Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 01:18 PM EDT

PDB ID	:	1UWB
Title	:	TYR 181 CYS HIV-1 RT/8-CL TIBO
Authors	:	Das, K.; Ding, J.; Hsiou, Y.; Arnold, E.
Deposited on	:	1996-11-21
Resolution	:	3.20 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:

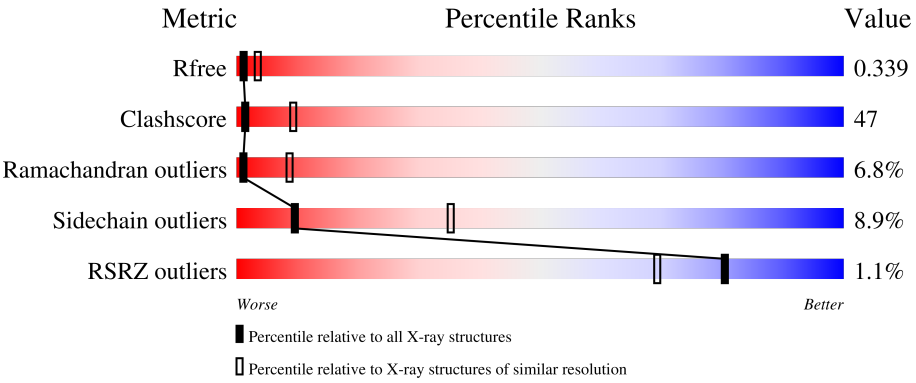
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	558	% 36% 56% 8%
2	B	427	% 29% 56% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7822 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
			4365	2822	725	812	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

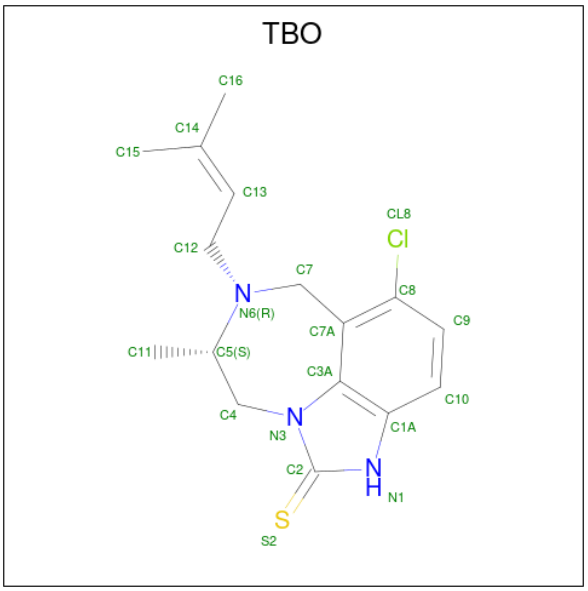
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3436	2234	567	629	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	181	CYS	TYR	engineered mutation	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 5-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: TBO) (formula: $C_{16}H_{20}ClN_3S$).



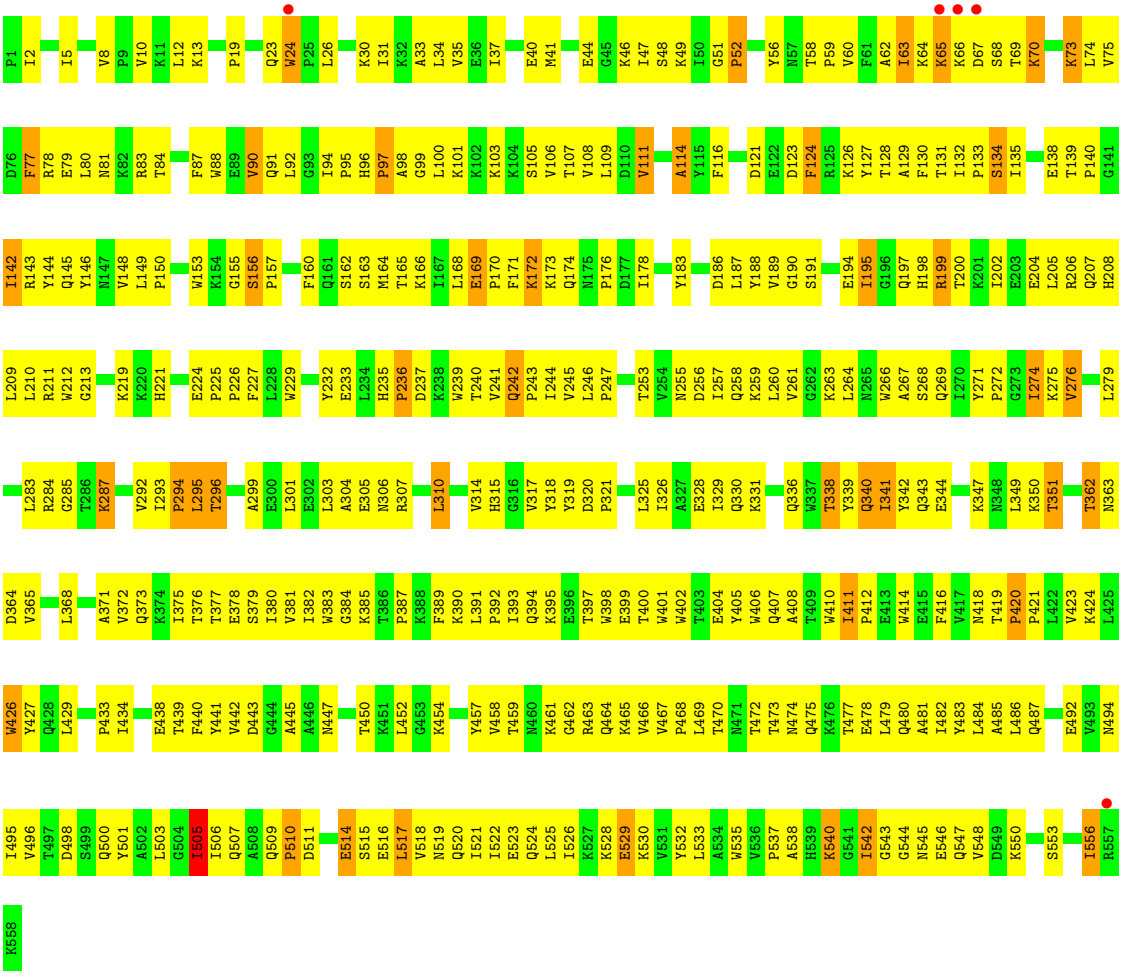
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	S		
3	A	1	21	16	1	3	1	0	0

3 Residue-property plots (i)

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

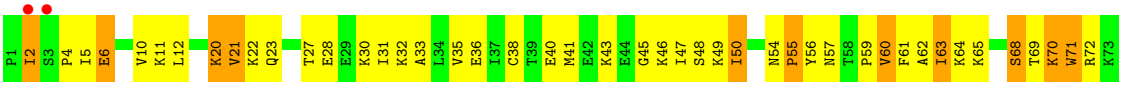
• Molecule 1: REVERSE TRANSCRIPTASE

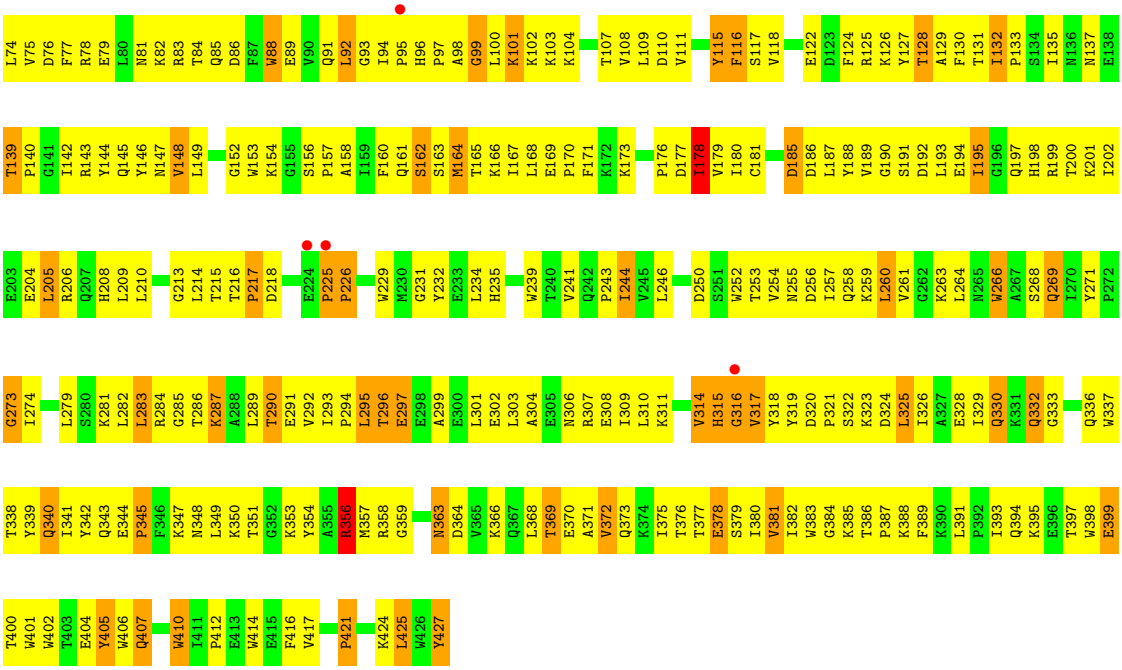
Chain A:



• Molecule 2: REVERSE TRANSCRIPTASE

Chain B:




L74 V75 D76 F77 R78 E79 L80 N81 K82 R83 T84 Q85 D86 F87 W88 E89 V90 Q91 L92 G93 I94 P95 H96 P97 A98 G99 L100 K101 K102 K103 K104 T107 V108 L109 D110 V111 Y115 F116 S117 V118 E122 D123 F124 R125 K126 Y127 T128 A129 F130 T131 I132 P133 S134 I135 N136 N137 E138
T139 P140 G141 I142 R143 Y144 Q145 Y146 N147 V148 L149 G152 W153 K154 G155 S156 P157 A158 I159 F160 Q161 S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 K172 K173 P176 D177 I178 V179 I180 C181 D185 D186 L187 Y188 V189 G190 S191 D192 L193 E194 I195 G196 Q197 H198 R199 T200 K201 I202
E203 E204 L205 R206 Q207 H208 L209 L210 G213 L214 T215 T216 P217 D218 E224 P225 P226 W229 M230 G231 Y232 E233 L234 H235 W239 T240 V241 Q242 P243 I244 V245 L246 D250 S251 W252 T253 V254 N255 D256 I257 Q258 K259 L260 V261 G262 K263 L264 N265 W266 A267 S268 Q269 I270 Y271 P272
G273 I274 L279 S280 K281 L282 L283 R284 G285 T286 K287 A288 L289 T290 E291 V292 I293 P294 L295 T296 E297 E298 A299 E300 L301 E302 L303 A304 E305 N306 R307 E308 I309 L310 K311 V314 H315 G316 V317 Y318 Y319 D320 P321 S322 K323 D324 L325 I326 A327 E328 I329 Q330 K331 Q332 G333 Q336 W337
T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 K347 N348 L349 K350 T351 G352 K353 Y354 A355 R356 M357 R358 G359 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377 E378 S379 I380 V381 I382 W383 G384 K385 T386 P387 K388 F389 K390 L391 P392 I393 Q394 K395 E396 T397 W398 E399
T400 W401 W402 T403 E404 Y405 W406 Q407 W410 I411 P412 E413 W414 E415 F416 V417 P421 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	225.70Å 69.20Å 104.90Å 90.00° 106.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20 14.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	85.0 ((Not available)-3.20) 85.0 (14.98-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 3.19Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.274 , 0.360 0.260 , 0.339	Depositor DCC
R_{free} test set	1059 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	68.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.14 , 14.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7822	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: TBO

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	0.55	0/4479	0.78	3/6108 (0.0%)
2	B	0.60	0/3534	0.85	5/4812 (0.1%)
All	All	0.57	0/8013	0.81	8/10920 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	LYS	N-CA-C	6.92	129.68	111.00
1	A	517	LEU	CA-CB-CG	5.82	128.69	115.30
2	B	226	PRO	N-CA-CB	5.54	109.95	103.30
2	B	225	PRO	N-CA-CB	5.50	109.89	103.30
2	B	260	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	24	TRP	N-CA-C	-5.45	96.30	111.00
2	B	295	LEU	N-CA-C	5.30	125.33	111.00
2	B	332	GLN	N-CA-C	5.19	125.02	111.00

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	4365	0	4260	397	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3436	0	3401	363	0
3	A	21	0	20	8	0
All	All	7822	0	7681	736	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 47.

All (736) 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	1.39	1.03
2:B:180:ILE:HG23	2:B:189:VAL:HG22	1.41	1.00
1:A:272:PRO:HA	1:A:351:THR:HG21	1.43	0.99
1:A:318:TYR:CE2	3:A:559:TBO:H10	2.03	0.93
2:B:12:LEU:HA	2:B:84:THR:HG22	1.48	0.92
1:A:543:GLY:H	2:B:284:ARG:HA	1.33	0.91
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.51	0.91
2:B:340:GLN:HB3	2:B:351:THR:HG22	1.54	0.90
1:A:373:GLN:NE2	2:B:397:THR:HA	1.87	0.90
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.51	0.89
1:A:241:VAL:HG11	1:A:266:TRP:HE1	1.37	0.89
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.53	0.89
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.55	0.88
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.09	0.88
2:B:263:LYS:HE2	2:B:425:LEU:HD13	1.58	0.86
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.11	0.85
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.59	0.85
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.42	0.84
1:A:543:GLY:HA2	1:A:546:GLU:HB3	1.61	0.83
1:A:63:ILE:HG22	1:A:64:LYS:H	1.43	0.82
1:A:399:GLU:HA	1:A:402:TRP:NE1	1.94	0.81
1:A:51:GLY:H	1:A:52:PRO:HD2	1.43	0.81
1:A:253:THR:HA	1:A:292:VAL:HA	1.63	0.81
2:B:258:GLN:HG2	2:B:283:LEU:HD13	1.61	0.81
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.63	0.81
2:B:344:GLU:HB2	2:B:347:LYS:HB2	1.62	0.80
1:A:341:ILE:HD13	1:A:350:LYS:HB3	1.62	0.80
2:B:326:ILE:HD12	2:B:388:LYS:HE2	1.63	0.80
1:A:101:LYS:HD3	1:A:321:PRO:HD3	1.63	0.80
1:A:257:ILE:HD11	1:A:295:LEU:HD11	1.63	0.80
2:B:132:ILE:CG2	2:B:142:ILE:HB	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:ILE:HG23	2:B:142:ILE:HB	1.62	0.80
2:B:306:ASN:HA	2:B:309:ILE:HB	1.64	0.79
2:B:328:GLU:O	2:B:339:TYR:HA	1.81	0.79
2:B:79:GLU:O	2:B:83:ARG:HG3	1.82	0.79
1:A:164:MET:SD	1:A:168:LEU:HD21	2.23	0.78
1:A:542:ILE:HG23	1:A:545:ASN:HB2	1.66	0.78
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.84	0.78
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.13	0.78
1:A:240:THR:CG2	1:A:315:HIS:HA	2.13	0.77
1:A:8:VAL:O	1:A:121:ASP:HB2	1.85	0.77
2:B:379:SER:HA	2:B:383:TRP:CZ3	2.20	0.77
1:A:106:VAL:HG12	1:A:107:THR:H	1.50	0.77
1:A:227:PHE:O	1:A:233:GLU:HA	1.86	0.76
1:A:317:VAL:HG23	1:A:349:LEU:HD13	1.66	0.76
2:B:79:GLU:HG3	2:B:83:ARG:HD2	1.66	0.76
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.67	0.76
1:A:267:ALA:HB1	1:A:271:TYR:CD2	2.21	0.75
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.21	0.75
1:A:398:TRP:HE1	1:A:411:ILE:HG12	1.50	0.75
1:A:427:TYR:OH	1:A:509:GLN:HA	1.86	0.74
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.69	0.74
2:B:425:LEU:HD12	2:B:427:TYR:HB3	1.69	0.74
2:B:319:TYR:O	2:B:321:PRO:HD3	1.87	0.74
1:A:543:GLY:HA3	2:B:284:ARG:O	1.88	0.74
2:B:65:LYS:HD2	2:B:407:GLN:HG2	1.70	0.73
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.70	0.73
1:A:503:LEU:O	1:A:507:GLN:HG3	1.86	0.73
1:A:239:TRP:HB3	1:A:318:TYR:HE1	1.53	0.73
1:A:459:THR:OG1	1:A:463:ARG:HB3	1.88	0.73
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.23	0.73
1:A:503:LEU:HD13	1:A:535:TRP:CB	2.18	0.73
2:B:281:LYS:HA	2:B:284:ARG:HG3	1.71	0.72
2:B:254:VAL:O	2:B:258:GLN:HG3	1.90	0.72
1:A:301:LEU:O	1:A:305:GLU:HB2	1.88	0.72
2:B:61:PHE:CE1	2:B:76:ASP:HB2	2.24	0.72
1:A:99:GLY:HA2	1:A:383:TRP:NE1	2.03	0.71
2:B:164:MET:SD	2:B:168:LEU:HD11	2.30	0.71
2:B:366:LYS:O	2:B:369:THR:HG22	1.91	0.71
2:B:257:ILE:O	2:B:261:VAL:HG23	1.90	0.71
1:A:169:GLU:O	1:A:172:LYS:HG3	1.91	0.71
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:CG2	1:A:144:TYR:HB3	2.21	0.70
1:A:256:ASP:HA	1:A:259:LYS:HE3	1.73	0.70
2:B:116:PHE:HA	2:B:148:VAL:HG21	1.74	0.70
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.26	0.70
1:A:246:LEU:HG	1:A:310:LEU:HD22	1.74	0.70
1:A:443:ASP:CB	1:A:548:VAL:HB	2.21	0.70
2:B:198:HIS:O	2:B:202:ILE:HG12	1.92	0.70
2:B:257:ILE:O	2:B:260:LEU:HB3	1.92	0.69
2:B:252:TRP:O	2:B:292:VAL:HA	1.93	0.69
2:B:260:LEU:O	2:B:264:LEU:HG	1.93	0.69
1:A:474:ASN:O	1:A:478:GLU:HG3	1.92	0.69
2:B:84:THR:HG21	2:B:124:PHE:CZ	2.26	0.69
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.73	0.69
2:B:241:VAL:HG13	2:B:351:THR:OG1	1.93	0.69
1:A:88:TRP:CE2	2:B:143:ARG:HD2	2.27	0.69
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.27	0.69
1:A:478:GLU:O	1:A:481:ALA:HB3	1.92	0.69
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.75	0.69
1:A:267:ALA:HB1	1:A:271:TYR:HD2	1.55	0.69
1:A:239:TRP:O	1:A:240:THR:HG23	1.92	0.69
1:A:92:LEU:HD11	2:B:22:LYS:HE3	1.74	0.68
1:A:443:ASP:HB2	1:A:548:VAL:HB	1.74	0.68
2:B:23:GLN:HG3	2:B:133:PRO:HG3	1.75	0.68
2:B:205:LEU:O	2:B:205:LEU:HD12	1.92	0.68
2:B:261:VAL:HA	2:B:264:LEU:HD12	1.75	0.68
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.76	0.68
1:A:397:THR:HG21	1:A:424:LYS:HA	1.76	0.68
1:A:128:THR:HG21	1:A:150:PRO:HG2	1.75	0.68
1:A:232:TYR:HA	1:A:241:VAL:HG22	1.74	0.68
2:B:201:LYS:O	2:B:204:GLU:HB3	1.93	0.68
2:B:125:ARG:HE	2:B:147:ASN:HA	1.59	0.68
2:B:398:TRP:O	2:B:402:TRP:HD1	1.76	0.68
2:B:166:LYS:O	2:B:170:PRO:HD2	1.94	0.67
1:A:521:ILE:O	1:A:525:LEU:HG	1.94	0.67
2:B:108:VAL:HA	2:B:187:LEU:O	1.94	0.67
1:A:90:VAL:HG23	1:A:91:GLN:H	1.58	0.67
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.30	0.67
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.24	0.67
1:A:326:ILE:O	1:A:341:ILE:HA	1.94	0.67
1:A:188:TYR:CB	3:A:559:TBO:H122	2.25	0.67
2:B:107:THR:HA	2:B:232:TYR:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ARG:O	2:B:202:ILE:HB	1.94	0.67
2:B:323:LYS:HB2	2:B:343:GLN:OE1	1.93	0.67
1:A:398:TRP:CE2	1:A:402:TRP:CD1	2.84	0.66
1:A:198:HIS:O	1:A:202:ILE:HG12	1.96	0.66
1:A:31:ILE:HG21	1:A:134:SER:O	1.96	0.66
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.31	0.66
1:A:399:GLU:HA	1:A:402:TRP:HE1	1.58	0.66
1:A:419:THR:HB	1:A:420:PRO:HD2	1.78	0.66
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.61	0.66
2:B:326:ILE:O	2:B:341:ILE:HA	1.96	0.66
1:A:398:TRP:NE1	1:A:411:ILE:HG12	2.11	0.66
2:B:393:ILE:HG12	2:B:394:GLN:N	2.11	0.66
2:B:40:GLU:O	2:B:43:LYS:HB3	1.96	0.65
1:A:207:GLN:HB3	1:A:211:ARG:HH12	1.59	0.65
1:A:240:THR:HG21	1:A:315:HIS:HA	1.76	0.65
2:B:101:LYS:HD2	2:B:382:ILE:HG23	1.79	0.65
2:B:128:THR:CB	2:B:146:TYR:HB2	2.27	0.65
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.78	0.65
2:B:115:TYR:HD2	2:B:156:SER:HB3	1.61	0.65
1:A:303:LEU:HD21	1:A:307:ARG:HH21	1.60	0.65
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.65
2:B:271:TYR:O	2:B:274:ILE:HG22	1.97	0.65
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.33	0.64
2:B:163:SER:O	2:B:167:ILE:HG12	1.98	0.64
2:B:160:PHE:HE2	2:B:164:MET:HG2	1.63	0.64
1:A:514:GLU:CD	1:A:514:GLU:H	2.00	0.64
2:B:379:SER:HA	2:B:383:TRP:CE3	2.32	0.64
2:B:99:GLY:HA2	2:B:102:LYS:HD2	1.80	0.64
1:A:146:TYR:CE2	1:A:150:PRO:HA	2.33	0.64
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.80	0.63
1:A:260:LEU:O	1:A:264:LEU:HG	1.98	0.63
2:B:380:ILE:O	2:B:384:GLY:N	2.31	0.63
1:A:188:TYR:CG	3:A:559:TBO:H122	2.33	0.63
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.34	0.63
1:A:439:THR:HA	1:A:494:ASN:HB2	1.79	0.63
2:B:257:ILE:HD13	2:B:283:LEU:HB3	1.81	0.63
2:B:329:ILE:HD11	2:B:375:ILE:HD11	1.79	0.63
1:A:241:VAL:HG11	1:A:266:TRP:NE1	2.11	0.63
2:B:378:GLU:O	2:B:381:VAL:HB	1.99	0.63
2:B:5:ILE:HG22	2:B:6:GLU:H	1.64	0.62
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:PHE:HD2	2:B:152:GLY:HA3	1.64	0.62
1:A:101:LYS:HD3	1:A:321:PRO:CD	2.28	0.62
1:A:479:LEU:HA	1:A:482:ILE:HD12	1.81	0.62
1:A:194:GLU:O	1:A:197:GLN:N	2.31	0.62
1:A:331:LYS:O	1:A:421:PRO:HG2	1.99	0.62
1:A:466:VAL:HG12	1:A:467:VAL:N	2.15	0.62
1:A:398:TRP:O	1:A:401:TRP:HB3	1.99	0.62
1:A:445:ALA:O	1:A:477:THR:HG21	1.99	0.62
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.33	0.62
1:A:304:ALA:HA	1:A:307:ARG:HB2	1.81	0.62
2:B:160:PHE:CE2	2:B:164:MET:HG2	2.34	0.62
1:A:341:ILE:O	1:A:349:LEU:HB3	1.99	0.62
1:A:420:PRO:HB2	1:A:421:PRO:HD3	1.82	0.61
1:A:478:GLU:O	1:A:482:ILE:HG13	2.00	0.61
1:A:482:ILE:O	1:A:485:ALA:HB3	2.00	0.61
1:A:500:GLN:OE1	1:A:500:GLN:HA	1.98	0.61
1:A:239:TRP:HB3	1:A:318:TYR:CE1	2.36	0.61
2:B:292:VAL:HG12	2:B:294:PRO:HD3	1.83	0.61
1:A:442:VAL:HG21	1:A:485:ALA:HB2	1.83	0.61
1:A:509:GLN:N	1:A:510:PRO:HD3	2.16	0.61
1:A:372:VAL:HA	1:A:375:ILE:HD12	1.82	0.61
2:B:99:GLY:HA2	2:B:102:LYS:CD	2.31	0.61
2:B:115:TYR:HE2	2:B:157:PRO:N	1.99	0.61
2:B:330:GLN:HB2	2:B:332:GLN:HE22	1.65	0.61
2:B:27:THR:HG23	2:B:30:LYS:H	1.65	0.60
2:B:261:VAL:HG22	2:B:279:LEU:HD23	1.83	0.60
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.36	0.60
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.65	0.60
1:A:368:LEU:O	1:A:371:ALA:HB3	2.02	0.60
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.67	0.60
1:A:90:VAL:HG23	1:A:91:GLN:N	2.15	0.60
1:A:373:GLN:HE21	2:B:397:THR:HA	1.67	0.60
2:B:315:HIS:O	2:B:317:VAL:N	2.35	0.60
2:B:31:ILE:HD13	2:B:133:PRO:O	2.02	0.60
1:A:63:ILE:HG22	1:A:64:LYS:N	2.16	0.60
1:A:317:VAL:HG11	1:A:347:LYS:HE3	1.82	0.60
1:A:441:TYR:O	1:A:548:VAL:HG11	2.02	0.60
2:B:375:ILE:O	2:B:378:GLU:HG2	2.02	0.60
1:A:34:LEU:HD22	1:A:60:VAL:HG12	1.82	0.59
2:B:379:SER:HA	2:B:383:TRP:HZ3	1.65	0.59
2:B:354:TYR:HD2	2:B:371:ALA:HB2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:LEU:H	2:B:325:LEU:CD2	2.15	0.59
1:A:92:LEU:HD11	2:B:22:LYS:CE	2.32	0.59
1:A:37:ILE:O	1:A:41:MET:HG3	2.02	0.59
1:A:268:SER:O	1:A:351:THR:HB	2.03	0.59
1:A:195:ILE:CG2	1:A:199:ARG:HH12	2.16	0.59
1:A:400:THR:O	1:A:404:GLU:HG3	2.02	0.59
1:A:106:VAL:HG12	1:A:107:THR:N	2.17	0.59
1:A:51:GLY:N	1:A:52:PRO:HD2	2.16	0.59
1:A:492:GLU:HG2	1:A:530:LYS:HD2	1.85	0.59
2:B:239:TRP:HB2	2:B:350:LYS:HE3	1.84	0.59
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.66	0.59
1:A:398:TRP:CE2	1:A:402:TRP:HD1	2.20	0.59
1:A:498:ASP:HB3	1:A:545:ASN:HD21	1.68	0.58
2:B:296:THR:HB	2:B:299:ALA:HB3	1.84	0.58
1:A:95:PRO:HG3	2:B:137:ASN:O	2.03	0.58
1:A:480:GLN:HE22	1:A:483:TYR:HD2	1.51	0.58
1:A:482:ILE:HG23	1:A:495:ILE:HG21	1.85	0.58
1:A:503:LEU:HD22	1:A:535:TRP:CG	2.38	0.58
1:A:468:PRO:C	1:A:469:LEU:HG	2.22	0.58
2:B:342:TYR:HB3	2:B:348:ASN:CA	2.34	0.58
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.85	0.58
2:B:32:LYS:O	2:B:35:VAL:HG22	2.04	0.58
2:B:64:LYS:HB3	2:B:68:SER:HA	1.85	0.58
1:A:123:ASP:O	1:A:126:LYS:HE3	2.01	0.58
1:A:40:GLU:O	1:A:44:GLU:HG2	2.04	0.58
1:A:56:TYR:O	1:A:129:ALA:HB3	2.04	0.58
1:A:257:ILE:CD1	1:A:295:LEU:HD11	2.32	0.58
1:A:269:GLN:O	1:A:351:THR:N	2.35	0.58
2:B:320:ASP:CG	2:B:323:LYS:HG2	2.23	0.58
1:A:163:SER:HA	1:A:166:LYS:HD2	1.85	0.58
2:B:81:ASN:ND2	2:B:154:LYS:HG3	2.18	0.57
1:A:325:LEU:HD11	1:A:383:TRP:HB2	1.85	0.57
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.22	0.57
1:A:447:ASN:HB3	1:A:450:THR:HG1	1.69	0.57
1:A:97:PRO:HA	1:A:100:LEU:HG	1.87	0.57
1:A:461:LYS:O	1:A:463:ARG:N	2.38	0.57
1:A:108:VAL:HA	1:A:187:LEU:O	2.04	0.57
1:A:543:GLY:N	2:B:284:ARG:HA	2.14	0.57
2:B:41:MET:CB	2:B:47:ILE:HG12	2.34	0.57
2:B:325:LEU:HG	2:B:387:PRO:HB3	1.85	0.57
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:CD2	3:A:559:TBO:H122	2.40	0.57
2:B:380:ILE:HA	2:B:385:LYS:H	1.68	0.57
1:A:162:SER:O	1:A:166:LYS:HG3	2.04	0.57
1:A:199:ARG:HB2	1:A:199:ARG:NH1	2.20	0.57
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.70	0.56
2:B:342:TYR:CB	2:B:348:ASN:HA	2.33	0.56
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.35	0.56
1:A:329:ILE:HG22	1:A:330:GLN:N	2.20	0.56
1:A:379:SER:CB	1:A:387:PRO:HD3	2.34	0.56
1:A:492:GLU:HG3	1:A:529:GLU:OE1	2.04	0.56
2:B:107:THR:O	2:B:188:TYR:HA	2.06	0.56
2:B:178:ILE:HG22	2:B:178:ILE:O	2.04	0.56
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.06	0.56
2:B:62:ALA:HB1	2:B:71:TRP:CE3	2.41	0.56
2:B:382:ILE:HB	2:B:383:TRP:CZ3	2.40	0.56
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.71	0.56
2:B:333:GLY:N	2:B:336:GLN:HB2	2.20	0.56
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.41	0.56
1:A:233:GLU:N	1:A:240:THR:O	2.35	0.56
2:B:393:ILE:HG12	2:B:394:GLN:H	1.69	0.56
1:A:472:THR:OG1	1:A:477:THR:HG23	2.05	0.56
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.87	0.56
2:B:169:GLU:O	2:B:173:LYS:HG3	2.06	0.56
1:A:255:ASN:HA	1:A:258:GLN:OE1	2.05	0.56
2:B:128:THR:HB	2:B:146:TYR:HB2	1.87	0.56
2:B:210:LEU:HD13	2:B:216:THR:HA	1.87	0.56
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.74	0.55
2:B:38:CYS:O	2:B:47:ILE:HD11	2.06	0.55
2:B:41:MET:HB2	2:B:47:ILE:HG12	1.88	0.55
1:A:97:PRO:HD2	1:A:232:TYR:CZ	2.41	0.55
1:A:438:GLU:HG2	1:A:459:THR:HB	1.88	0.55
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.40	0.55
2:B:296:THR:HG22	2:B:299:ALA:H	1.71	0.55
2:B:421:PRO:HG2	2:B:424:LYS:HB2	1.88	0.55
1:A:68:SER:HB2	1:A:70:LYS:CE	2.37	0.55
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.42	0.55
2:B:253:THR:HA	2:B:291:GLU:O	2.07	0.55
2:B:115:TYR:HD1	2:B:115:TYR:H	1.50	0.55
1:A:442:VAL:HA	1:A:457:TYR:HB3	1.88	0.55
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.41	0.55
1:A:368:LEU:HD22	1:A:423:VAL:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HB3	3:A:559:TBO:N1	2.22	0.55
1:A:31:ILE:HD13	1:A:133:PRO:O	2.07	0.55
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.42	0.55
2:B:177:ASP:O	2:B:179:VAL:HG23	2.07	0.55
2:B:198:HIS:O	2:B:201:LYS:HB3	2.06	0.55
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.88	0.54
1:A:49:LYS:O	1:A:49:LYS:HG3	2.08	0.54
2:B:380:ILE:HA	2:B:385:LYS:N	2.23	0.54
1:A:162:SER:O	1:A:165:THR:HB	2.08	0.54
1:A:271:TYR:HE1	1:A:314:VAL:H	1.55	0.54
2:B:12:LEU:HD23	2:B:83:ARG:O	2.07	0.54
2:B:59:PRO:HB2	2:B:76:ASP:CB	2.33	0.54
2:B:131:THR:HG23	2:B:143:ARG:HG3	1.90	0.54
2:B:320:ASP:OD1	2:B:322:SER:HB3	2.07	0.54
1:A:383:TRP:O	1:A:385:LYS:HG2	2.08	0.54
2:B:171:PHE:CE2	2:B:205:LEU:HA	2.42	0.54
1:A:19:PRO:HA	1:A:83:ARG:HH12	1.73	0.54
2:B:78:ARG:NH1	2:B:412:PRO:O	2.41	0.54
2:B:378:GLU:O	2:B:382:ILE:HD12	2.07	0.54
1:A:46:LYS:HG3	1:A:148:VAL:HG11	1.90	0.54
1:A:101:LYS:NZ	1:A:321:PRO:HG2	2.23	0.54
1:A:537:PRO:HB2	1:A:540:LYS:HB2	1.89	0.54
2:B:94:ILE:HG12	2:B:161:GLN:CD	2.28	0.54
2:B:299:ALA:O	2:B:302:GLU:HB2	2.08	0.54
1:A:377:THR:O	1:A:381:VAL:HG23	2.07	0.54
2:B:393:ILE:O	2:B:416:PHE:HB3	2.08	0.54
1:A:372:VAL:O	1:A:375:ILE:HB	2.08	0.53
1:A:466:VAL:CG1	1:A:467:VAL:N	2.71	0.53
1:A:320:ASP:O	1:A:343:GLN:NE2	2.41	0.53
1:A:372:VAL:HG13	1:A:389:PHE:CE2	2.43	0.53
2:B:127:TYR:C	2:B:129:ALA:H	2.12	0.53
2:B:338:THR:HG22	2:B:339:TYR:N	2.23	0.53
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.90	0.53
1:A:441:TYR:HA	1:A:496:VAL:HB	1.90	0.53
1:A:469:LEU:HB2	1:A:472:THR:HG21	1.91	0.53
2:B:167:ILE:O	2:B:208:HIS:NE2	2.41	0.53
2:B:406:TRP:HZ2	2:B:410:TRP:O	1.92	0.53
1:A:111:VAL:HG22	1:A:187:LEU:HD12	1.90	0.53
1:A:426:TRP:CE3	1:A:426:TRP:HA	2.43	0.53
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.89	0.53
2:B:332:GLN:HB3	2:B:336:GLN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TYR:O	1:A:143:ARG:NH2	2.42	0.53
2:B:329:ILE:HD11	2:B:375:ILE:CD1	2.38	0.53
1:A:268:SER:HA	1:A:274:ILE:HD12	1.89	0.53
2:B:59:PRO:O	2:B:75:VAL:HG13	2.08	0.53
1:A:23:GLN:HE22	1:A:26:LEU:HD23	1.73	0.52
1:A:473:THR:HG22	1:A:475:GLN:H	1.73	0.52
2:B:325:LEU:H	2:B:325:LEU:HD23	1.73	0.52
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.74	0.52
1:A:486:LEU:HD11	1:A:521:ILE:HG23	1.90	0.52
2:B:330:GLN:HB2	2:B:332:GLN:NE2	2.24	0.52
1:A:207:GLN:O	1:A:210:LEU:HB3	2.10	0.52
1:A:340:GLN:HA	1:A:350:LYS:O	2.08	0.52
2:B:234:LEU:HD13	2:B:377:THR:HG21	1.91	0.52
1:A:420:PRO:CB	1:A:421:PRO:HD3	2.40	0.52
2:B:324:ASP:O	2:B:343:GLN:HG2	2.09	0.52
1:A:325:LEU:HD12	1:A:385:LYS:HB2	1.92	0.52
1:A:408:ALA:O	2:B:393:ILE:HG13	2.09	0.52
2:B:244:ILE:HG12	2:B:427:TYR:HB2	1.90	0.52
2:B:253:THR:HG23	2:B:289:LEU:O	2.10	0.52
2:B:253:THR:HG23	2:B:291:GLU:H	1.75	0.52
1:A:275:LYS:HB3	1:A:336:GLN:HE22	1.74	0.52
2:B:400:THR:O	2:B:400:THR:HG22	2.10	0.52
2:B:368:LEU:O	2:B:372:VAL:HG23	2.09	0.52
1:A:328:GLU:O	1:A:339:TYR:HA	2.10	0.52
1:A:116:PHE:O	1:A:148:VAL:HB	2.10	0.52
1:A:170:PRO:O	1:A:173:LYS:HB3	2.10	0.52
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.39	0.52
1:A:81:ASN:O	1:A:84:THR:HB	2.10	0.51
2:B:115:TYR:HB3	2:B:149:LEU:HB3	1.92	0.51
2:B:382:ILE:HB	2:B:383:TRP:CE3	2.45	0.51
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.08	0.51
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.26	0.51
1:A:40:GLU:O	1:A:44:GLU:N	2.44	0.51
1:A:101:LYS:HG2	1:A:319:TYR:HB3	1.92	0.51
1:A:408:ALA:HB1	2:B:364:ASP:CB	2.41	0.51
2:B:344:GLU:HB2	2:B:347:LYS:CB	2.38	0.51
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.45	0.51
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.46	0.51
1:A:458:VAL:HA	1:A:463:ARG:O	2.09	0.51
1:A:362:THR:HG22	1:A:363:ASN:H	1.75	0.50
1:A:365:VAL:HG22	1:A:423:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:VAL:N	2:B:185:ASP:O	2.43	0.50
2:B:285:GLY:HA3	2:B:287:LYS:HD2	1.92	0.50
1:A:195:ILE:HG23	1:A:199:ARG:HH12	1.76	0.50
1:A:317:VAL:HG23	1:A:349:LEU:CD1	2.37	0.50
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.27	0.50
1:A:500:GLN:O	1:A:503:LEU:HB3	2.11	0.50
1:A:505:ILE:HG22	1:A:506:ILE:N	2.26	0.50
2:B:229:TRP:C	2:B:231:GLY:H	2.13	0.50
1:A:103:LYS:O	1:A:236:PRO:HB2	2.10	0.50
1:A:245:VAL:O	1:A:247:PRO:HD3	2.11	0.50
1:A:439:THR:CG2	1:A:441:TYR:CE1	2.94	0.50
2:B:69:THR:HG22	2:B:70:LYS:N	2.27	0.50
1:A:188:TYR:HB3	3:A:559:TBO:H122	1.92	0.50
1:A:452:LEU:HD22	1:A:470:THR:HA	1.93	0.50
2:B:99:GLY:O	2:B:102:LYS:HB2	2.11	0.50
1:A:153:TRP:CE3	1:A:156:SER:N	2.80	0.50
2:B:65:LYS:HB2	2:B:72:ARG:HG3	1.93	0.50
1:A:427:TYR:CZ	1:A:509:GLN:HA	2.47	0.50
2:B:156:SER:N	2:B:157:PRO:HD2	2.26	0.50
2:B:338:THR:HG22	2:B:339:TYR:H	1.76	0.50
1:A:153:TRP:HB3	1:A:156:SER:OG	2.12	0.49
1:A:394:GLN:HB3	1:A:397:THR:OG1	2.12	0.49
1:A:542:ILE:HG12	1:A:544:GLY:N	2.27	0.49
2:B:260:LEU:HD23	2:B:279:LEU:HD21	1.94	0.49
1:A:12:LEU:HD22	1:A:83:ARG:C	2.32	0.49
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.94	0.49
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.27	0.49
2:B:21:VAL:HG23	2:B:57:ASN:O	2.12	0.49
2:B:210:LEU:HD13	2:B:216:THR:CA	2.42	0.49
1:A:164:MET:SD	1:A:168:LEU:CD2	2.98	0.49
1:A:479:LEU:HA	1:A:482:ILE:CD1	2.40	0.49
2:B:239:TRP:HE3	2:B:350:LYS:HG3	1.78	0.49
2:B:320:ASP:H	2:B:343:GLN:HE22	1.60	0.49
2:B:253:THR:HB	2:B:256:ASP:CG	2.32	0.49
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.47	0.49
1:A:387:PRO:HG2	1:A:389:PHE:CE1	2.47	0.49
2:B:246:LEU:HD11	2:B:307:ARG:HA	1.94	0.49
2:B:319:TYR:CE2	2:B:383:TRP:HD1	2.31	0.49
1:A:314:VAL:HG12	1:A:315:HIS:N	2.28	0.49
1:A:328:GLU:HA	1:A:390:LYS:HB2	1.95	0.49
1:A:442:VAL:CG2	1:A:485:ALA:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ILE:HB	2:B:145:GLN:O	2.13	0.49
2:B:126:LYS:HA	2:B:145:GLN:NE2	2.27	0.49
1:A:131:THR:HG1	1:A:143:ARG:NH1	2.10	0.49
2:B:50:ILE:HD12	2:B:143:ARG:HB3	1.94	0.49
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.48	0.49
2:B:308:GLU:HG3	2:B:311:LYS:HD2	1.94	0.49
1:A:33:ALA:O	1:A:37:ILE:HG13	2.13	0.49
2:B:178:ILE:CD1	2:B:191:SER:HB3	2.43	0.49
2:B:179:VAL:O	2:B:189:VAL:HA	2.12	0.49
2:B:255:ASN:O	2:B:258:GLN:HB2	2.12	0.49
1:A:59:PRO:O	1:A:75:VAL:HG13	2.12	0.49
1:A:257:ILE:O	1:A:261:VAL:HG23	2.13	0.49
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.94	0.49
2:B:263:LYS:HE2	2:B:425:LEU:CD1	2.35	0.49
2:B:268:SER:HA	2:B:274:ILE:CG2	2.43	0.49
2:B:320:ASP:O	2:B:343:GLN:OE1	2.31	0.49
2:B:398:TRP:C	2:B:400:THR:H	2.15	0.49
1:A:495:ILE:HB	1:A:533:LEU:HD13	1.94	0.48
2:B:397:THR:O	2:B:401:TRP:HD1	1.95	0.48
1:A:19:PRO:HA	1:A:83:ARG:NH1	2.28	0.48
1:A:459:THR:CG2	1:A:463:ARG:HD2	2.44	0.48
2:B:115:TYR:C	2:B:117:SER:H	2.16	0.48
2:B:128:THR:HG21	2:B:146:TYR:HB2	1.94	0.48
2:B:193:LEU:HD22	2:B:197:GLN:CB	2.43	0.48
1:A:105:SER:HB3	1:A:198:HIS:CG	2.48	0.48
2:B:30:LYS:HG2	2:B:71:TRP:CZ3	2.48	0.48
2:B:391:LEU:HB2	2:B:416:PHE:CD2	2.47	0.48
2:B:340:GLN:HA	2:B:351:THR:HA	1.96	0.48
1:A:272:PRO:CA	1:A:351:THR:HG21	2.29	0.48
2:B:35:VAL:CG2	2:B:36:GLU:N	2.76	0.48
2:B:86:ASP:O	2:B:89:GLU:HG2	2.13	0.48
2:B:254:VAL:HG23	2:B:291:GLU:HB3	1.96	0.48
2:B:325:LEU:CD2	2:B:387:PRO:HA	2.44	0.48
1:A:12:LEU:HD23	1:A:124:PHE:HZ	1.78	0.48
1:A:60:VAL:HA	1:A:75:VAL:CG2	2.29	0.48
1:A:468:PRO:O	1:A:469:LEU:HD23	2.14	0.48
1:A:474:ASN:H	1:A:474:ASN:ND2	2.11	0.48
1:A:486:LEU:HB3	1:A:524:GLN:OE1	2.13	0.48
1:A:553:SER:HA	1:A:556:ILE:O	2.13	0.48
2:B:254:VAL:HG12	2:B:258:GLN:HE21	1.79	0.48
2:B:88:TRP:CZ3	2:B:92:LEU:HD12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:THR:CG2	2:B:289:LEU:O	2.62	0.48
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.49	0.48
1:A:274:ILE:HA	1:A:306:ASN:OD1	2.14	0.47
1:A:341:ILE:HD12	1:A:350:LYS:O	2.14	0.47
1:A:441:TYR:CD1	1:A:441:TYR:N	2.82	0.47
1:A:519:ASN:O	1:A:522:ILE:HB	2.13	0.47
2:B:206:ARG:O	2:B:209:LEU:HB2	2.14	0.47
1:A:23:GLN:HG2	1:A:24:TRP:N	2.28	0.47
2:B:62:ALA:HB1	2:B:71:TRP:HE3	1.78	0.47
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.44	0.47
2:B:27:THR:CG2	2:B:30:LYS:HG3	2.45	0.47
2:B:178:ILE:HD12	2:B:189:VAL:HG12	1.95	0.47
1:A:246:LEU:HD21	1:A:310:LEU:HD13	1.97	0.47
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.96	0.47
2:B:104:LYS:O	2:B:235:HIS:HA	2.14	0.47
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.47
2:B:164:MET:SD	2:B:168:LEU:CD1	3.01	0.47
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.15	0.47
1:A:34:LEU:HB3	1:A:132:ILE:HD13	1.97	0.47
1:A:433:PRO:HG2	2:B:290:THR:HG23	1.97	0.47
2:B:425:LEU:CD1	2:B:427:TYR:HB3	2.42	0.47
2:B:342:TYR:HB3	2:B:348:ASN:HB3	1.96	0.47
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.97	0.46
2:B:246:LEU:HD23	2:B:246:LEU:N	2.30	0.46
2:B:271:TYR:O	2:B:273:GLY:N	2.48	0.46
2:B:296:THR:HB	2:B:299:ALA:CB	2.45	0.46
1:A:378:GLU:O	1:A:382:ILE:HG13	2.15	0.46
1:A:474:ASN:H	1:A:474:ASN:HD22	1.63	0.46
2:B:5:ILE:HG22	2:B:6:GLU:N	2.29	0.46
2:B:64:LYS:HE3	2:B:71:TRP:CZ2	2.50	0.46
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.33	0.46
2:B:320:ASP:N	2:B:343:GLN:HE22	2.13	0.46
1:A:13:LYS:HG3	1:A:83:ARG:O	2.16	0.46
1:A:77:PHE:CB	1:A:80:LEU:HD23	2.45	0.46
1:A:199:ARG:HB2	1:A:199:ARG:CZ	2.46	0.46
2:B:10:VAL:HG12	2:B:11:LYS:N	2.31	0.46
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.97	0.46
2:B:304:ALA:O	2:B:307:ARG:HB3	2.16	0.46
1:A:47:ILE:HG22	1:A:48:SER:N	2.29	0.46
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.97	0.46
1:A:241:VAL:HG21	1:A:266:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:O	1:A:414:TRP:HD1	1.99	0.46
2:B:65:LYS:HE3	2:B:407:GLN:HE21	1.81	0.46
2:B:116:PHE:HA	2:B:148:VAL:CG2	2.45	0.46
2:B:12:LEU:HD23	2:B:84:THR:HG23	1.98	0.46
2:B:303:LEU:HD11	2:B:307:ARG:NH2	2.30	0.46
1:A:12:LEU:HD22	1:A:83:ARG:O	2.15	0.46
1:A:373:GLN:HE22	2:B:397:THR:HA	1.76	0.46
1:A:406:TRP:CH2	2:B:417:VAL:O	2.69	0.46
1:A:442:VAL:HG12	1:A:481:ALA:HB1	1.98	0.46
1:A:420:PRO:HG2	1:A:421:PRO:HD3	1.98	0.46
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.51	0.46
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.98	0.46
1:A:87:PHE:O	2:B:55:PRO:HB3	2.16	0.46
1:A:153:TRP:CH2	1:A:155:GLY:HA3	2.51	0.46
1:A:329:ILE:HG23	1:A:338:THR:O	2.16	0.46
1:A:194:GLU:HB2	1:A:197:GLN:HB3	1.98	0.45
1:A:547:GLN:HA	1:A:550:LYS:HB2	1.97	0.45
2:B:379:SER:O	2:B:383:TRP:HE3	1.98	0.45
1:A:375:ILE:HG21	1:A:389:PHE:CE2	2.50	0.45
2:B:163:SER:C	2:B:167:ILE:HG12	2.36	0.45
2:B:296:THR:HG22	2:B:299:ALA:N	2.31	0.45
1:A:65:LYS:HD2	1:A:66:LYS:N	2.30	0.45
1:A:545:ASN:HA	1:A:548:VAL:CG2	2.47	0.45
1:A:207:GLN:OE1	1:A:210:LEU:HD23	2.17	0.45
2:B:178:ILE:HG23	2:B:189:VAL:CG1	2.46	0.45
2:B:314:VAL:HG23	2:B:316:GLY:H	1.80	0.45
2:B:377:THR:HG22	2:B:381:VAL:CG2	2.46	0.45
1:A:244:ILE:HG22	1:A:310:LEU:HD11	1.97	0.45
1:A:283:LEU:O	1:A:285:GLY:N	2.50	0.45
1:A:341:ILE:HD12	1:A:341:ILE:N	2.32	0.45
1:A:365:VAL:O	1:A:368:LEU:HB3	2.17	0.45
2:B:375:ILE:HD12	2:B:389:PHE:HE1	1.81	0.45
1:A:168:LEU:HD23	1:A:209:LEU:HD21	1.99	0.45
1:A:317:VAL:O	1:A:349:LEU:HD12	2.17	0.45
1:A:318:TYR:CZ	3:A:559:TBO:H10	2.49	0.45
1:A:459:THR:HG21	1:A:463:ARG:HD2	1.98	0.45
2:B:78:ARG:O	2:B:82:LYS:HG3	2.17	0.45
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.30	0.45
2:B:373:GLN:NE2	2:B:406:TRP:CD2	2.84	0.45
1:A:106:VAL:O	1:A:107:THR:HB	2.17	0.45
1:A:418:ASN:O	1:A:419:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:THR:CG2	2:B:146:TYR:HB2	2.46	0.45
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.82	0.45
1:A:376:THR:O	1:A:380:ILE:HG12	2.16	0.45
1:A:479:LEU:HD13	1:A:517:LEU:HG	1.97	0.45
2:B:253:THR:O	2:B:257:ILE:HG22	2.17	0.45
1:A:195:ILE:HG22	1:A:199:ARG:HH12	1.81	0.45
2:B:74:LEU:C	2:B:74:LEU:HD23	2.37	0.45
2:B:132:ILE:HG23	2:B:142:ILE:CB	2.42	0.45
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.30	0.45
1:A:178:ILE:HG23	1:A:190:GLY:O	2.16	0.45
1:A:296:THR:O	1:A:299:ALA:HB3	2.17	0.45
1:A:341:ILE:CD1	1:A:350:LYS:HB3	2.42	0.45
1:A:419:THR:CB	1:A:420:PRO:HD2	2.46	0.45
1:A:438:GLU:CD	1:A:461:LYS:HD2	2.38	0.45
2:B:326:ILE:CD1	2:B:388:LYS:HE2	2.42	0.45
2:B:354:TYR:HE1	2:B:356:ARG:HD3	1.82	0.45
2:B:380:ILE:O	2:B:384:GLY:HA2	2.17	0.45
1:A:105:SER:HB3	1:A:198:HIS:ND1	2.32	0.44
1:A:174:GLN:O	1:A:176:PRO:HD3	2.17	0.44
2:B:170:PRO:HG2	2:B:171:PHE:H	1.82	0.44
2:B:234:LEU:CD1	2:B:377:THR:HG21	2.47	0.44
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.20	0.44
2:B:380:ILE:O	2:B:384:GLY:CA	2.65	0.44
1:A:142:ILE:HG13	1:A:142:ILE:O	2.18	0.44
1:A:194:GLU:O	1:A:195:ILE:C	2.55	0.44
1:A:260:LEU:HD23	1:A:279:LEU:HD13	1.98	0.44
1:A:532:TYR:CE2	2:B:289:LEU:HD13	2.52	0.44
2:B:303:LEU:O	2:B:307:ARG:HB2	2.17	0.44
1:A:183:TYR:O	1:A:186:ASP:HB2	2.17	0.44
2:B:126:LYS:HA	2:B:145:GLN:HE21	1.81	0.44
2:B:191:SER:OG	2:B:198:HIS:ND1	2.50	0.44
2:B:257:ILE:CD1	2:B:282:LEU:HB3	2.47	0.44
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.99	0.44
1:A:479:LEU:CD1	1:A:517:LEU:HG	2.46	0.44
2:B:2:ILE:O	2:B:2:ILE:HG22	2.16	0.44
2:B:96:HIS:CE1	2:B:382:ILE:O	2.71	0.44
1:A:188:TYR:HD2	3:A:559:TBO:H71	1.82	0.44
1:A:224:GLU:C	1:A:226:PRO:HD2	2.37	0.44
2:B:410:TRP:O	2:B:410:TRP:CE3	2.70	0.44
1:A:511:ASP:HA	1:A:522:ILE:HD13	1.99	0.44
2:B:131:THR:OG1	2:B:143:ARG:NH1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:LEU:O	2:B:215:THR:OG1	2.36	0.44
1:A:47:ILE:HG23	1:A:145:GLN:O	2.17	0.44
1:A:202:ILE:HG21	1:A:221:HIS:CB	2.47	0.44
2:B:21:VAL:CB	2:B:59:PRO:HD3	2.44	0.44
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.99	0.44
2:B:103:LYS:HD2	2:B:191:SER:CA	2.48	0.44
2:B:406:TRP:HH2	2:B:412:PRO:HD2	1.83	0.44
1:A:264:LEU:HD11	1:A:279:LEU:CD1	2.48	0.44
1:A:450:THR:O	1:A:452:LEU:HG	2.18	0.44
2:B:241:VAL:HG12	2:B:241:VAL:O	2.18	0.44
1:A:2:ILE:O	1:A:213:GLY:HA3	2.18	0.44
1:A:51:GLY:HA2	1:A:143:ARG:HD3	1.99	0.44
2:B:109:LEU:O	2:B:187:LEU:N	2.47	0.44
1:A:240:THR:HG22	1:A:315:HIS:HA	1.98	0.43
2:B:376:THR:HG22	2:B:380:ILE:HD11	2.00	0.43
1:A:373:GLN:O	1:A:376:THR:N	2.51	0.43
2:B:246:LEU:CD1	2:B:307:ARG:HA	2.48	0.43
2:B:401:TRP:O	2:B:404:GLU:HB3	2.18	0.43
1:A:149:LEU:HD22	1:A:156:SER:HA	1.99	0.43
1:A:259:LYS:O	1:A:263:LYS:HG3	2.18	0.43
2:B:125:ARG:NE	2:B:147:ASN:HA	2.30	0.43
2:B:188:TYR:CD1	2:B:188:TYR:N	2.86	0.43
2:B:371:ALA:O	2:B:372:VAL:C	2.57	0.43
1:A:465:LYS:O	1:A:466:VAL:HG23	2.17	0.43
2:B:63:ILE:O	2:B:72:ARG:N	2.51	0.43
2:B:171:PHE:CE2	2:B:205:LEU:CA	3.00	0.43
1:A:139:THR:HA	1:A:140:PRO:HD3	1.66	0.43
1:A:483:TYR:O	1:A:486:LEU:HB2	2.17	0.43
1:A:523:GLU:HA	1:A:526:ILE:HD12	1.99	0.43
2:B:60:VAL:HA	2:B:74:LEU:O	2.18	0.43
2:B:329:ILE:CG2	2:B:330:GLN:N	2.82	0.43
2:B:363:ASN:O	2:B:364:ASP:C	2.56	0.43
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.53	0.43
1:A:521:ILE:HG22	1:A:525:LEU:HD11	1.99	0.43
1:A:532:TYR:HE2	2:B:289:LEU:HD13	1.83	0.43
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.19	0.43
2:B:349:LEU:H	2:B:349:LEU:HG	1.54	0.43
1:A:380:ILE:O	1:A:384:GLY:HA2	2.18	0.43
1:A:473:THR:HG22	1:A:474:ASN:N	2.34	0.43
2:B:81:ASN:HD22	2:B:154:LYS:HG3	1.82	0.43
1:A:480:GLN:O	1:A:483:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ILE:O	2:B:35:VAL:HG13	2.18	0.43
2:B:206:ARG:HA	2:B:209:LEU:HD12	2.00	0.43
1:A:178:ILE:CG2	1:A:189:VAL:HG12	2.49	0.43
1:A:368:LEU:O	1:A:372:VAL:HG23	2.18	0.43
1:A:426:TRP:HA	1:A:426:TRP:HE3	1.84	0.43
2:B:108:VAL:CG1	2:B:186:ASP:HB3	2.49	0.43
2:B:342:TYR:HB3	2:B:348:ASN:CB	2.49	0.43
2:B:354:TYR:CE1	2:B:356:ARG:HD3	2.53	0.43
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.82	0.42
1:A:23:GLN:HG2	1:A:24:TRP:O	2.19	0.42
1:A:73:LYS:HG2	1:A:74:LEU:N	2.34	0.42
1:A:242:GLN:N	1:A:243:PRO:HD2	2.34	0.42
1:A:393:ILE:HG12	1:A:394:GLN:N	2.33	0.42
1:A:68:SER:HB2	1:A:70:LYS:HE2	2.02	0.42
1:A:206:ARG:NH1	1:A:219:LYS:O	2.50	0.42
1:A:543:GLY:HA2	1:A:546:GLU:CB	2.42	0.42
2:B:377:THR:O	2:B:381:VAL:HG23	2.19	0.42
1:A:79:GLU:HG3	1:A:83:ARG:HH11	1.84	0.42
1:A:433:PRO:HA	1:A:532:TYR:CE2	2.54	0.42
2:B:100:LEU:HD11	2:B:190:GLY:HA3	2.01	0.42
2:B:255:ASN:O	2:B:259:LYS:HG3	2.19	0.42
1:A:210:LEU:O	1:A:210:LEU:HD12	2.19	0.42
2:B:377:THR:HA	2:B:380:ILE:HD12	2.02	0.42
1:A:293:ILE:HA	1:A:294:PRO:HD3	1.79	0.42
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.02	0.42
2:B:195:ILE:HD12	2:B:195:ILE:H	1.85	0.42
2:B:373:GLN:HA	2:B:376:THR:OG1	2.19	0.42
1:A:30:LYS:HD3	1:A:62:ALA:O	2.20	0.42
1:A:46:LYS:HE2	1:A:116:PHE:HB3	2.00	0.42
1:A:342:TYR:OH	1:A:390:LYS:HD2	2.19	0.42
1:A:477:THR:O	1:A:480:GLN:HB3	2.20	0.42
2:B:65:LYS:HD2	2:B:65:LYS:HA	1.80	0.42
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.75	0.42
2:B:132:ILE:HA	2:B:133:PRO:HD3	1.56	0.42
2:B:143:ARG:HG2	2:B:143:ARG:NH1	2.33	0.42
2:B:153:TRP:HE3	2:B:156:SER:OG	2.03	0.42
2:B:200:THR:C	2:B:202:ILE:N	2.73	0.42
1:A:23:GLN:HB2	1:A:59:PRO:HB3	2.01	0.42
1:A:69:THR:H	1:A:70:LYS:HD3	1.84	0.42
1:A:171:PHE:CD1	1:A:205:LEU:HD13	2.54	0.42
1:A:229:TRP:O	1:A:232:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:GLU:O	2:B:301:LEU:HD13	2.20	0.42
2:B:325:LEU:HG	2:B:387:PRO:HA	2.02	0.42
2:B:329:ILE:CG2	2:B:337:TRP:HE3	2.32	0.42
2:B:375:ILE:O	2:B:376:THR:C	2.58	0.42
1:A:92:LEU:HD21	2:B:22:LYS:HD3	2.02	0.42
1:A:200:THR:O	1:A:204:GLU:HG3	2.20	0.42
1:A:543:GLY:CA	2:B:284:ARG:O	2.63	0.42
2:B:5:ILE:HD12	2:B:118:VAL:HG22	2.00	0.42
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.96	0.42
2:B:325:LEU:HG	2:B:387:PRO:CB	2.50	0.42
2:B:337:TRP:O	2:B:353:LYS:HG3	2.20	0.42
1:A:97:PRO:HG2	1:A:232:TYR:CG	2.54	0.42
1:A:235:HIS:O	1:A:237:ASP:N	2.53	0.42
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.55	0.42
1:A:510:PRO:O	1:A:511:ASP:HB3	2.20	0.42
2:B:27:THR:HG22	2:B:30:LYS:HG3	2.01	0.42
2:B:398:TRP:O	2:B:400:THR:N	2.53	0.42
2:B:65:LYS:CD	2:B:407:GLN:HG2	2.47	0.42
2:B:253:THR:H	2:B:256:ASP:HB2	1.85	0.42
2:B:377:THR:O	2:B:378:GLU:C	2.58	0.42
1:A:68:SER:HB2	1:A:70:LYS:NZ	2.35	0.41
2:B:48:SER:O	2:B:145:GLN:N	2.52	0.41
2:B:111:VAL:O	2:B:115:TYR:HE1	2.02	0.41
1:A:191:SER:OG	1:A:198:HIS:CE1	2.73	0.41
1:A:276:VAL:HG12	1:A:276:VAL:O	2.20	0.41
1:A:391:LEU:HB2	1:A:414:TRP:CE3	2.54	0.41
2:B:20:LYS:HG3	2:B:56:TYR:HA	2.02	0.41
1:A:483:TYR:O	1:A:487:GLN:HG3	2.20	0.41
2:B:23:GLN:CG	2:B:133:PRO:HG3	2.47	0.41
2:B:110:ASP:HA	2:B:185:ASP:O	2.20	0.41
1:A:329:ILE:O	1:A:392:PRO:HG3	2.20	0.41
1:A:443:ASP:HB3	1:A:548:VAL:HB	2.00	0.41
1:A:524:GLN:O	1:A:528:LYS:HG3	2.21	0.41
2:B:27:THR:O	2:B:31:ILE:HG13	2.20	0.41
2:B:410:TRP:O	2:B:410:TRP:HE3	2.03	0.41
1:A:69:THR:N	1:A:70:LYS:HD3	2.36	0.41
1:A:149:LEU:HD13	1:A:156:SER:O	2.21	0.41
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.81	0.41
2:B:162:SER:O	2:B:165:THR:HB	2.21	0.41
1:A:90:VAL:CG2	1:A:91:GLN:N	2.84	0.41
1:A:99:GLY:HA3	1:A:382:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:HA	1:A:521:ILE:HD12	2.02	0.41
2:B:380:ILE:O	2:B:381:VAL:C	2.59	0.41
1:A:205:LEU:O	1:A:208:HIS:HB3	2.21	0.41
1:A:440:PHE:CE2	1:A:459:THR:HG22	2.55	0.41
1:A:545:ASN:HA	1:A:548:VAL:HG22	2.03	0.41
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.56	0.41
2:B:264:LEU:HB3	2:B:274:ILE:HD11	2.03	0.41
2:B:329:ILE:HA	2:B:338:THR:O	2.20	0.41
2:B:330:GLN:O	2:B:338:THR:N	2.53	0.41
1:A:70:LYS:HD3	1:A:70:LYS:N	2.36	0.41
1:A:77:PHE:O	1:A:80:LEU:N	2.53	0.41
1:A:515:SER:O	1:A:516:GLU:C	2.59	0.41
2:B:125:ARG:O	2:B:128:THR:N	2.54	0.41
2:B:216:THR:HA	2:B:217:PRO:HD3	1.80	0.41
2:B:239:TRP:CE3	2:B:350:LYS:HG3	2.54	0.41
2:B:269:GLN:OE1	2:B:269:GLN:HA	2.21	0.41
2:B:308:GLU:C	2:B:310:LEU:N	2.75	0.41
2:B:77:PHE:CD2	2:B:152:GLY:HA3	2.51	0.41
2:B:100:LEU:CD1	2:B:190:GLY:HA3	2.51	0.41
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.44	0.41
2:B:369:THR:CG2	2:B:370:GLU:N	2.83	0.41
1:A:99:GLY:HA2	1:A:383:TRP:HE1	1.81	0.41
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.51	0.41
2:B:181:CYS:N	2:B:188:TYR:O	2.53	0.41
1:A:40:GLU:C	1:A:44:GLU:HG2	2.41	0.40
1:A:99:GLY:HA3	1:A:382:ILE:HG22	2.03	0.40
1:A:132:ILE:O	1:A:142:ILE:HG12	2.20	0.40
1:A:393:ILE:O	1:A:416:PHE:HB2	2.21	0.40
1:A:420:PRO:CG	1:A:421:PRO:HD3	2.51	0.40
2:B:33:ALA:O	2:B:36:GLU:HB2	2.20	0.40
2:B:103:LYS:HD2	2:B:191:SER:C	2.42	0.40
2:B:210:LEU:HD12	2:B:214:LEU:HA	2.03	0.40
2:B:368:LEU:HD12	2:B:368:LEU:HA	1.90	0.40
1:A:484:LEU:O	1:A:485:ALA:C	2.59	0.40
2:B:96:HIS:CD2	2:B:384:GLY:HA3	2.56	0.40
2:B:166:LYS:O	2:B:170:PRO:CD	2.66	0.40
2:B:193:LEU:HA	2:B:193:LEU:HD23	1.73	0.40
2:B:342:TYR:CD1	2:B:342:TYR:C	2.95	0.40
1:A:81:ASN:OD1	1:A:153:TRP:HA	2.22	0.40
1:A:90:VAL:CG2	1:A:91:GLN:H	2.30	0.40
1:A:350:LYS:HG2	1:A:351:THR:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:N	1:A:226:PRO:HD2	2.37	0.40
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.88	0.40
1:A:483:TYR:CE1	1:A:524:GLN:NE2	2.90	0.40
2:B:395:LYS:O	2:B:399:GLU:HG3	2.21	0.40
1:A:127:TYR:C	1:A:129:ALA:H	2.25	0.40
1:A:434:ILE:HG13	1:A:532:TYR:HB2	2.03	0.40
2:B:98:ALA:O	2:B:100:LEU:N	2.55	0.40
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.22	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%)	415 (75%)	114 (20%)	27 (5%)	2 17
2	B	425/427 (100%)	309 (73%)	76 (18%)	40 (9%)	0 3
All	All	981/985 (100%)	724 (74%)	190 (19%)	67 (7%)	1 9

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	287	LYS
1	A	420	PRO
1	A	556	ILE
2	B	71	TRP
2	B	116	PHE
2	B	195	ILE
2	B	226	PRO
2	B	295	LEU
2	B	316	GLY

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Mol	Chain	Res	Type
1	A	52	PRO
1	A	63	ILE
1	A	67	ASP
1	A	90	VAL
1	A	274	ILE
1	A	284	ARG
1	A	462	GLY
2	B	2	ILE
2	B	4	PRO
2	B	45	GLY
2	B	93	GLY
2	B	99	GLY
2	B	162	SER
2	B	244	ILE
2	B	296	THR
2	B	372	VAL
1	A	134	SER
1	A	429	LEU
1	A	501	TYR
2	B	68	SER
2	B	213	GLY
2	B	273	GLY
2	B	317	VAL
2	B	359	GLY
1	A	114	ALA
1	A	135	ILE
1	A	169	GLU
1	A	236	PRO
2	B	122	GLU
2	B	128	THR
2	B	178	ILE
2	B	345	PRO
2	B	381	VAL
1	A	111	VAL
1	A	138	GLU
1	A	295	LEU
2	B	92	LEU
2	B	115	TYR
2	B	356	ARG
1	A	510	PRO
2	B	225	PRO
2	B	357	MET

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Mol	Chain	Res	Type
2	B	358	ARG
2	B	363	ASN
2	B	399	GLU
2	B	55	PRO
2	B	148	VAL
2	B	176	PRO
2	B	243	PRO
1	A	142	ILE
1	A	156	SER
1	A	294	PRO
2	B	314	VAL
2	B	421	PRO
1	A	276	VAL
2	B	217	PRO
1	A	505	ILE

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	453/498 (91%)	424 (94%)	29 (6%)	17 52
2	B	367/389 (94%)	323 (88%)	44 (12%)	5 22
All	All	820/887 (92%)	747 (91%)	73 (9%)	9 35

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	70	LYS
1	A	73	LYS
1	A	77	PHE
1	A	78	ARG
1	A	94	ILE
1	A	97	PRO
1	A	109	LEU

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Mol	Chain	Res	Type
1	A	124	PHE
1	A	172	LYS
1	A	199	ARG
1	A	242	GLN
1	A	296	THR
1	A	310	LEU
1	A	338	THR
1	A	340	GLN
1	A	341	ILE
1	A	344	GLU
1	A	351	THR
1	A	362	THR
1	A	405	TYR
1	A	411	ILE
1	A	426	TRP
1	A	454	LYS
1	A	505	ILE
1	A	514	GLU
1	A	529	GLU
1	A	540	LYS
1	A	542	ILE
2	B	6	GLU
2	B	20	LYS
2	B	21	VAL
2	B	46	LYS
2	B	49	LYS
2	B	50	ILE
2	B	60	VAL
2	B	63	ILE
2	B	70	LYS
2	B	88	TRP
2	B	91	GLN
2	B	101	LYS
2	B	132	ILE
2	B	139	THR
2	B	164	MET
2	B	178	ILE
2	B	185	ASP
2	B	194	GLU
2	B	205	LEU
2	B	218	ASP
2	B	250	ASP

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Mol	Chain	Res	Type
2	B	266	TRP
2	B	269	GLN
2	B	283	LEU
2	B	287	LYS
2	B	290	THR
2	B	293	ILE
2	B	297	GLU
2	B	315	HIS
2	B	318	TYR
2	B	325	LEU
2	B	330	GLN
2	B	340	GLN
2	B	345	PRO
2	B	356	ARG
2	B	369	THR
2	B	378	GLU
2	B	386	THR
2	B	405	TYR
2	B	407	GLN
2	B	410	TRP
2	B	414	TRP
2	B	425	LEU
2	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	255	ASN
1	A	336	GLN
1	A	373	GLN
1	A	407	GLN
1	A	471	ASN
1	A	474	ASN
1	A	480	GLN
2	B	96	HIS
2	B	137	ASN
2	B	145	GLN
2	B	161	GLN
2	B	207	GLN
2	B	255	ASN
2	B	332	GLN

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Mol	Chain	Res	Type
2	B	340	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	TBO	A	559	-	19,23,23	4.40	9 (47%)	16,34,34	4.66	11 (68%)

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	TBO	A	559	-	-	1/4/17/17	0/2/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	559	TBO	C7A-C3A	-10.69	1.40	1.54
3	A	559	TBO	C9-C8	-8.60	1.41	1.52
3	A	559	TBO	C10-C1A	-6.47	1.41	1.53
3	A	559	TBO	C2-N1	6.44	1.43	1.34
3	A	559	TBO	C3A-N3	-6.13	1.39	1.47
3	A	559	TBO	C4-N3	-4.21	1.44	1.46
3	A	559	TBO	C12-N6	3.10	1.51	1.47
3	A	559	TBO	C10-C9	-2.98	1.45	1.52
3	A	559	TBO	C7-N6	-2.61	1.43	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	559	TBO	C9-C8-CL8	9.21	119.23	109.51
3	A	559	TBO	C1A-C3A-N3	7.60	112.68	102.58
3	A	559	TBO	C16-C14-C15	7.49	131.14	114.60
3	A	559	TBO	C4-N3-C3A	6.03	132.83	123.06
3	A	559	TBO	C15-C14-C13	-5.70	106.17	122.65
3	A	559	TBO	C9-C10-C1A	4.53	120.16	111.68
3	A	559	TBO	C10-C9-C8	3.76	118.88	112.22
3	A	559	TBO	C10-C1A-N1	3.72	135.49	118.95
3	A	559	TBO	C12-N6-C7	3.60	118.38	111.98
3	A	559	TBO	C3A-C1A-N1	3.42	106.32	102.22
3	A	559	TBO	C12-C13-C14	2.11	131.03	127.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	559	TBO	N6-C12-C13-C14

There are no ring outliers.

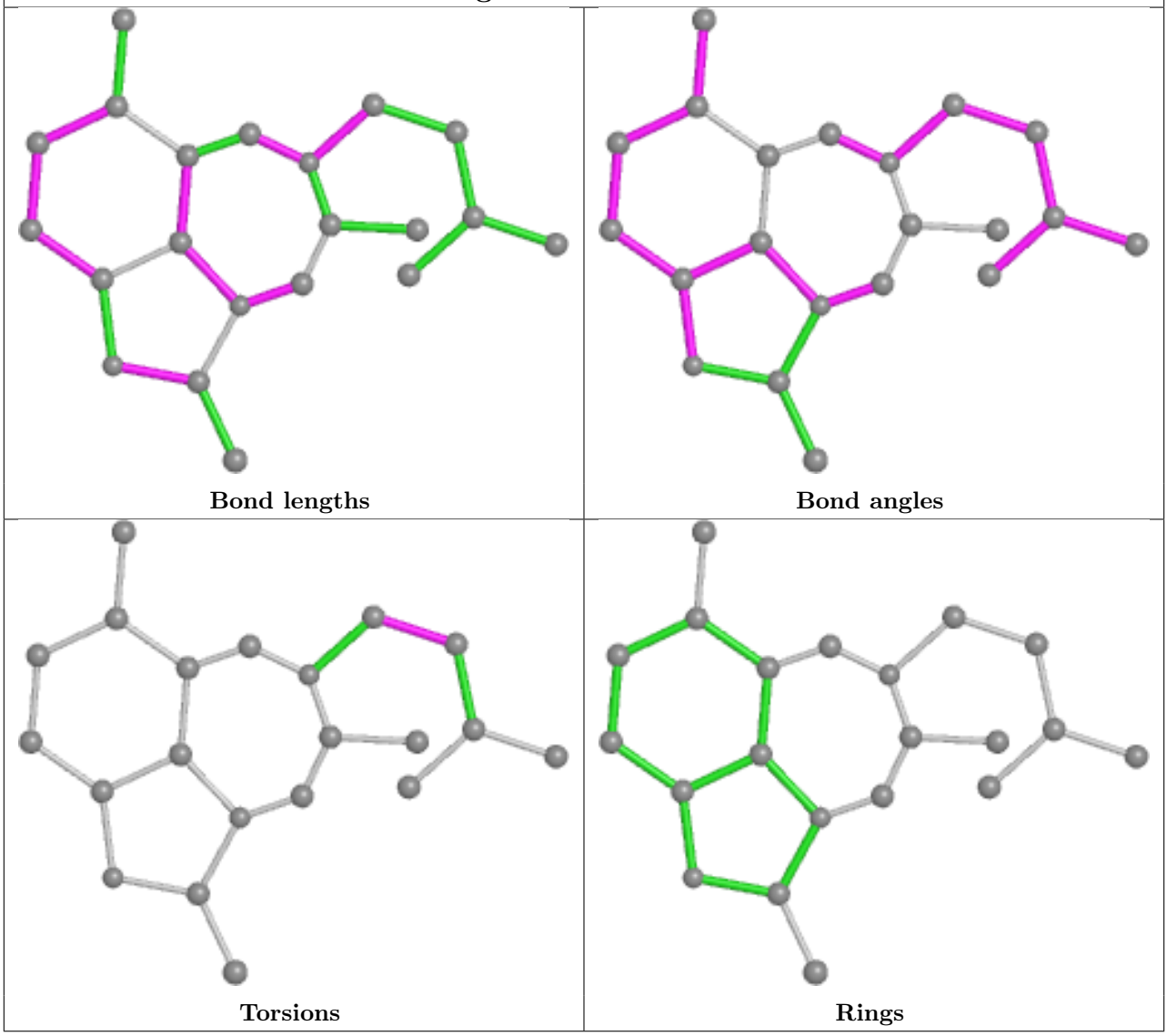
1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	559	TBO	8	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 TBO A 559



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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	558/558 (100%)	-0.46	5 (0%)	84	75	22, 71, 97, 100	0
2	B	427/427 (100%)	-0.47	6 (1%)	75	63	18, 59, 97, 100	0
All	All	985/985 (100%)	-0.46	11 (1%)	80	69	18, 68, 97, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	95	PRO	2.9
1	A	557	ARG	2.7
1	A	24	TRP	2.6
2	B	225	PRO	2.5
1	A	67	ASP	2.3
1	A	66	LYS	2.3
2	B	3	SER	2.2
2	B	2	ILE	2.2
1	A	65	LYS	2.1
2	B	224	GLU	2.1
2	B	316	GLY	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

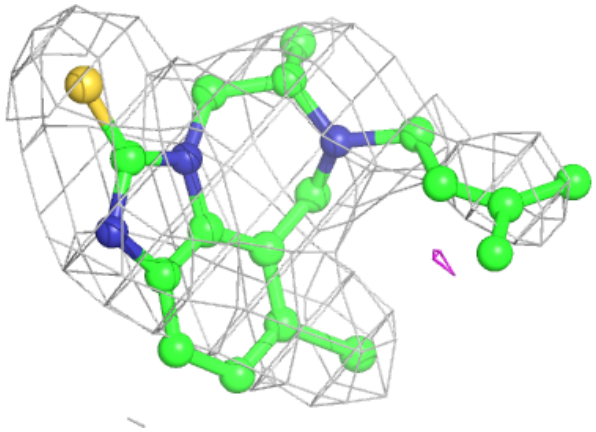
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

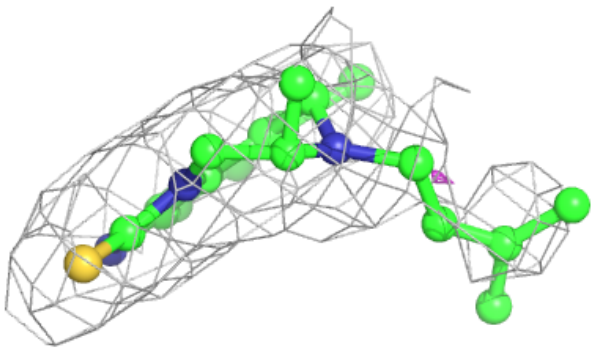
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TBO	A	559	21/21	0.96	0.17	59,67,70,73	0

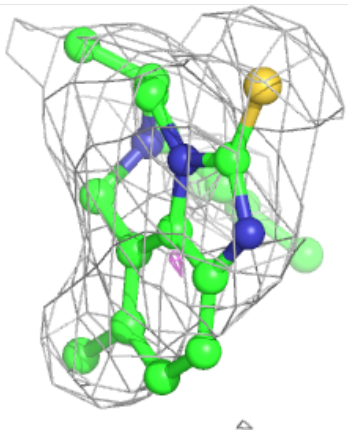
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TBO A 559:

$2mF_o$-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

There are no such residues in this entry.