	3:A:380:ILE:HA	1.83	0.42
3:A:179:VAL:O	3:A:189:VAL:HA	2.19	0.42
3:A:424:LYS:HE2	3:A:426:TRP:CE3	2.54	0.42
2:P:835:DG:H2"	2:P:836:DC:OP2	2.19	0.42
3:A:222:GLN:O	3:A:224:GLU:N	2.52	0.42
5:L:84:ALA:O	5:L:86:TYR:HD1	2.03	0.42
5:L:31:SER:HB2	5:L:50:TYR:CE1	2.55	0.42
6:H:32:SER:O	6:H:55:TRP:NE1	2.52	0.42
1:T:818:DA:H2"	1:T:819:DC:C6	2.55	0.42
3:A:19:PRO:O	3:A:57:ASN:N	2.53	0.42
3:A:279:LEU:CD1	3:A:279:LEU:N	2.79	0.42
3:A:59:PRO:O	3:A:75:VAL:HG13	2.19	0.42
3:A:90:VAL:O	3:A:91:GLN:CG	2.63	0.42
4:B:328:GLU:CD	4:B:430:GLU:HG2	2.40	0.42
4:B:245:VAL:CB	4:B:427:TYR:CE1	3.00	0.42
3:A:491:LEU:O	3:A:492:GLU:HG3	2.20	0.42
3:A:114:ALA:O	3:A:117:SER:HB2	2.19	0.42
3:A:218:ASP:C	3:A:220:LYS:H	2.22	0.42
2:P:831:DG:C4	2:P:832:DG:C5	3.08	0.42
5:L:113:PRO:HB3	5:L:139:PHE:HD2	1.83	0.42
3:A:459:THR:HG23	3:A:461:LYS:HB2	2.02	0.42
4:B:161:GLN:NE2	4:B:165:THR:HG21	2.35	0.42
5:L:86:TYR:CE1	5:L:104:LEU:HD23	2.55	0.42
4:B:126:LYS:HG3	4:B:127:TYR:CE2	2.55	0.42
5:L:179:LEU:HA	5:L:179:LEU:HD12	1.70	0.42
3:A:84:THR:HG22	3:A:85:GLN:N	2.35	0.42
3:A:274:ILE:HG22	3:A:275:LYS:N	2.34	0.42
4:B:72:ARG:CG	4:B:72:ARG:HH11	2.33	0.42
3:A:401:TRP:CZ2	3:A:405:TYR:CD2	3.07	0.42
3:A:523:GLU:HA	3:A:526:ILE:CD1	2.44	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:835:DG:H1'	2:P:836:DC:O5'	2.19	0.42
1:T:803:DG:C2'	1:T:804:DG:H5"	2.43	0.42
4:B:73:LYS:HD2	4:B:151:GLN:NE2	2.35	0.42
6:H:87:VAL:HG13	6:H:91:ASP:HB2	2.01	0.42
4:B:202:ILE:HD13	4:B:202:ILE:HA	1.92	0.42
4:B:203:GLU:HA	4:B:206:ARG:HD3	2.02	0.42
3:A:410:TRP:CE3	4:B:363:ASN:ND2	2.88	0.42
5:L:166:GLN:HB2	5:L:173:TYR:OH	2.20	0.42
3:A:64:LYS:HG2	3:A:72:ARG:N	2.33	0.42
6:H:61:TYR:HB2	6:H:66:LYS:HB2	2.02	0.42
3:A:156:SER:HB2	3:A:157:PRO:CD	2.46	0.42
3:A:165:THR:HG23	3:A:182:GLN:NE2	2.34	0.42
3:A:64:LYS:HG2	3:A:71:TRP:HA	2.00	0.42
2:P:829:DT:H2'	2:P:830:DC:C6	2.53	0.42
6:H:198:TRP:HB3	6:H:199:PRO:HD3	2.01	0.42
4:B:258:GLN:O	4:B:259:LYS:C	2.58	0.42
3:A:473:THR:OG1	3:A:476:LYS:HG3	2.20	0.42
4:B:121:ASP:OD2	4:B:123:ASP:N	2.53	0.42
5:L:167:ASP:C	5:L:169:LYS:N	2.73	0.42
2:P:827:DG:P	3:A:360:ALA:H	2.43	0.42
2:P:828:DT:H2'	2:P:829:DT:C7	2.49	0.42
6:H:162:VAL:HB	6:H:207:VAL:HG22	2.02	0.42
4:B:289:LEU:HD12	4:B:289:LEU:C	2.40	0.42
4:B:253:THR:HB	4:B:292:VAL:O	2.19	0.42
4:B:115:TYR:HE1	4:B:156:SER:C	2.23	0.42
6:H:152:VAL:N	6:H:187:LEU:O	2.39	0.42
5:L:203:SER:HA	5:L:204:PRO:HD3	1.64	0.42
5:L:121:SER:O	5:L:125:LEU:HG	2.20	0.42
5:L:122:SER:OG	5:L:123:GLU:N	2.53	0.42
1:T:805:DC:C5'	3:A:93:GLY:HA2	2.50	0.41
3:A:261:VAL:O	3:A:264:LEU:HB2	2.20	0.41
3:A:221:HIS:NE2	3:A:228:LEU:HB3	2.35	0.41
3:A:450:THR:O	3:A:451:LYS:HB2	2.20	0.41
3:A:155:GLY:O	3:A:156:SER:C	2.59	0.41
4:B:22:LYS:HZ3	4:B:23:GLN:CA	2.33	0.41
4:B:180:ILE:CG1	4:B:189:VAL:HG22	2.48	0.41
3:A:254:VAL:CG2	3:A:289:LEU:HA	2.50	0.41
3:A:474:ASN:HD22	3:A:474:ASN:N	2.16	0.41
3:A:519:ASN:HA	3:A:522:ILE:CD1	2.50	0.41
2:P:833:DG:O5'	2:P:833:DG:C2'	2.67	0.41
1:T:816:DG:H1	2:P:824:DC:H42	1.68	0.41
4:B:94:ILE:N	4:B:95:PRO:HD3	2.34	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:180:ILE:HA	3:A:188:TYR:O	2.19	0.41
3:A:412:PRO:HD3	4:B:401:TRP:CZ2	2.56	0.41
5:L:19:VAL:HG12	5:L:20:THR:N	2.35	0.41
4:B:424:LYS:C	4:B:426:TRP:N	2.69	0.41
4:B:224:GLU:OE2	5:L:96:TRP:HZ2	2.03	0.41
3:A:376:THR:O	3:A:377:THR:C	2.58	0.41
3:A:60:VAL:HG22	3:A:61:PHE:N	2.35	0.41
1:T:804:DG:N2	1:T:805:DC:O2	2.53	0.41
4:B:387:PRO:HG2	4:B:389:PHE:CZ	2.54	0.41
3:A:329:ILE:HD13	3:A:329:ILE:N	2.26	0.41
6:H:2:ILE:HD11	6:H:112:HIS:CD2	2.55	0.41
3:A:97:PRO:O	3:A:100:LEU:HB3	2.20	0.41
3:A:139:THR:N	3:A:140:PRO:CD	2.84	0.41
1:T:803:DG:N3	1:T:804:DG:C8	2.88	0.41
3:A:12:LEU:HD11	3:A:127:TYR:CE1	2.55	0.41
5:L:35:TRP:CH2	5:L:88:CYS:HB2	2.56	0.41
4:B:326:ILE:O	4:B:341:ILE:HG23	2.20	0.41
6:H:88:GLU:O	6:H:89:THR:C	2.58	0.41
3:A:149:LEU:HA	3:A:150:PRO:HD2	1.79	0.41
4:B:97:PRO:O	4:B:100:LEU:HB3	2.20	0.41
4:B:223:LYS:HE2	6:H:60:ARG:NH2	2.35	0.41
3:A:61:PHE:N	3:A:61:PHE:CD1	2.87	0.41
3:A:426:TRP:CE3	3:A:426:TRP:HA	2.56	0.41
5:L:106:ILE:HG22	5:L:107:LYS:N	2.35	0.41
4:B:202:ILE:CG2	4:B:203:GLU:N	2.84	0.41
5:L:55:HIS:O	5:L:58:VAL:HG23	2.20	0.41
3:A:329:ILE:HD11	3:A:392:PRO:CD	2.50	0.41
3:A:339:TYR:CE1	3:A:352:GLY:N	2.88	0.41
4:B:153:TRP:O	4:B:154:LYS:C	2.58	0.41
6:H:181:GLN:N	6:H:184:LEU:O	2.53	0.41
3:A:377:THR:CG2	3:A:378:GLU:N	2.83	0.41
3:A:517:LEU:O	3:A:520:GLN:HB2	2.19	0.41
3:A:312:GLU:HA	3:A:313:PRO:HD3	1.83	0.41
6:H:141:GLN:OE1	6:H:199:PRO:HG2	2.20	0.41
5:L:198:HIS:C	5:L:200:THR:N	2.73	0.41
3:A:371:ALA:O	3:A:375:ILE:HG13	2.21	0.41
3:A:10:VAL:HG23	3:A:87:PHE:HE2	1.85	0.41
4:B:124:PHE:CZ	4:B:153:TRP:CZ2	3.09	0.41
3:A:457:TYR:CD2	3:A:457:TYR:N	2.88	0.41
6:H:176:PHE:O	6:H:187:LEU:HG	2.20	0.41
4:B:97:PRO:HG2	4:B:100:LEU:HD22	2.02	0.41
4:B:266:TRP:CZ2	4:B:346:PHE:HE2	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:L:193:THR:CG2	5:L:194:CYS:N	2.83	0.41
3:A:167:ILE:N	3:A:167:ILE:CD1	2.83	0.41
4:B:258:GLN:NE2	4:B:283:LEU:HD21	2.35	0.41
4:B:96:HIS:CE1	4:B:382:ILE:O	2.73	0.41
5:L:204:PRO:O	5:L:206:VAL:HG23	2.20	0.41
4:B:223:LYS:CE	6:H:60:ARG:HH22	2.33	0.41
3:A:522:ILE:O	3:A:525:LEU:HB2	2.20	0.41
3:A:125:ARG:NH2	3:A:147:ASN:O	2.54	0.41
3:A:503:LEU:HD23	3:A:504:GLY:N	2.36	0.41
4:B:8:VAL:HA	4:B:9:PRO:HD3	1.80	0.41
1:T:802:DT:C2'	1:T:803:DG:OP2	2.69	0.41
4:B:205:LEU:O	4:B:205:LEU:HD23	2.21	0.41
4:B:61:PHE:O	4:B:74:LEU:HB2	2.20	0.41
4:B:365:VAL:O	4:B:366:LYS:C	2.58	0.41
3:A:119:PRO:HA	3:A:148:VAL:HA	2.03	0.41
4:B:406:TRP:O	4:B:407:GLN:OE1	2.39	0.41
4:B:89:GLU:HA	4:B:92:LEU:CD2	2.51	0.41
3:A:188:TYR:C	3:A:188:TYR:CD1	2.94	0.41
4:B:113:ASP:O	4:B:114:ALA:C	2.59	0.41
4:B:227:PHE:CZ	6:H:108:SER:HB2	2.55	0.41
4:B:319:TYR:HE2	4:B:321:PRO:HG3	1.80	0.41
3:A:325:LEU:HD11	3:A:383:TRP:CE3	2.56	0.41
3:A:362:THR:HG22	3:A:366:LYS:HZ2	1.83	0.41
6:H:39:ILE:HD11	6:H:110:MET:CE	2.51	0.41
3:A:171:PHE:HB2	3:A:208:HIS:CD2	2.54	0.41
3:A:454:LYS:CA	3:A:468:PRO:HA	2.39	0.41
4:B:31:ILE:O	4:B:32:LYS:C	2.59	0.41
4:B:88:TRP:O	4:B:92:LEU:HB3	2.21	0.41
3:A:307:ARG:CG	3:A:307:ARG:NH1	2.84	0.41
4:B:99:GLY:HA2	4:B:102:LYS:HD2	2.03	0.41
4:B:224:GLU:OE1	6:H:102:ILE:HD11	2.21	0.41
3:A:376:THR:HB	3:A:377:THR:H	1.73	0.41
6:H:41:GLN:HA	6:H:42:PRO:HD3	1.67	0.41
4:B:288:ALA:O	4:B:292:VAL:CB	2.69	0.40
3:A:372:VAL:HG13	3:A:389:PHE:CZ	2.56	0.40
5:L:205:ILE:H	5:L:205:ILE:CD1	2.19	0.40
3:A:75:VAL:HG12	3:A:76:ASP:N	2.35	0.40
4:B:46:LYS:C	4:B:147:ASN:HD22	2.24	0.40
3:A:442:VAL:CG1	3:A:481:ALA:HB1	2.50	0.40
4:B:266:TRP:CA	4:B:269:GLN:HE21	2.34	0.40
3:A:324:ASP:N	3:A:343:GLN:HE21	2.19	0.40
3:A:60:VAL:CG2	3:A:61:PHE:N	2.83	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:265:ASN:O	3:A:268:SER:OG	2.39	0.40
3:A:427:TYR:CE2	3:A:525:LEU:HD23	2.57	0.40
4:B:222:GLN:HE21	4:B:222:GLN:HB2	1.62	0.40
3:A:461:LYS:C	3:A:463:ARG:H	2.21	0.40
5:L:2:ILE:HD11	5:L:93:LYS:CB	2.49	0.40
4:B:260:LEU:HD23	4:B:260:LEU:C	2.42	0.40
3:A:209:LEU:O	3:A:214:LEU:HB2	2.20	0.40
4:B:12:LEU:HA	4:B:84:THR:HA	2.03	0.40
2:P:834:DC:C2	2:P:835:DG:N7	2.89	0.40
3:A:260:LEU:HD11	3:A:264:LEU:HD21	2.03	0.40
3:A:433:PRO:CB	4:B:289:LEU:HD11	2.52	0.40
5:L:58:VAL:HA	5:L:59:PRO:HD3	1.91	0.40
4:B:22:LYS:NZ	4:B:23:GLN:N	2.60	0.40
4:B:236:PRO:HA	4:B:239:TRP:CE2	2.56	0.40
3:A:131:THR:HA	3:A:142:ILE:O	2.21	0.40
1:T:817:DG:H2"	1:T:818:DA:C5'	2.35	0.40
3:A:30:LYS:O	3:A:33:ALA:HB3	2.22	0.40
4:B:363:ASN:O	4:B:364:ASP:C	2.60	0.40
5:L:11:LEU:HD23	5:L:11:LEU:N	2.36	0.40
4:B:64:LYS:HB2	4:B:71:TRP:CZ3	2.56	0.40
5:L:84:ALA:O	5:L:104:LEU:HB3	2.21	0.40
5:L:39:LYS:O	5:L:42:GLY:N	2.54	0.40
4:B:207:GLN:O	4:B:211:ARG:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	
3	A	556/558 (100%)	394 (71%)	121 (22%)	41 (7%)	2	24
4	B	428/430 (100%)	284 (66%)	96 (22%)	48 (11%)	1	13
5	L	212/214 (99%)	162 (76%)	35 (16%)	15 (7%)	2	25
6	H	218/220 (99%)	160 (73%)	42 (19%)	16 (7%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1414/1422 (99%)	1000 (71%)	294 (21%)	120 (8%)	1	20

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	63	ILE
3	A	66	LYS
3	A	136	ASN
3	A	195	ILE
3	A	223	LYS
3	A	251	SER
3	A	273	GLY
3	A	294	PRO
3	A	345	PRO
3	A	358	ARG
4	B	12	LEU
4	B	63	ILE
4	B	85	GLN
4	B	213	GLY
4	B	225	PRO
4	B	227	PHE
4	B	237	ASP
4	B	242	GLN
4	B	247	PRO
4	B	286	THR
4	B	332	GLN
4	B	395	LYS
4	B	400	THR
5	L	80	PRO
5	L	110	ASP
5	L	153	SER
6	H	180	LEU
3	A	91	GLN
3	A	114	ALA
3	A	137	ASN
3	A	184	ILE
3	A	252	TRP
3	A	376	THR
3	A	393	ILE
3	A	462	GLY
3	A	465	LYS
3	A	493	VAL

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Mol	Chain	Res	Type
3	A	513	SER
3	A	528	LYS
4	B	53	GLU
4	B	64	LYS
4	B	113	ASP
4	B	126	LYS
4	B	245	VAL
4	B	251	SER
4	B	382	ILE
4	B	396	GLU
4	B	399	GLU
4	B	426	TRP
4	B	429	LEU
5	L	101	GLY
5	L	138	ASN
6	H	76	SER
6	H	89	THR
6	H	116	GLY
3	A	128	THR
3	A	284	ARG
3	A	295	LEU
3	A	419	THR
3	A	445	ALA
3	A	484	LEU
3	A	539	HIS
4	B	17	ASP
4	B	70	LYS
4	B	124	PHE
4	B	153	TRP
4	B	160	PHE
4	B	175	ASN
4	B	358	ARG
5	L	52	SER
5	L	61	ALA
5	L	151	ASP
5	L	156	ALA
5	L	168	SER
6	H	115	GLN
6	H	124	ALA
6	H	126	THR
3	A	77	PHE
3	A	243	PRO

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Mol	Chain	Res	Type
3	A	244	ILE
4	B	99	GLY
4	B	119	PRO
4	B	136	ASN
4	B	184	ILE
4	B	272	PRO
4	B	360	ALA
5	L	199	LYS
6	H	17	PRO
6	H	105	VAL
6	H	160	VAL
6	H	213	SER
3	A	164	MET
3	A	177	ASP
4	B	20	LYS
4	B	148	VAL
4	B	317	VAL
4	B	404	GLU
5	L	68	GLY
5	L	144	ILE
6	H	90	ALA
3	A	156	SER
3	A	157	PRO
3	A	433	PRO
4	B	195	ILE
4	B	316	GLY
4	B	364	ASP
5	L	171	SER
6	H	26	GLY
6	H	66	LYS
6	H	156	PHE
4	B	236	PRO
3	A	10	VAL
3	A	490	GLY
4	B	133	PRO
5	L	94	PHE
3	A	261	VAL
4	B	90	VAL
3	A	541	GLY
4	B	294	PRO
6	H	44	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	434/498 (87%)	364 (84%)	70 (16%)	3	22
4	B	350/392 (89%)	290 (83%)	60 (17%)	3	18
5	L	182/182 (100%)	148 (81%)	34 (19%)	2	13
6	H	191/191 (100%)	168 (88%)	23 (12%)	7	37
All	All	1157/1263 (92%)	970 (84%)	187 (16%)	3	21

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LYS
3	A	16	MET
3	A	22	LYS
3	A	24	TRP
3	A	26	LEU
3	A	58	THR
3	A	87	PHE
3	A	89	GLU
3	A	94	ILE
3	A	101	LYS
3	A	110	ASP
3	A	147	ASN
3	A	157	PRO
3	A	162	SER
3	A	164	MET
3	A	165	THR
3	A	175	ASN
3	A	177	ASP
3	A	188	TYR
3	A	204	GLU
3	A	208	HIS
3	A	228	LEU
3	A	230	MET
3	A	234	LEU
3	A	237	ASP
3	A	240	THR

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Mol	Chain	Res	Type
3	A	246	LEU
3	A	256	ASP
3	A	279	LEU
3	A	307	ARG
3	A	310	LEU
3	A	326	ILE
3	A	329	ILE
3	A	339	TYR
3	A	341	ILE
3	A	345	PRO
3	A	348	ASN
3	A	349	LEU
3	A	353	LYS
3	A	364	ASP
3	A	365	VAL
3	A	377	THR
3	A	382	ILE
3	A	395	LYS
3	A	405	TYR
3	A	406	TRP
3	A	410	TRP
3	A	419	THR
3	A	420	PRO
3	A	424	LYS
3	A	425	LEU
3	A	429	LEU
3	A	439	THR
3	A	443	ASP
3	A	452	LEU
3	A	457	TYR
3	A	465	LYS
3	A	469	LEU
3	A	475	GLN
3	A	479	LEU
3	A	492	GLU
3	A	497	THR
3	A	500	GLN
3	A	506	ILE
3	A	507	GLN
3	A	512	LYS
3	A	518	VAL
3	A	525	LEU

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Mol	Chain	Res	Type
3	A	532	TYR
3	A	542	ILE
4	B	2	ILE
4	B	8	VAL
4	B	11	LYS
4	B	12	LEU
4	B	27	THR
4	B	36	GLU
4	B	42	GLU
4	B	50	ILE
4	B	52	PRO
4	B	63	ILE
4	B	64	LYS
4	B	67	ASP
4	B	70	LYS
4	B	72	ARG
4	B	73	LYS
4	B	88	TRP
4	B	92	LEU
4	B	104	LYS
4	B	108	VAL
4	B	109	LEU
4	B	131	THR
4	B	143	ARG
4	B	148	VAL
4	B	159	ILE
4	B	163	SER
4	B	166	LYS
4	B	174	GLN
4	B	175	ASN
4	B	179	VAL
4	B	191	SER
4	B	192	ASP
4	B	193	LEU
4	B	202	ILE
4	B	207	GLN
4	B	211	ARG
4	B	218	ASP
4	B	219	LYS
4	B	222	GLN
4	B	228	LEU
4	B	235	HIS

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Mol	Chain	Res	Type
4	B	255	ASN
4	B	256	ASP
4	B	264	LEU
4	B	271	TYR
4	B	279	LEU
4	B	289	LEU
4	B	326	ILE
4	B	330	GLN
4	B	348	ASN
4	B	356	ARG
4	B	364	ASP
4	B	365	VAL
4	B	377	THR
4	B	383	TRP
4	B	385	LYS
4	B	396	GLU
4	B	419	THR
4	B	422	LEU
4	B	425	LEU
4	B	427	TYR
5	L	3	GLN
5	L	8	THR
5	L	15	LEU
5	L	18	ARG
5	L	33	LEU
5	L	37	GLN
5	L	39	LYS
5	L	48	ILE
5	L	49	TYR
5	L	50	TYR
5	L	60	SER
5	L	75	ILE
5	L	77	ASN
5	L	90	GLN
5	L	91	TYR
5	L	97	THR
5	L	108	ARG
5	L	110	ASP
5	L	136	LEU
5	L	137	ASN
5	L	142	LYS
5	L	161	ASN

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Mol	Chain	Res	Type
5	L	165	ASP
5	L	168	SER
5	L	169	LYS
5	L	174	SER
5	L	175	MET
5	L	180	THR
5	L	185	GLU
5	L	187	GLU
5	L	197	THR
5	L	208	SER
5	L	210	ASN
5	L	214	CYS
6	H	2	ILE
6	H	4	LEU
6	H	6	GLU
6	H	13	GLN
6	H	59	ASN
6	H	66	LYS
6	H	68	ARG
6	H	73	LYS
6	H	81	PHE
6	H	85	MET
6	H	86	THR
6	H	95	TYR
6	H	96	TYR
6	H	100	SER
6	H	107	ASP
6	H	150	CYS
6	H	162	VAL
6	H	176	PHE
6	H	184	LEU
6	H	196	SER
6	H	205	CYS
6	H	206	ASN
6	H	219	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	147	ASN
3	A	175	ASN
3	A	182	GLN

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Mol	Chain	Res	Type
3	A	198	HIS
3	A	258	GLN
3	A	269	GLN
3	A	330	GLN
3	A	348	ASN
3	A	407	GLN
3	A	428	GLN
3	A	474	ASN
3	A	475	GLN
3	A	480	GLN
3	A	494	ASN
4	B	136	ASN
4	B	151	GLN
4	B	207	GLN
4	B	221	HIS
4	B	222	GLN
4	B	258	GLN
4	B	306	ASN
4	B	330	GLN
4	B	340	GLN
5	L	3	GLN
5	L	6	GLN
5	L	37	GLN
5	L	38	GLN
5	L	77	ASN
5	L	124	GLN
5	L	145	ASN
5	L	210	ASN
6	H	1	GLN
6	H	59	ASN
6	H	62	ASN
6	H	83	ASN
6	H	206	ASN

5.3.3　RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates 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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	T	19/19 (100%)	0.69	2 (10%)	7 5	59, 76, 94, 96	0
2	P	18/18 (100%)	0.12	1 (5%)	24 10	61, 74, 86, 87	0
3	A	558/558 (100%)	-0.08	0	100 100	11, 52, 75, 92	0
4	B	430/430 (100%)	-0.17	5 (1%)	75 42	6, 32, 75, 93	0
5	L	214/214 (100%)	-0.08	2 (0%)	81 51	17, 44, 66, 76	0
6	H	220/220 (100%)	-0.16	1 (0%)	88 64	14, 33, 57, 68	0
All	All	1459/1459 (100%)	-0.11	11 (0%)	83 53	6, 43, 75, 96	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	429	LEU	6.0
5	L	214	CYS	5.9
1	T	801	DA	4.7
4	B	427	TYR	3.7
4	B	428	GLN	2.8
4	B	93	GLY	2.7
6	H	141	GLN	2.7
5	L	213	GLU	2.6
4	B	430	GLU	2.3
2	P	821	DG	2.2
1	T	819	DC	2.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.