Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 02:13 PM EST

PDB ID	:	1DFC
Title	:	CRYSTAL STRUCTURE OF HUMAN FASCIN, AN ACTIN-CROSSLINKING PROTEIN
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Ono, S.; Matsumura, F.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	1999-11-18
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

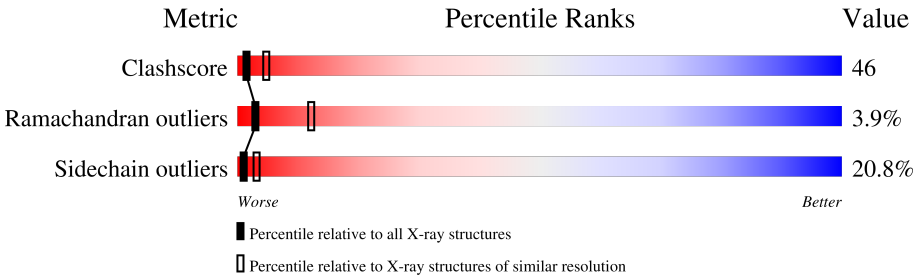
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	493	35% 46% 14%
1	B	493	35% 47% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7427 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 FASCIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3716	2326	663	714	13			
1	B	474	Total	C	N	O	S	0	0	0
			3711	2323	662	713	13			

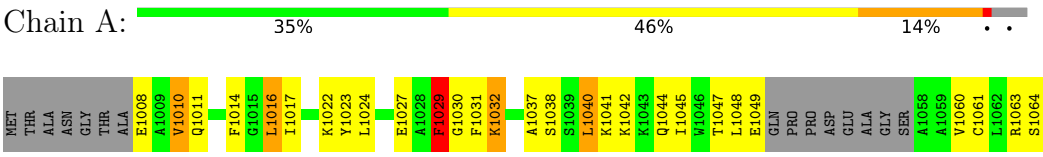
3 Residue-property plots (i)

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

Note EDS was not executed.

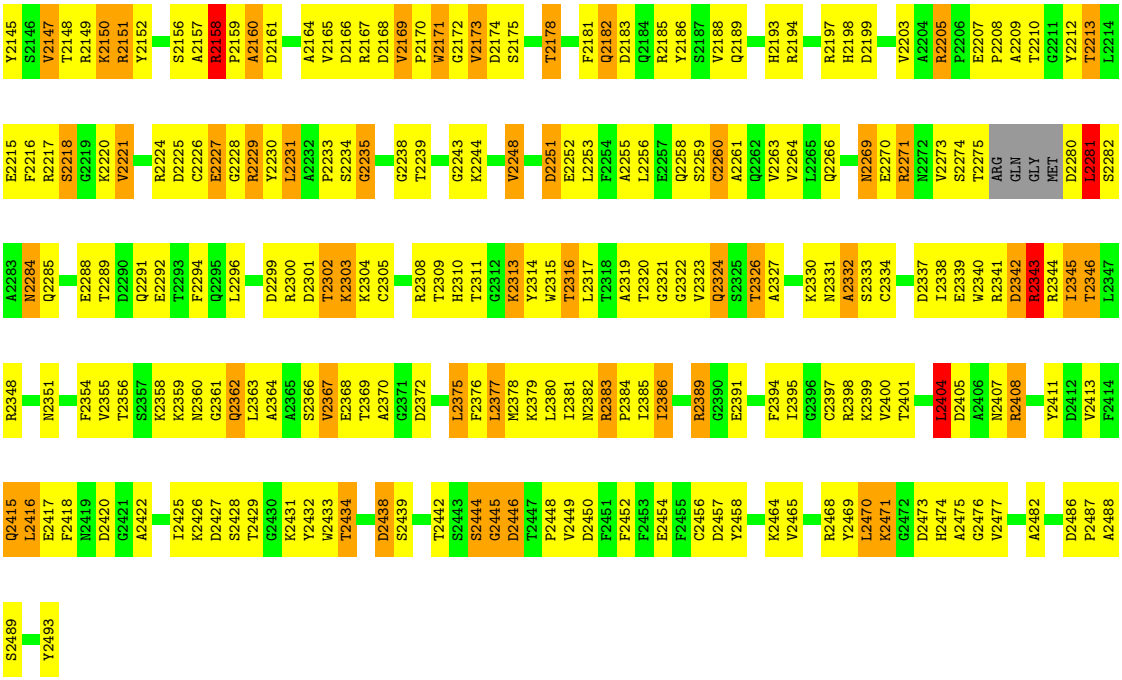
• Molecule 1: FASCIN

Chain A:



• Molecule 1: FASCIN

Chain B:


Y2145 S2146 V2147 T2148 R2149 K2150 R2151 Y2152 S2156 A2157 R2158 P2159 A2160 D2161 A2164 V2165 D2166 R2167 D2168 V2169 P2170 W2171 G2172 V2173 D2174 S2175 T2178 F2181 Q2182 D2183 Q2184 R2185 Y2186 S2187 V2188 Q2189 H2193 R2194 R2197 H2198 D2199 V2203 A2204 R2205 P2206 E2207 P2208 A2209 T2210 G2211 Y2212 T2213 L2214
E2215 F2216 R2217 S2218 G2219 K2220 V2221 R2224 D2225 C2226 E2227 G2228 R2229 Y2230 L2231 A2232 P2233 S2234 G2235 G2238 T2239 G2243 K2244 V2248 D2251 E2252 L2253 F2254 A2255 L2256 E2257 Q2258 S2259 C2260 A2261 Q2262 V2263 V2264 L2265 Q2266 N2269 E2270 R2271 N2272 V2273 S2274 T2275 ABG GLN GLY MET D2280 L2281 S2282
A2283 N2284 Q2285 E2288 T2289 D2290 Q2291 E2292 T2293 F2294 Q2295 L2296 D2299 R2300 D2301 T2302 K2303 K2304 C2305 R2308 T2309 H2310 T2311 G2312 K2313 Y2314 W2315 T2316 L2317 T2318 A2319 T2320 G2321 G2322 V2323 Q2324 S2325 T2326 A2327 K2330 N2331 A2332 S2333 C2334 D2337 I2338 E2339 W2340 R2341 D2342 R2343 R2344 I2345 T2346 L2347
R2348 W2351 F2354 V2355 T2356 S2357 K2358 K2359 N2360 G2361 Q2362 L2363 A2364 A2365 S2366 V2367 E2368 T2369 A2370 G2371 D2372 L2375 F2376 L2377 M2378 K2379 L2380 I2381 N2382 R2383 P2384 I2385 I2386 R2389 G2390 E2391 F2394 I2395 G2396 C2397 R2398 K2399 V2400 T2401 L2404 D2405 A2406 N2407 R2408 Y2411 D2412 V2413 F2414
Q2415 L2416 E2417 F2418 N2419 D2420 G2421 A2422 I2425 K2426 D2427 S2428 T2429 G2430 K2431 Y2432 W2433 T2434 D2438 S2439 T2442 S2443 S2444 G2445 D2446 T2447 P2448 V2449 D2450 F2451 F2452 F2453 E2454 F2455 C2456 D2457 Y2458 K2464 V2465 R2468 Y2469 L2470 K2471 G2472 D2473 H2474 A2475 G2476 V2477 A2482 D2486 P2487 A2488
S2489 Y2493

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	165.43Å 71.69Å 116.92Å 90.00° 132.17° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	83.6 (8.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.184 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7427	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.96	2/3793 (0.1%)	0.98	3/5126 (0.1%)
1	B	0.95	3/3788 (0.1%)	0.98	2/5119 (0.0%)
All	All	0.96	5/7581 (0.1%)	0.98	5/10245 (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	2
1	B	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2456	CYS	CB-SG	-6.68	1.70	1.82
1	A	1397	CYS	CB-SG	-6.12	1.71	1.82
1	B	2260	CYS	CB-SG	-5.68	1.72	1.81
1	A	1061	CYS	CB-SG	-5.42	1.73	1.81
1	B	2305	CYS	CB-SG	-5.34	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1383	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	B	2194	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	A	1387	VAL	N-CA-C	-5.67	95.70	111.00
1	A	1363	LEU	CA-CB-CG	5.30	127.50	115.30
1	B	2404	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1452	PHE	Sidechain
1	A	1493	TYR	Sidechain
1	B	2493	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3716	0	3599	343	1
1	B	3711	0	3597	336	1
All	All	7427	0	7196	679	1

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 (679) 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:1139:HIS:CE1	1:A:1141:GLN:HG3	1.61	1.36
1:A:1416:LEU:HD12	1:A:1416:LEU:H	1.15	1.12
1:A:1158:ARG:HB2	1:A:1159:PRO:HD3	1.14	1.10
1:B:2158:ARG:HB2	1:B:2159:PRO:HD3	1.11	1.10
1:B:2158:ARG:HB2	1:B:2159:PRO:CD	1.86	1.05
1:A:1269:ASN:OD1	1:A:1271:ARG:HB2	1.58	1.01
1:B:2100:ARG:HB2	1:B:2132:TRP:O	1.59	1.01
1:A:1100:ARG:HB2	1:A:1132:TRP:O	1.61	1.00
1:B:2282:SER:HB3	1:B:2362:GLN:HA	1.43	0.98
1:A:1158:ARG:HB2	1:A:1159:PRO:CD	1.93	0.98
1:B:2043:LYS:HA	1:B:2065:HIS:CD2	1.99	0.97
1:A:1282:SER:HB3	1:A:1362:GLN:HA	1.46	0.96
1:B:2416:LEU:HD12	1:B:2416:LEU:H	1.30	0.96
1:A:1205:ARG:NH1	1:A:1207:GLU:HB3	1.81	0.95
1:A:1127:SER:H	1:A:1130:GLU:HG2	1.29	0.94
1:B:2139:HIS:CE1	1:B:2141:GLN:HG3	2.05	0.91
1:A:1157:ALA:HB3	1:A:1158:ARG:NH1	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:HIS:HE1	1:A:1141:GLN:CG	1.85	0.89
1:A:1139:HIS:CE1	1:A:1141:GLN:CG	2.53	0.89
1:A:1416:LEU:HD12	1:A:1416:LEU:N	1.81	0.89
1:B:2205:ARG:NH1	1:B:2207:GLU:HB3	1.88	0.88
1:B:2150:LYS:HG3	1:B:2151:ARG:HE	1.36	0.88
1:B:2269:ASN:OD1	1:B:2271:ARG:HB2	1.74	0.88
1:B:2383:ARG:O	1:B:2416:LEU:HD11	1.74	0.87
1:A:1139:HIS:HE1	1:A:1141:GLN:HG3	1.04	0.87
1:B:2127:SER:H	1:B:2130:GLU:HG2	1.38	0.87
1:B:2136:ILE:HG23	1:B:2138:MET:SD	2.16	0.86
1:B:2097:ASP:HA	1:B:2224:ARG:NH1	1.92	0.85
1:B:2095:ALA:HB2	1:B:2215:GLU:HG3	1.57	0.84
1:B:2139:HIS:HE1	1:B:2141:GLN:HG3	1.38	0.84
1:A:1299:ASP:OD1	1:A:1302:THR:HG23	1.78	0.83
1:A:1010:VAL:HG12	1:A:1256:LEU:O	1.78	0.82
1:B:2043:LYS:HA	1:B:2065:HIS:HD2	1.43	0.82
1:A:1343:ARG:O	1:A:1344:ARG:HD2	1.79	0.82
1:A:1398:ARG:HH11	1:A:1403:THR:HG21	1.43	0.81
1:A:1150:LYS:HG3	1:A:1151:ARG:HE	1.43	0.81
1:A:1343:ARG:HH11	1:A:1343:ARG:HG3	1.43	0.80
1:B:2266:GLN:HG3	1:B:2271:ARG:O	1.80	0.80
1:B:2031:PHE:CD1	1:B:2081:GLU:HG3	2.16	0.80
1:A:1203:VAL:CG2	1:A:1205:ARG:HE	1.95	0.80
1:B:2158:ARG:CB	1:B:2159:PRO:HD3	2.04	0.79
1:A:1205:ARG:HH12	1:A:1207:GLU:HB3	1.46	0.79
1:B:2416:LEU:HD12	1:B:2416:LEU:N	1.97	0.78
1:B:2291:GLN:HB2	1:B:2292:GLU:OE1	1.84	0.78
1:B:2299:ASP:OD1	1:B:2302:THR:HG23	1.84	0.77
1:B:2205:ARG:HH22	1:B:2207:GLU:CD	1.88	0.77
1:A:1398:ARG:NH1	1:A:1403:THR:HG21	1.99	0.77
1:A:1354:PHE:HE2	1:A:1370:ALA:HB2	1.49	0.76
1:A:1207:GLU:HB2	1:A:1208:PRO:HD2	1.65	0.76
1:B:2207:GLU:HB2	1:B:2208:PRO:HD2	1.66	0.76
1:A:1203:VAL:HG21	1:A:1205:ARG:HH21	1.50	0.76
1:B:2400:VAL:HG13	1:B:2401:THR:H	1.51	0.75
1:A:1205:ARG:HH22	1:A:1207:GLU:CD	1.89	0.75
1:B:2205:ARG:NH2	1:B:2207:GLU:OE1	2.19	0.75
1:A:1031:PHE:CD1	1:A:1081:GLU:HG3	2.22	0.75
1:B:2111:TYR:CE2	1:B:2126:VAL:HG22	2.21	0.74
1:A:1474:HIS:O	1:A:1475:ALA:HB3	1.86	0.74
1:B:2438:ASP:OD1	1:B:2438:ASP:N	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1355:VAL:CG1	1:A:1363:LEU:HD13	2.18	0.74
1:B:2324:GLN:HG3	1:B:2326:THR:HB	1.69	0.73
1:A:1063:ARG:HE	1:A:1067:GLY:HA2	1.54	0.73
1:A:1165:VAL:HG12	1:A:1238:GLY:O	1.87	0.73
1:A:1011:GLN:O	1:A:1011:GLN:HG3	1.88	0.72
1:A:1205:ARG:HH22	1:A:1207:GLU:CG	2.01	0.72
1:B:2299:ASP:CG	1:B:2302:THR:HG23	2.09	0.72
1:A:1063:ARG:NE	1:A:1067:GLY:HA2	2.04	0.72
1:A:1205:ARG:NH2	1:A:1207:GLU:OE1	2.22	0.72
1:B:2097:ASP:HA	1:B:2224:ARG:HH12	1.53	0.72
1:B:2203:VAL:CG2	1:B:2205:ARG:HE	2.02	0.71
1:A:1339:GLU:O	1:A:1345:ILE:HD12	1.90	0.71
1:A:1299:ASP:OD1	1:A:1302:THR:N	2.23	0.70
1:A:1269:ASN:O	1:A:1270:GLU:HB2	1.91	0.70
1:B:2040:LEU:HD12	1:B:2041:LYS:N	2.06	0.70
1:A:1341:ARG:HH11	1:A:1375:LEU:HD11	1.55	0.70
1:B:2150:LYS:O	1:B:2151:ARG:HD3	1.90	0.70
1:B:2343:ARG:HG3	1:B:2343:ARG:HH11	1.56	0.70
1:A:1027:GLU:HB3	1:A:1029:PHE:HB2	1.72	0.70
1:A:1391:GLU:OE2	1:A:1487:PRO:HB2	1.91	0.70
1:B:2339:GLU:HB3	1:B:2346:THR:CG2	2.22	0.69
1:A:1386:ILE:HD11	1:A:1416:LEU:HG	1.73	0.69
1:B:2010:VAL:HG12	1:B:2256:LEU:O	1.91	0.69
1:B:2342:ASP:O	1:B:2343:ARG:HB2	1.89	0.69
1:A:1040:LEU:HD12	1:A:1041:LYS:N	2.08	0.69
1:A:1354:PHE:CE2	1:A:1370:ALA:HB2	2.27	0.69
1:B:2104:GLN:NE2	1:B:2111:TYR:HE1	1.90	0.69
1:A:1111:TYR:CE2	1:A:1126:VAL:HG22	2.28	0.69
1:A:1203:VAL:HG21	1:A:1205:ARG:HE	1.57	0.69
1:B:2150:LYS:HG3	1:B:2151:ARG:NE	2.08	0.69
1:A:1343:ARG:HD3	1:A:1420:ASP:O	1.93	0.69
1:B:2165:VAL:HG11	1:B:2233:PRO:HB3	1.75	0.69
1:B:2011:GLN:O	1:B:2011:GLN:HG3	1.92	0.68
1:B:2205:ARG:HH12	1:B:2207:GLU:HB3	1.56	0.68
1:A:1342:ASP:O	1:A:1343:ARG:HB2	1.93	0.68
1:A:1343:ARG:HG3	1:A:1343:ARG:NH1	2.08	0.68
1:B:2090:ARG:HH11	1:B:2090:ARG:HB3	1.58	0.68
1:A:1473:ASP:OD1	1:A:1477:VAL:HG22	1.93	0.68
1:A:1362:GLN:HG2	1:A:1363:LEU:N	2.08	0.68
1:A:1313:LYS:HG3	1:A:1327:ALA:O	1.93	0.67
1:B:2454:GLU:OE1	1:B:2464:LYS:HE3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2094:VAL:HB	1:B:2102:SER:HB3	1.77	0.67
1:B:2355:VAL:CG1	1:B:2363:LEU:HD13	2.25	0.67
1:B:2165:VAL:HG13	1:B:2165:VAL:O	1.95	0.67
1:B:2391:GLU:OE2	1:B:2487:PRO:HB2	1.93	0.67
1:A:1029:PHE:HB3	1:A:1032:LYS:HG3	1.76	0.67
1:A:1339:GLU:HB3	1:A:1346:THR:HB	1.75	0.67
1:B:2474:HIS:O	1:B:2475:ALA:HB3	1.95	0.67
1:B:2345:ILE:HG22	1:B:2376:PHE:HB2	1.78	0.66
1:A:1299:ASP:CG	1:A:1302:THR:HG23	2.16	0.66
1:B:2203:VAL:HG21	1:B:2205:ARG:HE	1.60	0.66
1:A:1266:GLN:HG3	1:A:1271:ARG:O	1.96	0.66
1:B:2027:GLU:HB3	1:B:2029:PHE:HB2	1.78	0.66
1:B:2299:ASP:OD1	1:B:2302:THR:N	2.29	0.66
1:A:1416:LEU:N	1:A:1416:LEU:CD1	2.58	0.66
1:A:1104:GLN:NE2	1:A:1111:TYR:HE1	1.92	0.65
1:B:2029:PHE:HB3	1:B:2032:LYS:HG3	1.79	0.65
1:A:1316:THR:HG22	1:A:1333:SER:HB3	1.79	0.65
1:B:2150:LYS:C	1:B:2151:ARG:HD3	2.16	0.65
1:A:1218:SER:C	1:A:1220:LYS:H	1.99	0.65
1:B:2398:ARG:HA	1:B:2408:ARG:HH12	1.61	0.65
1:B:2426:LYS:HA	1:B:2431:LYS:O	1.97	0.65
1:B:2457:ASP:OD1	1:B:2458:TYR:N	2.27	0.65
1:A:1203:VAL:HG21	1:A:1205:ARG:NH2	2.11	0.65
1:A:1136:ILE:HG23	1:A:1138:MET:SD	2.36	0.65
1:A:1339:GLU:HB3	1:A:1346:THR:CG2	2.27	0.65
1:B:2385:ILE:HG23	1:B:2413:VAL:CG1	2.27	0.65
1:A:1031:PHE:CZ	1:A:1068:ARG:CZ	2.80	0.64
1:B:2111:TYR:HE2	1:B:2126:VAL:HG22	1.62	0.64
1:B:2040:LEU:HD12	1:B:2040:LEU:C	2.17	0.64
1:B:2354:PHE:HE2	1:B:2370:ALA:HB2	1.63	0.64
1:B:2127:SER:N	1:B:2130:GLU:HG2	2.12	0.64
1:A:1216:PHE:CD1	1:A:1221:VAL:HG23	2.33	0.64
1:A:1338:ILE:CG2	1:A:1345:ILE:HD11	2.28	0.63
1:A:1182:GLN:NE2	1:A:1210:THR:OG1	2.31	0.63
1:B:2339:GLU:HB3	1:B:2346:THR:HB	1.79	0.63
1:B:2394:PHE:CG	1:B:2411:TYR:HB3	2.34	0.63
1:B:2147:VAL:HG23	1:B:2253:LEU:O	1.99	0.63
1:A:1341:ARG:NH1	1:A:1375:LEU:HD11	2.13	0.63
1:B:2338:ILE:HG21	1:B:2340:TRP:CZ2	2.34	0.63
1:B:2205:ARG:HH22	1:B:2207:GLU:CG	2.12	0.63
1:B:2362:GLN:HG2	1:B:2363:LEU:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1382:ASN:O	1:A:1383:ARG:HD3	1.98	0.62
1:A:1127:SER:N	1:A:1130:GLU:HG2	2.10	0.62
1:A:1139:HIS:ND1	1:A:1141:GLN:HG3	2.10	0.62
1:A:1008:GLU:HG2	1:A:1257:GLU:HB3	1.80	0.62
1:A:1425:ILE:HG21	1:A:1433:TRP:CE2	2.33	0.62
1:B:2316:THR:O	1:B:2323:VAL:HA	2.00	0.62
1:B:2382:ASN:O	1:B:2383:ARG:HD3	2.00	0.62
1:B:2426:LYS:HD3	1:B:2432:TYR:CZ	2.34	0.62
1:B:2203:VAL:HG21	1:B:2205:ARG:HH21	1.62	0.62
1:A:1396:GLY:HA3	1:A:1408:ARG:HD2	1.82	0.62
1:A:1042:LYS:O	1:A:1045:ILE:HG12	2.00	0.62
1:A:1122:PHE:O	1:A:1122:PHE:CD1	2.52	0.61
1:A:1426:LYS:HA	1:A:1431:LYS:O	1.99	0.61
1:B:2269:ASN:C	1:B:2269:ASN:OD1	2.38	0.61
1:B:2294:PHE:CE2	1:B:2309:THR:HG22	2.35	0.61
1:A:1198:HIS:CE1	1:A:1209:ALA:HB1	2.36	0.61
1:B:2343:ARG:O	1:B:2344:ARG:HD2	2.01	0.61
1:B:2252:GLU:OE2	1:B:2252:GLU:N	2.33	0.61
1:B:2294:PHE:HE2	1:B:2309:THR:HG22	1.65	0.61
1:B:2486:ASP:OD1	1:B:2488:ALA:HB3	2.00	0.61
1:A:1229:ARG:HG2	1:A:1243:GLY:O	2.01	0.61
1:A:1394:PHE:CG	1:A:1411:TYR:HB3	2.36	0.61
1:B:2400:VAL:HG22	1:B:2401:THR:N	2.16	0.61
1:B:2473:ASP:OD1	1:B:2474:HIS:O	2.19	0.61
1:A:1324:GLN:HG3	1:A:1326:THR:HB	1.83	0.60
1:A:1353:LYS:HB2	1:A:1365:ALA:O	2.00	0.60
1:B:2136:ILE:HD12	1:B:2138:MET:SD	2.41	0.60
1:A:1150:LYS:O	1:A:1151:ARG:HD3	2.01	0.60
1:B:2386:ILE:CG1	1:B:2416:LEU:HG	2.29	0.60
1:A:1183:ASP:C	1:A:1185:ARG:H	2.05	0.60
1:A:1383:ARG:O	1:A:1416:LEU:HD11	2.01	0.60
1:A:1438:ASP:N	1:A:1438:ASP:OD1	2.21	0.60
1:A:1474:HIS:O	1:A:1475:ALA:CB	2.48	0.60
1:A:1048:LEU:O	1:A:1049:GLU:HG3	2.01	0.60
1:B:2145:TYR:HB3	1:B:2255:ALA:HB3	1.84	0.60
1:B:2311:THR:O	1:B:2311:THR:HG22	2.02	0.60
1:A:1215:GLU:OE2	1:A:1230:TYR:OH	2.20	0.59
1:A:1385:ILE:HG23	1:A:1413:VAL:CG1	2.32	0.59
1:B:2152:TYR:CD2	1:B:2170:PRO:HG3	2.36	0.59
1:A:1416:LEU:HD13	1:A:1416:LEU:O	2.02	0.59
1:A:1040:LEU:C	1:A:1040:LEU:HD12	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:VAL:HG11	1:A:1233:PRO:HB3	1.83	0.59
1:A:1314:TYR:CZ	1:A:1330:LYS:HE2	2.38	0.59
1:B:2157:ALA:HB3	1:B:2158:ARG:NH1	2.17	0.59
1:B:2351:ASN:OD1	1:B:2351:ASN:C	2.40	0.59
1:B:2048:LEU:HD11	1:B:2060:VAL:HB	1.82	0.59
1:A:1111:TYR:HE2	1:A:1126:VAL:HG22	1.67	0.59
1:A:1217:ARG:CZ	1:A:1248:VAL:HG13	2.32	0.59
1:A:1048:LEU:HD11	1:A:1060:VAL:HB	1.85	0.59
1:A:1225:ASP:OD2	1:A:1229:ARG:NH2	2.36	0.59
1:B:2299:ASP:O	1:B:2303:LYS:HA	2.03	0.59
1:B:2321:GLY:O	1:B:2364:ALA:HB1	2.03	0.59
1:B:2434:THR:HG23	1:B:2449:VAL:CG1	2.32	0.59
1:B:2465:VAL:O	1:B:2465:VAL:HG13	2.01	0.59
1:A:1145:TYR:HB3	1:A:1255:ALA:HB3	1.85	0.59
1:A:1150:LYS:C	1:A:1151:ARG:HD3	2.23	0.58
1:A:1404:LEU:HD21	1:A:1433:TRP:CE2	2.38	0.58
1:B:2354:PHE:CE2	1:B:2370:ALA:HB2	2.37	0.58
1:A:1354:PHE:HD2	1:A:1370:ALA:HA	1.67	0.58
1:B:2275:THR:HG22	1:B:2281:LEU:HD23	1.85	0.58
1:B:2343:ARG:HD3	1:B:2420:ASP:O	2.03	0.58
1:A:1291:GLN:HB2	1:A:1292:GLU:OE1	2.03	0.58
1:B:2165:VAL:HG12	1:B:2238:GLY:O	2.03	0.58
1:A:1198:HIS:ND1	1:A:1209:ALA:HB1	2.18	0.58
1:A:1314:TYR:OH	1:A:1330:LYS:HE2	2.04	0.58
1:A:1389:ARG:CG	1:A:1394:PHE:CE2	2.86	0.58
1:A:1203:VAL:HG21	1:A:1205:ARG:NE	2.19	0.58
1:B:2386:ILE:HD11	1:B:2416:LEU:HG	1.86	0.58
1:A:1348:ARG:HB2	1:A:1354:PHE:CE1	2.38	0.58
1:A:1386:ILE:CG1	1:A:1416:LEU:HG	2.33	0.58
1:A:1358:LYS:HB3	1:A:1360:ASN:HD21	1.68	0.57
1:B:2266:GLN:HB3	1:B:2377:LEU:HB3	1.85	0.57
1:B:2148:THR:HG21	1:B:2251:ASP:CG	2.24	0.57
1:B:2269:ASN:O	1:B:2270:GLU:HB2	2.04	0.57
1:A:1379:LYS:HD3	1:A:1418:PHE:CD2	2.39	0.57
1:B:2229:ARG:HG2	1:B:2243:GLY:O	2.04	0.57
1:B:2425:ILE:HG21	1:B:2433:TRP:CE2	2.39	0.57
1:A:1234:SER:OG	1:A:1241:LYS:HD3	2.04	0.57
1:B:2348:ARG:HB2	1:B:2354:PHE:CE1	2.39	0.57
1:A:1203:VAL:CB	1:A:1205:ARG:HE	2.17	0.57
1:A:1040:LEU:HD23	1:A:1135:HIS:CE1	2.39	0.57
1:A:1345:ILE:HG22	1:A:1376:PHE:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2198:HIS:ND1	1:B:2209:ALA:HB1	2.19	0.57
1:B:2167:ARG:NH1	1:B:2174:ASP:HB2	2.20	0.57
1:B:2218:SER:C	1:B:2220:LYS:H	2.08	0.57
1:A:1205:ARG:HH22	1:A:1207:GLU:HG2	1.67	0.57
1:A:1031:PHE:CE2	1:A:1068:ARG:NE	2.73	0.57
1:A:1316:THR:O	1:A:1323:VAL:HA	2.06	0.56
1:B:2217:ARG:CZ	1:B:2248:VAL:HG13	2.34	0.56
1:B:2148:THR:HG21	1:B:2251:ASP:OD2	2.05	0.56
1:B:2324:GLN:CG	1:B:2326:THR:HB	2.35	0.56
1:A:1486:ASP:HB2	1:A:1487:PRO:HD2	1.88	0.56
1:B:2316:THR:N	1:B:2324:GLN:O	2.39	0.56
1:B:2398:ARG:NH1	1:B:2405:ASP:OD1	2.37	0.56
1:A:1049:GLU:OE2	1:A:1063:ARG:HG3	2.05	0.56
1:A:1205:ARG:NH2	1:A:1207:GLU:HG2	2.21	0.56
1:A:1269:ASN:HD21	1:A:1283:ALA:CB	2.19	0.56
1:A:1386:ILE:CD1	1:A:1416:LEU:HG	2.35	0.56
1:A:1090:ARG:HB3	1:A:1090:ARG:HH11	1.70	0.56
1:A:1183:ASP:C	1:A:1185:ARG:N	2.57	0.56
1:B:2358:LYS:HB3	1:B:2360:ASN:HD21	1.69	0.56
1:B:2422:ALA:HB1	1:B:2450:ASP:HB3	1.88	0.56
1:B:2097:ASP:HA	1:B:2224:ARG:CZ	2.35	0.56
1:A:1207:GLU:CB	1:A:1208:PRO:HD2	2.36	0.56
1:A:1313:LYS:CG	1:A:1327:ALA:O	2.53	0.56
1:A:1294:PHE:CE2	1:A:1309:THR:HG22	2.41	0.56
1:B:2203:VAL:HG21	1:B:2205:ARG:NH2	2.20	0.56
1:A:1159:PRO:O	1:A:1160:ALA:O	2.23	0.56
1:A:1165:VAL:HG13	1:A:1165:VAL:O	2.06	0.56
1:B:2197:ARG:HD2	1:B:2199:ASP:CG	2.27	0.55
1:B:2203:VAL:HG21	1:B:2205:ARG:NE	2.21	0.55
1:A:1096:HIS:NE2	1:A:1102:SER:HB2	2.22	0.55
1:B:2271:ARG:HG2	1:B:2271:ARG:HH11	1.71	0.55
1:B:2316:THR:HG22	1:B:2333:SER:HB3	1.89	0.55
1:A:1294:PHE:HE2	1:A:1309:THR:HG22	1.72	0.55
1:A:1398:ARG:HD2	1:A:1403:THR:HB	1.88	0.55
1:B:2048:LEU:O	1:B:2049:GLU:HG3	2.07	0.55
1:B:2188:VAL:O	1:B:2188:VAL:HG12	2.05	0.55
1:B:2041:LYS:O	1:B:2045:ILE:HG23	2.06	0.55
1:A:1271:ARG:HH11	1:A:1271:ARG:HG2	1.71	0.55
1:B:2063:ARG:NE	1:B:2067:GLY:HA2	2.22	0.55
1:B:2159:PRO:O	1:B:2160:ALA:O	2.25	0.55
1:B:2398:ARG:HA	1:B:2408:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2398:ARG:O	1:B:2400:VAL:N	2.39	0.55
1:A:1041:LYS:O	1:A:1045:ILE:HG23	2.07	0.55
1:A:1158:ARG:CB	1:A:1159:PRO:HD3	2.10	0.55
1:B:2093:ILE:HD13	1:B:2101:TRP:CH2	2.42	0.55
1:B:2198:HIS:CE1	1:B:2209:ALA:HB1	2.42	0.55
1:B:2358:LYS:O	1:B:2359:LYS:C	2.44	0.55
1:B:2207:GLU:CB	1:B:2208:PRO:HD2	2.35	0.54
1:A:1150:LYS:HG3	1:A:1151:ARG:NE	2.17	0.54
1:A:1315:TRP:O	1:A:1334:CYS:HB3	2.06	0.54
1:B:2339:GLU:HB3	1:B:2346:THR:HG22	1.89	0.54
1:A:1180:ALA:HA	1:A:1411:TYR:OH	2.07	0.54
1:B:2416:LEU:CD1	1:B:2416:LEU:N	2.70	0.54
1:B:2469:TYR:HB2	1:B:2482:ALA:HB3	1.89	0.54
1:A:1205:ARG:CZ	1:A:1207:GLU:HB3	2.38	0.54
1:A:1319:ALA:C	1:A:1321:GLY:H	2.10	0.54
1:B:2259:SER:HB3	1:B:2383:ARG:HH12	1.72	0.54
1:A:1203:VAL:HB	1:A:1205:ARG:HE	1.73	0.54
1:A:1331:ASN:O	1:A:1333:SER:N	2.42	0.54
1:A:1322:GLY:HA2	1:A:1364:ALA:HB2	1.89	0.54
1:A:1422:ALA:HB1	1:A:1450:ASP:HB3	1.90	0.54
1:A:1338:ILE:HG23	1:A:1345:ILE:HD11	1.89	0.53
1:A:1339:GLU:HB3	1:A:1346:THR:CB	2.38	0.53
1:B:2063:ARG:HG2	1:B:2069:TYR:CE1	2.43	0.53
1:B:2339:GLU:HB3	1:B:2346:THR:CB	2.37	0.53
1:A:1398:ARG:HG3	1:A:1408:ARG:HH12	1.73	0.53
1:B:2030:GLY:O	1:B:2032:LYS:HG2	2.07	0.53
1:A:1151:ARG:N	1:A:1151:ARG:HD3	2.18	0.53
1:A:1269:ASN:ND2	1:A:1283:ALA:HB3	2.23	0.53
1:B:2314:TYR:OH	1:B:2330:LYS:HE2	2.09	0.53
1:A:1341:ARG:O	1:A:1342:ASP:C	2.46	0.53
1:B:2049:GLU:OE2	1:B:2063:ARG:HG3	2.09	0.53
1:A:1304:LYS:HG2	1:A:1337:ASP:OD2	2.09	0.53
1:A:1477:VAL:HG23	1:A:1477:VAL:O	2.08	0.53
1:B:2338:ILE:CG2	1:B:2345:ILE:HD11	2.39	0.53
1:B:2434:THR:CG2	1:B:2449:VAL:HG11	2.38	0.53
1:B:2213:THR:OG1	1:B:2224:ARG:HB3	2.09	0.53
1:B:2355:VAL:HG13	1:B:2363:LEU:HD13	1.91	0.53
1:B:2474:HIS:O	1:B:2475:ALA:CB	2.57	0.53
1:A:1072:ALA:HA	1:A:1077:ASN:O	2.08	0.53
1:A:1185:ARG:NH2	1:A:1226:CYS:HA	2.23	0.53
1:B:2065:HIS:HE1	1:B:2066:LEU:HD21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2238:GLY:O	1:B:2239:THR:C	2.46	0.52
1:A:1136:ILE:HD12	1:A:1138:MET:SD	2.50	0.52
1:A:1229:ARG:HB2	1:A:1229:ARG:CZ	2.39	0.52
1:A:1275:THR:HG22	1:A:1281:LEU:HD23	1.92	0.52
1:A:1281:LEU:HD13	1:A:1315:TRP:CE2	2.45	0.52
1:B:2282:SER:HB3	1:B:2362:GLN:CA	2.29	0.52
1:B:2152:TYR:CG	1:B:2170:PRO:HG3	2.44	0.52
1:A:1377:LEU:HD23	1:A:1377:LEU:O	2.09	0.52
1:A:1474:HIS:C	1:A:1476:GLY:H	2.13	0.52
1:B:2346:THR:O	1:B:2346:THR:HG22	2.09	0.52
1:A:1348:ARG:NE	1:A:1354:PHE:HE1	2.08	0.52
1:B:2063:ARG:HD3	1:B:2069:TYR:CE2	2.45	0.52
1:B:2081:GLU:O	1:B:2081:GLU:HG2	2.10	0.52
1:B:2216:PHE:CD1	1:B:2221:VAL:HG23	2.45	0.52
1:A:1331:ASN:O	1:A:1332:ALA:C	2.47	0.52
1:A:1385:ILE:HG23	1:A:1413:VAL:HG13	1.90	0.52
1:B:2072:ALA:HA	1:B:2077:ASN:O	2.10	0.52
1:B:2149:ARG:HD2	1:B:2233:PRO:HB2	1.92	0.52
1:A:1167:ARG:NH2	1:A:1171:TRP:HB3	2.25	0.51
1:A:1205:ARG:NH2	1:A:1207:GLU:CG	2.71	0.51
1:A:1358:LYS:HB3	1:A:1360:ASN:ND2	2.25	0.51
1:B:2010:VAL:CG1	1:B:2256:LEU:O	2.59	0.51
1:A:1457:ASP:OD1	1:A:1458:TYR:N	2.35	0.51
1:A:1127:SER:H	1:A:1130:GLU:CG	2.11	0.51
1:B:2342:ASP:O	1:B:2343:ARG:CB	2.57	0.51
1:A:1201:ARG:HG2	1:A:1202:LEU:H	1.74	0.51
1:A:1266:GLN:HB3	1:A:1377:LEU:HB3	1.92	0.51
1:A:1299:ASP:O	1:A:1303:LYS:HA	2.10	0.51
1:A:1358:LYS:O	1:A:1359:LYS:C	2.48	0.51
1:B:2205:ARG:NH2	1:B:2207:GLU:HG2	2.26	0.51
1:A:1389:ARG:HG2	1:A:1394:PHE:CE2	2.45	0.51
1:B:2183:ASP:C	1:B:2185:ARG:N	2.63	0.51
1:B:2473:ASP:OD1	1:B:2477:VAL:HG22	2.10	0.51
1:B:2136:ILE:CG2	1:B:2138:MET:SD	2.95	0.51
1:A:1319:ALA:C	1:A:1321:GLY:N	2.64	0.51
1:B:2031:PHE:CZ	1:B:2068:ARG:CZ	2.93	0.51
1:B:2203:VAL:CB	1:B:2205:ARG:HE	2.23	0.51
1:B:2474:HIS:C	1:B:2476:GLY:H	2.14	0.51
1:A:1339:GLU:CB	1:A:1346:THR:HG22	2.41	0.50
1:B:2281:LEU:HD13	1:B:2315:TRP:CE2	2.46	0.50
1:B:2379:LYS:HB2	1:B:2418:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:ARG:HH22	1:A:1226:CYS:HA	1.75	0.50
1:A:1317:LEU:HD12	1:A:1322:GLY:O	2.10	0.50
1:A:1469:TYR:HB2	1:A:1482:ALA:HB3	1.93	0.50
1:B:2065:HIS:CE1	1:B:2066:LEU:HD21	2.47	0.50
1:B:2182:GLN:NE2	1:B:2210:THR:OG1	2.44	0.50
1:B:2269:ASN:OD1	1:B:2271:ARG:N	2.45	0.50
1:B:2343:ARG:HH11	1:B:2343:ARG:CG	2.22	0.50
1:A:1154:HIS:CE1	1:A:1164:ALA:HB3	2.47	0.50
1:A:1238:GLY:O	1:A:1239:THR:C	2.49	0.50
1:A:1342:ASP:HB2	1:A:1452:PHE:CG	2.46	0.50
1:B:2339:GLU:O	1:B:2345:ILE:HD12	2.10	0.50
1:B:2358:LYS:HB3	1:B:2360:ASN:ND2	2.27	0.50
1:A:1069:TYR:CD2	1:A:1069:TYR:N	2.78	0.50
1:A:1082:ARG:HH21	1:A:1086:GLY:HA3	1.77	0.50
1:A:1183:ASP:O	1:A:1185:ARG:N	2.45	0.50
1:A:1269:ASN:OD1	1:A:1271:ARG:CB	2.45	0.50
1:B:2205:ARG:O	1:B:2205:ARG:HG2	2.11	0.50
1:A:1218:SER:C	1:A:1220:LYS:N	2.64	0.50
1:A:1397:CYS:HB2	1:A:1412:ASP:OD1	2.12	0.50
1:A:1045:ILE:HD11	1:A:1065:HIS:CD2	2.46	0.50
1:A:1197:ARG:HD2	1:A:1199:ASP:CG	2.32	0.50
1:A:1471:LYS:HB2	1:A:1489:SER:HB3	1.93	0.50
1:B:2274:SER:HB3	1:B:2292:GLU:HG3	1.94	0.50
1:B:2432:TYR:CD1	1:B:2448:PRO:HB3	2.47	0.50
1:A:1387:VAL:CG2	1:A:1413:VAL:HG22	2.42	0.49
1:B:2314:TYR:CZ	1:B:2330:LYS:HE2	2.47	0.49
1:A:1010:VAL:CG1	1:A:1256:LEU:HB2	2.42	0.49
1:A:1339:GLU:CB	1:A:1346:THR:CG2	2.90	0.49
1:B:2093:ILE:HG21	1:B:2101:TRP:CE2	2.48	0.49
1:A:1149:ARG:HD2	1:A:1233:PRO:HB2	1.93	0.49
1:A:1181:PHE:HE1	1:A:1186:TYR:HH	1.58	0.49
1:B:2205:ARG:HH22	1:B:2207:GLU:HG2	1.76	0.49
1:A:1367:VAL:CG1	1:A:1368:GLU:N	2.76	0.49
1:B:2205:ARG:NH1	1:B:2207:GLU:OE1	2.45	0.49
1:B:2308:ARG:HB2	1:B:2314:TYR:CE2	2.48	0.49
1:A:1149:ARG:HD2	1:A:1233:PRO:CB	2.43	0.49
1:A:1224:ARG:HG3	1:A:1230:TYR:CE2	2.48	0.49
1:A:1148:THR:HG21	1:A:1251:ASP:OD2	2.12	0.49
1:B:2096:HIS:O	1:B:2097:ASP:C	2.50	0.49
1:B:2416:LEU:HD13	1:B:2416:LEU:O	2.13	0.49
1:B:2486:ASP:HB2	1:B:2487:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1486:ASP:OD1	1:A:1488:ALA:HB3	2.12	0.49
1:B:2150:LYS:CG	1:B:2150:LYS:O	2.61	0.49
1:B:2151:ARG:N	1:B:2151:ARG:HD3	2.19	0.49
1:B:2170:PRO:HA	1:B:2175:SER:OG	2.13	0.49
1:A:1205:ARG:HH12	1:A:1207:GLU:CB	2.19	0.49
1:A:1387:VAL:HG22	1:A:1413:VAL:HG22	1.95	0.49
1:A:1030:GLY:O	1:A:1031:PHE:C	2.51	0.48
1:A:1252:GLU:N	1:A:1252:GLU:OE2	2.47	0.48
1:A:1417:GLU:OE1	1:A:1432:TYR:OH	2.28	0.48
1:B:2008:GLU:O	1:B:2258:GLN:HG2	2.13	0.48
1:B:2100:ARG:CB	1:B:2132:TRP:O	2.48	0.48
1:B:2186:TYR:O	1:B:2212:TYR:N	2.44	0.48
1:B:2274:SER:CB	1:B:2292:GLU:HG3	2.43	0.48
1:B:2275:THR:HG22	1:B:2281:LEU:CD2	2.43	0.48
1:A:1339:GLU:HB3	1:A:1346:THR:HG22	1.95	0.48
1:A:1149:ARG:NH2	1:A:1235:GLY:O	2.47	0.48
1:A:1321:GLY:O	1:A:1364:ALA:HB1	2.14	0.48
1:B:2342:ASP:HB2	1:B:2452:PHE:CD2	2.49	0.48
1:B:2042:LYS:O	1:B:2045:ILE:HG12	2.13	0.48
1:B:2090:ARG:CB	1:B:2090:ARG:HH11	2.24	0.48
1:B:2384:PRO:O	1:B:2385:ILE:HD13	2.14	0.48
1:A:1022:LYS:HA	1:A:1037:ALA:O	2.13	0.48
1:A:1269:ASN:HD21	1:A:1283:ALA:HB3	1.77	0.48
1:B:2063:ARG:HG2	1:B:2069:TYR:CZ	2.49	0.48
1:B:2203:VAL:HB	1:B:2205:ARG:HE	1.78	0.48
1:B:2434:THR:HG23	1:B:2449:VAL:HG11	1.95	0.48
1:A:1261:ALA:HB2	1:A:1493:TYR:CE2	2.49	0.48
1:B:2115:THR:HG23	1:B:2116:GLU:N	2.28	0.48
1:B:2407:ASN:ND2	1:B:2476:GLY:HA3	2.29	0.48
1:A:1156:SER:HB2	1:A:1164:ALA:HB2	1.95	0.48
1:A:1269:ASN:CG	1:A:1271:ARG:HB2	2.32	0.48
1:B:2212:TYR:CZ	1:B:2231:LEU:HD21	2.49	0.48
1:B:2389:ARG:CG	1:B:2394:PHE:CE2	2.97	0.48
1:A:1215:GLU:OE2	1:A:1230:TYR:CZ	2.67	0.47
1:A:1343:ARG:CG	1:A:1343:ARG:NH1	2.75	0.47
1:B:2095:ALA:HB2	1:B:2215:GLU:CG	2.36	0.47
1:A:1355:VAL:HG13	1:A:1363:LEU:HD13	1.93	0.47
1:A:1351:ASN:C	1:A:1351:ASN:OD1	2.52	0.47
1:A:1373:SER:OG	1:A:1374:GLU:OE2	2.27	0.47
1:B:2197:ARG:HB3	1:B:2199:ASP:OD1	2.15	0.47
1:A:1158:ARG:H	1:A:1158:ARG:HH11	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2017:ILE:HA	1:B:2022:LYS:O	2.14	0.47
1:B:2313:LYS:HG3	1:B:2327:ALA:O	2.14	0.47
1:A:1078:VAL:HG12	1:A:1120:SER:HA	1.96	0.47
1:A:1048:LEU:HD12	1:A:1048:LEU:HA	1.48	0.47
1:B:2259:SER:CB	1:B:2383:ARG:HH12	2.28	0.47
1:A:1197:ARG:HA	1:A:1210:THR:HG22	1.95	0.47
1:B:2156:SER:HB2	1:B:2164:ALA:HB2	1.95	0.47
1:B:2252:GLU:N	1:B:2252:GLU:CD	2.68	0.47
1:B:2385:ILE:CD1	1:B:2415:GLN:HB3	2.44	0.47
1:A:1115:THR:O	1:A:1116:GLU:C	2.53	0.47
1:A:1339:GLU:OE2	1:A:1346:THR:HG21	2.15	0.47
1:B:2197:ARG:HA	1:B:2210:THR:HG22	1.96	0.47
1:B:2205:ARG:NH2	1:B:2207:GLU:CG	2.78	0.47
1:A:1132:TRP:CD1	1:A:1132:TRP:N	2.82	0.47
1:A:1269:ASN:O	1:A:1270:GLU:CB	2.57	0.47
1:B:2100:ARG:CD	1:B:2100:ARG:N	2.77	0.47
1:B:2386:ILE:CD1	1:B:2416:LEU:HG	2.44	0.47
1:A:1426:LYS:HG3	1:A:1431:LYS:O	2.15	0.47
1:B:2264:VAL:HG11	1:B:2288:GLU:HG2	1.97	0.47
1:A:1127:SER:O	1:A:1128:PRO:C	2.53	0.46
1:B:2063:ARG:HE	1:B:2067:GLY:HA2	1.79	0.46
1:B:2109:ARG:CG	1:B:2109:ARG:HH11	2.28	0.46
1:A:1127:SER:O	1:A:1129:ALA:N	2.47	0.46
1:A:1316:THR:N	1:A:1324:GLN:O	2.48	0.46
1:A:1150:LYS:O	1:A:1150:LYS:CG	2.62	0.46
1:B:2093:ILE:HG23	1:B:2101:TRP:CD2	2.51	0.46
1:B:2367:VAL:CG1	1:B:2369:THR:O	2.62	0.46
1:B:2300:ARG:NH2	1:B:2458:TYR:CZ	2.84	0.46
1:A:1063:ARG:HG2	1:A:1069:TYR:CE1	2.50	0.46
1:A:1167:ARG:NH1	1:A:1174:ASP:HB2	2.31	0.46
1:A:1207:GLU:HB2	1:A:1208:PRO:CD	2.42	0.46
1:B:2069:TYR:N	1:B:2069:TYR:CD2	2.83	0.46
1:B:2446:ASP:OD1	1:B:2446:ASP:N	2.45	0.46
1:A:1017:ILE:HA	1:A:1022:LYS:O	2.16	0.46
1:A:1076:GLY:HA2	1:A:1121:CYS:O	2.16	0.46
1:A:1008:GLU:CG	1:A:1257:GLU:HB3	2.45	0.46
1:A:1010:VAL:HG12	1:A:1256:LEU:C	2.35	0.46
1:A:1030:GLY:O	1:A:1032:LYS:HG2	2.16	0.46
1:A:1317:LEU:HD12	1:A:1317:LEU:HA	1.59	0.46
1:B:2205:ARG:HH12	1:B:2207:GLU:CB	2.25	0.46
1:A:1016:LEU:O	1:A:1023:TYR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:ARG:HG2	1:A:1202:LEU:N	2.31	0.46
1:A:1289:THR:C	1:A:1291:GLN:N	2.68	0.46
1:B:2045:ILE:HG13	1:B:2045:ILE:O	2.16	0.46
1:B:2471:LYS:HB2	1:B:2489:SER:HB3	1.98	0.46
1:A:1473:ASP:OD1	1:A:1474:HIS:O	2.34	0.46
1:B:2142:VAL:HG21	1:B:2256:LEU:HD22	1.98	0.46
1:B:2465:VAL:CG1	1:B:2465:VAL:O	2.63	0.46
1:A:1264:VAL:HG21	1:A:1288:GLU:HG2	1.96	0.46
1:B:2048:LEU:HD11	1:B:2060:VAL:CB	2.46	0.46
1:A:1269:ASN:OD1	1:A:1271:ARG:N	2.49	0.46
1:A:1041:LYS:H	1:A:1044:GLN:HB2	1.81	0.45
1:A:1105:SER:O	1:A:1109:ARG:N	2.45	0.45
1:A:1340:TRP:HA	1:A:1345:ILE:CD1	2.46	0.45
1:B:2389:ARG:HG3	1:B:2394:PHE:CE2	2.50	0.45
1:B:2379:LYS:HB2	1:B:2418:PHE:CE2	2.51	0.45
1:A:1322:GLY:HA2	1:A:1364:ALA:CB	2.46	0.45
1:A:1426:LYS:HD3	1:A:1432:TYR:CZ	2.52	0.45
1:B:2063:ARG:CG	1:B:2069:TYR:CZ	3.00	0.45
1:B:2071:ALA:O	1:B:2078:VAL:HA	2.17	0.45
1:A:1187:SER:HB3	1:A:1210:THR:O	2.16	0.45
1:A:1148:THR:HG21	1:A:1251:ASP:CG	2.36	0.45
1:A:1282:SER:CB	1:A:1362:GLN:HA	2.33	0.45
1:B:2284:ASN:ND2	1:B:2285:GLN:HG2	2.31	0.45
1:A:1093:ILE:HD13	1:A:1101:TRP:CH2	2.52	0.45
1:A:1111:TYR:N	1:A:1111:TYR:CD1	2.83	0.45
1:B:2031:PHE:CE2	1:B:2068:ARG:NE	2.83	0.45
1:B:2183:ASP:C	1:B:2185:ARG:H	2.18	0.45
1:B:2343:ARG:NH2	1:B:2450:ASP:OD2	2.50	0.45
1:B:2381:ILE:HG13	1:B:2382:ASN:N	2.32	0.45
1:A:1150:LYS:NZ	1:A:1168:ASP:OD1	2.48	0.45
1:A:1398:ARG:CG	1:A:1408:ARG:HH12	2.28	0.45
1:B:2339:GLU:CB	1:B:2346:THR:HG22	2.47	0.45
1:B:2379:LYS:HD3	1:B:2418:PHE:CD2	2.52	0.45
1:B:2224:ARG:HG3	1:B:2230:TYR:CE2	2.52	0.45
1:B:2275:THR:CG2	1:B:2281:LEU:CD2	2.94	0.45
1:A:1297:GLU:OE1	1:A:1330:LYS:NZ	2.32	0.45
1:A:1444:SER:HB2	1:A:1445:GLY:H	1.47	0.45
1:B:2149:ARG:HD2	1:B:2233:PRO:CB	2.46	0.45
1:B:2082:ARG:HH21	1:B:2086:GLY:HA3	1.83	0.44
1:B:2205:ARG:CZ	1:B:2207:GLU:OE1	2.65	0.44
1:B:2422:ALA:CB	1:B:2450:ASP:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:LYS:NZ	1:A:1407:ASN:HB2	2.32	0.44
1:B:2069:TYR:CE1	1:B:2085:PRO:HG3	2.52	0.44
1:B:2271:ARG:CG	1:B:2271:ARG:HH11	2.30	0.44
1:B:2227:GLU:HB2	1:B:2229:ARG:HE	1.83	0.44
1:A:1126:VAL:HA	1:A:1130:GLU:HG3	1.99	0.44
1:A:1354:PHE:CD2	1:A:1370:ALA:HA	2.50	0.44
1:B:2065:HIS:CE1	1:B:2066:LEU:CD2	3.01	0.44
1:B:2095:ALA:HB1	1:B:2224:ARG:HD2	2.00	0.44
1:B:2338:ILE:HG23	1:B:2345:ILE:HD11	1.98	0.44
1:A:1203:VAL:HG21	1:A:1205:ARG:CZ	2.46	0.44
1:A:1437:SER:C	1:A:1439:SER:H	2.20	0.44
1:B:2017:ILE:CG2	1:B:2021:ASN:HA	2.48	0.44
1:B:2169:VAL:HA	1:B:2170:PRO:HD3	1.82	0.44
1:B:2263:VAL:HG21	1:B:2378:MET:HE2	1.99	0.44
1:A:1213:THR:OG1	1:A:1224:ARG:HB3	2.17	0.44
1:B:2260:CYS:O	1:B:2261:ALA:C	2.54	0.44
1:A:1111:TYR:HD1	1:A:1111:TYR:N	2.16	0.44
1:A:1139:HIS:ND1	1:A:1140:PRO:HD2	2.33	0.44
1:A:1265:LEU:HB2	1:A:1273:VAL:HG13	1.99	0.44
1:B:2331:ASN:O	1:B:2332:ALA:C	2.54	0.44
1:B:2338:ILE:HG21	1:B:2340:TRP:CE2	2.52	0.44
1:A:1385:ILE:HA	1:A:1385:ILE:HD13	1.66	0.44
1:B:2331:ASN:O	1:B:2333:SER:N	2.51	0.44
1:B:2427:ASP:C	1:B:2427:ASP:OD1	2.55	0.44
1:A:1159:PRO:O	1:A:1160:ALA:C	2.56	0.44
1:A:1319:ALA:O	1:A:1321:GLY:N	2.51	0.44
1:A:1470:LEU:HD12	1:A:1470:LEU:HA	1.75	0.44
1:B:2043:LYS:HD2	1:B:2065:HIS:NE2	2.33	0.44
1:B:2074:LYS:HG2	1:B:2108:HIS:ND1	2.33	0.44
1:B:2361:GLY:C	1:B:2362:GLN:O	2.54	0.44
1:B:2426:LYS:HG3	1:B:2431:LYS:O	2.17	0.44
1:A:1269:ASN:C	1:A:1269:ASN:OD1	2.56	0.43
1:A:1017:ILE:HG23	1:A:1022:LYS:O	2.17	0.43
1:A:1063:ARG:HG2	1:A:1069:TYR:CZ	2.52	0.43
1:A:1155:LEU:HD23	1:A:1156:SER:N	2.33	0.43
1:A:1271:ARG:CG	1:A:1271:ARG:HH11	2.29	0.43
1:B:2096:HIS:NE2	1:B:2102:SER:HB2	2.33	0.43
1:B:2100:ARG:HB2	1:B:2101:TRP:H	1.45	0.43
1:A:1369:THR:O	1:A:1370:ALA:C	2.57	0.43
1:B:2048:LEU:HD12	1:B:2048:LEU:HA	1.77	0.43
1:B:2269:ASN:CG	1:B:2271:ARG:HB2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2339:GLU:CB	1:B:2346:THR:CG2	2.94	0.43
1:B:2395:ILE:HA	1:B:2405:ASP:O	2.17	0.43
1:A:1186:TYR:O	1:A:1212:TYR:N	2.51	0.43
1:A:1361:GLY:C	1:A:1362:GLN:O	2.55	0.43
1:B:2094:VAL:HB	1:B:2102:SER:CB	2.47	0.43
1:B:2343:ARG:HG2	1:B:2452:PHE:HE2	1.82	0.43
1:B:2367:VAL:CG1	1:B:2368:GLU:N	2.81	0.43
1:A:1045:ILE:O	1:A:1045:ILE:HG13	2.18	0.43
1:A:1232:ALA:HB1	1:A:1233:PRO:HD2	2.00	0.43
1:A:1324:GLN:CG	1:A:1326:THR:HB	2.49	0.43
1:B:2151:ARG:HA	1:B:2151:ARG:HD3	1.57	0.43
1:A:1169:VAL:HA	1:A:1170:PRO:HD3	1.76	0.43
1:A:1190:THR:HG21	1:A:1202:LEU:HD21	2.00	0.43
1:B:2386:ILE:HG12	1:B:2416:LEU:HG	2.00	0.43
1:A:1151:ARG:HH11	1:A:1151:ARG:CG	2.32	0.43
1:A:1380:LEU:HA	1:A:1380:LEU:HD23	1.72	0.43
1:B:2043:LYS:CA	1:B:2065:HIS:CD2	2.87	0.43
1:B:2166:ASP:OD1	1:B:2166:ASP:N	2.52	0.43
1:B:2282:SER:CB	1:B:2362:GLN:HA	2.31	0.43
1:B:2366:SER:O	1:B:2367:VAL:C	2.58	0.43
1:A:1152:TYR:CE2	1:A:1170:PRO:HG3	2.54	0.42
1:A:1269:ASN:ND2	1:A:1283:ALA:CB	2.81	0.42
1:B:2074:LYS:HG2	1:B:2108:HIS:CE1	2.54	0.42
1:B:2161:ASP:N	1:B:2161:ASP:OD1	2.52	0.42
1:B:2319:ALA:C	1:B:2321:GLY:H	2.22	0.42
1:B:2383:ARG:N	1:B:2384:PRO:CD	2.81	0.42
1:B:2289:THR:O	1:B:2291:GLN:N	2.52	0.42
1:B:2193:HIS:NE2	1:B:2385:ILE:HD11	2.34	0.42
1:A:1438:ASP:O	1:A:1439:SER:HB2	2.19	0.42
1:B:2275:THR:CG2	1:B:2281:LEU:HD22	2.49	0.42
1:A:1098:ASP:O	1:A:1099:GLY:O	2.38	0.42
1:B:2296:LEU:HD13	1:B:2378:MET:HE2	2.01	0.42
1:B:2382:ASN:O	1:B:2382:ASN:CG	2.57	0.42
1:B:2400:VAL:HG13	1:B:2401:THR:N	2.26	0.42
1:B:2432:TYR:CG	1:B:2448:PRO:HB3	2.54	0.42
1:B:2438:ASP:O	1:B:2439:SER:HB2	2.20	0.42
1:A:1071:ALA:O	1:A:1078:VAL:HA	2.19	0.42
1:A:1289:THR:C	1:A:1291:GLN:H	2.21	0.42
1:A:1407:ASN:ND2	1:A:1476:GLY:HA3	2.35	0.42
1:A:1150:LYS:CG	1:A:1151:ARG:HE	2.21	0.42
1:A:1289:THR:O	1:A:1291:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:THR:HG22	1:A:1311:THR:O	2.19	0.42
1:B:2135:HIS:C	1:B:2135:HIS:CD2	2.93	0.42
1:B:2225:ASP:C	1:B:2225:ASP:OD1	2.57	0.42
1:B:2400:VAL:HG13	1:B:2401:THR:HG23	2.01	0.42
1:A:1064:SER:C	1:A:1066:LEU:H	2.23	0.42
1:A:1282:SER:HB3	1:A:1362:GLN:CA	2.32	0.42
1:B:2181:PHE:CD1	1:B:2186:TYR:CE1	3.08	0.42
1:B:2341:ARG:NH1	1:B:2375:LEU:HD11	2.34	0.42
1:A:1073:ASP:C	1:A:1073:ASP:OD1	2.58	0.42
1:A:1266:GLN:HA	1:A:1271:ARG:O	2.20	0.42
1:B:2041:LYS:H	1:B:2044:GLN:HB2	1.84	0.42
1:B:2078:VAL:HG12	1:B:2120:SER:HA	2.02	0.42
1:A:1434:THR:HG23	1:A:1449:VAL:CG1	2.48	0.42
1:B:2096:HIS:O	1:B:2098:ASP:N	2.53	0.42
1:B:2158:ARG:HH11	1:B:2158:ARG:H	1.68	0.42
1:B:2289:THR:C	1:B:2291:GLN:N	2.73	0.42
1:B:2343:ARG:C	1:B:2344:ARG:HD2	2.39	0.42
1:A:1096:HIS:O	1:A:1097:ASP:C	2.58	0.42
1:A:1102:SER:OG	1:A:1126:VAL:CG1	2.68	0.42
1:A:1361:GLY:O	1:A:1362:GLN:O	2.38	0.42
1:A:1432:TYR:CE1	1:A:1448:PRO:HB3	2.55	0.42
1:A:1342:ASP:HB2	1:A:1452:PHE:CD2	2.55	0.42
1:A:1063:ARG:HG3	1:A:1063:ARG:HH11	1.83	0.41
1:A:1218:SER:O	1:A:1220:LYS:N	2.48	0.41
1:A:1343:ARG:NH2	1:A:1450:ASP:OD2	2.49	0.41
1:A:1454:GLU:OE1	1:A:1464:LYS:HE3	2.20	0.41
1:B:2127:SER:O	1:B:2129:ALA:N	2.52	0.41
1:B:2417:GLU:OE1	1:B:2432:TYR:OH	2.26	0.41
1:A:1040:LEU:HD11	1:A:1045:ILE:HG22	2.02	0.41
1:A:1100:ARG:HB3	1:A:1133:SER:HA	2.00	0.41
1:A:1490:LEU:HD23	1:A:1490:LEU:HA	1.76	0.41
1:B:2040:LEU:HD11	1:B:2045:ILE:HG22	2.02	0.41
1:B:2167:ARG:NH2	1:B:2171:TRP:HB3	2.35	0.41
1:A:1166:ASP:OD1	1:A:1166:ASP:N	2.52	0.41
1:A:1416:LEU:HA	1:A:1424:ASN:O	2.20	0.41
1:A:1432:TYR:CD1	1:A:1448:PRO:HB3	2.55	0.41
1:B:2160:ALA:O	1:B:2161:ASP:HB2	2.20	0.41
1:B:2359:LYS:HG3	1:B:2360:ASN:H	1.85	0.41
1:A:1029:PHE:HA	1:A:1029:PHE:HD2	1.77	0.41
1:A:1299:ASP:O	1:A:1300:ARG:C	2.59	0.41
1:A:1386:ILE:HG12	1:A:1416:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:LYS:O	1:A:1150:LYS:HG3	2.18	0.41
1:B:2208:PRO:HG2	1:B:2209:ALA:N	2.35	0.41
1:A:1010:VAL:CG1	1:A:1256:LEU:CB	2.98	0.41
1:A:1177:ILE:CG2	1:A:1188:VAL:HG13	2.51	0.41
1:B:2048:LEU:CD1	1:B:2060:VAL:HB	2.49	0.41
1:B:2317:LEU:HD12	1:B:2317:LEU:HA	1.68	0.41
1:A:1074:LYS:HG2	1:A:1108:HIS:ND1	2.36	0.41
1:A:1150:LYS:O	1:A:1150:LYS:HE3	2.20	0.41
1:B:2322:GLY:HA2	1:B:2364:ALA:HB2	2.02	0.41
1:B:2367:VAL:HG12	1:B:2368:GLU:N	2.35	0.41
1:B:2470:LEU:HD12	1:B:2470:LEU:HA	1.92	0.41
1:B:2093:ILE:CG2	1:B:2101:TRP:CE2	3.04	0.41
1:B:2141:GLN:NE2	1:B:2178:THR:HG23	2.36	0.41
1:B:2444:SER:HB2	1:B:2445:GLY:H	1.67	0.41
1:A:1109:ARG:HH11	1:A:1109:ARG:CG	2.33	0.41
1:A:1127:SER:C	1:A:1129:ALA:N	2.74	0.41
1:A:1205:ARG:NE	1:A:1205:ARG:O	2.54	0.41
1:B:2100:ARG:HB3	1:B:2133:SER:HA	2.01	0.41
1:B:2183:ASP:O	1:B:2185:ARG:N	2.54	0.41
1:A:1338:ILE:HG23	1:A:1345:ILE:CD1	2.50	0.41
1:B:2024:LEU:C	1:B:2024:LEU:CD2	2.89	0.41
1:B:2205:ARG:O	1:B:2205:ARG:CG	2.69	0.41
1:B:2319:ALA:C	1:B:2321:GLY:N	2.74	0.41
1:B:2361:GLY:O	1:B:2362:GLN:O	2.38	0.41
1:A:1048:LEU:HD11	1:A:1060:VAL:CB	2.51	0.40
1:A:1154:HIS:HE1	1:A:1164:ALA:HB3	1.85	0.40
1:A:1343:ARG:C	1:A:1344:ARG:HD2	2.38	0.40
1:B:2203:VAL:HG21	1:B:2205:ARG:CZ	2.51	0.40
1:B:2284:ASN:C	1:B:2284:ASN:HD22	2.24	0.40
1:A:1152:TYR:CD2	1:A:1170:PRO:HG3	2.56	0.40
1:B:2141:GLN:C	1:B:2142:VAL:CG1	2.89	0.40
1:B:2173:VAL:O	1:B:2174:ASP:C	2.60	0.40
1:B:2197:ARG:HD2	1:B:2199:ASP:OD2	2.21	0.40
1:B:2218:SER:C	1:B:2220:LYS:N	2.74	0.40
1:A:1063:ARG:HD3	1:A:1069:TYR:CE2	2.56	0.40
1:A:1197:ARG:HB3	1:A:1199:ASP:OD1	2.21	0.40
1:A:1346:THR:O	1:A:1346:THR:HG22	2.21	0.40
1:B:2304:LYS:HG2	1:B:2337:ASP:OD2	2.20	0.40
1:B:2385:ILE:HG23	1:B:2413:VAL:HG13	2.02	0.40
1:A:1212:TYR:CZ	1:A:1231:LEU:HD21	2.56	0.40
1:A:1262:GLN:HB2	1:A:1382:ASN:CG	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:THR:O	1:A:1312:GLY:C	2.58	0.40
1:A:1314:TYR:HH	1:A:1330:LYS:HE2	1.86	0.40
1:B:2185:ARG:HH22	1:B:2226:CYS:HA	1.86	0.40
1:B:2234:SER:O	1:B:2235:GLY:O	2.39	0.40
1:B:2017:ILE:HG23	1:B:2022:LYS:O	2.22	0.40
1:B:2404:LEU:HD22	1:B:2442:THR:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:ASP:OD1	1:B:2343:ARG:NH1[1_565]	2.15	0.05

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	469/493 (95%)	390 (83%)	61 (13%)	18 (4%)	3 13
1	B	468/493 (95%)	390 (83%)	59 (13%)	19 (4%)	3 11
All	All	937/986 (95%)	780 (83%)	120 (13%)	37 (4%)	3 12

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1029	PHE
1	A	1116	GLU
1	A	1158	ARG
1	A	1160	ALA
1	A	1227	GLU
1	A	1399	LYS
1	A	1445	GLY

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Mol	Chain	Res	Type
1	B	2029	PHE
1	B	2097	ASP
1	B	2116	GLU
1	B	2158	ARG
1	B	2160	ALA
1	B	2227	GLU
1	B	2281	LEU
1	B	2399	LYS
1	B	2445	GLY
1	A	1097	ASP
1	A	1099	GLY
1	A	1235	GLY
1	A	1332	ALA
1	A	1342	ASP
1	A	1362	GLN
1	B	2099	GLY
1	B	2235	GLY
1	B	2343	ARG
1	B	2362	GLN
1	A	1218	SER
1	B	2172	GLY
1	B	2332	ALA
1	B	2342	ASP
1	A	1080	CYS
1	A	1228	GLY
1	A	1367	VAL
1	B	2228	GLY
1	B	2367	VAL
1	B	2218	SER
1	A	1320	THR

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	391/404 (97%)	312 (80%)	79 (20%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	391/404 (97%)	307 (78%)	84 (22%)	1 3
All	All	782/808 (97%)	619 (79%)	163 (21%)	1 3

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1010	VAL
1	A	1014	PHE
1	A	1016	LEU
1	A	1024	LEU
1	A	1029	PHE
1	A	1032	LYS
1	A	1038	SER
1	A	1040	LEU
1	A	1047	THR
1	A	1066	LEU
1	A	1078	VAL
1	A	1090	ARG
1	A	1100	ARG
1	A	1102	SER
1	A	1103	LEU
1	A	1109	ARG
1	A	1116	GLU
1	A	1117	ASP
1	A	1126	VAL
1	A	1127	SER
1	A	1130	GLU
1	A	1138	MET
1	A	1140	PRO
1	A	1141	GLN
1	A	1147	VAL
1	A	1150	LYS
1	A	1151	ARG
1	A	1158	ARG
1	A	1168	ASP
1	A	1169	VAL
1	A	1171	TRP
1	A	1178	THR
1	A	1182	GLN
1	A	1189	GLN
1	A	1205	ARG
1	A	1213	THR

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Mol	Chain	Res	Type
1	A	1221	VAL
1	A	1229	ARG
1	A	1231	LEU
1	A	1244	LYS
1	A	1248	VAL
1	A	1251	ASP
1	A	1271	ARG
1	A	1273	VAL
1	A	1281	LEU
1	A	1301	ASP
1	A	1302	THR
1	A	1303	LYS
1	A	1310	HIS
1	A	1313	LYS
1	A	1316	THR
1	A	1320	THR
1	A	1324	GLN
1	A	1326	THR
1	A	1334	CYS
1	A	1343	ARG
1	A	1345	ILE
1	A	1346	THR
1	A	1356	THR
1	A	1372	ASP
1	A	1374	GLU
1	A	1375	LEU
1	A	1380	LEU
1	A	1383	ARG
1	A	1386	ILE
1	A	1389	ARG
1	A	1397	CYS
1	A	1404	LEU
1	A	1408	ARG
1	A	1415	GLN
1	A	1416	LEU
1	A	1428	SER
1	A	1434	THR
1	A	1438	ASP
1	A	1444	SER
1	A	1446	ASP
1	A	1468	ARG
1	A	1470	LEU

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Mol	Chain	Res	Type
1	A	1471	LYS
1	B	2010	VAL
1	B	2014	PHE
1	B	2016	LEU
1	B	2019	CYS
1	B	2024	LEU
1	B	2029	PHE
1	B	2032	LYS
1	B	2033	VAL
1	B	2040	LEU
1	B	2047	THR
1	B	2078	VAL
1	B	2090	ARG
1	B	2100	ARG
1	B	2102	SER
1	B	2103	LEU
1	B	2109	ARG
1	B	2116	GLU
1	B	2117	ASP
1	B	2126	VAL
1	B	2127	SER
1	B	2130	GLU
1	B	2138	MET
1	B	2140	PRO
1	B	2141	GLN
1	B	2147	VAL
1	B	2150	LYS
1	B	2151	ARG
1	B	2158	ARG
1	B	2168	ASP
1	B	2169	VAL
1	B	2171	TRP
1	B	2173	VAL
1	B	2178	THR
1	B	2182	GLN
1	B	2189	GLN
1	B	2205	ARG
1	B	2213	THR
1	B	2221	VAL
1	B	2229	ARG
1	B	2231	LEU
1	B	2244	LYS

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Mol	Chain	Res	Type
1	B	2248	VAL
1	B	2251	ASP
1	B	2269	ASN
1	B	2271	ARG
1	B	2273	VAL
1	B	2280	ASP
1	B	2281	LEU
1	B	2284	ASN
1	B	2301	ASP
1	B	2302	THR
1	B	2303	LYS
1	B	2310	HIS
1	B	2313	LYS
1	B	2316	THR
1	B	2320	THR
1	B	2324	GLN
1	B	2326	THR
1	B	2334	CYS
1	B	2343	ARG
1	B	2345	ILE
1	B	2346	THR
1	B	2356	THR
1	B	2372	ASP
1	B	2375	LEU
1	B	2377	LEU
1	B	2380	LEU
1	B	2383	ARG
1	B	2386	ILE
1	B	2389	ARG
1	B	2397	CYS
1	B	2404	LEU
1	B	2408	ARG
1	B	2415	GLN
1	B	2416	LEU
1	B	2428	SER
1	B	2429	THR
1	B	2434	THR
1	B	2438	ASP
1	B	2444	SER
1	B	2446	ASP
1	B	2468	ARG
1	B	2470	LEU

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Mol	Chain	Res	Type
1	B	2471	LYS

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

Mol	Chain	Res	Type
1	A	1011	GLN
1	A	1021	ASN
1	A	1124	GLN
1	A	1182	GLN
1	A	1324	GLN
1	A	1415	GLN
1	B	2011	GLN
1	B	2013	GLN
1	B	2021	ASN
1	B	2124	GLN
1	B	2141	GLN
1	B	2143	ASN
1	B	2182	GLN
1	B	2324	GLN
1	B	2415	GLN
1	B	2424	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.