Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 07:07 PM EDT

PDB ID	:	1SV5
Title	:	CRYSTAL STRUCTURE OF K103N MUTANT HIV-1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH JANSSEN-R165335
Authors	:	Das, K.; Arnold, E.
Deposited on	:	2004-03-27
Resolution	:	2.90 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:

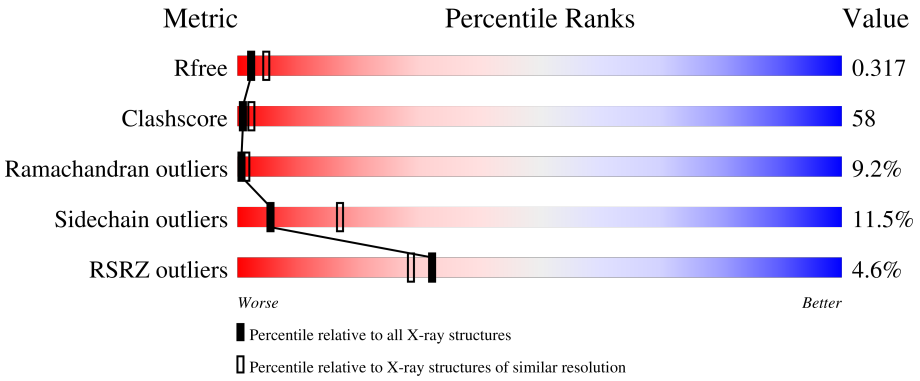
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	560	3% 27% 60% 11%
2	B	430	7% 34% 47% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	65B	A	600	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7905 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	552	Total	C	N	O	S	0	0	0
			4435	2873	739	816	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

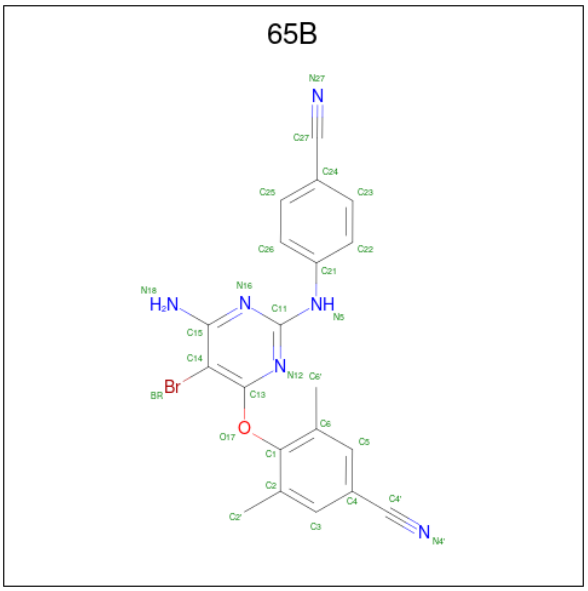
- Molecule 2 is a protein called Reverse Transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3442	2238	570	628	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	engineered mutation	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-({6-AMINO-5-BROMO-2-[(4-CYANOPHENYL)AMINO]PYRIMIDIN-4-YL}OXY)-3,5-DIMETHYLBENZONITRILE (three-letter code: 65B) (formula: $C_{20}H_{15}BrN_6O$).



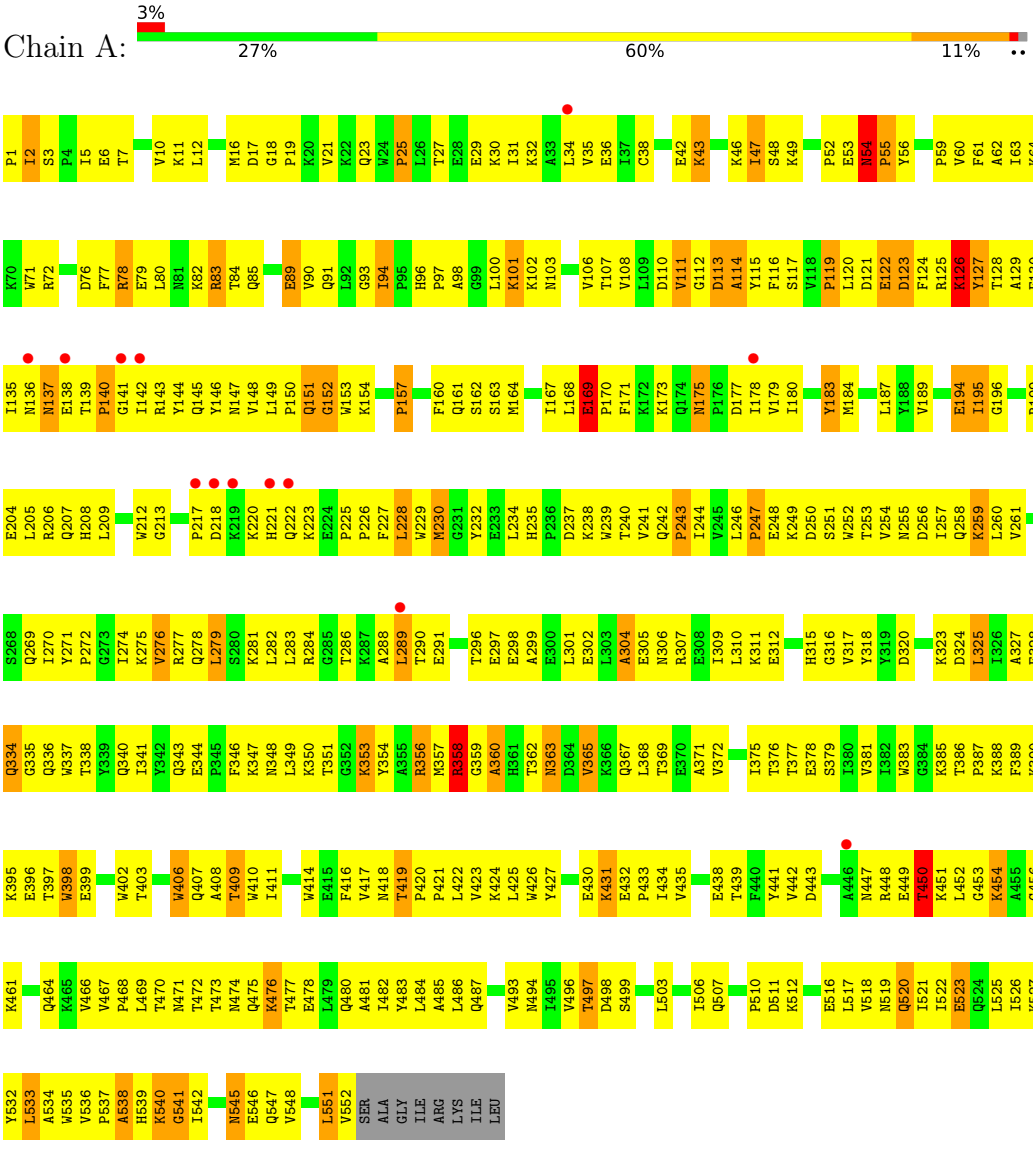
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
3	A	1	28	1	20	6	1	0	0

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.

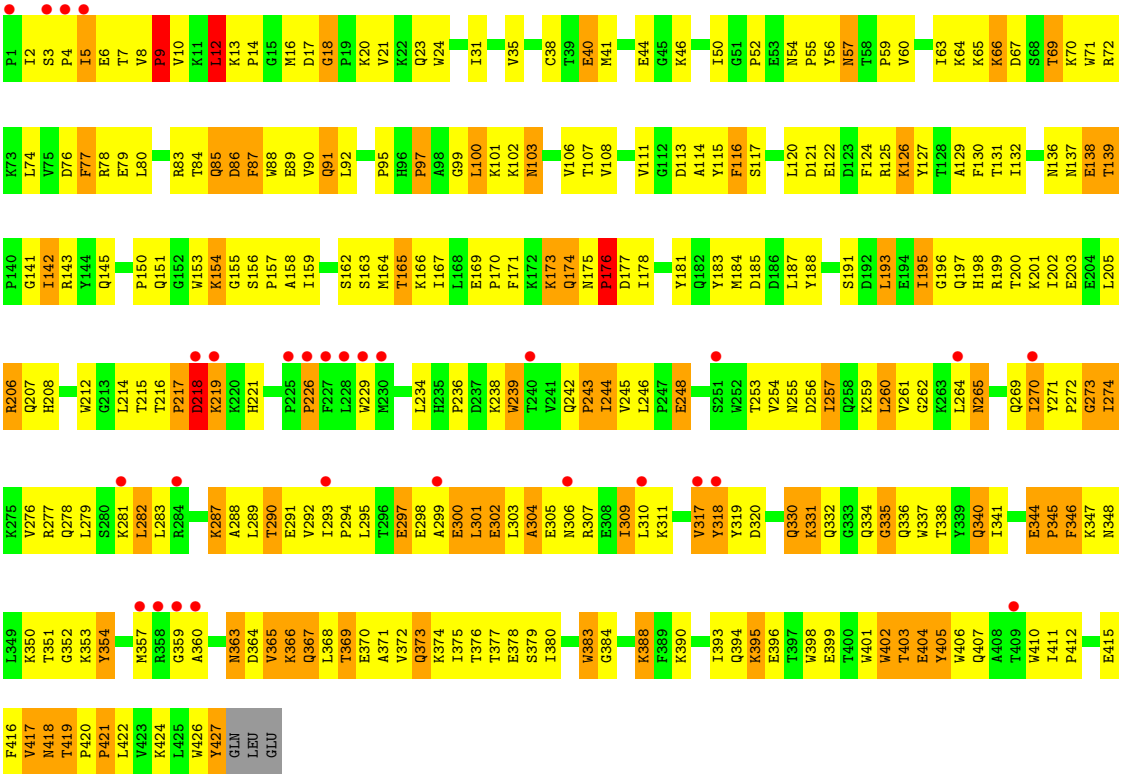
• Molecule 1: Reverse Transcriptase

Chain A:



• Molecule 2: Reverse Transcriptase

Chain B:


P1 I2 S3 P4 I5 E6 T7 V8 P9 V10 K11 L12 K13 P14 G15 M16 D17 G18 P19 K20 V21 K22 Q23 W24 I31 V35 C38 T39 E40 M41 E44 G45 K46 I50 G51 P52 E53 N54 P55 Y56 N57 T58 P59 V60 I63 K64 K65 K66 D67 S68 T69 K70 W71 R72
K73 L74 V75 D76 F77 R78 E79 L80 R83 T84 Q85 D86 F87 W88 E89 V90 Q91 L92 P95 H96 P97 A98 G99 L100 K101 K102 N103 V106 T107 V108 V111 G112 D113 A114 Y115 F116 S117 L120 D121 E122 D123 F124 R125 K126 Y127 T128 A129 F130 T131 I132 N136 N137 E138 T139
P140 G141 I142 R143 Y144 Q145 P150 Q151 G152 W153 K154 G155 S156 P157 A158 I159 S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 K172 K173 Q174 N175 P176 D177 I178 Y181 Q182 Y183 M184 D185 D186 L187 Y188 S191 D192 L193 E194 I195 G196 Q197 H198 R199 T200 K201 I202 E203 E204 L205
R206 Q207 H208 W212 G213 L214 T215 T216 P217 D218 K219 K220 H221 P226 P226 F227 L228 W229 W230 L234 H235 P236 D237 K238 W239 T240 V241 Q242 P243 I244 V245 L246 P247 E248 S251 W252 T253 V254 N255 D256 I257 Q258 K259 L260 V261 G262 K263 L264 N265 Q269 I270 Y271 P272 G273 I274
K275 V276 R277 Q278 L279 S280 K281 L282 L283 R284 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 V317 Y318 Y319 D320 Q330 K331 Q332 G333 Q334 G335 Q336 W337 T338 Y339 Q340 I341 E344 P345 F346 K347 N348
L349 K350 T351 G352 K353 Y354 M357 R358 G359 A360 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377 E378 S379 I380 W383 G384 K388 F389 K390 I393 Q394 K395 E396 T397 W398 E399 T400 W401 W402 T403 E404 Y405 W406 Q407 A408 T409 W410 I411 P412 E415
F416 V417 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427 GLN LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	222.51Å 67.74Å 103.29Å 90.00° 107.47° 90.00°	Depositor
Resolution (Å)	19.95 – 2.90 35.97 – 2.86	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.95-2.90) 94.1 (35.97-2.86)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.326 0.250 , 0.317	Depositor DCC
R_{free} test set	1624 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	79.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7905	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: 65B

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	0.59	2/4553 (0.0%)	0.83	5/6196 (0.1%)
2	B	0.63	0/3542	0.94	6/4826 (0.1%)
All	All	0.61	2/8095 (0.0%)	0.88	11/11022 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	TYR	CD2-CE2	8.00	1.51	1.39
1	A	183	TYR	CG-CD2	7.92	1.49	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	141	GLY	N-CA-C	-8.00	93.11	113.10
2	B	218	ASP	N-CA-C	7.79	132.03	111.00
2	B	331	LYS	CB-CA-C	6.86	124.11	110.40
2	B	219	LYS	N-CA-C	-6.39	93.76	111.00
1	A	347	LYS	N-CA-C	-5.92	95.00	111.00
2	B	226	PRO	N-CA-CB	5.84	110.31	103.30
1	A	228	LEU	CA-CB-CG	5.41	127.73	115.30
2	B	295	LEU	N-CA-C	5.28	125.27	111.00
1	A	183	TYR	CD1-CE1-CZ	5.26	124.53	119.80
1	A	54	ASN	N-CA-C	-5.20	96.97	111.00
2	B	12	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4435	0	4426	547	0
2	B	3442	0	3399	372	0
3	A	28	0	15	10	0
All	All	7905	0	7840	908	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 58.

All (908) 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)
2:B:274:ILE:HG12	2:B:306:ASN:HB3	1.21	1.15
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.27	1.09
2:B:13:LYS:HG2	2:B:87:PHE:HB2	1.37	1.06
2:B:85:GLN:HG3	2:B:154:LYS:HG2	1.31	1.06
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.33	1.06
1:A:246:LEU:HD11	1:A:260:LEU:HD12	1.42	1.00
1:A:240:THR:HG22	1:A:241:VAL:H	1.26	1.00
2:B:274:ILE:HG12	2:B:306:ASN:CB	1.92	0.99
1:A:249:LYS:HG3	1:A:251:SER:H	1.25	0.98
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.28	0.98
1:A:517:LEU:O	1:A:520:GLN:HB2	1.63	0.97
2:B:357:MET:HG2	2:B:360:ALA:HB2	1.46	0.97
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.41	0.97
1:A:406:TRP:CZ2	2:B:419:THR:HG22	2.01	0.96
2:B:90:VAL:HG23	2:B:91:GLN:H	1.28	0.96
1:A:170:PRO:O	1:A:173:LYS:HG2	1.65	0.95
1:A:140:PRO:HB3	1:A:142:ILE:HG13	1.47	0.95
1:A:356:ARG:NH2	1:A:359:GLY:HA3	1.81	0.94
2:B:242:GLN:HG3	2:B:243:PRO:HD2	1.48	0.93
1:A:96:HIS:HD2	1:A:98:ALA:H	1.10	0.92
1:A:102:LYS:N	3:A:600:65B:H181	1.66	0.92
1:A:84:THR:HG22	1:A:154:LYS:HE2	1.50	0.92
1:A:235:HIS:CD2	1:A:238:LYS:HE3	2.05	0.91
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:HE21	1:A:298:GLU:HB3	1.35	0.90
1:A:281:LYS:HA	1:A:358:ARG:HH22	1.38	0.89
1:A:101:LYS:C	3:A:600:65B:H181	1.75	0.89
2:B:66:LYS:HG3	2:B:218:ASP:OD2	1.71	0.89
1:A:473:THR:HG22	1:A:475:GLN:H	1.37	0.89
1:A:498:ASP:HB2	1:A:538:ALA:HA	1.53	0.89
1:A:460:ASN:HD21	1:A:461:LYS:HG3	1.36	0.88
1:A:320:ASP:OD2	1:A:323:LYS:HE3	1.73	0.88
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.56	0.87
1:A:394:GLN:HG3	1:A:397:THR:OG1	1.73	0.87
1:A:126:LYS:H	1:A:126:LYS:HD2	1.39	0.87
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.56	0.87
2:B:2:ILE:HG21	2:B:9:PRO:HD2	1.56	0.87
2:B:85:GLN:HG3	2:B:154:LYS:CG	2.04	0.87
2:B:332:GLN:HB3	2:B:336:GLN:HG2	1.57	0.86
1:A:1:PRO:HD2	1:A:213:GLY:HA2	1.55	0.86
1:A:48:SER:HB2	1:A:147:ASN:HD21	1.41	0.85
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.11	0.85
1:A:241:VAL:CG1	1:A:266:TRP:HE1	1.89	0.85
1:A:448:ARG:HH12	1:A:473:THR:HG23	1.40	0.85
1:A:356:ARG:HH22	1:A:359:GLY:HA3	1.41	0.85
1:A:452:LEU:HD23	1:A:470:THR:HA	1.59	0.85
1:A:371:ALA:O	1:A:375:ILE:HD12	1.75	0.84
1:A:96:HIS:CD2	1:A:98:ALA:H	1.95	0.84
2:B:174:GLN:O	2:B:176:PRO:HD3	1.76	0.84
2:B:332:GLN:HB3	2:B:336:GLN:CG	2.07	0.84
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.12	0.84
2:B:66:LYS:CG	2:B:218:ASP:OD2	2.26	0.84
1:A:3:SER:OG	1:A:5:ILE:HG13	1.77	0.84
1:A:334:GLN:HG2	1:A:336:GLN:HG3	1.56	0.84
2:B:305:GLU:O	2:B:309:ILE:HG22	1.78	0.84
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.60	0.83
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.13	0.83
1:A:10:VAL:HG12	1:A:11:LYS:N	1.91	0.83
1:A:3:SER:HB3	1:A:119:PRO:HD3	1.60	0.83
1:A:10:VAL:HG12	1:A:11:LYS:H	1.44	0.82
1:A:30:LYS:HG2	1:A:71:TRP:CZ3	2.13	0.82
2:B:131:THR:OG1	2:B:143:ARG:HD2	1.78	0.82
1:A:246:LEU:HD11	1:A:260:LEU:CD1	2.09	0.82
1:A:317:VAL:HG12	1:A:348:ASN:O	1.78	0.82
1:A:163:SER:O	1:A:167:ILE:HD13	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:HG23	2:B:290:THR:HG21	1.62	0.82
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.62	0.81
1:A:442:VAL:HG22	1:A:481:ALA:HB1	1.62	0.81
1:A:47:ILE:HD11	1:A:130:PHE:HE1	1.45	0.81
2:B:366:LYS:HB2	2:B:405:TYR:CE2	2.15	0.81
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.45	0.80
2:B:332:GLN:HG2	2:B:336:GLN:HE21	1.45	0.80
2:B:418:ASN:CG	2:B:419:THR:H	1.83	0.80
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.63	0.80
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.17	0.80
2:B:76:ASP:OD1	2:B:78:ARG:HD3	1.81	0.80
2:B:246:LEU:CD1	2:B:264:LEU:HD21	2.12	0.80
1:A:520:GLN:HE21	1:A:520:GLN:HA	1.47	0.79
2:B:31:ILE:O	2:B:35:VAL:HG23	1.82	0.79
1:A:356:ARG:CZ	1:A:359:GLY:HA3	2.13	0.79
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.63	0.79
1:A:64:LYS:HE3	1:A:69:THR:O	1.81	0.79
1:A:406:TRP:CE3	1:A:407:GLN:HB2	2.16	0.79
1:A:240:THR:HG22	1:A:241:VAL:N	1.96	0.78
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.14	0.78
1:A:164:MET:O	1:A:167:ILE:HB	1.83	0.78
1:A:460:ASN:ND2	1:A:461:LYS:N	2.32	0.77
1:A:167:ILE:O	1:A:170:PRO:HD2	1.84	0.77
2:B:357:MET:HG2	2:B:360:ALA:CB	2.15	0.77
1:A:239:TRP:HB3	1:A:318:TYR:HE2	1.50	0.76
2:B:368:LEU:O	2:B:372:VAL:HG23	1.86	0.76
2:B:287:LYS:HD3	2:B:291:GLU:OE2	1.85	0.76
1:A:441:TYR:HB2	1:A:458:VAL:HG12	1.67	0.76
2:B:218:ASP:OD1	2:B:218:ASP:N	2.18	0.75
1:A:281:LYS:O	1:A:284:ARG:HG3	1.86	0.75
1:A:31:ILE:O	1:A:35:VAL:HG23	1.85	0.75
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.52	0.75
2:B:97:PRO:HG3	2:B:181:TYR:HB2	1.69	0.75
1:A:84:THR:CG2	1:A:154:LYS:HE2	2.15	0.75
1:A:460:ASN:ND2	1:A:461:LYS:HG3	2.00	0.75
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.69	0.74
2:B:303:LEU:HA	2:B:306:ASN:OD1	1.87	0.74
1:A:239:TRP:HB3	1:A:318:TYR:CE2	2.22	0.74
2:B:20:LYS:HE2	2:B:55:PRO:HB2	1.69	0.74
2:B:163:SER:O	2:B:167:ILE:HG12	1.87	0.74
2:B:257:ILE:O	2:B:261:VAL:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HD2	1:A:98:ALA:N	1.84	0.74
1:A:333:GLY:O	1:A:335:GLY:N	2.20	0.73
1:A:448:ARG:HH22	1:A:473:THR:HG23	1.52	0.73
1:A:30:LYS:HG2	1:A:71:TRP:HZ3	1.51	0.73
2:B:279:LEU:HA	2:B:299:ALA:HB1	1.71	0.73
1:A:460:ASN:HD22	1:A:461:LYS:N	1.87	0.73
1:A:392:PRO:O	1:A:423:VAL:HG23	1.88	0.73
2:B:257:ILE:HG12	2:B:283:LEU:HD11	1.71	0.73
1:A:253:THR:O	1:A:256:ASP:HB2	1.88	0.73
2:B:85:GLN:CG	2:B:154:LYS:HG2	2.17	0.72
1:A:286:THR:O	1:A:286:THR:HG22	1.88	0.72
1:A:470:THR:HG23	1:A:471:ASN:ND2	2.04	0.72
2:B:7:THR:HB	2:B:121:ASP:HA	1.72	0.72
1:A:416:PHE:CD2	1:A:417:VAL:N	2.58	0.72
1:A:448:ARG:NH1	1:A:473:THR:HG23	2.04	0.72
2:B:395:LYS:O	2:B:399:GLU:HG3	1.89	0.72
1:A:350:LYS:HE3	1:A:378:GLU:OE2	1.89	0.71
2:B:297:GLU:HB3	2:B:300:GLU:H	1.54	0.71
2:B:306:ASN:HA	2:B:309:ILE:CG2	2.20	0.71
1:A:138:GLU:C	1:A:140:PRO:HD3	2.10	0.71
1:A:254:VAL:O	1:A:258:GLN:HG3	1.90	0.71
1:A:539:HIS:CG	1:A:540:LYS:H	2.06	0.71
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.24	0.71
1:A:254:VAL:CG1	1:A:286:THR:HG23	2.20	0.71
1:A:356:ARG:NH1	1:A:359:GLY:HA3	2.05	0.71
1:A:540:LYS:O	1:A:542:ILE:N	2.23	0.71
2:B:202:ILE:HG21	2:B:219:LYS:HD2	1.73	0.71
2:B:257:ILE:CG1	2:B:283:LEU:HD11	2.20	0.71
1:A:167:ILE:HG22	1:A:168:LEU:N	2.03	0.71
2:B:352:GLY:O	2:B:353:LYS:HG3	1.91	0.71
1:A:450:THR:O	1:A:451:LYS:HG2	1.90	0.71
2:B:107:THR:HG21	2:B:219:LYS:HD2	1.72	0.71
1:A:324:ASP:O	1:A:343:GLN:HG2	1.91	0.70
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.73	0.70
2:B:346:PHE:N	2:B:346:PHE:HD1	1.89	0.70
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.26	0.70
1:A:3:SER:HB2	1:A:117:SER:O	1.91	0.70
2:B:46:LYS:HD3	2:B:116:PHE:CD2	2.27	0.70
2:B:238:LYS:HG3	2:B:239:TRP:N	2.05	0.70
2:B:10:VAL:HA	2:B:88:TRP:HZ2	1.55	0.70
2:B:353:LYS:HZ3	2:B:427:TYR:HB2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.26	0.69
1:A:394:GLN:CG	1:A:397:THR:OG1	2.40	0.69
1:A:2:ILE:O	1:A:213:GLY:HA3	1.92	0.69
1:A:484:LEU:O	1:A:487:GLN:HB2	1.92	0.69
1:A:240:THR:CG2	1:A:241:VAL:H	2.03	0.69
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	2.79	0.69
1:A:102:LYS:N	3:A:600:65B:N18	2.40	0.69
1:A:284:ARG:C	1:A:286:THR:H	1.95	0.69
2:B:100:LEU:O	2:B:100:LEU:HD12	1.92	0.69
2:B:171:PHE:HB2	2:B:208:HIS:HD2	1.58	0.68
2:B:8:VAL:O	2:B:9:PRO:C	2.32	0.68
2:B:332:GLN:CG	2:B:336:GLN:HE21	2.06	0.68
1:A:101:LYS:CA	3:A:600:65B:H181	2.05	0.68
2:B:299:ALA:O	2:B:302:GLU:HB2	1.93	0.68
2:B:346:PHE:N	2:B:346:PHE:CD1	2.62	0.68
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.76	0.68
2:B:371:ALA:O	2:B:375:ILE:HG13	1.94	0.68
2:B:239:TRP:HD1	2:B:239:TRP:O	1.76	0.68
1:A:411:ILE:O	1:A:411:ILE:HG23	1.94	0.68
2:B:417:VAL:HG12	2:B:418:ASN:H	1.58	0.68
1:A:406:TRP:CE2	2:B:419:THR:HG22	2.29	0.67
1:A:126:LYS:HD2	1:A:126:LYS:N	2.08	0.67
2:B:301:LEU:HG	2:B:302:GLU:OE2	1.93	0.67
2:B:365:VAL:HG12	2:B:366:LYS:N	2.09	0.67
1:A:125:ARG:O	1:A:126:LYS:C	2.33	0.67
1:A:47:ILE:HD11	1:A:130:PHE:CE1	2.29	0.67
1:A:327:ALA:HB2	1:A:341:ILE:HG12	1.76	0.66
1:A:416:PHE:HD2	1:A:417:VAL:H	1.44	0.66
1:A:96:HIS:H	2:B:136:ASN:HD21	1.41	0.66
1:A:356:ARG:HH11	1:A:356:ARG:CG	2.08	0.66
1:A:474:ASN:O	1:A:478:GLU:HG3	1.96	0.66
2:B:419:THR:O	2:B:420:PRO:C	2.28	0.66
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.25	0.66
1:A:458:VAL:HG23	1:A:464:GLN:HG2	1.77	0.66
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.60	0.66
1:A:64:LYS:HD2	1:A:71:TRP:CE2	2.31	0.66
3:A:600:65B:H6'3	3:A:600:65B:N12	2.11	0.66
2:B:76:ASP:OD2	2:B:78:ARG:NH1	2.28	0.66
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.31	0.65
1:A:90:VAL:CG2	1:A:157:PRO:HB2	2.25	0.65
2:B:330:GLN:HG2	2:B:338:THR:OG1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:NE2	2:B:424:LYS:O	2.26	0.65
1:A:32:LYS:O	1:A:36:GLU:HG3	1.96	0.65
1:A:255:ASN:OD1	1:A:259:LYS:HE3	1.97	0.65
1:A:101:LYS:N	3:A:600:65B:N18	2.45	0.65
1:A:473:THR:C	1:A:475:GLN:N	2.48	0.65
2:B:380:ILE:O	2:B:384:GLY:HA2	1.96	0.65
1:A:64:LYS:HB2	1:A:71:TRP:CD2	2.32	0.65
1:A:235:HIS:NE2	1:A:238:LYS:HE3	2.11	0.65
2:B:76:ASP:OD1	2:B:78:ARG:CD	2.45	0.65
2:B:90:VAL:HG23	2:B:91:GLN:N	2.07	0.65
2:B:317:VAL:HG13	2:B:347:LYS:HB3	1.77	0.65
1:A:96:HIS:N	2:B:136:ASN:HD21	1.94	0.65
2:B:3:SER:OG	2:B:4:PRO:HD2	1.97	0.65
1:A:246:LEU:CD1	1:A:260:LEU:HD12	2.23	0.64
1:A:125:ARG:HG2	1:A:146:TYR:O	1.97	0.64
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.78	0.64
1:A:238:LYS:HB2	1:A:315:HIS:HB2	1.79	0.64
1:A:448:ARG:NH2	1:A:473:THR:HG23	2.12	0.64
1:A:542:ILE:HG12	1:A:546:GLU:HA	1.79	0.64
1:A:53:GLU:C	1:A:55:PRO:HD3	2.17	0.64
1:A:179:VAL:HG21	3:A:600:65B:BR	2.53	0.64
1:A:442:VAL:CG2	1:A:481:ALA:HB1	2.27	0.64
2:B:303:LEU:HD12	2:B:303:LEU:O	1.97	0.64
1:A:284:ARG:C	1:A:286:THR:N	2.49	0.64
2:B:57:ASN:HB2	2:B:143:ARG:HH12	1.62	0.64
2:B:21:VAL:O	2:B:57:ASN:ND2	2.30	0.64
1:A:350:LYS:HB2	1:A:350:LYS:HZ3	1.63	0.64
1:A:475:GLN:O	1:A:477:THR:N	2.31	0.64
2:B:281:LYS:C	2:B:283:LEU:H	2.01	0.64
2:B:3:SER:OG	2:B:4:PRO:CD	2.46	0.63
2:B:238:LYS:HG3	2:B:239:TRP:H	1.62	0.63
1:A:7:THR:HG22	1:A:119:PRO:CB	2.28	0.63
3:A:600:65B:BR	3:A:600:65B:H2'2	2.53	0.63
2:B:84:THR:HG21	2:B:124:PHE:CZ	2.34	0.63
2:B:239:TRP:O	2:B:239:TRP:CD1	2.51	0.63
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.34	0.63
1:A:148:VAL:O	1:A:150:PRO:HD3	1.99	0.63
2:B:217:PRO:HB2	2:B:218:ASP:OD1	1.98	0.63
2:B:421:PRO:HG2	2:B:422:LEU:H	1.63	0.63
1:A:249:LYS:HD2	1:A:250:ASP:H	1.62	0.63
1:A:10:VAL:CG1	1:A:11:LYS:N	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:C	1:A:475:GLN:H	2.01	0.63
2:B:84:THR:O	2:B:86:ASP:N	2.32	0.62
1:A:518:VAL:O	1:A:522:ILE:HG12	1.99	0.62
1:A:460:ASN:HD22	1:A:460:ASN:C	2.03	0.62
1:A:23:GLN:HG2	1:A:133:PRO:HD3	1.81	0.62
2:B:354:TYR:HD2	2:B:374:LYS:HG3	1.65	0.62
2:B:243:PRO:HB2	2:B:353:LYS:NZ	2.14	0.62
1:A:43:LYS:HD2	1:A:43:LYS:O	2.00	0.62
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.81	0.62
2:B:13:LYS:HB3	2:B:14:PRO:HD2	1.81	0.62
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.65	0.62
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.00	0.62
2:B:137:ASN:C	2:B:139:THR:H	2.04	0.62
2:B:301:LEU:O	2:B:304:ALA:HB3	2.00	0.62
1:A:10:VAL:CG1	1:A:11:LYS:H	2.12	0.61
1:A:63:ILE:HG13	1:A:63:ILE:O	1.99	0.61
2:B:282:LEU:HD13	2:B:297:GLU:OE2	2.00	0.61
1:A:477:THR:HA	1:A:480:GLN:HB2	1.83	0.61
2:B:273:GLY:C	2:B:274:ILE:HG13	2.21	0.61
1:A:94:ILE:HG13	1:A:229:TRP:CZ2	2.35	0.61
1:A:526:ILE:HG22	1:A:527:LYS:N	2.16	0.61
2:B:90:VAL:O	2:B:91:GLN:C	2.39	0.61
1:A:542:ILE:HG12	1:A:546:GLU:CB	2.31	0.61
1:A:416:PHE:HD2	1:A:417:VAL:N	1.97	0.61
2:B:376:THR:O	2:B:380:ILE:HG13	2.00	0.61
1:A:194:GLU:HG2	1:A:196:GLY:H	1.66	0.61
1:A:418:ASN:O	1:A:420:PRO:HD3	2.00	0.61
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.36	0.61
1:A:112:GLY:C	1:A:114:ALA:H	2.04	0.61
1:A:406:TRP:HZ2	2:B:419:THR:HG22	1.60	0.61
2:B:254:VAL:HG21	2:B:288:ALA:O	2.01	0.61
2:B:302:GLU:O	2:B:306:ASN:CG	2.39	0.61
1:A:523:GLU:O	1:A:526:ILE:HB	2.00	0.60
2:B:115:TYR:O	2:B:117:SER:N	2.34	0.60
1:A:257:ILE:O	1:A:260:LEU:HB3	2.00	0.60
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.31	0.60
1:A:111:VAL:HG11	1:A:164:MET:HE1	1.83	0.60
1:A:325:LEU:HD11	1:A:383:TRP:CG	2.36	0.60
2:B:10:VAL:HA	2:B:88:TRP:CZ2	2.37	0.60
2:B:419:THR:O	2:B:421:PRO:N	2.34	0.60
1:A:84:THR:HG1	1:A:153:TRP:HE1	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:CG	1:A:450:THR:HG23	2.21	0.60
2:B:50:ILE:HG23	2:B:145:GLN:HB3	1.84	0.60
1:A:78:ARG:O	1:A:82:LYS:HG3	2.01	0.60
1:A:17:ASP:CG	1:A:18:GLY:N	2.55	0.60
1:A:458:VAL:CG2	1:A:464:GLN:HG2	2.30	0.60
1:A:494:ASN:OD1	1:A:532:TYR:HB3	2.02	0.60
1:A:84:THR:HG22	1:A:154:LYS:CE	2.28	0.60
2:B:318:TYR:HD1	2:B:318:TYR:O	1.83	0.60
1:A:261:VAL:HG12	1:A:265:ASN:ND2	2.17	0.60
1:A:49:LYS:HG3	1:A:144:TYR:CE2	2.36	0.59
1:A:151:GLN:O	1:A:151:GLN:HG2	2.02	0.59
1:A:235:HIS:HB2	1:A:238:LYS:O	2.02	0.59
2:B:85:GLN:O	2:B:89:GLU:N	2.35	0.59
2:B:85:GLN:CA	2:B:88:TRP:HB2	2.21	0.59
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.37	0.59
1:A:276:VAL:HG12	1:A:276:VAL:O	2.01	0.59
2:B:243:PRO:HB2	2:B:353:LYS:HZ1	1.66	0.59
2:B:269:GLN:NE2	2:B:346:PHE:HE2	2.00	0.59
2:B:427:TYR:CG	2:B:427:TYR:O	2.55	0.59
1:A:16:MET:CE	1:A:83:ARG:HG2	2.32	0.59
1:A:522:ILE:O	1:A:526:ILE:HD13	2.02	0.59
1:A:542:ILE:HG23	1:A:542:ILE:O	2.03	0.59
2:B:13:LYS:CG	2:B:87:PHE:HB2	2.25	0.59
1:A:101:LYS:CA	3:A:600:65B:N18	2.64	0.59
1:A:134:SER:CB	1:A:140:PRO:HD2	2.32	0.59
1:A:241:VAL:CG1	1:A:266:TRP:NE1	2.64	0.58
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.66	0.58
2:B:173:LYS:O	2:B:174:GLN:C	2.42	0.58
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.38	0.58
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.85	0.58
1:A:53:GLU:O	1:A:55:PRO:HD3	2.03	0.58
1:A:442:VAL:CG1	1:A:497:THR:HG23	2.33	0.58
1:A:2:ILE:HG23	1:A:3:SER:N	2.19	0.58
1:A:542:ILE:HG12	1:A:546:GLU:HB2	1.86	0.58
1:A:442:VAL:HG22	1:A:481:ALA:CB	2.33	0.58
2:B:243:PRO:O	2:B:245:VAL:HG22	2.03	0.58
1:A:305:GLU:O	1:A:309:ILE:HG13	2.03	0.58
2:B:402:TRP:O	2:B:406:TRP:HB2	2.04	0.58
1:A:140:PRO:CB	1:A:142:ILE:HG13	2.30	0.58
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.39	0.58
1:A:235:HIS:CD2	1:A:238:LYS:HG3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:LYS:O	2:B:262:GLY:N	2.36	0.57
2:B:269:GLN:CB	2:B:346:PHE:HD2	2.16	0.57
1:A:123:ASP:HA	1:A:126:LYS:HE2	1.85	0.57
2:B:401:TRP:O	2:B:404:GLU:N	2.36	0.57
1:A:430:GLU:O	1:A:532:TYR:HD2	1.87	0.57
2:B:242:GLN:HG3	2:B:243:PRO:CD	2.27	0.57
2:B:269:GLN:HB3	2:B:346:PHE:HD2	1.69	0.57
2:B:156:SER:O	2:B:157:PRO:C	2.40	0.57
1:A:368:LEU:O	1:A:372:VAL:HG23	2.05	0.57
2:B:50:ILE:CG2	2:B:145:GLN:HB3	2.35	0.57
2:B:248:GLU:O	2:B:248:GLU:HG2	2.05	0.57
1:A:480:GLN:O	1:A:483:TYR:HB3	2.04	0.57
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.40	0.57
1:A:96:HIS:H	2:B:136:ASN:ND2	2.01	0.57
1:A:111:VAL:HG11	1:A:164:MET:CE	2.35	0.57
2:B:88:TRP:HZ3	2:B:159:ILE:CG1	2.17	0.57
1:A:356:ARG:HH12	1:A:359:GLY:HA3	1.70	0.57
1:A:391:LEU:HG	1:A:414:TRP:HB2	1.87	0.57
1:A:395:LYS:HA	1:A:414:TRP:HZ2	1.70	0.56
2:B:66:LYS:HG2	2:B:218:ASP:OD2	2.02	0.56
2:B:153:TRP:C	2:B:155:GLY:H	2.08	0.56
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.86	0.56
2:B:366:LYS:HE3	2:B:405:TYR:HD2	1.69	0.56
1:A:3:SER:HB3	1:A:119:PRO:CD	2.35	0.56
1:A:56:TYR:O	1:A:143:ARG:NH2	2.38	0.56
1:A:84:THR:HG22	1:A:85:GLN:O	2.06	0.56
1:A:277:ARG:HD3	1:A:334:GLN:HG3	1.87	0.56
1:A:278:GLN:HE21	1:A:298:GLU:CB	2.12	0.56
1:A:350:LYS:NZ	1:A:351:THR:O	2.39	0.56
1:A:448:ARG:HH12	1:A:473:THR:CG2	2.16	0.56
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.40	0.56
2:B:262:GLY:HA2	2:B:265:ASN:HB3	1.87	0.56
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.38	0.56
1:A:334:GLN:HG3	1:A:334:GLN:O	2.04	0.56
2:B:2:ILE:O	2:B:3:SER:C	2.44	0.56
2:B:122:GLU:O	2:B:122:GLU:HG3	2.06	0.56
1:A:283:LEU:HD22	1:A:286:THR:HG21	1.87	0.56
1:A:493:VAL:HG22	1:A:494:ASN:N	2.20	0.56
2:B:99:GLY:O	2:B:102:LYS:HB3	2.04	0.56
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.34	0.56
2:B:153:TRP:O	2:B:155:GLY:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:LYS:O	2:B:154:LYS:HG3	2.05	0.56
2:B:302:GLU:C	2:B:304:ALA:N	2.57	0.56
1:A:79:GLU:OE1	1:A:83:ARG:NH1	2.38	0.56
2:B:301:LEU:O	2:B:301:LEU:HD12	2.06	0.56
2:B:393:ILE:HG12	2:B:394:GLN:N	2.21	0.56
2:B:354:TYR:CD2	2:B:374:LYS:HG3	2.41	0.56
2:B:106:VAL:O	2:B:234:LEU:HB2	2.05	0.55
2:B:279:LEU:CA	2:B:299:ALA:HB1	2.35	0.55
2:B:390:LYS:HB3	2:B:417:VAL:HG21	1.88	0.55
2:B:165:THR:HG22	2:B:166:LYS:N	2.20	0.55
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.40	0.55
1:A:542:ILE:HG12	1:A:546:GLU:CA	2.35	0.55
2:B:150:PRO:HG2	2:B:153:TRP:HB3	1.88	0.55
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.88	0.55
2:B:341:ILE:HD11	2:B:375:ILE:CG2	2.36	0.55
2:B:306:ASN:HA	2:B:309:ILE:HG23	1.88	0.55
1:A:200:THR:O	1:A:204:GLU:HB2	2.06	0.55
1:A:17:ASP:CG	1:A:18:GLY:H	2.09	0.55
1:A:140:PRO:HB3	1:A:142:ILE:CG1	2.31	0.55
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.34	0.55
1:A:254:VAL:HG12	1:A:286:THR:HG23	1.88	0.55
1:A:456:GLY:HA2	1:A:484:LEU:HD23	1.88	0.55
1:A:469:LEU:CD1	1:A:480:GLN:HG2	2.19	0.55
2:B:64:LYS:HG3	2:B:71:TRP:CE3	2.42	0.55
1:A:180:ILE:HD11	1:A:187:LEU:HD22	1.89	0.54
1:A:301:LEU:O	1:A:304:ALA:HB3	2.06	0.54
2:B:175:ASN:OD1	2:B:201:LYS:CE	2.55	0.54
2:B:366:LYS:O	2:B:370:GLU:HB2	2.08	0.54
1:A:473:THR:O	1:A:475:GLN:N	2.41	0.54
1:A:356:ARG:NH1	1:A:356:ARG:CG	2.68	0.54
1:A:376:THR:HG23	1:A:386:THR:HG22	1.90	0.54
2:B:111:VAL:C	2:B:113:ASP:H	2.09	0.54
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.42	0.54
1:A:106:VAL:HG11	3:A:600:65B:H6'2	1.89	0.54
1:A:389:PHE:HB3	1:A:391:LEU:CD2	2.30	0.54
1:A:473:THR:HG22	1:A:475:GLN:N	2.14	0.54
1:A:498:ASP:HB2	1:A:538:ALA:CA	2.32	0.54
2:B:243:PRO:O	2:B:245:VAL:N	2.35	0.54
2:B:396:GLU:CD	2:B:396:GLU:H	2.11	0.54
1:A:120:LEU:O	1:A:121:ASP:C	2.46	0.54
1:A:254:VAL:HG23	1:A:255:ASN:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.36	0.54
1:A:443:ASP:HB3	1:A:548:VAL:HG12	1.90	0.54
1:A:453:GLY:C	1:A:454:LYS:HG2	2.28	0.54
1:A:306:ASN:O	1:A:310:LEU:HG	2.07	0.54
1:A:406:TRP:CH2	1:A:407:GLN:OE1	2.61	0.54
2:B:246:LEU:O	2:B:307:ARG:NH2	2.41	0.54
2:B:354:TYR:CD1	2:B:354:TYR:C	2.81	0.54
1:A:90:VAL:O	1:A:91:GLN:C	2.43	0.54
1:A:334:GLN:HG2	1:A:336:GLN:CG	2.34	0.54
1:A:372:VAL:HG11	1:A:411:ILE:HG13	1.87	0.54
2:B:352:GLY:O	2:B:353:LYS:CG	2.54	0.54
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.43	0.54
1:A:111:VAL:HB	1:A:114:ALA:HB2	1.90	0.54
1:A:18:GLY:HA3	1:A:127:TYR:HD2	1.73	0.53
1:A:288:ALA:HB1	1:A:291:GLU:HG2	1.89	0.53
1:A:441:TYR:O	1:A:548:VAL:HG21	2.07	0.53
2:B:87:PHE:O	2:B:88:TRP:CD1	2.61	0.53
2:B:253:THR:OG1	2:B:256:ASP:OD2	2.23	0.53
1:A:377:THR:O	1:A:381:VAL:HG23	2.08	0.53
1:A:442:VAL:HG12	1:A:496:VAL:O	2.07	0.53
1:A:498:ASP:HB2	1:A:538:ALA:O	2.08	0.53
2:B:124:PHE:O	2:B:125:ARG:C	2.45	0.53
2:B:242:GLN:CG	2:B:243:PRO:HD2	2.30	0.53
1:A:54:ASN:ND2	1:A:56:TYR:HD1	2.05	0.53
1:A:275:LYS:O	1:A:276:VAL:CG2	2.56	0.53
2:B:257:ILE:HG13	2:B:283:LEU:HD11	1.91	0.53
2:B:282:LEU:O	2:B:282:LEU:HD12	2.09	0.53
1:A:161:GLN:O	1:A:162:SER:C	2.43	0.53
1:A:257:ILE:HG22	1:A:283:LEU:HD11	1.89	0.53
2:B:254:VAL:HA	2:B:257:ILE:HG23	1.89	0.53
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.89	0.53
2:B:86:ASP:C	2:B:88:TRP:H	2.10	0.53
1:A:65:LYS:HD2	1:A:72:ARG:HH11	1.73	0.53
1:A:542:ILE:CG1	1:A:546:GLU:HA	2.38	0.53
2:B:120:LEU:O	2:B:125:ARG:NH1	2.42	0.53
2:B:238:LYS:CG	2:B:239:TRP:H	2.21	0.53
1:A:358:ARG:HG3	1:A:358:ARG:HH11	1.73	0.53
2:B:115:TYR:HE1	2:B:185:ASP:OD1	1.92	0.53
2:B:303:LEU:HD11	2:B:307:ARG:HD2	1.91	0.53
2:B:405:TYR:CD1	2:B:405:TYR:N	2.72	0.53
1:A:539:HIS:CD2	1:A:540:LYS:H	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HG22	2:B:277:ARG:HH22	1.73	0.53
2:B:303:LEU:CA	2:B:306:ASN:OD1	2.55	0.53
1:A:221:HIS:HD2	1:A:223:LYS:CB	2.21	0.52
1:A:324:ASP:OD2	1:A:388:LYS:NZ	2.39	0.52
1:A:460:ASN:ND2	1:A:460:ASN:C	2.62	0.52
1:A:399:GLU:O	1:A:403:THR:HB	2.08	0.52
2:B:244:ILE:HG23	2:B:244:ILE:O	2.08	0.52
1:A:270:ILE:O	1:A:272:PRO:HD3	2.10	0.52
1:A:275:LYS:HB2	1:A:302:GLU:HG3	1.91	0.52
1:A:137:ASN:O	1:A:140:PRO:HD2	2.10	0.52
1:A:240:THR:OG1	1:A:315:HIS:HA	2.09	0.52
2:B:254:VAL:CG2	2:B:288:ALA:O	2.57	0.52
1:A:94:ILE:HG23	1:A:229:TRP:HH2	1.73	0.52
1:A:150:PRO:O	1:A:152:GLY:N	2.41	0.52
1:A:358:ARG:HD2	1:A:358:ARG:N	2.25	0.52
1:A:460:ASN:ND2	1:A:461:LYS:CG	2.72	0.52
1:A:261:VAL:O	1:A:264:LEU:HB2	2.10	0.52
2:B:157:PRO:HG2	2:B:158:ALA:H	1.73	0.52
1:A:3:SER:OG	1:A:5:ILE:CG1	2.54	0.52
1:A:112:GLY:C	1:A:114:ALA:N	2.61	0.52
1:A:304:ALA:O	1:A:307:ARG:N	2.42	0.52
2:B:254:VAL:HB	2:B:289:LEU:HA	1.91	0.52
2:B:270:ILE:HG22	2:B:271:TYR:H	1.73	0.52
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.90	0.52
2:B:8:VAL:O	2:B:10:VAL:HG23	2.10	0.52
2:B:57:ASN:HA	2:B:129:ALA:O	2.10	0.52
2:B:78:ARG:HD2	2:B:411:ILE:HB	1.92	0.52
2:B:87:PHE:C	2:B:88:TRP:CD1	2.84	0.52
1:A:53:GLU:OE1	1:A:53:GLU:HA	2.10	0.52
1:A:124:PHE:HE2	1:A:153:TRP:CZ2	2.27	0.52
1:A:132:ILE:HG13	1:A:132:ILE:O	2.10	0.52
1:A:448:ARG:CZ	1:A:473:THR:HG23	2.39	0.52
1:A:460:ASN:HD21	1:A:461:LYS:CG	2.15	0.52
2:B:259:LYS:O	2:B:261:VAL:N	2.43	0.52
2:B:281:LYS:O	2:B:283:LEU:N	2.43	0.52
2:B:411:ILE:HG22	2:B:412:PRO:O	2.09	0.52
1:A:220:LYS:NZ	1:A:221:HIS:CE1	2.78	0.51
1:A:431:LYS:HE3	1:A:432:GLU:OE1	2.10	0.51
1:A:2:ILE:HG12	1:A:3:SER:H	1.75	0.51
1:A:107:THR:HG23	1:A:221:HIS:HB2	1.93	0.51
2:B:7:THR:CB	2:B:121:ASP:HA	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:LYS:CG	2:B:239:TRP:N	2.71	0.51
2:B:253:THR:O	2:B:257:ILE:HG22	2.10	0.51
1:A:271:TYR:O	1:A:274:ILE:HG12	2.10	0.51
1:A:296:THR:O	1:A:297:GLU:C	2.48	0.51
2:B:100:LEU:HD12	2:B:100:LEU:C	2.31	0.51
1:A:64:LYS:HB2	1:A:71:TRP:CE3	2.46	0.51
1:A:235:HIS:CD2	1:A:238:LYS:CE	2.89	0.51
2:B:60:VAL:O	2:B:60:VAL:HG23	2.09	0.51
2:B:69:THR:HG23	2:B:70:LYS:H	1.75	0.51
1:A:47:ILE:HD13	1:A:145:GLN:O	2.10	0.51
1:A:261:VAL:HG12	1:A:265:ASN:HD21	1.74	0.51
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.45	0.51
1:A:126:LYS:H	1:A:126:LYS:CD	2.19	0.51
1:A:450:THR:O	1:A:451:LYS:CG	2.57	0.51
2:B:354:TYR:OH	2:B:370:GLU:OE1	2.29	0.51
1:A:503:LEU:O	1:A:507:GLN:HB2	2.10	0.51
2:B:50:ILE:HD12	2:B:143:ARG:HH21	1.76	0.51
2:B:155:GLY:O	2:B:158:ALA:HB3	2.11	0.51
1:A:16:MET:CE	1:A:83:ARG:HA	2.41	0.51
2:B:101:LYS:O	2:B:236:PRO:HB3	2.11	0.51
2:B:376:THR:HB	2:B:410:TRP:CH2	2.46	0.51
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.46	0.51
1:A:510:PRO:HG2	1:A:522:ILE:HD11	1.92	0.51
2:B:126:LYS:HE2	2:B:127:TYR:CZ	2.46	0.51
2:B:369:THR:O	2:B:373:GLN:NE2	2.44	0.50
1:A:390:LYS:C	1:A:391:LEU:HD23	2.30	0.50
1:A:536:VAL:CG1	1:A:537:PRO:HD2	2.40	0.50
1:A:288:ALA:HB1	1:A:291:GLU:CG	2.42	0.50
1:A:442:VAL:HG13	1:A:497:THR:HG23	1.91	0.50
2:B:270:ILE:HG22	2:B:271:TYR:N	2.26	0.50
1:A:47:ILE:HD12	1:A:144:TYR:HB3	1.92	0.50
2:B:388:LYS:HE2	2:B:415:GLU:OE1	2.12	0.50
2:B:418:ASN:O	2:B:420:PRO:HD3	2.10	0.50
1:A:365:VAL:HG12	1:A:398:TRP:CD1	2.47	0.50
2:B:13:LYS:HD3	2:B:87:PHE:N	2.27	0.50
2:B:291:GLU:CG	2:B:292:VAL:N	2.75	0.50
2:B:376:THR:CG2	2:B:410:TRP:CZ3	2.91	0.50
2:B:390:LYS:HB3	2:B:417:VAL:CG2	2.42	0.50
2:B:66:LYS:HE2	2:B:66:LYS:HA	1.93	0.50
1:A:434:ILE:H	1:A:494:ASN:HD21	1.59	0.50
1:A:528:LYS:HB3	1:A:531:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ARG:HH11	2:B:125:ARG:CG	2.25	0.50
2:B:405:TYR:H	2:B:405:TYR:HD1	1.57	0.50
1:A:447:ASN:CB	1:A:450:THR:HG23	2.41	0.50
1:A:113:ASP:O	1:A:116:PHE:N	2.41	0.49
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.36	0.49
1:A:546:GLU:HG2	1:A:547:GLN:HE21	1.75	0.49
2:B:366:LYS:HE3	2:B:405:TYR:CD2	2.46	0.49
1:A:42:GLU:HB2	1:A:47:ILE:HG22	1.94	0.49
1:A:275:LYS:C	1:A:276:VAL:HG23	2.33	0.49
1:A:452:LEU:HD23	1:A:470:THR:CA	2.37	0.49
1:A:467:VAL:HG13	1:A:468:PRO:HD2	1.94	0.49
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.94	0.49
2:B:281:LYS:C	2:B:283:LEU:N	2.66	0.49
1:A:258:GLN:HG2	1:A:283:LEU:HD13	1.94	0.49
1:A:334:GLN:CG	1:A:336:GLN:HG3	2.37	0.49
1:A:447:ASN:HB3	1:A:450:THR:HG23	1.93	0.49
1:A:536:VAL:HG12	1:A:537:PRO:HD2	1.95	0.49
2:B:150:PRO:HD2	2:B:153:TRP:HE3	1.78	0.49
2:B:418:ASN:CG	2:B:419:THR:N	2.56	0.49
1:A:134:SER:CB	1:A:140:PRO:CD	2.90	0.49
1:A:356:ARG:HH22	1:A:359:GLY:CA	2.21	0.49
1:A:443:ASP:O	1:A:552:VAL:HG11	2.12	0.49
1:A:510:PRO:HG2	1:A:522:ILE:CD1	2.42	0.49
1:A:528:LYS:CB	1:A:531:VAL:HG23	2.43	0.49
1:A:357:MET:C	1:A:359:GLY:H	2.16	0.48
1:A:406:TRP:HE3	1:A:406:TRP:O	1.96	0.48
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.53	0.48
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.94	0.48
2:B:288:ALA:O	2:B:291:GLU:HB3	2.13	0.48
2:B:254:VAL:O	2:B:255:ASN:C	2.52	0.48
2:B:271:TYR:CD1	2:B:310:LEU:HD23	2.49	0.48
1:A:110:ASP:OD1	1:A:110:ASP:O	2.31	0.48
1:A:350:LYS:HB2	1:A:350:LYS:NZ	2.24	0.48
2:B:401:TRP:O	2:B:403:THR:N	2.46	0.48
1:A:498:ASP:CB	1:A:538:ALA:HA	2.33	0.48
1:A:418:ASN:O	1:A:420:PRO:CD	2.61	0.48
1:A:516:GLU:O	1:A:520:GLN:HG2	2.14	0.48
1:A:115:TYR:O	1:A:149:LEU:HB2	2.13	0.48
1:A:431:LYS:HD2	1:A:432:GLU:N	2.29	0.48
1:A:16:MET:HE2	1:A:83:ARG:HA	1.94	0.48
1:A:108:VAL:HG12	1:A:223:LYS:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:HE3	1:A:256:ASP:HB3	1.79	0.48
1:A:328:GLU:CG	1:A:329:ILE:N	2.77	0.48
2:B:7:THR:CG2	2:B:121:ASP:HA	2.43	0.48
2:B:111:VAL:C	2:B:113:ASP:N	2.67	0.48
1:A:153:TRP:CG	1:A:154:LYS:N	2.81	0.48
1:A:254:VAL:HG11	1:A:286:THR:HG23	1.96	0.48
2:B:193:LEU:HD12	2:B:198:HIS:CA	2.44	0.48
1:A:80:LEU:O	1:A:84:THR:N	2.46	0.48
1:A:241:VAL:HG12	1:A:242:GLN:N	2.29	0.48
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.49	0.48
1:A:528:LYS:HG3	1:A:531:VAL:CG2	2.43	0.48
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.95	0.48
2:B:238:LYS:O	2:B:239:TRP:C	2.50	0.48
1:A:175:ASN:CB	1:A:178:ILE:HG13	2.43	0.47
1:A:276:VAL:HA	1:A:302:GLU:OE1	2.13	0.47
2:B:379:SER:HA	2:B:383:TRP:CZ3	2.49	0.47
2:B:401:TRP:O	2:B:402:TRP:C	2.50	0.47
1:A:441:TYR:HB3	1:A:548:VAL:HG21	1.96	0.47
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.40	0.47
1:A:54:ASN:OD1	1:A:129:ALA:HB2	2.13	0.47
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.95	0.47
1:A:356:ARG:HB2	1:A:367:GLN:HE21	1.78	0.47
1:A:397:THR:HG21	1:A:424:LYS:HA	1.97	0.47
1:A:419:THR:O	1:A:419:THR:OG1	2.29	0.47
1:A:497:THR:HB	1:A:499:SER:H	1.80	0.47
1:A:449:GLU:O	1:A:451:LYS:N	2.46	0.47
2:B:153:TRP:CE2	2:B:155:GLY:HA3	2.49	0.47
2:B:330:GLN:NE2	2:B:340:GLN:OE1	2.47	0.47
1:A:358:ARG:N	1:A:358:ARG:CD	2.77	0.47
1:A:441:TYR:CB	1:A:548:VAL:HG21	2.43	0.47
2:B:242:GLN:CG	2:B:243:PRO:CD	2.90	0.47
1:A:78:ARG:HG3	1:A:79:GLU:N	2.29	0.47
1:A:328:GLU:HG2	1:A:329:ILE:N	2.29	0.47
1:A:357:MET:O	1:A:359:GLY:N	2.48	0.47
1:A:448:ARG:HH22	1:A:473:THR:CG2	2.21	0.47
2:B:50:ILE:CD1	2:B:143:ARG:HH21	2.28	0.47
1:A:80:LEU:O	1:A:83:ARG:N	2.45	0.47
1:A:94:ILE:HD11	1:A:183:TYR:CE1	2.50	0.47
1:A:94:ILE:HD11	1:A:183:TYR:CZ	2.50	0.47
1:A:175:ASN:HB3	1:A:178:ILE:HG13	1.97	0.47
1:A:278:GLN:NE2	1:A:298:GLU:HB3	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HD3	1:A:395:LYS:C	2.35	0.47
1:A:411:ILE:O	1:A:411:ILE:CG2	2.60	0.47
2:B:99:GLY:O	2:B:102:LYS:CB	2.63	0.47
2:B:107:THR:HG21	2:B:219:LYS:CD	2.43	0.47
2:B:120:LEU:HD23	2:B:125:ARG:HA	1.96	0.47
2:B:125:ARG:HH11	2:B:125:ARG:HG2	1.80	0.47
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.49	0.47
2:B:302:GLU:C	2:B:306:ASN:ND2	2.68	0.47
1:A:19:PRO:HB3	1:A:79:GLU:HB3	1.97	0.47
1:A:106:VAL:CG1	1:A:107:THR:N	2.77	0.47
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.96	0.47
1:A:286:THR:O	1:A:286:THR:CG2	2.59	0.47
2:B:5:ILE:C	2:B:7:THR:H	2.18	0.47
2:B:88:TRP:HZ3	2:B:159:ILE:HG13	1.80	0.47
2:B:175:ASN:OD1	2:B:201:LYS:HE3	2.14	0.47
1:A:451:LYS:HD2	1:A:471:ASN:HA	1.97	0.47
2:B:79:GLU:HG3	2:B:83:ARG:NE	2.28	0.47
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.48	0.47
2:B:242:GLN:NE2	2:B:426:TRP:HD1	2.13	0.46
2:B:260:LEU:HD11	2:B:264:LEU:HD11	1.97	0.46
2:B:300:GLU:C	2:B:302:GLU:H	2.19	0.46
2:B:301:LEU:C	2:B:304:ALA:HB3	2.35	0.46
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.53	0.46
1:A:23:GLN:O	1:A:25:PRO:HD3	2.14	0.46
1:A:78:ARG:HG3	1:A:79:GLU:H	1.80	0.46
1:A:241:VAL:HG11	1:A:244:ILE:HD11	1.96	0.46
2:B:74:LEU:HG	2:B:74:LEU:O	2.16	0.46
2:B:259:LYS:C	2:B:261:VAL:N	2.67	0.46
1:A:7:THR:CG2	1:A:119:PRO:CB	2.93	0.46
1:A:324:ASP:O	1:A:343:GLN:CG	2.63	0.46
1:A:356:ARG:HG3	1:A:357:MET:O	2.15	0.46
2:B:85:GLN:O	2:B:85:GLN:HG2	2.15	0.46
1:A:203:GLU:O	1:A:206:ARG:HB3	2.16	0.46
1:A:518:VAL:HA	1:A:521:ILE:HD12	1.98	0.46
1:A:539:HIS:ND1	1:A:539:HIS:N	2.63	0.46
2:B:88:TRP:CZ3	2:B:92:LEU:HD12	2.51	0.46
2:B:302:GLU:O	2:B:306:ASN:ND2	2.48	0.46
1:A:346:PHE:CD1	1:A:346:PHE:N	2.83	0.46
1:A:406:TRP:CZ2	2:B:419:THR:CG2	2.88	0.46
1:A:270:ILE:O	1:A:272:PRO:CD	2.64	0.46
2:B:278:GLN:NE2	2:B:302:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD23	1:A:341:ILE:CG2	2.46	0.46
2:B:300:GLU:C	2:B:302:GLU:N	2.66	0.46
2:B:334:GLN:O	2:B:336:GLN:N	2.48	0.46
1:A:107:THR:HG23	1:A:221:HIS:CB	2.45	0.46
1:A:540:LYS:O	1:A:541:GLY:C	2.55	0.46
2:B:242:GLN:HE22	2:B:426:TRP:HD1	1.63	0.46
1:A:225:PRO:HA	1:A:226:PRO:C	2.37	0.46
1:A:240:THR:CG2	1:A:241:VAL:N	2.66	0.46
2:B:332:GLN:HB3	2:B:336:GLN:HG3	1.93	0.46
1:A:48:SER:HB2	1:A:147:ASN:ND2	2.22	0.45
1:A:80:LEU:HD23	1:A:153:TRP:CD1	2.51	0.45
2:B:167:ILE:O	2:B:170:PRO:HD2	2.16	0.45
2:B:198:HIS:C	2:B:200:THR:H	2.20	0.45
2:B:418:ASN:C	2:B:420:PRO:HD3	2.36	0.45
1:A:330:GLN:HE21	1:A:330:GLN:HB3	1.52	0.45
1:A:451:LYS:HD2	1:A:471:ASN:HB3	1.97	0.45
1:A:481:ALA:O	1:A:482:ILE:C	2.53	0.45
1:A:71:TRP:CD1	1:A:71:TRP:N	2.85	0.45
1:A:442:VAL:HG21	1:A:481:ALA:C	2.37	0.45
1:A:545:ASN:OD1	1:A:548:VAL:HB	2.17	0.45
2:B:60:VAL:O	2:B:60:VAL:CG2	2.62	0.45
2:B:279:LEU:HD12	2:B:279:LEU:O	2.17	0.45
2:B:344:GLU:HA	2:B:345:PRO:HD2	1.79	0.45
1:A:94:ILE:HG23	1:A:229:TRP:CH2	2.50	0.45
1:A:108:VAL:HG11	1:A:227:PHE:CE1	2.52	0.45
1:A:125:ARG:O	1:A:128:THR:N	2.24	0.45
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.80	0.45
1:A:356:ARG:HB2	1:A:367:GLN:NE2	2.31	0.45
1:A:363:ASN:OD1	1:A:365:VAL:HG23	2.15	0.45
1:A:470:THR:O	1:A:471:ASN:CG	2.55	0.45
2:B:352:GLY:C	2:B:353:LYS:HG3	2.36	0.45
1:A:46:LYS:NZ	1:A:113:ASP:OD2	2.48	0.45
1:A:209:LEU:O	1:A:212:TRP:HB2	2.17	0.45
1:A:260:LEU:O	1:A:264:LEU:HG	2.17	0.45
2:B:111:VAL:O	2:B:113:ASP:N	2.49	0.45
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.51	0.45
1:A:417:VAL:CG1	1:A:419:THR:HG23	2.45	0.45
1:A:449:GLU:C	1:A:451:LYS:H	2.20	0.45
1:A:482:ILE:HD13	1:A:506:ILE:CD1	2.46	0.45
2:B:88:TRP:HZ3	2:B:159:ILE:HG12	1.80	0.45
2:B:116:PHE:CZ	2:B:151:GLN:NE2	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:GLN:HA	2:B:243:PRO:HD3	1.56	0.45
2:B:243:PRO:C	2:B:245:VAL:N	2.70	0.45
1:A:277:ARG:HB2	1:A:336:GLN:OE1	2.17	0.45
2:B:88:TRP:CZ3	2:B:159:ILE:CG1	2.99	0.45
2:B:164:MET:O	2:B:165:THR:C	2.55	0.45
2:B:205:LEU:O	2:B:208:HIS:HB3	2.16	0.45
2:B:303:LEU:HD12	2:B:307:ARG:HB2	1.99	0.45
1:A:106:VAL:HG12	1:A:107:THR:N	2.31	0.45
1:A:30:LYS:HE2	1:A:71:TRP:HZ3	1.81	0.45
1:A:90:VAL:HG21	1:A:157:PRO:CB	2.38	0.45
1:A:270:ILE:HD11	1:A:316:GLY:CA	2.47	0.45
2:B:7:THR:O	2:B:9:PRO:HD3	2.17	0.45
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.47	0.45
2:B:203:GLU:OE2	2:B:207:GLN:HG2	2.16	0.45
2:B:363:ASN:O	2:B:367:GLN:CG	2.65	0.45
2:B:369:THR:HB	2:B:398:TRP:CH2	2.51	0.45
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.51	0.45
1:A:115:TYR:HE2	1:A:157:PRO:HA	1.82	0.45
1:A:195:ILE:CD1	1:A:199:ARG:HG3	2.47	0.45
1:A:281:LYS:HA	1:A:358:ARG:NH2	2.19	0.45
1:A:283:LEU:CD2	1:A:286:THR:HG21	2.47	0.45
1:A:327:ALA:CB	1:A:341:ILE:HG12	2.47	0.45
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.98	0.45
1:A:466:VAL:HG21	1:A:551:LEU:O	2.17	0.45
2:B:320:ASP:OD1	2:B:320:ASP:C	2.56	0.45
2:B:366:LYS:HB2	2:B:405:TYR:CZ	2.49	0.45
1:A:241:VAL:HG11	1:A:266:TRP:NE1	2.32	0.44
1:A:426:TRP:O	1:A:427:TYR:HB3	2.17	0.44
1:A:498:ASP:C	1:A:535:TRP:HE1	2.20	0.44
2:B:23:GLN:HG3	2:B:24:TRP:O	2.16	0.44
2:B:66:LYS:HG3	2:B:218:ASP:CB	2.46	0.44
1:A:125:ARG:O	1:A:128:THR:OG1	2.26	0.44
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.47	0.44
1:A:255:ASN:ND2	1:A:259:LYS:HE3	2.32	0.44
2:B:214:LEU:HD12	2:B:214:LEU:O	2.18	0.44
2:B:303:LEU:O	2:B:307:ARG:HB2	2.18	0.44
2:B:373:GLN:HE21	2:B:373:GLN:HB2	1.65	0.44
1:A:38:CYS:CB	1:A:144:TYR:CE1	3.00	0.44
1:A:122:GLU:O	1:A:124:PHE:N	2.51	0.44
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.99	0.44
2:B:10:VAL:HG13	2:B:88:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ASP:CG	2:B:78:ARG:HD3	2.37	0.44
1:A:32:LYS:HD3	1:A:32:LYS:HA	1.73	0.44
1:A:510:PRO:O	1:A:522:ILE:HD12	2.18	0.44
2:B:138:GLU:O	2:B:139:THR:HG22	2.17	0.44
2:B:273:GLY:HA3	2:B:309:ILE:HG12	2.00	0.44
1:A:255:ASN:HD21	1:A:259:LYS:HE3	1.82	0.44
1:A:511:ASP:OD1	1:A:512:LYS:N	2.51	0.44
2:B:57:ASN:ND2	2:B:57:ASN:C	2.70	0.44
2:B:65:LYS:NZ	2:B:72:ARG:HE	2.16	0.44
2:B:203:GLU:HA	2:B:206:ARG:HB2	2.00	0.44
2:B:243:PRO:C	2:B:245:VAL:H	2.20	0.44
1:A:76:ASP:OD2	1:A:78:ARG:NE	2.51	0.44
1:A:106:VAL:HG13	1:A:189:VAL:O	2.17	0.44
1:A:475:GLN:O	1:A:476:LYS:C	2.56	0.44
2:B:18:GLY:HA3	2:B:56:TYR:CD1	2.52	0.44
2:B:366:LYS:HB2	2:B:405:TYR:CD2	2.52	0.44
1:A:61:PHE:HE1	1:A:76:ASP:HB2	1.81	0.44
1:A:64:LYS:HD2	1:A:71:TRP:CZ2	2.52	0.44
1:A:323:LYS:NZ	1:A:344:GLU:OE2	2.32	0.44
1:A:395:LYS:HD3	1:A:395:LYS:O	2.18	0.44
2:B:65:LYS:HB3	2:B:66:LYS:H	1.68	0.44
2:B:273:GLY:O	2:B:274:ILE:HG13	2.18	0.44
1:A:137:ASN:C	1:A:139:THR:H	2.21	0.44
1:A:208:HIS:O	1:A:212:TRP:HD1	2.00	0.44
1:A:457:TYR:C	1:A:457:TYR:CD2	2.91	0.44
2:B:2:ILE:O	2:B:4:PRO:O	2.36	0.44
2:B:137:ASN:C	2:B:139:THR:N	2.70	0.44
2:B:178:ILE:HD11	2:B:201:LYS:HG3	1.98	0.44
1:A:525:LEU:HD23	1:A:525:LEU:HA	1.81	0.43
2:B:175:ASN:OD1	2:B:201:LYS:HD2	2.17	0.43
2:B:318:TYR:O	2:B:318:TYR:CD1	2.68	0.43
2:B:350:LYS:CE	2:B:378:GLU:OE1	2.66	0.43
2:B:377:THR:O	2:B:378:GLU:C	2.57	0.43
1:A:27:THR:HG22	1:A:29:GLU:H	1.82	0.43
1:A:296:THR:H	1:A:299:ALA:HB3	1.83	0.43
1:A:391:LEU:HG	1:A:414:TRP:CB	2.48	0.43
1:A:453:GLY:O	1:A:469:LEU:O	2.35	0.43
2:B:85:GLN:O	2:B:88:TRP:N	2.47	0.43
2:B:242:GLN:HB2	2:B:351:THR:OG1	2.19	0.43
1:A:30:LYS:HD3	1:A:62:ALA:O	2.19	0.43
1:A:64:LYS:HA	1:A:71:TRP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:HG3	1:A:248:GLU:O	2.19	0.43
2:B:272:PRO:O	2:B:274:ILE:N	2.52	0.43
2:B:291:GLU:CG	2:B:292:VAL:H	2.31	0.43
1:A:246:LEU:CD1	1:A:260:LEU:CD1	2.91	0.43
2:B:282:LEU:O	2:B:283:LEU:HD23	2.19	0.43
1:A:5:ILE:HG22	1:A:6:GLU:N	2.33	0.43
1:A:27:THR:C	1:A:29:GLU:H	2.21	0.43
1:A:137:ASN:O	1:A:140:PRO:CD	2.66	0.43
1:A:439:THR:CG2	1:A:441:TYR:CE1	3.00	0.43
1:A:548:VAL:HG12	1:A:552:VAL:HG21	1.99	0.43
2:B:340:GLN:HB3	2:B:348:ASN:ND2	2.33	0.43
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.83	0.43
1:A:48:SER:N	1:A:145:GLN:O	2.45	0.43
1:A:108:VAL:CG1	1:A:227:PHE:CE1	3.01	0.43
1:A:416:PHE:HZ	1:A:422:LEU:HD11	1.83	0.43
1:A:420:PRO:HA	1:A:422:LEU:HD23	2.00	0.43
1:A:457:TYR:HE2	1:A:464:GLN:C	2.22	0.43
1:A:482:ILE:O	1:A:485:ALA:HB3	2.19	0.43
2:B:195:ILE:HG22	2:B:196:GLY:N	2.34	0.43
2:B:242:GLN:CG	2:B:243:PRO:N	2.82	0.43
2:B:270:ILE:CG2	2:B:271:TYR:H	2.31	0.43
1:A:2:ILE:HG23	1:A:3:SER:H	1.83	0.43
1:A:17:ASP:OD1	1:A:56:TYR:HE2	2.01	0.43
1:A:277:ARG:HB3	1:A:334:GLN:OE1	2.18	0.43
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.49	0.43
2:B:153:TRP:C	2:B:155:GLY:N	2.72	0.43
2:B:278:GLN:O	2:B:299:ALA:HB2	2.18	0.43
2:B:319:TYR:CG	2:B:320:ASP:N	2.87	0.43
1:A:434:ILE:HD13	1:A:530:LYS:CB	2.49	0.43
1:A:480:GLN:HA	1:A:480:GLN:NE2	2.33	0.43
1:A:77:PHE:O	1:A:78:ARG:C	2.57	0.43
1:A:453:GLY:O	1:A:469:LEU:HB2	2.19	0.43
1:A:457:TYR:C	1:A:457:TYR:HD2	2.23	0.43
2:B:131:THR:HG23	2:B:141:GLY:HA3	2.01	0.43
2:B:138:GLU:C	2:B:139:THR:HG22	2.39	0.43
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.92	0.43
2:B:193:LEU:HD12	2:B:198:HIS:N	2.34	0.43
1:A:94:ILE:HD12	1:A:94:ILE:HA	1.78	0.42
2:B:125:ARG:O	2:B:127:TYR:N	2.51	0.42
1:A:275:LYS:O	1:A:276:VAL:HG23	2.19	0.42
2:B:131:THR:OG1	2:B:143:ARG:CD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HA	1:A:144:TYR:HD2	1.84	0.42
1:A:410:TRP:CZ3	2:B:401:TRP:CE3	3.07	0.42
1:A:548:VAL:O	1:A:552:VAL:CG2	2.67	0.42
1:A:235:HIS:CB	1:A:238:LYS:HG2	2.50	0.42
1:A:337:TRP:O	1:A:354:TYR:N	2.52	0.42
1:A:420:PRO:HB2	1:A:421:PRO:HA	2.02	0.42
1:A:435:VAL:HA	2:B:290:THR:HG21	2.01	0.42
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.54	0.42
2:B:191:SER:OG	2:B:198:HIS:ND1	2.39	0.42
1:A:110:ASP:CB	1:A:222:GLN:NE2	2.82	0.42
1:A:254:VAL:CG2	1:A:255:ASN:N	2.83	0.42
1:A:341:ILE:O	1:A:349:LEU:HB2	2.20	0.42
1:A:391:LEU:O	1:A:416:PHE:HA	2.18	0.42
1:A:278:GLN:OE1	1:A:278:GLN:HA	2.20	0.42
1:A:456:GLY:HA2	1:A:484:LEU:CD2	2.50	0.42
2:B:197:GLN:O	2:B:200:THR:HB	2.20	0.42
2:B:279:LEU:HA	2:B:299:ALA:CB	2.47	0.42
1:A:229:TRP:NE1	1:A:230:MET:HG2	2.35	0.42
1:A:279:LEU:HA	1:A:282:LEU:HD12	2.02	0.42
1:A:317:VAL:HG22	1:A:318:TYR:H	1.85	0.42
1:A:317:VAL:HG22	1:A:318:TYR:N	2.33	0.42
1:A:363:ASN:OD1	1:A:363:ASN:C	2.58	0.42
1:A:539:HIS:CG	1:A:540:LYS:N	2.79	0.42
2:B:66:LYS:HG3	2:B:218:ASP:CG	2.38	0.42
2:B:85:GLN:O	2:B:88:TRP:C	2.58	0.42
2:B:142:ILE:H	2:B:142:ILE:HG12	1.72	0.42
1:A:93:GLY:HA3	2:B:137:ASN:ND2	2.35	0.42
1:A:485:ALA:O	1:A:486:LEU:C	2.58	0.42
2:B:52:PRO:C	2:B:54:ASN:H	2.22	0.42
1:A:338:THR:HA	1:A:353:LYS:HA	2.02	0.42
1:A:475:GLN:C	1:A:477:THR:N	2.73	0.42
2:B:66:LYS:HB3	2:B:221:HIS:CE1	2.55	0.42
2:B:156:SER:HB2	2:B:157:PRO:CD	2.50	0.42
1:A:221:HIS:C	1:A:223:LYS:H	2.22	0.42
1:A:359:GLY:O	1:A:360:ALA:C	2.58	0.42
2:B:5:ILE:C	2:B:7:THR:N	2.73	0.42
1:A:288:ALA:O	1:A:290:THR:N	2.53	0.41
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.20	0.41
1:A:442:VAL:HG21	1:A:482:ILE:HA	2.02	0.41
2:B:65:LYS:O	2:B:67:ASP:N	2.53	0.41
2:B:242:GLN:HG2	2:B:243:PRO:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LEU:CD1	2:B:282:LEU:HD23	2.50	0.41
2:B:331:LYS:CE	2:B:364:ASP:OD2	2.68	0.41
2:B:363:ASN:ND2	2:B:405:TYR:OH	2.53	0.41
2:B:379:SER:HA	2:B:383:TRP:HZ3	1.83	0.41
1:A:107:THR:HG21	1:A:202:ILE:HG21	2.03	0.41
1:A:206:ARG:NH2	1:A:207:GLN:OE1	2.49	0.41
1:A:324:ASP:O	1:A:343:GLN:NE2	2.47	0.41
1:A:340:GLN:HA	1:A:351:THR:HA	2.02	0.41
2:B:4:PRO:O	2:B:6:GLU:N	2.53	0.41
1:A:442:VAL:HG21	1:A:482:ILE:N	2.35	0.41
1:A:467:VAL:CG1	1:A:468:PRO:HD2	2.50	0.41
2:B:298:GLU:CG	2:B:299:ALA:N	2.83	0.41
1:A:134:SER:O	1:A:136:ASN:N	2.53	0.41
1:A:324:ASP:OD2	1:A:388:LYS:HE3	2.20	0.41
1:A:398:TRP:CH2	1:A:411:ILE:HG22	2.55	0.41
1:A:427:TYR:CE1	1:A:525:LEU:HD13	2.55	0.41
1:A:451:LYS:NZ	1:A:471:ASN:HB3	2.35	0.41
2:B:13:LYS:CE	2:B:86:ASP:HB2	2.50	0.41
2:B:376:THR:HG21	2:B:410:TRP:CE3	2.55	0.41
1:A:329:ILE:HD12	1:A:391:LEU:HD22	2.03	0.41
2:B:334:GLN:O	2:B:335:GLY:C	2.59	0.41
1:A:27:THR:HG22	1:A:29:GLU:CB	2.50	0.41
1:A:47:ILE:HD13	1:A:145:GLN:C	2.41	0.41
1:A:157:PRO:O	1:A:160:PHE:HB3	2.21	0.41
1:A:397:THR:HG23	1:A:424:LYS:HD2	2.03	0.41
1:A:296:THR:O	1:A:299:ALA:N	2.53	0.41
2:B:76:ASP:OD1	2:B:76:ASP:C	2.59	0.41
1:A:148:VAL:O	1:A:150:PRO:CD	2.67	0.41
1:A:175:ASN:C	1:A:177:ASP:H	2.24	0.41
1:A:424:LYS:HG3	1:A:425:LEU:N	2.36	0.41
1:A:447:ASN:C	1:A:449:GLU:H	2.23	0.41
1:A:517:LEU:O	1:A:521:ILE:HD12	2.21	0.41
2:B:3:SER:CB	2:B:4:PRO:CD	2.98	0.41
2:B:46:LYS:CD	2:B:116:PHE:CD2	3.03	0.41
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.56	0.41
2:B:373:GLN:OE1	2:B:407:GLN:N	2.34	0.41
1:A:134:SER:CB	1:A:140:PRO:HB2	2.51	0.41
1:A:138:GLU:O	1:A:138:GLU:HG2	2.21	0.41
1:A:482:ILE:HD13	1:A:506:ILE:HD12	2.03	0.41
2:B:12:LEU:HD21	2:B:127:TYR:CD2	2.55	0.41
2:B:260:LEU:CD1	2:B:264:LEU:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LYS:HE3	2:B:364:ASP:OD2	2.21	0.41
2:B:402:TRP:O	2:B:403:THR:C	2.59	0.41
1:A:221:HIS:CD2	1:A:223:LYS:CB	3.04	0.40
1:A:365:VAL:HG21	1:A:425:LEU:HD21	2.03	0.40
2:B:99:GLY:O	2:B:102:LYS:N	2.48	0.40
2:B:122:GLU:HA	2:B:125:ARG:HG3	2.02	0.40
2:B:298:GLU:H	2:B:298:GLU:HG2	1.62	0.40
1:A:202:ILE:HD13	1:A:202:ILE:HA	1.90	0.40
1:A:255:ASN:CG	1:A:259:LYS:HE3	2.41	0.40
1:A:296:THR:C	1:A:298:GLU:N	2.74	0.40
1:A:390:LYS:HB3	1:A:417:VAL:HG21	2.02	0.40
1:A:396:GLU:O	1:A:396:GLU:HG2	2.21	0.40
1:A:431:LYS:O	1:A:532:TYR:HE2	2.03	0.40
2:B:291:GLU:HG3	2:B:292:VAL:H	1.87	0.40
1:A:66:LYS:HE3	1:A:66:LYS:HB2	1.90	0.40
1:A:379:SER:HB3	1:A:385:LYS:O	2.21	0.40
1:A:520:GLN:HA	1:A:520:GLN:NE2	2.25	0.40
2:B:40:GLU:HB3	2:B:44:GLU:OE2	2.20	0.40
2:B:183:TYR:O	2:B:184:MET:HB2	2.20	0.40
1:A:472:THR:OG1	1:A:476:LYS:HB3	2.21	0.40
2:B:350:LYS:HE3	2:B:378:GLU:OE1	2.21	0.40
1:A:113:ASP:O	1:A:116:PHE:HB2	2.21	0.40
2:B:404:GLU:OE1	2:B:404:GLU:HA	2.21	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	550/560 (98%)	410 (74%)	94 (17%)	46 (8%)	1 2
2	B	425/430 (99%)	310 (73%)	71 (17%)	44 (10%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	975/990 (98%)	720 (74%)	165 (17%)	90 (9%)	1 1

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	289	LEU
1	A	334	GLN
1	A	360	ALA
1	A	433	PRO
1	A	540	LYS
2	B	5	ILE
2	B	85	GLN
2	B	154	LYS
2	B	195	ILE
2	B	273	GLY
2	B	366	LYS
2	B	404	GLU
1	A	78	ARG
1	A	123	ASP
1	A	137	ASN
1	A	237	ASP
1	A	247	PRO
1	A	276	VAL
1	A	358	ARG
1	A	406	TRP
1	A	450	THR
1	A	476	LYS
1	A	541	GLY
2	B	18	GLY
2	B	66	LYS
2	B	91	GLN
2	B	103	ASN
2	B	116	PHE
2	B	126	LYS
2	B	193	LEU
2	B	217	PRO
2	B	260	LEU
2	B	282	LEU
2	B	345	PRO
2	B	365	VAL
1	A	52	PRO

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Mol	Chain	Res	Type
1	A	126	LYS
1	A	151	GLN
1	A	152	GLY
1	A	169	GLU
1	A	195	ILE
1	A	230	MET
1	A	538	ALA
2	B	77	PHE
2	B	199	ARG
2	B	226	PRO
2	B	287	LYS
2	B	304	ALA
2	B	395	LYS
2	B	421	PRO
1	A	2	ILE
1	A	103	ASN
1	A	114	ALA
1	A	127	TYR
1	A	279	LEU
1	A	304	ALA
1	A	408	ALA
1	A	409	THR
1	A	419	THR
2	B	138	GLU
2	B	229	TRP
2	B	359	GLY
2	B	402	TRP
2	B	419	THR
1	A	25	PRO
1	A	122	GLU
1	A	157	PRO
1	A	184	MET
1	A	259	LYS
1	A	311	LYS
2	B	162	SER
2	B	174	GLN
2	B	270	ILE
2	B	335	GLY
1	A	111	VAL
2	B	173	LYS
2	B	418	ASN
1	A	135	ILE

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Mol	Chain	Res	Type
1	A	217	PRO
2	B	95	PRO
2	B	97	PRO
2	B	276	VAL
2	B	9	PRO
2	B	244	ILE
1	A	55	PRO
1	A	133	PRO
2	B	176	PRO
1	A	243	PRO
2	B	243	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	475/500 (95%)	431 (91%)	44 (9%)	9 27
2	B	367/392 (94%)	314 (86%)	53 (14%)	3 9
All	All	842/892 (94%)	745 (88%)	97 (12%)	5 17

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	47	ILE
1	A	54	ASN
1	A	83	ARG
1	A	89	GLU
1	A	94	ILE
1	A	113	ASP
1	A	119	PRO
1	A	126	LYS
1	A	133	PRO
1	A	140	PRO
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	175	ASN
1	A	194	GLU
1	A	218	ASP
1	A	228	LEU
1	A	243	PRO
1	A	289	LEU
1	A	312	GLU
1	A	325	LEU
1	A	330	GLN
1	A	353	LYS
1	A	356	ARG
1	A	358	ARG
1	A	362	THR
1	A	363	ASN
1	A	365	VAL
1	A	369	THR
1	A	387	PRO
1	A	398	TRP
1	A	409	THR
1	A	431	LYS
1	A	450	THR
1	A	454	LYS
1	A	457	TYR
1	A	458	VAL
1	A	460	ASN
1	A	497	THR
1	A	520	GLN
1	A	523	GLU
1	A	529	GLU
1	A	533	LEU
1	A	545	ASN
1	A	551	LEU
2	B	9	PRO
2	B	12	LEU
2	B	16	MET
2	B	17	ASP
2	B	40	GLU
2	B	41	MET
2	B	57	ASN
2	B	69	THR
2	B	86	ASP
2	B	87	PHE

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Mol	Chain	Res	Type
2	B	100	LEU
2	B	103	ASN
2	B	139	THR
2	B	142	ILE
2	B	165	THR
2	B	176	PRO
2	B	177	ASP
2	B	206	ARG
2	B	212	TRP
2	B	215	THR
2	B	216	THR
2	B	218	ASP
2	B	239	TRP
2	B	248	GLU
2	B	257	ILE
2	B	265	ASN
2	B	274	ILE
2	B	290	THR
2	B	293	ILE
2	B	294	PRO
2	B	297	GLU
2	B	300	GLU
2	B	301	LEU
2	B	302	GLU
2	B	309	ILE
2	B	311	LYS
2	B	317	VAL
2	B	318	TYR
2	B	330	GLN
2	B	340	GLN
2	B	344	GLU
2	B	346	PHE
2	B	354	TYR
2	B	363	ASN
2	B	367	GLN
2	B	369	THR
2	B	373	GLN
2	B	383	TRP
2	B	388	LYS
2	B	403	THR
2	B	405	TYR
2	B	417	VAL

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Mol	Chain	Res	Type
2	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	145	GLN
1	A	147	ASN
1	A	175	ASN
1	A	221	HIS
1	A	222	GLN
1	A	235	HIS
1	A	265	ASN
1	A	269	GLN
1	A	394	GLN
1	A	471	ASN
1	A	480	GLN
1	A	487	GLN
1	A	509	GLN
1	A	519	ASN
1	A	520	GLN
1	A	524	GLN
1	A	547	GLN
2	B	136	ASN
2	B	208	HIS
2	B	258	GLN
2	B	269	GLN
2	B	278	GLN
2	B	336	GLN
2	B	348	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	65B	A	600	-	29,30,30	2.93	15 (51%)	38,42,42	2.12	7 (18%)

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	65B	A	600	-	-	4/12/12/12	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	65B	C22-C21	7.91	1.52	1.39
3	A	600	65B	C1-C2	4.67	1.48	1.40
3	A	600	65B	C13-N12	4.61	1.39	1.32
3	A	600	65B	C1-C6	4.54	1.48	1.40
3	A	600	65B	BR-C14	-4.23	1.80	1.89
3	A	600	65B	C23-C22	3.84	1.45	1.38
3	A	600	65B	O17-C13	3.21	1.48	1.36
3	A	600	65B	C23-C24	3.04	1.45	1.39
3	A	600	65B	C5-C6	2.93	1.43	1.39
3	A	600	65B	C3-C2	2.74	1.43	1.39
3	A	600	65B	C26-C25	2.63	1.43	1.38
3	A	600	65B	C11-N12	2.58	1.42	1.34
3	A	600	65B	C15-N16	2.55	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	65B	C25-C24	2.32	1.44	1.39
3	A	600	65B	C13-C14	2.11	1.41	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	65B	C1-O17-C13	-6.01	110.71	116.88
3	A	600	65B	N16-C11-N12	-5.44	117.63	126.23
3	A	600	65B	C14-C13-N12	-5.29	117.57	123.72
3	A	600	65B	C11-N12-C13	4.76	123.70	115.18
3	A	600	65B	C15-C14-C13	2.62	119.67	117.41
3	A	600	65B	C22-C23-C24	-2.36	117.30	120.35
3	A	600	65B	C11-N16-C15	2.27	121.17	116.52

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	65B	C14-C13-O17-C1
3	A	600	65B	C26-C21-N5-C11
3	A	600	65B	C22-C21-N5-C11
3	A	600	65B	N12-C13-O17-C1

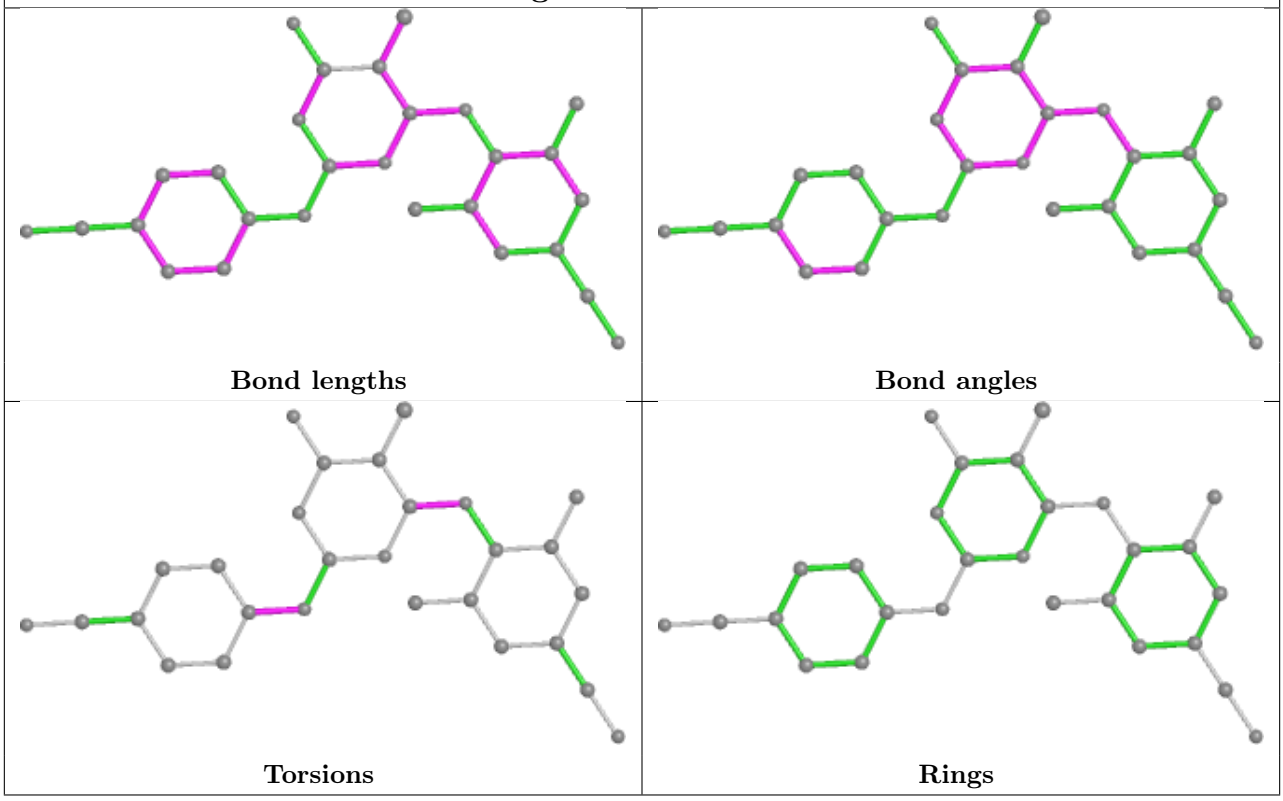
There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	65B	10	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 65B A 600



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.

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	552/560 (98%)	-0.06	16 (2%)	51	47	47, 87, 120, 120	0
2	B	427/430 (99%)	0.16	29 (6%)	17	13	36, 77, 120, 120	0
All	All	979/990 (98%)	0.04	45 (4%)	32	29	36, 83, 120, 120	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	5	ILE	8.2
2	B	358	ARG	7.3
2	B	228	LEU	7.2
2	B	219	LYS	5.7
2	B	229	TRP	5.2
2	B	1	PRO	5.2
2	B	227	PHE	5.1
1	A	133	PRO	5.0
2	B	218	ASP	4.8
2	B	359	GLY	4.7
1	A	217	PRO	4.3
2	B	360	ALA	4.1
2	B	226	PRO	4.0
1	A	142	ILE	3.9
2	B	4	PRO	3.9
2	B	317	VAL	3.7
1	A	218	ASP	3.7
2	B	3	SER	3.6
1	A	134	SER	3.5
2	B	225	PRO	3.3
1	A	222	GLN	3.3
2	B	306	ASN	3.3
2	B	318	TYR	3.2
2	B	284	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	409	THR	3.0
1	A	136	ASN	3.0
2	B	251	SER	2.7
1	A	221	HIS	2.6
2	B	270	ILE	2.6
1	A	446	ALA	2.6
1	A	219	LYS	2.5
2	B	240	THR	2.5
1	A	34	LEU	2.5
2	B	281	LYS	2.4
2	B	357	MET	2.4
2	B	310	LEU	2.3
1	A	141	GLY	2.2
2	B	293	ILE	2.2
1	A	178	ILE	2.2
2	B	299	ALA	2.2
1	A	66	LYS	2.2
2	B	264	LEU	2.2
1	A	138	GLU	2.1
2	B	230	MET	2.1
1	A	289	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

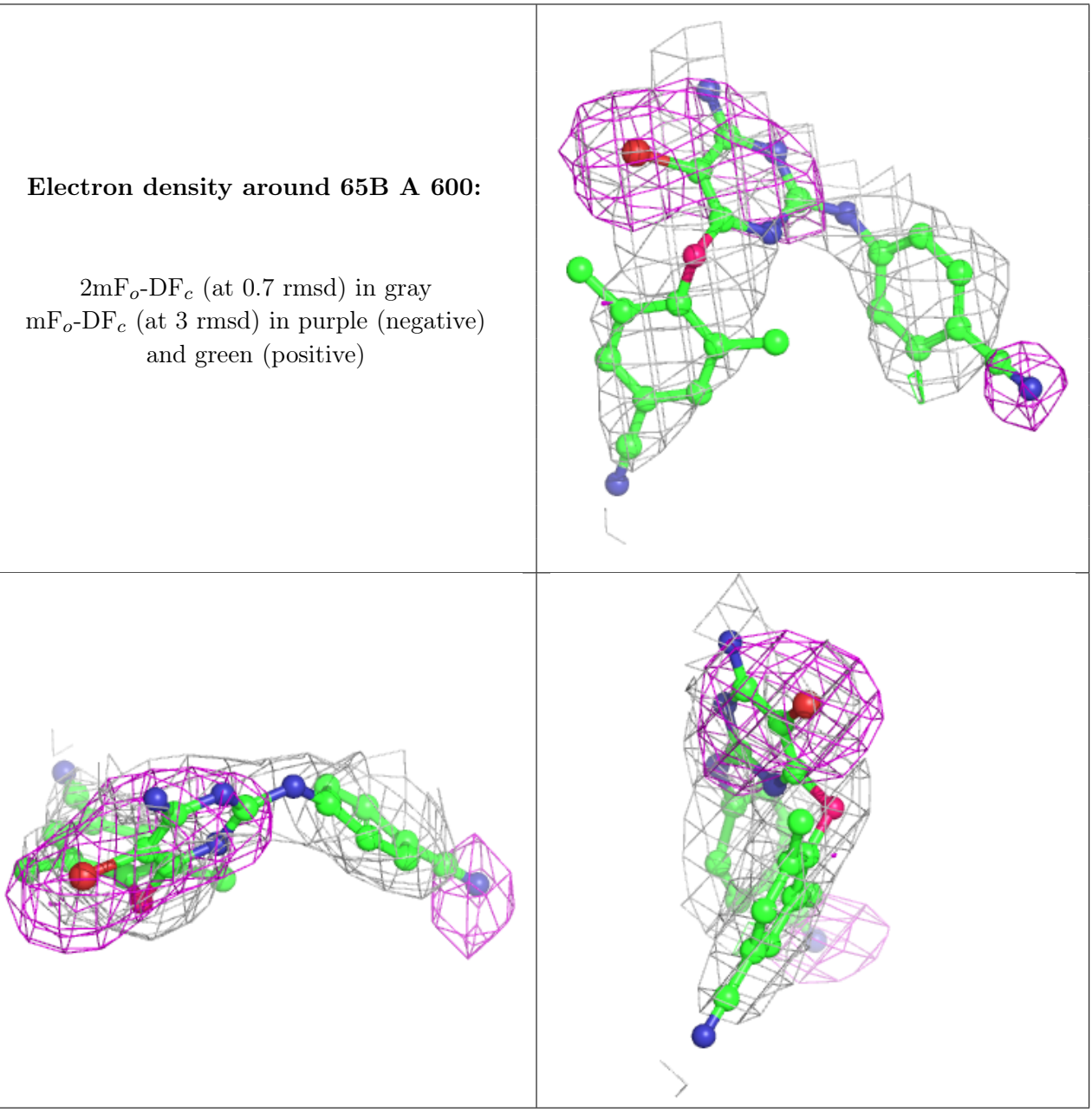
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	65B	A	600	28/28	0.85	0.37	58,72,83,108	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 65B A 600:

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



6.5 Other polymers (i)

There are no such residues in this entry.