Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 08:51 AM EDT

PDB ID	:	1TVR
Title	:	HIV-1 RT/9-CL TIBO
Authors	:	Das, K.; Ding, J.; Hsiou, Y.; Arnold, E.
Deposited on	:	1996-04-16
Resolution	:	3.00 Å(reported)

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

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

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

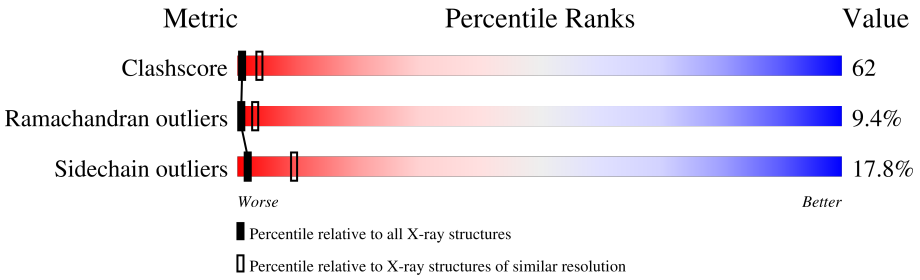
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	558	25% 58% 16%
2	B	427	24% 58% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TB9	A	600	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7845 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 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4382	2832	727	817	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

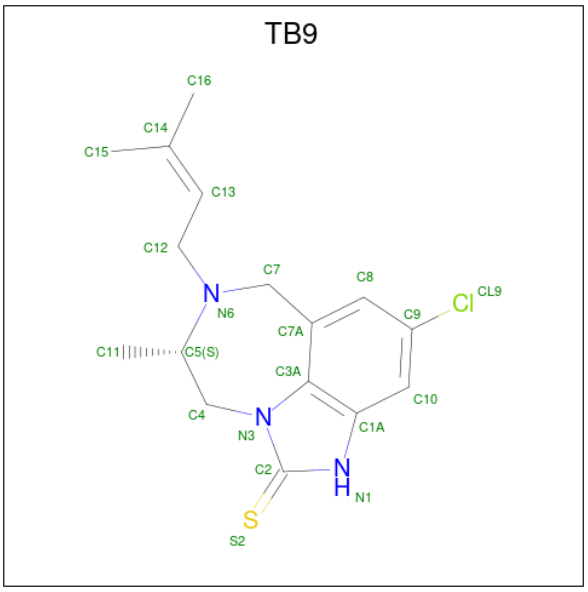
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3442	2240	567	630	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-CHLORO-8-METHYL-7-(3-METHYL-BUT-2-ENYL)-6,7,8,9-TETRAHYDRO-2H-2,7,9A-TRIAZA-BENZO[CD]AZULENE-1-THIONE (three-letter code: TB9) (formula: $C_{16}H_{20}ClN_3S$).



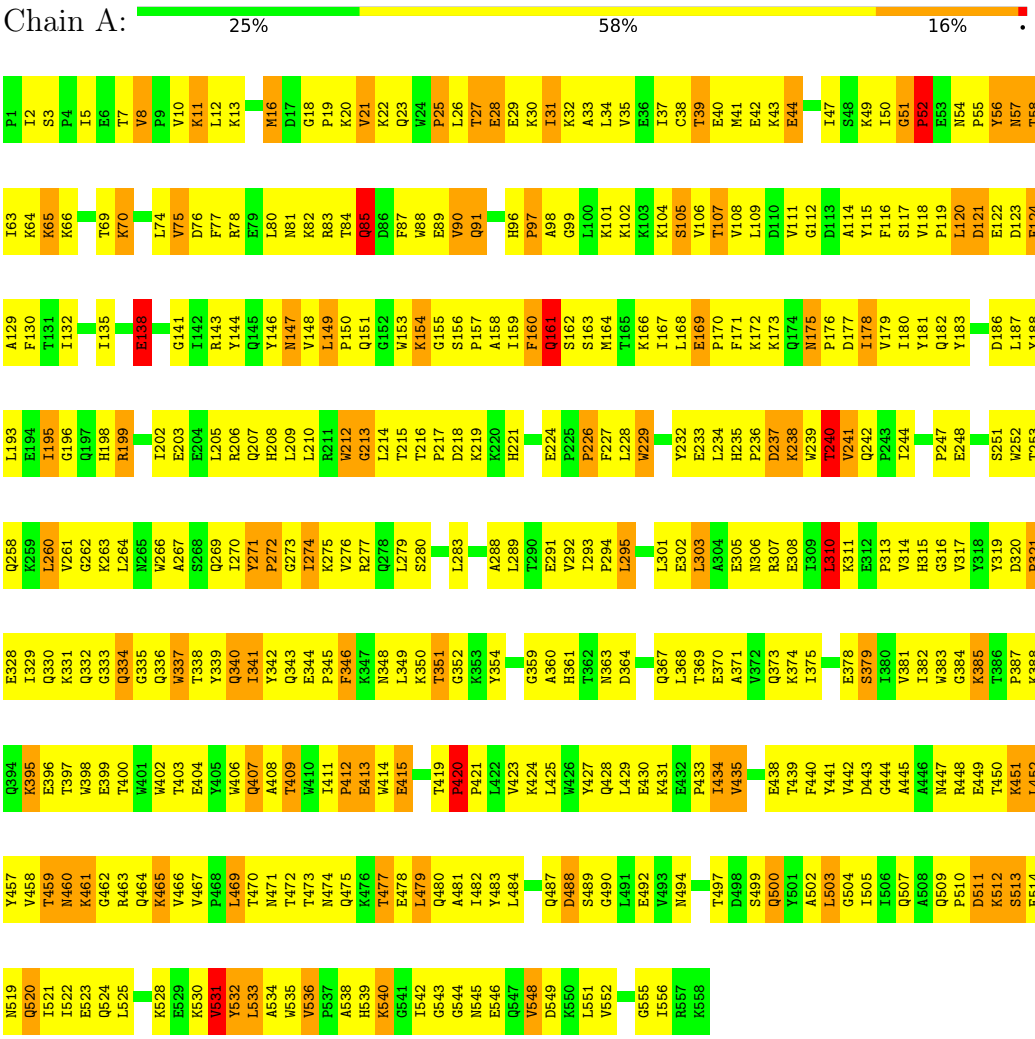
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	S	0	0
			21	16	1	3	1		

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. 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. 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.

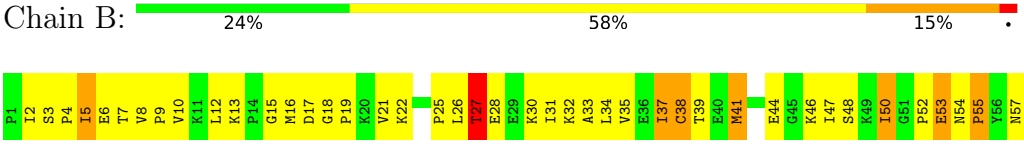
- Molecule 1: REVERSE TRANSCRIPTASE

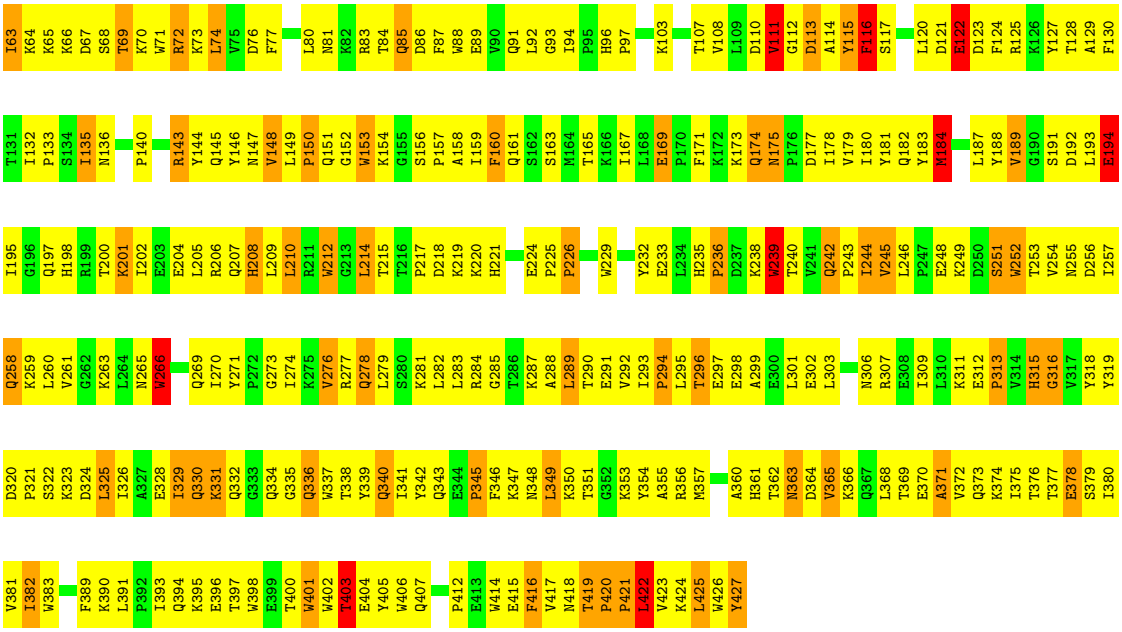
Chain A:



- Molecule 2: REVERSE TRANSCRIPTASE

Chain B:




I63 K64 K65 K66 D67 S68 T69 K70 W71 R72 K73 L74 V75 D76 F77 L80 N81 K82 R83 T84 Q85 D86 F87 W88 E89 V90 Q91 L92 G93 I94 P95 H96 P97 K103 T107 V108 L109 D110 V111 G112 D113 A114 Y115 F116 S117 L120 D121 E122 D123 F124 R125 K126 Y127 T128 A129 F130
T131 I132 P133 S134 I135 N136 P140 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 P176 D177 I178 V179 I180 Y181 Q182 Y183 M184 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 T216 P217 D218 K219 K220 H221 E224 P225 P226 W229 Y232 E233 L234 H235 P236 D237 K238 W239 T240 V241 Q242 P243 I244 V245 L246 P247 E248 K249 D250 S251 W252 T253 V254 N255 D256 I257
Q258 K259 L260 V261 G262 K263 L264 N265 W266 Q269 I270 Y271 P272 G273 I274 K275 V276 R277 Q278 L279 S280 K281 L282 L283 R284 G285 T286 K287 A288 L289 T290 E291 V292 I293 P294 L295 T296 E297 E298 A299 E300 L301 E302 L303 N306 R307 E308 I309 L310 K311 E312 P313 V314 H315 G316 V317 Y318 Y319
D320 P321 S322 K323 D324 L325 I326 A327 E328 I329 Q330 K331 Q332 G333 Q334 G335 Q336 W337 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 K347 N348 L349 K350 T351 G352 K353 Y354 A355 R356 M357 A360 H361 T362 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377 E378 S379 I380
V381 I382 W383 F389 K390 L391 P392 I393 Q394 K395 E396 T397 W398 E399 T400 W401 W402 T403 E404 Y405 W406 Q407 P412 E413 W414 E415 F416 V417 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	226.00Å 69.30Å 104.10Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.00) 82.5 (19.95-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.88Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.259 , (Not available) 0.302 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	78.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 200.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	7845	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TB9

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	0.71	1/4497 (0.0%)	0.98	10/6132 (0.2%)
2	B	0.77	3/3541 (0.1%)	0.99	7/4822 (0.1%)
All	All	0.74	4/8038 (0.0%)	0.98	17/10954 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	CYS	CB-SG	-5.32	1.73	1.81
1	A	337	TRP	CB-CG	-5.25	1.40	1.50
2	B	153	TRP	CB-CG	-5.21	1.40	1.50
2	B	266	TRP	CB-CG	5.09	1.59	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	325	LEU	CA-CB-CG	7.62	132.82	115.30
2	B	244	ILE	N-CA-C	-6.38	93.76	111.00
1	A	420	PRO	C-N-CD	6.19	141.40	128.40
1	A	420	PRO	N-CA-C	6.17	128.14	112.10
2	B	226	PRO	N-CA-CB	6.14	110.66	103.30
1	A	138	GLU	N-CA-C	5.96	127.09	111.00
1	A	479	LEU	CA-CB-CG	5.94	128.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	16	MET	CG-SD-CE	5.82	109.51	100.20
1	A	388	LYS	N-CA-C	-5.82	95.29	111.00
2	B	225	PRO	N-CA-CB	5.60	110.02	103.30
1	A	346	PHE	CB-CA-C	-5.50	99.40	110.40
1	A	213	GLY	N-CA-C	5.41	126.61	113.10
2	B	422	LEU	N-CA-C	-5.31	96.67	111.00
2	B	313	PRO	N-CA-C	5.29	125.85	112.10
1	A	52	PRO	N-CA-C	5.28	125.83	112.10
2	B	215	THR	N-CA-C	-5.12	97.18	111.00
1	A	513	SER	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	427	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4382	0	4279	576	0
2	B	3442	0	3405	410	0
3	A	21	0	20	15	0
All	All	7845	0	7704	962	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 62.

All (962) 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:60:VAL:HA	1:A:75:VAL:HG22	1.24	1.17
1:A:420:PRO:HG2	1:A:421:PRO:HD3	1.31	1.10
1:A:419:THR:HG22	1:A:420:PRO:HD3	1.09	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HG	2:B:293:ILE:HG22	1.32	1.09
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.36	1.07
2:B:38:CYS:HB3	2:B:144:TYR:HE2	1.12	1.07
1:A:344:GLU:HG2	1:A:345:PRO:CD	1.85	1.06
2:B:38:CYS:HB3	2:B:144:TYR:CE2	1.91	1.06
1:A:344:GLU:CG	1:A:345:PRO:HD2	1.88	1.04
2:B:34:LEU:HD21	2:B:62:ALA:HB2	1.38	1.02
1:A:419:THR:HG22	1:A:420:PRO:CD	1.91	0.99
2:B:34:LEU:HB2	2:B:132:ILE:HD11	1.45	0.98
1:A:344:GLU:HG2	1:A:345:PRO:HD2	1.00	0.97
1:A:264:LEU:HD22	1:A:306:ASN:HD22	1.30	0.97
1:A:540:LYS:HE3	1:A:540:LYS:HA	1.46	0.97
2:B:183:TYR:CD2	2:B:380:ILE:HG23	2.00	0.96
1:A:21:VAL:HB	1:A:58:THR:HA	1.50	0.93
1:A:254:VAL:HB	1:A:289:LEU:HA	1.52	0.92
1:A:56:TYR:HD1	1:A:56:TYR:H	1.18	0.91
2:B:183:TYR:CD2	2:B:380:ILE:HD12	2.07	0.90
1:A:164:MET:CE	1:A:187:LEU:HD11	2.01	0.90
1:A:10:VAL:HG13	1:A:87:PHE:HZ	1.35	0.90
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.08	0.89
1:A:181:TYR:HB3	3:A:600:TB9:H111	1.54	0.88
2:B:81:ASN:ND2	2:B:154:LYS:HG3	1.89	0.88
1:A:543:GLY:H	2:B:284:ARG:HG2	1.38	0.88
1:A:341:ILE:HD11	1:A:350:LYS:HG2	1.56	0.88
2:B:183:TYR:CE2	2:B:380:ILE:HD12	2.09	0.87
1:A:97:PRO:HG3	1:A:234:LEU:HD21	1.56	0.87
2:B:63:ILE:HD11	2:B:74:LEU:HD13	1.57	0.87
2:B:261:VAL:HG21	2:B:283:LEU:HD11	1.58	0.86
2:B:292:VAL:HG12	2:B:294:PRO:HD3	1.57	0.85
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.58	0.85
1:A:163:SER:HA	1:A:166:LYS:HE3	1.59	0.84
2:B:10:VAL:HG11	2:B:153:TRP:HH2	1.41	0.84
1:A:328:GLU:HB2	1:A:340:GLN:OE1	1.77	0.84
2:B:341:ILE:HD13	2:B:383:TRP:HZ3	1.42	0.84
2:B:125:ARG:HE	2:B:147:ASN:HA	1.40	0.84
2:B:183:TYR:HD2	2:B:380:ILE:HG23	1.39	0.83
1:A:164:MET:HE1	1:A:187:LEU:HD11	1.61	0.83
2:B:38:CYS:CB	2:B:144:TYR:HE2	1.92	0.83
1:A:435:VAL:HG12	2:B:290:THR:HG21	1.59	0.83
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.59	0.82
1:A:460:ASN:ND2	1:A:461:LYS:HE2	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.15	0.82
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.60	0.81
2:B:128:THR:HG21	2:B:150:PRO:HG2	1.63	0.81
1:A:517:LEU:HD12	1:A:518:VAL:HG23	1.63	0.81
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.16	0.80
1:A:228:LEU:HA	1:A:232:TYR:O	1.81	0.80
1:A:395:LYS:HG2	1:A:414:TRP:CH2	2.17	0.80
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.47	0.79
1:A:81:ASN:OD1	1:A:153:TRP:HA	1.82	0.79
1:A:490:GLY:O	1:A:528:LYS:HE2	1.83	0.78
1:A:252:TRP:CD1	1:A:295:LEU:HD22	2.18	0.78
1:A:108:VAL:HG22	1:A:188:TYR:CD2	2.19	0.78
1:A:455:ALA:H	1:A:469:LEU:HD11	1.49	0.78
2:B:397:THR:O	2:B:401:TRP:HD1	1.67	0.77
1:A:369:THR:HG21	1:A:409:THR:HG21	1.66	0.77
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.19	0.77
1:A:420:PRO:CG	1:A:421:PRO:HD3	2.13	0.77
1:A:387:PRO:HG2	1:A:389:PHE:HE1	1.47	0.77
2:B:389:PHE:O	2:B:415:GLU:HG2	1.85	0.77
1:A:235:HIS:HB2	1:A:238:LYS:HG3	1.67	0.76
1:A:12:LEU:HD22	1:A:83:ARG:O	1.86	0.76
1:A:542:ILE:HG23	1:A:545:ASN:HB3	1.66	0.76
1:A:109:LEU:HD13	1:A:216:THR:HG21	1.68	0.76
1:A:454:LYS:HG3	1:A:552:VAL:HG13	1.68	0.75
2:B:366:LYS:HE3	2:B:405:TYR:CE2	2.22	0.75
1:A:26:LEU:HB3	1:A:31:ILE:HG13	1.68	0.75
2:B:282:LEU:O	2:B:293:ILE:HG21	1.86	0.75
2:B:31:ILE:O	2:B:35:VAL:HG23	1.87	0.74
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.49	0.74
1:A:341:ILE:HG13	1:A:383:TRP:HH2	1.51	0.74
1:A:503:LEU:HD13	1:A:535:TRP:CB	2.18	0.73
2:B:319:TYR:CE2	2:B:383:TRP:HB3	2.23	0.73
1:A:419:THR:CG2	1:A:420:PRO:HD3	2.05	0.73
2:B:243:PRO:HA	2:B:245:VAL:HG12	1.69	0.73
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.70	0.73
1:A:23:GLN:NE2	1:A:26:LEU:HD13	2.03	0.73
1:A:173:LYS:O	1:A:176:PRO:HD3	1.88	0.73
1:A:10:VAL:HG13	1:A:87:PHE:CZ	2.20	0.73
1:A:276:VAL:HG12	1:A:276:VAL:O	1.88	0.73
1:A:515:SER:O	1:A:519:ASN:HB2	1.87	0.73
2:B:122:GLU:HG3	2:B:125:ARG:NH1	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LYS:O	2:B:424:LYS:HG3	1.87	0.73
2:B:253:THR:HA	2:B:291:GLU:O	1.88	0.73
2:B:66:LYS:O	2:B:69:THR:HG23	1.89	0.72
1:A:114:ALA:C	1:A:160:PHE:HE2	1.93	0.72
2:B:363:ASN:O	2:B:366:LYS:HB3	1.90	0.72
2:B:37:ILE:HG22	2:B:38:CYS:N	2.02	0.72
1:A:27:THR:HB	1:A:30:LYS:HB2	1.70	0.72
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.18	0.72
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.71	0.71
2:B:128:THR:HG21	2:B:150:PRO:CG	2.20	0.71
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.72	0.71
1:A:341:ILE:O	1:A:349:LEU:HB3	1.89	0.71
2:B:249:LYS:HB2	2:B:252:TRP:CZ3	2.25	0.71
1:A:254:VAL:HG12	1:A:258:GLN:HE21	1.55	0.71
1:A:483:TYR:CZ	1:A:520:GLN:HG2	2.25	0.71
1:A:227:PHE:O	1:A:233:GLU:HA	1.90	0.71
2:B:263:LYS:HD3	2:B:425:LEU:CD1	2.20	0.70
2:B:365:VAL:HG22	2:B:393:ILE:HD11	1.73	0.70
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.71	0.70
2:B:67:ASP:H	2:B:407:GLN:HE22	1.38	0.70
2:B:202:ILE:O	2:B:206:ARG:HG3	1.91	0.70
2:B:341:ILE:HD13	2:B:383:TRP:CZ3	2.25	0.70
1:A:3:SER:O	1:A:5:ILE:HG22	1.90	0.70
2:B:115:TYR:HE2	2:B:157:PRO:CA	2.04	0.70
2:B:125:ARG:NE	2:B:147:ASN:HA	2.07	0.70
2:B:328:GLU:O	2:B:339:TYR:HA	1.91	0.70
1:A:240:THR:HG21	1:A:314:VAL:O	1.91	0.70
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.74	0.70
1:A:389:PHE:O	1:A:414:TRP:HA	1.91	0.69
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.73	0.69
2:B:34:LEU:HB2	2:B:132:ILE:CD1	2.20	0.69
2:B:130:PHE:CZ	2:B:144:TYR:HD2	2.11	0.69
1:A:425:LEU:HD13	1:A:428:GLN:OE1	1.92	0.69
1:A:202:ILE:O	1:A:206:ARG:HB2	1.93	0.69
1:A:59:PRO:O	1:A:75:VAL:HG13	1.92	0.69
2:B:63:ILE:HG21	2:B:406:TRP:O	1.93	0.69
1:A:56:TYR:N	1:A:56:TYR:CD1	2.61	0.69
1:A:19:PRO:CD	1:A:80:LEU:HD13	2.23	0.69
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.28	0.68
2:B:61:PHE:HE2	2:B:76:ASP:HB2	1.58	0.68
2:B:400:THR:HB	2:B:401:TRP:CD1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:PHE:CE2	2:B:76:ASP:HB2	2.28	0.68
2:B:340:GLN:HG2	2:B:427:TYR:OH	1.93	0.68
1:A:235:HIS:ND1	1:A:238:LYS:HG3	2.09	0.68
1:A:97:PRO:CG	1:A:234:LEU:HD21	2.24	0.68
1:A:229:TRP:CH2	3:A:600:TB9:H151	2.28	0.68
1:A:483:TYR:HE1	1:A:524:GLN:HE21	1.40	0.68
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.24	0.67
1:A:181:TYR:CE1	3:A:600:TB9:H162	2.29	0.67
2:B:27:THR:HG22	2:B:28:GLU:H	1.58	0.67
1:A:181:TYR:CB	3:A:600:TB9:H111	2.22	0.67
2:B:201:LYS:O	2:B:204:GLU:HB3	1.95	0.67
2:B:281:LYS:HA	2:B:284:ARG:HG3	1.75	0.67
1:A:58:THR:HG22	1:A:59:PRO:CD	2.23	0.67
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.77	0.67
1:A:455:ALA:N	1:A:469:LEU:HD11	2.10	0.67
1:A:434:ILE:HG21	1:A:492:GLU:CG	2.24	0.67
2:B:7:THR:O	2:B:9:PRO:HD3	1.94	0.67
2:B:15:GLY:O	2:B:16:MET:HG2	1.94	0.67
1:A:264:LEU:HD22	1:A:306:ASN:ND2	2.04	0.67
2:B:354:TYR:CG	2:B:371:ALA:HB2	2.30	0.66
2:B:366:LYS:HE3	2:B:405:TYR:CD2	2.30	0.66
1:A:149:LEU:HD11	1:A:159:ILE:HG22	1.75	0.66
2:B:242:GLN:HG2	2:B:243:PRO:HD3	1.76	0.66
2:B:398:TRP:CD1	2:B:416:PHE:HE2	2.14	0.66
2:B:296:THR:HG22	2:B:299:ALA:H	1.61	0.66
1:A:96:HIS:HE1	1:A:269:GLN:HE21	1.43	0.66
1:A:344:GLU:CG	1:A:345:PRO:CD	2.61	0.66
1:A:411:ILE:HD13	1:A:414:TRP:HE1	1.59	0.66
1:A:521:ILE:HG22	1:A:525:LEU:HD11	1.78	0.65
2:B:183:TYR:HD2	2:B:380:ILE:CG2	2.07	0.65
1:A:3:SER:HB3	1:A:212:TRP:C	2.17	0.65
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.77	0.65
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.31	0.65
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.30	0.65
1:A:382:ILE:O	2:B:136:ASN:HB2	1.96	0.65
2:B:38:CYS:HG	2:B:130:PHE:HZ	1.43	0.65
2:B:282:LEU:HD11	2:B:295:LEU:H	1.61	0.65
2:B:285:GLY:O	2:B:287:LYS:HG3	1.95	0.65
2:B:254:VAL:HA	2:B:257:ILE:HG22	1.79	0.65
2:B:299:ALA:O	2:B:302:GLU:HB2	1.96	0.65
2:B:328:GLU:HG2	2:B:390:LYS:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:HD1	1:A:148:VAL:HG23	1.62	0.65
2:B:263:LYS:HD3	2:B:425:LEU:HD13	1.77	0.65
2:B:330:GLN:HG2	2:B:338:THR:HB	1.79	0.65
2:B:154:LYS:HG2	2:B:184:MET:CE	2.27	0.64
1:A:238:LYS:HZ2	1:A:315:HIS:HB2	1.62	0.64
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.32	0.64
2:B:67:ASP:H	2:B:407:GLN:NE2	1.96	0.64
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.79	0.64
2:B:122:GLU:HG3	2:B:125:ARG:HH11	1.60	0.64
2:B:70:LYS:O	2:B:70:LYS:HG3	1.98	0.64
1:A:26:LEU:HD23	1:A:34:LEU:HD11	1.79	0.64
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.79	0.63
1:A:109:LEU:HD22	1:A:216:THR:CG2	2.27	0.63
1:A:500:GLN:OE1	1:A:500:GLN:HA	1.98	0.63
1:A:23:GLN:HG3	1:A:61:PHE:HE1	1.63	0.63
1:A:78:ARG:NH1	1:A:81:ASN:HB3	2.14	0.63
1:A:124:PHE:HD1	1:A:124:PHE:O	1.80	0.63
1:A:434:ILE:HD11	1:A:530:LYS:O	1.98	0.63
2:B:10:VAL:HG11	2:B:153:TRP:CH2	2.29	0.63
2:B:371:ALA:O	2:B:375:ILE:HD12	1.99	0.63
1:A:106:VAL:HG13	1:A:189:VAL:O	1.99	0.63
1:A:164:MET:HE3	1:A:187:LEU:HD11	1.79	0.63
1:A:384:GLY:HA3	2:B:135:ILE:HD13	1.79	0.63
2:B:335:GLY:O	2:B:337:TRP:CD1	2.51	0.63
1:A:57:ASN:ND2	1:A:143:ARG:HH21	1.96	0.63
1:A:260:LEU:HD21	1:A:279:LEU:HD13	1.79	0.63
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.67	0.63
1:A:229:TRP:CZ3	3:A:600:TB9:H151	2.34	0.63
1:A:503:LEU:HG	1:A:507:GLN:HG3	1.81	0.62
1:A:34:LEU:HD12	1:A:132:ILE:HG23	1.81	0.62
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.14	0.62
1:A:340:GLN:CB	1:A:351:THR:HG23	2.29	0.62
1:A:123:ASP:O	1:A:126:LYS:HG2	1.99	0.62
1:A:311:LYS:O	1:A:313:PRO:HD3	2.00	0.62
1:A:545:ASN:O	1:A:548:VAL:HG22	1.98	0.62
1:A:49:LYS:HG2	1:A:50:ILE:N	2.14	0.62
2:B:335:GLY:O	2:B:337:TRP:HD1	1.83	0.62
2:B:242:GLN:H	2:B:243:PRO:HD2	1.64	0.62
1:A:460:ASN:HD21	1:A:461:LYS:HE2	1.62	0.62
2:B:254:VAL:HG22	2:B:293:ILE:HG13	1.82	0.62
1:A:444:GLY:O	1:A:477:THR:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LYS:CG	1:A:552:VAL:HG13	2.29	0.62
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.65	0.62
1:A:238:LYS:NZ	1:A:315:HIS:HB2	2.14	0.62
2:B:282:LEU:HG	2:B:293:ILE:CG2	2.22	0.62
1:A:60:VAL:CA	1:A:75:VAL:HG22	2.16	0.61
1:A:397:THR:HG21	1:A:423:VAL:O	1.99	0.61
1:A:341:ILE:HG13	1:A:383:TRP:CH2	2.33	0.61
2:B:143:ARG:HG2	2:B:143:ARG:NH1	2.15	0.61
2:B:325:LEU:HD11	2:B:383:TRP:CE3	2.35	0.61
2:B:63:ILE:HG23	2:B:403:THR:O	2.00	0.61
2:B:270:ILE:HA	2:B:346:PHE:HB3	1.82	0.61
1:A:178:ILE:HD12	1:A:191:SER:HB3	1.83	0.61
1:A:238:LYS:HA	1:A:316:GLY:O	2.00	0.61
2:B:120:LEU:HD22	2:B:150:PRO:CD	2.31	0.61
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.16	0.61
1:A:30:LYS:HA	1:A:33:ALA:HB3	1.83	0.61
1:A:13:LYS:O	1:A:16:MET:HB2	2.01	0.61
1:A:163:SER:HA	1:A:166:LYS:CE	2.31	0.61
1:A:326:ILE:CG2	1:A:390:LYS:HD2	2.30	0.61
1:A:30:LYS:NZ	1:A:64:LYS:HE2	2.16	0.60
2:B:30:LYS:HG2	2:B:71:TRP:CH2	2.36	0.60
2:B:329:ILE:HA	2:B:338:THR:O	2.01	0.60
1:A:397:THR:HG21	1:A:424:LYS:HA	1.83	0.60
1:A:270:ILE:O	1:A:272:PRO:HD3	2.01	0.60
2:B:368:LEU:O	2:B:372:VAL:HG23	2.01	0.60
1:A:188:TYR:CG	3:A:600:TB9:H122	2.35	0.60
1:A:395:LYS:HD2	1:A:399:GLU:HG3	1.84	0.60
1:A:333:GLY:HA3	1:A:336:GLN:HB2	1.84	0.60
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.83	0.60
2:B:249:LYS:HB2	2:B:252:TRP:CE3	2.37	0.60
1:A:434:ILE:HG21	1:A:492:GLU:HG3	1.84	0.60
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.82	0.60
2:B:403:THR:O	2:B:403:THR:HG23	2.00	0.60
1:A:163:SER:CA	1:A:166:LYS:HE3	2.31	0.60
1:A:341:ILE:HD11	1:A:350:LYS:CG	2.29	0.60
1:A:542:ILE:CG2	1:A:545:ASN:HB3	2.31	0.60
1:A:34:LEU:HB3	1:A:132:ILE:HD13	1.84	0.59
1:A:440:PHE:CE2	1:A:457:TYR:CE1	2.90	0.59
1:A:461:LYS:O	1:A:463:ARG:N	2.35	0.59
2:B:59:PRO:HD2	2:B:76:ASP:HB3	1.83	0.59
2:B:183:TYR:CE2	2:B:380:ILE:CD1	2.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TYR:HD2	2:B:380:ILE:HD12	1.60	0.59
1:A:160:PHE:O	1:A:162:SER:N	2.35	0.59
1:A:170:PRO:HG2	1:A:208:HIS:CE1	2.36	0.59
1:A:542:ILE:HG12	1:A:545:ASN:H	1.66	0.59
2:B:158:ALA:O	2:B:161:GLN:HB2	2.02	0.59
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.36	0.59
1:A:179:VAL:HG12	3:A:600:TB9:H112	1.83	0.59
1:A:205:LEU:O	1:A:208:HIS:N	2.35	0.59
1:A:191:SER:OG	1:A:198:HIS:ND1	2.36	0.59
2:B:404:GLU:HB3	2:B:405:TYR:CD1	2.38	0.59
1:A:23:GLN:HE21	1:A:26:LEU:HD13	1.67	0.59
1:A:59:PRO:O	1:A:75:VAL:HA	2.03	0.59
1:A:27:THR:O	1:A:31:ILE:N	2.36	0.59
1:A:331:LYS:HE3	1:A:333:GLY:O	2.03	0.59
2:B:115:TYR:CE2	2:B:157:PRO:HA	2.38	0.59
2:B:397:THR:O	2:B:401:TRP:CD1	2.53	0.59
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.38	0.58
1:A:178:ILE:HB	1:A:191:SER:HB3	1.85	0.58
1:A:178:ILE:HD11	1:A:189:VAL:HG12	1.84	0.58
1:A:439:THR:HG23	2:B:289:LEU:HG	1.85	0.58
2:B:52:PRO:O	2:B:54:ASN:N	2.36	0.58
2:B:115:TYR:HE2	2:B:157:PRO:N	2.00	0.58
2:B:252:TRP:CE3	2:B:252:TRP:HA	2.38	0.58
1:A:543:GLY:HA2	1:A:546:GLU:HB2	1.84	0.58
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.85	0.58
1:A:390:LYS:HA	1:A:415:GLU:O	2.03	0.58
1:A:434:ILE:HD12	1:A:494:ASN:OD1	2.03	0.58
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.84	0.58
1:A:438:GLU:HG2	1:A:459:THR:HB	1.86	0.58
2:B:13:LYS:HA	2:B:87:PHE:CD2	2.39	0.58
2:B:167:ILE:O	2:B:208:HIS:NE2	2.35	0.58
1:A:546:GLU:O	1:A:549:ASP:HB2	2.04	0.58
2:B:183:TYR:HE2	2:B:380:ILE:CD1	2.17	0.58
1:A:431:LYS:O	1:A:532:TYR:HE1	1.87	0.57
2:B:19:PRO:HG3	2:B:80:LEU:HB2	1.85	0.57
2:B:115:TYR:HE2	2:B:157:PRO:HA	1.69	0.57
2:B:160:PHE:O	2:B:160:PHE:CD2	2.57	0.57
1:A:101:LYS:NZ	1:A:321:PRO:HG2	2.19	0.57
1:A:518:VAL:HA	1:A:521:ILE:HD12	1.86	0.57
1:A:160:PHE:CD1	1:A:161:GLN:N	2.73	0.57
1:A:433:PRO:HG2	2:B:255:ASN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:HA	1:A:83:ARG:HH11	1.68	0.57
1:A:182:GLN:HA	1:A:187:LEU:HD23	1.87	0.57
1:A:288:ALA:HB1	1:A:291:GLU:CB	2.33	0.57
1:A:354:TYR:CE2	1:A:370:GLU:HG2	2.40	0.57
2:B:26:LEU:HD23	2:B:133:PRO:HG2	1.85	0.57
2:B:163:SER:O	2:B:167:ILE:HG13	2.04	0.57
1:A:56:TYR:HD1	1:A:56:TYR:N	1.95	0.57
1:A:420:PRO:HG2	1:A:421:PRO:CD	2.20	0.57
1:A:503:LEU:HD13	1:A:535:TRP:HB3	1.87	0.57
2:B:18:GLY:HA3	2:B:127:TYR:HD1	1.69	0.57
2:B:266:TRP:CH2	2:B:346:PHE:CZ	2.93	0.57
1:A:241:VAL:HG11	1:A:266:TRP:NE1	2.20	0.57
1:A:275:LYS:HB3	1:A:336:GLN:HE22	1.70	0.57
1:A:340:GLN:HB3	1:A:351:THR:HG23	1.86	0.57
2:B:46:LYS:HE2	2:B:116:PHE:CG	2.40	0.57
2:B:85:GLN:HG3	2:B:154:LYS:O	2.04	0.57
2:B:248:GLU:O	2:B:248:GLU:HG3	2.05	0.57
1:A:101:LYS:CE	1:A:321:PRO:HG2	2.35	0.57
1:A:317:VAL:HG22	1:A:348:ASN:O	2.05	0.57
2:B:194:GLU:O	2:B:197:GLN:N	2.38	0.57
2:B:417:VAL:HG23	2:B:417:VAL:O	2.04	0.57
1:A:168:LEU:HD22	1:A:180:ILE:CD1	2.35	0.57
1:A:188:TYR:HB3	3:A:600:TB9:C7	2.35	0.57
2:B:21:VAL:O	2:B:57:ASN:HB3	2.05	0.57
2:B:65:LYS:HG3	2:B:407:GLN:O	2.05	0.57
2:B:252:TRP:HA	2:B:252:TRP:HE3	1.69	0.57
2:B:316:GLY:HA3	2:B:347:LYS:HB3	1.86	0.57
1:A:19:PRO:HA	1:A:83:ARG:NH1	2.20	0.56
1:A:153:TRP:O	1:A:155:GLY:N	2.38	0.56
1:A:341:ILE:CD1	1:A:350:LYS:HG2	2.34	0.56
2:B:33:ALA:HB1	2:B:71:TRP:CG	2.39	0.56
2:B:112:GLY:HA2	2:B:115:TYR:CE1	2.40	0.56
2:B:330:GLN:HG3	2:B:332:GLN:NE2	2.19	0.56
1:A:168:LEU:O	1:A:172:LYS:HB2	2.05	0.56
1:A:261:VAL:HG12	1:A:261:VAL:O	2.05	0.56
1:A:511:ASP:O	1:A:522:ILE:HG12	2.05	0.56
2:B:279:LEU:HD11	2:B:303:LEU:HD13	1.85	0.56
2:B:319:TYR:CD2	2:B:383:TRP:CD1	2.93	0.56
1:A:114:ALA:O	1:A:160:PHE:HE2	1.88	0.56
1:A:149:LEU:HD11	1:A:159:ILE:CG2	2.35	0.56
1:A:240:THR:HG22	1:A:270:ILE:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:LEU:HD23	1:A:487:GLN:NE2	2.20	0.56
2:B:61:PHE:HD2	2:B:74:LEU:HD23	1.71	0.56
2:B:148:VAL:HG23	2:B:149:LEU:N	2.21	0.56
1:A:23:GLN:NE2	1:A:61:PHE:HD1	2.03	0.56
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.05	0.56
1:A:452:LEU:HA	1:A:472:THR:HG22	1.87	0.56
2:B:179:VAL:HG12	2:B:180:ILE:N	2.20	0.56
2:B:393:ILE:CG2	2:B:416:PHE:HD2	2.18	0.56
1:A:40:GLU:HG3	1:A:44:GLU:OE1	2.04	0.56
2:B:50:ILE:HD13	2:B:145:GLN:HB2	1.87	0.56
2:B:85:GLN:O	2:B:89:GLU:N	2.38	0.56
1:A:503:LEU:O	1:A:507:GLN:HB2	2.06	0.56
2:B:34:LEU:CD2	2:B:62:ALA:HB2	2.25	0.56
2:B:261:VAL:CG2	2:B:283:LEU:HD11	2.35	0.56
1:A:509:GLN:N	1:A:510:PRO:HD3	2.21	0.56
1:A:339:TYR:CD2	1:A:375:ILE:HG12	2.41	0.56
1:A:445:ALA:O	1:A:477:THR:HG21	2.06	0.56
2:B:41:MET:O	2:B:47:ILE:HG12	2.06	0.56
1:A:18:GLY:HA3	1:A:56:TYR:HD2	1.71	0.56
2:B:50:ILE:HD12	2:B:54:ASN:ND2	2.21	0.56
2:B:73:LYS:NZ	2:B:130:PHE:CZ	2.74	0.56
2:B:92:LEU:HB2	2:B:158:ALA:HB1	1.88	0.56
2:B:319:TYR:HE2	2:B:383:TRP:HB3	1.70	0.56
1:A:160:PHE:HD1	1:A:161:GLN:N	2.05	0.55
1:A:164:MET:SD	1:A:214:LEU:HD13	2.46	0.55
1:A:234:LEU:HB3	3:A:600:TB9:CL9	2.43	0.55
2:B:271:TYR:HE1	2:B:313:PRO:HA	1.70	0.55
1:A:2:ILE:HG23	1:A:117:SER:O	2.05	0.55
1:A:500:GLN:O	1:A:504:GLY:N	2.36	0.55
2:B:263:LYS:HD3	2:B:425:LEU:HD11	1.88	0.55
1:A:130:PHE:HE2	1:A:146:TYR:CE1	2.23	0.55
1:A:303:LEU:HD12	1:A:303:LEU:O	2.06	0.55
1:A:397:THR:CG2	1:A:424:LYS:HA	2.37	0.55
2:B:124:PHE:CE2	2:B:153:TRP:CH2	2.95	0.55
1:A:54:ASN:ND2	1:A:126:LYS:HA	2.21	0.55
1:A:130:PHE:O	1:A:143:ARG:HG3	2.07	0.55
1:A:328:GLU:HG3	1:A:342:TYR:HE1	1.71	0.55
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.89	0.55
1:A:126:LYS:HG3	1:A:127:TYR:CE1	2.42	0.55
1:A:406:TRP:CE3	1:A:407:GLN:N	2.75	0.55
2:B:365:VAL:HG12	2:B:365:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:N	1:A:170:PRO:HD2	2.22	0.55
1:A:430:GLU:CD	1:A:530:LYS:HG3	2.27	0.55
1:A:473:THR:O	1:A:475:GLN:N	2.39	0.55
2:B:70:LYS:HD3	2:B:72:ARG:NH2	2.21	0.55
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.89	0.55
2:B:390:LYS:HG2	2:B:415:GLU:OE2	2.07	0.55
1:A:329:ILE:HA	1:A:338:THR:O	2.06	0.54
2:B:54:ASN:HD21	2:B:129:ALA:CB	2.20	0.54
1:A:241:VAL:CG1	1:A:266:TRP:HE1	2.21	0.54
1:A:241:VAL:CG1	1:A:266:TRP:NE1	2.70	0.54
1:A:544:GLY:N	2:B:284:ARG:HA	2.22	0.54
2:B:198:HIS:O	2:B:202:ILE:HG12	2.07	0.54
1:A:135:ILE:CB	1:A:138:GLU:HB2	2.38	0.54
2:B:376:THR:HG22	2:B:376:THR:O	2.06	0.54
1:A:130:PHE:CE2	1:A:146:TYR:CE1	2.96	0.54
2:B:369:THR:HA	2:B:398:TRP:HH2	1.71	0.54
1:A:108:VAL:HG22	1:A:188:TYR:CE2	2.43	0.54
1:A:469:LEU:HD22	1:A:480:GLN:HG2	1.89	0.54
1:A:191:SER:HB2	1:A:193:LEU:HG	1.89	0.54
1:A:503:LEU:O	1:A:507:GLN:HG3	2.08	0.54
2:B:323:LYS:HB2	2:B:343:GLN:HE21	1.72	0.54
1:A:111:VAL:HG12	1:A:114:ALA:CB	2.37	0.54
1:A:162:SER:OG	1:A:163:SER:N	2.40	0.54
2:B:27:THR:O	2:B:31:ILE:HG13	2.08	0.54
2:B:400:THR:HB	2:B:401:TRP:NE1	2.22	0.54
2:B:401:TRP:CD1	2:B:401:TRP:N	2.75	0.54
2:B:125:ARG:HG2	2:B:146:TYR:O	2.08	0.54
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.06	0.54
2:B:122:GLU:CG	2:B:125:ARG:HH11	2.21	0.54
2:B:339:TYR:CE2	2:B:375:ILE:HG12	2.43	0.54
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.43	0.53
1:A:275:LYS:HG2	1:A:332:GLN:NE2	2.23	0.53
2:B:197:GLN:O	2:B:200:THR:HB	2.08	0.53
1:A:42:GLU:HG3	1:A:47:ILE:O	2.08	0.53
1:A:253:THR:HG22	1:A:292:VAL:HA	1.90	0.53
1:A:26:LEU:CD2	1:A:34:LEU:HD11	2.38	0.53
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.23	0.53
1:A:439:THR:OG1	2:B:288:ALA:HA	2.08	0.53
1:A:483:TYR:HE1	1:A:524:GLN:NE2	2.06	0.53
2:B:296:THR:O	2:B:299:ALA:HB3	2.08	0.53
1:A:30:LYS:HZ1	1:A:64:LYS:HE2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:CD1	1:A:518:VAL:HG22	2.38	0.53
2:B:330:GLN:HG3	2:B:332:GLN:HE22	1.73	0.53
1:A:454:LYS:HE2	1:A:555:GLY:HA3	1.90	0.53
1:A:126:LYS:HG3	1:A:127:TYR:CD1	2.43	0.53
1:A:320:ASP:H	1:A:343:GLN:HE22	1.54	0.53
1:A:459:THR:HG23	1:A:463:ARG:HB3	1.89	0.53
1:A:465:LYS:O	1:A:466:VAL:HG23	2.09	0.53
1:A:23:GLN:NE2	1:A:61:PHE:CD1	2.77	0.53
1:A:54:ASN:HD21	1:A:126:LYS:HA	1.73	0.53
1:A:375:ILE:HB	1:A:389:PHE:HZ	1.73	0.53
1:A:408:ALA:HB1	2:B:364:ASP:CB	2.39	0.53
2:B:266:TRP:CZ3	2:B:346:PHE:CE1	2.97	0.53
1:A:224:GLU:O	1:A:227:PHE:CE1	2.62	0.53
2:B:38:CYS:SG	2:B:130:PHE:HZ	2.32	0.53
1:A:235:HIS:HB2	1:A:238:LYS:HG2	1.90	0.53
2:B:115:TYR:O	2:B:117:SER:N	2.42	0.52
1:A:50:ILE:HG22	1:A:51:GLY:N	2.24	0.52
2:B:148:VAL:HG23	2:B:149:LEU:H	1.74	0.52
1:A:47:ILE:HG23	1:A:144:TYR:HB3	1.90	0.52
1:A:153:TRP:CZ3	1:A:159:ILE:HD12	2.44	0.52
2:B:28:GLU:HG2	2:B:32:LYS:CE	2.39	0.52
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.39	0.52
2:B:354:TYR:CD1	2:B:371:ALA:HB2	2.43	0.52
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.75	0.52
1:A:96:HIS:CE1	1:A:269:GLN:HE21	2.26	0.52
1:A:403:THR:HG23	2:B:334:GLN:HE21	1.74	0.52
2:B:61:PHE:CZ	2:B:402:TRP:HZ2	2.27	0.52
2:B:315:HIS:CG	2:B:316:GLY:N	2.76	0.52
1:A:277:ARG:CZ	1:A:334:GLN:HG3	2.39	0.52
1:A:325:LEU:HD13	1:A:383:TRP:CE3	2.44	0.52
2:B:393:ILE:HG22	2:B:416:PHE:HD2	1.74	0.52
1:A:196:GLY:HA2	1:A:199:ARG:HB2	1.92	0.52
2:B:254:VAL:HA	2:B:257:ILE:CG2	2.37	0.52
2:B:366:LYS:O	2:B:369:THR:HG22	2.10	0.52
1:A:275:LYS:HB3	1:A:336:GLN:NE2	2.24	0.52
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.91	0.52
1:A:23:GLN:HG3	1:A:61:PHE:CE1	2.42	0.52
1:A:218:ASP:O	1:A:221:HIS:N	2.43	0.52
1:A:310:LEU:HD23	1:A:310:LEU:O	2.09	0.52
2:B:26:LEU:HD12	2:B:30:LYS:HB3	1.92	0.52
2:B:120:LEU:HD22	2:B:150:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:HD2	1:A:374:LYS:O	2.10	0.51
2:B:50:ILE:CD1	2:B:145:GLN:HB2	2.40	0.51
2:B:156:SER:H	2:B:157:PRO:HD2	1.74	0.51
2:B:159:ILE:C	2:B:161:GLN:H	2.12	0.51
2:B:13:LYS:HA	2:B:87:PHE:HD2	1.75	0.51
1:A:274:ILE:HG23	1:A:306:ASN:ND2	2.25	0.51
1:A:379:SER:OG	1:A:387:PRO:HD2	2.10	0.51
2:B:81:ASN:OD1	2:B:153:TRP:HD1	1.93	0.51
2:B:115:TYR:CE2	2:B:157:PRO:CA	2.91	0.51
1:A:512:LYS:HD3	1:A:512:LYS:H	1.75	0.51
2:B:276:VAL:HG22	2:B:276:VAL:O	2.11	0.51
2:B:372:VAL:HG12	2:B:372:VAL:O	2.10	0.51
1:A:41:MET:HB2	1:A:47:ILE:HD12	1.91	0.51
1:A:247:PRO:HD3	1:A:263:LYS:NZ	2.25	0.51
2:B:48:SER:OG	2:B:147:ASN:ND2	2.43	0.51
1:A:124:PHE:O	1:A:124:PHE:CD1	2.61	0.51
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.46	0.51
2:B:273:GLY:O	2:B:309:ILE:HD13	2.11	0.51
1:A:31:ILE:O	1:A:34:LEU:HB2	2.10	0.51
1:A:384:GLY:C	1:A:385:LYS:HG2	2.31	0.51
2:B:62:ALA:HB1	2:B:71:TRP:CE3	2.46	0.51
2:B:361:HIS:O	2:B:363:ASN:N	2.45	0.50
2:B:394:GLN:O	2:B:395:LYS:C	2.50	0.50
1:A:180:ILE:HA	1:A:188:TYR:O	2.11	0.50
1:A:470:THR:HG22	1:A:471:ASN:N	2.26	0.50
2:B:236:PRO:HB3	2:B:381:VAL:HG11	1.94	0.50
2:B:406:TRP:CZ2	2:B:412:PRO:HD2	2.46	0.50
1:A:442:VAL:HG12	1:A:443:ASP:N	2.26	0.50
2:B:252:TRP:CH2	2:B:260:LEU:HD22	2.47	0.50
2:B:259:LYS:HG3	2:B:260:LEU:N	2.26	0.50
2:B:28:GLU:O	2:B:32:LYS:HE3	2.10	0.50
2:B:58:THR:HG22	2:B:76:ASP:O	2.11	0.50
1:A:121:ASP:OD1	1:A:123:ASP:HB2	2.12	0.50
2:B:149:LEU:O	2:B:150:PRO:C	2.50	0.50
2:B:297:GLU:O	2:B:301:LEU:HD13	2.12	0.50
2:B:323:LYS:CB	2:B:343:GLN:HE21	2.24	0.50
1:A:331:LYS:HG3	1:A:336:GLN:O	2.11	0.50
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.47	0.50
1:A:60:VAL:HG23	1:A:130:PHE:HB2	1.94	0.50
1:A:227:PHE:O	1:A:233:GLU:CA	2.58	0.50
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASN:O	2:B:309:ILE:HG22	2.11	0.50
2:B:345:PRO:HB2	2:B:346:PHE:CD2	2.47	0.50
2:B:393:ILE:O	2:B:416:PHE:HB3	2.12	0.50
1:A:188:TYR:CB	3:A:600:TB9:H122	2.41	0.50
1:A:328:GLU:O	1:A:339:TYR:HA	2.12	0.50
1:A:543:GLY:HA3	2:B:284:ARG:HB3	1.92	0.50
1:A:10:VAL:HB	1:A:124:PHE:CD2	2.47	0.49
1:A:412:PRO:HG3	2:B:401:TRP:CH2	2.47	0.49
1:A:475:GLN:HA	1:A:478:GLU:OE1	2.12	0.49
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.47	0.49
1:A:118:VAL:HG13	1:A:119:PRO:HD2	1.94	0.49
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.26	0.49
1:A:38:CYS:O	1:A:42:GLU:N	2.44	0.49
1:A:55:PRO:HD2	1:A:56:TYR:CD1	2.47	0.49
1:A:106:VAL:HA	1:A:189:VAL:O	2.12	0.49
1:A:164:MET:SD	1:A:214:LEU:CD1	3.00	0.49
1:A:479:LEU:HD22	1:A:521:ILE:HD13	1.95	0.49
2:B:160:PHE:O	2:B:160:PHE:CG	2.65	0.49
1:A:543:GLY:HA2	1:A:546:GLU:CB	2.43	0.49
1:A:454:LYS:CE	1:A:555:GLY:HA3	2.42	0.49
2:B:2:ILE:HG23	2:B:2:ILE:O	2.13	0.49
2:B:299:ALA:O	2:B:302:GLU:N	2.46	0.49
1:A:183:TYR:CE2	1:A:229:TRP:NE1	2.77	0.49
1:A:398:TRP:NE1	1:A:402:TRP:NE1	2.61	0.49
2:B:35:VAL:O	2:B:39:THR:HB	2.12	0.49
1:A:61:PHE:N	1:A:74:LEU:O	2.46	0.49
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.27	0.49
1:A:479:LEU:HD22	1:A:521:ILE:CD1	2.43	0.49
2:B:21:VAL:HG12	2:B:22:LYS:N	2.26	0.49
2:B:113:ASP:O	2:B:116:PHE:HB2	2.13	0.49
1:A:160:PHE:HE1	1:A:182:GLN:NE2	2.11	0.49
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.13	0.49
1:A:525:LEU:HD23	1:A:531:VAL:HG21	1.95	0.49
2:B:64:LYS:HB2	2:B:68:SER:HA	1.94	0.49
2:B:368:LEU:HD21	2:B:391:LEU:HD22	1.95	0.49
1:A:274:ILE:HA	1:A:306:ASN:OD1	2.12	0.49
2:B:26:LEU:CD2	2:B:133:PRO:HG2	2.43	0.49
2:B:121:ASP:C	2:B:123:ASP:H	2.16	0.49
2:B:253:THR:HB	2:B:256:ASP:OD2	2.12	0.49
1:A:118:VAL:O	1:A:148:VAL:HB	2.12	0.49
1:A:381:VAL:HG22	2:B:25:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LYS:O	1:A:471:ASN:N	2.43	0.49
2:B:34:LEU:HD21	2:B:62:ALA:CB	2.27	0.49
2:B:80:LEU:O	2:B:80:LEU:HG	2.12	0.49
2:B:364:ASP:C	2:B:366:LYS:H	2.16	0.49
1:A:121:ASP:O	1:A:125:ARG:HG3	2.13	0.48
1:A:483:TYR:CE1	1:A:524:GLN:NE2	2.81	0.48
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.13	0.48
2:B:282:LEU:HD11	2:B:295:LEU:N	2.27	0.48
2:B:319:TYR:CE2	2:B:383:TRP:CD1	3.01	0.48
1:A:332:GLN:HG3	1:A:333:GLY:N	2.27	0.48
2:B:27:THR:HG22	2:B:28:GLU:N	2.27	0.48
2:B:212:TRP:HA	2:B:212:TRP:CE3	2.48	0.48
2:B:329:ILE:HD11	2:B:389:PHE:CD2	2.49	0.48
1:A:382:ILE:O	2:B:135:ILE:HG22	2.13	0.48
2:B:258:GLN:CG	2:B:283:LEU:HD22	2.43	0.48
2:B:266:TRP:HE3	2:B:266:TRP:O	1.96	0.48
2:B:288:ALA:C	2:B:290:THR:H	2.16	0.48
1:A:229:TRP:CZ3	1:A:234:LEU:HD11	2.49	0.48
1:A:303:LEU:HD12	1:A:303:LEU:C	2.33	0.48
2:B:354:TYR:CE1	2:B:356:ARG:HG3	2.49	0.48
1:A:8:VAL:HG11	2:B:52:PRO:HD2	1.95	0.48
1:A:181:TYR:CD1	1:A:182:GLN:O	2.67	0.48
1:A:199:ARG:HB2	1:A:199:ARG:NH1	2.29	0.48
1:A:419:THR:CG2	1:A:420:PRO:CD	2.78	0.48
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.76	0.48
2:B:111:VAL:HG23	2:B:111:VAL:O	2.12	0.48
1:A:97:PRO:O	1:A:99:GLY:N	2.46	0.48
1:A:102:LYS:HD3	1:A:237:ASP:CB	2.44	0.48
1:A:196:GLY:HA2	1:A:199:ARG:CB	2.42	0.48
1:A:229:TRP:HE3	1:A:234:LEU:HD11	1.78	0.48
1:A:452:LEU:HB3	1:A:470:THR:HA	1.94	0.48
2:B:396:GLU:O	2:B:397:THR:C	2.50	0.48
1:A:337:TRP:NE1	1:A:367:GLN:HG2	2.29	0.48
1:A:434:ILE:HG12	1:A:530:LYS:HG2	1.95	0.48
2:B:169:GLU:OE1	2:B:173:LYS:HD2	2.13	0.48
1:A:27:THR:HG22	1:A:29:GLU:HG2	1.96	0.48
1:A:120:LEU:CD2	1:A:125:ARG:HG2	2.41	0.48
1:A:326:ILE:HD12	1:A:342:TYR:CE2	2.49	0.48
1:A:326:ILE:HG13	1:A:343:GLN:HA	1.96	0.48
1:A:340:GLN:HB2	1:A:351:THR:HG23	1.96	0.48
1:A:341:ILE:CG1	1:A:350:LYS:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ALA:HA	1:A:545:ASN:OD1	2.14	0.48
2:B:288:ALA:O	2:B:290:THR:N	2.47	0.48
1:A:57:ASN:HD22	1:A:143:ARG:HH21	1.61	0.48
1:A:28:GLU:HA	1:A:31:ILE:HB	1.95	0.48
1:A:305:GLU:O	1:A:308:GLU:HB3	2.14	0.48
1:A:387:PRO:HG2	1:A:389:PHE:CE1	2.38	0.48
1:A:453:GLY:H	1:A:472:THR:HG21	1.78	0.48
2:B:337:TRP:HB2	2:B:354:TYR:HB3	1.95	0.48
1:A:111:VAL:HG12	1:A:111:VAL:O	2.13	0.47
1:A:125:ARG:HB3	1:A:146:TYR:O	2.14	0.47
1:A:244:ILE:HG23	1:A:263:LYS:HB3	1.97	0.47
1:A:302:GLU:O	1:A:303:LEU:C	2.53	0.47
2:B:12:LEU:O	2:B:87:PHE:HD2	1.97	0.47
2:B:94:ILE:HG12	2:B:161:GLN:CD	2.34	0.47
2:B:311:LYS:O	2:B:313:PRO:HD3	2.14	0.47
2:B:425:LEU:HD12	2:B:426:TRP:H	1.79	0.47
1:A:78:ARG:HA	1:A:81:ASN:HB2	1.95	0.47
2:B:340:GLN:HG2	2:B:427:TYR:CZ	2.48	0.47
2:B:342:TYR:HB3	2:B:348:ASN:HB3	1.96	0.47
1:A:119:PRO:HA	1:A:148:VAL:HA	1.95	0.47
2:B:366:LYS:HE3	2:B:405:TYR:HE2	1.74	0.47
1:A:122:GLU:HG3	1:A:122:GLU:O	2.14	0.47
1:A:123:ASP:O	1:A:125:ARG:N	2.47	0.47
1:A:360:ALA:O	1:A:361:HIS:CG	2.67	0.47
1:A:453:GLY:H	1:A:472:THR:CG2	2.27	0.47
2:B:159:ILE:O	2:B:161:GLN:N	2.45	0.47
2:B:233:GLU:O	2:B:235:HIS:CE1	2.68	0.47
2:B:246:LEU:HD12	2:B:307:ARG:HE	1.80	0.47
2:B:261:VAL:HG21	2:B:283:LEU:CD1	2.37	0.47
2:B:422:LEU:HD12	2:B:422:LEU:N	2.29	0.47
1:A:171:PHE:O	1:A:175:ASN:HB2	2.15	0.47
1:A:270:ILE:HA	1:A:351:THR:OG1	2.14	0.47
1:A:434:ILE:CD1	1:A:530:LYS:O	2.61	0.47
2:B:188:TYR:CE1	2:B:380:ILE:HG21	2.49	0.47
2:B:257:ILE:O	2:B:261:VAL:HG23	2.14	0.47
1:A:125:ARG:HH12	1:A:147:ASN:HB3	1.79	0.47
1:A:153:TRP:HZ3	1:A:159:ILE:HD12	1.80	0.47
1:A:335:GLY:O	1:A:337:TRP:CD1	2.67	0.47
1:A:441:TYR:HB3	1:A:548:VAL:HG11	1.97	0.47
2:B:174:GLN:OE1	2:B:174:GLN:N	2.47	0.47
1:A:51:GLY:H	1:A:52:PRO:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:HA	1:A:125:ARG:NE	2.30	0.47
1:A:160:PHE:HE1	1:A:182:GLN:HE22	1.60	0.47
2:B:103:LYS:HE3	2:B:192:ASP:HB2	1.97	0.47
2:B:366:LYS:HA	2:B:369:THR:HG22	1.95	0.47
1:A:108:VAL:CG2	1:A:188:TYR:CE2	2.98	0.47
1:A:202:ILE:HG21	1:A:221:HIS:CB	2.45	0.47
1:A:235:HIS:CB	1:A:238:LYS:HG3	2.42	0.47
1:A:465:LYS:HD3	1:A:488:ASP:OD2	2.14	0.47
2:B:181:TYR:CD1	2:B:182:GLN:N	2.83	0.47
2:B:205:LEU:O	2:B:209:LEU:HD12	2.15	0.47
2:B:183:TYR:CD2	2:B:380:ILE:CG2	2.84	0.47
2:B:191:SER:HG	2:B:198:HIS:HD1	1.59	0.47
1:A:106:VAL:HG11	3:A:600:TB9:H72	1.97	0.46
1:A:18:GLY:H	1:A:56:TYR:HE2	1.63	0.46
1:A:51:GLY:N	1:A:52:PRO:HD2	2.30	0.46
1:A:114:ALA:O	1:A:160:PHE:CE2	2.67	0.46
1:A:248:GLU:HB3	1:A:307:ARG:NH2	2.30	0.46
1:A:440:PHE:CD2	1:A:457:TYR:CD1	3.03	0.46
1:A:32:LYS:O	1:A:35:VAL:N	2.49	0.46
1:A:120:LEU:O	1:A:121:ASP:C	2.53	0.46
1:A:122:GLU:HA	1:A:125:ARG:HE	1.80	0.46
1:A:163:SER:O	1:A:166:LYS:HB2	2.15	0.46
1:A:10:VAL:HG12	1:A:124:PHE:CE2	2.50	0.46
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.81	0.46
1:A:30:LYS:O	1:A:34:LEU:HG	2.15	0.46
2:B:377:THR:O	2:B:379:SER:N	2.49	0.46
1:A:266:TRP:O	1:A:269:GLN:HG3	2.15	0.46
1:A:441:TYR:O	1:A:548:VAL:CG1	2.64	0.46
1:A:455:ALA:HB3	1:A:469:LEU:HD21	1.97	0.46
1:A:483:TYR:OH	1:A:520:GLN:HG2	2.15	0.46
1:A:519:ASN:O	1:A:522:ILE:HB	2.16	0.46
1:A:543:GLY:N	2:B:284:ARG:HG2	2.20	0.46
1:A:57:ASN:ND2	1:A:143:ARG:NH2	2.62	0.46
1:A:120:LEU:HD21	1:A:125:ARG:HA	1.98	0.46
2:B:3:SER:N	2:B:4:PRO:HD3	2.30	0.46
2:B:292:VAL:O	2:B:293:ILE:CG1	2.64	0.46
1:A:58:THR:HG22	1:A:59:PRO:HD3	1.97	0.46
1:A:433:PRO:HB3	2:B:289:LEU:HB2	1.97	0.46
2:B:5:ILE:HG23	2:B:6:GLU:N	2.30	0.46
1:A:12:LEU:HD21	1:A:124:PHE:CZ	2.50	0.46
1:A:81:ASN:O	1:A:84:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:HB3	1:A:160:PHE:CZ	2.51	0.46
1:A:218:ASP:O	1:A:221:HIS:HA	2.16	0.46
2:B:110:ASP:O	2:B:112:GLY:N	2.49	0.46
2:B:122:GLU:CG	2:B:125:ARG:NH1	2.76	0.46
2:B:159:ILE:HG22	2:B:160:PHE:N	2.30	0.46
2:B:278:GLN:O	2:B:299:ALA:HB2	2.16	0.46
1:A:276:VAL:O	1:A:276:VAL:CG1	2.59	0.45
1:A:482:ILE:HD11	1:A:502:ALA:HB1	1.97	0.45
1:A:521:ILE:HG22	1:A:525:LEU:CD1	2.44	0.45
1:A:542:ILE:O	1:A:546:GLU:N	2.49	0.45
2:B:244:ILE:HG22	2:B:244:ILE:O	2.16	0.45
1:A:168:LEU:CD2	1:A:205:LEU:HD11	2.47	0.45
1:A:196:GLY:O	1:A:199:ARG:N	2.49	0.45
1:A:212:TRP:CD1	1:A:212:TRP:N	2.84	0.45
2:B:64:LYS:CB	2:B:68:SER:HA	2.45	0.45
1:A:233:GLU:O	1:A:239:TRP:HA	2.17	0.45
1:A:406:TRP:CD2	1:A:407:GLN:N	2.84	0.45
1:A:457:TYR:OH	1:A:488:ASP:HB2	2.15	0.45
2:B:114:ALA:O	2:B:116:PHE:N	2.50	0.45
1:A:340:GLN:HA	1:A:350:LYS:O	2.16	0.45
2:B:370:GLU:O	2:B:372:VAL:N	2.49	0.45
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.50	0.45
1:A:11:LYS:O	1:A:85:GLN:HB3	2.16	0.45
1:A:85:GLN:NE2	2:B:53:GLU:HA	2.32	0.45
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.52	0.45
1:A:188:TYR:HB2	3:A:600:TB9:H122	1.99	0.45
1:A:483:TYR:CE1	1:A:524:GLN:HG3	2.52	0.45
1:A:540:LYS:C	1:A:542:ILE:N	2.70	0.45
2:B:114:ALA:C	2:B:116:PHE:N	2.69	0.45
2:B:378:GLU:O	2:B:382:ILE:HG13	2.17	0.45
1:A:90:VAL:O	1:A:91:GLN:NE2	2.49	0.45
1:A:478:GLU:O	1:A:482:ILE:HG13	2.16	0.45
2:B:19:PRO:HD3	2:B:80:LEU:CD1	2.46	0.45
2:B:183:TYR:HE2	2:B:380:ILE:HD12	1.66	0.45
2:B:368:LEU:O	2:B:372:VAL:N	2.50	0.45
1:A:233:GLU:OE1	1:A:242:GLN:HB2	2.17	0.45
1:A:295:LEU:HD12	1:A:295:LEU:HA	1.79	0.45
1:A:55:PRO:HD2	1:A:56:TYR:CE1	2.52	0.45
1:A:101:LYS:HA	1:A:319:TYR:O	2.17	0.45
1:A:341:ILE:HG13	1:A:350:LYS:HB3	1.98	0.45
1:A:10:VAL:CG1	1:A:87:PHE:HZ	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.52	0.45
2:B:121:ASP:O	2:B:123:ASP:N	2.50	0.45
2:B:206:ARG:HA	2:B:209:LEU:HD12	1.99	0.45
2:B:425:LEU:CG	2:B:426:TRP:H	2.29	0.45
1:A:178:ILE:CG1	1:A:189:VAL:HG12	2.47	0.44
1:A:241:VAL:HG21	1:A:266:TRP:CD1	2.51	0.44
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.98	0.44
1:A:260:LEU:CD2	1:A:279:LEU:HD13	2.45	0.44
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.70	0.44
1:A:328:GLU:HG3	1:A:342:TYR:CE1	2.52	0.44
2:B:114:ALA:O	2:B:115:TYR:C	2.54	0.44
2:B:332:GLN:OE1	2:B:425:LEU:N	2.50	0.44
2:B:339:TYR:C	2:B:340:GLN:HG3	2.38	0.44
1:A:235:HIS:O	1:A:237:ASP:N	2.51	0.44
1:A:237:ASP:N	1:A:237:ASP:OD1	2.50	0.44
1:A:254:VAL:HG12	1:A:258:GLN:NE2	2.26	0.44
1:A:264:LEU:O	1:A:274:ILE:HG21	2.17	0.44
1:A:293:ILE:HA	1:A:294:PRO:HD2	1.74	0.44
2:B:153:TRP:HE3	2:B:156:SER:HG	1.63	0.44
2:B:154:LYS:HA	2:B:184:MET:CE	2.47	0.44
1:A:54:ASN:HD21	1:A:126:LYS:CA	2.29	0.44
1:A:105:SER:HB3	1:A:198:HIS:ND1	2.32	0.44
1:A:183:TYR:CD1	1:A:183:TYR:C	2.91	0.44
2:B:328:GLU:HB2	2:B:340:GLN:HE22	1.82	0.44
2:B:365:VAL:HG21	2:B:397:THR:HG22	2.00	0.44
1:A:389:PHE:HB2	1:A:413:GLU:O	2.17	0.44
2:B:191:SER:OG	2:B:198:HIS:ND1	2.48	0.44
2:B:424:LYS:O	2:B:424:LYS:HD3	2.18	0.44
1:A:34:LEU:CB	1:A:132:ILE:HD13	2.47	0.44
1:A:63:ILE:CD1	1:A:74:LEU:HD22	2.48	0.44
1:A:143:ARG:HH11	1:A:143:ARG:HB2	1.82	0.44
2:B:70:LYS:HE3	2:B:70:LYS:HB2	1.68	0.44
2:B:355:ALA:C	2:B:356:ARG:HG2	2.38	0.44
1:A:274:ILE:HG23	1:A:306:ASN:HD21	1.83	0.44
2:B:242:GLN:HG2	2:B:243:PRO:CD	2.44	0.44
2:B:296:THR:O	2:B:299:ALA:N	2.50	0.44
1:A:379:SER:CB	1:A:387:PRO:HD2	2.48	0.44
1:A:471:ASN:OD1	1:A:471:ASN:O	2.36	0.44
1:A:533:LEU:HD13	1:A:534:ALA:H	1.83	0.44
1:A:381:VAL:O	1:A:381:VAL:CG1	2.66	0.44
1:A:440:PHE:CD2	1:A:457:TYR:CE1	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.53	0.44
1:A:212:TRP:HD1	1:A:212:TRP:H	1.64	0.44
1:A:247:PRO:HD3	1:A:263:LYS:HZ2	1.83	0.44
1:A:340:GLN:OE1	1:A:340:GLN:O	2.35	0.44
2:B:220:LYS:O	2:B:221:HIS:CG	2.71	0.44
2:B:319:TYR:CE2	2:B:383:TRP:CG	3.06	0.44
1:A:111:VAL:HG12	1:A:114:ALA:HB2	2.00	0.43
1:A:253:THR:O	1:A:257:ILE:N	2.47	0.43
1:A:271:TYR:HE1	1:A:313:PRO:HA	1.83	0.43
1:A:427:TYR:CD2	1:A:525:LEU:HB3	2.52	0.43
1:A:483:TYR:O	1:A:487:GLN:HG3	2.18	0.43
2:B:279:LEU:HD21	2:B:303:LEU:CD1	2.48	0.43
2:B:391:LEU:N	2:B:415:GLU:O	2.44	0.43
1:A:99:GLY:HA2	1:A:383:TRP:CD1	2.53	0.43
1:A:354:TYR:CZ	1:A:370:GLU:HG2	2.52	0.43
2:B:67:ASP:O	2:B:68:SER:HB2	2.18	0.43
2:B:354:TYR:HE2	2:B:374:LYS:HE3	1.82	0.43
1:A:175:ASN:HB3	1:A:178:ILE:HG23	1.99	0.43
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.53	0.43
1:A:544:GLY:H	2:B:284:ARG:HA	1.83	0.43
2:B:295:LEU:O	2:B:296:THR:C	2.57	0.43
2:B:325:LEU:HD12	2:B:341:ILE:CG2	2.48	0.43
1:A:111:VAL:HG12	1:A:114:ALA:HB3	2.00	0.43
1:A:395:LYS:HE3	1:A:399:GLU:OE2	2.18	0.43
2:B:46:LYS:HE2	2:B:116:PHE:CD2	2.53	0.43
2:B:120:LEU:HB2	2:B:148:VAL:O	2.18	0.43
2:B:180:ILE:HG12	2:B:189:VAL:CG1	2.40	0.43
1:A:467:VAL:O	1:A:469:LEU:HG	2.18	0.43
2:B:271:TYR:CE1	2:B:313:PRO:HA	2.53	0.43
2:B:282:LEU:HD21	2:B:295:LEU:N	2.33	0.43
1:A:70:LYS:HD3	1:A:70:LYS:N	2.34	0.43
1:A:160:PHE:CD1	1:A:160:PHE:C	2.92	0.43
1:A:363:ASN:O	1:A:367:GLN:HB2	2.18	0.43
1:A:459:THR:HG21	1:A:463:ARG:HD2	2.00	0.43
2:B:347:LYS:HA	2:B:347:LYS:HD3	1.71	0.43
1:A:22:LYS:HB2	1:A:22:LYS:HE3	1.74	0.43
1:A:160:PHE:CE1	1:A:182:GLN:NE2	2.86	0.43
1:A:217:PRO:O	1:A:219:LYS:N	2.51	0.43
1:A:339:TYR:CD1	1:A:352:GLY:O	2.72	0.43
1:A:375:ILE:CG2	1:A:389:PHE:HZ	2.32	0.43
1:A:479:LEU:HD13	1:A:518:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:MET:HB3	2:B:47:ILE:CD1	2.49	0.43
2:B:84:THR:HG21	2:B:124:PHE:CZ	2.54	0.43
2:B:110:ASP:C	2:B:112:GLY:H	2.22	0.43
2:B:258:GLN:HG2	2:B:283:LEU:HD22	2.00	0.43
1:A:77:PHE:HB3	1:A:80:LEU:HB3	2.00	0.43
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.54	0.43
1:A:188:TYR:HB2	3:A:600:TB9:C12	2.49	0.43
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.52	0.43
2:B:63:ILE:HD13	2:B:406:TRP:O	2.19	0.43
2:B:175:ASN:OD1	2:B:201:LYS:HD2	2.18	0.43
2:B:393:ILE:HG21	2:B:398:TRP:HB2	2.01	0.43
1:A:115:TYR:O	1:A:149:LEU:HB2	2.19	0.43
1:A:156:SER:O	1:A:158:ALA:N	2.51	0.43
1:A:203:GLU:O	1:A:207:GLN:HG2	2.18	0.43
1:A:326:ILE:O	1:A:341:ILE:HG22	2.18	0.43
1:A:441:TYR:O	1:A:548:VAL:HG11	2.18	0.43
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.48	0.43
1:A:472:THR:O	1:A:473:THR:HG23	2.19	0.43
2:B:128:THR:HB	2:B:146:TYR:HD2	1.84	0.43
2:B:366:LYS:O	2:B:368:LEU:N	2.52	0.43
1:A:120:LEU:O	1:A:125:ARG:NE	2.52	0.43
1:A:363:ASN:OD1	1:A:364:ASP:N	2.52	0.43
1:A:540:LYS:C	1:A:542:ILE:H	2.21	0.43
2:B:279:LEU:HD21	2:B:303:LEU:HD12	2.01	0.42
1:A:479:LEU:HD11	1:A:518:VAL:HG22	2.01	0.42
2:B:350:LYS:HD3	2:B:351:THR:N	2.35	0.42
1:A:60:VAL:HG22	1:A:75:VAL:HG21	2.02	0.42
1:A:275:LYS:HD3	1:A:336:GLN:NE2	2.33	0.42
1:A:521:ILE:O	1:A:525:LEU:HG	2.19	0.42
1:A:26:LEU:HD22	1:A:60:VAL:O	2.19	0.42
1:A:156:SER:O	1:A:157:PRO:C	2.57	0.42
1:A:438:GLU:HB3	1:A:440:PHE:HE1	1.84	0.42
1:A:443:ASP:OD2	1:A:548:VAL:HG23	2.19	0.42
2:B:320:ASP:O	2:B:322:SER:N	2.52	0.42
1:A:50:ILE:CG2	1:A:51:GLY:N	2.82	0.42
2:B:85:GLN:O	2:B:85:GLN:CG	2.67	0.42
2:B:214:LEU:HD13	2:B:214:LEU:HA	1.87	0.42
1:A:37:ILE:O	1:A:41:MET:HG3	2.20	0.42
1:A:492:GLU:O	1:A:492:GLU:HG2	2.20	0.42
2:B:28:GLU:HG2	2:B:32:LYS:HE2	2.01	0.42
1:A:12:LEU:HD23	1:A:84:THR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLN:O	1:A:151:GLN:HG2	2.20	0.42
2:B:132:ILE:HA	2:B:133:PRO:HD3	1.75	0.42
2:B:298:GLU:HA	2:B:301:LEU:HD22	2.01	0.42
2:B:319:TYR:CE2	2:B:383:TRP:CB	2.99	0.42
1:A:104:LYS:HB2	1:A:192:ASP:HA	2.01	0.42
2:B:107:THR:HG1	2:B:198:HIS:CD2	2.38	0.42
2:B:154:LYS:HG2	2:B:184:MET:HE3	2.00	0.42
1:A:59:PRO:C	1:A:75:VAL:HG13	2.40	0.42
1:A:326:ILE:HG21	1:A:390:LYS:HD2	2.00	0.42
1:A:379:SER:HB2	1:A:383:TRP:CE3	2.55	0.42
2:B:84:THR:OG1	2:B:85:GLN:N	2.53	0.42
1:A:101:LYS:HD3	1:A:321:PRO:CD	2.50	0.42
1:A:129:ALA:HB1	1:A:143:ARG:HD3	2.02	0.42
1:A:408:ALA:CB	2:B:364:ASP:HB3	2.49	0.42
2:B:46:LYS:HD3	2:B:116:PHE:CE1	2.54	0.42
2:B:337:TRP:CE3	2:B:368:LEU:HD13	2.53	0.42
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.01	0.42
2:B:417:VAL:C	2:B:419:THR:H	2.23	0.42
2:B:87:PHE:O	2:B:87:PHE:CD1	2.73	0.41
2:B:128:THR:O	2:B:129:ALA:C	2.58	0.41
2:B:239:TRP:HB2	2:B:350:LYS:HE2	2.01	0.41
2:B:249:LYS:C	2:B:251:SER:H	2.21	0.41
2:B:281:LYS:HA	2:B:284:ARG:CG	2.45	0.41
2:B:292:VAL:HG12	2:B:293:ILE:N	2.35	0.41
2:B:376:THR:O	2:B:376:THR:CG2	2.68	0.41
1:A:10:VAL:HG22	1:A:159:ILE:HD11	2.01	0.41
1:A:85:GLN:O	1:A:154:LYS:HE3	2.20	0.41
1:A:195:ILE:H	1:A:195:ILE:HG12	1.64	0.41
1:A:235:HIS:CG	1:A:238:LYS:HG3	2.55	0.41
1:A:252:TRP:HZ3	1:A:256:ASP:OD1	2.04	0.41
1:A:326:ILE:HB	1:A:342:TYR:O	2.20	0.41
2:B:85:GLN:O	2:B:85:GLN:HG2	2.20	0.41
1:A:155:GLY:O	1:A:156:SER:C	2.58	0.41
1:A:171:PHE:CD1	1:A:205:LEU:HD13	2.55	0.41
1:A:276:VAL:O	1:A:280:SER:HB2	2.20	0.41
2:B:73:LYS:HG3	2:B:74:LEU:N	2.35	0.41
2:B:306:ASN:CA	2:B:309:ILE:HG22	2.46	0.41
2:B:326:ILE:CB	2:B:342:TYR:CE1	3.03	0.41
2:B:336:GLN:OE1	2:B:353:LYS:HE2	2.19	0.41
1:A:65:LYS:HD3	1:A:66:LYS:H	1.85	0.41
1:A:319:TYR:CE1	1:A:325:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:HG22	1:A:390:LYS:HD2	2.02	0.41
1:A:373:GLN:O	1:A:374:LYS:C	2.59	0.41
1:A:536:VAL:HB	1:A:542:ILE:CD1	2.51	0.41
2:B:10:VAL:HA	2:B:88:TRP:CH2	2.56	0.41
2:B:249:LYS:HA	2:B:249:LYS:HD2	1.93	0.41
2:B:349:LEU:O	2:B:350:LYS:HB2	2.21	0.41
1:A:39:THR:HG23	1:A:43:LYS:HE3	2.02	0.41
1:A:96:HIS:HE1	1:A:269:GLN:NE2	2.15	0.41
1:A:109:LEU:O	1:A:186:ASP:HA	2.20	0.41
1:A:153:TRP:CE3	1:A:156:SER:N	2.89	0.41
1:A:180:ILE:HG22	1:A:181:TYR:N	2.36	0.41
2:B:48:SER:N	2:B:147:ASN:HD21	2.19	0.41
2:B:292:VAL:O	2:B:293:ILE:HG13	2.21	0.41
2:B:332:GLN:NE2	2:B:427:TYR:OXT	2.53	0.41
1:A:12:LEU:CD2	1:A:84:THR:HA	2.50	0.41
1:A:188:TYR:HB3	3:A:600:TB9:H71	2.02	0.41
1:A:196:GLY:O	1:A:199:ARG:HB3	2.20	0.41
1:A:407:GLN:OE1	2:B:418:ASN:HA	2.21	0.41
2:B:96:HIS:ND1	2:B:181:TYR:CE2	2.81	0.41
2:B:417:VAL:C	2:B:419:THR:N	2.72	0.41
1:A:19:PRO:HD3	1:A:80:LEU:CD1	2.40	0.41
1:A:107:THR:OG1	1:A:202:ILE:CD1	2.68	0.41
1:A:167:ILE:HD13	1:A:212:TRP:HB2	2.03	0.41
1:A:229:TRP:O	1:A:232:TYR:HB2	2.20	0.41
1:A:279:LEU:CD2	1:A:295:LEU:HD11	2.51	0.41
2:B:377:THR:C	2:B:379:SER:H	2.24	0.41
2:B:419:THR:HA	2:B:420:PRO:HD3	1.59	0.41
1:A:26:LEU:HB3	1:A:31:ILE:CG1	2.45	0.41
1:A:123:ASP:C	1:A:125:ARG:H	2.23	0.41
1:A:307:ARG:O	1:A:308:GLU:C	2.59	0.41
1:A:311:LYS:O	1:A:313:PRO:CD	2.68	0.41
1:A:368:LEU:O	1:A:371:ALA:HB3	2.20	0.41
1:A:399:GLU:HG2	1:A:402:TRP:CZ2	2.55	0.41
2:B:8:VAL:O	2:B:9:PRO:C	2.58	0.41
2:B:73:LYS:HG3	2:B:74:LEU:H	1.86	0.41
2:B:130:PHE:CD1	2:B:144:TYR:HB2	2.55	0.41
2:B:339:TYR:CZ	2:B:375:ILE:HG12	2.55	0.41
1:A:65:LYS:CD	1:A:66:LYS:H	2.34	0.41
1:A:109:LEU:HD22	1:A:216:THR:HG22	2.02	0.41
1:A:130:PHE:CE2	1:A:146:TYR:HE1	2.37	0.41
1:A:269:GLN:O	1:A:351:THR:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLY:O	1:A:274:ILE:C	2.59	0.41
1:A:317:VAL:HG23	1:A:349:LEU:HD12	2.03	0.41
2:B:296:THR:HG22	2:B:299:ALA:N	2.32	0.41
2:B:312:GLU:HA	2:B:313:PRO:HD3	1.83	0.41
2:B:354:TYR:CE2	2:B:374:LYS:HE3	2.55	0.41
1:A:10:VAL:O	1:A:124:PHE:HD2	2.04	0.41
1:A:65:LYS:HD3	1:A:66:LYS:N	2.35	0.41
1:A:148:VAL:O	1:A:149:LEU:C	2.59	0.41
1:A:161:GLN:O	1:A:161:GLN:HG2	2.21	0.41
1:A:178:ILE:CD1	1:A:189:VAL:HG12	2.49	0.41
1:A:301:LEU:O	1:A:305:GLU:HB2	2.20	0.41
1:A:340:GLN:HA	1:A:351:THR:HA	2.03	0.41
1:A:400:THR:O	1:A:404:GLU:HG2	2.20	0.41
2:B:46:LYS:HE2	2:B:116:PHE:CD1	2.56	0.41
2:B:77:PHE:HD2	2:B:152:GLY:HA3	1.86	0.41
2:B:149:LEU:O	2:B:151:GLN:N	2.53	0.41
2:B:156:SER:N	2:B:157:PRO:HD2	2.36	0.41
2:B:181:TYR:HD1	2:B:182:GLN:H	1.69	0.41
2:B:207:GLN:O	2:B:210:LEU:HB3	2.20	0.41
2:B:238:LYS:C	2:B:239:TRP:HD1	2.24	0.41
2:B:315:HIS:ND1	2:B:316:GLY:N	2.69	0.41
2:B:377:THR:C	2:B:379:SER:N	2.74	0.41
1:A:105:SER:O	1:A:198:HIS:CE1	2.74	0.40
1:A:181:TYR:HB3	3:A:600:TB9:H121	2.02	0.40
1:A:460:ASN:OD1	1:A:460:ASN:N	2.53	0.40
2:B:238:LYS:C	2:B:239:TRP:CD1	2.94	0.40
2:B:257:ILE:HG23	2:B:283:LEU:CD2	2.51	0.40
1:A:3:SER:HB3	1:A:212:TRP:O	2.20	0.40
1:A:57:ASN:HA	1:A:129:ALA:O	2.21	0.40
1:A:233:GLU:CD	1:A:242:GLN:HB2	2.42	0.40
1:A:262:GLY:O	1:A:263:LYS:C	2.59	0.40
1:A:484:LEU:HD23	1:A:487:GLN:HE21	1.85	0.40
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.86	0.40
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.56	0.40
2:B:206:ARG:NH1	2:B:217:PRO:CG	2.85	0.40
2:B:281:LYS:HA	2:B:284:ARG:CD	2.51	0.40
2:B:368:LEU:O	2:B:371:ALA:N	2.54	0.40
1:A:89:GLU:O	1:A:90:VAL:C	2.59	0.40
1:A:162:SER:O	1:A:163:SER:C	2.59	0.40
1:A:216:THR:HG22	1:A:216:THR:O	2.21	0.40
1:A:350:LYS:HD3	1:A:378:GLU:OE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:THR:O	1:A:452:LEU:N	2.54	0.40
1:A:494:ASN:HA	1:A:532:TYR:HB3	2.04	0.40
1:A:18:GLY:O	1:A:20:LYS:HD2	2.22	0.40
1:A:77:PHE:N	1:A:77:PHE:CD1	2.89	0.40
1:A:183:TYR:HE2	1:A:229:TRP:HE1	1.64	0.40
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.86	0.40
1:A:277:ARG:NH1	1:A:334:GLN:HG3	2.37	0.40
2:B:167:ILE:O	2:B:208:HIS:CE1	2.75	0.40
2:B:363:ASN:O	2:B:366:LYS:N	2.54	0.40
1:A:40:GLU:O	1:A:44:GLU:HB2	2.21	0.40
1:A:332:GLN:CG	1:A:333:GLY:N	2.85	0.40
1:A:452:LEU:HD12	1:A:452:LEU:O	2.22	0.40
1:A:503:LEU:O	1:A:507:GLN:CB	2.70	0.40
2:B:34:LEU:HD21	2:B:61:PHE:O	2.21	0.40
2:B:154:LYS:HA	2:B:184:MET:HE3	2.04	0.40
2:B:281:LYS:CA	2:B:284:ARG:HG3	2.47	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	556/558 (100%)	381 (68%)	129 (23%)	46 (8%)	1	4
2	B	425/427 (100%)	291 (68%)	88 (21%)	46 (11%)	0	2
All	All	981/985 (100%)	672 (68%)	217 (22%)	92 (9%)	0	3

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
1	A	213	GLY

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Mol	Chain	Res	Type
1	A	412	PRO
1	A	462	GLY
1	A	474	ASN
2	B	27	THR
2	B	53	GLU
2	B	116	PHE
2	B	242	GLN
2	B	277	ARG
2	B	289	LEU
2	B	294	PRO
2	B	296	THR
2	B	321	PRO
2	B	360	ALA
2	B	362	THR
2	B	382	ILE
1	A	98	ALA
1	A	112	GLY
1	A	124	PHE
1	A	141	GLY
1	A	160	PHE
1	A	161	GLN
1	A	272	PRO
1	A	274	ILE
1	A	420	PRO
1	A	556	ILE
2	B	37	ILE
2	B	41	MET
2	B	69	THR
2	B	93	GLY
2	B	160	PHE
2	B	194	GLU
2	B	195	ILE
2	B	210	LEU
2	B	276	VAL
2	B	278	GLN
2	B	316	GLY
2	B	357	MET
2	B	371	ALA
2	B	420	PRO
1	A	85	GLN
1	A	283	LEU
1	A	295	LEU

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Mol	Chain	Res	Type
1	A	393	ILE
1	A	452	LEU
1	A	532	TYR
2	B	55	PRO
2	B	236	PRO
2	B	403	THR
2	B	421	PRO
1	A	51	GLY
1	A	121	ASP
1	A	150	PRO
1	A	236	PRO
1	A	240	THR
1	A	251	SER
1	A	310	LEU
1	A	465	LYS
2	B	111	VAL
2	B	226	PRO
1	A	21	VAL
1	A	90	VAL
1	A	237	ASP
1	A	451	LYS
2	B	115	TYR
2	B	122	GLU
2	B	148	VAL
2	B	219	LYS
2	B	229	TRP
2	B	239	TRP
2	B	331	LYS
2	B	336	GLN
2	B	345	PRO
2	B	363	ASN
1	A	52	PRO
1	A	149	LEU
1	A	175	ASN
1	A	321	PRO
2	B	184	MET
2	B	224	GLU
2	B	365	VAL
1	A	75	VAL
1	A	226	PRO
1	A	505	ILE
1	A	25	PRO

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Mol	Chain	Res	Type
1	A	195	ILE
1	A	271	TYR
2	B	140	PRO
1	A	359	GLY
1	A	531	VAL
1	A	241	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	457/498 (92%)	372 (81%)	85 (19%)	1 8
2	B	367/389 (94%)	305 (83%)	62 (17%)	2 11
All	All	824/887 (93%)	677 (82%)	147 (18%)	2 9

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	8	VAL
1	A	11	LYS
1	A	25	PRO
1	A	27	THR
1	A	28	GLU
1	A	31	ILE
1	A	39	THR
1	A	44	GLU
1	A	56	TYR
1	A	57	ASN
1	A	58	THR
1	A	59	PRO
1	A	65	LYS
1	A	69	THR
1	A	70	LYS
1	A	76	ASP

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Mol	Chain	Res	Type
1	A	82	LYS
1	A	85	GLN
1	A	91	GLN
1	A	97	PRO
1	A	105	SER
1	A	107	THR
1	A	120	LEU
1	A	128	THR
1	A	138	GLU
1	A	147	ASN
1	A	161	GLN
1	A	169	GLU
1	A	177	ASP
1	A	178	ILE
1	A	199	ARG
1	A	210	LEU
1	A	212	TRP
1	A	215	THR
1	A	226	PRO
1	A	229	TRP
1	A	238	LYS
1	A	240	THR
1	A	257	ILE
1	A	260	LEU
1	A	303	LEU
1	A	310	LEU
1	A	330	GLN
1	A	334	GLN
1	A	340	GLN
1	A	341	ILE
1	A	346	PHE
1	A	351	THR
1	A	379	SER
1	A	385	LYS
1	A	395	LYS
1	A	396	GLU
1	A	407	GLN
1	A	409	THR
1	A	413	GLU
1	A	415	GLU
1	A	429	LEU
1	A	434	ILE

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Mol	Chain	Res	Type
1	A	435	VAL
1	A	448	ARG
1	A	449	GLU
1	A	459	THR
1	A	460	ASN
1	A	461	LYS
1	A	469	LEU
1	A	477	THR
1	A	488	ASP
1	A	497	THR
1	A	499	SER
1	A	500	GLN
1	A	503	LEU
1	A	511	ASP
1	A	512	LYS
1	A	513	SER
1	A	514	GLU
1	A	520	GLN
1	A	523	GLU
1	A	531	VAL
1	A	533	LEU
1	A	536	VAL
1	A	539	HIS
1	A	540	LYS
1	A	548	VAL
1	A	551	LEU
2	B	5	ILE
2	B	17	ASP
2	B	27	THR
2	B	44	GLU
2	B	50	ILE
2	B	55	PRO
2	B	63	ILE
2	B	72	ARG
2	B	74	LEU
2	B	83	ARG
2	B	85	GLN
2	B	86	ASP
2	B	91	GLN
2	B	111	VAL
2	B	113	ASP
2	B	116	PHE

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Mol	Chain	Res	Type
2	B	122	GLU
2	B	135	ILE
2	B	143	ARG
2	B	150	PRO
2	B	165	THR
2	B	169	GLU
2	B	174	GLN
2	B	175	ASN
2	B	177	ASP
2	B	184	MET
2	B	189	VAL
2	B	193	LEU
2	B	194	GLU
2	B	201	LYS
2	B	208	HIS
2	B	212	TRP
2	B	214	LEU
2	B	218	ASP
2	B	232	TYR
2	B	239	TRP
2	B	240	THR
2	B	245	VAL
2	B	251	SER
2	B	252	TRP
2	B	258	GLN
2	B	265	ASN
2	B	266	TRP
2	B	269	GLN
2	B	274	ILE
2	B	315	HIS
2	B	318	TYR
2	B	324	ASP
2	B	329	ILE
2	B	330	GLN
2	B	340	GLN
2	B	349	LEU
2	B	378	GLU
2	B	401	TRP
2	B	403	THR
2	B	414	TRP
2	B	416	PHE
2	B	419	THR

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Mol	Chain	Res	Type
2	B	421	PRO
2	B	422	LEU
2	B	423	VAL
2	B	425	LEU

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	258	GLN
1	A	269	GLN
1	A	334	GLN
1	A	343	GLN
1	A	487	GLN
2	B	54	ASN
2	B	57	ASN
2	B	145	GLN
2	B	147	ASN
2	B	151	GLN
2	B	207	GLN
2	B	255	ASN
2	B	334	GLN
2	B	407	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TB9	A	600	-	19,23,23	4.20	12 (63%)	18,34,34	5.71	14 (77%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TB9	A	600	-	-	0/4/17/17	0/2/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	TB9	C10-C1A	-9.58	1.38	1.53
3	A	600	TB9	C2-N1	7.57	1.44	1.34
3	A	600	TB9	C10-C9	-6.92	1.43	1.52
3	A	600	TB9	C2-S2	5.97	1.77	1.67
3	A	600	TB9	C7A-C3A	-5.14	1.44	1.53
3	A	600	TB9	C1A-N1	-3.70	1.40	1.46
3	A	600	TB9	C12-C13	-3.63	1.46	1.50
3	A	600	TB9	C3A-N3	-3.44	1.42	1.47
3	A	600	TB9	C8-C7A	-3.28	1.45	1.53
3	A	600	TB9	C8-C9	-3.14	1.48	1.52
3	A	600	TB9	C15-C14	2.13	1.56	1.50
3	A	600	TB9	C9-CL9	-2.07	1.76	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	TB9	C8-C9-CL9	12.50	121.09	109.77
3	A	600	TB9	C16-C14-C15	9.39	135.34	114.60
3	A	600	TB9	C10-C9-CL9	9.11	118.02	109.77
3	A	600	TB9	C10-C9-C8	7.61	120.70	111.79
3	A	600	TB9	C1A-C3A-N3	7.58	112.66	102.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	TB9	C15-C14-C13	-5.20	107.63	122.65
3	A	600	TB9	C4-N3-C3A	5.17	131.45	123.06
3	A	600	TB9	C12-N6-C7	5.09	121.04	111.98
3	A	600	TB9	C3A-C1A-N1	4.42	107.52	102.22
3	A	600	TB9	C10-C1A-N1	3.16	132.81	118.26
3	A	600	TB9	C13-C12-N6	-3.01	106.02	112.55
3	A	600	TB9	C7A-C7-N6	2.77	119.91	114.43
3	A	600	TB9	C8-C7A-C3A	2.15	115.44	109.47
3	A	600	TB9	C3A-N3-C2	-2.13	103.67	109.91

There are no chirality outliers.

There are no torsion outliers.

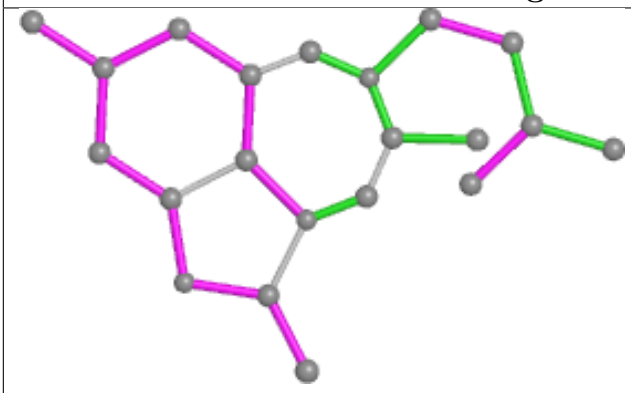
There are no ring outliers.

1 monomer is involved in 15 short contacts:

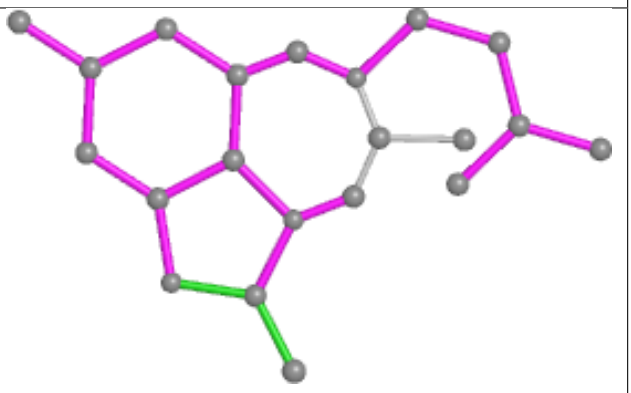
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	TB9	15	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

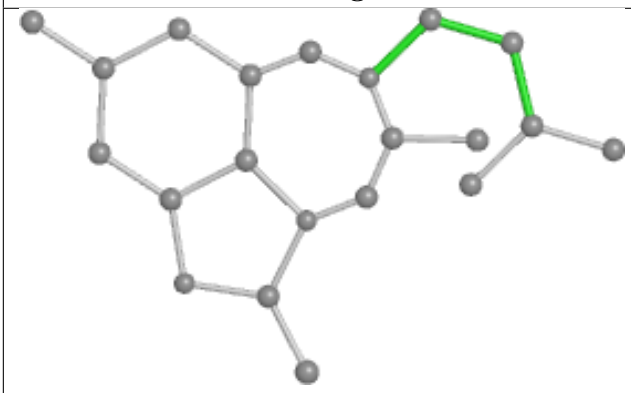
Ligand TB9 A 600



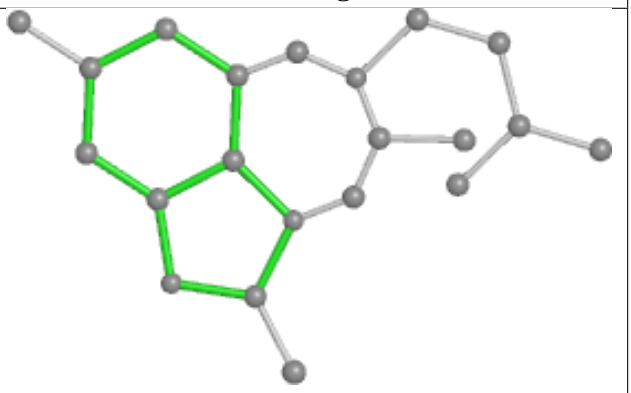
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

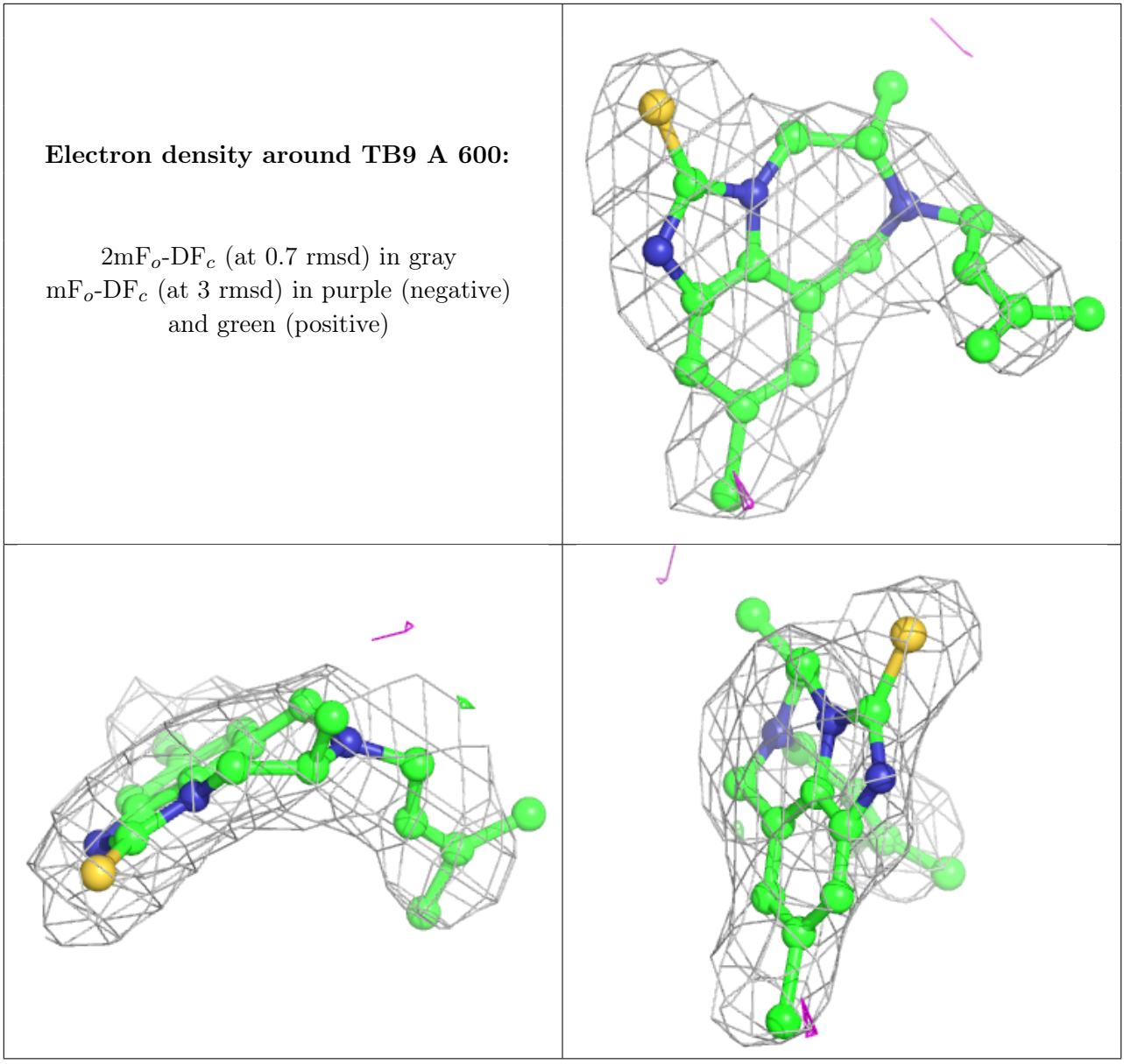
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TB9 A 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.