Full wwPDB EM Validation Report ⓘ

Aug 15, 2023 – 04:23 AM EDT

PDB ID	:	1TVK
Title	:	The binding mode of epothilone A on a,b-tubulin by electron crystallography
Authors	:	Nettles, J.H.; Li, H.; Cornett, B.; Krahn, J.M.; Snyder, J.P.; Downing, K.H.
Deposited on	:	2004-06-29
Resolution	:	2.89 Å(reported)
Based on initial model	:	1JFF

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

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

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

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

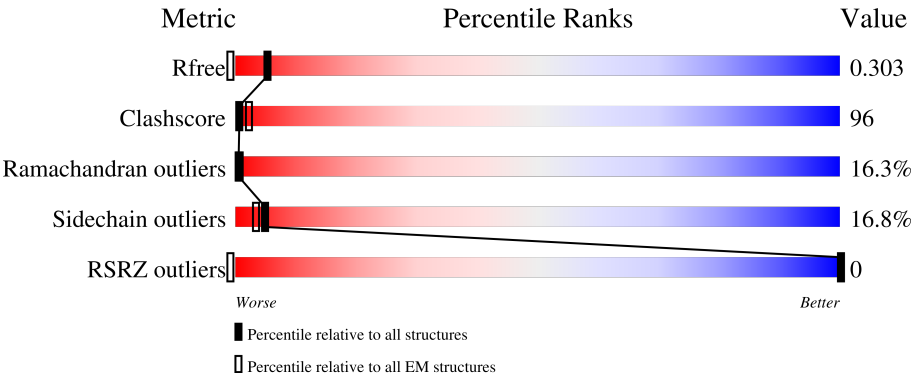
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 2.89 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)	EM structures (#Entries)
R_{free}	130704	0
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RSRZ outliers	127900	0

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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	440	9% 61% 22% · 6%
2	B	427	14% 61% 23% ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6672 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	412	3227	2043	551	613	20	0	0

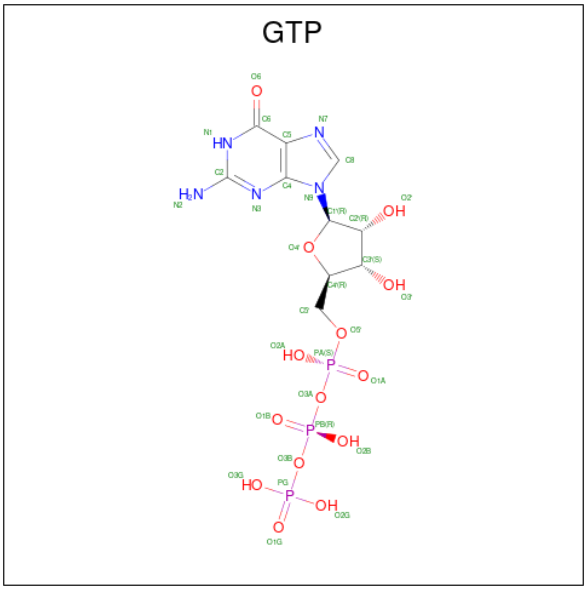
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

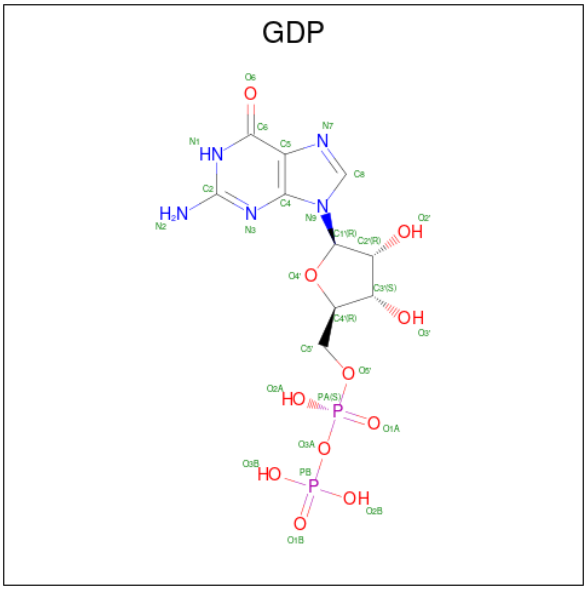
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3351	2105	575	646	25	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



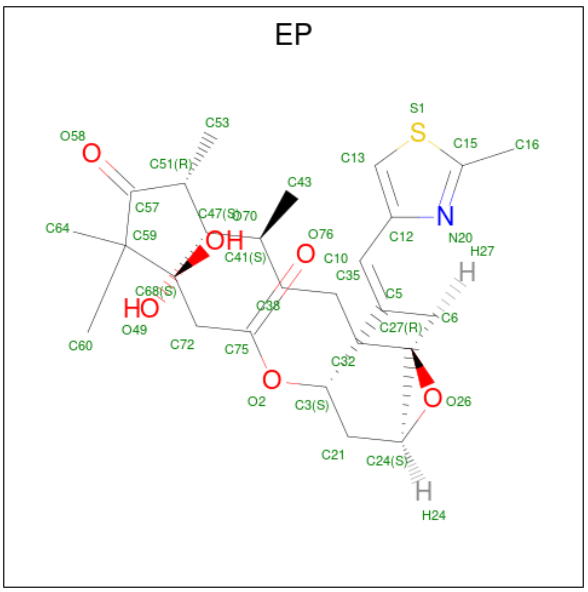
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 5 is EPOTHILONE A (three-letter code: EP) (formula: $C_{26}H_{39}NO_6S$).



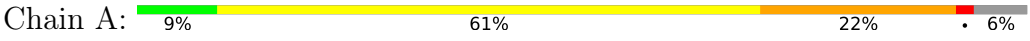
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	S	0
			34	26	1	6	1	

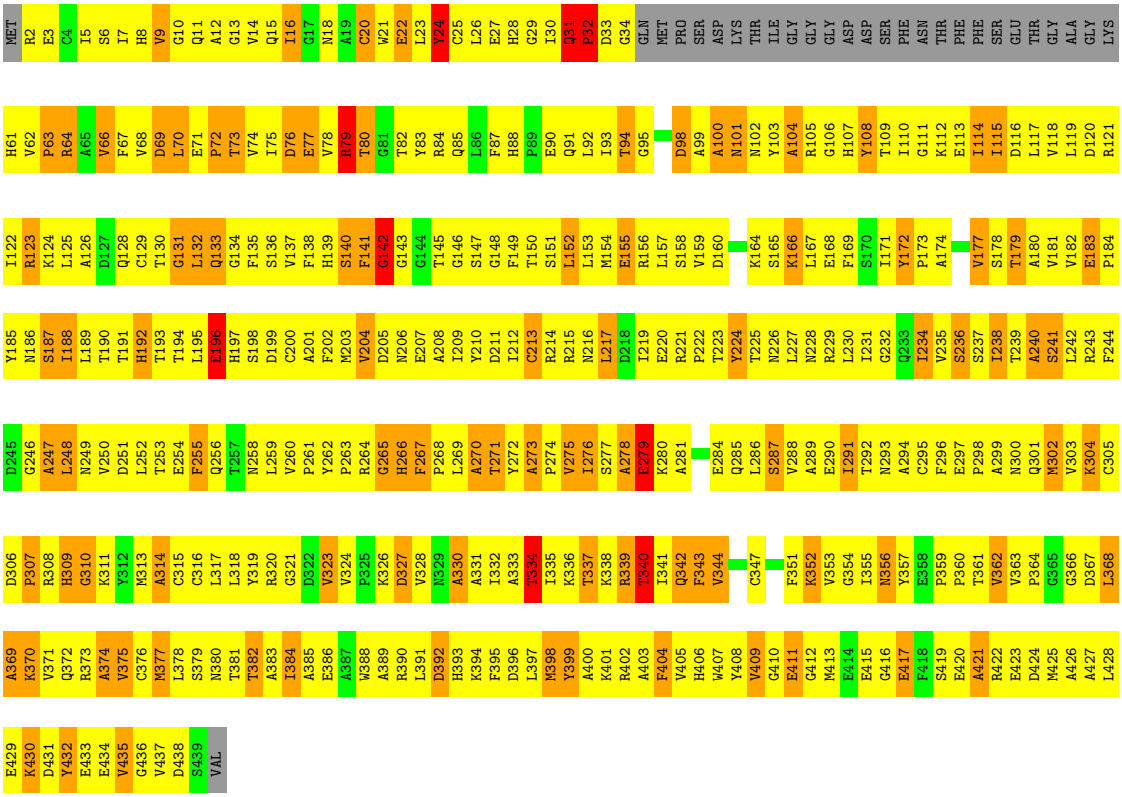
3 Residue-property plots (i)

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: Tubulin alpha chain

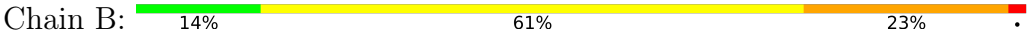
Chain A:

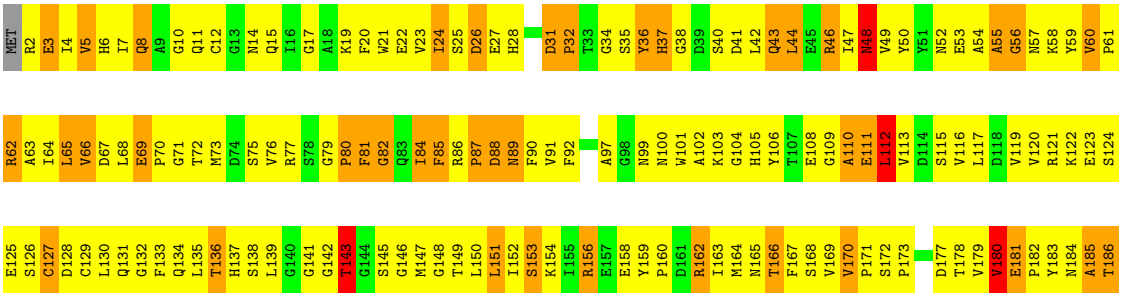


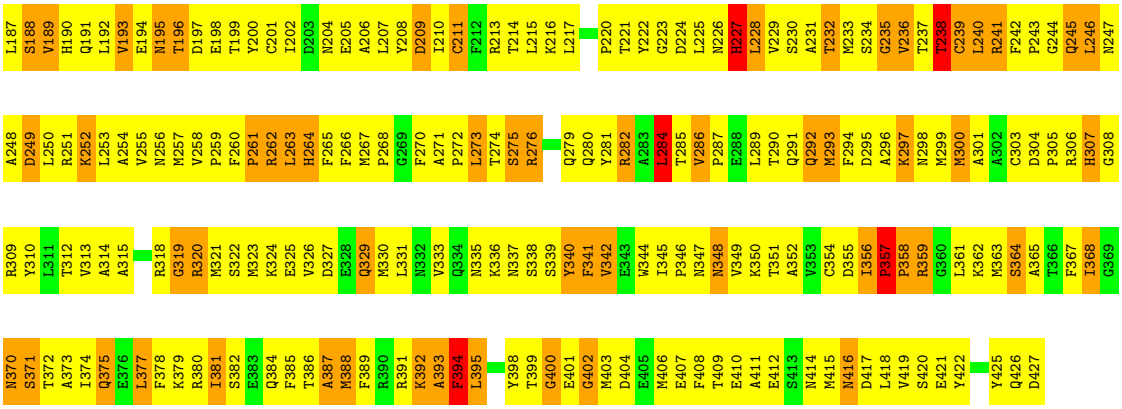


- Molecule 2: Tubulin beta chain

Chain B:






L187 S188 V189 H190 Q191 L192 V193 E194 N195 T196 D197 E198 T199 Y200 C201 I202 D203 N204 E205 A206 L207 Y208 D209 I210 C211 F212 R213 T214 L215 K216 L217 P220 T221 Y222 G223 D224 L225 N226 H227 L228 V229 S230 A231 T232 M233 S234 G235 V236 T237 T238 C239 L240 R241 F242 P243 G244 Q245 L246 N247
A248 D249 L250 R251 K252 L253 A254 V255 N256 M257 V258 P259 F260 P261 R262 L263 H264 F265 F266 M267 P268 G269 F270 A271 P272 L273 T274 S275 R276 Q279 Q280 Y281 R282 A283 L284 T285 V286 P287 E288 L289 T290 Q291 Q292 M293 F294 D295 A296 K297 N298 M299 M300 A301 A302 C303 D304 P305 R306 H307 G308
R309 Y310 L311 T312 V313 A314 A315 R318 G319 R320 M321 S322 M323 K324 E325 V326 D327 E328 Q329 M330 L331 N332 V333 Q334 N335 K336 N337 S338 S339 Y340 F341 V342 E343 W344 I345 P346 N347 N348 V349 K350 T351 A352 V353 C354 D355 I356 P357 P358 R359 G360 L361 K362 M363 S364 A365 T366 F367 I368 G369
M370 S371 T372 A373 I374 Q375 E376 L377 F378 K379 R380 I381 S382 E383 Q384 F385 T386 A387 M388 F389 R390 R391 K392 A393 F394 L395 Y398 T399 G400 E401 G402 M403 D404 E405 M406 E407 F408 T409 E410 A411 E412 S413 N414 M415 N416 D417 L418 V419 S420 E421 Y422 Y425 Q426 D427

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.20Å 93.50Å 90.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.89 23.84 – 2.89	Depositor EDS
% Data completeness (in resolution range)	67.0 (91.29-2.89) 63.9 (23.84-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.43 (at 2.89Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.333 , 0.321 0.314 , 0.303	Depositor DCC
R_{free} test set	967 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.096 for -h,-l,-k 0.070 for -h,l,k 0.118 for h,-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	6672	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8280e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GDP, EP, GTP

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	0.48	0/3300	0.71	2/4482 (0.0%)
2	B	0.51	0/3426	0.76	3/4642 (0.1%)
All	All	0.50	0/6726	0.73	5/9124 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	152	LEU	CA-CB-CG	6.52	130.30	115.30
2	B	282	ARG	CG-CD-NE	-6.12	98.96	111.80
1	A	142	GLY	N-CA-C	5.35	126.46	113.10
2	B	227	HIS	CG-CD2-NE2	-5.22	99.27	109.20
2	B	282	ARG	N-CA-CB	-5.22	101.20	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3227	0	3143	668	0
2	B	3351	0	3229	620	0
3	A	32	0	12	4	0
4	B	28	0	12	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	34	0	39	4	0
All	All	6672	0	6435	1260	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 96.

All (1260) 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:11:GLN:HG2	1:A:15:GLN:HE21	1.04	1.12
2:B:172:SER:HB3	2:B:205:GLU:HG2	1.16	1.10
2:B:286:VAL:H	2:B:287:PRO:HD2	1.11	1.09
1:A:229:ARG:HD3	1:A:363:VAL:HG21	1.33	1.08
2:B:285:THR:HB	2:B:287:PRO:HD2	1.31	1.07
1:A:242:LEU:HD12	1:A:250:VAL:HB	1.39	1.04
1:A:119:LEU:HD21	1:A:156:ARG:HB3	1.38	1.03
2:B:377:LEU:HG	2:B:381:ILE:HD11	1.40	1.00
2:B:40:SER:HB3	2:B:43:GLN:HG3	1.41	1.00
1:A:331:ALA:O	1:A:335:ILE:HG12	1.64	0.98
1:A:69:ASP:HB2	1:A:75:ILE:HD11	1.46	0.97
2:B:5:VAL:HG13	2:B:62:ARG:HG2	1.43	0.96
1:A:79:ARG:HA	1:A:84:ARG:HG3	1.47	0.95
1:A:217:LEU:HD12	1:A:277:SER:HA	1.47	0.95
2:B:113:VAL:HG21	2:B:150:LEU:HD23	1.46	0.95
1:A:276:ILE:HD11	1:A:281:ALA:HB3	1.48	0.93
1:A:23:LEU:HD12	1:A:26:LEU:HD23	1.49	0.93
2:B:139:LEU:HD13	2:B:168:SER:HB2	1.51	0.93
1:A:247:ALA:HB3	1:A:355:ILE:HB	1.47	0.93
2:B:286:VAL:H	2:B:287:PRO:CD	1.79	0.93
1:A:11:GLN:HG2	1:A:15:GLN:NE2	1.83	0.92
2:B:211:CYS:SG	2:B:220:PRO:HB3	2.08	0.92
2:B:356:ILE:HD12	2:B:357:PRO:HD2	1.52	0.92
1:A:107:HIS:CE1	1:A:152:LEU:HB3	2.06	0.91
2:B:329:GLN:O	2:B:333:VAL:HG23	1.71	0.91
2:B:241:ARG:HG3	2:B:241:ARG:HH11	1.36	0.91
2:B:236:VAL:HG22	2:B:368:ILE:HD11	1.52	0.91
1:A:359:PRO:HB3	1:A:372:GLN:O	1.71	0.90
1:A:259:LEU:HD21	1:A:316:CYS:HB2	1.53	0.90
2:B:3:GLU:HG3	2:B:130:LEU:HA	1.54	0.90
2:B:228:LEU:HD11	2:B:273:LEU:HD21	1.52	0.90
2:B:172:SER:CB	2:B:205:GLU:HG2	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:CD1	1:A:250:VAL:HB	2.03	0.89
1:A:179:THR:HG21	2:B:246:LEU:HD21	1.55	0.89
2:B:172:SER:HB3	2:B:205:GLU:CG	2.02	0.89
1:A:210:TYR:OH	2:B:323:MET:HB2	1.73	0.89
1:A:229:ARG:CD	1:A:363:VAL:HG21	2.02	0.89
2:B:226:ASN:ND2	4:B:1500:GDP:HN1	1.70	0.89
1:A:145:THR:O	1:A:149:PHE:HB3	1.74	0.88
2:B:254:ALA:O	2:B:258:VAL:HG22	1.72	0.88
2:B:271:ALA:CB	2:B:365:ALA:HB3	2.04	0.88
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.56	0.88
2:B:226:ASN:HD21	4:B:1500:GDP:HN1	0.88	0.87
2:B:77:ARG:HD3	2:B:90:PHE:CE2	2.09	0.87
2:B:287:PRO:O	2:B:291:GLN:HB2	1.72	0.87
2:B:221:THR:HG22	2:B:222:TYR:H	1.40	0.86
2:B:308:GLY:CA	2:B:426:GLN:HE21	1.89	0.86
1:A:178:SER:HB3	2:B:347:ASN:ND2	1.91	0.86
1:A:188:ILE:HG23	1:A:421:ALA:O	1.75	0.85
1:A:179:THR:O	2:B:350:LYS:HA	1.76	0.85
1:A:111:GLY:O	1:A:114:ILE:HD13	1.76	0.85
2:B:14:ASN:HD21	2:B:65:LEU:HB3	1.41	0.84
2:B:46:ARG:O	2:B:49:VAL:HG23	1.77	0.84
2:B:358:PRO:HB2	2:B:361:LEU:HB3	1.57	0.84
1:A:223:THR:HB	1:A:225:THR:HG22	1.58	0.83
1:A:115:ILE:HG13	1:A:152:LEU:CD1	2.08	0.83
2:B:190:HIS:ND1	2:B:411:ALA:HA	1.94	0.82
2:B:121:ARG:HD3	2:B:158:GLU:OE1	1.79	0.82
1:A:294:ALA:O	1:A:297:GLU:HG2	1.79	0.82
2:B:6:HIS:HB3	2:B:63:ALA:HB2	1.60	0.82
1:A:155:GLU:HG2	1:A:197:HIS:NE2	1.94	0.82
1:A:276:ILE:HG23	1:A:369:ALA:HB3	1.61	0.81
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.60	0.81
2:B:132:GLY:HA3	2:B:163:ILE:HD12	1.62	0.81
2:B:32:PRO:O	2:B:84:ILE:HB	1.79	0.81
1:A:243:ARG:NH2	1:A:252:LEU:HG	1.95	0.81
1:A:9:VAL:HG23	1:A:145:THR:HG22	1.63	0.81
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.63	0.81
2:B:361:LEU:HB2	5:B:1001:EP:H432	1.63	0.80
2:B:24:ILE:HD11	2:B:238:THR:HG21	1.64	0.80
1:A:167:LEU:HD23	1:A:200:CYS:HB3	1.62	0.80
1:A:234:ILE:HD13	1:A:234:ILE:O	1.81	0.80
1:A:339:ARG:C	1:A:341:ILE:H	1.83	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:VAL:HB	2:B:377:LEU:HD11	1.63	0.80
1:A:141:PHE:HB2	1:A:173:PRO:HD3	1.63	0.80
1:A:238:ILE:HG12	1:A:378:LEU:CD2	2.12	0.79
2:B:8:GLN:CD	2:B:65:LEU:HD22	2.03	0.79
1:A:123:ARG:HB2	1:A:123:ARG:HH11	1.48	0.79
1:A:151:SER:HB3	1:A:193:THR:HG21	1.65	0.79
1:A:195:LEU:HD11	1:A:264:ARG:HD2	1.63	0.79
2:B:271:ALA:HB3	2:B:365:ALA:HB3	1.66	0.78
1:A:148:GLY:O	1:A:151:SER:HB2	1.83	0.78
2:B:104:GLY:O	2:B:109:GLY:HA3	1.83	0.78
1:A:7:ILE:HD12	1:A:137:VAL:HG22	1.66	0.78
1:A:278:ALA:O	1:A:279:GLU:HG2	1.84	0.78
2:B:286:VAL:HG22	2:B:321:MET:HE3	1.65	0.78
2:B:102:ALA:O	2:B:106:TYR:HB2	1.83	0.77
1:A:84:ARG:HH12	1:A:85:GLN:HG2	1.48	0.77
1:A:182:VAL:HG23	1:A:186:ASN:HD21	1.49	0.77
1:A:250:VAL:HA	1:A:254:GLU:OE1	1.83	0.77
1:A:238:ILE:C	1:A:242:LEU:HD23	2.04	0.77
1:A:308:ARG:O	1:A:309:HIS:HB3	1.84	0.77
2:B:237:THR:HG22	2:B:238:THR:H	1.49	0.77
1:A:276:ILE:CD1	1:A:281:ALA:HB3	2.14	0.77
2:B:293:MET:SD	2:B:365:ALA:HB1	2.24	0.77
2:B:152:ILE:HB	2:B:164:MET:HE1	1.67	0.77
1:A:420:GLU:O	1:A:422:ARG:N	2.18	0.76
2:B:282:ARG:NH1	5:B:1001:EP:O49	2.18	0.76
2:B:197:ASP:HA	2:B:263:LEU:HB2	1.67	0.76
1:A:167:LEU:HD13	1:A:252:LEU:HD22	1.67	0.76
1:A:243:ARG:HH21	1:A:252:LEU:HG	1.50	0.76
1:A:278:ALA:HB2	1:A:369:ALA:N	2.01	0.76
1:A:120:ASP:HA	1:A:123:ARG:HH12	1.48	0.76
2:B:110:ALA:O	2:B:112:LEU:N	2.17	0.76
1:A:69:ASP:HA	1:A:145:THR:HG21	1.67	0.76
1:A:391:LEU:HD23	1:A:391:LEU:O	1.85	0.76
2:B:55:ALA:HB3	2:B:58:LYS:HB2	1.67	0.76
2:B:287:PRO:HB3	2:B:329:GLN:OE1	1.85	0.76
2:B:221:THR:HG22	2:B:222:TYR:N	2.01	0.76
1:A:412:GLY:O	1:A:413:MET:HG2	1.86	0.75
2:B:166:THR:HG22	2:B:199:THR:HG23	1.67	0.75
1:A:201:ALA:HB3	1:A:267:PHE:HB3	1.68	0.75
2:B:177:ASP:HB2	4:B:1500:GDP:O3'	1.87	0.75
1:A:151:SER:HB3	1:A:193:THR:CG2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ILE:CD1	2:B:131:GLN:HB3	2.16	0.75
2:B:240:LEU:HD22	2:B:248:ALA:O	1.86	0.75
2:B:196:THR:O	2:B:263:LEU:HB2	1.86	0.75
2:B:139:LEU:CD1	2:B:168:SER:HB2	2.17	0.75
1:A:241:SER:OG	1:A:242:LEU:HD22	1.87	0.74
2:B:154:LYS:NZ	2:B:154:LYS:HB3	2.02	0.74
2:B:183:TYR:HA	2:B:385:PHE:HE1	1.53	0.74
2:B:315:ALA:HB3	2:B:330:MET:HE1	1.69	0.74
2:B:19:LYS:O	2:B:23:VAL:HG23	1.88	0.73
2:B:145:SER:O	2:B:149:THR:HG23	1.88	0.73
1:A:237:SER:O	1:A:239:THR:N	2.22	0.73
1:A:296:PHE:CD2	1:A:341:ILE:HD11	2.24	0.73
1:A:184:PRO:HG2	1:A:398:MET:CE	2.19	0.73
2:B:315:ALA:HB3	2:B:330:MET:CE	2.17	0.73
1:A:368:LEU:O	1:A:370:LYS:N	2.21	0.73
1:A:362:VAL:HG21	1:A:368:LEU:O	1.88	0.73
2:B:206:ALA:O	2:B:210:ILE:HG13	1.87	0.73
1:A:155:GLU:O	1:A:159:VAL:HG12	1.89	0.72
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.19	0.72
2:B:286:VAL:N	2:B:287:PRO:HD2	1.96	0.72
1:A:79:ARG:CA	1:A:84:ARG:HG3	2.19	0.72
1:A:271:THR:CG2	1:A:272:TYR:N	2.51	0.72
2:B:132:GLY:HA3	2:B:163:ILE:CD1	2.19	0.72
1:A:420:GLU:C	1:A:422:ARG:H	1.90	0.72
2:B:308:GLY:HA2	2:B:426:GLN:HE21	1.53	0.72
1:A:238:ILE:O	1:A:242:LEU:HD23	1.89	0.72
1:A:271:THR:HG23	1:A:272:TYR:H	1.55	0.72
2:B:221:THR:O	2:B:225:LEU:HD23	1.89	0.72
1:A:311:LYS:H	1:A:382:THR:HB	1.55	0.72
2:B:310:TYR:HB2	2:B:340:TYR:O	1.90	0.72
1:A:229:ARG:HD3	1:A:363:VAL:CG2	2.18	0.72
1:A:238:ILE:HG12	1:A:378:LEU:HD22	1.72	0.71
2:B:308:GLY:HA3	2:B:426:GLN:HE21	1.52	0.71
1:A:88:HIS:H	1:A:91:GLN:NE2	1.87	0.71
1:A:195:LEU:HD21	1:A:264:ARG:NH1	2.05	0.71
1:A:402:ARG:O	1:A:405:VAL:HG23	1.88	0.71
2:B:77:ARG:HD3	2:B:90:PHE:HE2	1.54	0.71
2:B:164:MET:HB3	2:B:196:THR:HA	1.70	0.71
2:B:240:LEU:CD2	2:B:248:ALA:H	2.02	0.71
2:B:258:VAL:HG23	2:B:258:VAL:O	1.90	0.71
2:B:64:ILE:HD13	2:B:120:VAL:HG12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:PHE:CE1	2:B:418:LEU:HD21	2.26	0.71
1:A:16:ILE:HD11	1:A:138:PHE:HD2	1.56	0.71
1:A:115:ILE:HG13	1:A:152:LEU:HD12	1.71	0.70
2:B:326:VAL:HG11	2:B:351:THR:HG21	1.73	0.70
2:B:11:GLN:HG3	2:B:72:THR:OG1	1.91	0.70
1:A:252:LEU:O	1:A:255:PHE:HB2	1.92	0.70
1:A:84:ARG:NH1	1:A:85:GLN:HG2	2.05	0.70
2:B:48:ASN:HD22	2:B:48:ASN:N	1.89	0.70
2:B:66:VAL:HA	2:B:91:VAL:HG23	1.74	0.70
1:A:132:LEU:HD23	1:A:132:LEU:H	1.57	0.70
1:A:141:PHE:O	1:A:147:SER:HB3	1.90	0.70
2:B:285:THR:CB	2:B:287:PRO:HD2	2.15	0.70
1:A:264:ARG:C	1:A:266:HIS:H	1.95	0.70
2:B:181:GLU:HB3	2:B:182:PRO:CD	2.22	0.70
1:A:393:HIS:HA	1:A:396:ASP:OD2	1.92	0.70
2:B:10:GLY:HA2	2:B:67:ASP:OD1	1.91	0.70
1:A:102:ASN:HD21	1:A:411:GLU:HG2	1.57	0.69
1:A:106:GLY:O	1:A:111:GLY:HA3	1.92	0.69
1:A:404:PHE:HZ	2:B:312:THR:HG21	1.57	0.69
1:A:267:PHE:CD1	1:A:267:PHE:N	2.60	0.69
1:A:239:THR:HG22	1:A:240:ALA:N	2.07	0.69
2:B:253:LEU:O	2:B:257:MET:N	2.25	0.69
1:A:62:VAL:CG2	1:A:63:PRO:HD2	2.22	0.69
1:A:69:ASP:HB2	1:A:75:ILE:CD1	2.20	0.69
1:A:381:THR:HG23	1:A:383:ALA:HB3	1.73	0.69
2:B:66:VAL:HA	2:B:91:VAL:O	1.92	0.69
1:A:221:ARG:N	1:A:222:PRO:HD3	2.07	0.69
2:B:117:LEU:O	2:B:120:VAL:HG22	1.93	0.69
1:A:11:GLN:HA	1:A:74:VAL:HG11	1.75	0.69
1:A:217:LEU:HA	1:A:277:SER:HB2	1.75	0.69
1:A:384:ILE:HD13	1:A:384:ILE:H	1.58	0.69
2:B:64:ILE:C	2:B:65:LEU:HD23	2.13	0.69
1:A:14:VAL:HG21	1:A:75:ILE:HD13	1.74	0.69
1:A:311:LYS:CD	1:A:342:GLN:HE22	2.06	0.69
1:A:319:TYR:O	1:A:355:ILE:HA	1.93	0.69
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.28	0.69
1:A:73:THR:HG23	1:A:77:GLU:OE2	1.93	0.68
1:A:279:GLU:HA	1:A:279:GLU:OE1	1.94	0.68
2:B:177:ASP:OD2	4:B:1500:GDP:H2'	1.94	0.68
1:A:272:TYR:CE2	1:A:274:PRO:HG2	2.29	0.68
2:B:356:ILE:HD12	2:B:357:PRO:CD	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:HE2	2:B:223:GLY:HA2	1.75	0.68
2:B:103:LYS:HE3	2:B:108:GLU:OE2	1.93	0.68
1:A:220:GLU:C	1:A:222:PRO:HD3	2.14	0.68
2:B:154:LYS:HB3	2:B:154:LYS:HZ2	1.59	0.68
1:A:167:LEU:HD11	1:A:252:LEU:HB3	1.74	0.68
2:B:183:TYR:HA	2:B:385:PHE:CE1	2.29	0.68
2:B:149:THR:HB	2:B:191:GLN:HG2	1.75	0.67
2:B:149:THR:HB	2:B:191:GLN:CB	2.24	0.67
1:A:291:ILE:HG21	1:A:373:ARG:HD2	1.74	0.67
1:A:241:SER:O	1:A:244:PHE:N	2.25	0.67
1:A:284:GLU:O	1:A:286:LEU:N	2.27	0.67
1:A:306:ASP:O	1:A:308:ARG:N	2.26	0.67
2:B:60:VAL:HG11	2:B:86:ARG:HG2	1.77	0.67
2:B:185:ALA:O	2:B:188:SER:N	2.26	0.67
2:B:130:LEU:HD23	2:B:162:ARG:NH1	2.10	0.67
1:A:120:ASP:HA	1:A:123:ARG:NH1	2.10	0.67
1:A:195:LEU:HG	1:A:196:GLU:OE1	1.93	0.67
1:A:291:ILE:CD1	1:A:375:VAL:HG22	2.25	0.67
1:A:297:GLU:OE2	1:A:299:ALA:HB3	1.94	0.67
2:B:392:LYS:O	2:B:393:ALA:O	2.12	0.67
1:A:2:ARG:O	1:A:2:ARG:HG2	1.94	0.67
1:A:406:HIS:HA	1:A:409:VAL:HG23	1.76	0.67
2:B:248:ALA:HA	2:B:252:LYS:HD3	1.77	0.67
2:B:178:THR:HG22	2:B:179:VAL:H	1.60	0.66
2:B:290:THR:HA	2:B:293:MET:CE	2.25	0.66
2:B:333:VAL:O	2:B:337:ASN:HB3	1.95	0.66
2:B:47:ILE:C	2:B:49:VAL:H	1.98	0.66
2:B:227:HIS:O	2:B:229:VAL:N	2.27	0.66
1:A:235:VAL:C	1:A:237:SER:H	1.96	0.66
1:A:252:LEU:HA	1:A:255:PHE:CD1	2.29	0.66
2:B:6:HIS:HE1	2:B:8:GLN:HB3	1.61	0.66
1:A:242:LEU:HB3	1:A:250:VAL:O	1.94	0.66
1:A:276:ILE:CG1	1:A:281:ALA:HB3	2.25	0.66
2:B:115:SER:O	2:B:119:VAL:HG23	1.96	0.66
2:B:184:ASN:O	2:B:188:SER:HB2	1.94	0.66
2:B:217:LEU:HD21	2:B:224:ASP:OD2	1.95	0.66
1:A:234:ILE:HG13	1:A:270:ALA:HB1	1.77	0.66
2:B:193:VAL:HG22	2:B:262:ARG:HH11	1.58	0.66
1:A:105:ARG:O	1:A:110:ILE:HG12	1.95	0.66
1:A:371:VAL:HG12	1:A:372:GLN:H	1.59	0.66
1:A:14:VAL:HG21	1:A:75:ILE:CD1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TYR:CE1	1:A:413:MET:SD	2.89	0.66
1:A:119:LEU:HD13	1:A:156:ARG:CZ	2.26	0.66
2:B:4:ILE:HD13	2:B:131:GLN:HB3	1.75	0.65
2:B:113:VAL:HG21	2:B:150:LEU:CD2	2.21	0.65
1:A:123:ARG:O	1:A:126:ALA:N	2.28	0.65
1:A:138:PHE:HZ	1:A:235:VAL:HG11	1.61	0.65
2:B:286:VAL:HG22	2:B:321:MET:CE	2.26	0.65
1:A:244:PHE:CB	1:A:356:ASN:HD21	2.08	0.65
1:A:255:PHE:O	1:A:259:LEU:N	2.29	0.65
2:B:137:HIS:CE1	2:B:168:SER:HB3	2.31	0.65
1:A:324:VAL:HG12	1:A:326:LYS:H	1.62	0.65
2:B:205:GLU:O	2:B:208:TYR:HB2	1.96	0.65
2:B:210:ILE:CG2	2:B:298:ASN:HA	2.26	0.65
1:A:173:PRO:HB2	1:A:391:LEU:HD11	1.79	0.65
2:B:290:THR:HA	2:B:293:MET:HE2	1.79	0.65
2:B:199:THR:HB	2:B:265:PHE:CD2	2.32	0.65
2:B:322:SER:HB3	2:B:325:GLU:CD	2.17	0.65
1:A:381:THR:C	1:A:383:ALA:H	2.00	0.64
1:A:273:ALA:H	1:A:274:PRO:HD2	1.62	0.64
1:A:309:HIS:CG	1:A:310:GLY:N	2.64	0.64
1:A:373:ARG:O	1:A:374:ALA:HB2	1.98	0.64
1:A:27:GLU:O	1:A:28:HIS:HD2	1.79	0.64
1:A:114:ILE:O	1:A:118:VAL:HG23	1.97	0.64
1:A:242:LEU:HD22	1:A:242:LEU:H	1.62	0.64
2:B:53:GLU:HG2	2:B:59:TYR:HE2	1.62	0.64
2:B:73:MET:HE1	2:B:92:PHE:HD2	1.63	0.64
2:B:127:CYS:O	2:B:128:ASP:HB2	1.97	0.64
1:A:167:LEU:HD12	1:A:252:LEU:HD13	1.78	0.64
2:B:190:HIS:HA	2:B:414:ASN:HD22	1.63	0.64
2:B:210:ILE:HG23	2:B:298:ASN:HA	1.80	0.64
2:B:211:CYS:O	2:B:215:LEU:HB2	1.97	0.64
1:A:288:VAL:HG22	1:A:323:VAL:HG13	1.77	0.64
2:B:166:THR:CG2	2:B:199:THR:HG23	2.28	0.64
2:B:377:LEU:HG	2:B:381:ILE:CD1	2.24	0.64
1:A:202:PHE:CE2	1:A:378:LEU:HD13	2.32	0.64
1:A:420:GLU:N	1:A:420:GLU:OE2	2.31	0.64
2:B:102:ALA:HB2	2:B:403:MET:SD	2.37	0.64
2:B:200:TYR:HB3	2:B:268:PRO:CG	2.28	0.64
1:A:172:TYR:OH	1:A:388:TRP:CE3	2.51	0.64
1:A:239:THR:O	1:A:240:ALA:C	2.36	0.64
2:B:80:PRO:O	2:B:82:GLY:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:O	1:A:16:ILE:HG22	1.98	0.63
2:B:249:ASP:H	2:B:252:LYS:HG3	1.64	0.63
1:A:7:ILE:HG21	1:A:153:LEU:CD2	2.25	0.63
1:A:71:GLU:HG2	2:B:2:ARG:NH1	2.12	0.63
1:A:98:ASP:HB3	2:B:251:ARG:HG3	1.80	0.63
1:A:269:LEU:O	1:A:269:LEU:HD12	1.97	0.63
2:B:3:GLU:HG3	2:B:130:LEU:CA	2.28	0.63
1:A:102:ASN:HD21	1:A:105:ARG:HB2	1.64	0.63
1:A:132:LEU:HD23	1:A:132:LEU:N	2.14	0.63
2:B:14:ASN:ND2	2:B:65:LEU:HB3	2.12	0.63
1:A:208:ALA:HB2	1:A:304:LYS:N	2.14	0.63
1:A:311:LYS:HD3	1:A:342:GLN:HE22	1.63	0.63
2:B:245:GLN:O	2:B:246:LEU:HB2	1.99	0.63
1:A:167:LEU:CD1	1:A:252:LEU:HD13	2.29	0.63
2:B:263:LEU:O	2:B:264:HIS:O	2.17	0.63
1:A:66:VAL:HG23	1:A:91:GLN:O	1.99	0.63
1:A:184:PRO:HG2	1:A:398:MET:HE2	1.79	0.63
1:A:336:LYS:O	1:A:341:ILE:HG21	1.99	0.63
2:B:241:ARG:HH11	2:B:241:ARG:CG	2.09	0.63
2:B:344:TRP:CZ3	2:B:345:ILE:HD11	2.34	0.63
2:B:271:ALA:HB2	2:B:365:ALA:HB3	1.80	0.63
2:B:358:PRO:HG2	2:B:364:SER:OG	1.99	0.63
1:A:242:LEU:HD12	1:A:250:VAL:CB	2.25	0.62
2:B:190:HIS:CG	2:B:411:ALA:HA	2.34	0.62
2:B:285:THR:HB	2:B:287:PRO:CD	2.18	0.62
1:A:147:SER:O	1:A:190:THR:HG23	1.98	0.62
2:B:103:LYS:HG3	2:B:401:GLU:HG3	1.81	0.62
2:B:181:GLU:OE2	2:B:181:GLU:HA	1.99	0.62
2:B:231:ALA:O	2:B:234:SER:HB3	1.98	0.62
1:A:2:ARG:N	1:A:131:GLY:O	2.33	0.62
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.34	0.62
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.81	0.62
2:B:112:LEU:O	2:B:116:VAL:HG23	1.99	0.62
2:B:275:SER:OG	2:B:279:GLN:HB2	2.00	0.62
2:B:377:LEU:O	2:B:381:ILE:HG12	1.99	0.62
2:B:86:ARG:O	2:B:89:ASN:HB2	2.00	0.62
2:B:137:HIS:HE1	2:B:168:SER:HB3	1.64	0.62
1:A:267:PHE:CZ	1:A:428:LEU:HD21	2.35	0.62
1:A:311:LYS:HE2	1:A:437:VAL:H	1.63	0.62
2:B:171:PRO:HB3	2:B:181:GLU:CG	2.29	0.62
1:A:9:VAL:CG2	1:A:145:THR:HG22	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:THR:HB	2:B:265:PHE:HD2	1.64	0.62
1:A:138:PHE:CE2	1:A:235:VAL:HG21	2.35	0.62
1:A:237:SER:O	1:A:238:ILE:C	2.37	0.62
1:A:244:PHE:HB3	1:A:356:ASN:HD21	1.65	0.62
1:A:290:GLU:CD	1:A:290:GLU:H	2.04	0.62
2:B:87:PRO:HG2	2:B:88:ASP:H	1.63	0.61
1:A:354:GLY:O	1:A:355:ILE:HG13	2.00	0.61
1:A:115:ILE:HG23	1:A:116:ASP:N	2.15	0.61
2:B:88:ASP:OD2	2:B:88:ASP:N	2.34	0.61
2:B:180:VAL:HG12	2:B:183:TYR:HD1	1.66	0.61
2:B:193:VAL:HG13	2:B:194:GLU:CG	2.30	0.61
1:A:362:VAL:CG2	1:A:370:LYS:HB2	2.29	0.61
1:A:429:GLU:C	1:A:431:ASP:H	2.02	0.61
2:B:248:ALA:HA	2:B:252:LYS:CD	2.31	0.61
1:A:273:ALA:O	1:A:275:VAL:HG23	2.00	0.61
2:B:50:TYR:OH	2:B:134:GLN:HG3	2.01	0.61
1:A:172:TYR:CZ	1:A:391:LEU:HD13	2.35	0.61
1:A:101:ASN:OD1	2:B:252:LYS:HE3	2.01	0.61
1:A:109:THR:HG22	1:A:110:ILE:HG23	1.83	0.61
2:B:280:GLN:O	2:B:282:ARG:HG3	2.01	0.61
1:A:16:ILE:HD11	1:A:138:PHE:CD2	2.36	0.61
1:A:133:GLN:O	1:A:164:LYS:HB3	2.00	0.61
2:B:395:LEU:O	2:B:395:LEU:HD13	2.01	0.61
2:B:101:TRP:HB2	2:B:184:ASN:OD1	2.01	0.61
1:A:178:SER:HB3	2:B:347:ASN:CG	2.20	0.61
2:B:131:GLN:O	2:B:163:ILE:HG13	2.01	0.61
1:A:256:GLN:O	1:A:260:VAL:HG12	2.01	0.60
2:B:2:ARG:HD2	2:B:131:GLN:NE2	2.16	0.60
2:B:244:GLY:C	2:B:246:LEU:H	2.05	0.60
1:A:264:ARG:O	1:A:266:HIS:N	2.32	0.60
2:B:52:ASN:HB3	2:B:60:VAL:HG23	1.83	0.60
2:B:210:ILE:HD12	2:B:300:MET:HE3	1.83	0.60
2:B:116:VAL:O	2:B:120:VAL:HG13	2.01	0.60
2:B:375:GLN:O	2:B:379:LYS:HB2	2.02	0.60
2:B:193:VAL:HG13	2:B:194:GLU:HG3	1.83	0.60
1:A:315:CYS:HG	1:A:343:PHE:HZ	1.47	0.60
2:B:36:TYR:C	2:B:38:GLY:H	2.04	0.60
2:B:322:SER:HB3	2:B:325:GLU:HG2	1.83	0.60
1:A:71:GLU:HG2	2:B:2:ARG:HH12	1.66	0.60
1:A:93:ILE:HD13	1:A:117:LEU:HG	1.83	0.60
1:A:110:ILE:O	1:A:113:GLU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:H	1:A:132:LEU:CD2	2.14	0.60
1:A:404:PHE:N	1:A:404:PHE:CD1	2.67	0.60
1:A:214:ARG:HG3	1:A:220:GLU:OE1	2.01	0.60
2:B:240:LEU:HD22	2:B:248:ALA:H	1.64	0.60
1:A:72:PRO:O	1:A:74:VAL:N	2.34	0.60
1:A:227:LEU:O	1:A:231:ILE:HG12	2.01	0.60
1:A:294:ALA:HB1	1:A:300:ASN:HD21	1.66	0.60
1:A:242:LEU:HD21	1:A:318:LEU:CD1	2.31	0.59
1:A:249:ASN:H	1:A:249:ASN:HD22	1.49	0.59
1:A:376:CYS:O	1:A:377:MET:C	2.38	0.59
2:B:177:ASP:HB2	4:B:1500:GDP:C3'	2.33	0.59
2:B:341:PHE:O	2:B:348:ASN:ND2	2.35	0.59
2:B:105:HIS:CD2	2:B:150:LEU:HB2	2.37	0.59
1:A:298:PRO:HB3	1:A:307:PRO:HD2	1.85	0.59
1:A:303:VAL:C	1:A:305:CYS:H	2.06	0.59
1:A:316:CYS:SG	1:A:318:LEU:HD21	2.43	0.59
1:A:434:GLU:O	1:A:436:GLY:O	2.20	0.59
1:A:339:ARG:C	1:A:341:ILE:N	2.55	0.59
1:A:371:VAL:HG12	1:A:372:GLN:N	2.17	0.59
2:B:68:LEU:O	2:B:97:ALA:HB2	2.03	0.59
1:A:103:TYR:O	1:A:105:ARG:N	2.36	0.59
1:A:177:VAL:HB	2:B:327:ASP:HB3	1.85	0.59
1:A:359:PRO:HB2	1:A:360:PRO:HD2	1.85	0.59
2:B:23:VAL:HG21	2:B:230:SER:HB3	1.83	0.59
2:B:100:ASN:HB3	2:B:103:LYS:HB2	1.85	0.59
2:B:335:ASN:C	2:B:337:ASN:H	2.04	0.59
2:B:394:PHE:HD1	2:B:394:PHE:H	1.49	0.59
1:A:16:ILE:CD1	1:A:138:PHE:HD2	2.16	0.59
2:B:121:ARG:HA	2:B:124:SER:HB2	1.85	0.59
1:A:101:ASN:O	1:A:182:VAL:HG21	2.03	0.59
2:B:4:ILE:HD11	2:B:131:GLN:HB3	1.84	0.59
1:A:362:VAL:HB	1:A:370:LYS:HB2	1.84	0.59
1:A:384:ILE:HD13	1:A:384:ILE:N	2.18	0.59
2:B:42:LEU:C	2:B:44:LEU:H	2.06	0.59
2:B:121:ARG:O	2:B:125:GLU:HG2	2.01	0.59
2:B:163:ILE:HD12	2:B:163:ILE:O	2.03	0.59
1:A:61:HIS:CD2	1:A:62:VAL:HG12	2.37	0.58
2:B:46:ARG:HG2	2:B:241:ARG:O	2.03	0.58
2:B:149:THR:HB	2:B:191:GLN:CG	2.32	0.58
1:A:62:VAL:HG23	1:A:63:PRO:HD2	1.85	0.58
1:A:142:GLY:H	1:A:173:PRO:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:THR:CG2	2:B:222:TYR:H	2.15	0.58
2:B:248:ALA:HA	2:B:252:LYS:CE	2.33	0.58
1:A:210:TYR:CE2	1:A:227:LEU:HD11	2.38	0.58
2:B:335:ASN:O	2:B:337:ASN:N	2.36	0.58
1:A:104:ALA:CB	1:A:413:MET:HG3	2.34	0.58
1:A:184:PRO:HG2	1:A:398:MET:HE1	1.85	0.58
1:A:188:ILE:HD11	1:A:392:ASP:HA	1.85	0.58
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.32	0.58
1:A:276:ILE:HD13	1:A:277:SER:C	2.24	0.58
1:A:287:SER:HA	1:A:373:ARG:HH21	1.68	0.58
1:A:398:MET:O	1:A:400:ALA:N	2.36	0.58
2:B:377:LEU:HD23	2:B:378:PHE:N	2.18	0.58
1:A:11:GLN:HG3	1:A:74:VAL:CG1	2.34	0.58
1:A:309:HIS:NE2	1:A:382:THR:O	2.37	0.58
2:B:206:ALA:HB3	2:B:300:MET:O	2.02	0.58
1:A:192:HIS:ND1	1:A:193:THR:N	2.52	0.58
1:A:195:LEU:HD21	1:A:264:ARG:CZ	2.34	0.58
1:A:277:SER:HB3	1:A:280:LYS:HB3	1.84	0.58
1:A:278:ALA:O	1:A:279:GLU:CG	2.52	0.58
1:A:362:VAL:HG22	1:A:368:LEU:HD12	1.86	0.58
1:A:381:THR:O	1:A:383:ALA:N	2.33	0.58
2:B:261:PRO:O	2:B:263:LEU:N	2.36	0.58
2:B:359:ARG:CA	2:B:359:ARG:HH11	2.16	0.58
1:A:24:TYR:CE2	1:A:240:ALA:HB2	2.38	0.58
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.85	0.58
1:A:71:GLU:HB2	1:A:99:ALA:HB2	1.86	0.58
1:A:138:PHE:HZ	1:A:235:VAL:CG1	2.16	0.58
1:A:189:LEU:HD23	1:A:421:ALA:CB	2.33	0.58
2:B:23:VAL:HG21	2:B:230:SER:CB	2.34	0.58
2:B:399:THR:O	2:B:402:GLY:N	2.37	0.58
1:A:70:LEU:HG	1:A:145:THR:OG1	2.03	0.58
1:A:404:PHE:HD1	1:A:404:PHE:H	1.52	0.58
2:B:262:ARG:C	2:B:264:HIS:H	2.06	0.58
1:A:7:ILE:HD13	1:A:153:LEU:HD21	1.84	0.57
1:A:7:ILE:CD1	1:A:157:LEU:HD11	2.34	0.57
2:B:19:LYS:HG2	2:B:226:ASN:HB2	1.84	0.57
2:B:36:TYR:CD2	2:B:44:LEU:HD22	2.39	0.57
2:B:152:ILE:CB	2:B:164:MET:HE1	2.32	0.57
2:B:192:LEU:O	2:B:194:GLU:N	2.37	0.57
2:B:253:LEU:O	2:B:257:MET:HB2	2.04	0.57
2:B:319:GLY:O	2:B:320:ARG:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:HG22	1:A:83:TYR:CD1	2.40	0.57
1:A:141:PHE:CE2	1:A:191:THR:HB	2.40	0.57
2:B:19:LYS:HB2	2:B:226:ASN:HB3	1.87	0.57
1:A:195:LEU:O	1:A:197:HIS:N	2.36	0.57
1:A:195:LEU:HD12	1:A:265:GLY:H	1.68	0.57
1:A:420:GLU:C	1:A:422:ARG:N	2.58	0.57
1:A:12:ALA:O	1:A:15:GLN:N	2.38	0.57
1:A:241:SER:O	1:A:244:PHE:HB2	2.04	0.57
1:A:291:ILE:CG2	1:A:373:ARG:HD2	2.34	0.57
1:A:344:VAL:HG23	1:A:347:CYS:HB3	1.86	0.57
2:B:24:ILE:CD1	2:B:238:THR:HG21	2.33	0.57
2:B:164:MET:O	2:B:197:ASP:OD2	2.21	0.57
2:B:136:THR:HG23	2:B:233:MET:CE	2.35	0.57
2:B:237:THR:O	2:B:239:CYS:N	2.38	0.57
2:B:263:LEU:O	2:B:263:LEU:HD12	2.05	0.57
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.69	0.57
1:A:138:PHE:HE2	1:A:235:VAL:HG21	1.69	0.57
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.87	0.57
1:A:260:VAL:HG23	1:A:266:HIS:HB2	1.87	0.56
2:B:113:VAL:CG2	2:B:150:LEU:HD23	2.30	0.56
2:B:164:MET:HG3	2:B:195:ASN:O	2.05	0.56
1:A:270:ALA:O	1:A:302:MET:HB2	2.05	0.56
1:A:427:ALA:C	1:A:429:GLU:H	2.07	0.56
2:B:44:LEU:HD11	2:B:47:ILE:HD13	1.87	0.56
1:A:179:THR:CG2	2:B:246:LEU:HD21	2.32	0.56
2:B:54:ALA:C	2:B:56:GLY:H	2.08	0.56
1:A:182:VAL:CG2	1:A:186:ASN:HD21	2.17	0.56
1:A:310:GLY:HA2	1:A:382:THR:O	2.05	0.56
2:B:106:TYR:HE2	2:B:403:MET:SD	2.28	0.56
2:B:216:LYS:HD3	2:B:275:SER:HB3	1.86	0.56
2:B:241:ARG:HG3	2:B:241:ARG:NH1	2.15	0.56
2:B:337:ASN:O	2:B:337:ASN:ND2	2.39	0.56
2:B:384:GLN:O	2:B:387:ALA:HB3	2.06	0.56
1:A:71:GLU:O	1:A:71:GLU:OE2	2.24	0.56
2:B:270:PHE:CE2	2:B:272:PRO:HG2	2.41	0.56
1:A:384:ILE:H	1:A:384:ILE:CD1	2.15	0.56
1:A:406:HIS:C	1:A:408:TYR:H	2.07	0.56
2:B:170:VAL:CB	2:B:377:LEU:HD11	2.34	0.56
2:B:236:VAL:CG2	2:B:368:ILE:HD11	2.31	0.56
1:A:77:GLU:HG2	2:B:243:PRO:HB3	1.88	0.56
1:A:104:ALA:HB1	1:A:413:MET:HG3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:CYS:SG	2:B:138:SER:HB3	2.46	0.56
1:A:247:ALA:CB	1:A:355:ILE:HB	2.29	0.56
2:B:173:PRO:O	2:B:380:ARG:NH2	2.39	0.56
2:B:190:HIS:CE1	2:B:411:ALA:HA	2.40	0.56
1:A:119:LEU:HD13	1:A:156:ARG:NH2	2.21	0.56
1:A:241:SER:OG	1:A:242:LEU:N	2.38	0.56
1:A:362:VAL:HG22	1:A:368:LEU:HB2	1.87	0.56
2:B:44:LEU:CD1	2:B:47:ILE:HD13	2.36	0.56
2:B:375:GLN:HG2	2:B:419:VAL:HG13	1.87	0.56
1:A:419:SER:O	1:A:422:ARG:HB3	2.06	0.56
1:A:195:LEU:C	1:A:197:HIS:H	2.09	0.55
1:A:250:VAL:HG22	1:A:352:LYS:HE3	1.88	0.55
1:A:291:ILE:CG1	1:A:292:THR:N	2.68	0.55
1:A:334:THR:O	1:A:338:LYS:HB2	2.06	0.55
2:B:6:HIS:HB3	2:B:63:ALA:CB	2.32	0.55
2:B:191:GLN:O	2:B:195:ASN:HB2	2.05	0.55
1:A:104:ALA:HB2	1:A:413:MET:CE	2.37	0.55
1:A:308:ARG:NH1	1:A:390:ARG:HH22	2.04	0.55
2:B:152:ILE:CG2	2:B:164:MET:HE1	2.36	0.55
2:B:248:ALA:HA	2:B:252:LYS:HE2	1.88	0.55
2:B:289:LEU:HG	2:B:365:ALA:HB2	1.88	0.55
2:B:375:GLN:CG	2:B:419:VAL:HG13	2.36	0.55
1:A:8:HIS:ND1	1:A:138:PHE:HB2	2.21	0.55
1:A:20:CYS:HA	1:A:232:GLY:HA3	1.89	0.55
1:A:291:ILE:HD12	1:A:375:VAL:HG22	1.87	0.55
2:B:44:LEU:HD21	2:B:59:TYR:OH	2.06	0.55
1:A:115:ILE:CG2	1:A:116:ASP:N	2.69	0.55
2:B:4:ILE:HG21	2:B:134:GLN:HG2	1.88	0.55
2:B:106:TYR:CE2	2:B:403:MET:SD	2.99	0.55
2:B:227:HIS:O	2:B:230:SER:N	2.38	0.55
2:B:241:ARG:HE	2:B:249:ASP:HB3	1.71	0.55
1:A:417:GLU:OE2	1:A:417:GLU:HA	2.07	0.55
2:B:109:GLY:O	2:B:113:VAL:HG23	2.07	0.55
2:B:335:ASN:C	2:B:337:ASN:N	2.59	0.55
1:A:266:HIS:HB3	1:A:380:ASN:HD21	1.70	0.55
1:A:173:PRO:HB2	1:A:391:LEU:CD1	2.36	0.55
1:A:242:LEU:HD21	1:A:318:LEU:HD13	1.88	0.55
1:A:313:MET:HE3	1:A:380:ASN:O	2.07	0.55
2:B:73:MET:O	2:B:77:ARG:HG2	2.06	0.55
2:B:394:PHE:N	2:B:394:PHE:CD1	2.72	0.55
1:A:5:ILE:HB	1:A:135:PHE:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:CE	1:A:437:VAL:H	2.20	0.55
1:A:382:THR:O	1:A:382:THR:HG22	2.06	0.55
1:A:419:SER:HB2	1:A:420:GLU:OE2	2.05	0.55
2:B:102:ALA:CB	2:B:403:MET:SD	2.95	0.55
1:A:152:LEU:HD12	1:A:152:LEU:O	2.06	0.55
1:A:308:ARG:O	1:A:309:HIS:CB	2.55	0.55
1:A:102:ASN:ND2	1:A:105:ARG:HB2	2.22	0.55
1:A:138:PHE:CZ	1:A:235:VAL:HG11	2.41	0.55
2:B:149:THR:HB	2:B:191:GLN:HB2	1.88	0.55
1:A:276:ILE:HD13	1:A:277:SER:N	2.21	0.54
1:A:334:THR:HA	1:A:337:THR:OG1	2.07	0.54
2:B:20:PHE:CE2	2:B:233:MET:HG2	2.42	0.54
2:B:88:ASP:C	2:B:90:PHE:H	2.10	0.54
2:B:103:LYS:CG	2:B:401:GLU:HG3	2.37	0.54
1:A:83:TYR:HB3	1:A:87:PHE:HE1	1.71	0.54
1:A:276:ILE:HD13	1:A:277:SER:O	2.07	0.54
1:A:296:PHE:HD2	1:A:341:ILE:HD11	1.72	0.54
2:B:407:GLU:HA	2:B:407:GLU:OE2	2.07	0.54
1:A:6:SER:HA	1:A:136:SER:OG	2.07	0.54
1:A:147:SER:HB2	1:A:190:THR:OG1	2.07	0.54
1:A:210:TYR:C	1:A:212:ILE:H	2.11	0.54
2:B:101:TRP:HD1	2:B:145:SER:HB2	1.73	0.54
2:B:322:SER:HB3	2:B:325:GLU:CG	2.36	0.54
1:A:22:GLU:HG2	1:A:83:TYR:CZ	2.43	0.54
1:A:25:CYS:SG	1:A:83:TYR:HE2	2.30	0.54
1:A:256:GLN:O	1:A:260:VAL:CG1	2.55	0.54
2:B:48:ASN:N	2:B:48:ASN:ND2	2.56	0.54
2:B:207:LEU:CD2	2:B:300:MET:HG3	2.37	0.54
2:B:263:LEU:HD12	2:B:263:LEU:C	2.28	0.54
1:A:305:CYS:SG	1:A:384:ILE:HA	2.47	0.54
1:A:381:THR:C	1:A:383:ALA:N	2.61	0.54
2:B:323:MET:SD	2:B:323:MET:N	2.81	0.54
2:B:358:PRO:HD2	2:B:361:LEU:HD12	1.89	0.54
1:A:319:TYR:CE1	1:A:328:VAL:HG13	2.43	0.54
2:B:202:ILE:HD13	2:B:229:VAL:HG22	1.88	0.54
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.42	0.54
1:A:126:ALA:O	1:A:129:CYS:SG	2.66	0.54
1:A:190:THR:O	1:A:194:THR:HG22	2.08	0.54
2:B:290:THR:CG2	2:B:333:VAL:HG21	2.38	0.54
2:B:36:TYR:OH	2:B:40:SER:O	2.26	0.54
2:B:67:ASP:HA	2:B:143:THR:OG1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TRP:HE1	2:B:258:VAL:HG23	1.73	0.54
2:B:6:HIS:O	2:B:63:ALA:HA	2.07	0.54
2:B:65:LEU:HD23	2:B:65:LEU:N	2.23	0.54
2:B:171:PRO:HB3	2:B:181:GLU:HG3	1.90	0.54
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.48	0.54
2:B:306:ARG:HG2	2:B:340:TYR:OH	2.08	0.54
1:A:100:ALA:O	1:A:102:ASN:N	2.39	0.53
1:A:168:GLU:OE1	1:A:198:SER:HB3	2.07	0.53
1:A:180:ALA:HA	2:B:350:LYS:HE2	1.89	0.53
1:A:368:LEU:N	1:A:368:LEU:HD23	2.24	0.53
2:B:236:VAL:O	2:B:240:LEU:HB2	2.08	0.53
1:A:159:VAL:O	1:A:159:VAL:HG13	2.08	0.53
1:A:191:THR:HG21	1:A:425:MET:CE	2.37	0.53
1:A:273:ALA:HB1	1:A:294:ALA:HB3	1.89	0.53
2:B:198:GLU:OE1	2:B:254:ALA:HB2	2.09	0.53
1:A:62:VAL:HG22	1:A:63:PRO:HD2	1.89	0.53
2:B:167:PHE:CZ	2:B:233:MET:HA	2.42	0.53
1:A:191:THR:HG23	1:A:192:HIS:N	2.22	0.53
1:A:339:ARG:O	1:A:341:ILE:N	2.40	0.53
1:A:426:ALA:O	1:A:429:GLU:HB3	2.09	0.53
2:B:100:ASN:ND2	2:B:102:ALA:HB3	2.23	0.53
2:B:211:CYS:SG	2:B:220:PRO:CB	2.89	0.53
1:A:123:ARG:HB2	1:A:123:ARG:NH1	2.19	0.53
1:A:182:VAL:HG23	1:A:186:ASN:ND2	2.21	0.53
1:A:426:ALA:O	1:A:430:LYS:HG3	2.08	0.53
2:B:163:ILE:CD1	2:B:250:LEU:HD12	2.39	0.53
2:B:193:VAL:CG2	2:B:262:ARG:HH11	2.22	0.53
2:B:172:SER:OG	2:B:204:ASN:HB2	2.08	0.53
2:B:337:ASN:O	2:B:339:SER:N	2.42	0.53
2:B:387:ALA:O	2:B:389:PHE:N	2.42	0.53
1:A:70:LEU:HD13	1:A:110:ILE:HG13	1.91	0.53
1:A:199:ASP:HB3	1:A:256:GLN:NE2	2.24	0.53
1:A:201:ALA:O	1:A:267:PHE:HB3	2.09	0.53
2:B:50:TYR:HE1	2:B:238:THR:HG22	1.73	0.53
2:B:130:LEU:HD23	2:B:130:LEU:H	1.73	0.53
1:A:29:GLY:C	1:A:30:ILE:HG13	2.29	0.53
1:A:121:ARG:O	1:A:124:LYS:HB2	2.07	0.53
1:A:187:SER:O	1:A:190:THR:N	2.41	0.53
2:B:289:LEU:O	2:B:293:MET:HG3	2.09	0.53
1:A:153:LEU:O	1:A:157:LEU:HG	2.08	0.53
2:B:342:VAL:HG13	2:B:344:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:THR:O	2:B:401:GLU:N	2.42	0.53
1:A:103:TYR:HB2	1:A:186:ASN:HA	1.91	0.52
1:A:122:ILE:O	1:A:126:ALA:N	2.41	0.52
1:A:177:VAL:CG2	1:A:207:GLU:HB2	2.40	0.52
1:A:223:THR:N	1:A:226:ASN:HD22	2.07	0.52
1:A:256:GLN:CA	1:A:260:VAL:HG12	2.39	0.52
2:B:359:ARG:NH1	2:B:359:ARG:HB3	2.24	0.52
1:A:172:TYR:HH	1:A:388:TRP:HE3	1.51	0.52
1:A:264:ARG:C	1:A:266:HIS:N	2.62	0.52
1:A:401:LYS:C	1:A:403:ALA:H	2.12	0.52
2:B:73:MET:SD	2:B:92:PHE:HB3	2.50	0.52
2:B:284:LEU:HD13	2:B:289:LEU:HD13	1.91	0.52
2:B:421:GLU:HG2	2:B:421:GLU:O	2.09	0.52
1:A:21:TRP:HH2	1:A:64:ARG:HG2	1.74	0.52
1:A:182:VAL:O	1:A:184:PRO:N	2.41	0.52
2:B:200:TYR:CD1	2:B:200:TYR:N	2.76	0.52
2:B:249:ASP:OD1	2:B:252:LYS:HD3	2.10	0.52
2:B:358:PRO:HB2	2:B:361:LEU:CB	2.36	0.52
1:A:16:ILE:HD12	1:A:171:ILE:HD11	1.92	0.52
1:A:77:GLU:CG	2:B:243:PRO:HB3	2.39	0.52
1:A:271:THR:HG23	1:A:272:TYR:N	2.16	0.52
2:B:412:GLU:O	2:B:416:ASN:N	2.42	0.52
2:B:377:LEU:CG	2:B:381:ILE:HD11	2.25	0.52
1:A:93:ILE:CD1	1:A:118:VAL:HA	2.40	0.52
1:A:154:MET:HE3	1:A:166:LYS:HB3	1.92	0.52
1:A:378:LEU:O	1:A:378:LEU:HD12	2.10	0.52
2:B:44:LEU:HD12	2:B:47:ILE:HG21	1.91	0.52
2:B:255:VAL:HG12	2:B:255:VAL:O	2.08	0.52
2:B:4:ILE:CG2	2:B:134:GLN:HG2	2.40	0.52
2:B:86:ARG:HB3	2:B:87:PRO:HD2	1.92	0.52
1:A:317:LEU:C	1:A:318:LEU:HD23	2.30	0.52
2:B:6:HIS:CE1	2:B:8:GLN:HB3	2.44	0.52
2:B:306:ARG:HA	2:B:340:TYR:CE2	2.45	0.52
1:A:116:ASP:HA	1:A:119:LEU:HD12	1.92	0.52
1:A:427:ALA:C	1:A:429:GLU:N	2.61	0.52
2:B:117:LEU:HD11	2:B:154:LYS:HZ2	1.75	0.52
2:B:257:MET:HE2	2:B:368:ILE:HG22	1.91	0.52
2:B:361:LEU:HD23	5:B:1001:EP:H431	1.91	0.52
2:B:113:VAL:HG12	2:B:117:LEU:CD1	2.40	0.52
2:B:139:LEU:HG	2:B:188:SER:HB3	1.92	0.52
2:B:232:THR:OG1	2:B:233:MET:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:PHE:HB3	2:B:261:PRO:HD2	1.91	0.52
1:A:107:HIS:O	1:A:152:LEU:HD21	2.10	0.51
1:A:189:LEU:HD23	1:A:421:ALA:HB3	1.91	0.51
1:A:217:LEU:HD12	1:A:277:SER:CA	2.30	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.91	0.51
1:A:23:LEU:O	1:A:26:LEU:HB3	2.11	0.51
1:A:69:ASP:C	1:A:70:LEU:HD23	2.30	0.51
1:A:117:LEU:HD12	1:A:117:LEU:O	2.10	0.51
1:A:167:LEU:CD2	1:A:200:CYS:HB3	2.37	0.51
1:A:221:ARG:HG2	1:A:221:ARG:O	2.09	0.51
2:B:372:THR:CB	2:B:426:GLN:HB2	2.40	0.51
2:B:3:GLU:HA	2:B:49:VAL:HA	1.91	0.51
2:B:133:PHE:O	2:B:165:ASN:HB2	2.10	0.51
2:B:149:THR:HG21	2:B:188:SER:HA	1.93	0.51
2:B:251:ARG:O	2:B:255:VAL:HG23	2.11	0.51
2:B:393:ALA:C	2:B:395:LEU:H	2.13	0.51
2:B:394:PHE:HD1	2:B:394:PHE:N	2.09	0.51
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.45	0.51
1:A:223:THR:H	1:A:226:ASN:HD22	1.58	0.51
2:B:21:TRP:O	2:B:25:SER:HB3	2.10	0.51
1:A:209:ILE:HG21	1:A:227:LEU:HD22	1.93	0.51
2:B:53:GLU:HG2	2:B:59:TYR:CE2	2.44	0.51
2:B:70:PRO:O	2:B:72:THR:N	2.44	0.51
1:A:274:PRO:HG3	1:A:374:ALA:HA	1.92	0.51
2:B:406:MET:O	2:B:409:THR:HB	2.10	0.51
1:A:114:ILE:HD11	1:A:149:PHE:CE2	2.46	0.51
1:A:223:THR:HG22	1:A:224:TYR:N	2.25	0.51
1:A:344:VAL:CG2	1:A:347:CYS:HB3	2.40	0.51
2:B:47:ILE:C	2:B:49:VAL:N	2.64	0.51
2:B:193:VAL:C	2:B:263:LEU:HD23	2.31	0.51
1:A:191:THR:HG21	1:A:425:MET:HE1	1.93	0.51
1:A:296:PHE:N	1:A:296:PHE:CD1	2.79	0.51
1:A:399:TYR:CE2	1:A:402:ARG:NH2	2.79	0.51
2:B:207:LEU:HB2	2:B:225:LEU:CD1	2.41	0.51
1:A:181:VAL:HG11	1:A:404:PHE:CZ	2.46	0.51
2:B:11:GLN:HA	2:B:72:THR:HG21	1.93	0.51
2:B:341:PHE:O	2:B:342:VAL:O	2.29	0.51
1:A:263:PRO:O	1:A:264:ARG:C	2.49	0.50
2:B:42:LEU:O	2:B:44:LEU:N	2.43	0.50
2:B:415:MET:O	2:B:415:MET:SD	2.69	0.50
2:B:417:ASP:O	2:B:420:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG22	1:A:146:GLY:HA2	1.92	0.50
2:B:3:GLU:HB2	2:B:62:ARG:CZ	2.41	0.50
2:B:66:VAL:HG13	2:B:91:VAL:HG23	1.92	0.50
2:B:187:LEU:HD11	2:B:408:PHE:CZ	2.46	0.50
2:B:265:PHE:CD1	2:B:265:PHE:N	2.78	0.50
2:B:271:ALA:O	2:B:292:GLN:OE1	2.29	0.50
1:A:192:HIS:ND1	1:A:192:HIS:C	2.64	0.50
1:A:313:MET:HE1	1:A:380:ASN:OD1	2.12	0.50
2:B:271:ALA:H	2:B:272:PRO:HD2	1.76	0.50
2:B:303:CYS:HB3	2:B:373:ALA:O	2.11	0.50
1:A:256:GLN:HA	1:A:260:VAL:HG12	1.93	0.50
1:A:287:SER:HA	1:A:373:ARG:NH2	2.26	0.50
1:A:351:PHE:O	1:A:353:VAL:N	2.45	0.50
1:A:300:ASN:O	1:A:301:GLN:C	2.49	0.50
1:A:309:HIS:NE2	1:A:382:THR:HG22	2.27	0.50
1:A:404:PHE:N	1:A:404:PHE:HD1	2.08	0.50
2:B:3:GLU:O	2:B:131:GLN:N	2.43	0.50
2:B:17:GLY:O	2:B:20:PHE:N	2.45	0.50
2:B:66:VAL:CA	2:B:91:VAL:HG23	2.40	0.50
2:B:153:SER:HA	2:B:195:ASN:OD1	2.11	0.50
2:B:304:ASP:HB2	2:B:307:HIS:HB2	1.92	0.50
1:A:273:ALA:O	1:A:275:VAL:N	2.39	0.50
1:A:336:LYS:C	1:A:338:LYS:H	2.14	0.50
1:A:12:ALA:O	1:A:16:ILE:CG2	2.60	0.50
1:A:264:ARG:CB	1:A:266:HIS:CD2	2.94	0.50
1:A:330:ALA:O	1:A:334:THR:CG2	2.60	0.50
2:B:6:HIS:HA	2:B:134:GLN:O	2.12	0.50
2:B:28:HIS:HA	2:B:43:GLN:HB3	1.93	0.50
2:B:163:ILE:HD11	2:B:250:LEU:HD12	1.93	0.50
2:B:193:VAL:O	2:B:194:GLU:HG2	2.11	0.50
2:B:200:TYR:CE2	2:B:266:PHE:HD1	2.29	0.50
2:B:240:LEU:HD21	2:B:248:ALA:H	1.75	0.50
2:B:280:GLN:O	2:B:282:ARG:CG	2.60	0.50
2:B:322:SER:O	2:B:326:VAL:HG23	2.11	0.50
1:A:271:THR:HG22	1:A:272:TYR:N	2.27	0.50
2:B:257:MET:HE3	2:B:370:ASN:HB2	1.93	0.50
1:A:21:TRP:CH2	1:A:64:ARG:HG2	2.46	0.50
1:A:109:THR:HG22	1:A:110:ILE:CG2	2.42	0.50
1:A:178:SER:HB3	2:B:347:ASN:HD21	1.76	0.50
1:A:286:LEU:HD11	1:A:290:GLU:HG2	1.94	0.50
1:A:383:ALA:C	1:A:385:ALA:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ALA:O	2:B:57:ASN:N	2.45	0.50
2:B:181:GLU:HB3	2:B:182:PRO:HD3	1.93	0.50
1:A:12:ALA:HB3	1:A:140:SER:OG	2.12	0.49
1:A:386:GLU:O	1:A:389:ALA:N	2.45	0.49
2:B:240:LEU:HD11	2:B:248:ALA:HB3	1.94	0.49
2:B:313:VAL:HG12	2:B:314:ALA:N	2.27	0.49
1:A:69:ASP:HB2	1:A:75:ILE:CG1	2.42	0.49
2:B:64:ILE:CD1	2:B:120:VAL:HG12	2.40	0.49
2:B:290:THR:HA	2:B:293:MET:HE3	1.94	0.49
2:B:361:LEU:HB2	5:B:1001:EP:C43	2.39	0.49
1:A:104:ALA:HB2	1:A:413:MET:HE2	1.94	0.49
1:A:134:GLY:HA3	1:A:165:SER:OG	2.12	0.49
1:A:169:PHE:HZ	1:A:238:ILE:HD12	1.75	0.49
1:A:269:LEU:O	1:A:269:LEU:CD1	2.60	0.49
1:A:273:ALA:C	1:A:275:VAL:H	2.14	0.49
2:B:190:HIS:HA	2:B:414:ASN:ND2	2.27	0.49
1:A:9:VAL:O	1:A:13:GLY:HA3	2.12	0.49
1:A:276:ILE:HD13	1:A:276:ILE:C	2.32	0.49
1:A:315:CYS:SG	1:A:343:PHE:HZ	2.33	0.49
1:A:422:ARG:O	1:A:423:GLU:C	2.50	0.49
1:A:423:GLU:O	1:A:426:ALA:HB3	2.12	0.49
1:A:427:ALA:O	1:A:429:GLU:N	2.46	0.49
2:B:36:TYR:HE1	2:B:43:GLN:HB2	1.78	0.49
2:B:65:LEU:O	2:B:73:MET:HE3	2.12	0.49
2:B:271:ALA:HB2	2:B:293:MET:CG	2.41	0.49
2:B:385:PHE:O	2:B:386:THR:C	2.51	0.49
1:A:132:LEU:HG	1:A:133:GLN:N	2.27	0.49
1:A:207:GLU:O	1:A:208:ALA:C	2.51	0.49
1:A:237:SER:C	1:A:239:THR:N	2.64	0.49
1:A:402:ARG:O	1:A:403:ALA:C	2.51	0.49
2:B:351:THR:HG22	2:B:352:ALA:N	2.28	0.49
2:B:361:LEU:HD11	2:B:363:MET:O	2.12	0.49
2:B:389:PHE:C	2:B:391:ARG:H	2.16	0.49
1:A:84:ARG:HG2	1:A:84:ARG:HH11	1.77	0.49
1:A:202:PHE:HE2	1:A:378:LEU:HD13	1.75	0.49
1:A:235:VAL:C	1:A:237:SER:N	2.64	0.49
1:A:264:ARG:HB2	1:A:266:HIS:CD2	2.48	0.49
2:B:73:MET:CE	2:B:92:PHE:HD2	2.26	0.49
2:B:119:VAL:O	2:B:122:LYS:HB3	2.13	0.49
2:B:148:GLY:O	2:B:151:LEU:HB2	2.13	0.49
1:A:139:HIS:CG	1:A:140:SER:N	2.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:VAL:O	1:A:183:GLU:C	2.50	0.49
1:A:332:ILE:O	1:A:336:LYS:HB3	2.12	0.49
1:A:362:VAL:CB	1:A:370:LYS:HB2	2.42	0.49
2:B:23:VAL:O	2:B:27:GLU:HB2	2.13	0.49
2:B:130:LEU:CD2	2:B:162:ARG:NH1	2.75	0.49
2:B:287:PRO:O	2:B:291:GLN:CB	2.55	0.49
2:B:308:GLY:HA3	2:B:426:GLN:NE2	2.23	0.49
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.95	0.49
1:A:434:GLU:O	1:A:435:VAL:C	2.51	0.49
2:B:24:ILE:CG1	2:B:238:THR:HG21	2.43	0.49
2:B:117:LEU:CD1	2:B:154:LYS:HZ2	2.26	0.49
2:B:198:GLU:HB3	2:B:266:PHE:CE1	2.48	0.49
1:A:112:LYS:HD3	1:A:115:ILE:HG21	1.95	0.48
1:A:141:PHE:O	1:A:143:GLY:N	2.45	0.48
1:A:203:MET:HG3	1:A:384:ILE:HG21	1.94	0.48
1:A:210:TYR:CG	2:B:324:LYS:HD3	2.46	0.48
1:A:273:ALA:N	1:A:274:PRO:HD2	2.28	0.48
1:A:294:ALA:HB1	1:A:300:ASN:ND2	2.28	0.48
2:B:72:THR:HA	2:B:75:SER:OG	2.13	0.48
1:A:90:GLU:O	1:A:121:ARG:NE	2.43	0.48
1:A:93:ILE:HD12	1:A:118:VAL:HA	1.95	0.48
1:A:149:PHE:O	1:A:150:THR:C	2.51	0.48
1:A:319:TYR:CD2	1:A:323:VAL:HG11	2.48	0.48
1:A:278:ALA:HB2	1:A:369:ALA:CA	2.42	0.48
2:B:76:VAL:O	2:B:82:GLY:HA3	2.13	0.48
1:A:78:VAL:O	1:A:80:THR:N	2.42	0.48
1:A:123:ARG:HA	1:A:126:ALA:HB3	1.94	0.48
1:A:295:CYS:SG	1:A:375:VAL:HG21	2.53	0.48
2:B:108:GLU:O	2:B:111:GLU:HG2	2.13	0.48
1:A:321:GLY:HA2	1:A:357:TYR:O	2.13	0.48
2:B:135:LEU:HD13	2:B:152:ILE:HG23	1.95	0.48
2:B:341:PHE:CD2	2:B:348:ASN:ND2	2.82	0.48
1:A:5:ILE:O	1:A:135:PHE:HA	2.14	0.48
1:A:425:MET:O	1:A:426:ALA:C	2.52	0.48
2:B:289:LEU:HD22	2:B:363:MET:HB3	1.95	0.48
1:A:228:ASN:HA	1:A:231:ILE:HG12	1.94	0.48
1:A:235:VAL:O	1:A:237:SER:N	2.43	0.48
1:A:31:GLN:HB2	1:A:32:PRO:HD2	1.96	0.48
1:A:261:PRO:HB2	1:A:262:TYR:HD1	1.79	0.48
1:A:362:VAL:CG2	1:A:368:LEU:HB2	2.43	0.48
2:B:79:GLY:O	2:B:80:PRO:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:LEU:HD21	2:B:300:MET:HG3	1.95	0.48
2:B:241:ARG:CG	2:B:241:ARG:NH1	2.71	0.48
1:A:99:ALA:HB1	3:A:9500:GTP:O3G	2.14	0.48
1:A:187:SER:O	1:A:188:ILE:C	2.51	0.48
1:A:354:GLY:C	1:A:355:ILE:HG13	2.33	0.48
1:A:404:PHE:CZ	2:B:312:THR:HG21	2.44	0.48
2:B:91:VAL:HG21	2:B:116:VAL:HG22	1.95	0.48
1:A:152:LEU:CD1	1:A:152:LEU:O	2.61	0.48
1:A:178:SER:CB	2:B:347:ASN:ND2	2.73	0.48
1:A:343:PHE:CE1	1:A:351:PHE:CZ	3.02	0.48
1:A:209:ILE:O	1:A:212:ILE:HB	2.13	0.47
1:A:244:PHE:HB2	1:A:356:ASN:HD21	1.78	0.47
2:B:256:ASN:CB	2:B:350:LYS:HG3	2.44	0.47
2:B:265:PHE:CD1	2:B:378:PHE:HE1	2.31	0.47
1:A:68:VAL:HG22	1:A:93:ILE:HB	1.96	0.47
1:A:104:ALA:HB1	1:A:413:MET:CG	2.43	0.47
1:A:150:THR:O	1:A:153:LEU:HB3	2.14	0.47
1:A:191:THR:CG2	1:A:192:HIS:N	2.78	0.47
1:A:296:PHE:HD1	1:A:296:PHE:H	1.61	0.47
1:A:406:HIS:C	1:A:408:TYR:N	2.67	0.47
2:B:412:GLU:O	2:B:416:ASN:HB2	2.14	0.47
1:A:151:SER:OG	1:A:190:THR:HG23	2.15	0.47
1:A:171:ILE:HA	1:A:204:VAL:O	2.13	0.47
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.94	0.47
1:A:332:ILE:C	1:A:334:THR:H	2.18	0.47
2:B:205:GLU:HA	2:B:208:TYR:CD1	2.49	0.47
1:A:14:VAL:O	1:A:18:ASN:HB2	2.14	0.47
1:A:166:LYS:HE3	1:A:166:LYS:N	2.29	0.47
1:A:188:ILE:HG22	1:A:189:LEU:N	2.29	0.47
1:A:210:TYR:HA	1:A:213:CYS:SG	2.55	0.47
1:A:254:GLU:O	1:A:258:ASN:ND2	2.47	0.47
2:B:40:SER:HB3	2:B:43:GLN:CG	2.29	0.47
2:B:100:ASN:HD21	2:B:102:ALA:HB3	1.79	0.47
2:B:104:GLY:C	2:B:109:GLY:HA3	2.35	0.47
2:B:205:GLU:O	2:B:208:TYR:N	2.44	0.47
2:B:357:PRO:HB2	2:B:358:PRO:HD2	1.97	0.47
1:A:27:GLU:O	1:A:28:HIS:CD2	2.66	0.47
2:B:8:GLN:CG	2:B:65:LEU:HD22	2.44	0.47
2:B:77:ARG:NH1	2:B:90:PHE:CD2	2.82	0.47
2:B:326:VAL:HG11	2:B:351:THR:CG2	2.43	0.47
1:A:11:GLN:O	1:A:15:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:CB	1:A:32:PRO:HD2	2.43	0.47
1:A:239:THR:CG2	1:A:240:ALA:N	2.73	0.47
2:B:313:VAL:HG13	2:B:367:PHE:CE1	2.48	0.47
2:B:337:ASN:O	2:B:337:ASN:CG	2.53	0.47
1:A:277:SER:O	1:A:279:GLU:N	2.45	0.47
1:A:403:ALA:HB1	1:A:404:PHE:HD1	1.79	0.47
2:B:143:THR:HG23	4:B:1500:GDP:PB	2.54	0.47
2:B:235:GLY:O	2:B:236:VAL:C	2.52	0.47
2:B:252:LYS:H	2:B:252:LYS:HG2	1.49	0.47
2:B:371:SER:C	2:B:373:ALA:H	2.18	0.47
1:A:234:ILE:CD1	1:A:270:ALA:HB1	2.45	0.47
2:B:135:LEU:HD13	2:B:152:ILE:CG2	2.44	0.47
2:B:185:ALA:O	2:B:186:THR:C	2.53	0.47
2:B:244:GLY:C	2:B:246:LEU:N	2.69	0.47
1:A:261:PRO:HB2	1:A:262:TYR:CD1	2.50	0.47
1:A:291:ILE:HG13	1:A:292:THR:N	2.30	0.47
2:B:66:VAL:HG13	2:B:91:VAL:CG2	2.44	0.47
1:A:66:VAL:HA	1:A:91:GLN:HB3	1.97	0.47
1:A:102:ASN:ND2	1:A:411:GLU:HG2	2.27	0.46
1:A:311:LYS:NZ	1:A:437:VAL:H	2.12	0.46
2:B:377:LEU:C	2:B:379:LYS:N	2.68	0.46
1:A:368:LEU:C	1:A:370:LYS:H	2.18	0.46
1:A:381:THR:HG23	1:A:383:ALA:CB	2.44	0.46
1:A:429:GLU:C	1:A:431:ASP:N	2.68	0.46
2:B:186:THR:HG22	2:B:187:LEU:N	2.31	0.46
2:B:210:ILE:HG21	2:B:298:ASN:HA	1.97	0.46
2:B:282:ARG:HH22	2:B:361:LEU:CD2	2.29	0.46
2:B:319:GLY:O	2:B:320:ARG:C	2.53	0.46
1:A:11:GLN:HB3	3:A:9500:GTP:O2A	2.15	0.46
1:A:31:GLN:H	1:A:31:GLN:HG2	1.30	0.46
1:A:410:GLY:C	1:A:412:GLY:H	2.17	0.46
2:B:197:ASP:O	2:B:198:GLU:HG3	2.15	0.46
2:B:215:LEU:O	2:B:216:LYS:HG3	2.16	0.46
1:A:7:ILE:HD11	1:A:157:LEU:HD11	1.97	0.46
1:A:404:PHE:O	1:A:407:TRP:HB2	2.14	0.46
2:B:7:ILE:O	2:B:8:GLN:C	2.53	0.46
2:B:344:TRP:HZ2	2:B:425:TYR:HB3	1.81	0.46
1:A:128:GLN:O	1:A:128:GLN:HG3	2.15	0.46
1:A:188:ILE:CG2	1:A:421:ALA:O	2.57	0.46
1:A:407:TRP:HZ2	2:B:258:VAL:CG2	2.28	0.46
1:A:416:GLY:O	1:A:417:GLU:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ASP:O	2:B:331:LEU:N	2.49	0.46
1:A:62:VAL:HG23	1:A:88:HIS:CE1	2.50	0.46
1:A:246:GLY:O	1:A:247:ALA:C	2.54	0.46
1:A:396:ASP:O	1:A:397:LEU:C	2.54	0.46
2:B:187:LEU:HD11	2:B:408:PHE:CE1	2.50	0.46
1:A:313:MET:O	1:A:314:ALA:HB2	2.16	0.46
2:B:2:ARG:HD2	2:B:131:GLN:HE22	1.79	0.46
2:B:192:LEU:C	2:B:194:GLU:N	2.69	0.46
2:B:209:ASP:OD2	2:B:213:ARG:HD2	2.16	0.46
1:A:276:ILE:HG21	1:A:284:GLU:OE1	2.16	0.46
1:A:390:ARG:C	1:A:392:ASP:H	2.18	0.46
2:B:22:GLU:O	2:B:22:GLU:HG2	2.15	0.46
2:B:106:TYR:CE2	2:B:403:MET:HG3	2.51	0.46
2:B:171:PRO:CB	2:B:181:GLU:HG3	2.45	0.46
1:A:184:PRO:O	1:A:185:TYR:C	2.53	0.46
1:A:271:THR:OG1	1:A:301:GLN:HA	2.15	0.46
1:A:384:ILE:C	1:A:386:GLU:N	2.67	0.46
1:A:412:GLY:C	1:A:413:MET:HG2	2.35	0.46
2:B:11:GLN:O	2:B:15:GLN:N	2.48	0.46
2:B:196:THR:OG1	2:B:263:LEU:HD22	2.16	0.46
2:B:238:THR:OG1	2:B:239:CYS:N	2.47	0.46
2:B:282:ARG:HE	2:B:282:ARG:HB3	1.27	0.46
1:A:199:ASP:CB	1:A:256:GLN:NE2	2.78	0.46
1:A:207:GLU:O	1:A:210:TYR:N	2.49	0.46
1:A:234:ILE:O	1:A:234:ILE:CD1	2.59	0.46
1:A:300:ASN:O	1:A:302:MET:HE3	2.16	0.46
2:B:112:LEU:O	2:B:112:LEU:HD13	2.16	0.46
2:B:293:MET:SD	2:B:315:ALA:HB1	2.56	0.46
1:A:62:VAL:HG23	1:A:88:HIS:HE1	1.81	0.45
1:A:242:LEU:HD13	1:A:242:LEU:HA	1.68	0.45
2:B:121:ARG:HG2	2:B:159:TYR:OH	2.17	0.45
2:B:270:PHE:HE2	2:B:272:PRO:HG2	1.81	0.45
2:B:377:LEU:C	2:B:379:LYS:H	2.18	0.45
2:B:399:THR:O	2:B:400:GLY:C	2.55	0.45
1:A:72:PRO:HD3	1:A:95:GLY:O	2.16	0.45
1:A:115:ILE:HA	1:A:118:VAL:HG23	1.97	0.45
1:A:216:ASN:N	1:A:216:ASN:HD22	2.14	0.45
1:A:274:PRO:HG3	1:A:374:ALA:CB	2.47	0.45
1:A:297:GLU:HG3	1:A:299:ALA:H	1.82	0.45
2:B:121:ARG:C	2:B:123:GLU:N	2.67	0.45
2:B:289:LEU:HG	2:B:365:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:LEU:HD11	2:B:363:MET:C	2.37	0.45
1:A:115:ILE:HD13	1:A:115:ILE:O	2.15	0.45
1:A:139:HIS:O	1:A:140:SER:HB3	2.17	0.45
1:A:150:THR:CG2	1:A:151:SER:N	2.80	0.45
1:A:193:THR:O	1:A:193:THR:HG23	2.16	0.45
1:A:195:LEU:CD1	1:A:265:GLY:H	2.29	0.45
1:A:237:SER:O	1:A:242:LEU:HD23	2.16	0.45
1:A:264:ARG:HB3	1:A:266:HIS:CD2	2.51	0.45
1:A:408:TYR:O	1:A:411:GLU:N	2.49	0.45
2:B:113:VAL:HG12	2:B:117:LEU:HD12	1.97	0.45
2:B:319:GLY:HA2	2:B:355:ASP:O	2.15	0.45
1:A:12:ALA:C	1:A:16:ILE:HG22	2.37	0.45
1:A:76:ASP:HA	1:A:79:ARG:HG3	1.99	0.45
2:B:2:ARG:HG2	2:B:46:ARG:HH12	1.81	0.45
2:B:113:VAL:HG13	2:B:151:LEU:CD1	2.46	0.45
1:A:33:ASP:OD1	1:A:85:GLN:HB3	2.17	0.45
1:A:252:LEU:HA	1:A:255:PHE:HD1	1.76	0.45
1:A:267:PHE:H	1:A:267:PHE:HD1	1.59	0.45
1:A:215:ARG:C	1:A:216:ASN:HD22	2.20	0.45
1:A:268:PRO:CB	1:A:379:SER:O	2.65	0.45
1:A:426:ALA:HB1	1:A:430:LYS:NZ	2.31	0.45
2:B:61:PRO:CD	2:B:84:ILE:HG12	2.47	0.45
2:B:136:THR:HG23	2:B:233:MET:HE3	1.98	0.45
2:B:209:ASP:CG	2:B:213:ARG:HD2	2.37	0.45
1:A:180:ALA:HA	2:B:350:LYS:HG2	1.99	0.45
1:A:219:ILE:HG21	1:A:367:ASP:OD2	2.17	0.45
1:A:373:ARG:HB3	1:A:373:ARG:NH1	2.31	0.45
1:A:386:GLU:OE1	1:A:390:ARG:NH2	2.49	0.45
2:B:3:GLU:H	2:B:130:LEU:HA	1.81	0.45
2:B:292:GLN:O	2:B:293:MET:C	2.55	0.45
2:B:294:PHE:CZ	2:B:313:VAL:HG11	2.52	0.45
1:A:169:PHE:CZ	1:A:235:VAL:HG22	2.52	0.45
1:A:234:ILE:CG1	1:A:270:ALA:HB1	2.45	0.45
1:A:291:ILE:O	1:A:294:ALA:HB3	2.17	0.45
1:A:373:ARG:O	1:A:374:ALA:CB	2.63	0.45
2:B:2:ARG:HA	2:B:129:CYS:O	2.16	0.45
2:B:221:THR:CG2	2:B:222:TYR:N	2.70	0.45
2:B:253:LEU:O	2:B:257:MET:CB	2.64	0.45
2:B:272:PRO:O	2:B:274:THR:HG23	2.16	0.45
1:A:259:LEU:HD21	1:A:316:CYS:CB	2.37	0.45
1:A:287:SER:HB2	1:A:290:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:C	1:A:370:LYS:N	2.69	0.45
2:B:117:LEU:CD1	2:B:154:LYS:NZ	2.79	0.45
1:A:259:LEU:HD11	1:A:378:LEU:CD1	2.46	0.45
2:B:205:GLU:HA	2:B:208:TYR:HD1	1.82	0.45
2:B:240:LEU:HD13	2:B:248:ALA:C	2.37	0.45
2:B:324:LYS:HD2	2:B:324:LYS:O	2.17	0.45
1:A:8:HIS:CE1	1:A:138:PHE:CD1	3.05	0.44
1:A:31:GLN:CB	1:A:32:PRO:CD	2.95	0.44
1:A:203:MET:HG2	1:A:268:PRO:O	2.16	0.44
1:A:210:TYR:O	1:A:212:ILE:N	2.48	0.44
2:B:61:PRO:HG2	2:B:85:PHE:CD2	2.52	0.44
2:B:88:ASP:C	2:B:90:PHE:N	2.70	0.44
2:B:130:LEU:HD23	2:B:130:LEU:N	2.31	0.44
2:B:130:LEU:O	2:B:130:LEU:HG	2.17	0.44
2:B:249:ASP:OD2	2:B:251:ARG:HB2	2.18	0.44
1:A:417:GLU:OE2	1:A:417:GLU:CA	2.65	0.44
2:B:35:SER:O	2:B:37:HIS:N	2.49	0.44
2:B:81:PHE:O	2:B:84:ILE:HG22	2.17	0.44
1:A:20:CYS:HA	1:A:232:GLY:CA	2.47	0.44
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.52	0.44
1:A:122:ILE:O	1:A:125:LEU:N	2.49	0.44
1:A:248:LEU:CD1	1:A:355:ILE:HD12	2.46	0.44
1:A:276:ILE:CG2	1:A:369:ALA:HB3	2.39	0.44
1:A:292:THR:HG22	1:A:335:ILE:HD11	1.99	0.44
2:B:210:ILE:CG2	2:B:298:ASN:HD22	2.30	0.44
1:A:228:ASN:HA	1:A:231:ILE:CG1	2.48	0.44
2:B:42:LEU:C	2:B:44:LEU:N	2.70	0.44
2:B:73:MET:HE1	2:B:91:VAL:O	2.17	0.44
2:B:210:ILE:HD11	2:B:299:MET:O	2.17	0.44
2:B:322:SER:O	2:B:325:GLU:HG2	2.18	0.44
1:A:356:ASN:HD22	1:A:356:ASN:HA	1.54	0.44
2:B:36:TYR:C	2:B:38:GLY:N	2.69	0.44
2:B:52:ASN:CB	2:B:60:VAL:HG23	2.46	0.44
1:A:184:PRO:HG3	1:A:394:LYS:HB3	2.00	0.44
1:A:384:ILE:C	1:A:386:GLU:H	2.19	0.44
1:A:436:GLY:O	1:A:437:VAL:HB	2.18	0.44
2:B:193:VAL:CA	2:B:263:LEU:HD23	2.48	0.44
1:A:115:ILE:O	1:A:118:VAL:N	2.49	0.44
2:B:146:GLY:HA2	2:B:149:THR:OG1	2.17	0.44
2:B:150:LEU:O	2:B:154:LYS:HG3	2.17	0.44
2:B:265:PHE:HE1	2:B:418:LEU:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:C	1:A:105:ARG:H	2.21	0.44
1:A:384:ILE:N	1:A:384:ILE:CD1	2.80	0.44
1:A:429:GLU:O	1:A:431:ASP:N	2.47	0.44
1:A:359:PRO:CB	1:A:372:GLN:O	2.55	0.44
2:B:100:ASN:HD21	2:B:398:TYR:HA	1.83	0.44
2:B:165:ASN:OD1	2:B:250:LEU:HD13	2.18	0.44
2:B:262:ARG:C	2:B:264:HIS:N	2.72	0.44
2:B:399:THR:HG22	2:B:400:GLY:N	2.32	0.44
1:A:132:LEU:N	1:A:132:LEU:CD2	2.78	0.43
2:B:105:HIS:HB2	2:B:146:GLY:CA	2.48	0.43
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.83	0.43
1:A:172:TYR:CE2	1:A:391:LEU:HD13	2.53	0.43
2:B:201:CYS:SG	2:B:374:ILE:HD11	2.58	0.43
2:B:282:ARG:HH22	2:B:361:LEU:HD23	1.83	0.43
2:B:322:SER:HB3	2:B:325:GLU:OE1	2.18	0.43
1:A:217:LEU:HG	1:A:367:ASP:OD1	2.18	0.43
1:A:265:GLY:O	1:A:266:HIS:C	2.56	0.43
1:A:382:THR:HG23	1:A:432:TYR:O	2.18	0.43
2:B:44:LEU:HG	2:B:47:ILE:CD1	2.49	0.43
2:B:101:TRP:CD1	2:B:146:GLY:N	2.87	0.43
2:B:295:ASP:OD1	2:B:297:LYS:HG2	2.17	0.43
2:B:341:PHE:HB3	2:B:348:ASN:ND2	2.33	0.43
2:B:359:ARG:HH11	2:B:359:ARG:HA	1.82	0.43
2:B:393:ALA:O	2:B:395:LEU:N	2.51	0.43
1:A:10:GLY:O	1:A:11:GLN:C	2.56	0.43
1:A:277:SER:C	1:A:279:GLU:H	2.19	0.43
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.48	0.43
2:B:258:VAL:HA	2:B:259:PRO:HD2	1.83	0.43
1:A:217:LEU:HA	1:A:277:SER:CB	2.47	0.43
1:A:296:PHE:CE1	1:A:317:LEU:HD21	2.53	0.43
1:A:303:VAL:O	1:A:305:CYS:N	2.49	0.43
1:A:436:GLY:C	1:A:438:ASP:H	2.20	0.43
2:B:104:GLY:O	2:B:147:MET:HA	2.18	0.43
2:B:120:VAL:HG23	2:B:121:ARG:N	2.33	0.43
2:B:120:VAL:O	2:B:123:GLU:HB2	2.19	0.43
2:B:190:HIS:ND1	2:B:414:ASN:ND2	2.67	0.43
2:B:193:VAL:C	2:B:194:GLU:HG2	2.38	0.43
2:B:242:PHE:HB3	2:B:243:PRO:CD	2.49	0.43
2:B:271:ALA:HB2	2:B:293:MET:HG2	2.01	0.43
2:B:112:LEU:HD22	2:B:112:LEU:HA	1.69	0.43
2:B:163:ILE:HD13	2:B:250:LEU:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:MET:CE	2:B:367:PHE:CE2	3.01	0.43
1:A:201:ALA:O	1:A:267:PHE:CB	2.67	0.43
1:A:206:ASN:OD1	3:A:9500:GTP:N3	2.52	0.43
1:A:236:SER:O	1:A:320:ARG:NH1	2.49	0.43
1:A:303:VAL:C	1:A:305:CYS:N	2.72	0.43
1:A:390:ARG:C	1:A:392:ASP:N	2.71	0.43
2:B:19:LYS:CG	2:B:226:ASN:HB2	2.47	0.43
2:B:60:VAL:CG1	2:B:86:ARG:HG2	2.46	0.43
2:B:113:VAL:HG13	2:B:151:LEU:HD12	2.00	0.43
2:B:258:VAL:O	2:B:258:VAL:CG2	2.62	0.43
2:B:271:ALA:HB2	2:B:293:MET:HG3	2.00	0.43
1:A:15:GLN:O	1:A:16:ILE:C	2.57	0.43
1:A:29:GLY:O	1:A:30:ILE:HG13	2.19	0.43
1:A:194:THR:O	1:A:197:HIS:HB2	2.19	0.43
1:A:383:ALA:C	1:A:385:ALA:H	2.22	0.43
1:A:407:TRP:CZ2	2:B:258:VAL:CG2	3.01	0.43
2:B:36:TYR:CZ	2:B:44:LEU:HB2	2.54	0.43
2:B:80:PRO:O	2:B:81:PHE:C	2.57	0.43
2:B:156:ARG:HH21	2:B:164:MET:HB2	1.84	0.43
2:B:232:THR:O	2:B:233:MET:C	2.57	0.43
2:B:257:MET:CE	2:B:368:ILE:HG22	2.48	0.43
2:B:267:MET:SD	2:B:301:ALA:HB3	2.58	0.43
2:B:299:MET:HG3	2:B:305:PRO:HG2	1.99	0.43
2:B:361:LEU:HD13	2:B:362:LYS:N	2.34	0.43
1:A:8:HIS:HE1	1:A:138:PHE:CD1	2.37	0.43
1:A:139:HIS:CG	1:A:140:SER:H	2.37	0.43
1:A:167:LEU:CD1	1:A:252:LEU:HB3	2.45	0.43
1:A:188:ILE:O	1:A:191:THR:HG22	2.19	0.43
1:A:336:LYS:O	1:A:338:LYS:N	2.52	0.43
1:A:411:GLU:N	1:A:411:GLU:OE1	2.52	0.43
2:B:117:LEU:HD11	2:B:154:LYS:NZ	2.34	0.43
2:B:138:SER:HA	2:B:169:VAL:HB	2.01	0.43
2:B:359:ARG:HH11	2:B:359:ARG:CB	2.32	0.43
1:A:205:ASP:HB3	1:A:208:ALA:HB3	2.00	0.42
2:B:54:ALA:C	2:B:56:GLY:N	2.72	0.42
2:B:69:GLU:CG	2:B:69:GLU:O	2.67	0.42
2:B:158:GLU:C	2:B:159:TYR:CD1	2.92	0.42
2:B:192:LEU:C	2:B:194:GLU:H	2.23	0.42
2:B:240:LEU:HD22	2:B:248:ALA:N	2.33	0.42
1:A:242:LEU:HG	1:A:255:PHE:CZ	2.54	0.42
1:A:362:VAL:HG21	1:A:370:LYS:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:HE1	2:B:8:GLN:CB	2.30	0.42
2:B:64:ILE:HG22	2:B:91:VAL:HG22	2.02	0.42
2:B:169:VAL:O	2:B:169:VAL:HG12	2.18	0.42
2:B:193:VAL:HG22	2:B:193:VAL:O	2.20	0.42
2:B:389:PHE:C	2:B:391:ARG:N	2.73	0.42
1:A:209:ILE:O	1:A:210:TYR:C	2.57	0.42
1:A:224:TYR:HD2	1:A:224:TYR:HA	1.75	0.42
1:A:392:ASP:OD1	1:A:392:ASP:C	2.58	0.42
1:A:422:ARG:O	1:A:425:MET:N	2.52	0.42
2:B:26:ASP:OD1	2:B:26:ASP:C	2.56	0.42
2:B:36:TYR:CE1	2:B:43:GLN:HB2	2.54	0.42
2:B:130:LEU:HD11	2:B:162:ARG:HG3	2.02	0.42
2:B:163:ILE:HG13	2:B:163:ILE:H	1.67	0.42
2:B:193:VAL:HA	2:B:263:LEU:HD23	2.01	0.42
2:B:350:LYS:O	2:B:350:LYS:HD3	2.18	0.42
1:A:169:PHE:CZ	1:A:238:ILE:HD12	2.53	0.42
1:A:192:HIS:CD2	1:A:421:ALA:HA	2.54	0.42
1:A:241:SER:O	1:A:242:LEU:C	2.57	0.42
2:B:28:HIS:C	2:B:43:GLN:HE21	2.22	0.42
2:B:289:LEU:HD21	2:B:364:SER:C	2.40	0.42
2:B:425:TYR:C	2:B:427:ASP:H	2.22	0.42
1:A:276:ILE:CD1	1:A:277:SER:O	2.67	0.42
1:A:284:GLU:HB3	1:A:371:VAL:HG13	2.02	0.42
1:A:341:ILE:O	1:A:342:GLN:O	2.38	0.42
1:A:407:TRP:CE3	2:B:255:VAL:HG22	2.54	0.42
2:B:80:PRO:C	2:B:82:GLY:N	2.72	0.42
2:B:49:VAL:C	2:B:62:ARG:NH2	2.73	0.42
2:B:183:TYR:HD2	2:B:385:PHE:CE1	2.37	0.42
2:B:200:TYR:HB3	2:B:268:PRO:HG3	2.02	0.42
2:B:398:TYR:CD2	2:B:408:PHE:HZ	2.38	0.42
1:A:18:ASN:O	1:A:22:GLU:HB2	2.20	0.42
1:A:75:ILE:HG13	1:A:94:THR:OG1	2.19	0.42
2:B:244:GLY:H	2:B:247:ASN:HD22	1.68	0.42
1:A:33:ASP:O	1:A:34:GLY:O	2.37	0.42
1:A:71:GLU:CG	2:B:2:ARG:HH12	2.32	0.42
1:A:83:TYR:O	1:A:84:ARG:C	2.58	0.42
1:A:238:ILE:CA	1:A:242:LEU:HD23	2.49	0.42
1:A:303:VAL:HG12	1:A:305:CYS:N	2.34	0.42
1:A:313:MET:HG2	1:A:344:VAL:HG11	2.02	0.42
1:A:416:GLY:O	1:A:419:SER:N	2.53	0.42
1:A:16:ILE:HG13	1:A:231:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLN:NE2	1:A:253:THR:HG23	2.35	0.42
1:A:338:LYS:O	1:A:340:THR:N	2.49	0.42
2:B:60:VAL:O	2:B:61:PRO:C	2.58	0.42
2:B:183:TYR:OH	2:B:388:MET:O	2.36	0.42
2:B:242:PHE:HB2	2:B:354:CYS:SG	2.59	0.42
2:B:368:ILE:HG22	2:B:368:ILE:O	2.20	0.42
2:B:372:THR:OG1	2:B:426:GLN:HB2	2.20	0.42
1:A:12:ALA:O	1:A:15:GLN:HB2	2.20	0.42
1:A:122:ILE:O	1:A:123:ARG:C	2.57	0.42
1:A:155:GLU:O	1:A:155:GLU:OE1	2.37	0.42
1:A:239:THR:O	1:A:241:SER:N	2.53	0.42
1:A:296:PHE:CZ	1:A:317:LEU:HD21	2.55	0.42
2:B:228:LEU:CD1	2:B:273:LEU:HD21	2.38	0.42
1:A:70:LEU:HD23	1:A:70:LEU:N	2.35	0.41
1:A:103:TYR:CD1	1:A:148:GLY:CA	3.03	0.41
1:A:242:LEU:H	1:A:242:LEU:CD2	2.32	0.41
1:A:267:PHE:CE1	1:A:428:LEU:HD21	2.55	0.41
2:B:69:GLU:O	2:B:69:GLU:HG2	2.20	0.41
2:B:84:ILE:HG12	2:B:84:ILE:O	2.20	0.41
2:B:88:ASP:O	2:B:90:PHE:N	2.53	0.41
2:B:193:VAL:HA	2:B:265:PHE:HZ	1.85	0.41
2:B:313:VAL:CG1	2:B:314:ALA:N	2.83	0.41
1:A:14:VAL:O	1:A:14:VAL:HG12	2.20	0.41
2:B:197:ASP:HA	2:B:263:LEU:CB	2.45	0.41
1:A:3:GLU:H	1:A:132:LEU:HA	1.84	0.41
1:A:14:VAL:HG22	1:A:67:PHE:HD2	1.84	0.41
1:A:207:GLU:O	1:A:210:TYR:HB2	2.21	0.41
1:A:327:ASP:OD1	1:A:327:ASP:N	2.54	0.41
2:B:265:PHE:CD1	2:B:378:PHE:CE1	3.08	0.41
2:B:322:SER:OG	2:B:324:LYS:HB3	2.20	0.41
1:A:259:LEU:O	1:A:261:PRO:HD3	2.19	0.41
1:A:309:HIS:CG	1:A:310:GLY:H	2.38	0.41
2:B:37:HIS:N	2:B:37:HIS:ND1	2.69	0.41
2:B:54:ALA:O	2:B:56:GLY:N	2.49	0.41
2:B:204:ASN:OD1	4:B:1500:GDP:N3	2.53	0.41
2:B:304:ASP:O	2:B:307:HIS:HB2	2.21	0.41
1:A:11:GLN:O	1:A:15:GLN:N	2.54	0.41
1:A:93:ILE:CD1	1:A:117:LEU:HG	2.49	0.41
1:A:177:VAL:HG23	1:A:177:VAL:O	2.20	0.41
1:A:214:ARG:CG	1:A:220:GLU:OE1	2.67	0.41
1:A:269:LEU:HD23	1:A:384:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:ILE:HG22	2:B:65:LEU:N	2.36	0.41
2:B:197:ASP:O	2:B:258:VAL:HG11	2.20	0.41
1:A:22:GLU:HG2	1:A:83:TYR:CE1	2.54	0.41
1:A:115:ILE:HD13	1:A:115:ILE:C	2.41	0.41
1:A:195:LEU:C	1:A:197:HIS:N	2.73	0.41
2:B:101:TRP:HE1	2:B:188:SER:HA	1.86	0.41
2:B:244:GLY:O	2:B:246:LEU:N	2.54	0.41
2:B:257:MET:CE	2:B:370:ASN:HB2	2.50	0.41
2:B:299:MET:HE1	2:B:367:PHE:CE2	2.55	0.41
2:B:318:ARG:HG3	2:B:318:ARG:O	2.21	0.41
1:A:115:ILE:CG2	1:A:116:ASP:H	2.33	0.41
1:A:203:MET:O	1:A:204:VAL:HG23	2.21	0.41
1:A:242:LEU:HD11	1:A:250:VAL:HB	1.97	0.41
2:B:85:PHE:HB2	2:B:90:PHE:HE1	1.84	0.41
2:B:170:VAL:CG2	2:B:377:LEU:HD11	2.51	0.41
2:B:197:ASP:O	2:B:198:GLU:CG	2.69	0.41
2:B:309:ARG:HB3	2:B:342:VAL:HG23	2.03	0.41
2:B:313:VAL:CG1	2:B:367:PHE:CE1	3.03	0.41
2:B:344:TRP:CE3	2:B:345:ILE:HG13	2.55	0.41
1:A:154:MET:SD	1:A:168:GLU:OE1	2.79	0.41
2:B:403:MET:CE	2:B:408:PHE:HE1	2.33	0.41
1:A:23:LEU:CD1	1:A:26:LEU:HD23	2.34	0.41
1:A:70:LEU:HD22	1:A:114:ILE:CD1	2.51	0.41
1:A:76:ASP:O	1:A:80:THR:CG2	2.69	0.41
1:A:201:ALA:HB3	1:A:267:PHE:CD2	2.56	0.41
1:A:416:GLY:O	1:A:419:SER:HB2	2.21	0.41
2:B:99:ASN:HD22	2:B:99:ASN:HA	1.67	0.41
2:B:101:TRP:NE1	2:B:146:GLY:HA2	2.36	0.41
2:B:159:TYR:N	2:B:160:PRO:CD	2.84	0.41
2:B:181:GLU:CB	2:B:182:PRO:CD	2.94	0.41
2:B:207:LEU:HB2	2:B:225:LEU:HD13	2.02	0.41
2:B:255:VAL:O	2:B:255:VAL:CG1	2.68	0.41
2:B:262:ARG:NH2	2:B:417:ASP:OD1	2.54	0.41
2:B:263:LEU:HG	2:B:264:HIS:N	2.36	0.41
2:B:312:THR:O	2:B:312:THR:OG1	2.38	0.41
2:B:374:ILE:O	2:B:374:ILE:HG23	2.21	0.41
2:B:379:LYS:O	2:B:382:SER:HB3	2.21	0.41
2:B:399:THR:C	2:B:401:GLU:N	2.75	0.41
2:B:403:MET:HG2	2:B:404:ASP:H	1.86	0.41
1:A:11:GLN:O	1:A:12:ALA:C	2.58	0.41
1:A:173:PRO:HG2	1:A:187:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:HB3	1:A:184:PRO:HD2	2.02	0.41
1:A:209:ILE:O	1:A:213:CYS:SG	2.78	0.41
1:A:216:ASN:N	1:A:216:ASN:ND2	2.69	0.41
1:A:262:TYR:HB3	1:A:263:PRO:CD	2.44	0.41
1:A:404:PHE:HE2	2:B:256:ASN:HA	1.85	0.41
2:B:91:VAL:CB	2:B:116:VAL:HG22	2.51	0.41
2:B:230:SER:O	2:B:234:SER:CB	2.69	0.41
1:A:15:GLN:OE1	3:A:9500:GTP:O6	2.38	0.40
1:A:181:VAL:HG23	2:B:256:ASN:OD1	2.21	0.40
1:A:214:ARG:CD	1:A:220:GLU:OE1	2.69	0.40
1:A:333:ALA:C	1:A:334:THR:HG22	2.42	0.40
2:B:117:LEU:HD11	2:B:154:LYS:CE	2.51	0.40
2:B:169:VAL:HG11	2:B:204:ASN:HD21	1.86	0.40
2:B:234:SER:O	2:B:235:GLY:C	2.58	0.40
2:B:241:ARG:NH2	2:B:250:LEU:HG	2.36	0.40
1:A:71:GLU:HB2	1:A:99:ALA:CB	2.50	0.40
1:A:209:ILE:O	1:A:212:ILE:N	2.55	0.40
2:B:36:TYR:CG	2:B:44:LEU:HD22	2.56	0.40
2:B:189:VAL:O	2:B:190:HIS:C	2.58	0.40
2:B:193:VAL:CG2	2:B:262:ARG:NH1	2.84	0.40
2:B:271:ALA:HB3	2:B:272:PRO:HD3	2.02	0.40
1:A:91:GLN:O	1:A:93:ILE:N	2.50	0.40
1:A:289:ALA:HB3	1:A:290:GLU:OE2	2.21	0.40
2:B:141:GLY:O	2:B:184:ASN:ND2	2.54	0.40
1:A:84:ARG:NH1	1:A:84:ARG:HG2	2.36	0.40
1:A:191:THR:O	1:A:194:THR:HG22	2.21	0.40
1:A:217:LEU:CA	1:A:277:SER:HB2	2.46	0.40
1:A:291:ILE:O	1:A:294:ALA:N	2.54	0.40
1:A:392:ASP:O	1:A:395:PHE:HB3	2.22	0.40
2:B:31:ASP:OD2	2:B:37:HIS:CE1	2.75	0.40
2:B:136:THR:HG22	2:B:167:PHE:HB2	2.03	0.40
2:B:204:ASN:HD21	4:B:1500:GDP:H1'	1.86	0.40
2:B:310:TYR:CD2	2:B:371:SER:HB3	2.57	0.40
1:A:5:ILE:O	1:A:136:SER:N	2.51	0.40
1:A:167:LEU:HD22	1:A:202:PHE:CE1	2.56	0.40
1:A:210:TYR:HH	2:B:323:MET:HB2	1.79	0.40
2:B:11:GLN:O	2:B:15:GLN:HG3	2.22	0.40
2:B:111:GLU:HG3	2:B:111:GLU:O	2.21	0.40
2:B:337:ASN:HD21	2:B:340:TYR:HD1	1.67	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 PDB entries followed by that with respect to all EM entries.

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	408/440 (93%)	223 (55%)	113 (28%)	72 (18%)	0	0
2	B	424/427 (99%)	251 (59%)	109 (26%)	64 (15%)	0	0
All	All	832/867 (96%)	474 (57%)	222 (27%)	136 (16%)	0	0

All (136) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	72	PRO
1	A	73	THR
1	A	100	ALA
1	A	101	ASN
1	A	104	ALA
1	A	132	LEU
1	A	141	PHE
1	A	142	GLY
1	A	183	GLU
1	A	238	ILE
1	A	240	ALA
1	A	247	ALA
1	A	287	SER
1	A	342	GLN
1	A	369	ALA
1	A	399	TYR
1	A	421	ALA
2	B	80	PRO
2	B	81	PHE
2	B	84	ILE
2	B	111	GLU
2	B	112	LEU
2	B	126	SER
2	B	185	ALA

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Mol	Chain	Res	Type
2	B	227	HIS
2	B	228	LEU
2	B	236	VAL
2	B	238	THR
2	B	246	LEU
2	B	262	ARG
2	B	264	HIS
2	B	286	VAL
2	B	293	MET
2	B	320	ARG
2	B	359	ARG
2	B	387	ALA
2	B	388	MET
2	B	393	ALA
1	A	24	TYR
1	A	79	ARG
1	A	80	THR
1	A	92	LEU
1	A	108	TYR
1	A	131	GLY
1	A	196	GLU
1	A	211	ASP
1	A	241	SER
1	A	255	PHE
1	A	266	HIS
1	A	270	ALA
1	A	278	ALA
1	A	279	GLU
1	A	309	HIS
1	A	310	GLY
1	A	330	ALA
1	A	337	THR
1	A	344	VAL
1	A	352	LYS
1	A	370	LYS
1	A	374	ALA
2	B	34	GLY
2	B	36	TYR
2	B	43	GLN
2	B	56	GLY
2	B	71	GLY
2	B	82	GLY

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Mol	Chain	Res	Type
2	B	166	THR
2	B	193	VAL
2	B	275	SER
2	B	284	LEU
2	B	292	GLN
2	B	296	ALA
2	B	338	SER
2	B	342	VAL
2	B	368	ILE
2	B	394	PHE
2	B	400	GLY
2	B	402	GLY
1	A	158	SER
1	A	187	SER
1	A	217	LEU
1	A	285	GLN
1	A	314	ALA
1	A	339	ARG
1	A	377	MET
1	A	398	MET
1	A	430	LYS
2	B	8	GLN
2	B	48	ASN
2	B	62	ARG
2	B	89	ASN
2	B	276	ARG
2	B	281	TYR
2	B	336	LYS
2	B	349	VAL
2	B	392	LYS
2	B	410	GLU
1	A	133	GLN
1	A	140	SER
1	A	179	THR
1	A	188	ILE
1	A	304	LYS
1	A	334	THR
1	A	340	THR
1	A	364	PRO
1	A	382	THR
2	B	55	ALA
2	B	110	ALA

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Mol	Chain	Res	Type
2	B	162	ARG
2	B	195	ASN
2	B	235	GLY
2	B	245	GLN
2	B	348	ASN
2	B	357	PRO
1	A	31	GLN
1	A	236	SER
1	A	265	GLY
1	A	362	VAL
2	B	143	THR
2	B	180	VAL
2	B	346	PRO
1	A	32	PRO
1	A	160	ASP
1	A	307	PRO
1	A	435	VAL
2	B	142	GLY
2	B	319	GLY
1	A	63	PRO
1	A	174	ALA
1	A	366	GLY
1	A	177	VAL
2	B	261	PRO
1	A	204	VAL
1	A	273	ALA
2	B	87	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	347/369 (94%)	291 (84%)	56 (16%)	2 7
2	B	367/368 (100%)	303 (83%)	64 (17%)	2 6
All	All	714/737 (97%)	594 (83%)	120 (17%)	5 6

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	16	ILE
1	A	20	CYS
1	A	22	GLU
1	A	24	TYR
1	A	31	GLN
1	A	32	PRO
1	A	64	ARG
1	A	69	ASP
1	A	70	LEU
1	A	76	ASP
1	A	77	GLU
1	A	79	ARG
1	A	94	THR
1	A	98	ASP
1	A	114	ILE
1	A	115	ILE
1	A	123	ARG
1	A	130	THR
1	A	155	GLU
1	A	166	LYS
1	A	172	TYR
1	A	192	HIS
1	A	196	GLU
1	A	213	CYS
1	A	224	TYR
1	A	234	ILE
1	A	248	LEU
1	A	251	ASP
1	A	267	PHE
1	A	271	THR
1	A	275	VAL
1	A	276	ILE
1	A	279	GLU
1	A	291	ILE
1	A	293	ASN
1	A	302	MET
1	A	323	VAL
1	A	327	ASP
1	A	334	THR
1	A	340	THR
1	A	343	PHE

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Mol	Chain	Res	Type
1	A	356	ASN
1	A	361	THR
1	A	368	LEU
1	A	375	VAL
1	A	384	ILE
1	A	392	ASP
1	A	404	PHE
1	A	409	VAL
1	A	411	GLU
1	A	415	GLU
1	A	417	GLU
1	A	424	ASP
1	A	432	TYR
1	A	433	GLU
2	B	3	GLU
2	B	5	VAL
2	B	24	ILE
2	B	26	ASP
2	B	31	ASP
2	B	32	PRO
2	B	37	HIS
2	B	41	ASP
2	B	44	LEU
2	B	46	ARG
2	B	48	ASN
2	B	60	VAL
2	B	65	LEU
2	B	66	VAL
2	B	69	GLU
2	B	85	PHE
2	B	88	ASP
2	B	112	LEU
2	B	127	CYS
2	B	136	THR
2	B	143	THR
2	B	151	LEU
2	B	153	SER
2	B	156	ARG
2	B	170	VAL
2	B	180	VAL
2	B	181	GLU
2	B	186	THR

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Mol	Chain	Res	Type
2	B	188	SER
2	B	189	VAL
2	B	196	THR
2	B	209	ASP
2	B	211	CYS
2	B	214	THR
2	B	232	THR
2	B	238	THR
2	B	239	CYS
2	B	240	LEU
2	B	241	ARG
2	B	249	ASP
2	B	252	LYS
2	B	263	LEU
2	B	273	LEU
2	B	276	ARG
2	B	284	LEU
2	B	297	LYS
2	B	300	MET
2	B	307	HIS
2	B	329	GLN
2	B	340	TYR
2	B	341	PHE
2	B	356	ILE
2	B	357	PRO
2	B	358	PRO
2	B	364	SER
2	B	370	ASN
2	B	371	SER
2	B	375	GLN
2	B	377	LEU
2	B	381	ILE
2	B	394	PHE
2	B	395	LEU
2	B	416	ASN
2	B	422	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN

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Mol	Chain	Res	Type
1	A	28	HIS
1	A	61	HIS
1	A	85	GLN
1	A	88	HIS
1	A	91	GLN
1	A	139	HIS
1	A	216	ASN
1	A	226	ASN
1	A	249	ASN
1	A	256	GLN
1	A	266	HIS
1	A	293	ASN
1	A	300	ASN
1	A	329	ASN
1	A	356	ASN
1	A	406	HIS
2	B	8	GLN
2	B	14	ASN
2	B	43	GLN
2	B	48	ASN
2	B	99	ASN
2	B	100	ASN
2	B	105	HIS
2	B	131	GLN
2	B	137	HIS
2	B	191	GLN
2	B	204	ASN
2	B	226	ASN
2	B	247	ASN
2	B	264	HIS
2	B	298	ASN
2	B	332	ASN
2	B	337	ASN
2	B	347	ASN
2	B	370	ASN
2	B	414	ASN
2	B	416	ASN
2	B	423	GLN
2	B	426	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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EP	B	1001	-	32,36,36	2.15	7 (21%)	39,53,53	2.76	7 (17%)
4	GDP	B	1500	-	24,30,30	1.03	2 (8%)	30,47,47	1.00	3 (10%)
3	GTP	A	9500	-	26,34,34	1.10	2 (7%)	32,54,54	0.95	3 (9%)

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
5	EP	B	1001	-	-	13/49/55/55	0/2/3/3
4	GDP	B	1500	-	-	2/12/32/32	0/3/3/3
3	GTP	A	9500	-	-	2/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	EP	C27-C24	7.79	1.60	1.46
5	B	1001	EP	C13-S1	5.88	1.79	1.70
3	A	9500	GTP	C5-C6	-2.98	1.41	1.47
5	B	1001	EP	C72-C68	2.76	1.56	1.53
3	A	9500	GTP	C8-N7	-2.44	1.30	1.35
4	B	1500	GDP	C5-C6	-2.39	1.42	1.47
5	B	1001	EP	O26-C24	-2.38	1.40	1.45
4	B	1500	GDP	C8-N7	-2.37	1.31	1.35
5	B	1001	EP	O26-C27	-2.23	1.40	1.45
5	B	1001	EP	C12-N20	2.20	1.44	1.37
5	B	1001	EP	C41-C47	2.18	1.57	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1001	EP	C27-O26-C24	12.26	69.53	60.69
5	B	1001	EP	O26-C27-C24	-7.05	55.15	59.65
5	B	1001	EP	O26-C24-C27	-6.77	55.32	59.65
3	A	9500	GTP	PB-O3B-PG	-2.77	123.33	132.83
5	B	1001	EP	O2-C75-C72	2.54	116.13	111.46
5	B	1001	EP	C38-C41-C47	2.49	115.43	111.39
3	A	9500	GTP	O2G-PG-O1G	2.33	119.80	110.68
4	B	1500	GDP	O2B-PB-O1B	2.32	119.75	110.68
5	B	1001	EP	O26-C24-C21	-2.25	111.57	116.33
4	B	1500	GDP	O6-C6-C5	2.19	128.66	124.37
5	B	1001	EP	O2-C3-C5	2.18	115.44	109.48
3	A	9500	GTP	O6-C6-C5	2.14	128.56	124.37
4	B	1500	GDP	PA-O3A-PB	-2.12	125.56	132.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1001	EP	C5-C10-C12-N20
5	B	1001	EP	C59-C68-C72-C75
5	B	1001	EP	O70-C68-C72-C75
5	B	1001	EP	C41-C47-C51-C53
5	B	1001	EP	O49-C47-C51-C57
5	B	1001	EP	C35-C38-C41-C43
5	B	1001	EP	O26-C27-C32-C35
5	B	1001	EP	C41-C47-C51-C57
3	A	9500	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
5	B	1001	EP	C5-C3-O2-C75
5	B	1001	EP	C51-C57-C59-C68
5	B	1001	EP	O58-C57-C59-C68
4	B	1500	GDP	C3'-C4'-C5'-O5'
5	B	1001	EP	C38-C41-C47-O49
5	B	1001	EP	O58-C57-C59-C60
4	B	1500	GDP	O4'-C4'-C5'-O5'
3	A	9500	GTP	PA-O3A-PB-O1B

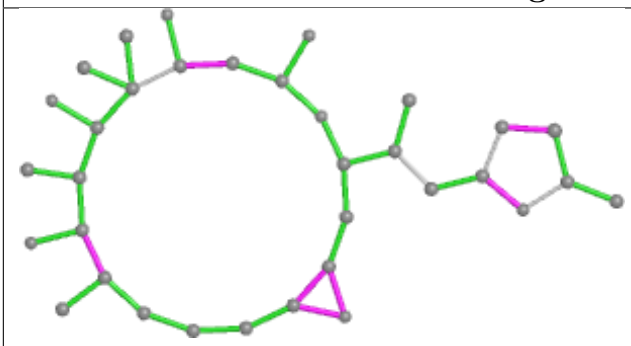
There are no ring outliers.

3 monomers are involved in 16 short contacts:

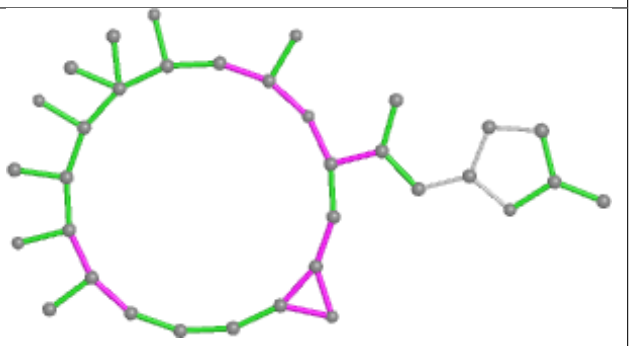
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	EP	4	0
4	B	1500	GDP	8	0
3	A	9500	GTP	4	0

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.

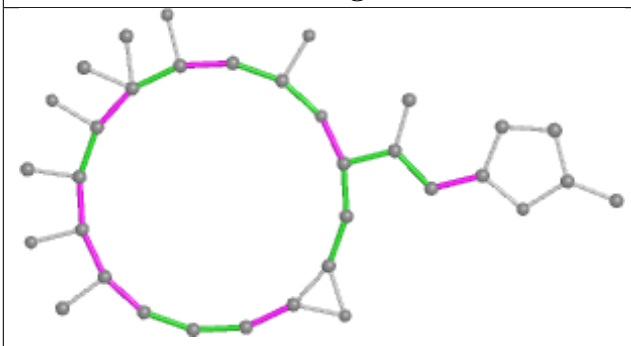
Ligand EP B 1001



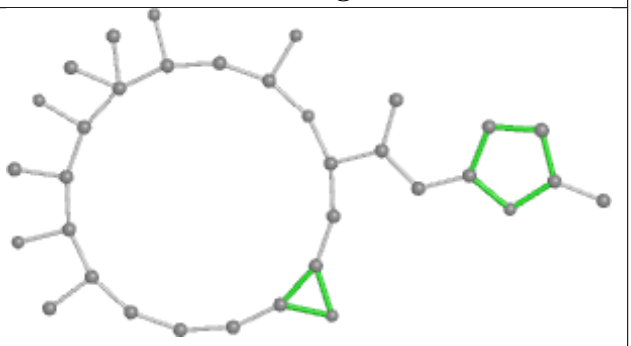
Bond lengths



Bond angles

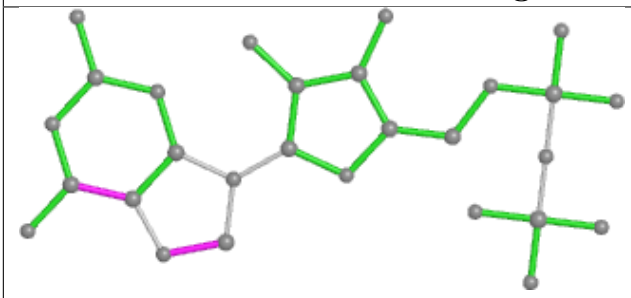


Torsions

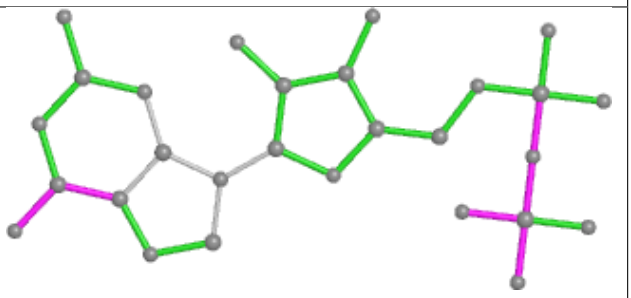


Rings

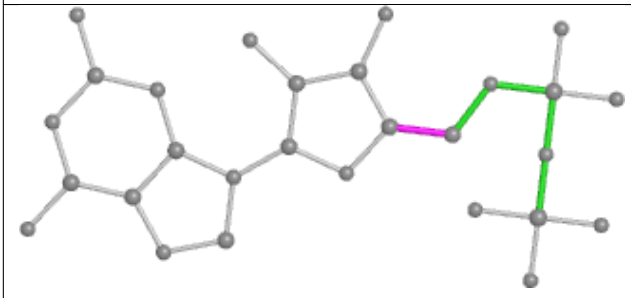
Ligand GDP B 1500



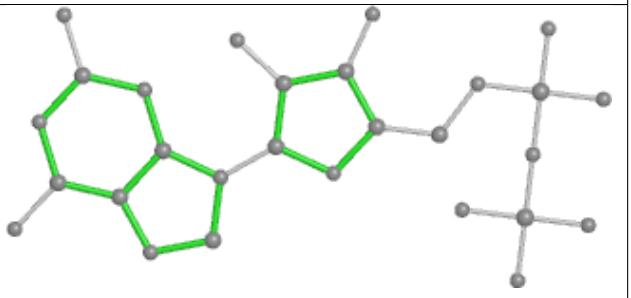
Bond lengths



Bond angles

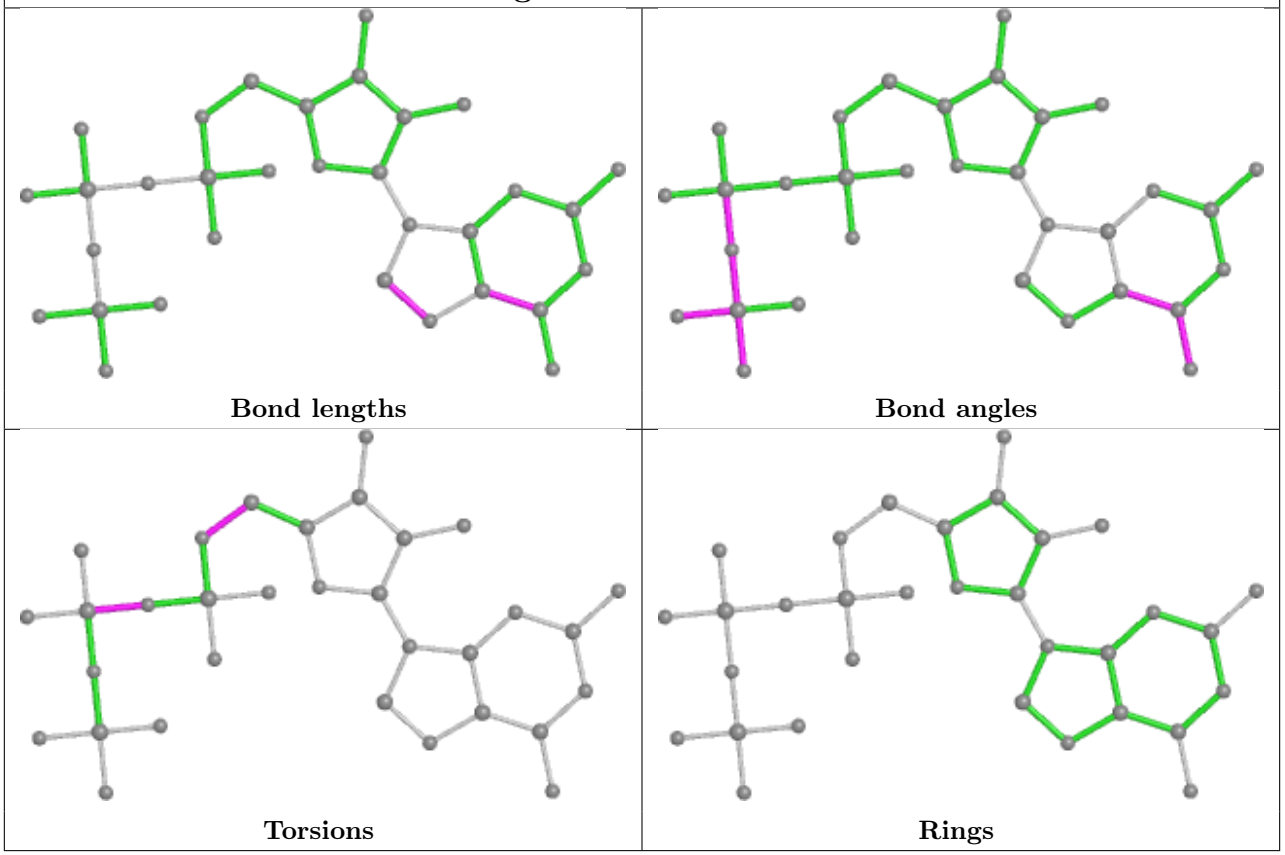


Torsions



Rings

Ligand GTP A 9500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.