W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 12:16 pm GMT

PDB ID	:	3I0R
Title	:	crystal structure of HIV reverse transcriptase in complex with inhibitor 3
Authors	:	Yan, Y.; Prasad, S.
Deposited on	:	2009-06-25
Resolution	:	2.98 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.
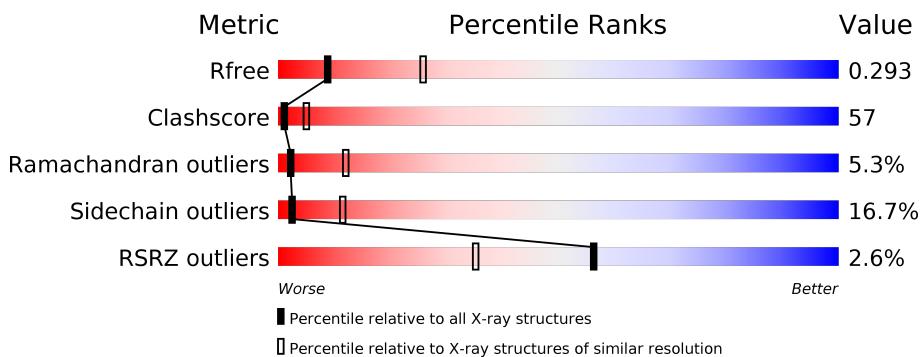
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
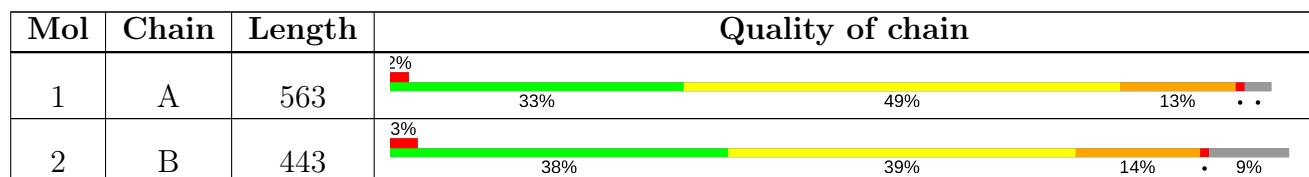
The reported resolution of this entry is 2.98 Å.

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	Percentile Ranks	Value
Rfree		0.293
Clashscore		57
Ramachandran outliers		5.3%
Sidechain outliers		16.7%
RSRZ outliers		2.6%

Worse .... *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	2168 (3.00-2.96)
Clashscore	112137	2535 (3.00-2.96)
Ramachandran outliers	110173	2451 (3.00-2.96)
Sidechain outliers	110143	2454 (3.00-2.96)
RSRZ outliers	101464	2192 (3.00-2.96)

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	563	2% | 33% | 49% | 13% | · ·
2	B	443	3% | 38% | 39% | 14% | · | 9%

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	RT3	A	601	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7823 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/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total 4442	C 2874	N 741	O 819	S 8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P04585
A	-1	ASN	-	EXPRESSION TAG	UNP P04585
A	0	SER	-	EXPRESSION TAG	UNP P04585
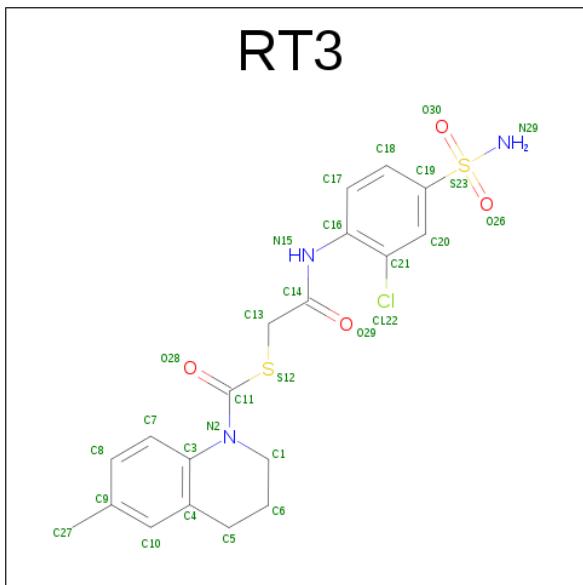
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total 3352	C 2182	N 555	O 609	S 6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP P04585
B	-1	ASN	-	EXPRESSION TAG	UNP P04585
B	0	SER	-	EXPRESSION TAG	UNP P04585

- Molecule 3 is S-{2-[(2-CHLORO-4-SULFAMOYLPHENYL)AMINO]-2-OXOETHYL} 6-METHYL-3,4-DIHYDROQUINOLINE-1(2H)-CARBOTHIOATE (three-letter code: RT3) (formula: $C_{19}H_{20}ClN_3O_4S_2$).

RT3
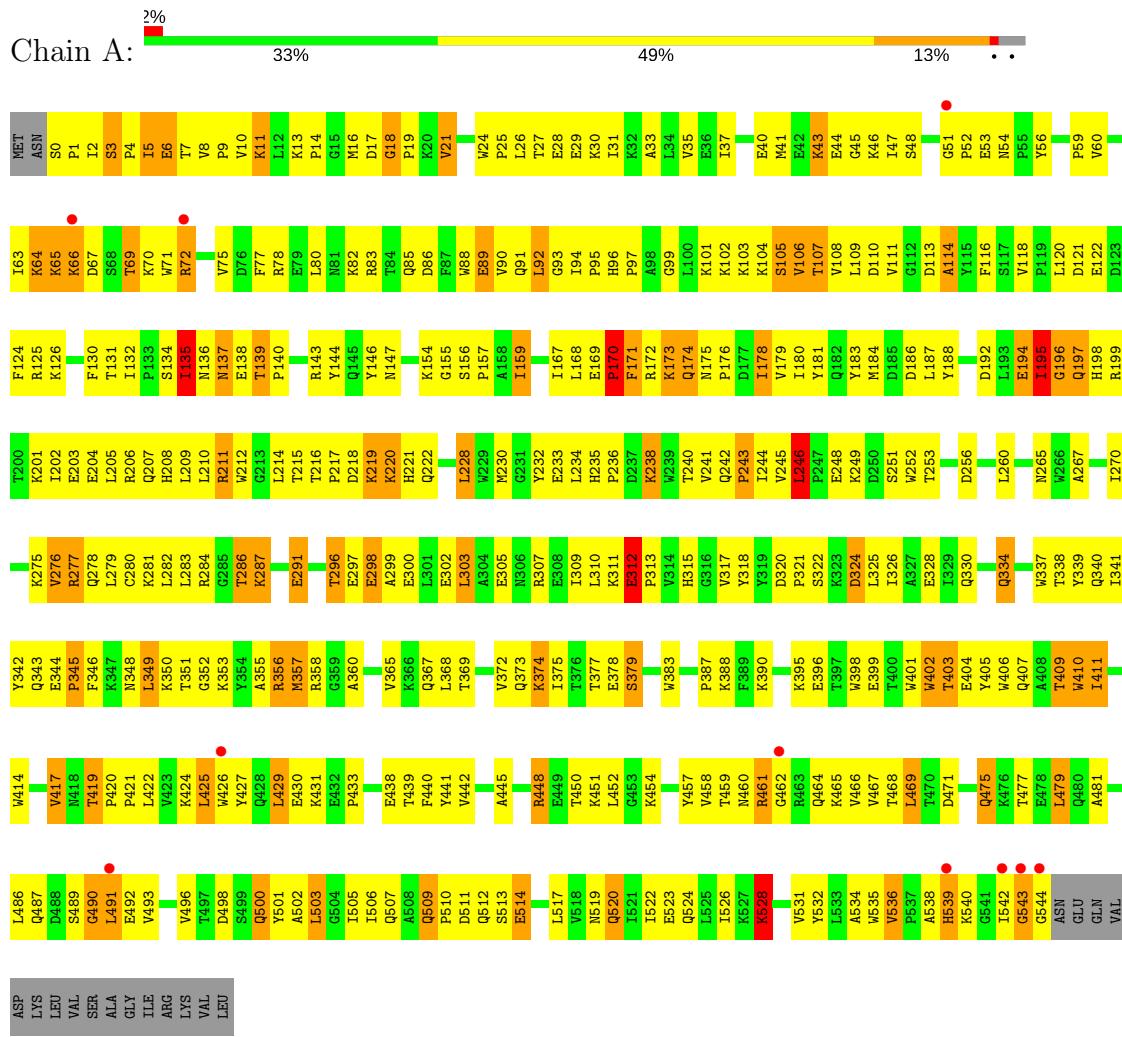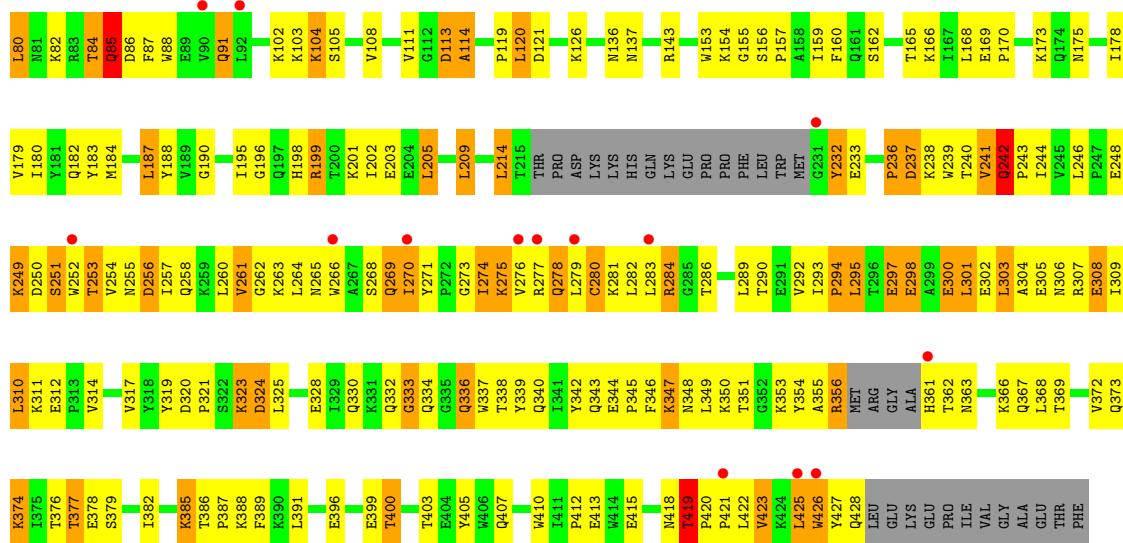
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
3	A	1	29	19	1	3	4	2	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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/ribonuclease H

• Molecule 2: p51 RT

L80 N81 K82 R83 T84 Q85 D86 F87 W88 E89 V90 Q91 L92 K102 K103 K104 S105 V108 V111 G112 D113 A114 P119 L120 D121 K126 N136 N137 R143 W153 K154 G155 S156 P157 A158 I159 F160 Q161 S162 T165 K166 I167 L168 E169 P170 K173 Q174 N175 I178

V179 I180 Y181 Q182 Y183 M184 L187 Y188 V189 G190 I195 G196 Q197 H198 R199 T200 K201 I202 E203 E204 L205 L209 L214 T215 THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET G231 Y232 E233 P236 D237 K238 W239 T240 V241 Q242 P243 I244 V245 L246 P247 E248

K249 D250 S251 W252 T253 V254 N255 D256 I257 Q258 K259 L260 V261 G262 K263 L264 N265 W266 A267 S268 Q269 I270 Y271 P272 G273 I274 K275 V276 R277 Q278 L279 C280 K281 L282 L283 R284 G285 T286 L289 T290 E291 V292 I293 P294 L295 T296 E297 E298 A299 E300 L301 E302 L303 A304 E305 N306 R307 E308 I309

L310 K311 E312 P313 V314 V317 Y318 Y319 D320 P321 S322 K323 D324 L325 E328 I329 Q330 K331 Q332 G333 Q334 G335 Q336 W337 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 K347 N348 L349 K350 T351 G352 K353 Y354 A355 R356 MET ARG GLY ALA H361 T362 N363 K366 Q367 L368 T369 V372 Q373

K374 I375 T376 T377 E378 S379 I382 K385 T386 P387 K388 F389 K390 L391 E396 E399 T400 T403 E404 Y405 W406 Q407 W410 I411 P412 E413 W414 E415 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427 Q428 LEU GLU LYS GLU PRO ILE VAL GLY ALA GLU THR PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.33Å 155.31Å 154.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.98 47.49 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.98) 99.3 (47.49-2.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.220 , 0.295 0.222 , 0.293	Depositor DCC
R_{free} test set	1494 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	76.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7823	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: RT3

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	0.60	0/4559	0.72	0/6196
2	B	0.63	1/3446 (0.0%)	0.72	0/4682
All	All	0.61	1/8005 (0.0%)	0.72	0/10878

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24	TRP	CB-CG	-5.02	1.41	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	HIS	Peptide

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	4442	0	4489	550	0
2	B	3352	0	3380	383	0
3	A	29	0	20	17	0
All	All	7823	0	7889	899	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 57.

All (899) 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:244:ILE:CD1	2:B:266:TRP:CZ3	2.03	1.41
2:B:244:ILE:CD1	2:B:266:TRP:CH2	2.21	1.23
1:A:1:PRO:O	1:A:2:ILE:HD13	1.36	1.21
1:A:206:ARG:NH2	1:A:218:ASP:HB3	1.57	1.19
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	1.69	1.18
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.21	1.17
2:B:244:ILE:CD1	2:B:266:TRP:HZ3	1.47	1.17
1:A:355:ALA:O	1:A:356:ARG:O	1.62	1.15
1:A:195:ILE:HD13	1:A:199:ARG:NH2	1.63	1.14
1:A:220:LYS:C	1:A:220:LYS:HD3	1.67	1.13
1:A:220:LYS:HE2	1:A:221:HIS:CE1	1.84	1.13
2:B:344:GLU:HB3	2:B:347:LYS:HE2	1.28	1.11
2:B:241:VAL:CG2	2:B:243:PRO:HD3	1.80	1.10
1:A:406:TRP:HZ2	2:B:418:ASN:OD1	1.34	1.10
2:B:66:LYS:HG3	2:B:407:GLN:HE22	1.10	1.09
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.22	1.09
2:B:244:ILE:HD12	2:B:266:TRP:HZ3	1.15	1.09
2:B:283:LEU:O	2:B:284:ARG:HG3	1.53	1.08
1:A:220:LYS:CE	1:A:221:HIS:CD2	2.37	1.08
1:A:107:THR:HG21	1:A:202:ILE:CD1	1.84	1.08
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.35	1.08
1:A:3:SER:OG	1:A:5:ILE:HG23	1.53	1.07
1:A:107:THR:HG21	1:A:202:ILE:HD11	1.14	1.07
1:A:194:GLU:H	1:A:194:GLU:CD	1.53	1.06
1:A:220:LYS:HE2	1:A:221:HIS:CG	1.90	1.06
1:A:406:TRP:CZ2	2:B:418:ASN:OD1	2.09	1.06
2:B:366:LYS:HD3	2:B:405:TYR:CE1	1.91	1.05
1:A:298:GLU:OE2	1:A:298:GLU:N	1.89	1.05
1:A:498:ASP:OD2	1:A:538:ALA:HB2	1.55	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.39	1.05
1:A:94:ILE:HD12	1:A:94:ILE:O	1.57	1.04
2:B:244:ILE:HD11	2:B:266:TRP:CH2	1.88	1.04
2:B:242:GLN:H	2:B:243:PRO:HD3	1.20	1.04
2:B:298:GLU:CD	2:B:298:GLU:H	1.53	1.04
1:A:197:GLN:OE1	1:A:197:GLN:N	1.90	1.03
1:A:489:SER:HB2	1:A:493:VAL:CG2	1.89	1.02
2:B:420:PRO:HG2	2:B:423:VAL:CG2	1.89	1.02
2:B:253:THR:HG22	2:B:255:ASN:N	1.74	1.01
1:A:3:SER:OG	1:A:5:ILE:CG2	2.10	1.00
2:B:253:THR:HG23	2:B:289:LEU:O	1.61	1.00
1:A:220:LYS:HE2	1:A:221:HIS:ND1	1.77	1.00
1:A:107:THR:CG2	1:A:202:ILE:HD11	1.91	0.99
2:B:344:GLU:HB3	2:B:347:LYS:CE	1.92	0.99
2:B:268:SER:O	2:B:269:GLN:HB2	1.58	0.98
2:B:271:TYR:HB3	2:B:274:ILE:HD11	1.46	0.98
2:B:244:ILE:HD12	2:B:266:TRP:CZ3	1.88	0.98
1:A:27:THR:O	1:A:31:ILE:HG13	1.63	0.98
2:B:420:PRO:HG2	2:B:423:VAL:HG21	1.46	0.97
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	1.99	0.97
2:B:260:LEU:CD1	2:B:264:LEU:CD1	2.42	0.97
2:B:241:VAL:HG23	2:B:243:PRO:HD3	1.44	0.96
1:A:460:ASN:HB2	2:B:286:THR:O	1.64	0.95
1:A:175:ASN:HB3	1:A:178:ILE:CD1	1.95	0.95
2:B:260:LEU:HD13	2:B:264:LEU:HD12	1.48	0.95
1:A:220:LYS:CE	1:A:221:HIS:NE2	2.31	0.94
1:A:296:THR:HG22	1:A:299:ALA:H	1.31	0.94
1:A:277:ARG:HH12	1:A:334:GLN:HE21	0.97	0.94
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.46	0.94
1:A:220:LYS:HE3	1:A:221:HIS:CD2	2.02	0.94
2:B:66:LYS:HG3	2:B:407:GLN:NE2	1.82	0.94
1:A:51:GLY:HA3	1:A:53:GLU:OE1	1.65	0.93
2:B:65:LYS:HA	2:B:407:GLN:HG2	1.50	0.93
2:B:356:ARG:HH11	2:B:356:ARG:HB2	1.30	0.93
1:A:277:ARG:NH1	1:A:334:GLN:HE21	1.67	0.92
1:A:372:VAL:HG11	1:A:411:ILE:CG2	1.99	0.92
2:B:420:PRO:CG	2:B:423:VAL:HG21	1.99	0.92
1:A:199:ARG:O	1:A:203:GLU:HG2	1.70	0.92
2:B:242:GLN:H	2:B:243:PRO:CD	1.83	0.92
1:A:10:VAL:O	1:A:11:LYS:HG2	1.69	0.92
1:A:220:LYS:HE3	1:A:221:HIS:NE2	1.85	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:GLU:HA	2:B:300:GLU:HB2	1.49	0.91
1:A:194:GLU:N	1:A:194:GLU:OE1	2.03	0.91
2:B:298:GLU:N	2:B:298:GLU:CD	2.22	0.91
2:B:260:LEU:CD1	2:B:264:LEU:HD11	2.00	0.91
2:B:373:GLN:NE2	2:B:407:GLN:H	1.69	0.91
2:B:244:ILE:HD11	2:B:266:TRP:HH2	1.26	0.91
1:A:433:PRO:HB2	2:B:290:THR:HG22	1.52	0.91
1:A:543:GLY:HA2	2:B:284:ARG:CA	2.00	0.91
1:A:195:ILE:HG23	1:A:199:ARG:NE	1.87	0.90
2:B:373:GLN:HE22	2:B:407:GLN:H	1.07	0.90
2:B:373:GLN:O	2:B:377:THR:HG22	1.70	0.90
1:A:233:GLU:HG2	1:A:235:HIS:CE1	2.07	0.89
2:B:244:ILE:HD13	2:B:266:TRP:CH2	1.95	0.89
2:B:356:ARG:HH11	2:B:356:ARG:CB	1.86	0.89
1:A:220:LYS:CE	1:A:221:HIS:CE1	2.55	0.89
2:B:271:TYR:O	2:B:274:ILE:HG12	1.73	0.88
1:A:220:LYS:HE2	1:A:221:HIS:CD2	2.01	0.88
1:A:183:TYR:CZ	1:A:230:MET:HE3	2.09	0.88
2:B:268:SER:HB3	2:B:274:ILE:HB	1.55	0.88
1:A:357:MET:HG2	1:A:357:MET:O	1.74	0.88
2:B:160:PHE:CD2	2:B:160:PHE:O	2.27	0.87
1:A:173:LYS:CE	1:A:173:LYS:HA	2.05	0.87
3:A:601:RT3:H7	3:A:601:RT3:O28	1.71	0.87
1:A:220:LYS:HD3	1:A:221:HIS:N	1.89	0.87
2:B:11:LYS:HB3	2:B:11:LYS:NZ	1.89	0.87
1:A:228:LEU:CD2	1:A:228:LEU:N	2.37	0.87
2:B:253:THR:HG22	2:B:255:ASN:H	1.38	0.86
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.57	0.86
2:B:236:PRO:O	2:B:238:LYS:N	2.08	0.86
1:A:186:ASP:O	1:A:187:LEU:HD23	1.74	0.86
1:A:489:SER:HB2	1:A:493:VAL:HG21	1.58	0.86
2:B:270:ILE:HB	2:B:346:PHE:O	1.74	0.86
1:A:489:SER:CB	1:A:493:VAL:HG21	2.06	0.85
1:A:206:ARG:HH22	1:A:218:ASP:HB3	1.37	0.85
1:A:498:ASP:OD2	1:A:538:ALA:CB	2.25	0.85
2:B:308:GLU:O	2:B:311:LYS:HG2	1.78	0.84
1:A:287:LYS:HD3	1:A:291:GLU:OE2	1.77	0.84
1:A:51:GLY:CA	1:A:53:GLU:OE1	2.26	0.83
1:A:433:PRO:HB2	2:B:290:THR:CG2	2.08	0.83
1:A:296:THR:CG2	1:A:299:ALA:H	1.92	0.83
1:A:103:LYS:O	3:A:601:RT3:H17	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:CD1	1:A:199:ARG:NH2	2.42	0.82
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.27	0.82
2:B:271:TYR:CB	2:B:274:ILE:HD11	2.08	0.82
2:B:283:LEU:O	2:B:284:ARG:CG	2.28	0.82
2:B:396:GLU:O	2:B:400:THR:HG22	1.78	0.82
1:A:206:ARG:NH2	1:A:218:ASP:CB	2.41	0.82
1:A:220:LYS:C	1:A:220:LYS:CD	2.43	0.82
2:B:260:LEU:CD1	2:B:264:LEU:HD12	2.05	0.82
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.61	0.81
1:A:194:GLU:N	1:A:194:GLU:CD	2.33	0.81
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.62	0.81
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.62	0.81
1:A:10:VAL:HG12	1:A:11:LYS:N	1.96	0.81
2:B:422:LEU:CD2	2:B:425:LEU:HD11	2.10	0.81
2:B:260:LEU:HD11	2:B:264:LEU:HD11	1.62	0.81
1:A:500:GLN:HG3	2:B:422:LEU:HD12	1.60	0.81
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.44	0.80
2:B:242:GLN:HG3	2:B:242:GLN:O	1.78	0.80
2:B:374:LYS:HD3	2:B:378:GLU:OE2	1.81	0.80
2:B:257:ILE:O	2:B:261:VAL:HG12	1.79	0.80
2:B:260:LEU:HD13	2:B:264:LEU:CD1	2.06	0.80
2:B:420:PRO:CG	2:B:423:VAL:CG2	2.55	0.80
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.12	0.80
1:A:175:ASN:CB	1:A:178:ILE:HD12	2.11	0.80
2:B:344:GLU:CB	2:B:347:LYS:HD3	2.12	0.80
1:A:0:SER:CB	1:A:113:ASP:OD2	2.30	0.80
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.64	0.80
1:A:464:GLN:HG2	1:A:465:LYS:N	1.95	0.80
1:A:543:GLY:HA2	2:B:284:ARG:HA	1.63	0.79
1:A:233:GLU:C	1:A:234:LEU:HD23	2.02	0.79
1:A:303:LEU:O	1:A:307:ARG:HG3	1.82	0.79
2:B:65:LYS:CA	2:B:407:GLN:HG2	2.13	0.79
1:A:104:LYS:N	1:A:192:ASP:OD2	2.15	0.79
1:A:277:ARG:HH12	1:A:334:GLN:NE2	1.80	0.79
2:B:241:VAL:HG23	2:B:242:GLN:H	1.48	0.78
1:A:330:GLN:NE2	1:A:338:THR:HG23	1.98	0.78
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.18	0.78
1:A:93:GLY:HA3	2:B:137:ASN:ND2	1.98	0.78
2:B:373:GLN:O	2:B:377:THR:CG2	2.32	0.78
1:A:10:VAL:HG12	1:A:11:LYS:H	1.47	0.78
2:B:209:LEU:HB3	2:B:214:LEU:HB2	1.63	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:CZ3	2:B:363:ASN:HB3	2.19	0.78
1:A:194:GLU:O	1:A:196:GLY:N	2.17	0.77
1:A:195:ILE:HG23	1:A:199:ARG:CZ	2.15	0.77
2:B:366:LYS:CD	2:B:405:TYR:CD1	2.67	0.77
1:A:175:ASN:ND2	1:A:178:ILE:HD11	2.00	0.77
1:A:72:ARG:NH1	1:A:72:ARG:HB3	2.01	0.76
1:A:424:LYS:HE3	1:A:426:TRP:NE1	2.00	0.76
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.10	0.76
2:B:162:SER:O	2:B:166:LYS:HE3	1.85	0.76
1:A:197:GLN:CD	1:A:197:GLN:H	1.88	0.76
1:A:298:GLU:CD	1:A:298:GLU:H	1.87	0.76
1:A:95:PRO:HA	2:B:136:ASN:OD1	1.85	0.76
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.20	0.76
1:A:457:TYR:C	1:A:457:TYR:CD1	2.60	0.76
2:B:12:LEU:HD23	2:B:17:ASP:HA	1.68	0.75
2:B:209:LEU:HG	2:B:214:LEU:HD12	1.68	0.75
1:A:356:ARG:HH21	1:A:358:ARG:HG3	1.50	0.75
1:A:228:LEU:HD23	1:A:228:LEU:H	1.50	0.75
1:A:296:THR:HG22	1:A:299:ALA:N	2.01	0.75
1:A:475:GLN:HG2	1:A:501:TYR:CE2	2.21	0.75
1:A:210:LEU:O	1:A:212:TRP:N	2.20	0.75
2:B:253:THR:CG2	2:B:255:ASN:H	1.99	0.75
2:B:344:GLU:O	2:B:347:LYS:HD2	1.87	0.75
2:B:356:ARG:NH1	2:B:356:ARG:CB	2.50	0.75
1:A:210:LEU:C	1:A:212:TRP:H	1.89	0.75
2:B:268:SER:O	2:B:269:GLN:CB	2.35	0.74
1:A:220:LYS:HE2	1:A:221:HIS:NE2	1.96	0.74
2:B:241:VAL:CB	2:B:243:PRO:HD3	2.17	0.74
1:A:64:LYS:HD2	1:A:70:LYS:O	1.87	0.74
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.88	0.74
2:B:319:TYR:O	2:B:321:PRO:HD3	1.88	0.74
1:A:45:GLY:O	1:A:147:ASN:OD1	2.06	0.74
1:A:228:LEU:HD22	1:A:228:LEU:N	2.01	0.74
2:B:5:ILE:HD12	2:B:5:ILE:N	2.02	0.74
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.08	0.74
1:A:503:LEU:HD22	1:A:507:GLN:HG3	1.70	0.74
1:A:430:GLU:HG2	1:A:531:VAL:O	1.88	0.74
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.70	0.74
1:A:173:LYS:HE3	1:A:173:LYS:HA	1.68	0.73
1:A:403:THR:HG22	1:A:404:GLU:HG3	1.69	0.73
1:A:125:ARG:HD3	1:A:146:TYR:O	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.23	0.73
2:B:388:LYS:HE3	2:B:415:GLU:HG3	1.70	0.73
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.70	0.73
2:B:254:VAL:O	2:B:258:GLN:HG3	1.89	0.73
2:B:330:GLN:OE1	2:B:338:THR:OG1	2.07	0.73
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.54	0.73
2:B:298:GLU:HA	2:B:301:LEU:HD12	1.71	0.73
2:B:280:CYS:O	2:B:283:LEU:N	2.19	0.72
2:B:361:HIS:CD2	2:B:361:HIS:O	2.42	0.72
2:B:366:LYS:HD3	2:B:405:TYR:CD1	2.23	0.72
1:A:233:GLU:HG2	1:A:235:HIS:HE1	1.54	0.72
2:B:332:GLN:O	2:B:333:GLY:O	2.08	0.72
1:A:543:GLY:HA2	2:B:284:ARG:N	2.04	0.72
2:B:266:TRP:HE1	2:B:346:PHE:HE2	1.36	0.72
1:A:441:TYR:CD2	1:A:544:GLY:CA	2.73	0.72
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.71	0.72
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.71	0.72
1:A:10:VAL:O	1:A:11:LYS:CG	2.38	0.72
2:B:209:LEU:CD1	2:B:214:LEU:HD12	2.19	0.72
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.72	0.72
2:B:366:LYS:HD2	2:B:405:TYR:CD1	2.24	0.72
2:B:345:PRO:O	2:B:347:LYS:HD2	1.89	0.71
2:B:373:GLN:HE22	2:B:407:GLN:N	1.86	0.71
1:A:139:THR:HG22	1:A:140:PRO:CD	2.16	0.71
1:A:51:GLY:C	1:A:53:GLU:OE1	2.28	0.71
2:B:274:ILE:HA	2:B:306:ASN:HD21	1.55	0.71
2:B:422:LEU:HD22	2:B:425:LEU:HD11	1.73	0.71
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.70	0.71
3:A:601:RT3:C7	3:A:601:RT3:O28	2.38	0.71
2:B:239:TRP:O	2:B:240:THR:HG23	1.91	0.71
2:B:274:ILE:C	2:B:275:LYS:HG2	2.11	0.71
1:A:17:ASP:O	1:A:83:ARG:NH1	2.23	0.70
2:B:11:LYS:HB3	2:B:11:LYS:HZ3	1.54	0.70
2:B:344:GLU:HB3	2:B:347:LYS:CD	2.20	0.70
1:A:402:TRP:CD1	1:A:402:TRP:C	2.65	0.70
2:B:362:THR:HG23	2:B:366:LYS:HG2	1.71	0.70
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.26	0.70
1:A:468:THR:C	1:A:469:LEU:HG	2.10	0.70
1:A:173:LYS:CA	1:A:173:LYS:HE3	2.20	0.70
1:A:175:ASN:CB	1:A:178:ILE:CD1	2.66	0.70
1:A:175:ASN:HD21	1:A:201:LYS:CE	2.04	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:CE	1:A:221:HIS:CG	2.64	0.70
1:A:489:SER:OG	1:A:493:VAL:HG21	1.92	0.70
1:A:467:VAL:HG12	1:A:468:THR:N	2.07	0.70
1:A:64:LYS:O	1:A:65:LYS:CB	2.38	0.70
2:B:242:GLN:N	2:B:243:PRO:HD3	2.02	0.70
1:A:53:GLU:OE1	1:A:53:GLU:N	2.23	0.70
1:A:173:LYS:CA	1:A:173:LYS:CE	2.69	0.69
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.27	0.69
1:A:134:SER:OG	1:A:138:GLU:O	2.08	0.69
1:A:51:GLY:HA3	1:A:53:GLU:CD	2.13	0.69
2:B:250:ASP:O	2:B:251:SER:HB2	1.90	0.69
1:A:197:GLN:O	1:A:201:LYS:HB2	1.91	0.69
1:A:350:LYS:HE3	1:A:378:GLU:OE2	1.91	0.69
1:A:406:TRP:CH2	1:A:407:GLN:HB2	2.27	0.69
1:A:277:ARG:NH1	1:A:334:GLN:NE2	2.40	0.69
1:A:195:ILE:CD1	1:A:199:ARG:HH21	2.04	0.69
2:B:253:THR:CG2	2:B:289:LEU:O	2.37	0.69
2:B:46:LYS:HA	2:B:46:LYS:HE2	1.74	0.69
1:A:64:LYS:O	1:A:65:LYS:HB2	1.92	0.69
1:A:369:THR:CG2	1:A:398:TRP:CZ3	2.75	0.69
1:A:500:GLN:CG	2:B:422:LEU:HD12	2.23	0.69
2:B:244:ILE:CD1	2:B:266:TRP:HH2	1.85	0.69
1:A:63:ILE:HD11	1:A:72:ARG:HD3	1.75	0.68
1:A:330:GLN:HE21	1:A:338:THR:HG23	1.58	0.68
2:B:241:VAL:O	2:B:242:GLN:CB	2.42	0.68
1:A:1:PRO:O	1:A:2:ILE:CD1	2.28	0.68
1:A:445:ALA:O	1:A:477:THR:HG21	1.93	0.68
2:B:243:PRO:HB3	2:B:311:LYS:HA	1.76	0.68
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.20	0.68
2:B:11:LYS:HG3	2:B:12:LEU:O	1.94	0.67
1:A:458:VAL:HG23	1:A:458:VAL:O	1.94	0.67
1:A:342:TYR:HA	1:A:349:LEU:CD1	2.23	0.67
1:A:406:TRP:CZ3	1:A:407:GLN:CB	2.76	0.67
2:B:366:LYS:CD	2:B:405:TYR:CE1	2.72	0.67
2:B:344:GLU:O	2:B:347:LYS:CD	2.42	0.67
2:B:356:ARG:NH1	2:B:356:ARG:HB3	2.10	0.67
1:A:2:ILE:HD12	1:A:116:PHE:O	1.95	0.67
2:B:308:GLU:HA	2:B:311:LYS:CE	2.25	0.67
1:A:175:ASN:ND2	1:A:201:LYS:CE	2.58	0.67
1:A:458:VAL:HG23	2:B:286:THR:HG21	1.76	0.67
2:B:420:PRO:HG2	2:B:423:VAL:CB	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:HB3	1:A:146:TYR:O	1.94	0.67
1:A:513:SER:N	1:A:519:ASN:HD21	1.94	0.66
1:A:360:ALA:HA	1:A:514:GLU:OE1	1.96	0.66
2:B:66:LYS:CG	2:B:407:GLN:NE2	2.55	0.66
1:A:82:LYS:HG2	1:A:82:LYS:O	1.95	0.66
1:A:410:TRP:CE3	2:B:363:ASN:CB	2.79	0.66
2:B:298:GLU:O	2:B:301:LEU:HB2	1.95	0.66
1:A:24:TRP:CD2	1:A:25:PRO:HD2	2.31	0.66
2:B:305:GLU:O	2:B:309:ILE:HG13	1.96	0.66
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.26	0.66
2:B:86:ASP:O	2:B:91:GLN:HB2	1.96	0.66
2:B:344:GLU:CB	2:B:347:LYS:CD	2.74	0.65
1:A:406:TRP:CE3	1:A:407:GLN:HB2	2.31	0.65
1:A:181:TYR:HB2	3:A:601:RT3:H15	1.79	0.65
2:B:241:VAL:HB	2:B:243:PRO:HD3	1.78	0.65
2:B:308:GLU:HA	2:B:311:LYS:HE2	1.79	0.65
1:A:460:ASN:CB	2:B:286:THR:O	2.43	0.65
1:A:369:THR:CG2	1:A:398:TRP:HZ3	2.10	0.65
1:A:43:LYS:HE2	1:A:43:LYS:HA	1.78	0.65
2:B:241:VAL:CG2	2:B:243:PRO:CD	2.67	0.65
1:A:24:TRP:CG	1:A:25:PRO:HD2	2.32	0.65
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.79	0.65
2:B:156:SER:N	2:B:157:PRO:HD2	2.12	0.65
1:A:173:LYS:N	1:A:173:LYS:HE3	2.11	0.64
1:A:175:ASN:HD21	1:A:201:LYS:NZ	1.95	0.64
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.78	0.64
1:A:406:TRP:CE3	1:A:407:GLN:CA	2.81	0.64
2:B:425:LEU:O	2:B:428:GLN:N	2.29	0.64
1:A:105:SER:OG	1:A:198:HIS:CD2	2.50	0.64
1:A:195:ILE:HD13	1:A:199:ARG:HH22	1.60	0.64
1:A:173:LYS:HE2	1:A:173:LYS:HA	1.78	0.64
2:B:303:LEU:HD22	2:B:307:ARG:NH2	2.13	0.64
1:A:131:THR:OG1	1:A:143:ARG:HD2	1.98	0.64
1:A:238:LYS:HB2	1:A:315:HIS:HB3	1.79	0.64
1:A:66:LYS:O	1:A:67:ASP:HB3	1.97	0.64
1:A:535:TRP:CE3	2:B:422:LEU:HD13	2.33	0.64
1:A:175:ASN:CG	1:A:178:ILE:HD11	2.17	0.63
2:B:425:LEU:O	2:B:427:TYR:N	2.32	0.63
1:A:219:LYS:O	1:A:220:LYS:HB3	1.98	0.63
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.34	0.63
1:A:398:TRP:CH2	1:A:411:ILE:HD11	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLN:HA	1:A:523:GLU:HG2	1.81	0.63
2:B:244:ILE:HG22	2:B:263:LYS:NZ	2.14	0.63
1:A:245:VAL:O	1:A:245:VAL:HG22	1.98	0.63
2:B:209:LEU:CG	2:B:214:LEU:HD12	2.28	0.63
1:A:138:GLU:H	1:A:138:GLU:CD	2.01	0.63
2:B:241:VAL:HG23	2:B:243:PRO:CD	2.23	0.63
1:A:102:LYS:HG3	3:A:601:RT3:O29	1.98	0.63
1:A:29:GLU:HG3	1:A:30:LYS:N	2.14	0.63
1:A:486:LEU:O	1:A:528:LYS:NZ	2.32	0.63
1:A:441:TYR:HD2	1:A:544:GLY:HA3	1.60	0.63
1:A:228:LEU:HD23	1:A:228:LEU:N	2.11	0.63
1:A:104:LYS:O	3:A:601:RT3:H18	1.98	0.63
2:B:102:LYS:O	2:B:237:ASP:HB3	1.99	0.63
1:A:355:ALA:O	1:A:356:ARG:C	2.34	0.62
1:A:28:GLU:HG2	1:A:135:ILE:HG23	1.80	0.62
1:A:210:LEU:C	1:A:212:TRP:N	2.52	0.62
2:B:361:HIS:O	2:B:361:HIS:CG	2.53	0.62
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.82	0.62
1:A:134:SER:O	1:A:136:ASN:O	2.17	0.62
1:A:28:GLU:HG2	1:A:135:ILE:CG2	2.30	0.62
1:A:175:ASN:CG	1:A:178:ILE:CD1	2.67	0.62
1:A:234:LEU:HD23	1:A:234:LEU:N	2.13	0.62
1:A:60:VAL:CG2	1:A:130:PHE:CD2	2.82	0.62
1:A:441:TYR:CD2	1:A:544:GLY:HA2	2.34	0.62
2:B:268:SER:HB3	2:B:274:ILE:CB	2.28	0.62
1:A:543:GLY:H	2:B:283:LEU:HB3	1.64	0.62
1:A:311:LYS:O	1:A:312:GLU:OE1	2.17	0.62
1:A:41:MET:HB3	1:A:47:ILE:HG12	1.80	0.62
1:A:137:ASN:C	1:A:137:ASN:ND2	2.50	0.62
1:A:168:LEU:HD22	1:A:180:ILE:HD13	1.81	0.62
1:A:369:THR:HG22	1:A:398:TRP:CZ3	2.35	0.62
1:A:475:GLN:HG2	1:A:501:TYR:CD2	2.35	0.62
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.98	0.62
1:A:503:LEU:HD22	1:A:507:GLN:CG	2.30	0.62
2:B:11:LYS:HB3	2:B:11:LYS:HZ2	1.62	0.62
1:A:10:VAL:CG1	1:A:11:LYS:H	2.13	0.62
1:A:2:ILE:HG22	1:A:2:ILE:O	1.98	0.62
1:A:69:THR:HG23	1:A:69:THR:O	1.99	0.62
1:A:183:TYR:CZ	1:A:230:MET:CE	2.83	0.61
1:A:457:TYR:O	1:A:457:TYR:CD1	2.53	0.61
2:B:253:THR:CG2	2:B:254:VAL:N	2.62	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.30	0.61
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.35	0.61
1:A:219:LYS:O	1:A:220:LYS:HD2	2.00	0.61
1:A:410:TRP:O	1:A:410:TRP:CD1	2.54	0.61
1:A:542:ILE:CG2	1:A:543:GLY:N	2.63	0.61
1:A:60:VAL:CG2	1:A:130:PHE:HD2	2.14	0.61
2:B:236:PRO:O	2:B:239:TRP:N	2.32	0.61
2:B:309:ILE:O	2:B:312:GLU:HG2	2.01	0.61
2:B:420:PRO:HG3	2:B:423:VAL:HG21	1.80	0.61
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.30	0.60
1:A:1:PRO:C	1:A:2:ILE:HD13	2.18	0.60
1:A:365:VAL:O	1:A:369:THR:HG23	2.00	0.60
1:A:175:ASN:ND2	1:A:201:LYS:HE2	2.15	0.60
1:A:10:VAL:CG1	1:A:11:LYS:N	2.65	0.60
1:A:137:ASN:C	1:A:137:ASN:HD22	2.04	0.60
1:A:356:ARG:HH21	1:A:358:ARG:CG	2.13	0.60
1:A:458:VAL:O	1:A:458:VAL:CG2	2.49	0.60
1:A:369:THR:HG21	1:A:398:TRP:CH2	2.36	0.60
1:A:369:THR:HG21	1:A:398:TRP:CZ3	2.36	0.60
1:A:395:LYS:NZ	1:A:414:TRP:CE2	2.67	0.60
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.84	0.60
2:B:241:VAL:O	2:B:242:GLN:HB3	2.02	0.60
2:B:355:ALA:O	2:B:356:ARG:C	2.40	0.60
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.37	0.60
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.14	0.59
2:B:256:ASP:O	2:B:260:LEU:HB2	2.02	0.59
1:A:520:GLN:O	1:A:523:GLU:HG2	2.03	0.59
1:A:77:PHE:O	1:A:78:ARG:C	2.41	0.59
2:B:111:VAL:O	2:B:111:VAL:CG1	2.50	0.59
2:B:24:TRP:O	2:B:26:LEU:HD13	2.02	0.59
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.17	0.59
2:B:422:LEU:HB3	2:B:426:TRP:CZ2	2.37	0.59
1:A:195:ILE:CG1	1:A:199:ARG:HH21	2.16	0.59
2:B:111:VAL:HG13	2:B:111:VAL:O	2.02	0.59
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.37	0.59
1:A:205:LEU:CD1	1:A:209:LEU:HD11	2.33	0.59
2:B:162:SER:O	2:B:166:LYS:HG2	2.02	0.59
2:B:274:ILE:HA	2:B:306:ASN:ND2	2.18	0.59
1:A:70:LYS:NZ	1:A:72:ARG:HH12	2.00	0.58
1:A:417:VAL:HG22	1:A:419:THR:CG2	2.30	0.58
2:B:66:LYS:CB	2:B:407:GLN:NE2	2.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:N	1:A:157:PRO:CD	2.65	0.58
1:A:107:THR:HG22	1:A:198:HIS:HE1	1.68	0.58
1:A:72:ARG:NH1	1:A:72:ARG:CB	2.65	0.58
2:B:113:ASP:O	2:B:114:ALA:C	2.39	0.58
1:A:17:ASP:OD2	1:A:56:TYR:OH	2.18	0.58
1:A:424:LYS:CE	1:A:426:TRP:CE2	2.86	0.58
1:A:183:TYR:OH	1:A:230:MET:HE3	2.04	0.58
1:A:513:SER:H	1:A:519:ASN:HD21	1.50	0.58
2:B:248:GLU:O	2:B:249:LYS:HB3	2.03	0.58
2:B:244:ILE:HG22	2:B:263:LYS:HZ3	1.67	0.58
2:B:425:LEU:HD23	2:B:425:LEU:N	2.19	0.58
1:A:70:LYS:HZ3	1:A:72:ARG:HH12	1.52	0.58
2:B:64:LYS:HD2	2:B:69:THR:O	2.03	0.58
1:A:195:ILE:HD13	1:A:199:ARG:HH21	1.54	0.57
1:A:70:LYS:NZ	1:A:72:ARG:NH1	2.51	0.57
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.39	0.57
1:A:406:TRP:CE3	1:A:407:GLN:N	2.73	0.57
2:B:396:GLU:O	2:B:400:THR:CG2	2.49	0.57
1:A:409:THR:O	1:A:410:TRP:HB2	2.05	0.57
2:B:214:LEU:N	2:B:214:LEU:HD23	2.18	0.57
1:A:216:THR:HB	1:A:217:PRO:HD2	1.86	0.57
2:B:344:GLU:CB	2:B:347:LYS:CE	2.77	0.57
2:B:420:PRO:HG2	2:B:423:VAL:HB	1.87	0.57
2:B:422:LEU:HD23	2:B:425:LEU:HD11	1.84	0.57
2:B:50:ILE:HD12	2:B:54:ASN:HB3	1.87	0.57
1:A:64:LYS:NZ	1:A:69:THR:HA	2.19	0.57
2:B:236:PRO:O	2:B:237:ASP:C	2.43	0.57
2:B:241:VAL:CG2	2:B:242:GLN:H	2.13	0.57
2:B:280:CYS:O	2:B:282:LEU:N	2.38	0.56
1:A:170:PRO:O	1:A:172:ARG:N	2.38	0.56
1:A:398:TRP:CZ2	1:A:411:ILE:HG13	2.39	0.56
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.20	0.56
1:A:54:ASN:C	1:A:54:ASN:OD1	2.42	0.56
2:B:256:ASP:O	2:B:260:LEU:N	2.38	0.56
1:A:5:ILE:HG12	1:A:6:GLU:N	2.14	0.56
1:A:104:LYS:HG3	1:A:192:ASP:HB3	1.88	0.56
2:B:203:GLU:OE1	2:B:203:GLU:HA	2.05	0.56
1:A:430:GLU:CB	1:A:532:TYR:HB2	2.36	0.56
2:B:277:ARG:NH1	2:B:277:ARG:HB3	2.20	0.56
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.41	0.56
1:A:246:LEU:O	1:A:307:ARG:NH2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:TRP:O	1:A:536:VAL:HG12	2.06	0.56
2:B:209:LEU:HD12	2:B:214:LEU:HD12	1.88	0.56
2:B:314:VAL:CG1	2:B:317:VAL:HG23	2.36	0.56
1:A:175:ASN:HB3	1:A:178:ILE:CG1	2.35	0.56
1:A:94:ILE:C	1:A:94:ILE:HD12	2.26	0.56
1:A:5:ILE:HG12	1:A:6:GLU:O	2.06	0.55
2:B:121:ASP:C	2:B:121:ASP:OD2	2.45	0.55
2:B:277:ARG:HA	2:B:280:CYS:HB2	1.88	0.55
1:A:134:SER:OG	1:A:139:THR:HB	2.05	0.55
1:A:63:ILE:HD12	1:A:72:ARG:HG3	1.89	0.55
2:B:253:THR:HB	2:B:256:ASP:OD2	2.05	0.55
1:A:410:TRP:CE2	2:B:363:ASN:ND2	2.72	0.55
2:B:183:TYR:OH	2:B:386:THR:HG23	2.06	0.55
1:A:543:GLY:CA	2:B:284:ARG:N	2.69	0.55
2:B:344:GLU:O	2:B:345:PRO:C	2.44	0.55
2:B:425:LEU:C	2:B:427:TYR:N	2.58	0.55
1:A:195:ILE:HG23	1:A:199:ARG:HE	1.67	0.55
1:A:305:GLU:O	1:A:309:ILE:HG13	2.06	0.55
1:A:233:GLU:O	1:A:234:LEU:HD23	2.06	0.55
1:A:519:ASN:O	1:A:522:ILE:HB	2.07	0.55
2:B:266:TRP:NE1	2:B:346:PHE:HE2	2.03	0.55
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.42	0.55
2:B:257:ILE:HG23	2:B:279:LEU:HD11	1.89	0.55
1:A:542:ILE:CG2	2:B:283:LEU:HD13	2.37	0.55
2:B:256:ASP:N	2:B:256:ASP:OD2	2.39	0.55
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.42	0.55
1:A:511:ASP:C	1:A:511:ASP:OD2	2.45	0.55
2:B:241:VAL:HG23	2:B:242:GLN:N	2.18	0.55
2:B:273:GLY:O	2:B:274:ILE:O	2.25	0.55
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.08	0.54
1:A:542:ILE:O	1:A:544:GLY:N	2.40	0.54
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.89	0.54
1:A:406:TRP:C	1:A:406:TRP:CE3	2.81	0.54
2:B:283:LEU:O	2:B:284:ARG:CB	2.56	0.54
2:B:37:ILE:O	2:B:41:MET:HG3	2.07	0.54
1:A:296:THR:HG23	1:A:298:GLU:OE2	2.07	0.54
1:A:88:TRP:NE1	2:B:143:ARG:HD3	2.23	0.54
1:A:220:LYS:O	1:A:220:LYS:HD3	2.04	0.54
1:A:409:THR:HG23	1:A:410:TRP:N	2.21	0.54
1:A:430:GLU:HG2	1:A:531:VAL:C	2.28	0.54
1:A:410:TRP:CD2	2:B:363:ASN:ND2	2.76	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:SER:OG	2:B:387:PRO:HD3	2.08	0.54
1:A:155:GLY:O	1:A:159:ILE:HG13	2.08	0.54
2:B:120:LEU:HD22	2:B:121:ASP:N	2.23	0.54
1:A:86:ASP:HA	1:A:154:LYS:NZ	2.23	0.54
1:A:324:ASP:O	1:A:343:GLN:HG2	2.08	0.54
1:A:330:GLN:HE21	1:A:338:THR:CG2	2.20	0.54
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.89	0.54
2:B:277:ARG:HB3	2:B:277:ARG:HH11	1.73	0.54
1:A:113:ASP:O	1:A:114:ALA:C	2.44	0.54
1:A:19:PRO:O	1:A:56:TYR:HD1	1.90	0.54
1:A:467:VAL:HG12	1:A:468:THR:H	1.70	0.54
1:A:101:LYS:HD3	1:A:321:PRO:HD3	1.89	0.53
2:B:199:ARG:NH1	2:B:233:GLU:OE2	2.41	0.53
2:B:306:ASN:O	2:B:310:LEU:N	2.34	0.53
2:B:425:LEU:C	2:B:427:TYR:H	2.12	0.53
1:A:104:LYS:CB	1:A:192:ASP:HA	2.34	0.53
2:B:46:LYS:HA	2:B:46:LYS:CE	2.39	0.53
1:A:48:SER:O	1:A:144:TYR:HD1	1.91	0.53
2:B:80:LEU:O	2:B:84:THR:OG1	2.25	0.53
1:A:17:ASP:O	1:A:83:ARG:HD3	2.09	0.53
2:B:260:LEU:HD13	2:B:260:LEU:C	2.29	0.53
1:A:208:HIS:O	1:A:212:TRP:HD1	1.91	0.53
2:B:309:ILE:HA	2:B:312:GLU:HG2	1.91	0.53
2:B:78:ARG:NH1	2:B:412:PRO:O	2.39	0.53
1:A:106:VAL:CG1	3:A:601:RT3:C20	2.87	0.53
2:B:274:ILE:HG22	2:B:275:LYS:H	1.74	0.53
2:B:298:GLU:O	2:B:301:LEU:N	2.37	0.53
1:A:29:GLU:HG3	1:A:30:LYS:H	1.73	0.53
1:A:106:VAL:CG1	3:A:601:RT3:C21	2.87	0.53
1:A:467:VAL:CG1	1:A:468:THR:N	2.71	0.53
1:A:72:ARG:CZ	1:A:72:ARG:CB	2.87	0.53
1:A:406:TRP:CE3	1:A:407:GLN:HA	2.44	0.53
2:B:274:ILE:HG22	2:B:275:LYS:N	2.24	0.53
1:A:277:ARG:O	1:A:281:LYS:HG3	2.09	0.52
1:A:517:LEU:HA	1:A:520:GLN:HG3	1.90	0.52
2:B:428:GLN:O	2:B:428:GLN:HG3	2.08	0.52
2:B:252:TRP:HE3	2:B:256:ASP:HB2	1.74	0.52
1:A:325:LEU:HD11	1:A:383:TRP:CE3	2.45	0.52
2:B:273:GLY:O	2:B:275:LYS:HG2	2.09	0.52
1:A:439:THR:CG2	1:A:441:TYR:CE1	2.92	0.52
2:B:199:ARG:HD3	2:B:233:GLU:OE1	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:THR:HG21	2:B:367:GLN:HG3	1.91	0.52
2:B:421:PRO:O	2:B:425:LEU:HD21	2.10	0.52
1:A:320:ASP:O	1:A:322:SER:N	2.43	0.52
1:A:398:TRP:CZ3	1:A:411:ILE:HD11	2.45	0.52
2:B:160:PHE:CG	2:B:160:PHE:O	2.60	0.52
2:B:242:GLN:CG	2:B:242:GLN:O	2.53	0.52
1:A:138:GLU:CD	1:A:138:GLU:N	2.63	0.52
1:A:96:HIS:N	2:B:136:ASN:OD1	2.39	0.52
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.34	0.52
2:B:262:GLY:O	2:B:265:ASN:HB3	2.09	0.52
1:A:420:PRO:HA	1:A:421:PRO:C	2.30	0.52
2:B:242:GLN:O	2:B:243:PRO:C	2.49	0.52
2:B:84:THR:O	2:B:86:ASP:N	2.42	0.52
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.45	0.51
1:A:349:LEU:H	1:A:349:LEU:HD12	1.74	0.51
1:A:349:LEU:O	1:A:350:LYS:HB3	2.11	0.51
1:A:326:ILE:CD1	1:A:388:LYS:HE3	2.40	0.51
1:A:466:VAL:O	1:A:467:VAL:CG2	2.57	0.51
1:A:51:GLY:HA3	1:A:53:GLU:OE2	2.10	0.51
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.93	0.51
1:A:172:ARG:HH21	1:A:180:ILE:HB	1.74	0.51
1:A:104:LYS:HG3	1:A:192:ASP:CB	2.40	0.51
2:B:266:TRP:CZ2	2:B:427:TYR:CE1	2.98	0.51
1:A:103:LYS:O	3:A:601:RT3:C17	2.56	0.51
1:A:357:MET:CE	1:A:514:GLU:OE2	2.58	0.51
1:A:438:GLU:HG2	1:A:459:THR:HB	1.93	0.51
2:B:72:ARG:O	2:B:72:ARG:HG3	2.11	0.51
1:A:377:THR:O	1:A:378:GLU:C	2.49	0.51
1:A:498:ASP:HB2	1:A:536:VAL:O	2.11	0.51
1:A:63:ILE:CD1	1:A:72:ARG:HD3	2.41	0.51
2:B:169:GLU:N	2:B:170:PRO:HD2	2.25	0.51
2:B:337:TRP:CD1	2:B:337:TRP:N	2.79	0.51
2:B:297:GLU:CA	2:B:300:GLU:HB2	2.31	0.51
2:B:378:GLU:O	2:B:382:ILE:HG13	2.11	0.51
1:A:487:GLN:HA	1:A:524:GLN:HE22	1.77	0.50
1:A:106:VAL:HG13	3:A:601:RT3:C20	2.41	0.50
2:B:242:GLN:N	2:B:243:PRO:CD	2.55	0.50
1:A:535:TRP:CD2	2:B:422:LEU:CD1	2.94	0.50
2:B:88:TRP:CH2	2:B:154:LYS:HD3	2.46	0.50
1:A:33:ALA:O	1:A:37:ILE:HG13	2.11	0.50
2:B:350:LYS:C	2:B:351:THR:CG2	2.79	0.50

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:VAL:CG1	2:B:317:VAL:CG2	2.89	0.50
2:B:300:GLU:HA	2:B:303:LEU:HD12	1.93	0.50
1:A:395:LYS:HE2	1:A:414:TRP:CH2	2.47	0.50
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.94	0.50
1:A:218:ASP:O	1:A:219:LYS:C	2.50	0.50
2:B:120:LEU:O	2:B:121:ASP:C	2.50	0.50
2:B:165:THR:HB	2:B:166:LYS:HE2	1.92	0.50
2:B:240:THR:O	2:B:241:VAL:O	2.30	0.50
2:B:314:VAL:HG11	2:B:317:VAL:CG2	2.42	0.50
2:B:332:GLN:O	2:B:333:GLY:C	2.49	0.50
2:B:254:VAL:C	2:B:258:GLN:HG3	2.32	0.50
1:A:110:ASP:C	1:A:111:VAL:HG23	2.32	0.50
1:A:240:THR:OG1	1:A:241:VAL:N	2.44	0.49
1:A:296:THR:HG22	1:A:298:GLU:N	2.27	0.49
2:B:24:TRP:O	2:B:25:PRO:C	2.49	0.49
1:A:31:ILE:O	1:A:35:VAL:HG23	2.11	0.49
2:B:350:LYS:C	2:B:351:THR:HG23	2.32	0.49
1:A:296:THR:O	1:A:300:GLU:HG2	2.12	0.49
2:B:328:GLU:OE2	2:B:342:TYR:OH	2.22	0.49
2:B:195:ILE:O	2:B:198:HIS:HB3	2.12	0.49
2:B:5:ILE:CD1	2:B:5:ILE:N	2.72	0.49
1:A:296:THR:CG2	1:A:297:GLU:N	2.76	0.49
1:A:252:TRP:CE3	1:A:256:ASP:HB3	2.47	0.49
1:A:43:LYS:CE	1:A:43:LYS:HA	2.38	0.49
1:A:464:GLN:CG	1:A:465:LYS:N	2.72	0.49
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.47	0.49
1:A:277:ARG:NH1	1:A:334:GLN:HB2	2.26	0.49
1:A:109:LEU:HB2	1:A:187:LEU:HB2	1.96	0.48
1:A:195:ILE:HG12	1:A:199:ARG:HH21	1.78	0.48
1:A:424:LYS:NZ	1:A:426:TRP:CE2	2.81	0.48
1:A:424:LYS:NZ	1:A:426:TRP:CZ2	2.80	0.48
1:A:181:TYR:CD2	3:A:601:RT3:H10	2.48	0.48
2:B:302:GLU:O	2:B:303:LEU:C	2.51	0.48
2:B:85:GLN:HA	2:B:88:TRP:CD1	2.48	0.48
1:A:11:LYS:HB3	1:A:11:LYS:HE2	1.47	0.48
1:A:170:PRO:O	1:A:173:LYS:N	2.46	0.48
1:A:137:ASN:O	1:A:137:ASN:ND2	2.45	0.48
1:A:207:GLN:O	1:A:208:HIS:C	2.51	0.48
1:A:219:LYS:O	1:A:220:LYS:CB	2.61	0.48
1:A:296:THR:HG23	1:A:298:GLU:CD	2.34	0.48
2:B:301:LEU:HD23	2:B:305:GLU:OE1	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:THR:CG2	2:B:367:GLN:OE1	2.61	0.48
1:A:13:LYS:O	1:A:16:MET:HB2	2.13	0.48
1:A:350:LYS:CE	1:A:378:GLU:OE2	2.58	0.48
2:B:246:LEU:CD2	2:B:260:LEU:HD21	2.43	0.48
1:A:278:GLN:HB2	1:A:302:GLU:CG	2.44	0.48
1:A:43:LYS:HE2	1:A:43:LYS:CA	2.41	0.48
1:A:109:LEU:O	1:A:187:LEU:N	2.41	0.48
1:A:454:LYS:HA	1:A:467:VAL:O	2.14	0.48
1:A:542:ILE:HG22	1:A:543:GLY:N	2.29	0.48
2:B:389:PHE:HB3	2:B:391:LEU:HD21	1.95	0.48
2:B:418:ASN:O	2:B:419:THR:C	2.51	0.48
1:A:72:ARG:HH11	1:A:72:ARG:CG	2.27	0.48
2:B:304:ALA:O	2:B:308:GLU:N	2.35	0.48
1:A:52:PRO:N	1:A:53:GLU:OE1	2.47	0.48
2:B:334:GLN:O	2:B:336:GLN:HG3	2.13	0.48
2:B:324:ASP:O	2:B:343:GLN:HG2	2.14	0.48
2:B:65:LYS:NZ	2:B:72:ARG:HE	2.12	0.48
1:A:70:LYS:HZ3	1:A:72:ARG:NH1	2.11	0.48
1:A:337:TRP:NE1	1:A:367:GLN:OE1	2.32	0.47
2:B:82:LYS:HE3	2:B:413:GLU:OE2	2.14	0.47
2:B:13:LYS:NZ	2:B:85:GLN:HG2	2.29	0.47
1:A:205:LEU:HD13	1:A:209:LEU:CD1	2.44	0.47
1:A:467:VAL:CG1	1:A:468:THR:H	2.27	0.47
2:B:376:THR:HG21	2:B:410:TRP:CH2	2.49	0.47
1:A:369:THR:CG2	1:A:398:TRP:CH2	2.96	0.47
1:A:466:VAL:CG1	1:A:467:VAL:N	2.77	0.47
1:A:296:THR:O	1:A:300:GLU:CG	2.62	0.47
2:B:54:ASN:HD21	2:B:126:LYS:CA	2.28	0.47
2:B:209:LEU:HA	2:B:209:LEU:HD12	1.76	0.47
1:A:401:TRP:HB2	1:A:425:LEU:HD21	1.96	0.47
1:A:426:TRP:HE3	1:A:526:ILE:HD13	1.79	0.47
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.50	0.47
1:A:194:GLU:O	1:A:195:ILE:C	2.52	0.47
1:A:357:MET:CG	1:A:357:MET:O	2.57	0.47
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.61	0.47
1:A:283:LEU:O	1:A:286:THR:HB	2.14	0.47
1:A:410:TRP:CG	1:A:410:TRP:O	2.63	0.47
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.50	0.47
2:B:271:TYR:HB2	2:B:274:ILE:HD11	1.94	0.47
2:B:344:GLU:O	2:B:347:LYS:HD3	2.15	0.47
1:A:24:TRP:CG	1:A:25:PRO:CD	2.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HA	1:A:351:THR:HG23	1.95	0.46
2:B:306:ASN:O	2:B:310:LEU:HB2	2.15	0.46
1:A:234:LEU:HD12	3:A:601:RT3:H8	1.98	0.46
1:A:457:TYR:HD1	1:A:457:TYR:C	2.14	0.46
2:B:253:THR:HG23	2:B:254:VAL:N	2.29	0.46
1:A:175:ASN:HD21	1:A:201:LYS:HE2	1.72	0.46
1:A:342:TYR:C	1:A:342:TYR:CD1	2.89	0.46
1:A:438:GLU:HG3	1:A:461:ARG:HG2	1.98	0.46
1:A:63:ILE:HD12	1:A:72:ARG:CG	2.45	0.46
2:B:238:LYS:HE2	2:B:238:LYS:HB2	1.66	0.46
1:A:170:PRO:C	1:A:174:GLN:NE2	2.69	0.46
1:A:171:PHE:CD1	1:A:171:PHE:O	2.69	0.46
1:A:175:ASN:CG	1:A:178:ILE:HD12	2.35	0.46
1:A:450:THR:O	1:A:451:LYS:CB	2.63	0.46
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.57	0.46
1:A:532:TYR:C	1:A:532:TYR:CD2	2.88	0.46
2:B:314:VAL:HG12	2:B:317:VAL:HG23	1.97	0.46
1:A:107:THR:CG2	1:A:202:ILE:CD1	2.69	0.46
1:A:406:TRP:CE3	1:A:407:GLN:CB	2.96	0.46
1:A:134:SER:O	1:A:135:ILE:C	2.54	0.46
1:A:468:THR:O	1:A:469:LEU:HG	2.16	0.46
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.50	0.46
2:B:266:TRP:CZ2	2:B:427:TYR:CZ	3.03	0.46
2:B:309:ILE:HA	2:B:312:GLU:CG	2.45	0.46
1:A:202:ILE:O	1:A:205:LEU:HB3	2.16	0.46
1:A:466:VAL:C	1:A:467:VAL:HG23	2.36	0.46
1:A:491:LEU:H	1:A:491:LEU:CD1	2.28	0.46
1:A:102:LYS:HA	3:A:601:RT3:O29	2.16	0.46
1:A:94:ILE:O	1:A:94:ILE:CD1	2.47	0.46
1:A:410:TRP:CZ3	2:B:363:ASN:CB	2.92	0.46
2:B:209:LEU:CB	2:B:214:LEU:HB2	2.41	0.45
2:B:305:GLU:HA	2:B:308:GLU:HB2	1.98	0.45
1:A:5:ILE:HG22	1:A:212:TRP:HE3	1.80	0.45
2:B:23:GLN:OE1	2:B:60:VAL:N	2.49	0.45
1:A:244:ILE:HG22	1:A:246:LEU:HD23	1.98	0.45
1:A:64:LYS:HD3	1:A:71:TRP:CE2	2.52	0.45
1:A:99:GLY:HA3	2:B:136:ASN:ND2	2.32	0.45
2:B:423:VAL:O	2:B:427:TYR:HD2	2.00	0.45
1:A:105:SER:HG	1:A:198:HIS:CD2	2.34	0.45
1:A:538:ALA:C	1:A:540:LYS:N	2.70	0.45
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:O	2:B:85:GLN:HG3	2.13	0.45
1:A:186:ASP:C	1:A:187:LEU:HD23	2.34	0.45
2:B:277:ARG:NH1	2:B:277:ARG:CB	2.79	0.45
2:B:243:PRO:CB	2:B:311:LYS:HA	2.45	0.45
2:B:339:TYR:CD1	2:B:339:TYR:C	2.89	0.45
1:A:492:GLU:O	1:A:493:VAL:HG23	2.16	0.45
1:A:535:TRP:CD2	2:B:422:LEU:HD13	2.52	0.45
2:B:236:PRO:C	2:B:238:LYS:N	2.70	0.45
2:B:356:ARG:HG3	2:B:356:ARG:O	2.17	0.45
2:B:66:LYS:N	2:B:407:GLN:HG2	2.32	0.45
1:A:181:TYR:CB	3:A:601:RT3:H15	2.44	0.45
2:B:156:SER:N	2:B:157:PRO:CD	2.80	0.45
2:B:280:CYS:C	2:B:282:LEU:N	2.70	0.45
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.52	0.45
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.51	0.45
2:B:241:VAL:HG11	2:B:311:LYS:O	2.17	0.45
2:B:248:GLU:O	2:B:249:LYS:CB	2.64	0.45
1:A:296:THR:CG2	1:A:298:GLU:N	2.80	0.45
1:A:302:GLU:O	1:A:303:LEU:C	2.53	0.45
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.99	0.45
1:A:86:ASP:HA	1:A:154:LYS:HZ3	1.82	0.45
2:B:320:ASP:OD2	2:B:323:LYS:HG3	2.17	0.45
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.99	0.45
1:A:120:LEU:O	1:A:121:ASP:C	2.55	0.44
1:A:172:ARG:O	1:A:175:ASN:N	2.47	0.44
1:A:17:ASP:O	1:A:18:GLY:O	2.35	0.44
1:A:228:LEU:CD2	1:A:228:LEU:H	2.07	0.44
1:A:330:GLN:HE22	1:A:340:GLN:NE2	2.07	0.44
1:A:489:SER:CB	1:A:493:VAL:CG2	2.68	0.44
1:A:63:ILE:CD1	1:A:72:ARG:CD	2.94	0.44
2:B:120:LEU:HA	2:B:120:LEU:HD23	1.73	0.44
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.47	0.44
2:B:205:LEU:O	2:B:205:LEU:HD22	2.18	0.44
1:A:11:LYS:O	1:A:85:GLN:HB3	2.16	0.44
1:A:13:LYS:HA	1:A:14:PRO:HD2	1.79	0.44
1:A:3:SER:HA	1:A:212:TRP:O	2.17	0.44
1:A:236:PRO:HA	3:A:601:RT3:C16	2.48	0.44
2:B:298:GLU:N	2:B:298:GLU:OE2	2.39	0.44
2:B:422:LEU:HB3	2:B:426:TRP:CE2	2.52	0.44
2:B:65:LYS:HA	2:B:407:GLN:CG	2.33	0.44
1:A:195:ILE:HG23	1:A:199:ARG:NH2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:C	1:A:322:SER:H	2.20	0.44
1:A:171:PHE:O	1:A:175:ASN:HB2	2.18	0.44
1:A:40:GLU:O	1:A:43:LYS:HB2	2.17	0.44
2:B:278:GLN:HE21	2:B:278:GLN:CA	2.27	0.44
1:A:122:GLU:C	1:A:124:PHE:N	2.71	0.44
1:A:37:ILE:O	1:A:40:GLU:HB3	2.18	0.44
2:B:309:ILE:CA	2:B:312:GLU:HG2	2.47	0.44
1:A:131:THR:HG23	1:A:143:ARG:HG2	2.00	0.44
1:A:277:ARG:HB3	1:A:277:ARG:HE	1.05	0.44
1:A:280:CYS:O	1:A:281:LYS:C	2.54	0.44
2:B:273:GLY:C	2:B:274:ILE:O	2.55	0.44
2:B:295:LEU:O	2:B:297:GLU:OE2	2.36	0.44
2:B:344:GLU:O	2:B:345:PRO:O	2.36	0.44
2:B:422:LEU:O	2:B:423:VAL:C	2.56	0.44
1:A:8:VAL:HB	1:A:159:ILE:HD13	1.99	0.44
1:A:439:THR:HG21	1:A:441:TYR:CE1	2.53	0.44
1:A:502:ALA:O	1:A:506:ILE:HD12	2.18	0.44
1:A:89:GLU:HB2	1:A:92:LEU:HD22	2.00	0.44
2:B:253:THR:HG21	2:B:255:ASN:HB2	2.00	0.44
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.99	0.44
1:A:236:PRO:HA	3:A:601:RT3:C21	2.48	0.44
2:B:246:LEU:HD22	2:B:260:LEU:HD21	1.99	0.44
2:B:330:GLN:HE22	2:B:340:GLN:NE2	2.16	0.44
1:A:103:LYS:HA	1:A:192:ASP:OD2	2.18	0.43
1:A:344:GLU:O	1:A:345:PRO:C	2.56	0.43
1:A:500:GLN:HB3	1:A:500:GLN:HE21	1.67	0.43
2:B:279:LEU:O	2:B:282:LEU:HB2	2.17	0.43
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.98	0.43
1:A:419:THR:HA	1:A:420:PRO:HD3	1.85	0.43
1:A:426:TRP:CE3	1:A:526:ILE:HD13	2.53	0.43
1:A:46:LYS:HE3	1:A:116:PHE:HB3	1.99	0.43
1:A:429:LEU:HD21	1:A:506:ILE:HG22	1.99	0.43
2:B:422:LEU:CB	2:B:426:TRP:CZ2	3.00	0.43
1:A:303:LEU:O	1:A:303:LEU:HD23	2.18	0.43
1:A:375:ILE:O	1:A:379:SER:HB2	2.18	0.43
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.51	0.43
2:B:13:LYS:HE3	2:B:85:GLN:CB	2.48	0.43
1:A:48:SER:O	1:A:144:TYR:HA	2.18	0.43
1:A:542:ILE:HG23	1:A:543:GLY:H	1.84	0.43
1:A:95:PRO:HA	2:B:136:ASN:O	2.19	0.43
2:B:105:SER:O	2:B:190:GLY:HA2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:LEU:HA	2:B:310:LEU:HD12	1.81	0.43
2:B:88:TRP:CZ3	2:B:154:LYS:HD3	2.53	0.43
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.64	0.43
1:A:475:GLN:HG2	1:A:501:TYR:CZ	2.53	0.43
2:B:354:TYR:HD2	2:B:374:LYS:HZ2	1.64	0.43
1:A:339:TYR:CE1	1:A:352:GLY:HA3	2.54	0.43
2:B:420:PRO:HB2	2:B:423:VAL:HG23	2.01	0.43
2:B:64:LYS:O	2:B:65:LYS:CB	2.66	0.43
1:A:206:ARG:CZ	1:A:218:ASP:CB	2.96	0.43
2:B:274:ILE:N	2:B:274:ILE:HD13	2.33	0.43
1:A:175:ASN:HB3	1:A:178:ILE:HG13	2.01	0.43
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.17	0.43
2:B:425:LEU:HD23	2:B:425:LEU:H	1.81	0.43
2:B:6:GLU:O	2:B:6:GLU:OE1	2.37	0.43
1:A:93:GLY:HA3	2:B:137:ASN:CG	2.39	0.43
2:B:202:ILE:HA	2:B:202:ILE:HD13	1.85	0.43
1:A:1:PRO:HD2	1:A:215:THR:CG2	2.49	0.42
1:A:279:LEU:HD23	1:A:302:GLU:OE1	2.19	0.42
1:A:505:ILE:O	1:A:510:PRO:CG	2.67	0.42
2:B:307:ARG:O	2:B:308:GLU:C	2.56	0.42
2:B:325:LEU:HD12	2:B:385:LYS:HG2	2.01	0.42
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.54	0.42
2:B:368:LEU:O	2:B:372:VAL:HG23	2.19	0.42
1:A:170:PRO:C	1:A:174:GLN:HE21	2.23	0.42
1:A:183:TYR:OH	1:A:230:MET:CE	2.67	0.42
1:A:430:GLU:HB2	1:A:532:TYR:CB	2.44	0.42
1:A:70:LYS:HZ1	1:A:72:ARG:NH1	2.16	0.42
1:A:88:TRP:O	1:A:89:GLU:C	2.57	0.42
2:B:332:GLN:O	2:B:336:GLN:OE1	2.37	0.42
2:B:54:ASN:HD21	2:B:126:LYS:HA	1.83	0.42
1:A:108:VAL:HG22	1:A:188:TYR:CE2	2.53	0.42
1:A:8:VAL:CG1	1:A:159:ILE:HD13	2.50	0.42
2:B:87:PHE:HZ	2:B:159:ILE:HG13	1.83	0.42
1:A:320:ASP:C	1:A:320:ASP:OD1	2.57	0.42
2:B:308:GLU:O	2:B:311:LYS:HE3	2.19	0.42
1:A:169:GLU:HB3	1:A:170:PRO:HD2	2.02	0.42
1:A:1:PRO:HD3	1:A:215:THR:HG21	2.02	0.42
1:A:426:TRP:O	1:A:427:TYR:HB3	2.20	0.42
1:A:396:GLU:HA	1:A:399:GLU:HG2	2.02	0.42
1:A:520:GLN:C	1:A:522:ILE:N	2.72	0.42
2:B:199:ARG:HH11	2:B:233:GLU:CD	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:HG13	2:B:277:ARG:N	2.35	0.42
1:A:110:ASP:C	1:A:111:VAL:CG2	2.88	0.42
1:A:183:TYR:CE2	1:A:184:MET:HG3	2.54	0.42
1:A:204:GLU:O	1:A:204:GLU:HG2	2.19	0.42
1:A:220:LYS:CD	1:A:221:HIS:CD2	3.01	0.42
1:A:395:LYS:HE2	1:A:414:TRP:CZ3	2.55	0.42
1:A:5:ILE:CG1	1:A:6:GLU:N	2.82	0.42
2:B:195:ILE:HG23	2:B:196:GLY:N	2.35	0.42
1:A:244:ILE:HG22	1:A:246:LEU:CD2	2.50	0.42
1:A:91:GLN:HG3	1:A:93:GLY:O	2.20	0.42
1:A:94:ILE:C	1:A:94:ILE:CD1	2.89	0.42
2:B:168:LEU:HD13	2:B:180:ILE:HG21	2.01	0.42
2:B:277:ARG:CB	2:B:277:ARG:CZ	2.98	0.42
2:B:309:ILE:C	2:B:312:GLU:HG2	2.40	0.42
2:B:374:LYS:O	2:B:377:THR:HG23	2.20	0.42
1:A:121:ASP:OD1	1:A:121:ASP:C	2.57	0.41
1:A:253:THR:HA	1:A:291:GLU:O	2.20	0.41
2:B:103:LYS:CE	2:B:179:VAL:HG23	2.46	0.41
2:B:293:ILE:HA	2:B:294:PRO:HD2	1.81	0.41
1:A:167:ILE:HD12	1:A:214:LEU:CD1	2.49	0.41
2:B:253:THR:HG22	2:B:254:VAL:N	2.35	0.41
2:B:65:LYS:C	2:B:407:GLN:HG2	2.40	0.41
1:A:8:VAL:HG11	1:A:159:ILE:HD13	2.02	0.41
1:A:424:LYS:CE	1:A:426:TRP:CZ2	3.03	0.41
1:A:528:LYS:HD2	1:A:528:LYS:HA	1.79	0.41
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.56	0.41
1:A:72:ARG:HH11	1:A:72:ARG:HB3	1.79	0.41
2:B:203:GLU:OE1	2:B:203:GLU:CA	2.65	0.41
2:B:273:GLY:O	2:B:274:ILE:C	2.57	0.41
2:B:298:GLU:C	2:B:300:GLU:N	2.74	0.41
1:A:121:ASP:OD1	1:A:122:GLU:N	2.54	0.41
1:A:402:TRP:CG	1:A:403:THR:N	2.87	0.41
1:A:395:LYS:HE2	1:A:414:TRP:CZ2	2.56	0.41
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.56	0.41
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.24	0.41
2:B:363:ASN:OD1	2:B:366:LYS:CB	2.68	0.41
2:B:65:LYS:HZ3	2:B:72:ARG:HE	1.68	0.41
1:A:317:VAL:HG23	1:A:318:TYR:O	2.20	0.41
1:A:487:GLN:HA	1:A:524:GLN:NE2	2.35	0.41
1:A:3:SER:HA	1:A:4:PRO:HD2	1.86	0.41
1:A:519:ASN:HA	1:A:522:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PRO:C	1:A:178:ILE:H	2.24	0.41
1:A:194:GLU:C	1:A:196:GLY:N	2.74	0.41
1:A:21:VAL:CG1	1:A:59:PRO:CD	2.99	0.41
1:A:63:ILE:HD11	1:A:72:ARG:CD	2.47	0.41
2:B:7:THR:HG22	2:B:119:PRO:HB2	2.02	0.41
2:B:330:GLN:HE22	2:B:340:GLN:HE22	1.68	0.41
1:A:242:GLN:O	1:A:243:PRO:C	2.58	0.41
1:A:278:GLN:HB2	1:A:302:GLU:HG3	2.03	0.41
1:A:342:TYR:CA	1:A:349:LEU:HD12	2.44	0.41
2:B:239:TRP:O	2:B:240:THR:CG2	2.66	0.41
2:B:330:GLN:HE22	2:B:340:GLN:CD	2.22	0.41
2:B:183:TYR:OH	2:B:386:THR:CG2	2.68	0.41
2:B:263:LYS:HG3	2:B:426:TRP:HA	2.01	0.41
1:A:276:VAL:CG1	1:A:276:VAL:O	2.69	0.41
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.47	0.41
1:A:512:GLN:O	1:A:512:GLN:HG2	2.19	0.41
1:A:522:ILE:O	1:A:526:ILE:HG13	2.21	0.41
1:A:168:LEU:O	1:A:169:GLU:C	2.58	0.41
1:A:244:ILE:HD11	1:A:267:ALA:HB2	1.99	0.41
1:A:542:ILE:HG23	2:B:283:LEU:HB3	2.01	0.41
2:B:275:LYS:HB3	2:B:302:GLU:OE2	2.20	0.41
1:A:374:LYS:CD	1:A:374:LYS:C	2.88	0.41
1:A:103:LYS:HG3	3:A:601:RT3:H113	2.03	0.41
1:A:275:LYS:O	1:A:276:VAL:HG23	2.21	0.41
1:A:489:SER:O	1:A:490:GLY:O	2.38	0.41
2:B:63:ILE:HD13	2:B:74:LEU:CD2	2.44	0.41
1:A:122:GLU:O	1:A:124:PHE:N	2.54	0.40
1:A:21:VAL:HG13	1:A:59:PRO:CD	2.46	0.40
1:A:459:THR:OG1	1:A:460:ASN:N	2.54	0.40
1:A:538:ALA:C	1:A:540:LYS:H	2.24	0.40
2:B:253:THR:HG22	2:B:255:ASN:CA	2.48	0.40
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.75	0.40
1:A:233:GLU:HB3	1:A:240:THR:CG2	2.50	0.40
1:A:282:LEU:HA	1:A:282:LEU:HD23	1.85	0.40
1:A:479:LEU:HB3	1:A:517:LEU:HD21	2.02	0.40
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.90	0.40
2:B:261:VAL:HG23	2:B:276:VAL:HG21	2.03	0.40
2:B:65:LYS:NZ	2:B:72:ARG:NE	2.68	0.40
1:A:169:GLU:CB	1:A:170:PRO:CD	2.99	0.40
1:A:40:GLU:OE1	1:A:40:GLU:HA	2.22	0.40
2:B:13:LYS:CE	2:B:85:GLN:HG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:SER:O	2:B:166:LYS:CE	2.63	0.40
2:B:350:LYS:HG3	2:B:351:THR:H	1.87	0.40
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.57	0.40
1:A:406:TRP:CH2	2:B:418:ASN:OD1	2.68	0.40
2:B:51:GLY:O	2:B:53:GLU:N	2.54	0.40
1:A:448:ARG:HH11	1:A:448:ARG:CG	2.34	0.40
1:A:460:ASN:C	1:A:462:GLY:H	2.25	0.40
1:A:509:GLN:N	1:A:510:PRO:HD3	2.36	0.40
2:B:24:TRP:HE3	2:B:25:PRO:HD2	1.87	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	543/563 (96%)	442 (81%)	72 (13%)	29 (5%)	2	12
2	B	399/443 (90%)	331 (83%)	47 (12%)	21 (5%)	2	12
All	All	942/1006 (94%)	773 (82%)	119 (13%)	50 (5%)	2	12

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	90	VAL
1	A	195	ILE
1	A	345	PRO
1	A	356	ARG
1	A	410	TRP
1	A	491	LEU
2	B	85	GLN
2	B	237	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	241	VAL
2	B	242	GLN
2	B	269	GLN
2	B	274	ILE
2	B	284	ARG
2	B	333	GLY
1	A	18	GLY
1	A	114	ALA
1	A	171	PHE
1	A	196	GLY
1	A	211	ARG
1	A	276	VAL
1	A	346	PHE
1	A	490	GLY
1	A	528	LYS
1	A	543	GLY
2	B	114	ALA
2	B	249	LYS
2	B	281	LYS
2	B	324	ASP
2	B	426	TRP
1	A	3	SER
1	A	6	GLU
1	A	135	ILE
1	A	539	HIS
2	B	236	PRO
2	B	308	GLU
1	A	66	LYS
1	A	89	GLU
1	A	243	PRO
1	A	312	GLU
1	A	334	GLN
2	B	294	PRO
2	B	423	VAL
2	B	214	LEU
2	B	303	LEU
1	A	170	PRO
1	A	287	LYS
2	B	419	THR
2	B	18	GLY
1	A	246	LEU

5.3.2 Protein sidechains ⓘ

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	486/503 (97%)	405 (83%)	81 (17%)	2	11
2	B	369/403 (92%)	307 (83%)	62 (17%)	2	11
All	All	855/906 (94%)	712 (83%)	143 (17%)	2	11

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	11	LYS
1	A	21	VAL
1	A	26	LEU
1	A	43	LYS
1	A	44	GLU
1	A	64	LYS
1	A	69	THR
1	A	72	ARG
1	A	92	LEU
1	A	105	SER
1	A	106	VAL
1	A	107	THR
1	A	118	VAL
1	A	126	LYS
1	A	132	ILE
1	A	135	ILE
1	A	137	ASN
1	A	139	THR
1	A	159	ILE
1	A	170	PRO
1	A	173	LYS
1	A	174	GLN
1	A	178	ILE
1	A	179	VAL
1	A	194	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	ILE
1	A	197	GLN
1	A	211	ARG
1	A	219	LYS
1	A	220	LYS
1	A	222	GLN
1	A	228	LEU
1	A	238	LYS
1	A	246	LEU
1	A	248	GLU
1	A	249	LYS
1	A	251	SER
1	A	260	LEU
1	A	277	ARG
1	A	284	ARG
1	A	286	THR
1	A	291	GLU
1	A	296	THR
1	A	298	GLU
1	A	303	LEU
1	A	312	GLU
1	A	324	ASP
1	A	341	ILE
1	A	349	LEU
1	A	357	MET
1	A	368	LEU
1	A	373	GLN
1	A	374	LYS
1	A	379	SER
1	A	402	TRP
1	A	403	THR
1	A	409	THR
1	A	411	ILE
1	A	417	VAL
1	A	419	THR
1	A	422	LEU
1	A	425	LEU
1	A	429	LEU
1	A	431	LYS
1	A	448	ARG
1	A	452	LEU
1	A	461	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	469	LEU
1	A	471	ASP
1	A	475	GLN
1	A	479	LEU
1	A	496	VAL
1	A	500	GLN
1	A	503	LEU
1	A	509	GLN
1	A	514	GLU
1	A	520	GLN
1	A	528	LYS
1	A	536	VAL
2	B	6	GLU
2	B	8	VAL
2	B	11	LYS
2	B	17	ASP
2	B	22	LYS
2	B	26	LEU
2	B	29	GLU
2	B	30	LYS
2	B	48	SER
2	B	60	VAL
2	B	64	LYS
2	B	65	LYS
2	B	66	LYS
2	B	68	SER
2	B	72	ARG
2	B	73	LYS
2	B	79	GLU
2	B	80	LEU
2	B	84	THR
2	B	85	GLN
2	B	91	GLN
2	B	104	LYS
2	B	113	ASP
2	B	120	LEU
2	B	173	LYS
2	B	178	ILE
2	B	184	MET
2	B	187	LEU
2	B	199	ARG
2	B	205	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	209	LEU
2	B	232	TYR
2	B	242	GLN
2	B	251	SER
2	B	253	THR
2	B	256	ASP
2	B	261	VAL
2	B	270	ILE
2	B	275	LYS
2	B	278	GLN
2	B	280	CYS
2	B	292	VAL
2	B	295	LEU
2	B	297	GLU
2	B	298	GLU
2	B	300	GLU
2	B	301	LEU
2	B	310	LEU
2	B	323	LYS
2	B	336	GLN
2	B	347	LYS
2	B	349	LEU
2	B	353	LYS
2	B	356	ARG
2	B	374	LYS
2	B	377	THR
2	B	385	LYS
2	B	399	GLU
2	B	400	THR
2	B	403	THR
2	B	419	THR
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	136	ASN
1	A	137	ASN
1	A	147	ASN
1	A	174	GLN
1	A	175	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	198	HIS
1	A	221	HIS
1	A	235	HIS
1	A	242	GLN
1	A	258	GLN
1	A	330	GLN
1	A	334	GLN
1	A	407	GLN
1	A	480	GLN
1	A	512	GLN
1	A	519	ASN
1	A	524	GLN
2	B	137	ASN
2	B	147	ASN
2	B	161	GLN
2	B	175	ASN
2	B	255	ASN
2	B	278	GLN
2	B	306	ASN
2	B	361	HIS
2	B	373	GLN
2	B	407	GLN
2	B	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	RT3	A	601	-	30,31,31	2.39	7 (23%)	42,45,45	1.87	11 (26%)

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	RT3	A	601	-	-	1/17/29/29	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	RT3	C19-S23	-9.59	1.61	1.77
3	A	601	RT3	C11-S12	-4.76	1.67	1.78
3	A	601	RT3	C16-N15	-2.57	1.36	1.41
3	A	601	RT3	C13-S12	-2.34	1.77	1.80
3	A	601	RT3	C21-CL22	2.18	1.78	1.73
3	A	601	RT3	C16-C21	3.65	1.49	1.39
3	A	601	RT3	C3-C4	4.57	1.46	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	RT3	O26-S23-O30	-5.30	108.97	118.70
3	A	601	RT3	C6-C5-C4	-2.55	106.39	112.44
3	A	601	RT3	C1-N2-C3	2.10	120.85	115.14
3	A	601	RT3	C21-C20-C19	2.27	120.26	118.82
3	A	601	RT3	C13-C14-N15	2.33	117.87	114.39
3	A	601	RT3	C17-C18-C19	2.35	122.01	119.46
3	A	601	RT3	O26-S23-C19	2.53	110.35	107.39
3	A	601	RT3	O26-S23-N29	2.57	111.37	107.34
3	A	601	RT3	C1-N2-C11	2.62	126.08	118.21
3	A	601	RT3	C13-S12-C11	3.46	109.36	100.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	RT3	C4-C3-N2	4.89	121.83	117.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	RT3	C13-C14-N15-C16

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	RT3	17	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, 95th 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(Å²)	Q<0.9
1	A	545/563 (96%)	0.14	10 (1%)	69	48	44, 71, 91, 113	0
2	B	405/443 (91%)	0.21	15 (3%)	42	25	45, 64, 108, 114	0
All	All	950/1006 (94%)	0.17	25 (2%)	56	35	44, 69, 104, 114	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	LYS	4.7
2	B	252	TRP	4.6
1	A	542	ILE	4.4
2	B	270	ILE	3.9
1	A	426	TRP	3.7
2	B	276	VAL	3.4
2	B	277	ARG	3.0
2	B	426	TRP	2.8
2	B	279	LEU	2.7
1	A	539	HIS	2.7
2	B	231	GLY	2.7
1	A	51	GLY	2.6
2	B	283	LEU	2.6
2	B	425	LEU	2.6
2	B	67	ASP	2.5
2	B	266	TRP	2.4
1	A	543	GLY	2.4
1	A	544	GLY	2.4
1	A	491	LEU	2.2
2	B	92	LEU	2.2
1	A	462	GLY	2.1
2	B	421	PRO	2.1
2	B	90	VAL	2.1
2	B	361	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	72	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95th 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	RT3	A	601	29/29	0.86	0.26	1.41	86,100,107,107	0

6.5 Other polymers ⓘ

There are no such residues in this entry.