Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:16 PM GMT

PDB ID	:	1JLC
Title	:	CRYSTAL STRUCTURE OF Y181C MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH PETT-2
Authors	:	Ren, J.; Nichols, C.; Bird, L.; Chamberlain, P.; Weaver, K.; Short, S.; Stuart, D.I.; Stammers, D.K.
Deposited on	:	2001-07-16
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

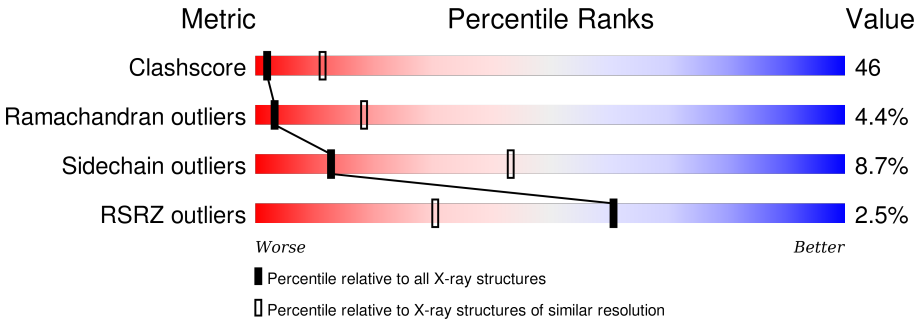
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%, 31%, 54%, 10%
2	B	440	2%, 44%, 41%, 6%, 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7711 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 HIV-1 RT A-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4361	2821	726	805	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	CYS	TYR	ENGINEERED	UNP P04585
A	280	CSD	CYS	OXIDIZED CYS	UNP P04585

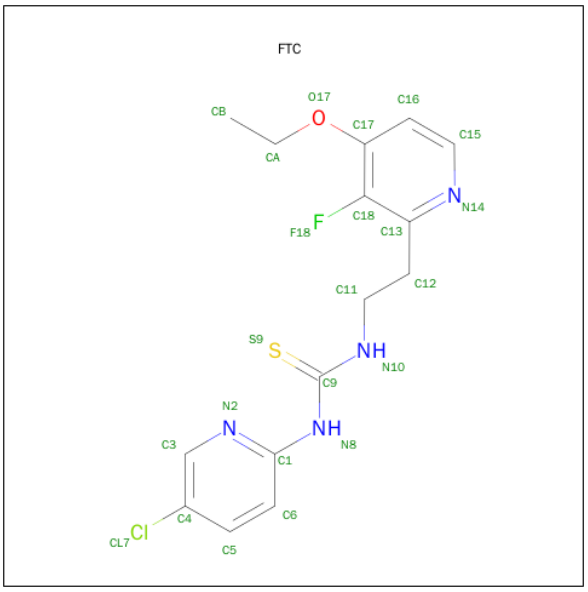
- Molecule 2 is a protein called HIV-1 RT B-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3327	2158	555	606	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	181	CYS	TYR	ENGINEERED	UNP P04585

- Molecule 3 is N-[[3-FLUORO-4-ETHOXY-PYRID-2-YL]ETHYL]-N'-[5-CHLORO-PYRIDYL]-THIOUREA (three-letter code: FTC) (formula: $C_{15}H_{16}ClFN_4OS$).

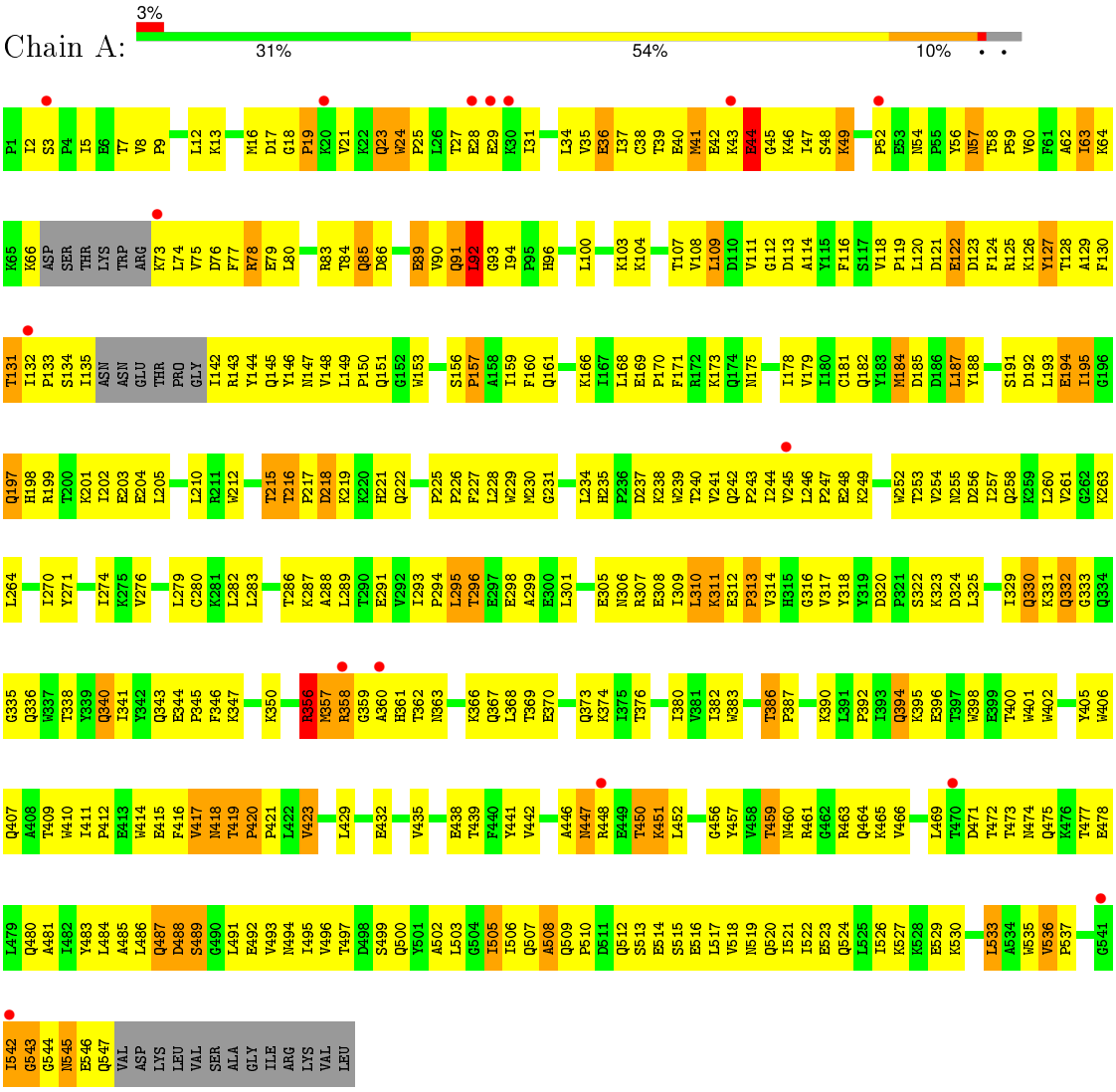


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	N	O	S		
3	A	1	23	15	1	1	4	1	1	0	0

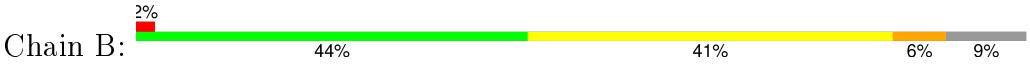
3 Residue-property plots (i)

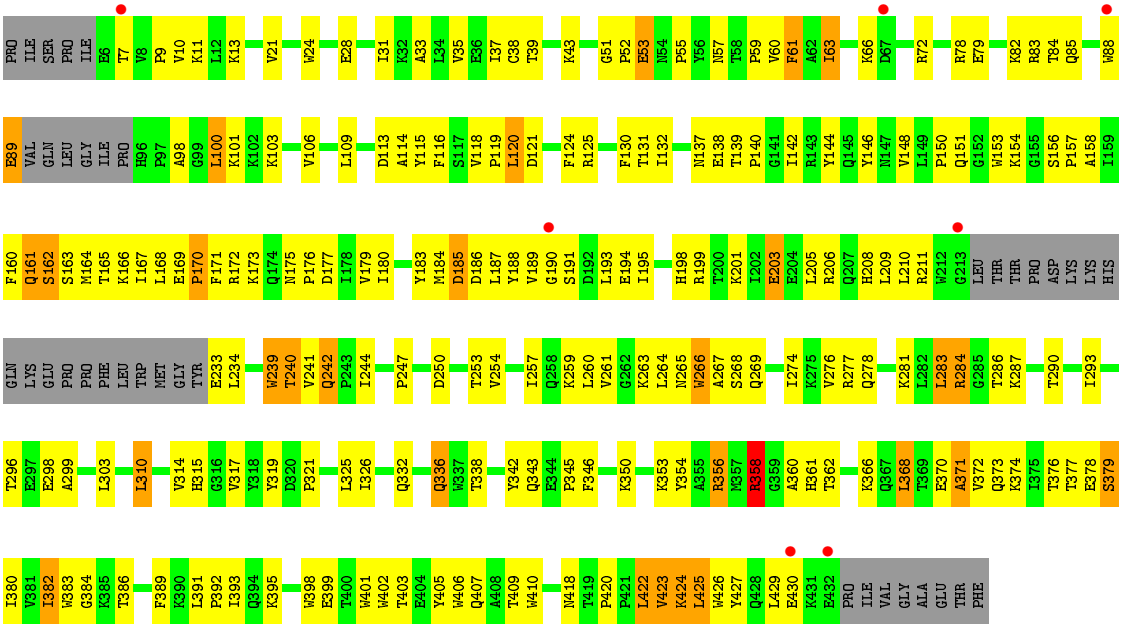
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: HIV-1 RT A-chain



- Molecule 2: HIV-1 RT B-chain




PRO ILE SER PRO ILE E6 T7 V8 P9 V10 K11 L12 K13 V21 W24 E28 I31 K32 A33 I34 V35 E36 I37 C38 T39 K43 G51 P52 E53 N54 P55 Y56 N57 T58 P59 V60 F61 A62 I63 K66 D67 R72 R78 E79 K82 R83 T84 Q85 W88
E89 VAL GLN LEU GLY ILE PRO H96 P97 A98 G99 L100 K101 K102 K103 V106 L109 D113 A114 Y115 F116 S117 V118 P119 L120 D121 F124 R125 F130 T131 I132 N137 E138 T139 P140 G141 I142 R143 Y144 Q145 Y146 N147 V148 I149 P150 Q151 G152 W153 K154 G155 S156 P157 A158 I159
F160 Q161 S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 R172 K173 Q174 N175 P176 D177 I178 V179 I180 Y183 M184 D185 D186 L187 Y188 V189 G190 S191 D192 L193 E194 I195 H198 R199 T200 K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 R211 W212 G213 LEU THR THR PRO ASP LYS LYS HIS
GLN LYS GLU PRO PRO PHE LEU TRP MET GLY TYR E233 L234 W239 T240 V241 Q242 P243 I244 P247 D250 T253 V254 I257 Q258 K259 L260 V261 G262 K263 L264 N265 W266 A267 S268 Q269 I274 K275 V276 R277 Q278 K281 L282 L283 R284 G285 T286 K287 T290 I293
T296 E297 E298 A299 L303 L310 V314 H315 G316 V317 Y318 Y319 D320 P321 L325 I326 Q332 Q336 W337 T338 Y342 Q343 E344 P345 F346 K350 K353 Y354 A355 R356 N357 R358 G359 A360 H361 T362 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377 E378 S379
I380 V381 I382 W383 G384 K385 T386 F389 K390 L391 P392 I393 Q394 K395 W398 E399 T400 W401 W402 T403 E404 Y405 W406 Q407 A408 T409 W410 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427 Q428 L429 E430 K431 E432 PRO ILE VAL GLY ALA GLU THR PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.20Å 109.30Å 73.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 3.00 29.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.79-3.00) 97.0 (29.79-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.282 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	83.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 83.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 22418 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7711	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CSD, FTC

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	0.56	0/4464	0.77	1/6061 (0.0%)
2	B	0.54	0/3418	0.74	1/4638 (0.0%)
All	All	0.55	0/7882	0.76	2/10699 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	356	ARG	N-CA-C	6.03	127.27	111.00
2	B	88	TRP	CA-CB-CG	-5.33	103.58	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	TYR	Sidechain

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	4361	0	4413	501	0
2	B	3327	0	3352	230	0
3	A	23	0	16	4	0
All	All	7711	0	7781	715	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 46.

All (715) 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:228:LEU:HD23	1:A:228:LEU:H	1.04	1.20
1:A:41:MET:HB3	1:A:47:ILE:HD13	1.25	1.13
1:A:216:THR:HG22	1:A:217:PRO:HD2	1.28	1.09
1:A:41:MET:HG2	1:A:46:LYS:HD2	1.32	1.09
1:A:41:MET:HB3	1:A:47:ILE:CD1	1.86	1.05
2:B:98:ALA:HA	2:B:101:LYS:HD3	1.40	1.03
1:A:536:VAL:HG21	1:A:542:ILE:HG21	1.38	1.02
1:A:274:ILE:HD11	1:A:310:LEU:HD11	1.43	1.01
1:A:46:LYS:HB3	1:A:47:ILE:HD12	1.40	1.01
1:A:244:ILE:HD11	1:A:263:LYS:HD3	1.39	0.99
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.46	0.97
1:A:132:ILE:HB	1:A:142:ILE:HG22	1.48	0.95
1:A:123:ASP:O	1:A:126:LYS:HD3	1.67	0.95
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.50	0.94
1:A:418:ASN:O	1:A:420:PRO:HD3	1.67	0.93
1:A:358:ARG:NH2	1:A:514:GLU:N	2.18	0.92
1:A:417:VAL:HG12	1:A:419:THR:HG22	1.52	0.92
1:A:228:LEU:CD2	1:A:228:LEU:H	1.80	0.92
1:A:499:SER:HB2	1:A:502:ALA:HB3	1.51	0.92
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.69	0.91
1:A:356:ARG:HH12	1:A:374:LYS:HZ3	1.16	0.90
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.54	0.90
1:A:358:ARG:HH22	1:A:514:GLU:N	1.67	0.90
1:A:75:VAL:HG12	1:A:76:ASP:H	1.32	0.90
1:A:120:LEU:HD12	1:A:121:ASP:H	1.33	0.90
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.52	0.89
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.54	0.89
1:A:356:ARG:HH22	1:A:374:LYS:NZ	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:HB3	1:A:450:THR:HG23	1.54	0.89
1:A:46:LYS:HE3	1:A:116:PHE:CD2	2.08	0.89
1:A:130:PHE:HB2	1:A:144:TYR:H	1.38	0.88
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.08	0.88
1:A:41:MET:HG2	1:A:46:LYS:CD	2.04	0.87
1:A:228:LEU:HD23	1:A:228:LEU:N	1.90	0.86
1:A:356:ARG:HH22	1:A:374:LYS:HZ1	1.20	0.84
1:A:47:ILE:HG23	1:A:145:GLN:O	1.78	0.84
1:A:47:ILE:CG2	1:A:144:TYR:HB3	2.08	0.83
1:A:47:ILE:HG22	1:A:48:SER:N	1.92	0.83
1:A:57:ASN:HD22	1:A:58:THR:H	1.24	0.83
2:B:175:ASN:HD21	2:B:201:LYS:HZ1	1.28	0.82
1:A:523:GLU:HB3	1:A:527:LYS:NZ	1.94	0.81
1:A:130:PHE:CD1	1:A:144:TYR:HB2	2.16	0.81
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.63	0.81
1:A:57:ASN:HD22	1:A:58:THR:N	1.79	0.80
1:A:390:LYS:HE2	1:A:415:GLU:OE2	1.82	0.80
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.63	0.79
2:B:98:ALA:HA	2:B:101:LYS:CD	2.12	0.79
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.18	0.79
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.46	0.78
1:A:41:MET:CB	1:A:47:ILE:HD13	2.11	0.78
2:B:109:LEU:HB2	2:B:187:LEU:HB3	1.63	0.78
1:A:296:THR:HG22	1:A:298:GLU:OE2	1.84	0.78
2:B:233:GLU:C	2:B:234:LEU:HD12	2.05	0.77
2:B:98:ALA:CA	2:B:101:LYS:HD3	2.12	0.76
2:B:119:PRO:HA	2:B:148:VAL:HA	1.67	0.76
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.13	0.76
1:A:75:VAL:HG12	1:A:76:ASP:N	2.00	0.76
1:A:358:ARG:HD3	1:A:512:GLN:HG3	1.66	0.76
2:B:163:SER:HA	2:B:166:LYS:HE2	1.67	0.75
1:A:370:GLU:O	1:A:374:LYS:HG3	1.86	0.75
1:A:210:LEU:CD1	1:A:215:THR:HA	2.16	0.74
2:B:242:GLN:HB2	2:B:430:GLU:OE1	1.87	0.74
1:A:283:LEU:O	1:A:286:THR:HG23	1.86	0.74
1:A:235:HIS:HB2	1:A:238:LYS:HG3	1.68	0.74
1:A:2:ILE:HD11	1:A:45:GLY:HA3	1.70	0.74
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.70	0.74
1:A:23:GLN:HG2	1:A:131:THR:CG2	2.18	0.74
2:B:89:GLU:O	2:B:89:GLU:HG2	1.87	0.74
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD13	1:A:73:LYS:HB2	1.68	0.73
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.70	0.73
1:A:56:TYR:O	1:A:129:ALA:HB3	1.88	0.73
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.89	0.73
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.70	0.73
2:B:239:TRP:HZ3	2:B:382:ILE:HD11	1.53	0.73
1:A:452:LEU:HA	1:A:469:LEU:O	1.87	0.73
2:B:206:ARG:O	2:B:210:LEU:HD13	1.88	0.72
1:A:356:ARG:HH22	1:A:374:LYS:CE	2.02	0.72
1:A:23:GLN:HG2	1:A:131:THR:HG21	1.71	0.72
2:B:31:ILE:O	2:B:35:VAL:HG23	1.90	0.72
1:A:57:ASN:ND2	1:A:58:THR:N	2.37	0.71
1:A:47:ILE:N	1:A:47:ILE:HD12	2.05	0.71
1:A:47:ILE:HG22	1:A:48:SER:H	1.53	0.71
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.70	0.71
1:A:125:ARG:HB3	1:A:146:TYR:O	1.91	0.71
1:A:243:PRO:HG3	1:A:313:PRO:CG	2.21	0.71
2:B:266:TRP:CD1	2:B:267:ALA:N	2.58	0.71
1:A:170:PRO:HG2	1:A:171:PHE:H	1.55	0.71
1:A:5:ILE:HD11	1:A:166:LYS:HE3	1.73	0.71
2:B:296:THR:HG22	2:B:298:GLU:OE1	1.91	0.71
1:A:465:LYS:NZ	1:A:488:ASP:OD2	2.24	0.71
1:A:39:THR:O	1:A:42:GLU:HG2	1.91	0.71
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.73	0.71
1:A:457:TYR:HE2	1:A:465:LYS:HD2	1.56	0.70
2:B:358:ARG:H	2:B:358:ARG:HD3	1.55	0.70
1:A:66:LYS:HD2	1:A:66:LYS:H	1.56	0.70
1:A:356:ARG:NH2	1:A:374:LYS:HZ1	1.89	0.70
1:A:120:LEU:HD12	1:A:121:ASP:N	2.07	0.70
2:B:332:GLN:HB2	2:B:336:GLN:HB3	1.73	0.70
1:A:451:LYS:HB3	1:A:472:THR:N	2.06	0.69
1:A:118:VAL:O	1:A:148:VAL:HG22	1.93	0.69
1:A:358:ARG:CD	1:A:512:GLN:HG3	2.21	0.69
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.22	0.69
1:A:485:ALA:O	1:A:489:SER:HB3	1.92	0.69
1:A:317:VAL:HG22	1:A:318:TYR:H	1.58	0.69
2:B:420:PRO:O	2:B:423:VAL:HG22	1.93	0.69
1:A:331:LYS:HG2	1:A:333:GLY:O	1.92	0.69
1:A:516:GLU:HG3	1:A:517:LEU:N	2.08	0.69
1:A:246:LEU:O	1:A:307:ARG:NH1	2.26	0.69
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:LEU:O	2:B:429:LEU:HD13	1.93	0.68
2:B:233:GLU:O	2:B:234:LEU:HD12	1.94	0.68
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.75	0.68
1:A:35:VAL:O	1:A:39:THR:HG23	1.93	0.68
1:A:114:ALA:HB1	1:A:160:PHE:HE2	1.59	0.67
2:B:194:GLU:HG2	2:B:195:ILE:N	2.07	0.67
2:B:296:THR:HG22	2:B:298:GLU:H	1.58	0.67
1:A:254:VAL:CG2	1:A:291:GLU:HB3	2.24	0.67
1:A:358:ARG:NH2	1:A:513:SER:C	2.47	0.67
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.09	0.67
1:A:435:VAL:HA	2:B:290:THR:HG21	1.76	0.67
2:B:11:LYS:O	2:B:85:GLN:HG2	1.95	0.67
1:A:109:LEU:N	1:A:109:LEU:HD12	2.09	0.67
1:A:90:VAL:O	1:A:91:GLN:HB2	1.94	0.67
2:B:281:LYS:O	2:B:284:ARG:HG2	1.94	0.67
1:A:546:GLU:HG3	1:A:547:GLN:NE2	2.09	0.67
1:A:132:ILE:HB	1:A:142:ILE:CG2	2.23	0.66
1:A:282:LEU:H	1:A:282:LEU:HD22	1.60	0.66
2:B:422:LEU:HD12	2:B:422:LEU:H	1.60	0.66
1:A:8:VAL:HG21	1:A:159:ILE:HG12	1.77	0.66
1:A:356:ARG:HH12	1:A:374:LYS:NZ	1.92	0.66
1:A:441:TYR:HA	1:A:496:VAL:HG22	1.77	0.66
1:A:362:THR:HG22	1:A:363:ASN:N	2.11	0.66
1:A:500:GLN:HE22	2:B:422:LEU:HD11	1.60	0.66
1:A:47:ILE:HG21	1:A:144:TYR:CB	2.25	0.66
1:A:418:ASN:C	1:A:420:PRO:HD3	2.15	0.66
1:A:460:ASN:HD21	1:A:461:ARG:NH1	1.94	0.66
1:A:451:LYS:HB3	1:A:472:THR:H	1.61	0.65
1:A:118:VAL:O	1:A:148:VAL:CG2	2.44	0.65
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.30	0.65
1:A:480:GLN:HE21	1:A:484:LEU:HG	1.61	0.65
2:B:173:LYS:O	2:B:176:PRO:HD3	1.96	0.65
2:B:389:PHE:HB3	2:B:391:LEU:HD21	1.79	0.65
1:A:188:TYR:HB3	3:A:999:FTC:C18	2.27	0.65
1:A:27:THR:O	1:A:31:ILE:HG12	1.95	0.65
1:A:491:LEU:HB3	1:A:529:GLU:CB	2.26	0.65
1:A:100:LEU:O	1:A:318:TYR:HB3	1.96	0.64
1:A:118:VAL:HB	1:A:149:LEU:HD13	1.78	0.64
1:A:518:VAL:O	1:A:522:ILE:HG13	1.97	0.64
1:A:254:VAL:HB	1:A:289:LEU:O	1.98	0.64
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.64
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.32	0.64
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.13	0.64
1:A:122:GLU:CD	1:A:122:GLU:H	2.02	0.64
1:A:366:LYS:O	1:A:369:THR:HB	1.98	0.64
1:A:356:ARG:NH2	1:A:374:LYS:NZ	2.46	0.64
1:A:31:ILE:HD12	1:A:133:PRO:O	1.97	0.64
1:A:500:GLN:NE2	2:B:422:LEU:HD11	2.12	0.64
1:A:362:THR:HG22	1:A:363:ASN:H	1.63	0.63
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.33	0.63
1:A:500:GLN:OE1	2:B:422:LEU:HD11	1.99	0.63
1:A:330:GLN:HG2	1:A:338:THR:OG1	1.97	0.63
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.34	0.63
1:A:451:LYS:O	1:A:471:ASP:N	2.30	0.63
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.29	0.63
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.34	0.63
1:A:513:SER:HB3	1:A:519:ASN:ND2	2.13	0.63
1:A:47:ILE:CG2	1:A:48:SER:N	2.59	0.63
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.79	0.63
1:A:37:ILE:O	1:A:40:GLU:HB3	1.99	0.62
1:A:210:LEU:C	1:A:212:TRP:H	2.03	0.62
2:B:239:TRP:CZ3	2:B:382:ILE:HD11	2.34	0.62
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.33	0.62
1:A:73:LYS:HD3	1:A:74:LEU:H	1.64	0.62
1:A:104:LYS:HD2	1:A:192:ASP:O	1.99	0.62
1:A:438:GLU:OE1	1:A:459:THR:HG21	1.98	0.62
1:A:181:CYS:HB2	2:B:138:GLU:OE2	1.99	0.62
1:A:332:GLN:HG3	1:A:338:THR:CG2	2.28	0.62
1:A:249:LYS:HB3	1:A:252:TRP:CE2	2.34	0.62
1:A:473:THR:O	1:A:477:THR:HG23	1.99	0.62
1:A:500:GLN:HE22	2:B:422:LEU:HD21	1.63	0.62
1:A:358:ARG:NH2	1:A:513:SER:HA	2.15	0.62
1:A:47:ILE:CG2	1:A:48:SER:H	2.12	0.62
2:B:179:VAL:HG12	2:B:190:GLY:O	2.00	0.62
1:A:254:VAL:HG23	1:A:291:GLU:HB3	1.80	0.62
1:A:60:VAL:HG12	1:A:60:VAL:O	2.00	0.62
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.81	0.62
1:A:228:LEU:HG	1:A:228:LEU:O	1.99	0.61
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.82	0.61
2:B:169:GLU:O	2:B:173:LYS:HG2	1.98	0.61
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLN:HE22	1:A:289:LEU:HD11	1.64	0.61
2:B:130:PHE:CE2	2:B:144:TYR:HB2	2.34	0.61
1:A:13:LYS:HE3	1:A:84:THR:O	2.00	0.61
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.30	0.61
2:B:120:LEU:HD23	2:B:121:ASP:N	2.15	0.61
1:A:38:CYS:SG	1:A:73:LYS:HE3	2.40	0.61
1:A:358:ARG:CZ	1:A:513:SER:HA	2.30	0.61
2:B:163:SER:O	2:B:167:ILE:HG13	2.01	0.61
1:A:254:VAL:HG21	1:A:288:ALA:O	2.00	0.61
1:A:407:GLN:HG3	2:B:393:ILE:HA	1.83	0.61
2:B:84:THR:HG21	2:B:153:TRP:NE1	2.16	0.61
1:A:75:VAL:CG1	1:A:76:ASP:H	2.10	0.60
2:B:368:LEU:O	2:B:371:ALA:HB3	2.01	0.60
1:A:270:ILE:HG22	1:A:314:VAL:HG21	1.84	0.60
1:A:474:ASN:O	1:A:477:THR:OG1	2.11	0.60
2:B:287:LYS:HD3	2:B:293:ILE:HD11	1.83	0.60
2:B:79:GLU:O	2:B:82:LYS:HB2	2.02	0.60
1:A:123:ASP:C	1:A:126:LYS:HD3	2.22	0.60
1:A:181:CYS:HB3	1:A:188:TYR:HB2	1.84	0.60
2:B:376:THR:O	2:B:380:ILE:HG12	2.02	0.60
2:B:376:THR:CG2	2:B:386:THR:HG22	2.31	0.60
1:A:235:HIS:HB2	1:A:238:LYS:O	2.01	0.59
1:A:451:LYS:O	1:A:471:ASP:HA	2.00	0.59
1:A:332:GLN:HG3	1:A:338:THR:HG23	1.83	0.59
1:A:517:LEU:O	1:A:520:GLN:HB2	2.01	0.59
1:A:122:GLU:N	1:A:122:GLU:OE1	2.35	0.59
1:A:295:LEU:HD13	1:A:299:ALA:CB	2.33	0.59
2:B:239:TRP:O	2:B:240:THR:HG23	2.02	0.59
1:A:312:GLU:HG3	1:A:312:GLU:O	2.02	0.58
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.85	0.58
1:A:225:PRO:HA	1:A:226:PRO:C	2.24	0.58
1:A:130:PHE:O	1:A:143:ARG:HG3	2.03	0.58
1:A:497:THR:O	1:A:535:TRP:HA	2.03	0.58
2:B:356:ARG:HH12	2:B:358:ARG:HA	1.68	0.58
1:A:36:GLU:O	1:A:36:GLU:HG2	2.03	0.58
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.84	0.58
2:B:266:TRP:NE1	2:B:426:TRP:CD2	2.71	0.58
2:B:78:ARG:O	2:B:82:LYS:HG3	2.03	0.58
1:A:500:GLN:NE2	2:B:422:LEU:HD21	2.19	0.58
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.38	0.58
1:A:495:ILE:O	1:A:533:LEU:HD23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.86	0.58
1:A:506:ILE:H	1:A:506:ILE:HD12	1.68	0.58
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.38	0.58
2:B:424:LYS:HD3	2:B:425:LEU:N	2.18	0.58
1:A:317:VAL:HG22	1:A:318:TYR:N	2.18	0.58
1:A:243:PRO:HG3	1:A:313:PRO:HG2	1.85	0.57
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.85	0.57
1:A:361:HIS:CD2	1:A:510:PRO:HB3	2.39	0.57
2:B:264:LEU:O	2:B:267:ALA:HB3	2.03	0.57
1:A:451:LYS:CB	1:A:471:ASP:HA	2.33	0.57
1:A:356:ARG:NH1	1:A:374:LYS:HZ3	1.95	0.57
1:A:47:ILE:H	1:A:47:ILE:HD12	1.68	0.57
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.87	0.57
1:A:27:THR:HG22	1:A:29:GLU:H	1.69	0.57
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.47	0.57
1:A:96:HIS:CD2	1:A:230:MET:HE1	2.40	0.57
2:B:153:TRP:O	2:B:157:PRO:HD3	2.04	0.57
2:B:168:LEU:O	2:B:172:ARG:HG3	2.05	0.57
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.87	0.57
1:A:480:GLN:HE22	1:A:483:TYR:HD2	1.53	0.57
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.69	0.57
2:B:191:SER:HB2	2:B:193:LEU:HD23	1.85	0.57
1:A:135:ILE:HD12	1:A:135:ILE:N	2.19	0.57
1:A:77:PHE:O	1:A:80:LEU:N	2.38	0.56
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.87	0.56
2:B:61:PHE:CD2	2:B:61:PHE:N	2.73	0.56
1:A:253:THR:O	1:A:257:ILE:HG12	2.06	0.56
2:B:72:ARG:HH22	2:B:409:THR:HG22	1.71	0.56
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.41	0.56
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.85	0.56
1:A:57:ASN:ND2	1:A:58:THR:H	1.96	0.56
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.41	0.56
1:A:12:LEU:O	1:A:13:LYS:C	2.44	0.56
1:A:94:ILE:HD12	1:A:94:ILE:N	2.20	0.56
1:A:42:GLU:HG3	1:A:43:LYS:H	1.71	0.55
1:A:282:LEU:N	1:A:282:LEU:HD22	2.22	0.55
1:A:7:THR:HG22	1:A:119:PRO:O	2.07	0.55
2:B:84:THR:OG1	2:B:154:LYS:HE2	2.06	0.55
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.42	0.55
2:B:60:VAL:HG11	2:B:130:PHE:CD1	2.42	0.55
2:B:380:ILE:O	2:B:384:GLY:HA2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PRO:HA	1:A:421:PRO:C	2.27	0.55
1:A:358:ARG:HD2	1:A:362:THR:HB	1.87	0.55
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.33	0.55
1:A:17:ASP:O	1:A:83:ARG:HD3	2.07	0.55
1:A:42:GLU:HG3	1:A:43:LYS:N	2.21	0.55
1:A:451:LYS:O	1:A:471:ASP:CA	2.55	0.55
2:B:66:LYS:HG3	2:B:407:GLN:NE2	2.22	0.55
1:A:506:ILE:O	1:A:507:GLN:C	2.45	0.55
2:B:106:VAL:O	2:B:234:LEU:HB2	2.07	0.55
1:A:132:ILE:O	1:A:142:ILE:HG21	2.07	0.55
1:A:506:ILE:N	1:A:506:ILE:HD12	2.22	0.55
1:A:308:GLU:O	1:A:311:LYS:HB2	2.07	0.55
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.42	0.55
1:A:517:LEU:HA	1:A:520:GLN:CG	2.35	0.55
1:A:179:VAL:HG11	3:A:999:FTC:H112	1.87	0.55
1:A:320:ASP:OD2	1:A:322:SER:HB3	2.07	0.55
1:A:130:PHE:O	1:A:131:THR:OG1	2.25	0.55
1:A:23:GLN:HG2	1:A:131:THR:HG22	1.89	0.55
1:A:310:LEU:N	1:A:310:LEU:HD12	2.22	0.55
1:A:306:ASN:O	1:A:310:LEU:HD13	2.06	0.55
2:B:360:ALA:O	2:B:362:THR:N	2.40	0.55
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.22	0.55
2:B:33:ALA:O	2:B:37:ILE:HG13	2.06	0.54
2:B:253:THR:O	2:B:257:ILE:HG12	2.08	0.54
2:B:380:ILE:O	2:B:384:GLY:CA	2.55	0.54
1:A:362:THR:HG23	1:A:366:LYS:CE	2.36	0.54
1:A:474:ASN:CG	1:A:475:GLN:N	2.60	0.54
2:B:358:ARG:HG2	2:B:358:ARG:HH11	1.72	0.54
2:B:113:ASP:O	2:B:114:ALA:C	2.45	0.54
2:B:120:LEU:HD22	2:B:121:ASP:O	2.08	0.54
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.43	0.54
1:A:48:SER:O	1:A:49:LYS:HB2	2.07	0.54
1:A:474:ASN:OD1	1:A:475:GLN:HG3	2.08	0.54
1:A:330:GLN:OE1	1:A:340:GLN:OE1	2.25	0.54
2:B:84:THR:HG22	2:B:124:PHE:HZ	1.73	0.53
2:B:423:VAL:O	2:B:427:TYR:HD2	1.91	0.53
1:A:246:LEU:C	1:A:307:ARG:NH1	2.62	0.53
2:B:52:PRO:HD2	2:B:53:GLU:OE2	2.07	0.53
1:A:116:PHE:O	1:A:148:VAL:HG21	2.09	0.53
1:A:120:LEU:CD1	1:A:121:ASP:H	2.13	0.53
1:A:111:VAL:O	1:A:111:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:HD21	2:B:201:LYS:HZ3	1.51	0.53
2:B:132:ILE:HB	2:B:142:ILE:HB	1.90	0.53
2:B:39:THR:O	2:B:43:LYS:HG2	2.08	0.53
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.90	0.53
1:A:39:THR:C	1:A:42:GLU:HG2	2.29	0.53
1:A:416:PHE:CD1	1:A:417:VAL:N	2.76	0.53
1:A:91:GLN:C	1:A:93:GLY:H	2.12	0.53
2:B:424:LYS:C	2:B:424:LYS:HD3	2.28	0.53
1:A:407:GLN:CG	2:B:393:ILE:HA	2.38	0.53
1:A:503:LEU:O	1:A:507:GLN:HB2	2.08	0.53
1:A:546:GLU:HG3	1:A:547:GLN:HE21	1.72	0.53
1:A:418:ASN:O	1:A:420:PRO:CD	2.51	0.53
1:A:519:ASN:N	1:A:519:ASN:HD22	2.04	0.53
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.91	0.53
1:A:124:PHE:O	1:A:125:ARG:C	2.47	0.53
1:A:60:VAL:HG11	1:A:73:LYS:NZ	2.24	0.53
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.89	0.53
2:B:380:ILE:O	2:B:384:GLY:N	2.42	0.52
1:A:260:LEU:O	1:A:264:LEU:HD23	2.10	0.52
1:A:243:PRO:HB3	1:A:313:PRO:HG3	1.92	0.52
1:A:460:ASN:HA	2:B:286:THR:O	2.10	0.52
1:A:31:ILE:HG21	1:A:134:SER:HA	1.92	0.52
1:A:499:SER:CB	1:A:502:ALA:HB3	2.34	0.52
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.45	0.52
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.74	0.52
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.92	0.52
1:A:344:GLU:O	1:A:347:LYS:HB2	2.10	0.52
1:A:295:LEU:HD13	1:A:299:ALA:HB3	1.91	0.52
1:A:463:ARG:C	1:A:464:GLN:HG3	2.29	0.52
1:A:46:LYS:CB	1:A:47:ILE:HD12	2.27	0.52
1:A:235:HIS:CD2	1:A:238:LYS:HE3	2.45	0.52
1:A:253:THR:HG23	1:A:256:ASP:OD1	2.09	0.52
1:A:536:VAL:HG23	1:A:542:ILE:HD13	1.91	0.52
1:A:324:ASP:O	1:A:343:GLN:HG2	2.10	0.52
1:A:241:VAL:O	1:A:243:PRO:N	2.43	0.52
2:B:85:GLN:HG3	2:B:85:GLN:O	2.08	0.52
1:A:168:LEU:C	1:A:170:PRO:HD2	2.30	0.52
1:A:522:ILE:O	1:A:526:ILE:HG13	2.09	0.52
1:A:358:ARG:HD2	1:A:362:THR:CB	2.40	0.51
1:A:358:ARG:NH2	1:A:513:SER:CA	2.72	0.51
1:A:500:GLN:CD	2:B:422:LEU:HD11	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HB3	1:A:197:GLN:HB3	1.92	0.51
2:B:325:LEU:HD12	2:B:343:GLN:HG2	1.91	0.51
1:A:516:GLU:O	1:A:519:ASN:HB2	2.09	0.51
1:A:516:GLU:O	1:A:520:GLN:HG2	2.10	0.51
2:B:199:ARG:O	2:B:203:GLU:HB2	2.10	0.51
1:A:489:SER:HB2	1:A:493:VAL:HG21	1.92	0.51
1:A:7:THR:HG21	1:A:120:LEU:O	2.11	0.51
2:B:193:LEU:N	2:B:193:LEU:HD22	2.26	0.51
1:A:47:ILE:HG21	1:A:144:TYR:CD2	2.46	0.51
2:B:389:PHE:HB3	2:B:391:LEU:CD2	2.40	0.51
2:B:264:LEU:O	2:B:267:ALA:N	2.44	0.51
2:B:241:VAL:C	2:B:242:GLN:OE1	2.49	0.51
1:A:296:THR:CG2	1:A:298:GLU:OE2	2.57	0.51
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.46	0.51
1:A:274:ILE:CD1	1:A:310:LEU:HD11	2.29	0.51
1:A:282:LEU:O	1:A:293:ILE:HD13	2.11	0.50
1:A:439:THR:O	1:A:459:THR:HA	2.10	0.50
1:A:344:GLU:HB2	1:A:347:LYS:HB2	1.93	0.50
1:A:194:GLU:HG2	1:A:195:ILE:N	2.26	0.50
1:A:356:ARG:HH22	1:A:374:LYS:HE3	1.77	0.50
1:A:447:ASN:CB	1:A:450:THR:HG23	2.36	0.50
1:A:345:PRO:O	1:A:346:PHE:HB2	2.11	0.50
1:A:60:VAL:CG1	1:A:73:LYS:NZ	2.75	0.50
1:A:296:THR:O	1:A:299:ALA:HB3	2.12	0.50
2:B:276:VAL:HG22	2:B:276:VAL:O	2.11	0.50
2:B:406:TRP:HZ2	2:B:410:TRP:O	1.95	0.50
1:A:17:ASP:OD2	1:A:18:GLY:N	2.44	0.50
1:A:451:LYS:HB2	1:A:471:ASP:HA	1.94	0.50
2:B:100:LEU:HD23	2:B:100:LEU:N	2.27	0.50
2:B:7:THR:HG23	2:B:7:THR:O	2.12	0.50
2:B:332:GLN:OE1	2:B:424:LYS:HE3	2.12	0.50
1:A:543:GLY:HA2	1:A:546:GLU:HG2	1.93	0.50
1:A:246:LEU:C	1:A:307:ARG:HH11	2.14	0.50
2:B:368:LEU:O	2:B:372:VAL:HG23	2.11	0.50
1:A:60:VAL:HG11	1:A:73:LYS:HZ1	1.76	0.50
1:A:90:VAL:O	1:A:91:GLN:CB	2.59	0.50
2:B:193:LEU:H	2:B:193:LEU:HD22	1.77	0.50
1:A:24:TRP:H	1:A:24:TRP:HD1	1.59	0.50
1:A:417:VAL:CG1	1:A:419:THR:HG22	2.35	0.49
2:B:171:PHE:CG	2:B:205:LEU:HD23	2.47	0.49
1:A:356:ARG:HG2	1:A:357:MET:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:PRO:O	2:B:346:PHE:HB2	2.12	0.49
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.47	0.49
2:B:168:LEU:C	2:B:172:ARG:HG3	2.33	0.49
2:B:423:VAL:O	2:B:427:TYR:CD2	2.66	0.49
2:B:326:ILE:HB	2:B:342:TYR:O	2.11	0.49
1:A:114:ALA:CB	1:A:160:PHE:CE2	2.95	0.49
2:B:205:LEU:C	2:B:205:LEU:HD13	2.33	0.49
1:A:500:GLN:HE22	2:B:422:LEU:CD1	2.24	0.49
1:A:111:VAL:O	1:A:114:ALA:HB2	2.13	0.49
1:A:34:LEU:HA	1:A:37:ILE:HG22	1.94	0.49
2:B:100:LEU:HD23	2:B:101:LYS:H	1.78	0.49
1:A:54:ASN:HD22	1:A:126:LYS:HB3	1.78	0.49
1:A:513:SER:HB3	1:A:519:ASN:HD21	1.76	0.49
1:A:210:LEU:HD12	1:A:215:THR:HA	1.91	0.49
1:A:63:ILE:HD12	1:A:64:LYS:H	1.78	0.49
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.12	0.49
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.13	0.48
2:B:118:VAL:HG13	2:B:119:PRO:HD2	1.95	0.48
2:B:296:THR:CG2	2:B:298:GLU:OE1	2.60	0.48
2:B:426:TRP:O	2:B:429:LEU:HB2	2.13	0.48
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.81	0.48
1:A:173:LYS:HD3	1:A:173:LYS:O	2.13	0.48
1:A:126:LYS:O	1:A:128:THR:N	2.46	0.48
1:A:282:LEU:CD2	1:A:282:LEU:H	2.26	0.48
2:B:296:THR:CG2	2:B:298:GLU:HB2	2.43	0.48
2:B:61:PHE:CE1	2:B:403:THR:HG22	2.47	0.48
1:A:46:LYS:HE3	1:A:116:PHE:CG	2.46	0.48
2:B:60:VAL:HG11	2:B:130:PHE:HD1	1.76	0.48
1:A:49:LYS:HA	1:A:144:TYR:HA	1.96	0.48
1:A:502:ALA:O	1:A:506:ILE:HD13	2.12	0.48
2:B:240:THR:O	2:B:350:LYS:HG3	2.12	0.48
2:B:183:TYR:O	2:B:186:ASP:HB2	2.14	0.48
1:A:301:LEU:O	1:A:301:LEU:HD23	2.14	0.48
1:A:113:ASP:O	1:A:113:ASP:OD1	2.32	0.48
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.28	0.48
2:B:371:ALA:O	2:B:372:VAL:C	2.52	0.48
1:A:329:ILE:HG22	1:A:330:GLN:N	2.28	0.48
1:A:376:THR:HG23	1:A:386:THR:HB	1.95	0.48
1:A:92:LEU:HD21	2:B:137:ASN:OD1	2.13	0.48
1:A:517:LEU:HA	1:A:520:GLN:HG3	1.95	0.48
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:HG22	1:A:294:PRO:O	2.14	0.48
1:A:246:LEU:HB2	1:A:307:ARG:HH11	1.78	0.48
1:A:396:GLU:O	1:A:400:THR:HG23	2.14	0.48
1:A:34:LEU:HD21	1:A:62:ALA:CB	2.35	0.48
1:A:447:ASN:HD22	1:A:448:ARG:N	2.11	0.48
2:B:154:LYS:O	2:B:157:PRO:HD2	2.13	0.48
1:A:111:VAL:HG22	1:A:185:ASP:O	2.13	0.48
1:A:279:LEU:O	1:A:280:CSD:C	2.62	0.48
1:A:465:LYS:O	1:A:466:VAL:HG23	2.14	0.48
1:A:258:GLN:HE22	1:A:289:LEU:CD1	2.26	0.48
1:A:500:GLN:HE22	2:B:422:LEU:CD2	2.26	0.48
2:B:28:GLU:O	2:B:31:ILE:N	2.47	0.47
2:B:63:ILE:H	2:B:63:ILE:HD13	1.78	0.47
1:A:394:GLN:HG2	1:A:396:GLU:OE2	2.13	0.47
2:B:370:GLU:O	2:B:373:GLN:HB2	2.14	0.47
1:A:358:ARG:HH22	1:A:514:GLU:CA	2.24	0.47
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.44	0.47
1:A:92:LEU:C	1:A:92:LEU:HD22	2.35	0.47
1:A:46:LYS:O	1:A:147:ASN:ND2	2.46	0.47
1:A:34:LEU:CD2	1:A:73:LYS:HA	2.44	0.47
2:B:254:VAL:HG21	2:B:287:LYS:HB2	1.96	0.47
1:A:37:ILE:HD13	1:A:73:LYS:N	2.30	0.47
1:A:536:VAL:CG2	1:A:542:ILE:HD13	2.44	0.47
2:B:175:ASN:ND2	2:B:201:LYS:HZ3	2.10	0.47
1:A:235:HIS:CG	1:A:238:LYS:HE3	2.49	0.47
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.97	0.47
1:A:2:ILE:HD11	1:A:45:GLY:CA	2.42	0.47
2:B:100:LEU:HA	2:B:103:LYS:HB2	1.96	0.47
2:B:66:LYS:HG3	2:B:407:GLN:CD	2.35	0.47
2:B:277:ARG:NE	2:B:277:ARG:HA	2.28	0.47
1:A:411:ILE:HG22	1:A:412:PRO:O	2.14	0.47
1:A:46:LYS:CE	1:A:116:PHE:CD2	2.90	0.47
1:A:77:PHE:O	1:A:79:GLU:N	2.47	0.47
2:B:278:GLN:HE21	2:B:278:GLN:CA	2.27	0.47
1:A:34:LEU:HD22	1:A:73:LYS:HG2	1.96	0.47
1:A:47:ILE:HG22	1:A:48:SER:O	2.14	0.47
1:A:19:PRO:O	1:A:56:TYR:HA	2.14	0.47
2:B:171:PHE:CD2	2:B:205:LEU:HD23	2.50	0.47
1:A:124:PHE:O	1:A:127:TYR:N	2.48	0.47
1:A:356:ARG:HB2	1:A:356:ARG:CZ	2.45	0.47
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:TYR:CE2	1:A:465:LYS:HD2	2.43	0.47
1:A:66:LYS:N	1:A:66:LYS:HD2	2.27	0.47
1:A:484:LEU:HD23	1:A:487:GLN:OE1	2.14	0.47
1:A:122:GLU:HA	1:A:125:ARG:NE	2.30	0.47
2:B:296:THR:HB	2:B:299:ALA:H	1.79	0.47
2:B:53:GLU:H	2:B:53:GLU:CD	2.18	0.47
1:A:244:ILE:HG12	1:A:245:VAL:N	2.29	0.46
1:A:474:ASN:CG	1:A:475:GLN:H	2.18	0.46
1:A:60:VAL:HG13	1:A:73:LYS:HZ3	1.80	0.46
1:A:481:ALA:O	1:A:484:LEU:HB2	2.14	0.46
1:A:234:LEU:HD12	3:A:999:FTC:HB1	1.96	0.46
1:A:257:ILE:O	1:A:261:VAL:HG23	2.14	0.46
2:B:72:ARG:HH21	2:B:151:GLN:NE2	2.13	0.46
1:A:463:ARG:O	1:A:464:GLN:HG3	2.15	0.46
1:A:499:SER:HB2	1:A:502:ALA:CB	2.35	0.46
2:B:278:GLN:HB3	2:B:299:ALA:HA	1.95	0.46
1:A:252:TRP:HB3	1:A:257:ILE:HD11	1.97	0.46
2:B:120:LEU:HD23	2:B:121:ASP:H	1.78	0.46
1:A:109:LEU:H	1:A:109:LEU:HD12	1.78	0.46
1:A:486:LEU:CB	1:A:524:GLN:HG2	2.43	0.46
1:A:493:VAL:HG12	1:A:494:ASN:N	2.31	0.46
1:A:126:LYS:C	1:A:128:THR:H	2.18	0.46
1:A:358:ARG:NH2	1:A:514:GLU:H	2.08	0.46
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.44	0.46
2:B:158:ALA:O	2:B:161:GLN:HB2	2.16	0.46
1:A:382:ILE:HG22	1:A:383:TRP:CE2	2.50	0.46
2:B:266:TRP:C	2:B:266:TRP:CD1	2.89	0.46
1:A:447:ASN:O	1:A:450:THR:O	2.33	0.46
1:A:295:LEU:HD13	1:A:299:ALA:HB1	1.97	0.46
2:B:185:ASP:N	2:B:185:ASP:OD2	2.49	0.46
1:A:253:THR:O	1:A:256:ASP:HB2	2.16	0.46
1:A:218:ASP:O	1:A:221:HIS:N	2.39	0.46
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.46	0.45
1:A:34:LEU:HA	1:A:37:ILE:CG2	2.45	0.45
2:B:198:HIS:O	2:B:201:LYS:N	2.49	0.45
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.51	0.45
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.68	0.45
1:A:508:ALA:O	1:A:509:GLN:C	2.55	0.45
1:A:27:THR:HG22	1:A:28:GLU:N	2.31	0.45
1:A:506:ILE:CD1	1:A:506:ILE:H	2.28	0.45
2:B:201:LYS:HA	2:B:201:LYS:HD2	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:HB3	1:A:45:GLY:H	1.48	0.45
1:A:329:ILE:O	1:A:392:PRO:HD3	2.17	0.45
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.97	0.45
1:A:191:SER:OG	1:A:198:HIS:ND1	2.43	0.45
2:B:374:LYS:O	2:B:378:GLU:HG3	2.17	0.45
1:A:361:HIS:NE2	1:A:508:ALA:HB1	2.31	0.45
2:B:395:LYS:HG2	2:B:399:GLU:OE2	2.17	0.45
1:A:122:GLU:CD	1:A:122:GLU:N	2.70	0.45
1:A:241:VAL:CG2	1:A:270:ILE:HD13	2.45	0.45
2:B:121:ASP:O	2:B:125:ARG:HG3	2.17	0.45
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.16	0.45
2:B:374:LYS:O	2:B:377:THR:HB	2.15	0.45
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.45	0.45
1:A:456:GLY:HA3	1:A:466:VAL:HG22	1.97	0.45
1:A:248:GLU:OE2	1:A:307:ARG:NH2	2.50	0.45
2:B:63:ILE:O	2:B:72:ARG:HB3	2.17	0.45
1:A:358:ARG:HD2	1:A:362:THR:OG1	2.16	0.45
2:B:195:ILE:HA	2:B:198:HIS:HB3	1.99	0.45
2:B:162:SER:OG	2:B:163:SER:N	2.50	0.45
2:B:53:GLU:O	2:B:55:PRO:HD3	2.16	0.45
1:A:47:ILE:CD1	1:A:47:ILE:N	2.77	0.45
1:A:489:SER:CB	1:A:493:VAL:HG21	2.47	0.45
1:A:169:GLU:N	1:A:170:PRO:HD2	2.31	0.45
1:A:376:THR:O	1:A:380:ILE:HD12	2.17	0.45
2:B:317:VAL:O	2:B:317:VAL:HG23	2.16	0.45
1:A:40:GLU:O	1:A:42:GLU:N	2.50	0.45
1:A:356:ARG:CZ	1:A:356:ARG:CB	2.94	0.45
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.73	0.45
2:B:115:TYR:HE1	2:B:157:PRO:HA	1.81	0.44
1:A:228:LEU:CD2	1:A:228:LEU:N	2.60	0.44
1:A:332:GLN:HG3	1:A:338:THR:HG21	1.98	0.44
1:A:96:HIS:NE2	1:A:350:LYS:HE2	2.32	0.44
2:B:106:VAL:HG22	2:B:190:GLY:HA3	2.00	0.44
1:A:23:GLN:OE1	1:A:133:PRO:HG3	2.17	0.44
1:A:184:MET:HB3	1:A:185:ASP:H	1.41	0.44
1:A:2:ILE:HG22	1:A:3:SER:N	2.33	0.44
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.47	0.44
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.99	0.44
1:A:423:VAL:O	1:A:423:VAL:CG2	2.65	0.44
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.99	0.44
1:A:129:ALA:HA	1:A:144:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:THR:OG1	1:A:473:THR:N	2.50	0.44
1:A:287:LYS:HG3	1:A:288:ALA:N	2.33	0.44
1:A:405:TYR:HE2	1:A:407:GLN:HB3	1.80	0.44
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.53	0.44
2:B:398:TRP:O	2:B:402:TRP:HD1	2.01	0.44
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.99	0.44
1:A:46:LYS:HB3	1:A:47:ILE:CD1	2.29	0.44
1:A:311:LYS:O	1:A:313:PRO:HD3	2.18	0.44
2:B:208:HIS:O	2:B:211:ARG:HB3	2.18	0.44
1:A:477:THR:O	1:A:480:GLN:HB3	2.16	0.44
2:B:13:LYS:HG2	2:B:85:GLN:HA	1.99	0.44
1:A:130:PHE:HB2	1:A:144:TYR:N	2.20	0.44
2:B:296:THR:HG21	2:B:298:GLU:HB2	2.00	0.44
1:A:345:PRO:C	1:A:346:PHE:HD1	2.21	0.44
1:A:366:LYS:HE2	1:A:366:LYS:HB3	1.81	0.44
1:A:309:ILE:C	1:A:311:LYS:H	2.20	0.44
1:A:210:LEU:C	1:A:212:TRP:N	2.70	0.44
1:A:452:LEU:HD12	1:A:469:LEU:O	2.18	0.44
1:A:543:GLY:O	1:A:545:ASN:N	2.48	0.44
1:A:124:PHE:O	1:A:126:LYS:N	2.51	0.44
1:A:390:LYS:HE2	1:A:415:GLU:CD	2.39	0.43
1:A:170:PRO:CG	1:A:171:PHE:H	2.27	0.43
1:A:247:PRO:C	1:A:307:ARG:HH12	2.22	0.43
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.83	0.43
2:B:167:ILE:O	2:B:208:HIS:NE2	2.40	0.43
1:A:451:LYS:HA	1:A:472:THR:O	2.18	0.43
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.53	0.43
2:B:399:GLU:HA	2:B:402:TRP:HD1	1.83	0.43
1:A:114:ALA:O	1:A:118:VAL:HG23	2.17	0.43
1:A:310:LEU:CD1	1:A:310:LEU:N	2.81	0.43
1:A:243:PRO:CG	1:A:313:PRO:HG2	2.48	0.43
1:A:515:SER:CB	1:A:518:VAL:HG23	2.48	0.43
1:A:218:ASP:O	1:A:222:GLN:HG3	2.18	0.43
1:A:517:LEU:HA	1:A:520:GLN:HG2	1.98	0.43
2:B:358:ARG:HG2	2:B:358:ARG:NH1	2.33	0.43
1:A:358:ARG:CZ	1:A:513:SER:CA	2.95	0.43
1:A:419:THR:O	1:A:419:THR:HG23	2.19	0.43
1:A:58:THR:HG22	1:A:76:ASP:O	2.19	0.43
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.91	0.43
1:A:460:ASN:HD21	1:A:461:ARG:HH11	1.66	0.43
1:A:447:ASN:C	1:A:447:ASN:HD22	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ILE:HG12	2:B:189:VAL:HG13	2.00	0.43
1:A:237:ASP:OD2	1:A:237:ASP:N	2.51	0.43
1:A:77:PHE:HD2	1:A:80:LEU:CD2	2.31	0.43
2:B:263:LYS:O	2:B:266:TRP:HD1	2.02	0.43
1:A:64:LYS:HB2	1:A:66:LYS:NZ	2.34	0.43
1:A:77:PHE:O	1:A:78:ARG:C	2.57	0.43
2:B:120:LEU:CD2	2:B:121:ASP:N	2.81	0.43
1:A:201:LYS:HD3	1:A:204:GLU:OE1	2.19	0.43
1:A:203:GLU:O	1:A:204:GLU:C	2.56	0.43
1:A:118:VAL:CG1	1:A:119:PRO:HD2	2.49	0.43
2:B:100:LEU:N	2:B:100:LEU:CD2	2.82	0.43
1:A:361:HIS:HE2	1:A:508:ALA:HB1	1.83	0.43
2:B:264:LEU:O	2:B:265:ASN:C	2.57	0.43
2:B:211:ARG:HH11	2:B:211:ARG:HG3	1.83	0.43
1:A:255:ASN:HB2	1:A:289:LEU:HG	2.01	0.43
2:B:165:THR:OG1	2:B:166:LYS:N	2.52	0.43
2:B:84:THR:HG22	2:B:124:PHE:CZ	2.54	0.42
2:B:206:ARG:HG2	2:B:206:ARG:NH1	2.34	0.42
2:B:366:LYS:HG2	2:B:370:GLU:OE2	2.18	0.42
1:A:85:GLN:HG3	1:A:86:ASP:N	2.33	0.42
1:A:125:ARG:O	1:A:126:LYS:C	2.57	0.42
1:A:523:GLU:HB3	1:A:527:LYS:HZ3	1.78	0.42
2:B:209:LEU:C	2:B:211:ARG:N	2.71	0.42
2:B:188:TYR:CE1	2:B:380:ILE:HG21	2.54	0.42
2:B:184:MET:HB3	2:B:185:ASP:H	1.65	0.42
2:B:401:TRP:HB3	2:B:405:TYR:HE1	1.84	0.42
2:B:267:ALA:O	2:B:269:GLN:N	2.51	0.42
1:A:332:GLN:HB3	1:A:332:GLN:HE21	1.47	0.42
2:B:193:LEU:H	2:B:193:LEU:CD2	2.32	0.42
2:B:314:VAL:HG22	2:B:315:HIS:N	2.34	0.42
1:A:41:MET:CB	1:A:47:ILE:CD1	2.76	0.42
1:A:362:THR:HG23	1:A:366:LYS:HE3	2.02	0.42
1:A:493:VAL:CG1	1:A:494:ASN:N	2.83	0.42
2:B:72:ARG:NH2	2:B:409:THR:HG22	2.34	0.42
2:B:57:ASN:HD21	2:B:131:THR:N	2.18	0.42
1:A:505:ILE:O	1:A:510:PRO:HD3	2.20	0.42
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.50	0.42
1:A:124:PHE:C	1:A:126:LYS:N	2.72	0.42
1:A:516:GLU:CG	1:A:517:LEU:N	2.79	0.42
2:B:120:LEU:HD21	2:B:124:PHE:HB3	2.00	0.42
1:A:91:GLN:O	1:A:93:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:HB1	1:A:143:ARG:NH2	2.34	0.42
1:A:358:ARG:HD2	1:A:512:GLN:HG3	2.01	0.42
1:A:356:ARG:NH1	1:A:374:LYS:NZ	2.61	0.42
1:A:260:LEU:HD23	1:A:279:LEU:HD13	2.01	0.42
2:B:353:LYS:HG2	2:B:354:TYR:N	2.34	0.42
1:A:34:LEU:O	1:A:37:ILE:HG22	2.20	0.42
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.20	0.42
1:A:438:GLU:HG2	1:A:459:THR:HB	2.00	0.42
2:B:116:PHE:CE2	2:B:151:GLN:OE1	2.73	0.42
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.60	0.42
1:A:40:GLU:O	1:A:41:MET:C	2.58	0.42
1:A:243:PRO:CG	1:A:313:PRO:CG	2.95	0.42
2:B:259:LYS:O	2:B:260:LEU:C	2.58	0.42
1:A:122:GLU:HA	1:A:125:ARG:HE	1.83	0.42
1:A:491:LEU:HD12	1:A:491:LEU:N	2.34	0.42
1:A:296:THR:HB	1:A:299:ALA:H	1.83	0.42
2:B:171:PHE:HZ	2:B:201:LYS:HG3	1.85	0.41
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.50	0.41
1:A:402:TRP:HB2	1:A:409:THR:CG2	2.50	0.41
1:A:492:GLU:HA	1:A:530:LYS:O	2.20	0.41
1:A:118:VAL:O	1:A:149:LEU:HD13	2.19	0.41
1:A:170:PRO:HG2	1:A:171:PHE:N	2.28	0.41
1:A:179:VAL:CG1	3:A:999:FTC:H112	2.49	0.41
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.56	0.41
1:A:325:LEU:HD22	1:A:341:ILE:CG2	2.51	0.41
1:A:376:THR:HG22	1:A:380:ILE:CD1	2.50	0.41
1:A:130:PHE:O	1:A:143:ARG:NH1	2.53	0.41
1:A:358:ARG:NH2	1:A:359:GLY:O	2.48	0.41
2:B:422:LEU:HD12	2:B:422:LEU:N	2.33	0.41
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.50	0.41
2:B:185:ASP:HB2	2:B:409:THR:HG21	2.02	0.41
1:A:358:ARG:HD3	1:A:512:GLN:HE21	1.85	0.41
2:B:160:PHE:O	2:B:161:GLN:C	2.59	0.41
1:A:229:TRP:C	1:A:231:GLY:H	2.23	0.41
1:A:18:GLY:HA2	1:A:19:PRO:HD3	1.94	0.41
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.20	0.41
1:A:77:PHE:HD2	1:A:80:LEU:HD23	1.84	0.41
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.35	0.41
1:A:410:TRP:CG	1:A:411:ILE:N	2.89	0.41
1:A:41:MET:SD	1:A:47:ILE:HD11	2.60	0.41
1:A:362:THR:CG2	1:A:363:ASN:N	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:CZ	1:A:513:SER:C	2.89	0.41
1:A:447:ASN:O	1:A:448:ARG:C	2.59	0.41
1:A:279:LEU:CA	1:A:282:LEU:HD23	2.43	0.41
1:A:241:VAL:O	1:A:242:GLN:C	2.60	0.41
2:B:164:MET:O	2:B:167:ILE:HB	2.21	0.41
1:A:477:THR:O	1:A:478:GLU:C	2.59	0.41
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.56	0.41
1:A:94:ILE:CD1	1:A:94:ILE:N	2.83	0.41
2:B:378:GLU:O	2:B:379:SER:C	2.59	0.41
1:A:199:ARG:O	1:A:202:ILE:HB	2.20	0.41
2:B:392:PRO:HG2	2:B:392:PRO:O	2.21	0.41
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.51	0.41
1:A:210:LEU:HD11	1:A:215:THR:HB	2.02	0.41
2:B:139:THR:HG22	2:B:140:PRO:CD	2.50	0.41
1:A:359:GLY:C	1:A:361:HIS:H	2.24	0.40
1:A:246:LEU:H	1:A:246:LEU:HG	1.54	0.40
2:B:13:LYS:HG3	2:B:83:ARG:O	2.21	0.40
1:A:91:GLN:C	1:A:93:GLY:N	2.73	0.40
2:B:66:LYS:HB2	2:B:66:LYS:HE2	1.89	0.40
1:A:320:ASP:OD1	1:A:323:LYS:HG2	2.21	0.40
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.37	0.40
1:A:258:GLN:NE2	1:A:289:LEU:HD11	2.33	0.40
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.57	0.40
1:A:243:PRO:HG3	1:A:313:PRO:CB	2.50	0.40
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.52	0.40
2:B:109:LEU:N	2:B:187:LEU:O	2.44	0.40
1:A:205:LEU:O	1:A:205:LEU:HD12	2.22	0.40
2:B:175:ASN:C	2:B:177:ASP:H	2.24	0.40
1:A:79:GLU:O	1:A:80:LEU:C	2.60	0.40
1:A:305:GLU:O	1:A:309:ILE:HG12	2.22	0.40
2:B:10:VAL:HG12	2:B:11:LYS:N	2.37	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	528/560 (94%)	409 (78%)	89 (17%)	30 (6%)	2 12
2	B	396/440 (90%)	336 (85%)	49 (12%)	11 (3%)	6 30
All	All	924/1000 (92%)	745 (81%)	138 (15%)	41 (4%)	3 18

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	112	GLY
1	A	127	TYR
1	A	195	ILE
2	B	356	ARG
2	B	361	HIS
1	A	44	GLU
1	A	78	ARG
1	A	89	GLU
1	A	92	LEU
1	A	360	ALA
1	A	505	ILE
1	A	508	ALA
2	B	268	SER
2	B	358	ARG
2	B	382	ILE
1	A	41	MET
1	A	49	LYS
1	A	52	PRO
1	A	131	THR
1	A	451	LYS
1	A	85	GLN
1	A	310	LEU
1	A	313	PRO
1	A	420	PRO
1	A	487	GLN
2	B	162	SER
1	A	19	PRO
1	A	419	THR
1	A	489	SER
1	A	543	GLY
2	B	240	THR
2	B	310	LEU

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Mol	Chain	Res	Type
2	B	371	ALA
2	B	423	VAL
1	A	25	PRO
1	A	157	PRO
1	A	311	LYS
2	B	170	PRO
1	A	542	ILE
1	A	276	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	477/499 (96%)	429 (90%)	48 (10%)	9 34
2	B	366/400 (92%)	341 (93%)	25 (7%)	20 56
All	All	843/899 (94%)	770 (91%)	73 (9%)	13 43

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

Mol	Chain	Res	Type
1	A	16	MET
1	A	23	GLN
1	A	24	TRP
1	A	36	GLU
1	A	44	GLU
1	A	57	ASN
1	A	63	ILE
1	A	89	GLU
1	A	92	LEU
1	A	107	THR
1	A	108	VAL
1	A	109	LEU
1	A	122	GLU
1	A	151	GLN
1	A	184	MET

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Mol	Chain	Res	Type
1	A	187	LEU
1	A	194	GLU
1	A	197	GLN
1	A	215	THR
1	A	216	THR
1	A	218	ASP
1	A	219	LYS
1	A	240	THR
1	A	295	LEU
1	A	296	THR
1	A	330	GLN
1	A	332	GLN
1	A	336	GLN
1	A	340	GLN
1	A	356	ARG
1	A	357	MET
1	A	358	ARG
1	A	368	LEU
1	A	373	GLN
1	A	386	THR
1	A	394	GLN
1	A	417	VAL
1	A	418	ASN
1	A	423	VAL
1	A	432	GLU
1	A	447	ASN
1	A	450	THR
1	A	459	THR
1	A	488	ASP
1	A	533	LEU
1	A	536	VAL
1	A	537	PRO
1	A	545	ASN
2	B	24	TRP
2	B	53	GLU
2	B	61	PHE
2	B	63	ILE
2	B	89	GLU
2	B	100	LEU
2	B	120	LEU
2	B	161	GLN
2	B	185	ASP

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Mol	Chain	Res	Type
2	B	203	GLU
2	B	239	TRP
2	B	242	GLN
2	B	247	PRO
2	B	250	ASP
2	B	266	TRP
2	B	283	LEU
2	B	284	ARG
2	B	303	LEU
2	B	336	GLN
2	B	358	ARG
2	B	368	LEU
2	B	379	SER
2	B	422	LEU
2	B	424	LYS
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	222	GLN
1	A	235	HIS
1	A	258	GLN
1	A	278	GLN
1	A	332	GLN
1	A	334	GLN
1	A	340	GLN
1	A	394	GLN
1	A	418	ASN
1	A	428	GLN
1	A	447	ASN
1	A	475	GLN
1	A	480	GLN
1	A	509	GLN
1	A	512	GLN
1	A	519	ASN
1	A	545	ASN

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Mol	Chain	Res	Type
1	A	547	GLN
2	B	57	ASN
2	B	96	HIS
2	B	151	GLN
2	B	174	GLN
2	B	175	ASN
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	394	GLN
2	B	428	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
1	CSD	A	280	1	3,7,8	1.17	0	3,8,10	5.71	2 (66%)

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
1	CSD	A	280	1	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	CSD	O-C-CA	-2.04	120.17	125.49
1	A	280	CSD	OD1-SG-CB	9.68	121.53	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	FTC	A	999	-	23,24,24	1.83	5 (21%)	29,31,31	2.00	11 (37%)

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	FTC	A	999	-	-	0/13/13/13	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FTC	C18-C13	2.19	1.41	1.38
3	A	999	FTC	C3-N2	2.34	1.39	1.34
3	A	999	FTC	C9-S9	2.39	1.73	1.68
3	A	999	FTC	C1-N2	3.07	1.39	1.34
3	A	999	FTC	C13-N14	4.96	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	FTC	C16-C15-N14	-4.48	118.78	123.90
3	A	999	FTC	C4-C3-N2	-2.25	119.53	122.32
3	A	999	FTC	C6-C1-N2	-2.22	118.86	122.49
3	A	999	FTC	S9-C9-N8	-2.09	117.87	124.22
3	A	999	FTC	O17-C17-C16	-2.05	119.73	124.01
3	A	999	FTC	C18-C13-N14	-2.01	118.26	122.89
3	A	999	FTC	N8-C9-N10	2.07	119.40	114.34
3	A	999	FTC	C1-N8-C9	2.15	133.25	130.72
3	A	999	FTC	N8-C1-N2	2.66	122.49	114.83
3	A	999	FTC	C15-N14-C13	4.08	123.67	117.73
3	A	999	FTC	C3-N2-C1	4.20	122.49	117.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	FTC	4	0

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	534/560 (95%)	-0.35	16 (2%) 54 25	36, 84, 140, 150	0
2	B	402/440 (91%)	-0.37	7 (1%) 73 45	37, 77, 136, 150	0
All	All	936/1000 (93%)	-0.36	23 (2%) 61 30	36, 81, 139, 150	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	LYS	4.8
1	A	29	GLU	4.4
2	B	67	ASP	3.8
2	B	190	GLY	3.8
1	A	73	LYS	3.4
1	A	52	PRO	3.1
2	B	432	GLU	2.7
1	A	358	ARG	2.7
2	B	213	GLY	2.7
1	A	541	GLY	2.6
1	A	28	GLU	2.6
1	A	43	LYS	2.4
2	B	7	THR	2.4
2	B	430	GLU	2.4
1	A	542	ILE	2.3
1	A	360	ALA	2.2
1	A	245	VAL	2.2
1	A	20	LYS	2.1
1	A	3	SER	2.1
1	A	448	ARG	2.1
1	A	470	THR	2.1
1	A	132	ILE	2.0
2	B	88	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	CSD	A	280	8/9	0.97	0.12	-	56,70,77,85	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	FTC	A	999	23/23	0.96	0.15	-0.14	66,72,78,82	0

6.5 Other polymers (i)

There are no such residues in this entry.