Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 11:22 am GMT

PDB ID	:	3ZEF
Title	:	Crystal structure of Prp8:Aar2 complex: second crystal form at 3.1 Angstrom resolution
Authors	:	Galej, W.P.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on	:	2012-12-05
Resolution	:	3.10 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

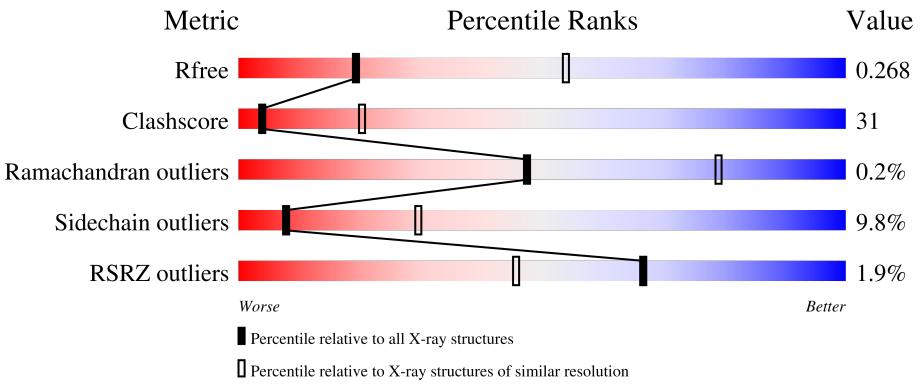
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	355	.% 75% 15% • 8%
1	D	355	67% 18% • 11%
2	B	1531	2% 52% 33% 6% 9%
2	E	1531	2% 58% 29% 5% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28285 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 A1 CISTRON-SPLICING FACTOR AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2684	1722	438	508	16	0	0	0
1	D	317	2618	1682	426	493	17	0	0	0

- Molecule 2 is a protein called PRE-MRNA-SPLICING FACTOR 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1398	11401	7329	1926	2109	37	0	0	0
2	E	1420	11582	7445	1958	2142	37	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

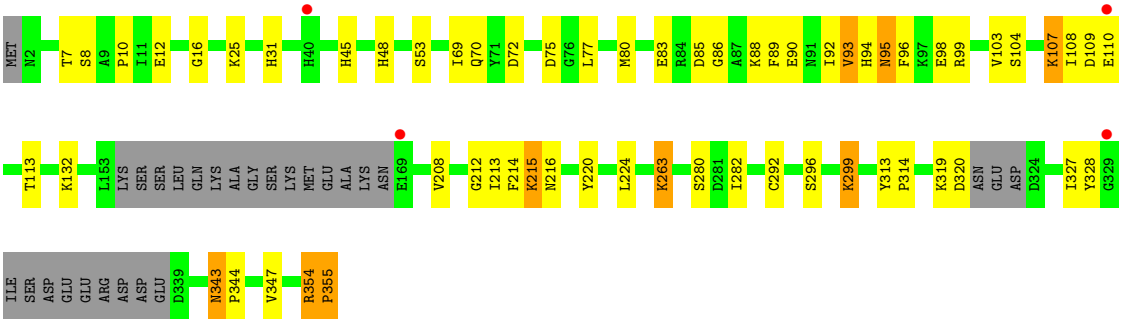
Chain	Residue	Modelled	Actual	Comment	Reference
B	883	SER	-	expression tag	UNP P33334
B	884	GLY	-	expression tag	UNP P33334
B	1961	ASN	LEU	engineered mutation	UNP P33334
B	1999	LEU	ILE	engineered mutation	UNP P33334
E	883	SER	-	expression tag	UNP P33334
E	884	GLY	-	expression tag	UNP P33334
E	1961	ASN	LEU	engineered mutation	UNP P33334
E	1999	LEU	ILE	engineered mutation	UNP P33334

3 Residue-property plots (i)

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

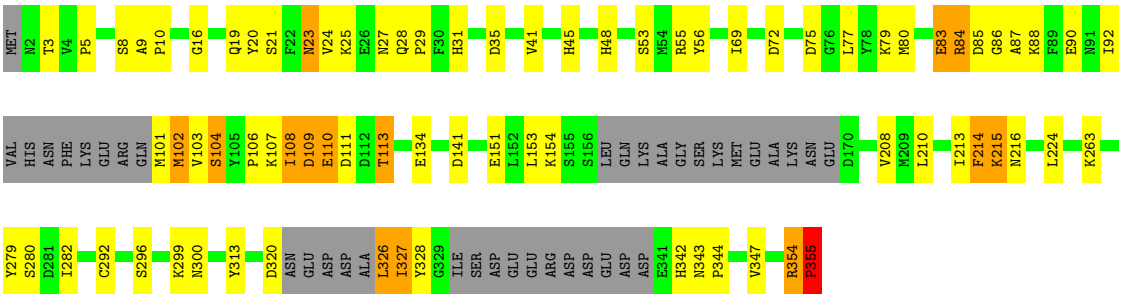
• Molecule 1: A1 CISTRON-SPLICING FACTOR AAR2

Chain A:



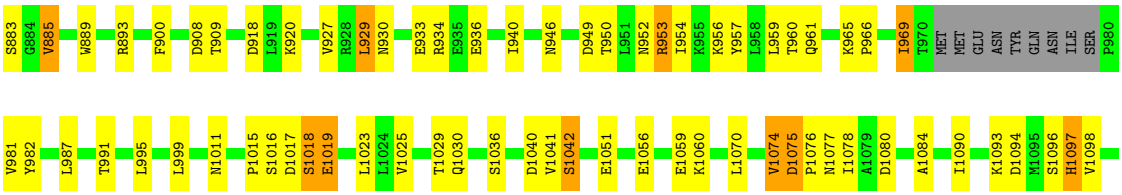
• Molecule 1: A1 CISTRON-SPLICING FACTOR AAR2

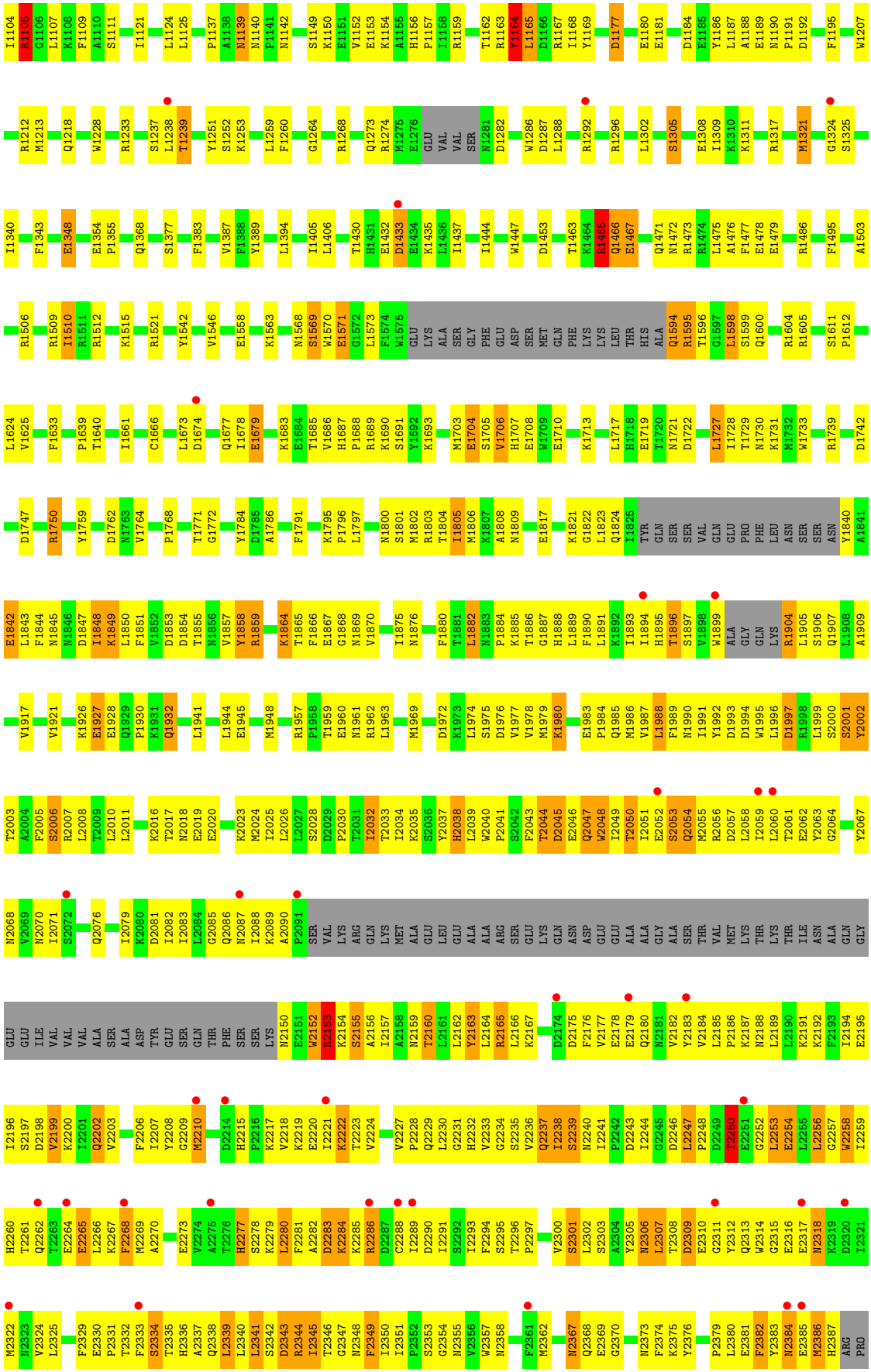
Chain D:

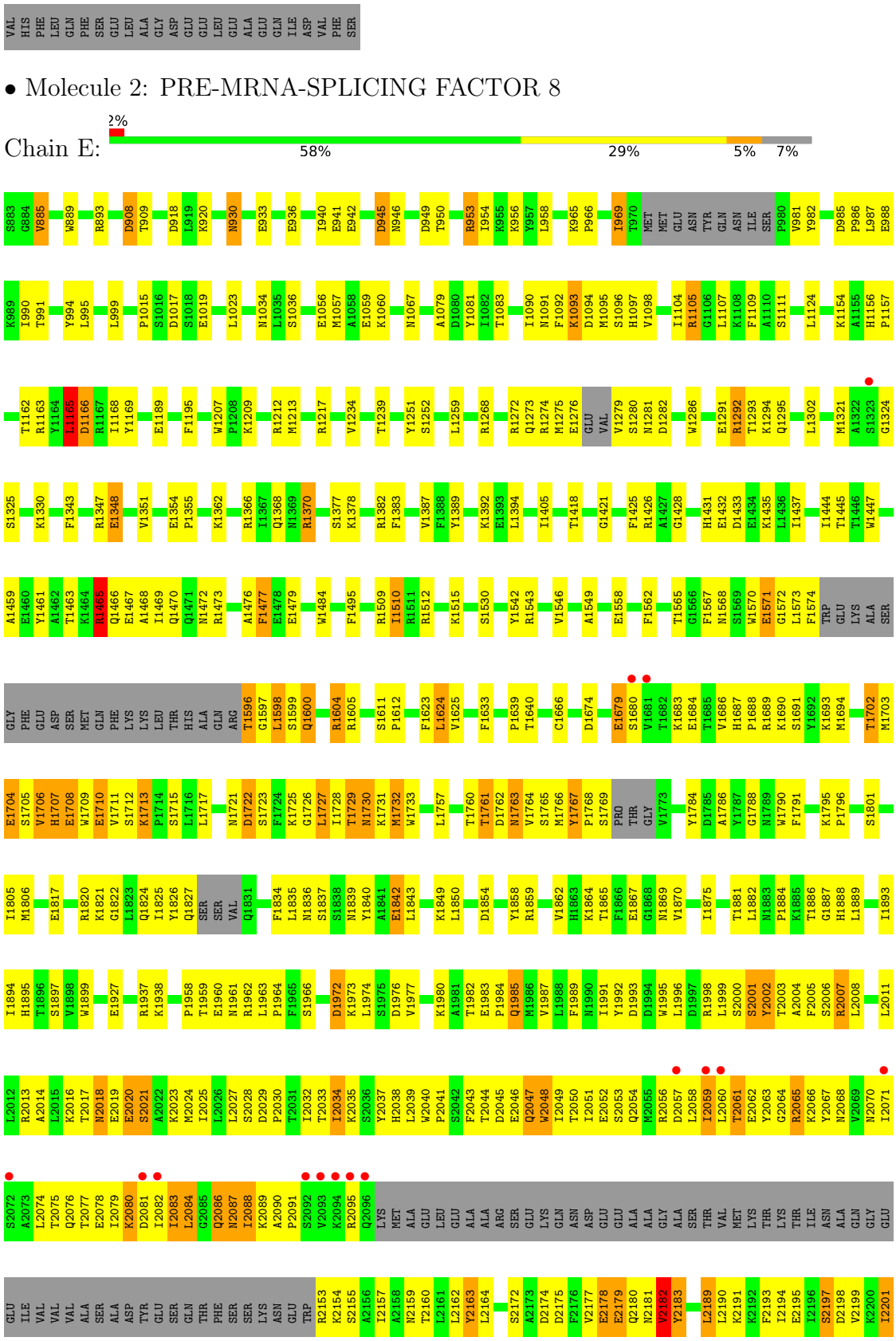


• Molecule 2: PRE-MRNA-SPLICING FACTOR 8

Chain B:

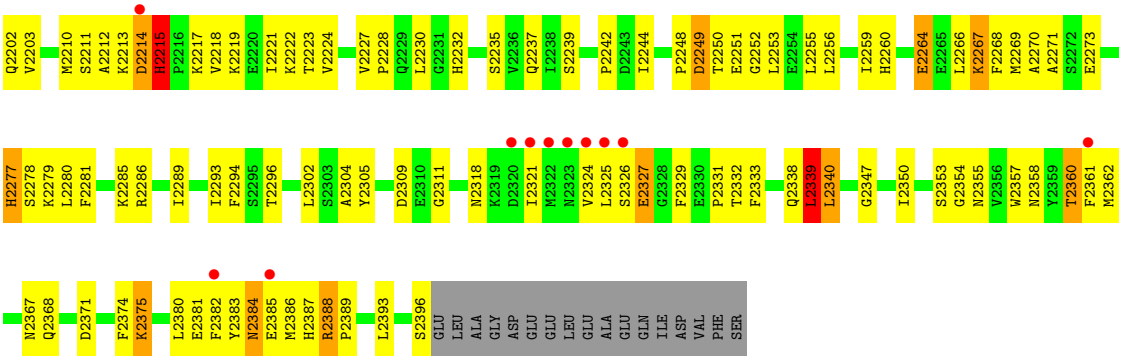



I1104 R1105 G1106 L1107 K1108 F1109 A1110 S1111 I1121 L1124 L1125 P1137 A1138 N1139 N1140 P1141 N1142 S1149 K1150 E1151 V1152 E1153 K1154 A1155 H1156 P1157 I1158 R1159 T1162 R1163 Y1164 L1165 D1166 R1167 I1168 Y1169 D1177 E1180 E1181 D1184 E1185 Y1186 L1187 A1188 E1189 N1190 P1191 D1192 F1195 W1207
R1212 M1213 Q1218 W1228 R1233 S1237 L1238 T1239 Y1251 S1252 K1253 L1259 F1260 G1264 R1268 Q1273 R1274 M1275 E1276 GLU VAL VAL SER N1281 D1282 W1286 D1287 L1288 R1292 R1296 L1302 S1305 E1308 I1309 K1310 K1311 R1317 M1321 G1324 S1325
I1340 F1343 E1348 E1354 P1355 Q1368 S1377 F1383 V1387 F1388 Y1389 L1394 I1405 L1406 T1430 H1431 E1432 D1433 E1434 K1435 L1436 I1437 I1444 W1447 D1453 T1463 K1464 R1465 Q1466 E1467 Q1471 N1472 R1473 R1474 L1475 A1476 F1477 E1478 E1479 R1486 F1495 A1503
R1506 R1509 I1510 R1511 R1512 K1515 R1521 Y1542 V1546 E1558 K1563 N1568 S1569 W1570 E1571 G1572 L1573 F1574 W1575 GLU LYS ALA SER GLY PHE GLU ASP SER MET GLN PHE LYS LYS LEU THR HIS ALA Q1594 R1595 T1596 G1597 L1598 S1599 Q1600 R1604 R1605 S1611 P1612
L1624 V1625 F1633 P1639 T1640 I1661 C1666 L1673 D1674 Q1677 I1678 E1679 K1683 E1684 T1685 V1686 H1687 P1688 R1689 K1690 S1691 Y1692 K1693 M1703 E1704 S1705 V1706 H1707 E1708 W1709 E1710 K1713 L1717 H1718 E1719 T1720 N1721 D1722 L1727 I1728 T1729 N1730 K1731 N1732 W1733 R1739 D1742
D1747 R1750 Y1759 D1762 N1763 V1764 P1768 T1771 G1772 Y1784 D1785 A1786 F1791 K1795 P1796 L1797 N1800 S1801 M1802 R1803 T1804 I1805 M1806 K1807 A1808 N1809 E1817 K1821 G1822 L1823 Q1824 I1825 TYR GLN SER SER VAL GLN GLU PRO PHE LEU ASN SER SER ASN Y1840 A1841
E1842 L1843 F1844 N1845 N1846 D1847 I1848 K1849 L1850 F1851 V1852 D1853 D1854 T1855 N1856 V1857 Y1858 R1859 K1864 T1865 F1866 E1867 G1868 N1869 V1870 I1875 N1876 F1880 T1881 L1882 N1883 P1884 K1885 T1886 G1887 H1888 L1889 F1890 L1891 K1892 I1893 I1894 H1895 T1896 S1897 V1898 W1899 ALA GLY GLN LYS R1904 L1905 S1906 Q1907 L1908 A1909
V1917 V1921 K1926 E1927 E1928 Q1929 P1930 K1931 Q1932 L1941 L1944 E1945 M1948 R1957 P1958 T1959 E1960 N1961 N1962 L1963 M1969 D1972 K1973 L1974 S1975 D1976 V1977 V1978 M1979 K1980 E1983 P1984 Q1985 M1986 V1987 L1988 F1989 N1990 I1991 Y1992 D1993 D1994 W1995 L1996 D1997 R1998 L1999 S2000 S2001 Y2002
T2003 A2004 F2005 S2006 R2007 L2008 T2009 L2010 L2011 K2016 T2017 N2018 E2019 E2020 K2023 M2024 I2025 L2026 L2027 S2028 D2029 P2030 T2031 I2032 T2033 I2034 K2035 S2036 Y2037 H2038 L2039 W2040 P2041 S2042 F2043 T2044 D2045 E2046 Q2047 W2048 I2049 T2050 I2051 E2052 S2053 Q2054 M2055 R2056 D2057 I2058 I2059 L2060 T2061 E2062 Y2063 G2064 Y2067
N2068 V2069 N2070 I2071 S2072 Q2076 I2079 K2080 D2081 I2082 I2083 L2084 G2085 Q2086 N2087 I2088 K2089 A2090 P2091 SER VAL LYS ARG GLN LYS MET ALA GLU LEU GLU ALA GLY ALA ASN ASP GLU GLU ALA ALA GLY ALA SER THR VAL MET LYS THR LYS GLN THR ILE ASN ALA GLN GLY
GLU GLU ILE VAL VAL VAL ALA SER ALA ASP TYR GLU SER GLN THR PHE SER SER SER LYS N2150 E2151 W2152 R2153 K2154 S2155 A2156 I2157 A2158 N2159 T2160 L2161 L2162 Y2163 L2164 R2165 L2166 K2167 D2174 D2175 F2176 V2177 E2178 E2179 Q2180 N2181 V2182 Y2183 V2184 L2185 P2186 K2187 N2188 L2189 L2190 K2191 K2192 F2193 I2194 E2195
I2196 S2197 D2198 V2199 K2200 I2201 Q2202 V2203 F2206 I2207 Y2208 G2209 M2210 D2214 H2215 P2216 K2217 V2218 K2219 E2220 I2221 K2222 T2223 V2224 V2227 P2228 Q2229 L2230 G2231 H2232 V2233 G2234 S2235 V2236 Q2237 I2238 S2239 N2240 I2241 P2242 D2243 I2244 G2245 D2246 L2247 P2248 D2249 T2250 E2251 G2252 L2253 E2254 L2255 L2256 G2257 W2258 I2259
H2260 T2261 Q2262 T2263 E2264 E2265 L2266 K2267 F2268 M2269 A2270 E2273 V2274 A2275 T2276 H2277 S2278 K2279 L2280 F2281 A2282 D2283 K2284 K2285 R2286 D2287 C2288 I2289 D2290 I2291 S2292 I2293 F2294 S2295 T2296 P2297 V2300 S2301 L2302 S2303 A2304 Y2305 N2306 L2307 T2308 D2309 E2310 G2311 Y2312 Q2313 W2314 G2315 E2316 E2317 N2318 K2319 D2320 I2321
M2322 N2323 V2324 L2325 F2329 E2330 P2331 T2332 F2333 S2334 T2335 H2336 A2337 Q2338 L2339 L2340 L2341 S2342 D2343 R2344 I2345 T2346 G2347 N2348 F2349 I2350 I2351 P2352 S2353 G2354 N2355 V2356 W2357 N2358 F2361 M2362 N2367 Q2368 E2369 G2370 N2373 F2374 K2375 Y2376 P2379 L2380 E2381 F2382 Y2383 N2384 E2385 M2386 H2387 ARG PRO



• Molecule 2: PRE-MRNA-SPLICING FACTOR 8

Chain E: 2% 58% 29% 5% 7%


Q2202 V2203 M2210 S2211 A2212 K2213 D2214 H2215 P2216 K2217 V2218 K2219 E2220 I2221 K2222 T2223 V2224 V2227 P2228 Q2229 L2230 G2231 H2232 S2235 V2236 Q2237 I2238 S2239 P2242 D2243 I2244 P2248 D2249 T2250 E2251 G2252 L2253 E2254 L2255 L2256 I2259 H2260 E2264 E2265 L2266 K2267 F2268 M2269 A2270 A2271 S2272 E2273
H2277 S2278 K2279 L2280 F2281 K2285 R2286 I2289 I2293 F2294 S2295 T2296 L2302 S2303 A2304 Y2305 D2309 E2310 G2311 N2318 K2319 D2320 I2321 M2322 N2323 V2324 L2325 S2326 E2327 G2328 F2329 E2330 P2331 T2332 F2333 Q2338 L2339 L2340 G2347 I2350 S2353 G2354 N2355 V2356 W2357 N2358 Y2359 T2360 F2361 M2362
N2367 Q2368 D2371 F2374 K2375 L2380 E2381 F2382 Y2383 N2384 E2385 M2386 H2387 R2388 P2389 L2393 S2396 GLU LEU ALA GLY ASP GLU GLU GLU LEU GLU ALA GLU GLN ILE ASP VAL PHE SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.42Å 177.84Å 216.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	137.45 – 3.10 92.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (137.45-3.10) 99.8 (92.50-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0016	Depositor
R, R_{free}	0.220 , 0.267 0.221 , 0.268	Depositor DCC
R_{free} test set	4874 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	79.1	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28285	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5812e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.55	0/2754	0.72	2/3725 (0.1%)
1	D	0.56	0/2685	0.75	4/3626 (0.1%)
2	B	0.59	1/11671 (0.0%)	0.79	5/15827 (0.0%)
2	E	0.58	3/11856 (0.0%)	0.77	8/16074 (0.0%)
All	All	0.58	4/28966 (0.0%)	0.77	19/39252 (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	D	0	1
2	B	0	6
2	E	0	5
All	All	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1708	GLU	CD-OE1	8.75	1.35	1.25
2	E	1571	GLU	CD-OE1	7.11	1.33	1.25
2	B	1164	TYR	CE2-CZ	-6.19	1.30	1.38
2	E	1708	GLU	CD-OE2	6.10	1.32	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2339	LEU	CA-CB-CG	7.05	131.52	115.30
2	E	1105	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	D	355	PRO	CA-N-CD	-6.36	102.59	111.50
1	A	354	ARG	C-N-CD	6.34	141.71	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1465	ARG	NE-CZ-NH1	6.09	123.35	120.30
2	E	1963	LEU	CA-CB-CG	-6.00	101.50	115.30
1	D	354	ARG	C-N-CD	5.73	140.43	128.40
2	E	1165	LEU	CA-CB-CG	5.71	128.43	115.30
2	E	1604	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	B	1988	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	355	PRO	CA-N-CD	-5.42	103.91	111.50
2	E	1105	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	B	1105	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	B	1075	ASP	C-N-CD	5.32	139.56	128.40
2	B	1465	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	B	927	VAL	CB-CA-C	-5.25	101.43	111.40
1	D	41	VAL	N-CA-C	-5.23	96.88	111.00
2	E	2182	VAL	CB-CA-C	-5.23	101.47	111.40
1	D	214	PHE	N-CA-C	-5.16	97.06	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	LYS	Peptide
1	A	93	VAL	Peptide
2	B	1164	TYR	Peptide
2	B	1433	ASP	Peptide
2	B	1704	GLU	Peptide
2	B	2152	TRP	Peptide
2	B	2153	ARG	Peptide
2	B	2250	THR	Peptide
1	D	110	GLU	Peptide
2	E	1092	PHE	Peptide
2	E	1572	GLY	Peptide
2	E	1706	VAL	Peptide
2	E	2083	ILE	Peptide
2	E	2215	HIS	Peptide

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	2684	0	2530	54	0
1	D	2618	0	2494	81	0
2	B	11401	0	11345	879	1
2	E	11582	0	11528	721	1
All	All	28285	0	27897	1719	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 31.

All (1719) 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:2043:PHE:CE2	2:B:2051:ILE:HD11	1.31	1.63
2:B:2259:ILE:HD13	2:B:2291:ILE:CB	1.30	1.60
2:B:2183:TYR:CE1	2:B:2219:LYS:HD3	1.45	1.49
2:B:2183:TYR:HE1	2:B:2219:LYS:CD	1.26	1.47
2:B:2236:VAL:HG22	2:B:2238:ILE:CD1	1.44	1.47
2:E:2210:MET:HE1	2:E:2253:LEU:N	1.11	1.43
2:E:2210:MET:HE1	2:E:2252:GLY:C	1.06	1.41
2:B:2259:ILE:CD1	2:B:2291:ILE:HB	1.48	1.40
2:E:2034:ILE:HD12	2:E:2041:PRO:N	1.12	1.40
2:E:2210:MET:CE	2:E:2252:GLY:C	1.89	1.39
2:E:2034:ILE:CD1	2:E:2041:PRO:CA	1.99	1.39
2:E:2080:LYS:HD2	2:E:2083:ILE:CG1	1.49	1.38
2:B:2308:THR:HG23	2:B:2333:PHE:O	1.23	1.36
2:E:2304:ALA:HB2	2:E:2339:LEU:CD2	1.55	1.35
2:E:2011:LEU:HD13	2:E:2040:TRP:CZ3	1.59	1.34
2:E:1995:TRP:CZ3	2:E:2007:ARG:HG2	1.63	1.33
2:B:2044:THR:HG23	2:B:2047:GLN:NE2	1.40	1.33
2:E:2041:PRO:HB2	2:E:2043:PHE:CE1	1.61	1.32
2:B:2182:VAL:HG12	2:B:2338:GLN:CB	1.59	1.32
2:E:1998:ARG:CZ	2:E:2045:ASP:OD2	1.75	1.31
2:B:1125:LEU:O	2:B:1233:ARG:NH1	1.62	1.31
2:E:2018:ASN:ND2	2:E:2058:LEU:HD11	1.41	1.30
2:B:2210:MET:CE	2:B:2253:LEU:HA	1.61	1.29
2:B:2259:ILE:CD1	2:B:2291:ILE:CB	2.04	1.28
2:E:2046:GLU:O	2:E:2049:ILE:HG22	1.24	1.28
2:E:2210:MET:SD	2:E:2252:GLY:O	1.92	1.27
2:E:1392:LYS:NZ	2:E:1599:SER:O	1.67	1.27
2:E:2178:GLU:O	2:E:2217:LYS:NZ	1.68	1.26
2:B:900:PHE:HB2	2:B:1075:ASP:OD2	1.09	1.26
2:E:1472:ASN:O	2:E:2325:LEU:HB2	1.11	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1865:THR:HB	2:E:1867:GLU:OE1	1.20	1.25
2:E:2034:ILE:CD1	2:E:2041:PRO:N	1.98	1.25
2:B:2259:ILE:CD1	2:B:2291:ILE:CG2	2.15	1.24
2:E:2011:LEU:CD1	2:E:2040:TRP:CZ3	2.20	1.24
2:E:2043:PHE:CD2	2:E:2051:ILE:HG13	1.71	1.23
2:B:2043:PHE:CE2	2:B:2051:ILE:CD1	2.20	1.23
2:E:2034:ILE:HD11	2:E:2041:PRO:CG	1.68	1.23
2:E:2047:GLN:O	2:E:2050:THR:N	1.70	1.23
2:E:2080:LYS:CD	2:E:2083:ILE:CD1	2.17	1.23
2:B:2259:ILE:HD13	2:B:2291:ILE:CG2	1.68	1.22
2:B:2259:ILE:HD12	2:B:2291:ILE:O	1.39	1.22
2:B:2281:PHE:O	2:B:2286:ARG:HA	1.39	1.22
2:B:2236:VAL:CG2	2:B:2238:ILE:CD1	2.16	1.22
2:B:1604:ARG:NH2	2:B:1822:GLY:O	1.72	1.22
2:E:2018:ASN:HD21	2:E:2058:LEU:CD1	1.51	1.22
2:B:900:PHE:CB	2:B:1075:ASP:OD2	1.87	1.21
2:E:2210:MET:CE	2:E:2253:LEU:N	1.99	1.21
2:B:1993:ASP:OD2	2:B:2038:HIS:HB3	1.39	1.21
2:E:2080:LYS:CD	2:E:2083:ILE:HD11	1.69	1.21
2:E:2043:PHE:CE2	2:E:2051:ILE:HG13	1.74	1.20
2:E:2046:GLU:O	2:E:2049:ILE:CG2	1.90	1.20
2:E:2034:ILE:HD11	2:E:2041:PRO:HG3	1.19	1.19
2:E:2034:ILE:HG23	2:E:2040:TRP:O	1.04	1.18
2:B:1729:THR:HG21	2:B:1771:THR:CG2	1.74	1.18
1:D:86:GLY:O	1:D:90:GLU:HB2	1.43	1.18
2:B:2182:VAL:CG1	2:B:2338:GLN:HB3	1.74	1.18
2:E:2024:MET:CE	2:E:2157:ILE:CG2	2.21	1.18
1:D:19:GLN:NE2	1:D:110:GLU:HG2	1.58	1.17
2:B:2358:ASN:HB3	2:B:2387:HIS:ND1	1.57	1.17
2:B:1993:ASP:CG	2:B:2038:HIS:HB3	1.64	1.16
2:E:2034:ILE:HD12	2:E:2040:TRP:C	1.64	1.16
2:E:2034:ILE:HG23	2:E:2040:TRP:C	1.62	1.16
2:B:2259:ILE:HD11	2:B:2291:ILE:HG22	1.25	1.16
2:B:2281:PHE:O	2:B:2286:ARG:CA	1.93	1.16
2:B:2339:LEU:HD12	2:B:2340:LEU:N	1.57	1.16
2:B:1729:THR:CG2	2:B:1771:THR:HG21	1.75	1.15
2:B:2357:TRP:HH2	2:B:2382:PHE:CE1	1.63	1.15
2:B:2358:ASN:HB3	2:B:2387:HIS:CE1	1.82	1.14
2:B:2052:GLU:O	2:B:2056:ARG:HG3	1.48	1.14
2:E:2034:ILE:HD12	2:E:2041:PRO:CA	1.67	1.14
2:B:2034:ILE:CG1	2:B:2041:PRO:HA	1.75	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2037:TYR:CD1	2:E:2038:HIS:CD2	2.36	1.13
2:B:2224:VAL:CG1	2:B:2349:PHE:CZ	2.32	1.13
2:B:2210:MET:HG3	2:B:2222:LYS:HD2	1.15	1.13
2:E:1731:LYS:CE	2:E:1768:PRO:HB2	1.77	1.12
2:B:1729:THR:HG21	2:B:1771:THR:HG21	1.19	1.12
2:E:1472:ASN:O	2:E:2325:LEU:CB	1.96	1.12
2:E:2034:ILE:HD13	2:E:2041:PRO:HA	1.13	1.12
2:E:1998:ARG:NE	2:E:2045:ASP:OD2	1.84	1.11
2:E:2018:ASN:HD22	2:E:2058:LEU:HD21	1.10	1.11
2:B:2182:VAL:HG13	2:B:2338:GLN:OE1	1.49	1.10
2:E:2034:ILE:CG2	2:E:2040:TRP:O	1.98	1.10
2:E:1763:ASN:C	2:E:1766:MET:CE	2.20	1.10
2:B:2208:TYR:HB3	2:B:2253:LEU:CD2	1.82	1.10
2:E:1865:THR:CB	2:E:1867:GLU:OE1	1.98	1.10
2:B:2236:VAL:HG22	2:B:2238:ILE:HD13	1.26	1.09
2:E:2080:LYS:HD3	2:E:2083:ILE:HD11	1.10	1.09
2:B:2191:LYS:O	2:B:2195:GLU:HG3	1.51	1.09
2:E:1998:ARG:NH1	2:E:2045:ASP:OD2	1.86	1.08
2:E:2048:TRP:O	2:E:2052:GLU:HB3	1.51	1.08
2:E:2385:GLU:O	2:E:2388:ARG:HB2	1.53	1.08
2:B:2224:VAL:O	2:B:2349:PHE:CD1	2.06	1.08
2:B:2358:ASN:N	2:B:2387:HIS:HE1	1.51	1.08
2:E:2037:TYR:HD1	2:E:2038:HIS:CD2	1.71	1.08
2:B:2339:LEU:O	2:B:2340:LEU:HD12	1.51	1.08
2:B:2357:TRP:CH2	2:B:2382:PHE:CE1	2.42	1.08
2:E:1763:ASN:C	2:E:1766:MET:HE2	1.73	1.07
2:B:2314:TRP:O	2:B:2318:ASN:ND2	1.87	1.07
2:E:2080:LYS:CD	2:E:2083:ILE:CG1	2.33	1.06
2:B:2183:TYR:CE1	2:B:2219:LYS:CD	2.15	1.06
2:B:2208:TYR:HB3	2:B:2253:LEU:HD21	1.34	1.06
2:E:2080:LYS:CD	2:E:2083:ILE:HG13	1.84	1.06
2:B:2159:ASN:OD1	2:B:2199:VAL:HG13	1.56	1.06
2:E:2018:ASN:ND2	2:E:2058:LEU:CD1	2.11	1.05
2:B:2150:ASN:HA	2:B:2152:TRP:CZ3	1.90	1.05
2:B:2210:MET:CE	2:B:2253:LEU:CA	2.34	1.05
2:E:1604:ARG:NH2	2:E:1822:GLY:O	1.90	1.05
2:B:2157:ILE:O	2:B:2160:THR:OG1	1.75	1.05
2:E:1291:GLU:O	2:E:1294:LYS:HE3	1.55	1.05
2:E:2064:GLY:O	2:E:2067:TYR:N	1.89	1.05
2:B:2043:PHE:CZ	2:B:2051:ILE:HD11	1.92	1.04
2:B:2307:LEU:HD12	2:B:2308:THR:N	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2039:LEU:HB2	2:E:2040:TRP:NE1	1.71	1.04
2:B:2281:PHE:O	2:B:2286:ARG:N	1.90	1.04
2:B:2358:ASN:H	2:B:2387:HIS:CE1	1.74	1.04
2:B:2358:ASN:CB	2:B:2387:HIS:CE1	2.41	1.04
2:E:2255:LEU:O	2:E:2285:LYS:NZ	1.91	1.04
2:B:2034:ILE:HG12	2:B:2041:PRO:HA	1.36	1.04
2:B:2210:MET:HE3	2:B:2253:LEU:CA	1.87	1.03
2:B:2210:MET:SD	2:B:2222:LYS:HD3	1.99	1.03
2:E:1597:GLY:HA2	2:E:1598:LEU:HB3	1.37	1.03
2:E:2039:LEU:HB2	2:E:2040:TRP:CD1	1.94	1.02
2:B:1859:ARG:HD2	2:B:1876:ASN:O	1.59	1.02
2:B:2268:PHE:HD2	2:B:2331:PRO:HB3	1.23	1.02
2:E:1465:ARG:HG2	2:E:1465:ARG:HH11	1.24	1.02
2:E:2024:MET:HE3	2:E:2157:ILE:CG2	1.86	1.02
2:E:2034:ILE:CD1	2:E:2041:PRO:HA	1.71	1.02
2:E:1727:LEU:C	2:E:1728:ILE:HD13	1.81	1.01
2:B:1885:LYS:O	2:B:2001:SER:OG	1.76	1.01
2:E:2048:TRP:O	2:E:2052:GLU:CB	2.08	1.01
2:B:2224:VAL:HB	2:B:2349:PHE:CZ	1.96	1.00
2:E:1731:LYS:HE2	2:E:1768:PRO:HB2	1.02	1.00
1:D:109:ASP:OD1	1:D:111:ASP:N	1.94	1.00
2:E:2024:MET:HE1	2:E:2157:ILE:HG22	1.44	1.00
2:E:2230:LEU:HD12	2:E:2360:THR:HA	1.42	0.99
2:B:2350:ILE:HD13	2:B:2376:TYR:HA	1.44	0.99
2:E:1995:TRP:CZ3	2:E:2007:ARG:CG	2.45	0.99
2:E:1995:TRP:CH2	2:E:2007:ARG:HG2	1.96	0.99
2:E:1705:SER:OG	2:E:1730:ASN:O	1.80	0.99
2:E:2304:ALA:HB2	2:E:2339:LEU:HD23	1.44	0.99
2:E:2353:SER:O	2:E:2375:LYS:NZ	1.95	0.99
2:B:2030:PRO:O	2:B:2033:THR:OG1	1.79	0.99
2:E:2041:PRO:CB	2:E:2043:PHE:CE1	2.44	0.99
2:B:2037:TYR:HB2	2:B:2038:HIS:CD2	1.96	0.99
2:B:2381:GLU:OE1	2:B:2381:GLU:N	1.95	0.99
2:E:2304:ALA:HB2	2:E:2339:LEU:HD22	1.42	0.99
2:B:2024:MET:O	2:B:2028:SER:HB2	1.63	0.99
2:B:2210:MET:CG	2:B:2222:LYS:HD2	1.93	0.98
2:B:2182:VAL:HA	2:B:2338:GLN:HB2	1.43	0.98
2:B:2224:VAL:HG12	2:B:2349:PHE:CE1	1.97	0.98
2:E:2018:ASN:HD21	2:E:2058:LEU:CG	1.76	0.98
2:E:2304:ALA:CB	2:E:2339:LEU:CD2	2.41	0.98
2:B:2224:VAL:HB	2:B:2349:PHE:CE1	1.99	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2294:PHE:HD2	2:B:2301:SER:OG	1.45	0.98
2:B:1011:ASN:ND2	2:B:1142:ASN:O	1.97	0.98
2:E:2034:ILE:CG2	2:E:2040:TRP:C	2.32	0.98
2:E:2024:MET:HE1	2:E:2157:ILE:CG2	1.90	0.97
2:E:2213:LYS:HA	2:E:2215:HIS:H	1.30	0.97
2:B:2236:VAL:CG2	2:B:2238:ILE:HD11	1.94	0.97
2:B:2358:ASN:H	2:B:2387:HIS:HE1	0.98	0.97
2:E:1207:TRP:O	2:E:1212:ARG:NH1	1.96	0.97
2:E:2080:LYS:HD2	2:E:2083:ILE:CD1	1.86	0.97
2:E:1834:PHE:CE2	2:E:1960:GLU:OE2	2.17	0.97
2:B:2236:VAL:HG22	2:B:2238:ILE:HD11	1.41	0.97
2:E:1067:ASN:HD22	2:E:1083:THR:HG21	1.27	0.97
2:E:2024:MET:HE3	2:E:2157:ILE:HG23	1.47	0.96
1:D:327:ILE:HB	1:D:328:TYR:HD1	1.27	0.96
2:B:2259:ILE:CD1	2:B:2291:ILE:HG22	1.84	0.96
2:E:2154:LYS:O	2:E:2157:ILE:N	1.98	0.96
2:E:1324:GLY:HA2	2:E:1325:SER:OG	1.62	0.96
2:B:2224:VAL:CB	2:B:2349:PHE:CE1	2.49	0.96
2:E:2034:ILE:CD1	2:E:2041:PRO:CG	2.44	0.96
2:B:1568:ASN:OD1	2:B:1569:SER:OG	1.84	0.95
2:E:1966:SER:OG	2:E:2016:LYS:HE3	1.66	0.95
2:E:1702:THR:CG2	2:E:1768:PRO:HG3	1.97	0.95
2:E:1762:ASP:OD1	2:E:1763:ASN:ND2	1.99	0.95
2:B:1887:GLY:HA3	2:B:1992:TYR:CD2	2.01	0.95
2:B:2210:MET:HG3	2:B:2222:LYS:CD	1.96	0.95
2:B:2224:VAL:CB	2:B:2349:PHE:CZ	2.50	0.95
2:E:2278:SER:O	2:E:2281:PHE:N	1.98	0.95
2:B:1707:HIS:CD2	2:B:1708:GLU:HB2	2.01	0.95
2:B:2034:ILE:HG12	2:B:2041:PRO:CA	1.97	0.95
2:B:2230:LEU:O	2:B:2236:VAL:HG23	1.66	0.95
2:E:2018:ASN:ND2	2:E:2058:LEU:CG	2.29	0.95
2:B:2043:PHE:HE2	2:B:2051:ILE:HD11	1.24	0.94
2:B:2357:TRP:CH2	2:B:2382:PHE:CD1	2.55	0.94
1:D:151:GLU:OE2	1:D:154:LYS:HE3	1.67	0.94
2:B:2210:MET:HE3	2:B:2253:LEU:HA	0.95	0.94
2:E:2011:LEU:HD13	2:E:2040:TRP:CE3	2.03	0.94
2:E:2041:PRO:HB2	2:E:2043:PHE:HE1	1.23	0.94
2:E:1567:PHE:CZ	2:E:1820:ARG:NH1	2.36	0.94
1:D:107:LYS:HB3	1:D:108:ILE:HG22	1.50	0.94
2:E:1711:VAL:HG12	2:E:1790:TRP:O	1.68	0.94
2:B:2310:GLU:OE1	2:B:2310:GLU:N	2.00	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1252:SER:O	2:B:1274:ARG:NH1	1.99	0.93
2:E:2043:PHE:CD2	2:E:2051:ILE:CG1	2.50	0.93
2:E:1826:TYR:OH	2:E:1938:LYS:NZ	1.99	0.93
2:E:2011:LEU:HD13	2:E:2040:TRP:HZ3	1.23	0.93
2:B:2224:VAL:CG1	2:B:2349:PHE:CE1	2.50	0.93
2:E:1998:ARG:CD	2:E:2045:ASP:OD2	2.16	0.93
2:E:1709:TRP:O	2:E:1729:THR:N	2.01	0.93
1:A:86:GLY:O	1:A:90:GLU:HG2	1.66	0.93
2:B:2011:LEU:HD13	2:B:2040:TRP:CZ3	2.04	0.93
2:E:1684:GLU:OE2	2:E:1702:THR:OG1	1.85	0.93
2:E:2267:LYS:O	2:E:2305:TYR:OH	1.86	0.93
1:D:19:GLN:HE21	1:D:110:GLU:HG2	1.25	0.93
2:B:2192:LYS:O	2:B:2195:GLU:N	2.02	0.92
2:B:1993:ASP:OD2	2:B:2038:HIS:CB	2.17	0.92
2:E:2034:ILE:CD1	2:E:2041:PRO:CB	2.46	0.92
2:E:1731:LYS:HE2	2:E:1768:PRO:CB	1.97	0.92
2:E:2210:MET:CE	2:E:2253:LEU:CA	2.47	0.92
2:E:2034:ILE:HG21	2:E:2040:TRP:N	1.84	0.92
2:E:2304:ALA:CB	2:E:2339:LEU:HD23	2.00	0.92
2:E:2210:MET:HE1	2:E:2253:LEU:CA	1.99	0.92
2:B:1961:ASN:OD1	2:B:2079:ILE:HD11	1.68	0.92
2:E:1826:TYR:H	2:E:1827:GLN:HG3	1.35	0.92
2:B:1887:GLY:HA3	2:B:1992:TYR:HD2	1.33	0.92
2:B:2315:GLY:O	2:B:2318:ASN:N	2.03	0.92
2:E:2210:MET:CE	2:E:2252:GLY:O	2.14	0.92
2:B:2183:TYR:HE1	2:B:2219:LYS:HD2	1.34	0.91
2:E:2041:PRO:CB	2:E:2043:PHE:HE1	1.80	0.91
2:B:2339:LEU:CD1	2:B:2340:LEU:N	2.33	0.91
2:E:2028:SER:O	2:E:2030:PRO:HD3	1.70	0.91
2:E:2019:GLU:O	2:E:2023:LYS:HG3	1.68	0.91
2:E:2030:PRO:HB2	2:E:2153:ARG:NH2	1.85	0.91
2:B:2282:ALA:HB2	2:B:2316:GLU:OE2	1.70	0.91
2:B:2034:ILE:HG13	2:B:2041:PRO:HA	1.51	0.91
2:B:2182:VAL:HG12	2:B:2338:GLN:HB3	0.92	0.90
2:B:2286:ARG:HD3	2:B:2312:TYR:CZ	2.07	0.90
2:E:2202:GLN:HE22	2:E:2235:SER:CA	1.84	0.90
2:B:2357:TRP:HH2	2:B:2382:PHE:CD1	1.87	0.90
2:B:2183:TYR:HE1	2:B:2219:LYS:HD3	0.77	0.90
2:B:2259:ILE:HD11	2:B:2291:ILE:CG2	1.91	0.90
2:B:2182:VAL:CG1	2:B:2338:GLN:CB	2.42	0.90
2:B:2237:GLN:C	2:B:2238:ILE:HD13	1.92	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2224:VAL:HG11	2:B:2349:PHE:HZ	1.35	0.89
2:E:1292:ARG:HD3	2:E:1293:THR:HG23	1.54	0.89
2:B:2339:LEU:CD1	2:B:2340:LEU:H	1.85	0.89
2:E:2050:THR:O	2:E:2053:SER:OG	1.90	0.89
2:B:1961:ASN:OD1	2:B:2079:ILE:CD1	2.20	0.89
2:B:2044:THR:OG1	2:B:2047:GLN:HG3	1.72	0.89
2:E:1834:PHE:HE2	2:E:1960:GLU:OE2	1.51	0.89
2:E:2014:ALA:HA	2:E:2059:ILE:CD1	2.03	0.89
2:B:1983:GLU:HB2	2:B:1984:PRO:HD2	1.52	0.89
2:B:2236:VAL:CG2	2:B:2238:ILE:HD12	2.02	0.89
2:E:2210:MET:HE1	2:E:2252:GLY:O	1.72	0.89
2:B:950:THR:O	2:B:954:ILE:HG13	1.72	0.89
2:B:1848:ILE:HD13	2:B:1928:GLU:O	1.72	0.89
2:E:2011:LEU:HD12	2:E:2040:TRP:CZ3	2.06	0.89
2:B:2182:VAL:CA	2:B:2338:GLN:HB2	2.03	0.88
2:E:1324:GLY:CA	2:E:1325:SER:OG	2.21	0.88
2:B:2019:GLU:O	2:B:2023:LYS:HG3	1.74	0.88
2:B:2259:ILE:HD12	2:B:2291:ILE:C	1.93	0.88
2:B:1594:GLN:OE1	2:B:1595:ARG:N	2.06	0.88
1:D:106:PRO:O	1:D:107:LYS:HG2	1.71	0.88
1:D:31:HIS:O	1:D:102:MET:SD	2.31	0.88
2:E:2037:TYR:CD1	2:E:2038:HIS:NE2	2.42	0.88
2:B:1016:SER:OG	2:B:1018:SER:OG	1.92	0.87
2:B:2282:ALA:CB	2:B:2316:GLU:OE2	2.21	0.87
2:E:2018:ASN:ND2	2:E:2058:LEU:HD21	1.87	0.87
2:E:2018:ASN:HD22	2:E:2058:LEU:CD2	1.86	0.87
1:A:347:VAL:HG21	2:B:1875:ILE:HD11	1.56	0.87
2:E:1762:ASP:OD2	2:E:1764:VAL:HG22	1.75	0.87
2:E:941:GLU:O	2:E:945:ASP:OD1	1.93	0.87
2:B:1849:LYS:O	2:B:1850:LEU:HD23	1.75	0.87
2:B:1015:PRO:HD2	2:B:1165:LEU:HD23	1.54	0.86
2:E:1998:ARG:HD2	2:E:2045:ASP:OD2	1.74	0.86
2:E:2080:LYS:HD2	2:E:2083:ILE:HG13	0.88	0.86
2:B:2286:ARG:HD3	2:B:2312:TYR:CE2	2.11	0.86
2:B:2358:ASN:HB3	2:B:2387:HIS:HD1	1.37	0.86
2:E:1466:GLN:O	2:E:1469:ILE:N	2.09	0.86
2:E:1992:TYR:OH	2:E:2005:PHE:HB2	1.76	0.86
2:B:2020:GLU:OE1	2:B:2165:ARG:NH2	2.07	0.86
2:B:1137:PRO:HG2	2:B:1140:ASN:O	1.76	0.85
2:E:2014:ALA:CA	2:E:2059:ILE:HD11	2.06	0.85
2:E:2030:PRO:HB2	2:E:2153:ARG:HH21	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:HIS:O	1:A:98:GLU:CB	2.24	0.85
2:B:2203:VAL:CG2	2:B:2382:PHE:CE1	2.59	0.85
2:B:2207:ILE:N	2:B:2257:GLY:O	2.09	0.85
1:D:106:PRO:C	1:D:107:LYS:HG2	1.93	0.85
2:B:1868:GLY:O	2:B:1870:VAL:HG23	1.75	0.85
2:B:2182:VAL:CG1	2:B:2338:GLN:OE1	2.24	0.85
2:E:1252:SER:O	2:E:1274:ARG:NH1	2.08	0.85
2:E:2177:VAL:HG23	2:E:2180:GLN:H	1.41	0.85
2:B:2350:ILE:HG23	2:B:2375:LYS:O	1.76	0.85
2:B:2256:LEU:O	2:B:2288:CYS:SG	2.34	0.85
2:E:2011:LEU:CD1	2:E:2040:TRP:CE3	2.59	0.85
2:E:2037:TYR:CD1	2:E:2038:HIS:HD2	1.95	0.85
2:B:2357:TRP:HH2	2:B:2382:PHE:HE1	1.18	0.85
2:E:1757:LEU:O	2:E:1761:THR:HG23	1.77	0.84
2:B:2034:ILE:CG1	2:B:2041:PRO:CA	2.55	0.84
2:B:2178:GLU:O	2:B:2217:LYS:CD	2.24	0.84
2:B:2210:MET:SD	2:B:2222:LYS:CD	2.65	0.84
1:D:327:ILE:HB	1:D:328:TYR:CD1	2.12	0.84
2:E:2065:ARG:NH1	2:E:2065:ARG:HB3	1.93	0.84
2:B:1887:GLY:CA	2:B:1992:TYR:CD2	2.60	0.84
2:B:2157:ILE:O	2:B:2160:THR:N	2.08	0.84
2:B:2281:PHE:CE1	2:B:2288:CYS:HB2	2.13	0.84
2:B:1994:ASP:O	2:B:1997:ASP:HB2	1.78	0.84
2:B:2049:ILE:O	2:B:2053:SER:OG	1.93	0.84
2:B:1686:VAL:HG11	2:B:1690:LYS:HD2	1.60	0.83
2:E:1763:ASN:CA	2:E:1766:MET:HE2	2.08	0.83
2:E:2174:ASP:OD1	2:E:2175:ASP:N	2.10	0.83
2:B:1895:HIS:CD2	2:B:1896:THR:H	1.94	0.83
2:B:2203:VAL:HG22	2:B:2382:PHE:HE1	1.43	0.83
2:B:2208:TYR:CD2	2:B:2253:LEU:HD13	2.12	0.83
2:B:2183:TYR:CE1	2:B:2219:LYS:HD2	2.09	0.83
2:B:2294:PHE:CZ	2:B:2296:THR:CG2	2.61	0.83
2:E:1712:SER:OG	2:E:1713:LYS:O	1.94	0.83
2:E:1763:ASN:O	2:E:1766:MET:CE	2.25	0.83
2:E:2034:ILE:HD13	2:E:2041:PRO:CA	1.80	0.83
2:E:2064:GLY:O	2:E:2068:ASN:N	2.11	0.83
2:E:2210:MET:HE2	2:E:2253:LEU:HA	1.59	0.83
2:B:1999:LEU:HD12	2:B:2000:SER:H	1.43	0.83
2:B:2182:VAL:HA	2:B:2338:GLN:CB	2.08	0.83
2:B:2210:MET:CG	2:B:2222:LYS:CD	2.54	0.83
2:B:2294:PHE:CZ	2:B:2296:THR:HG21	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2034:ILE:HD12	2:E:2041:PRO:CD	2.09	0.83
2:E:2381:GLU:OE1	2:E:2381:GLU:N	2.10	0.83
2:B:1853:ASP:OD1	2:B:1855:THR:OG1	1.97	0.82
2:B:2256:LEU:C	2:B:2288:CYS:SG	2.58	0.82
2:E:2189:LEU:CD1	2:E:2224:VAL:HG23	2.09	0.82
2:B:2380:LEU:HD13	2:B:2384:ASN:OD1	1.77	0.82
2:E:1711:VAL:CG1	2:E:1790:TRP:O	2.28	0.82
2:B:2224:VAL:O	2:B:2349:PHE:HD1	1.63	0.82
2:B:2224:VAL:C	2:B:2349:PHE:CE1	2.53	0.82
2:B:1848:ILE:CD1	2:B:1928:GLU:O	2.27	0.82
2:B:1999:LEU:HD21	2:B:2003:THR:HG22	1.60	0.82
2:E:2034:ILE:HD11	2:E:2041:PRO:CB	2.07	0.82
2:B:1999:LEU:HD11	2:B:2003:THR:HB	1.60	0.82
2:B:1568:ASN:OD1	2:B:1569:SER:N	2.13	0.82
2:B:2339:LEU:HD12	2:B:2340:LEU:H	1.35	0.82
2:E:1705:SER:OG	2:E:1730:ASN:CA	2.28	0.82
2:E:1987:VAL:HG12	2:E:1989:PHE:CE1	2.15	0.82
2:E:2083:ILE:HG22	2:E:2084:LEU:HD13	1.62	0.81
2:E:2080:LYS:HD3	2:E:2083:ILE:CD1	1.92	0.81
2:B:2192:LYS:O	2:B:2195:GLU:HB2	1.80	0.81
2:E:2024:MET:CE	2:E:2157:ILE:HG23	2.01	0.81
2:B:2224:VAL:HG12	2:B:2349:PHE:HE1	1.45	0.81
2:E:1711:VAL:CB	2:E:1790:TRP:O	2.28	0.81
2:E:2074:LEU:O	2:E:2075:THR:OG1	1.98	0.81
2:B:1895:HIS:CD2	2:B:1896:THR:OG1	2.33	0.81
2:B:1941:LEU:O	2:B:1945:GLU:HG3	1.81	0.81
2:B:2044:THR:HG23	2:B:2047:GLN:CD	2.00	0.81
2:B:2060:LEU:O	2:B:2063:TYR:HB3	1.80	0.81
2:B:2224:VAL:HG11	2:B:2349:PHE:CZ	2.09	0.81
2:B:2358:ASN:CA	2:B:2387:HIS:CE1	2.63	0.81
2:E:1974:LEU:O	2:E:1977:VAL:HG22	1.80	0.81
2:E:2177:VAL:CG2	2:E:2180:GLN:HB2	2.09	0.81
2:B:2047:GLN:O	2:B:2051:ILE:N	2.13	0.81
1:D:107:LYS:HB3	1:D:108:ILE:CG2	2.10	0.81
2:E:1727:LEU:O	2:E:1728:ILE:HD13	1.80	0.81
2:E:2018:ASN:HD21	2:E:2058:LEU:HD11	1.07	0.81
1:D:210:LEU:O	1:D:214:PHE:O	1.99	0.81
2:E:2030:PRO:HG2	2:E:2153:ARG:NE	1.95	0.81
2:B:2182:VAL:HG12	2:B:2338:GLN:CG	2.11	0.81
2:B:2198:ASP:OD1	2:B:2200:LYS:N	2.14	0.81
2:B:2259:ILE:HD12	2:B:2291:ILE:HB	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2178:GLU:O	2:B:2217:LYS:HD3	1.79	0.80
2:E:1849:LYS:O	2:E:1850:LEU:HD23	1.81	0.80
2:B:2259:ILE:HD13	2:B:2291:ILE:HB	0.81	0.80
2:E:1711:VAL:CG1	2:E:1791:PHE:HB3	2.11	0.80
2:B:1707:HIS:NE2	2:B:1708:GLU:HB2	1.97	0.80
2:E:2202:GLN:NE2	2:E:2235:SER:C	2.34	0.80
2:B:900:PHE:CA	2:B:1075:ASP:OD2	2.28	0.80
2:B:2367:ASN:OD1	2:B:2370:GLY:N	2.15	0.80
2:E:2384:ASN:HD22	2:E:2386:MET:H	1.30	0.80
2:B:2279:LYS:HZ3	2:B:2368:GLN:HE22	1.30	0.80
2:B:2308:THR:CG2	2:B:2333:PHE:O	2.19	0.80
2:E:2037:TYR:HD1	2:E:2038:HIS:NE2	1.77	0.80
2:E:1995:TRP:CE2	2:E:2007:ARG:HD2	2.17	0.80
2:E:2034:ILE:CD1	2:E:2041:PRO:CD	2.59	0.80
2:E:2084:LEU:O	2:E:2084:LEU:HD22	1.81	0.80
2:B:2044:THR:CG2	2:B:2047:GLN:NE2	2.36	0.80
2:E:1995:TRP:CH2	2:E:2007:ARG:CG	2.62	0.80
2:B:2358:ASN:CA	2:B:2387:HIS:HE1	1.95	0.79
2:B:1843:LEU:HD11	2:B:1884:PRO:CG	2.12	0.79
2:E:1987:VAL:CG1	2:E:1989:PHE:CE1	2.65	0.79
2:B:1961:ASN:CG	2:B:2079:ILE:HD11	2.03	0.79
2:B:1976:ASP:O	2:B:1980:LYS:HG3	1.83	0.79
2:B:2176:PHE:HA	2:B:2338:GLN:NE2	1.97	0.79
2:E:2065:ARG:HB3	2:E:2065:ARG:CZ	2.12	0.79
2:B:2035:LYS:HD2	2:B:2037:TYR:CE1	2.17	0.79
2:B:2176:PHE:HA	2:B:2338:GLN:HE21	1.47	0.79
2:E:2202:GLN:NE2	2:E:2235:SER:CA	2.46	0.79
1:D:75:ASP:OD2	1:D:79:LYS:CE	2.31	0.79
2:B:2184:VAL:HG23	2:B:2219:LYS:O	1.83	0.79
2:E:1995:TRP:CD2	2:E:2007:ARG:HD2	2.17	0.79
2:E:2353:SER:HA	2:E:2375:LYS:CD	2.13	0.79
2:B:1895:HIS:CD2	2:B:1896:THR:N	2.51	0.78
2:B:2224:VAL:CG1	2:B:2349:PHE:HZ	1.86	0.78
2:E:2384:ASN:ND2	2:E:2386:MET:H	1.81	0.78
2:E:1703:MET:N	2:E:1732:MET:O	2.17	0.78
2:B:2183:TYR:CD2	2:B:2289:ILE:HD13	2.19	0.78
2:B:1843:LEU:HD12	2:B:1843:LEU:O	1.84	0.78
2:B:2154:LYS:O	2:B:2157:ILE:HB	1.82	0.78
2:E:2034:ILE:CG2	2:E:2040:TRP:N	2.47	0.78
2:E:2043:PHE:HB3	2:E:2047:GLN:HG3	1.66	0.78
2:B:2358:ASN:N	2:B:2387:HIS:CE1	2.39	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ARG:NH2	1:D:279:TYR:CE1	2.51	0.78
2:B:1111:SER:HB2	2:B:1510:ILE:HG12	1.65	0.78
2:B:1348:GLU:OE1	2:B:1447:TRP:N	2.15	0.78
2:E:1727:LEU:HD23	2:E:1728:ILE:H	1.49	0.78
2:B:1797:LEU:O	2:B:1801:SER:OG	2.00	0.77
2:B:1503:ALA:O	2:B:1506:ARG:NH1	2.17	0.77
2:B:2224:VAL:O	2:B:2349:PHE:CE1	2.36	0.77
2:E:2087:ASN:HD22	2:E:2089:LYS:H	1.31	0.77
2:B:2236:VAL:HG21	2:B:2238:ILE:HD12	1.65	0.77
2:B:2279:LYS:NZ	2:B:2368:GLN:NE2	2.33	0.77
2:B:1983:GLU:HB2	2:B:1984:PRO:CD	2.14	0.77
2:B:2268:PHE:CD2	2:B:2331:PRO:HB3	2.15	0.77
1:D:108:ILE:HD13	1:D:109:ASP:H	1.48	0.77
2:E:1562:PHE:O	2:E:1565:THR:OG1	2.02	0.77
2:E:1565:THR:O	2:E:1820:ARG:NH2	2.17	0.77
2:E:2078:GLU:C	2:E:2079:ILE:HD13	2.05	0.77
2:E:2210:MET:CE	2:E:2253:LEU:HA	2.14	0.77
2:B:2157:ILE:C	2:B:2160:THR:HG1	1.85	0.77
2:B:2283:ASP:OD1	2:B:2284:LYS:HA	1.84	0.77
2:E:2080:LYS:CE	2:E:2083:ILE:CD1	2.63	0.77
2:E:1163:ARG:HG3	2:E:1168:ILE:HG22	1.67	0.77
2:E:2201:ILE:HG21	2:E:2382:PHE:CZ	2.20	0.77
2:B:1999:LEU:HD21	2:B:2003:THR:CG2	2.15	0.77
2:B:2357:TRP:CH2	2:B:2382:PHE:HE1	1.95	0.77
2:E:2087:ASN:HD22	2:E:2089:LYS:N	1.83	0.77
2:B:2294:PHE:HD2	2:B:2301:SER:HG	0.78	0.76
2:B:2247:LEU:HD12	2:B:2248:PRO:CD	2.16	0.76
2:E:2201:ILE:HG21	2:E:2382:PHE:HZ	1.49	0.76
2:B:2281:PHE:C	2:B:2286:ARG:HA	2.04	0.76
2:B:2286:ARG:CD	2:B:2312:TYR:CE2	2.68	0.76
2:E:1111:SER:HB2	2:E:1510:ILE:HG12	1.66	0.76
2:E:2057:ASP:O	2:E:2061:THR:N	2.17	0.76
2:B:2244:ILE:O	2:B:2250:THR:HG21	1.85	0.76
1:A:344:PRO:HB3	2:B:1858:TYR:CE1	2.21	0.76
2:B:2280:LEU:HD12	2:B:2281:PHE:CE2	2.21	0.76
2:E:1348:GLU:OE1	2:E:1447:TRP:N	2.19	0.76
2:E:2018:ASN:ND2	2:E:2058:LEU:CD2	2.44	0.76
2:E:2039:LEU:C	2:E:2040:TRP:CD1	2.59	0.76
2:E:2080:LYS:HE3	2:E:2083:ILE:HD12	1.68	0.76
2:E:2210:MET:HE2	2:E:2253:LEU:CA	2.16	0.76
1:A:292:CYS:O	1:A:296:SER:OG	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1729:THR:HG22	2:B:1771:THR:HG21	1.67	0.75
2:B:1843:LEU:O	2:B:1849:LYS:HE3	1.86	0.75
2:B:1605:ARG:NH2	2:B:1824:GLN:OE1	2.17	0.75
2:B:2177:VAL:H	2:B:2338:GLN:NE2	1.84	0.75
2:B:1477:PHE:CD2	2:B:1495:PHE:CD2	2.73	0.75
2:B:2227:VAL:O	2:B:2229:GLN:HG2	1.87	0.75
2:B:2309:ASP:HA	2:B:2312:TYR:HB2	1.66	0.75
1:D:292:CYS:O	1:D:296:SER:OG	2.04	0.75
2:E:1995:TRP:CH2	2:E:2007:ARG:CD	2.69	0.75
2:E:2189:LEU:HD13	2:E:2224:VAL:HG23	1.66	0.75
2:E:1292:ARG:HD3	2:E:1293:THR:CG2	2.16	0.75
2:B:1207:TRP:O	2:B:1212:ARG:NH1	2.19	0.75
2:E:2041:PRO:CG	2:E:2043:PHE:HE1	1.98	0.75
2:B:1287:ASP:OD2	2:B:1296:ARG:NH2	2.18	0.75
2:B:2183:TYR:CD1	2:B:2219:LYS:HD3	2.20	0.75
2:E:1702:THR:HG21	2:E:1768:PRO:HG3	1.66	0.75
2:E:1964:PRO:HG3	2:E:2013:ARG:NH1	2.02	0.75
2:E:1324:GLY:HA2	2:E:1325:SER:CB	2.16	0.75
2:E:1093:LYS:HG3	2:E:1094:ASP:OD1	1.87	0.74
2:E:1570:TRP:O	2:E:1571:GLU:CD	2.25	0.74
2:B:1895:HIS:HD2	2:B:1896:THR:H	1.32	0.74
2:E:2047:GLN:O	2:E:2050:THR:CA	2.34	0.74
1:A:212:GLY:O	1:A:215:LYS:NZ	2.19	0.74
2:B:1859:ARG:CD	2:B:1876:ASN:O	2.35	0.74
2:B:2232:HIS:N	2:B:2235:SER:O	2.20	0.74
2:B:2236:VAL:CG1	2:B:2238:ILE:HD11	2.17	0.74
2:E:1995:TRP:CE3	2:E:2007:ARG:HD2	2.22	0.74
2:E:2157:ILE:O	2:E:2160:THR:CB	2.34	0.74
2:E:2227:VAL:CG1	2:E:2239:SER:OG	2.35	0.74
2:B:2203:VAL:HG22	2:B:2382:PHE:CE1	2.20	0.74
2:E:1570:TRP:O	2:E:1571:GLU:OE2	2.04	0.74
2:E:2034:ILE:HG21	2:E:2040:TRP:CA	2.17	0.74
2:E:2066:LYS:HB2	2:E:2067:TYR:CD1	2.21	0.74
2:B:2210:MET:HE1	2:B:2253:LEU:CA	2.16	0.74
2:E:2041:PRO:HB2	2:E:2043:PHE:CD1	2.23	0.74
2:E:2162:LEU:CD1	2:E:2194:ILE:O	2.36	0.74
2:E:1418:THR:OG1	2:E:1421:GLY:O	2.05	0.74
2:B:1999:LEU:HG	2:B:2000:SER:O	1.87	0.74
2:B:2309:ASP:OD1	2:B:2309:ASP:N	2.18	0.74
2:B:2185:LEU:HG	2:B:2186:PRO:N	2.00	0.73
2:B:1932:GLN:OE1	2:B:1957:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1834:PHE:CD1	2:E:1958:PRO:HG2	2.23	0.73
2:E:1597:GLY:CA	2:E:1598:LEU:HB3	2.18	0.73
2:B:2238:ILE:HD13	2:B:2238:ILE:N	2.03	0.73
2:E:2230:LEU:CD1	2:E:2360:THR:HA	2.17	0.73
2:B:2309:ASP:HA	2:B:2312:TYR:HD2	1.54	0.73
2:E:2047:GLN:C	2:E:2050:THR:H	1.92	0.73
2:B:2034:ILE:HG12	2:B:2040:TRP:C	2.09	0.73
2:B:2209:GLY:HA3	2:B:2256:LEU:HD21	1.70	0.73
2:E:2202:GLN:HE22	2:E:2235:SER:HA	1.53	0.73
2:E:1705:SER:OG	2:E:1730:ASN:C	2.27	0.73
2:E:1987:VAL:HG11	2:E:1989:PHE:CZ	2.23	0.73
2:B:1993:ASP:OD1	2:B:2038:HIS:HB3	1.88	0.73
1:A:88:LYS:O	1:A:92:ILE:HD13	1.89	0.72
2:B:2306:ASN:N	2:B:2335:THR:O	2.17	0.72
2:E:1733:TRP:CE2	2:E:1767:TYR:HD2	2.07	0.72
2:E:2024:MET:CE	2:E:2157:ILE:HG21	2.18	0.72
2:E:2177:VAL:HG21	2:E:2180:GLN:HG3	1.70	0.72
2:B:1679:GLU:N	2:B:1704:GLU:O	2.22	0.72
2:B:2045:ASP:N	2:B:2045:ASP:OD1	2.21	0.72
2:E:1973:LYS:O	2:E:1977:VAL:HG13	1.89	0.72
1:D:75:ASP:OD2	1:D:79:LYS:NZ	2.23	0.72
2:E:2277:HIS:HD1	2:E:2281:PHE:HD2	1.35	0.72
2:E:1711:VAL:HG12	2:E:1791:PHE:HB3	1.70	0.72
2:E:2021:SER:O	2:E:2024:MET:N	2.22	0.72
2:E:2084:LEU:HD13	2:E:2084:LEU:H	1.55	0.72
2:E:1428:GLY:N	2:E:1433:ASP:OD2	2.19	0.72
2:B:2011:LEU:HD13	2:B:2040:TRP:CE3	2.24	0.72
2:B:2037:TYR:HB2	2:B:2038:HIS:HD2	1.55	0.72
2:B:2230:LEU:HD23	2:B:2237:GLN:HG3	1.72	0.72
1:D:19:GLN:NE2	1:D:110:GLU:CG	2.49	0.72
2:B:2034:ILE:HG12	2:B:2040:TRP:O	1.88	0.72
2:E:2178:GLU:C	2:E:2217:LYS:HZ2	1.87	0.72
2:B:2046:GLU:O	2:B:2049:ILE:HG22	1.89	0.71
2:B:2165:ARG:O	2:B:2300:VAL:HG13	1.90	0.71
2:B:1308:GLU:OE2	2:B:1311:LYS:HE3	1.90	0.71
2:B:2247:LEU:HG	2:B:2375:LYS:HA	1.72	0.71
2:B:2279:LYS:HZ3	2:B:2368:GLN:NE2	1.87	0.71
2:E:2162:LEU:HD13	2:E:2194:ILE:O	1.89	0.71
2:B:1996:LEU:HA	2:B:1999:LEU:O	1.89	0.71
2:E:2017:THR:HG22	2:E:2018:ASN:OD1	1.91	0.71
2:E:2048:TRP:O	2:E:2052:GLU:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2014:ALA:HA	2:E:2059:ILE:HD11	1.68	0.71
1:D:19:GLN:HE22	1:D:110:GLU:HG2	1.52	0.71
2:E:2043:PHE:CE2	2:E:2051:ILE:CG1	2.64	0.71
2:B:1983:GLU:HG3	2:B:1985:GLN:HE21	1.56	0.71
2:B:2159:ASN:OD1	2:B:2199:VAL:CG1	2.37	0.71
2:E:1291:GLU:O	2:E:1294:LYS:CE	2.37	0.71
2:E:1465:ARG:HG2	2:E:1465:ARG:NH1	1.97	0.71
2:E:1763:ASN:CA	2:E:1766:MET:CE	2.68	0.71
2:B:1731:LYS:HE3	2:B:1768:PRO:HB2	1.73	0.70
2:B:1927:GLU:OE1	2:B:1927:GLU:N	2.24	0.70
2:B:1180:GLU:O	2:B:1184:ASP:OD1	2.09	0.70
2:B:2207:ILE:HB	2:B:2221:ILE:HG23	1.71	0.70
2:E:2210:MET:SD	2:E:2252:GLY:C	2.57	0.70
2:B:2247:LEU:HD12	2:B:2248:PRO:HD2	1.73	0.70
2:E:1679:GLU:HB2	2:E:1706:VAL:HG13	1.74	0.70
2:B:1729:THR:HG21	2:B:1771:THR:HG23	1.73	0.70
2:B:2048:TRP:O	2:B:2052:GLU:HG3	1.92	0.70
1:D:48:HIS:CD2	1:D:53:SER:OG	2.45	0.70
2:B:2044:THR:OG1	2:B:2047:GLN:CG	2.39	0.70
2:B:1974:LEU:O	2:B:1977:VAL:HG12	1.91	0.70
2:B:2188:ASN:HD21	2:B:2346:THR:HB	1.56	0.70
2:B:2224:VAL:HG12	2:B:2349:PHE:CZ	2.17	0.70
2:B:2230:LEU:HB3	2:B:2237:GLN:CG	2.22	0.70
2:B:2307:LEU:HD12	2:B:2308:THR:H	1.55	0.70
2:E:1093:LYS:CG	2:E:1094:ASP:HA	2.21	0.70
2:B:2236:VAL:HG13	2:B:2238:ILE:HD11	1.73	0.70
2:E:1731:LYS:CE	2:E:1768:PRO:CB	2.64	0.70
2:E:2024:MET:HE3	2:E:2157:ILE:HG21	1.74	0.70
2:B:1704:GLU:HG3	2:B:1730:ASN:O	1.92	0.70
2:E:1763:ASN:O	2:E:1766:MET:HE1	1.91	0.70
2:E:1995:TRP:CZ2	2:E:2007:ARG:HD2	2.27	0.70
2:B:1687:HIS:ND1	2:B:1688:PRO:HD2	2.06	0.69
2:B:2044:THR:HG23	2:B:2047:GLN:HE21	1.50	0.69
2:E:2030:PRO:HG2	2:E:2153:ARG:CZ	2.21	0.69
2:E:1093:LYS:HG3	2:E:1094:ASP:HA	1.74	0.69
2:E:1687:HIS:ND1	2:E:1688:PRO:HD2	2.07	0.69
2:B:1722:ASP:OD1	2:B:1722:ASP:N	2.26	0.69
2:E:1711:VAL:HB	2:E:1790:TRP:O	1.92	0.69
2:B:2223:THR:HG23	2:B:2348:ASN:O	1.92	0.69
2:B:2314:TRP:O	2:B:2317:GLU:HB2	1.93	0.69
2:E:2213:LYS:HA	2:E:2215:HIS:N	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2084:LEU:H	2:E:2084:LEU:CD1	2.05	0.69
2:B:954:ILE:HG23	2:B:991:THR:HG22	1.73	0.69
2:E:1705:SER:HG	2:E:1730:ASN:C	1.93	0.69
2:E:1763:ASN:HA	2:E:1766:MET:HE2	1.75	0.69
2:E:2157:ILE:O	2:E:2160:THR:HB	1.92	0.69
2:B:1017:ASP:HA	2:B:1509:ARG:HG3	1.75	0.69
2:B:2281:PHE:CD1	2:B:2288:CYS:HB2	2.27	0.69
2:E:1274:ARG:O	2:E:1276:GLU:HB3	1.93	0.69
2:B:2152:TRP:HA	2:B:2154:LYS:N	2.07	0.69
2:B:2210:MET:HE2	2:B:2252:GLY:O	1.93	0.69
2:E:2327:GLU:OE1	2:E:2327:GLU:HA	1.93	0.69
2:B:2182:VAL:CG1	2:B:2338:GLN:CD	2.62	0.69
2:B:2207:ILE:HG22	2:B:2224:VAL:HG22	1.75	0.69
2:B:2286:ARG:HD3	2:B:2312:TYR:CE1	2.28	0.69
2:E:1472:ASN:C	2:E:2325:LEU:HB2	2.09	0.69
2:E:2201:ILE:CG2	2:E:2382:PHE:CZ	2.76	0.69
2:B:2268:PHE:HD2	2:B:2331:PRO:CB	2.03	0.68
2:B:1475:LEU:HD12	2:B:1479:GLU:OE2	1.94	0.68
2:B:1704:GLU:HG2	2:B:1705:SER:H	1.58	0.68
2:B:2294:PHE:CZ	2:B:2296:THR:HG23	2.29	0.68
2:E:1705:SER:OG	2:E:1730:ASN:HA	1.92	0.68
2:B:2350:ILE:HD11	2:B:2376:TYR:CD1	2.29	0.68
2:E:2189:LEU:HD13	2:E:2224:VAL:CG2	2.23	0.68
2:B:1961:ASN:CG	2:B:2079:ILE:CD1	2.63	0.68
2:B:2198:ASP:OD1	2:B:2199:VAL:N	2.27	0.68
2:B:2339:LEU:HD12	2:B:2340:LEU:O	1.94	0.68
2:B:1192:ASP:OD2	2:B:1195:PHE:HA	1.94	0.67
2:B:1163:ARG:HG3	2:B:1168:ILE:HG22	1.77	0.67
2:E:1763:ASN:HA	2:E:1766:MET:CE	2.24	0.67
2:E:2018:ASN:HD21	2:E:2058:LEU:HG	1.57	0.67
2:B:1858:TYR:HB2	2:B:1899:TRP:CZ2	2.29	0.67
2:B:1880:PHE:CE2	2:B:1889:LEU:HD11	2.30	0.67
2:B:2309:ASP:HA	2:B:2312:TYR:CD2	2.29	0.67
2:E:1573:LEU:HD22	2:E:1826:TYR:HD2	1.60	0.67
2:E:1834:PHE:CD2	2:E:1960:GLU:HG2	2.28	0.67
2:E:2385:GLU:O	2:E:2388:ARG:CB	2.36	0.67
2:E:1976:ASP:O	2:E:1980:LYS:HG2	1.94	0.67
2:E:1995:TRP:CZ3	2:E:2007:ARG:HD2	2.29	0.67
2:E:2179:GLU:O	2:E:2217:LYS:HD3	1.93	0.67
2:B:1188:ALA:O	2:B:1191:PRO:HD3	1.95	0.67
2:B:2044:THR:N	2:B:2047:GLN:OE1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2056:ARG:O	2:E:2060:LEU:HG	1.94	0.67
2:B:1686:VAL:HG11	2:B:1690:LYS:CD	2.25	0.67
2:E:1727:LEU:CD2	2:E:1728:ILE:H	2.06	0.67
2:B:2192:LYS:O	2:B:2195:GLU:CB	2.43	0.67
2:E:1707:HIS:HB3	2:E:1730:ASN:HB3	1.76	0.67
1:D:110:GLU:HB2	1:D:113:THR:H	1.59	0.67
2:B:1187:LEU:O	2:B:1191:PRO:HG3	1.95	0.66
1:D:347:VAL:HG21	2:E:1875:ILE:HD11	1.76	0.66
2:E:1017:ASP:HA	2:E:1509:ARG:HG3	1.76	0.66
2:E:2049:ILE:O	2:E:2053:SER:N	2.28	0.66
2:B:1987:VAL:HG12	2:B:1989:PHE:CE2	2.29	0.66
2:B:2277:HIS:HB3	2:B:2307:LEU:HD23	1.75	0.66
2:B:2343:ASP:HB3	2:B:2344:ARG:NH2	2.11	0.66
2:E:2025:ILE:HG23	2:E:2054:GLN:NE2	2.10	0.66
1:D:327:ILE:H	1:D:327:ILE:HD12	1.59	0.66
2:E:1995:TRP:CH2	2:E:2007:ARG:HD2	2.31	0.66
2:B:1040:ASP:OD1	2:B:1042:SER:OG	2.13	0.66
2:E:2014:ALA:HB2	2:E:2059:ILE:HD11	1.78	0.66
2:B:2178:GLU:O	2:B:2217:LYS:CE	2.43	0.66
2:E:1597:GLY:CA	2:E:1599:SER:H	2.08	0.66
2:B:909:THR:OG1	2:B:2175:ASP:OD1	2.13	0.66
2:B:2192:LYS:HA	2:B:2195:GLU:HB2	1.78	0.66
2:B:2277:HIS:NE2	2:B:2288:CYS:O	2.28	0.66
2:E:2202:GLN:NE2	2:E:2235:SER:N	2.43	0.66
2:B:946:ASN:HB3	2:B:949:ASP:OD2	1.96	0.66
2:B:1886:THR:OG1	2:B:1888:HIS:CE1	2.48	0.66
2:E:2014:ALA:CB	2:E:2059:ILE:HD11	2.26	0.66
2:E:2039:LEU:CB	2:E:2040:TRP:CD1	2.77	0.66
2:B:2306:ASN:OD1	2:B:2337:ALA:HB2	1.95	0.66
2:B:2259:ILE:HD12	2:B:2291:ILE:CB	2.17	0.66
2:E:1987:VAL:CG1	2:E:1989:PHE:CZ	2.79	0.66
2:E:2159:ASN:ND2	2:E:2197:SER:O	2.29	0.66
2:B:1727:LEU:HD23	2:B:1728:ILE:H	1.59	0.66
2:B:2208:TYR:CB	2:B:2253:LEU:HD21	2.22	0.66
2:B:2379:PRO:O	2:B:2380:LEU:HD23	1.96	0.66
2:B:2230:LEU:O	2:B:2237:GLN:N	2.27	0.65
1:D:84:ARG:HG3	1:D:84:ARG:HH11	1.60	0.65
2:E:2221:ILE:HD13	2:E:2256:LEU:HD12	1.76	0.65
2:E:1711:VAL:HG12	2:E:1790:TRP:C	2.17	0.65
2:E:2381:GLU:H	2:E:2381:GLU:CD	1.99	0.65
1:A:319:LYS:O	1:A:320:ASP:OD1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1186:TYR:HB2	2:B:1228:TRP:CE3	2.30	0.65
2:B:2203:VAL:CG2	2:B:2382:PHE:HE1	2.00	0.65
2:B:2177:VAL:O	2:B:2180:GLN:O	2.14	0.65
2:B:2260:HIS:CD2	2:B:2290:ASP:OD1	2.50	0.65
2:B:2087:ASN:HB3	2:B:2089:LYS:HG3	1.78	0.65
2:B:2368:GLN:HB3	2:B:2369:GLU:OE2	1.95	0.65
2:B:2182:VAL:CA	2:B:2338:GLN:CB	2.71	0.65
1:D:25:LYS:O	1:D:28:GLN:N	2.30	0.65
2:E:2087:ASN:C	2:E:2088:ILE:HG12	2.16	0.65
2:B:2259:ILE:CD1	2:B:2291:ILE:C	2.63	0.65
2:E:1709:TRP:O	2:E:1728:ILE:HA	1.97	0.65
2:E:1097:HIS:HD2	2:E:1098:VAL:O	1.80	0.65
2:E:1763:ASN:C	2:E:1766:MET:HE1	2.17	0.65
2:E:2034:ILE:CG2	2:E:2040:TRP:CA	2.73	0.65
1:A:327:ILE:HG23	2:B:1340:ILE:HD11	1.79	0.65
2:E:1886:THR:HB	2:E:1888:HIS:CE1	2.32	0.65
2:E:1995:TRP:CZ3	2:E:2007:ARG:CD	2.80	0.64
2:B:1598:LEU:O	2:B:1598:LEU:HD22	1.97	0.64
2:B:2182:VAL:CB	2:B:2338:GLN:HB3	2.25	0.64
2:E:1836:ASN:HB2	2:E:1839:ASN:OD1	1.98	0.64
2:B:2192:LYS:O	2:B:2195:GLU:CA	2.44	0.64
2:E:2080:LYS:CE	2:E:2083:ILE:HD12	2.25	0.64
2:E:2178:GLU:O	2:E:2217:LYS:CE	2.46	0.64
2:E:2037:TYR:CE1	2:E:2038:HIS:NE2	2.66	0.64
2:B:2203:VAL:HG21	2:B:2382:PHE:CE1	2.32	0.64
2:B:1605:ARG:NE	2:B:1824:GLN:OE1	2.30	0.64
2:B:1162:THR:HG22	2:B:1169:TYR:HB2	1.79	0.64
2:B:2044:THR:H	2:B:2047:GLN:CD	2.01	0.64
2:E:1763:ASN:ND2	2:E:1763:ASN:H	1.93	0.64
2:E:1867:GLU:CD	2:E:1867:GLU:H	2.01	0.64
1:D:108:ILE:HD13	1:D:109:ASP:N	2.12	0.64
2:B:1961:ASN:OD1	2:B:2079:ILE:HD12	1.96	0.63
2:B:2007:ARG:HG2	2:B:2052:GLU:OE2	1.98	0.63
2:B:2339:LEU:CD1	2:B:2340:LEU:O	2.46	0.63
2:B:2035:LYS:HB3	2:B:2037:TYR:HD1	1.62	0.63
2:B:1149:SER:OG	2:B:1152:VAL:HG12	1.97	0.63
2:B:2230:LEU:HB3	2:B:2237:GLN:HG3	1.79	0.63
1:D:134:GLU:OE1	1:D:134:GLU:N	2.22	0.63
2:E:2384:ASN:HD22	2:E:2385:GLU:N	1.96	0.63
2:B:1105:ARG:HH11	2:B:1105:ARG:HG3	1.62	0.63
2:B:2208:TYR:HB3	2:B:2253:LEU:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1091:ASN:HB3	2:E:1093:LYS:CE	2.28	0.63
2:E:2277:HIS:ND1	2:E:2281:PHE:CD2	2.66	0.63
2:B:1999:LEU:HD12	2:B:2000:SER:N	2.12	0.63
2:B:1886:THR:OG1	2:B:1888:HIS:ND1	2.32	0.63
2:B:1999:LEU:HD11	2:B:2003:THR:CB	2.28	0.63
2:B:2159:ASN:ND2	2:B:2198:ASP:HA	2.13	0.63
2:E:2177:VAL:HG22	2:E:2180:GLN:HB2	1.80	0.63
2:E:1961:ASN:OD1	2:E:2079:ILE:HD12	1.98	0.62
2:E:1972:ASP:OD1	2:E:1972:ASP:N	2.32	0.62
2:E:1995:TRP:CZ2	2:E:2007:ARG:CD	2.82	0.62
2:B:2177:VAL:H	2:B:2338:GLN:HE22	1.47	0.62
2:B:2247:LEU:HD12	2:B:2248:PRO:HD3	1.82	0.62
2:E:1887:GLY:HA3	2:E:1992:TYR:CD2	2.34	0.62
2:B:2037:TYR:C	2:B:2038:HIS:HD2	2.03	0.62
1:D:110:GLU:HB3	1:D:113:THR:OG1	1.99	0.62
2:E:1573:LEU:HD22	2:E:1826:TYR:CD2	2.33	0.62
2:B:1477:PHE:CE2	2:B:1495:PHE:HD2	2.17	0.62
2:E:1707:HIS:HB2	2:E:1708:GLU:HG3	1.79	0.62
1:A:94:HIS:O	1:A:98:GLU:N	2.28	0.62
2:B:2153:ARG:HH11	2:B:2153:ARG:CG	2.12	0.62
2:B:2206:PHE:O	2:B:2224:VAL:HA	2.00	0.62
1:D:109:ASP:O	1:D:110:GLU:HB2	1.99	0.62
2:E:950:THR:O	2:E:954:ILE:HG13	2.00	0.62
2:E:1826:TYR:N	2:E:1827:GLN:HG3	2.11	0.62
2:E:1834:PHE:CE1	2:E:1958:PRO:HG2	2.35	0.62
2:E:1991:ILE:CG2	2:E:2008:LEU:HD22	2.29	0.62
2:E:2090:ALA:HB1	2:E:2091:PRO:HD2	1.82	0.62
2:B:918:ASP:OD1	2:B:1515:LYS:NZ	2.27	0.62
2:B:2286:ARG:CD	2:B:2312:TYR:CD2	2.83	0.62
2:E:1162:THR:HG22	2:E:1169:TYR:HB2	1.82	0.62
2:B:1324:GLY:HA2	2:B:1325:SER:CB	2.29	0.61
2:B:1983:GLU:CB	2:B:1984:PRO:HD2	2.27	0.61
2:B:2294:PHE:HZ	2:B:2296:THR:HG21	1.63	0.61
2:E:1839:ASN:O	2:E:1842:GLU:HG3	2.00	0.61
2:B:2046:GLU:O	2:B:2050:THR:N	2.33	0.61
2:E:2157:ILE:O	2:E:2160:THR:OG1	2.18	0.61
2:B:2278:SER:OG	2:B:2316:GLU:HG3	2.00	0.61
1:D:83:GLU:OE1	1:D:83:GLU:HA	1.99	0.61
2:E:1834:PHE:CD2	2:E:1960:GLU:CG	2.84	0.61
2:B:2043:PHE:CD2	2:B:2051:ILE:CD1	2.82	0.61
2:B:2286:ARG:HD3	2:B:2312:TYR:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1853:ASP:OD1	2:B:1855:THR:N	2.19	0.61
2:E:2039:LEU:HB2	2:E:2040:TRP:HE1	1.59	0.61
2:B:2185:LEU:O	2:B:2341:LEU:HA	2.00	0.61
2:B:2224:VAL:C	2:B:2349:PHE:HE1	2.04	0.61
2:E:2028:SER:O	2:E:2030:PRO:CD	2.46	0.61
2:E:2353:SER:HA	2:E:2375:LYS:HD3	1.82	0.61
2:B:2011:LEU:HD13	2:B:2040:TRP:CH2	2.35	0.61
2:E:1709:TRP:N	2:E:1729:THR:O	2.32	0.61
2:E:2084:LEU:HD13	2:E:2084:LEU:N	2.14	0.61
2:B:1759:TYR:HA	2:B:1762:ASP:HB2	1.82	0.61
2:B:2154:LYS:O	2:B:2157:ILE:HD13	2.01	0.61
2:E:1324:GLY:CA	2:E:1325:SER:CB	2.76	0.60
2:E:1710:GLU:OE2	2:E:1725:LYS:HA	2.01	0.60
2:E:1966:SER:OG	2:E:2016:LYS:CE	2.46	0.60
2:E:2177:VAL:HG21	2:E:2180:GLN:CG	2.31	0.60
2:E:2358:ASN:HB3	2:E:2387:HIS:ND1	2.15	0.60
2:B:1137:PRO:CG	2:B:1140:ASN:O	2.48	0.60
2:B:2305:TYR:HB3	2:B:2334:SER:HB3	1.82	0.60
1:A:354:ARG:HB2	1:A:355:PRO:HD3	1.83	0.60
2:B:1849:LYS:C	2:B:1850:LEU:HD23	2.22	0.60
2:E:1056:GLU:O	2:E:1060:LYS:HG2	2.01	0.60
2:B:1823:LEU:O	2:B:1824:GLN:HB2	2.01	0.60
2:B:1858:TYR:HB2	2:B:1899:TRP:CH2	2.37	0.60
2:E:2304:ALA:CB	2:E:2339:LEU:HD22	2.20	0.60
2:B:2152:TRP:HA	2:B:2154:LYS:H	1.67	0.60
2:B:2277:HIS:HB3	2:B:2307:LEU:CD2	2.31	0.60
2:E:2177:VAL:CG2	2:E:2180:GLN:CB	2.80	0.60
2:E:2214:ASP:N	2:E:2214:ASP:OD1	2.34	0.60
2:B:1030:GLN:HE22	2:B:1288:LEU:HA	1.64	0.60
2:B:1705:SER:HB2	2:B:1730:ASN:O	2.00	0.60
2:E:1467:GLU:OE1	2:E:1470:GLN:NE2	2.35	0.60
2:E:1468:ALA:HB1	2:E:1473:ARG:O	2.02	0.60
2:B:2236:VAL:HG21	2:B:2238:ILE:CD1	2.16	0.60
1:D:342:HIS:O	1:D:343:ASN:ND2	2.31	0.60
2:E:1999:LEU:HD11	2:E:2004:ALA:HB2	1.84	0.60
2:B:2227:VAL:HG12	2:B:2239:SER:HB3	1.84	0.60
2:E:1476:ALA:HB3	2:E:1479:GLU:HG3	1.84	0.60
2:E:1639:PRO:C	2:E:1640:THR:HG23	2.22	0.60
2:E:1706:VAL:HG23	2:E:1706:VAL:O	2.01	0.60
2:B:2182:VAL:HG12	2:B:2338:GLN:CD	2.21	0.59
2:B:2034:ILE:HG12	2:B:2041:PRO:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2309:ASP:O	2:B:2312:TYR:HB2	2.02	0.59
1:A:95:ASN:O	1:A:99:ARG:CB	2.51	0.59
1:A:319:LYS:N	1:A:319:LYS:HD2	2.18	0.59
2:B:900:PHE:N	2:B:1075:ASP:OD2	2.35	0.59
2:B:2353:SER:O	2:B:2375:LYS:NZ	2.30	0.59
1:A:314:PRO:HB2	1:A:319:LYS:HB2	1.84	0.59
2:B:1747:ASP:CG	2:B:1750:ARG:HG3	2.23	0.59
2:B:1840:TYR:HH	2:B:2005:PHE:HD2	1.50	0.59
2:E:1731:LYS:NZ	2:E:1768:PRO:HB2	2.17	0.59
1:A:86:GLY:O	1:A:90:GLU:CG	2.46	0.59
2:B:2268:PHE:HA	2:B:2305:TYR:CE2	2.37	0.59
2:E:1702:THR:CG2	2:E:1768:PRO:CG	2.77	0.59
2:E:1761:THR:O	2:E:1761:THR:OG1	2.21	0.59
2:B:2269:MET:HE3	2:B:2273:GLU:HB3	1.82	0.59
2:B:2309:ASP:O	2:B:2313:GLN:N	2.34	0.59
2:E:2080:LYS:CE	2:E:2083:ILE:HD11	2.30	0.59
2:B:1070:LEU:O	2:B:1074:VAL:HG22	2.03	0.59
2:B:1843:LEU:HD11	2:B:1884:PRO:HG2	1.84	0.59
2:B:1887:GLY:O	2:B:1991:ILE:HG22	2.03	0.59
2:E:2353:SER:HA	2:E:2375:LYS:HD2	1.84	0.59
2:B:1324:GLY:HA2	2:B:1325:SER:OG	2.03	0.59
2:B:1733:TRP:NE1	2:B:1771:THR:O	2.35	0.59
2:B:2209:GLY:N	2:B:2254:GLU:O	2.35	0.59
2:B:2302:LEU:HD12	2:B:2302:LEU:N	2.18	0.59
2:B:2350:ILE:HG23	2:B:2375:LYS:C	2.23	0.59
2:E:1034:ASN:OD1	2:E:1291:GLU:N	2.27	0.59
2:E:1067:ASN:HD22	2:E:1083:THR:CG2	2.11	0.59
2:B:1453:ASP:OD2	2:B:1486:ARG:HD2	2.03	0.58
2:B:1690:LYS:HA	2:B:1693:LYS:HG3	1.85	0.58
2:B:2230:LEU:O	2:B:2236:VAL:CG2	2.47	0.58
2:E:1893:ILE:HG12	2:E:1985:GLN:O	2.03	0.58
2:E:2039:LEU:C	2:E:2040:TRP:CG	2.76	0.58
2:B:2041:PRO:HG2	2:B:2043:PHE:CD1	2.38	0.58
2:B:2227:VAL:CG1	2:B:2239:SER:HB3	2.34	0.58
2:B:2265:GLU:O	2:B:2266:LEU:HD23	2.03	0.58
2:E:889:TRP:O	2:E:893:ARG:HG2	2.04	0.58
2:E:1015:PRO:HD2	2:E:1165:LEU:HD23	1.85	0.58
1:A:214:PHE:O	1:A:215:LYS:HB2	2.04	0.58
2:B:1687:HIS:HE1	2:B:1689:ARG:HG3	1.68	0.58
2:E:2267:LYS:O	2:E:2305:TYR:CZ	2.56	0.58
2:B:1727:LEU:CD2	2:B:1728:ILE:H	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2183:TYR:HD2	2:B:2289:ILE:HD13	1.67	0.58
2:E:2268:PHE:CD2	2:E:2331:PRO:HB3	2.38	0.58
2:E:1999:LEU:HD13	2:E:2003:THR:HB	1.85	0.58
2:B:1983:GLU:CB	2:B:1984:PRO:CD	2.80	0.58
2:B:2221:ILE:HD13	2:B:2256:LEU:HD12	1.85	0.58
2:B:1476:ALA:O	2:B:1479:GLU:HB2	2.03	0.58
2:B:1731:LYS:O	2:B:1771:THR:OG1	2.21	0.58
2:B:2053:SER:HA	2:B:2056:ARG:HD2	1.86	0.58
2:B:1025:VAL:O	2:B:1029:THR:HG23	2.04	0.58
2:B:1056:GLU:O	2:B:1060:LYS:HG2	2.03	0.58
2:B:2038:HIS:CD2	2:B:2038:HIS:N	2.72	0.58
2:E:1091:ASN:HB3	2:E:1093:LYS:HE3	1.84	0.58
1:D:344:PRO:HB3	2:E:1858:TYR:CE2	2.39	0.57
2:B:1186:TYR:HB2	2:B:1228:TRP:CZ3	2.39	0.57
2:E:1709:TRP:HB2	2:E:1729:THR:O	2.04	0.57
2:E:1834:PHE:O	2:E:1839:ASN:ND2	2.34	0.57
2:E:2041:PRO:CG	2:E:2043:PHE:CE1	2.80	0.57
2:E:2066:LYS:HB2	2:E:2067:TYR:HD1	1.69	0.57
2:E:2304:ALA:HB2	2:E:2339:LEU:HD21	1.73	0.57
2:E:1704:GLU:OE1	2:E:1704:GLU:HA	2.05	0.57
2:B:2268:PHE:O	2:B:2268:PHE:HD1	1.88	0.57
2:E:2021:SER:O	2:E:2024:MET:CB	2.53	0.57
2:B:1019:GLU:HB2	2:B:1023:LEU:HD23	1.87	0.57
2:B:2309:ASP:CA	2:B:2312:TYR:HB2	2.35	0.57
1:D:8:SER:OG	1:D:10:PRO:HD3	2.04	0.57
2:E:1251:TYR:OH	2:E:1274:ARG:HD3	2.05	0.57
2:E:1826:TYR:HA	2:E:1827:GLN:HB2	1.86	0.57
2:E:2162:LEU:HD21	2:E:2199:VAL:HG12	1.86	0.57
1:A:327:ILE:HG23	2:B:1340:ILE:CD1	2.34	0.57
2:B:1015:PRO:CD	2:B:1165:LEU:HD23	2.29	0.57
2:B:2185:LEU:HG	2:B:2186:PRO:CD	2.33	0.57
2:B:2194:ILE:HA	2:B:2197:SER:OG	2.04	0.57
2:B:1639:PRO:C	2:B:1640:THR:HG23	2.25	0.57
2:B:2259:ILE:CD1	2:B:2291:ILE:O	2.33	0.57
1:A:8:SER:OG	1:A:10:PRO:HD3	2.05	0.57
2:B:1251:TYR:OH	2:B:1274:ARG:HD3	2.04	0.57
2:B:889:TRP:O	2:B:893:ARG:HG2	2.05	0.57
2:B:2152:TRP:CA	2:B:2154:LYS:H	2.18	0.57
2:B:2221:ILE:HD13	2:B:2256:LEU:CD1	2.35	0.57
1:D:87:ALA:O	1:D:90:GLU:HB3	2.04	0.57
2:E:1324:GLY:HA3	2:E:1325:SER:OG	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1721:ASN:OD1	2:E:1722:ASP:N	2.38	0.57
2:B:1477:PHE:CE2	2:B:1495:PHE:CD2	2.93	0.57
2:B:2228:PRO:O	2:B:2239:SER:HB3	2.05	0.57
2:E:1687:HIS:HE1	2:E:1689:ARG:HG3	1.69	0.57
2:B:2046:GLU:O	2:B:2049:ILE:N	2.38	0.56
2:E:2018:ASN:CG	2:E:2058:LEU:HD11	2.20	0.56
2:B:1976:ASP:OD1	2:B:1980:LYS:HG3	2.05	0.56
2:B:1977:VAL:HG13	2:B:1978:VAL:N	2.19	0.56
2:B:2191:LYS:C	2:B:2195:GLU:HG3	2.25	0.56
2:B:2307:LEU:HD11	2:B:2311:GLY:HA3	1.88	0.56
2:E:930:ASN:HD22	2:E:933:GLU:HB2	1.70	0.56
2:E:2358:ASN:H	2:E:2387:HIS:CE1	2.22	0.56
2:B:1887:GLY:HA2	2:B:1992:TYR:CE2	2.40	0.56
2:B:2035:LYS:HD2	2:B:2037:TYR:HE1	1.68	0.56
2:B:2281:PHE:CE1	2:B:2288:CYS:CB	2.87	0.56
2:E:1468:ALA:O	2:E:1472:ASN:N	2.38	0.56
2:E:1687:HIS:CE1	2:E:1688:PRO:HD2	2.41	0.56
2:E:1826:TYR:OH	2:E:1938:LYS:CE	2.53	0.56
2:B:2060:LEU:O	2:B:2064:GLY:N	2.38	0.56
2:B:2210:MET:CE	2:B:2253:LEU:N	2.69	0.56
2:E:2277:HIS:CE1	2:E:2281:PHE:CD2	2.94	0.56
2:B:1075:ASP:OD1	2:B:1076:PRO:HD2	2.05	0.56
2:B:1264:GLY:O	2:B:1305:SER:OG	2.24	0.56
2:B:1605:ARG:CZ	2:B:1824:GLN:OE1	2.53	0.56
2:B:1995:TRP:HH2	2:B:2011:LEU:HD11	1.71	0.56
2:E:1431:HIS:C	2:E:1433:ASP:H	2.07	0.56
2:E:2162:LEU:HD12	2:E:2194:ILE:O	2.06	0.56
1:A:108:ILE:HG22	1:A:109:ASP:O	2.04	0.56
2:B:2208:TYR:CB	2:B:2253:LEU:HD11	2.35	0.56
2:B:2235:SER:HB3	2:B:2322:MET:HA	1.88	0.56
2:B:2315:GLY:C	2:B:2318:ASN:H	2.08	0.56
2:E:1973:LYS:HE3	2:E:2038:HIS:O	2.06	0.56
2:E:2182:VAL:HG12	2:E:2338:GLN:CB	2.36	0.56
2:B:2037:TYR:CB	2:B:2038:HIS:CD2	2.79	0.56
2:B:2208:TYR:HB3	2:B:2253:LEU:HD22	1.84	0.56
2:B:2282:ALA:HB1	2:B:2316:GLU:OE2	2.03	0.56
2:E:1711:VAL:HG12	2:E:1791:PHE:CA	2.36	0.56
2:E:1711:VAL:HG12	2:E:1791:PHE:CB	2.34	0.56
2:E:2210:MET:HE1	2:E:2252:GLY:CA	2.22	0.56
2:B:2024:MET:SD	2:B:2157:ILE:HG22	2.46	0.56
2:E:1826:TYR:CZ	2:E:1938:LYS:NZ	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2043:PHE:CD2	2:B:2047:GLN:OE1	2.59	0.55
2:B:2247:LEU:CG	2:B:2375:LYS:HA	2.35	0.55
2:B:2258:TRP:HD1	2:B:2258:TRP:H	1.52	0.55
2:B:2003:THR:O	2:B:2006:SER:N	2.38	0.55
2:B:2358:ASN:CB	2:B:2387:HIS:ND1	2.47	0.55
1:A:31:HIS:HB3	1:A:96:PHE:CD2	2.41	0.55
2:E:1293:THR:O	2:E:1295:GLN:N	2.39	0.55
2:B:1598:LEU:C	2:B:1598:LEU:HD13	2.26	0.55
2:E:1731:LYS:NZ	2:E:1768:PRO:CB	2.68	0.55
2:E:2178:GLU:O	2:E:2217:LYS:CD	2.55	0.55
1:A:85:ASP:OD1	1:A:88:LYS:N	2.22	0.55
2:B:1687:HIS:CE1	2:B:1688:PRO:HD2	2.41	0.55
2:B:1887:GLY:CA	2:B:1992:TYR:CE2	2.90	0.55
2:E:1293:THR:O	2:E:1293:THR:OG1	2.24	0.55
2:E:2025:ILE:HG23	2:E:2054:GLN:CD	2.26	0.55
2:E:2087:ASN:HD22	2:E:2088:ILE:N	2.04	0.55
2:E:2213:LYS:CA	2:E:2215:HIS:H	2.12	0.55
2:B:1795:LYS:HB3	2:B:1796:PRO:HD3	1.89	0.55
2:B:2183:TYR:HD1	2:B:2219:LYS:HB2	1.71	0.55
2:E:1998:ARG:HD2	2:E:2045:ASP:CG	2.27	0.55
2:E:2278:SER:OG	2:E:2279:LYS:N	2.39	0.55
2:E:1259:LEU:HD23	2:E:1268:ARG:HG3	1.89	0.55
2:B:1866:PHE:HD1	2:B:1866:PHE:H	1.53	0.55
2:B:1895:HIS:NE2	2:B:1896:THR:OG1	2.38	0.55
2:B:2037:TYR:CB	2:B:2038:HIS:HD2	2.15	0.55
1:D:69:ILE:HD13	1:D:80:MET:HA	1.89	0.55
1:A:48:HIS:CE1	1:A:53:SER:HG	2.25	0.55
2:B:2017:THR:CG2	2:B:2062:GLU:HG3	2.37	0.55
2:B:2024:MET:SD	2:B:2157:ILE:CG2	2.95	0.55
2:E:1991:ILE:HG23	2:E:2008:LEU:HD22	1.89	0.55
2:E:2232:HIS:HE1	2:E:2237:GLN:HE21	1.55	0.55
2:B:2208:TYR:CG	2:B:2253:LEU:HD13	2.42	0.55
2:E:2193:PHE:CZ	2:E:2203:VAL:HG12	2.42	0.55
2:E:2244:ILE:O	2:E:2250:THR:HG21	2.06	0.55
2:B:2002:TYR:C	2:B:2002:TYR:CD1	2.80	0.54
2:B:1679:GLU:HB3	2:B:1704:GLU:O	2.07	0.54
2:B:1733:TRP:CE2	2:B:1772:GLY:HA3	2.41	0.54
2:B:2037:TYR:C	2:B:2038:HIS:CD2	2.80	0.54
2:B:2386:MET:HE2	2:B:2387:HIS:N	2.22	0.54
2:E:2034:ILE:CD1	2:E:2040:TRP:C	2.58	0.54
2:B:2061:THR:O	2:B:2064:GLY:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2182:VAL:N	2:B:2338:GLN:HB2	2.22	0.54
2:B:934:ARG:HG2	2:B:934:ARG:HH11	1.73	0.54
2:B:1704:GLU:CG	2:B:1705:SER:H	2.20	0.54
2:B:2037:TYR:CD1	2:B:2037:TYR:N	2.76	0.54
2:B:2183:TYR:HD1	2:B:2219:LYS:CB	2.20	0.54
2:B:2209:GLY:HA3	2:B:2256:LEU:CD2	2.35	0.54
2:B:2259:ILE:CD1	2:B:2291:ILE:CA	2.84	0.54
2:B:2262:GLN:N	2:B:2293:ILE:O	2.41	0.54
2:B:2382:PHE:HB3	2:B:2383:TYR:HD1	1.72	0.54
2:E:1598:LEU:C	2:E:1598:LEU:HD22	2.28	0.54
2:E:2179:GLU:HG2	2:E:2180:GLN:N	2.22	0.54
2:B:2192:LYS:HA	2:B:2195:GLU:CG	2.37	0.54
2:E:1710:GLU:HA	2:E:1728:ILE:HA	1.90	0.54
1:A:347:VAL:HG21	2:B:1875:ILE:CD1	2.33	0.54
2:B:1259:LEU:HD23	2:B:1268:ARG:HG3	1.90	0.54
2:B:2192:LYS:CA	2:B:2195:GLU:HB2	2.37	0.54
2:E:1624:LEU:HD23	2:E:1625:VAL:N	2.22	0.54
1:A:12:GLU:HG3	1:A:25:LYS:HA	1.89	0.54
2:B:885:VAL:HG21	2:B:1124:LEU:HD21	1.90	0.54
1:D:35:ASP:OD2	1:D:104:SER:OG	2.25	0.54
2:E:1466:GLN:O	2:E:1469:ILE:HB	2.07	0.54
2:E:1825:ILE:O	2:E:1826:TYR:HB3	2.08	0.54
2:B:1139:ASN:H	2:B:1139:ASN:ND2	2.05	0.54
2:B:2208:TYR:HB3	2:B:2253:LEU:HD11	1.90	0.54
2:E:2079:ILE:HD13	2:E:2079:ILE:N	2.23	0.54
2:B:1598:LEU:H	2:B:1598:LEU:HD12	1.72	0.54
2:B:2050:THR:HA	2:B:2053:SER:OG	2.06	0.54
2:B:2209:GLY:O	2:B:2254:GLU:O	2.25	0.54
2:B:2358:ASN:O	2:B:2387:HIS:ND1	2.41	0.54
1:D:354:ARG:HB2	1:D:355:PRO:HD3	1.89	0.54
2:E:1292:ARG:HG2	2:E:1292:ARG:HH11	1.72	0.54
2:B:1801:SER:O	2:B:1805:ILE:HG23	2.08	0.54
2:B:1882:LEU:CD1	2:B:1991:ILE:HG21	2.37	0.54
2:B:1070:LEU:O	2:B:1074:VAL:CG2	2.56	0.53
2:B:1961:ASN:HA	2:B:2079:ILE:HD12	1.89	0.53
2:B:2007:ARG:HG2	2:B:2052:GLU:CD	2.28	0.53
2:B:2188:ASN:ND2	2:B:2346:THR:HB	2.20	0.53
2:B:2210:MET:HE2	2:B:2252:GLY:C	2.27	0.53
2:B:2278:SER:HB3	2:B:2316:GLU:CG	2.38	0.53
2:B:1190:ASN:N	2:B:1191:PRO:HD3	2.22	0.53
2:B:1866:PHE:N	2:B:1866:PHE:CD1	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2296:THR:O	2:B:2297:PRO:C	2.44	0.53
2:B:2386:MET:HE2	2:B:2387:HIS:H	1.73	0.53
2:E:1702:THR:HG23	2:E:1768:PRO:HG3	1.85	0.53
2:E:1899:TRP:HA	2:E:1899:TRP:CE3	2.43	0.53
2:B:2007:ARG:NE	2:B:2052:GLU:OE2	2.41	0.53
2:B:2184:VAL:O	2:B:2221:ILE:HG12	2.08	0.53
2:B:2256:LEU:C	2:B:2288:CYS:HG	2.03	0.53
1:A:208:VAL:O	1:A:213:ILE:HD12	2.08	0.53
1:D:347:VAL:HG21	2:E:1875:ILE:CD1	2.38	0.53
2:B:2202:GLN:HG2	2:B:2261:THR:O	2.09	0.53
2:E:1259:LEU:CD2	2:E:1268:ARG:HG3	2.38	0.53
2:E:1801:SER:O	2:E:1805:ILE:HG12	2.09	0.53
2:E:2202:GLN:NE2	2:E:2235:SER:O	2.37	0.53
2:B:950:THR:O	2:B:954:ILE:N	2.40	0.53
2:B:2233:VAL:HG23	2:B:2234:GLY:N	2.24	0.53
2:E:2227:VAL:HG13	2:E:2228:PRO:HD2	1.91	0.53
1:A:109:ASP:OD2	1:A:113:THR:OG1	2.27	0.53
1:D:109:ASP:OD1	1:D:110:GLU:N	2.42	0.53
2:B:2035:LYS:HB3	2:B:2037:TYR:CD1	2.43	0.53
2:E:2003:THR:O	2:E:2006:SER:N	2.42	0.53
2:B:1624:LEU:C	2:B:1624:LEU:HD23	2.29	0.53
2:B:2185:LEU:O	2:B:2342:SER:N	2.37	0.53
2:B:2202:GLN:CG	2:B:2261:THR:O	2.57	0.53
1:A:69:ILE:HD13	1:A:80:MET:HA	1.90	0.53
2:B:1598:LEU:H	2:B:1598:LEU:CD1	2.21	0.53
2:B:2339:LEU:HD12	2:B:2339:LEU:C	2.26	0.53
2:B:2339:LEU:HD13	2:B:2340:LEU:H	1.68	0.53
2:E:1104:ILE:CG2	2:E:1107:LEU:HD13	2.39	0.53
2:E:2384:ASN:ND2	2:E:2385:GLU:N	2.57	0.53
2:B:1259:LEU:CD2	2:B:1268:ARG:HG3	2.39	0.52
2:B:2339:LEU:C	2:B:2340:LEU:HD12	2.24	0.52
1:A:214:PHE:CE1	1:A:220:TYR:HA	2.44	0.52
2:B:1107:LEU:HD23	2:B:1109:PHE:CE1	2.44	0.52
2:B:2273:GLU:OE2	2:B:2290:ASP:OD2	2.26	0.52
2:B:2294:PHE:CD2	2:B:2301:SER:OG	2.36	0.52
2:B:1466:GLN:OE1	2:B:1466:GLN:HA	2.08	0.52
2:B:1719:GLU:OE1	2:B:1719:GLU:HA	2.09	0.52
2:B:2350:ILE:HD13	2:B:2376:TYR:CA	2.30	0.52
2:E:1279:VAL:HG12	2:E:1280:SER:O	2.09	0.52
2:E:2024:MET:O	2:E:2027:LEU:N	2.42	0.52
2:B:1383:PHE:HE2	2:B:1387:VAL:HG21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1599:SER:C	2:B:1600:GLN:HG2	2.29	0.52
2:B:1721:ASN:CB	2:E:1463:THR:HB	2.39	0.52
2:B:2223:THR:OG1	2:B:2348:ASN:OD1	2.08	0.52
2:E:1966:SER:HG	2:E:2016:LYS:HE3	1.72	0.52
2:E:2014:ALA:HA	2:E:2059:ILE:HD12	1.87	0.52
2:E:2083:ILE:HG22	2:E:2084:LEU:CD1	2.38	0.52
2:E:2043:PHE:HA	2:E:2047:GLN:OE1	2.10	0.52
2:B:1104:ILE:CG2	2:B:1107:LEU:HD13	2.39	0.52
2:B:2183:TYR:CE2	2:B:2289:ILE:HD13	2.44	0.52
2:E:1324:GLY:HA2	2:E:1325:SER:HG	1.71	0.52
2:E:1864:LYS:HG3	2:E:1870:VAL:HG22	1.90	0.52
2:E:2182:VAL:HG12	2:E:2338:GLN:HB2	1.91	0.52
2:E:2267:LYS:O	2:E:2305:TYR:CE1	2.63	0.52
2:E:1767:TYR:N	2:E:1767:TYR:CD1	2.77	0.52
2:E:2060:LEU:O	2:E:2063:TYR:HB3	2.09	0.52
2:B:1848:ILE:O	2:B:1930:PRO:HA	2.09	0.52
2:B:2060:LEU:O	2:B:2063:TYR:CB	2.53	0.52
2:B:2280:LEU:CD1	2:B:2281:PHE:CE2	2.91	0.52
1:D:88:LYS:O	1:D:92:ILE:HG13	2.10	0.52
1:D:106:PRO:C	1:D:107:LYS:CG	2.72	0.52
2:E:918:ASP:OD1	2:E:1515:LYS:NZ	2.39	0.52
2:E:1286:TRP:CE2	2:E:1302:LEU:HD11	2.45	0.52
2:E:1666:CYS:SG	2:E:1683:LYS:HE3	2.50	0.52
2:E:2384:ASN:HD22	2:E:2386:MET:N	2.02	0.52
2:B:1595:ARG:HG3	2:B:1596:THR:N	2.24	0.52
2:B:2357:TRP:CH2	2:B:2382:PHE:HD1	2.22	0.52
2:E:1212:ARG:HG2	2:E:1212:ARG:HH11	1.74	0.52
2:B:2233:VAL:CG2	2:B:2234:GLY:N	2.73	0.52
2:E:2074:LEU:C	2:E:2075:THR:HG1	2.09	0.52
1:A:296:SER:O	1:A:299:LYS:HG2	2.10	0.51
2:B:1093:LYS:HE2	2:B:1094:ASP:OD1	2.10	0.51
2:E:2011:LEU:O	2:E:2014:ALA:HB3	2.09	0.51
2:E:2302:LEU:HD12	2:E:2302:LEU:N	2.24	0.51
2:B:2035:LYS:CD	2:B:2037:TYR:HE1	2.22	0.51
2:B:2152:TRP:HA	2:B:2153:ARG:C	2.29	0.51
2:B:2182:VAL:HG13	2:B:2338:GLN:CD	2.23	0.51
2:B:2286:ARG:HD2	2:B:2312:TYR:CE2	2.45	0.51
2:E:1093:LYS:CD	2:E:1094:ASP:HA	2.41	0.51
1:D:20:TYR:CZ	1:D:106:PRO:HG2	2.44	0.51
2:E:1107:LEU:HD23	2:E:1109:PHE:CE1	2.45	0.51
2:B:2162:LEU:HD23	2:B:2165:ARG:NE	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2189:LEU:HD21	2:B:2347:GLY:CA	2.40	0.51
2:E:1763:ASN:H	2:E:1763:ASN:HD22	1.58	0.51
2:E:1991:ILE:HG21	2:E:2008:LEU:HD22	1.92	0.51
2:E:2062:GLU:OE2	2:E:2065:ARG:NH2	2.34	0.51
2:E:2064:GLY:O	2:E:2067:TYR:CA	2.58	0.51
2:E:2361:PHE:CZ	2:E:2383:TYR:CE1	2.98	0.51
2:E:1097:HIS:CD2	2:E:1098:VAL:O	2.63	0.51
2:E:1899:TRP:HA	2:E:1899:TRP:HE3	1.75	0.51
2:B:959:LEU:HD12	2:B:1077:ASN:OD1	2.11	0.51
2:E:1767:TYR:N	2:E:1767:TYR:HD1	2.09	0.51
2:B:1041:VAL:HG21	2:B:1253:LYS:HA	1.91	0.51
2:B:2017:THR:HG23	2:B:2062:GLU:OE2	2.11	0.51
2:B:2037:TYR:HB2	2:B:2038:HIS:NE2	2.26	0.51
2:E:1843:LEU:HD22	2:E:1884:PRO:HG3	1.93	0.51
2:E:2357:TRP:H	2:E:2387:HIS:CE1	2.28	0.51
2:B:2155:SER:O	2:B:2156:ALA:HB3	2.10	0.51
2:E:920:LYS:HG3	2:E:940:ILE:HG21	1.92	0.51
2:E:1292:ARG:HG2	2:E:1292:ARG:NH1	2.26	0.51
2:B:1029:THR:HG22	2:B:1260:PHE:CZ	2.46	0.51
2:B:1029:THR:HG22	2:B:1260:PHE:HZ	1.75	0.51
2:B:1105:ARG:HG3	2:B:1105:ARG:NH1	2.25	0.51
2:B:2019:GLU:OE2	2:B:2167:LYS:NZ	2.44	0.51
2:B:2210:MET:HE1	2:B:2253:LEU:CB	2.40	0.51
2:E:1472:ASN:C	2:E:2325:LEU:CB	2.75	0.51
2:E:2025:ILE:CG2	2:E:2054:GLN:CD	2.79	0.51
2:E:2050:THR:HA	2:E:2053:SER:HB3	1.93	0.51
2:B:1687:HIS:CE1	2:B:1689:ARG:HG3	2.46	0.50
2:B:2208:TYR:CB	2:B:2253:LEU:CD1	2.88	0.50
2:E:2041:PRO:HG2	2:E:2043:PHE:CE1	2.46	0.50
2:E:2049:ILE:O	2:E:2053:SER:HB3	2.11	0.50
2:B:1075:ASP:HB3	2:B:1078:ILE:HD12	1.93	0.50
2:B:1317:ARG:O	2:B:1321:MET:HB2	2.12	0.50
2:B:1661:ILE:HG23	2:B:1805:ILE:CD1	2.41	0.50
2:B:2157:ILE:HA	2:B:2160:THR:OG1	2.10	0.50
2:B:2236:VAL:CB	2:B:2238:ILE:HD11	2.41	0.50
2:E:1605:ARG:NH2	2:E:1824:GLN:OE1	2.44	0.50
2:E:2034:ILE:CG2	2:E:2040:TRP:H	2.22	0.50
2:B:1999:LEU:CD1	2:B:2003:THR:HB	2.36	0.50
2:B:2194:ILE:O	2:B:2197:SER:OG	2.28	0.50
2:B:2350:ILE:CD1	2:B:2376:TYR:HA	2.31	0.50
2:E:1599:SER:C	2:E:1600:GLN:HG2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2183:TYR:OH	2:B:2219:LYS:NZ	2.37	0.50
2:B:2247:LEU:CD1	2:B:2248:PRO:HD3	2.41	0.50
1:D:55:ARG:NH2	1:D:279:TYR:CZ	2.79	0.50
2:E:1057:MET:CE	2:E:1166:ASP:HB2	2.41	0.50
2:E:1687:HIS:CE1	2:E:1689:ARG:HG3	2.46	0.50
2:E:2227:VAL:HG13	2:E:2239:SER:OG	2.10	0.50
2:E:1343:PHE:HB3	2:E:1444:ILE:CD1	2.40	0.50
2:E:1795:LYS:HB3	2:E:1796:PRO:HD3	1.94	0.50
2:B:1854:ASP:HA	2:B:1857:VAL:HG23	1.94	0.50
2:B:2157:ILE:CA	2:B:2160:THR:OG1	2.60	0.50
2:B:2162:LEU:CD2	2:B:2165:ARG:NE	2.74	0.50
2:E:885:VAL:HG21	2:E:1124:LEU:HD21	1.94	0.50
2:E:1983:GLU:HB2	2:E:1984:PRO:HD2	1.94	0.50
2:E:2040:TRP:CD1	2:E:2040:TRP:N	2.80	0.50
1:A:327:ILE:HB	1:A:328:TYR:CD2	2.47	0.50
2:B:1969:MET:O	2:B:1975:SER:OG	2.30	0.50
2:B:2032:ILE:CD1	2:B:2047:GLN:HE22	2.24	0.50
2:B:2350:ILE:CD1	2:B:2376:TYR:CD1	2.95	0.50
2:E:2018:ASN:ND2	2:E:2058:LEU:HG	2.17	0.50
1:D:153:LEU:HD23	1:D:153:LEU:C	2.32	0.50
1:D:280:SER:HB2	1:D:313:TYR:CE1	2.47	0.50
2:E:1764:VAL:N	2:E:1766:MET:HE2	2.24	0.50
1:A:215:LYS:O	1:A:216:ASN:OD1	2.29	0.50
2:B:1036:SER:HB3	2:B:1154:LYS:HE2	1.93	0.50
2:B:2278:SER:CB	2:B:2316:GLU:HG3	2.42	0.50
2:E:945:ASP:OD1	2:E:945:ASP:N	2.45	0.50
1:D:19:GLN:HE22	1:D:110:GLU:CG	2.18	0.49
2:E:1854:ASP:OD1	2:E:1937:ARG:HD3	2.11	0.49
2:E:2051:ILE:HD13	2:E:2051:ILE:N	2.27	0.49
2:E:2083:ILE:HG22	2:E:2084:LEU:H	1.77	0.49
2:E:2177:VAL:CG2	2:E:2180:GLN:HG3	2.42	0.49
2:E:2182:VAL:HA	2:E:2338:GLN:HB2	1.92	0.49
2:E:2311:GLY:HA2	2:E:2333:PHE:CD1	2.46	0.49
2:B:969:ILE:HA	2:B:981:VAL:O	2.12	0.49
2:B:1666:CYS:SG	2:B:1683:LYS:HE3	2.52	0.49
2:B:1890:PHE:HB3	2:B:1986:MET:SD	2.52	0.49
2:B:2182:VAL:HG23	2:B:2182:VAL:O	2.11	0.49
2:E:1015:PRO:CD	2:E:1165:LEU:HD23	2.42	0.49
2:E:1705:SER:OG	2:E:1730:ASN:CB	2.60	0.49
2:E:2064:GLY:C	2:E:2067:TYR:H	2.11	0.49
2:E:2083:ILE:HG22	2:E:2084:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:SER:HB2	1:A:313:TYR:CE1	2.48	0.49
2:B:1604:ARG:HH22	2:B:1822:GLY:C	2.14	0.49
2:B:2192:LYS:HA	2:B:2195:GLU:CB	2.41	0.49
1:D:151:GLU:OE2	1:D:154:LYS:CE	2.49	0.49
2:B:1015:PRO:CD	2:B:1165:LEU:CD2	2.90	0.49
2:B:2041:PRO:CG	2:B:2043:PHE:CE1	2.96	0.49
2:B:2052:GLU:O	2:B:2056:ARG:CG	2.40	0.49
1:D:77:LEU:C	1:D:77:LEU:HD12	2.33	0.49
2:E:988:GLU:O	2:E:991:THR:HG22	2.12	0.49
2:E:1711:VAL:CA	2:E:1790:TRP:O	2.60	0.49
2:E:2201:ILE:HG22	2:E:2382:PHE:CZ	2.48	0.49
2:B:1463:THR:O	2:B:1467:GLU:HG2	2.12	0.49
2:B:2208:TYR:C	2:B:2253:LEU:HD21	2.33	0.49
2:B:2247:LEU:CD1	2:B:2375:LYS:HA	2.42	0.49
2:E:1394:LEU:HD23	2:E:1570:TRP:CZ2	2.47	0.49
2:E:2163:TYR:CE1	2:E:2164:LEU:CD2	2.96	0.49
2:B:2055:MET:O	2:B:2058:LEU:N	2.45	0.49
2:B:2153:ARG:HA	2:B:2155:SER:O	2.12	0.49
1:D:88:LYS:NZ	1:D:92:ILE:HD11	2.27	0.49
1:D:326:LEU:O	1:D:326:LEU:HG	2.13	0.49
2:E:1766:MET:C	2:E:1767:TYR:HD1	2.16	0.49
1:A:72:ASP:OD2	1:A:75:ASP:HB2	2.13	0.49
1:A:83:GLU:CG	1:A:89:PHE:HB2	2.42	0.49
2:B:1687:HIS:ND1	2:B:1688:PRO:CD	2.76	0.49
2:B:2064:GLY:O	2:B:2068:ASN:N	2.45	0.49
1:D:110:GLU:O	1:D:111:ASP:CB	2.60	0.49
2:E:1036:SER:HB3	2:E:1154:LYS:HE2	1.95	0.49
2:E:1368:GLN:NE2	2:E:1389:TYR:OH	2.44	0.49
2:E:1383:PHE:HE2	2:E:1387:VAL:HG21	1.75	0.49
2:B:1097:HIS:ND1	2:B:1098:VAL:N	2.60	0.49
2:B:1137:PRO:CD	2:B:1140:ASN:O	2.61	0.49
2:B:1324:GLY:CA	2:B:1325:SER:CB	2.91	0.49
2:B:2182:VAL:CB	2:B:2338:GLN:CB	2.89	0.49
2:B:2183:TYR:N	2:B:2338:GLN:O	2.40	0.49
2:B:2284:LYS:HE2	2:B:2285:LYS:CA	2.42	0.49
2:E:1461:TYR:O	2:E:1465:ARG:N	2.44	0.49
2:E:2177:VAL:HG23	2:E:2180:GLN:N	2.19	0.49
2:E:2251:GLU:OE1	2:E:2251:GLU:N	2.46	0.49
2:B:920:LYS:HG3	2:B:940:ILE:HG21	1.94	0.49
2:B:930:ASN:N	2:B:933:GLU:OE1	2.46	0.49
2:B:1624:LEU:HD21	2:B:1633:PHE:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1808:ALA:O	2:B:1809:ASN:C	2.51	0.49
2:B:1993:ASP:CG	2:B:2038:HIS:CB	2.58	0.49
2:B:2381:GLU:H	2:B:2381:GLU:CD	2.00	0.49
2:E:2087:ASN:ND2	2:E:2088:ILE:N	2.61	0.49
2:B:1465:ARG:HG3	2:B:1465:ARG:NH1	2.28	0.48
2:B:1729:THR:CG2	2:B:1771:THR:CG2	2.54	0.48
2:B:2044:THR:H	2:B:2047:GLN:NE2	2.11	0.48
2:B:2259:ILE:HD13	2:B:2291:ILE:HG21	1.82	0.48
2:B:2259:ILE:HD12	2:B:2291:ILE:CA	2.42	0.48
2:B:2379:PRO:C	2:B:2380:LEU:HD23	2.33	0.48
2:E:2163:TYR:CD1	2:E:2164:LEU:N	2.81	0.48
2:E:2384:ASN:HD22	2:E:2384:ASN:C	2.16	0.48
2:B:2282:ALA:O	2:B:2286:ARG:HG2	2.14	0.48
2:E:1733:TRP:CE2	2:E:1767:TYR:CD2	2.97	0.48
2:E:2163:TYR:CE1	2:E:2164:LEU:HD23	2.48	0.48
2:E:2177:VAL:CG2	2:E:2180:GLN:CG	2.91	0.48
2:E:2183:TYR:CD1	2:E:2289:ILE:HD13	2.48	0.48
2:B:2342:SER:HG	2:B:2344:ARG:H	1.59	0.48
2:B:2208:TYR:OH	2:B:2244:ILE:HG23	2.13	0.48
2:B:2307:LEU:HD12	2:B:2307:LEU:C	2.28	0.48
2:E:1209:LYS:HG2	2:E:1212:ARG:NH2	2.27	0.48
2:E:2269:MET:HE3	2:E:2273:GLU:HB3	1.95	0.48
2:E:2270:ALA:HB1	2:E:2324:VAL:HA	1.95	0.48
2:B:1432:GLU:O	2:B:1433:ASP:CB	2.61	0.48
2:B:2044:THR:O	2:B:2048:TRP:CD1	2.66	0.48
2:B:2284:LYS:C	2:B:2284:LYS:HE3	2.34	0.48
1:D:224:LEU:HD23	1:D:224:LEU:C	2.33	0.48
2:E:1709:TRP:O	2:E:1728:ILE:CA	2.62	0.48
2:E:2183:TYR:CE1	2:E:2289:ILE:HG21	2.48	0.48
2:B:930:ASN:O	2:B:934:ARG:HB2	2.14	0.48
2:B:2280:LEU:HD12	2:B:2281:PHE:CD2	2.49	0.48
2:B:2386:MET:CE	2:B:2387:HIS:N	2.76	0.48
2:B:2210:MET:CE	2:B:2252:GLY:C	2.82	0.48
2:E:1343:PHE:HB3	2:E:1444:ILE:HD13	1.96	0.48
2:E:1762:ASP:CG	2:E:1763:ASN:N	2.66	0.48
2:E:2271:ALA:HA	2:E:2329:PHE:CE1	2.48	0.48
1:A:77:LEU:C	1:A:77:LEU:HD12	2.33	0.48
1:A:77:LEU:HD12	1:A:77:LEU:O	2.14	0.48
2:B:1687:HIS:CG	2:B:1688:PRO:HD2	2.49	0.48
2:B:1899:TRP:HB3	2:B:1905:LEU:HD21	1.95	0.48
2:B:2278:SER:HB3	2:B:2316:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2384:ASN:HD22	2:B:2385:GLU:N	2.11	0.48
1:D:280:SER:CB	1:D:313:TYR:CE1	2.97	0.48
2:E:1865:THR:OG1	2:E:1867:GLU:OE1	2.31	0.48
2:E:2019:GLU:O	2:E:2019:GLU:HG2	2.14	0.48
2:B:1164:TYR:O	2:B:1167:ARG:N	2.42	0.48
2:B:1188:ALA:O	2:B:1191:PRO:CD	2.62	0.48
2:B:1368:GLN:NE2	2:B:1389:TYR:OH	2.47	0.48
2:B:1959:THR:OG1	2:B:1960:GLU:N	2.47	0.48
2:B:2183:TYR:HE2	2:B:2289:ILE:HG21	1.79	0.48
2:B:2307:LEU:CD1	2:B:2308:THR:O	2.62	0.48
2:B:2358:ASN:CB	2:B:2387:HIS:HE1	2.04	0.48
2:E:2037:TYR:C	2:E:2038:HIS:CD2	2.88	0.48
2:E:2066:LYS:HB2	2:E:2067:TYR:CE1	2.49	0.48
1:A:108:ILE:HD12	1:A:108:ILE:N	2.29	0.47
2:B:936:GLU:O	2:B:940:ILE:CD1	2.61	0.47
2:B:1041:VAL:HG23	2:B:1041:VAL:O	2.13	0.47
2:B:1570:TRP:O	2:B:1571:GLU:HG3	2.14	0.47
2:B:2177:VAL:N	2:B:2338:GLN:NE2	2.59	0.47
2:E:2268:PHE:CD1	2:E:2268:PHE:C	2.87	0.47
2:B:1759:TYR:O	2:B:1762:ASP:CB	2.62	0.47
2:B:2186:PRO:HG3	2:B:2345:ILE:HD12	1.95	0.47
2:B:2267:LYS:O	2:B:2305:TYR:HE2	1.96	0.47
2:E:2277:HIS:O	2:E:2281:PHE:HD2	1.96	0.47
2:B:1895:HIS:CD2	2:B:1896:THR:HG1	2.26	0.47
2:B:2294:PHE:CE1	2:B:2296:THR:HG23	2.48	0.47
2:B:2350:ILE:HD11	2:B:2376:TYR:CE1	2.49	0.47
2:B:1394:LEU:HD23	2:B:1570:TRP:CZ2	2.49	0.47
2:B:1558:GLU:CD	2:B:1563:LYS:HZ1	2.17	0.47
2:B:1624:LEU:HD23	2:B:1625:VAL:N	2.30	0.47
2:B:1677:GLN:OE1	2:B:1706:VAL:HG11	2.15	0.47
2:B:2058:LEU:O	2:B:2059:ILE:C	2.52	0.47
2:B:1189:GLU:C	2:B:1191:PRO:HD3	2.35	0.47
2:B:2025:ILE:HG22	2:B:2025:ILE:O	2.12	0.47
2:B:2268:PHE:CE2	2:B:2331:PRO:HG3	2.49	0.47
1:D:108:ILE:HD13	1:D:108:ILE:H	1.78	0.47
2:E:936:GLU:O	2:E:940:ILE:CD1	2.61	0.47
2:B:953:ARG:HH11	2:B:953:ARG:HG3	1.79	0.47
2:B:2302:LEU:N	2:B:2302:LEU:CD1	2.77	0.47
2:E:1472:ASN:HB3	2:E:2325:LEU:O	2.14	0.47
2:E:1791:PHE:CD1	2:E:1791:PHE:C	2.87	0.47
2:E:2053:SER:OG	2:E:2054:GLN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1075:ASP:CB	2:B:1078:ILE:HD12	2.45	0.47
2:B:1097:HIS:ND1	2:B:1098:VAL:O	2.48	0.47
2:B:2163:TYR:CD1	2:B:2164:LEU:N	2.83	0.47
2:B:2192:LYS:O	2:B:2196:ILE:N	2.46	0.47
2:B:2215:HIS:HB3	2:B:2218:VAL:HB	1.97	0.47
2:B:2230:LEU:CD2	2:B:2237:GLN:HG3	2.44	0.47
2:B:2247:LEU:HA	2:B:2247:LEU:HD13	1.74	0.47
2:B:2306:ASN:HB2	2:B:2335:THR:OG1	2.14	0.47
1:D:77:LEU:HD12	1:D:77:LEU:O	2.14	0.47
1:D:215:LYS:HD2	1:D:215:LYS:N	2.29	0.47
1:D:320:ASP:OD1	2:E:1330:LYS:HE2	2.15	0.47
2:E:969:ILE:HA	2:E:981:VAL:O	2.15	0.47
2:E:1079:ALA:O	2:E:1083:THR:HG22	2.15	0.47
2:E:1686:VAL:HG11	2:E:1690:LYS:HD2	1.95	0.47
2:E:1886:THR:CB	2:E:1888:HIS:CE1	2.96	0.47
2:E:2004:ALA:O	2:E:2007:ARG:HB3	2.14	0.47
2:E:2339:LEU:O	2:E:2340:LEU:HD12	2.14	0.47
2:B:1471:GLN:O	2:B:1473:ARG:HG3	2.15	0.47
2:B:1791:PHE:CD1	2:B:1791:PHE:C	2.87	0.47
2:B:1857:VAL:HG13	2:B:1894:ILE:HG13	1.97	0.47
2:B:2178:GLU:O	2:B:2217:LYS:CG	2.62	0.47
2:E:1019:GLU:HB2	2:E:1023:LEU:HD23	1.97	0.47
2:E:1687:HIS:ND1	2:E:1688:PRO:CD	2.78	0.47
2:E:2037:TYR:C	2:E:2038:HIS:HD2	2.17	0.47
2:E:2177:VAL:HG23	2:E:2180:GLN:HB2	1.93	0.47
2:B:1984:PRO:O	2:B:1985:GLN:NE2	2.48	0.47
2:B:2208:TYR:CE2	2:B:2244:ILE:HD13	2.50	0.47
2:E:1680:SER:OG	2:E:1704:GLU:HB2	2.15	0.47
2:B:1721:ASN:HB2	2:E:1463:THR:HB	1.96	0.47
2:B:2007:ARG:CG	2:B:2052:GLU:OE2	2.62	0.47
2:E:1067:ASN:ND2	2:E:1083:THR:HG21	2.11	0.47
2:E:2011:LEU:HD12	2:E:2040:TRP:CH2	2.49	0.47
2:E:2210:MET:CE	2:E:2252:GLY:CA	2.85	0.47
2:B:1707:HIS:CG	2:B:1708:GLU:N	2.83	0.46
2:B:1733:TRP:CD1	2:B:1771:THR:O	2.68	0.46
2:B:1840:TYR:OH	2:B:2005:PHE:HD2	1.98	0.46
2:B:2184:VAL:CG2	2:B:2219:LYS:O	2.60	0.46
1:D:208:VAL:O	1:D:213:ILE:HD12	2.15	0.46
2:E:1999:LEU:HD12	2:E:2000:SER:O	2.15	0.46
2:E:2056:ARG:O	2:E:2060:LEU:N	2.42	0.46
2:E:2260:HIS:HE1	2:E:2273:GLU:OE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HD12	1:A:108:ILE:H	1.80	0.46
2:B:2032:ILE:HD11	2:B:2047:GLN:HE22	1.80	0.46
2:B:2034:ILE:HG23	2:B:2040:TRP:O	2.15	0.46
2:B:2210:MET:CE	2:B:2253:LEU:CB	2.93	0.46
1:D:75:ASP:OD2	1:D:79:LYS:HE2	2.11	0.46
2:E:1687:HIS:CG	2:E:1688:PRO:HD2	2.50	0.46
2:E:1760:THR:C	2:E:1762:ASP:H	2.19	0.46
2:B:2007:ARG:CD	2:B:2052:GLU:OE2	2.63	0.46
2:B:2153:ARG:CG	2:B:2153:ARG:NH1	2.74	0.46
2:E:1405:ILE:HB	2:E:1437:ILE:HB	1.98	0.46
2:E:1728:ILE:HD13	2:E:1728:ILE:N	2.26	0.46
2:E:1834:PHE:HD2	2:E:1960:GLU:CG	2.28	0.46
1:A:292:CYS:HA	1:A:296:SER:OG	2.15	0.46
2:B:1059:GLU:OE1	2:B:1059:GLU:N	2.48	0.46
2:B:1570:TRP:C	2:B:1571:GLU:HG3	2.36	0.46
2:B:1679:GLU:HB3	2:B:1704:GLU:C	2.36	0.46
1:D:327:ILE:CB	1:D:328:TYR:HD1	2.13	0.46
2:E:965:LYS:HB3	2:E:966:PRO:HD2	1.98	0.46
2:E:1370:ARG:HH11	2:E:1370:ARG:CG	2.28	0.46
2:E:1730:ASN:OD1	2:E:1730:ASN:N	2.49	0.46
2:E:2044:THR:H	2:E:2047:GLN:CD	2.18	0.46
2:E:2047:GLN:O	2:E:2051:ILE:N	2.48	0.46
2:B:1324:GLY:CA	2:B:1325:SER:OG	2.64	0.46
2:B:2227:VAL:CG1	2:B:2239:SER:CB	2.94	0.46
2:B:2247:LEU:CD1	2:B:2248:PRO:CD	2.91	0.46
1:D:354:ARG:HB2	1:D:355:PRO:CD	2.45	0.46
2:E:1378:LYS:HE3	2:E:1623:PHE:CE2	2.50	0.46
2:E:1733:TRP:CZ2	2:E:1767:TYR:CD2	3.04	0.46
2:B:929:LEU:HA	2:B:933:GLU:OE1	2.16	0.46
2:B:1104:ILE:HG22	2:B:1107:LEU:HD13	1.97	0.46
2:B:1465:ARG:HG3	2:B:1465:ARG:HH11	1.81	0.46
2:B:2198:ASP:CG	2:B:2199:VAL:N	2.68	0.46
2:E:1679:GLU:HB3	2:E:1704:GLU:O	2.16	0.46
2:E:1895:HIS:CD2	2:E:1982:THR:C	2.89	0.46
2:E:2159:ASN:HD21	2:E:2198:ASP:HA	1.81	0.46
2:B:936:GLU:O	2:B:940:ILE:HD13	2.15	0.46
2:B:1286:TRP:CE2	2:B:1302:LEU:HD11	2.50	0.46
2:B:2163:TYR:CE1	2:B:2164:LEU:CD2	2.99	0.46
2:E:1104:ILE:HG22	2:E:1107:LEU:HD13	1.97	0.46
2:E:1565:THR:O	2:E:1820:ARG:CZ	2.64	0.46
2:E:2182:VAL:CG1	2:E:2338:GLN:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1137:PRO:HD2	2:B:1140:ASN:O	2.14	0.46
2:B:1156:HIS:ND1	2:B:1157:PRO:HD2	2.31	0.46
2:B:1991:ILE:HD11	2:B:2008:LEU:HD11	1.98	0.46
2:B:2265:GLU:HG3	2:B:2294:PHE:CG	2.50	0.46
2:B:2367:ASN:OD1	2:B:2370:GLY:CA	2.64	0.46
2:E:1763:ASN:HD22	2:E:1763:ASN:N	2.13	0.46
2:E:2081:ASP:CG	2:E:2082:ILE:HG23	2.37	0.46
2:E:2354:GLY:O	2:E:2355:ASN:HB2	2.16	0.46
2:B:1188:ALA:O	2:B:1191:PRO:CG	2.64	0.46
2:B:1611:SER:N	2:B:1612:PRO:CD	2.79	0.46
2:B:2081:ASP:CG	2:B:2082:ILE:HG23	2.36	0.46
2:B:2209:GLY:HA2	2:B:2220:GLU:O	2.16	0.46
2:E:1542:TYR:CE2	2:E:1546:VAL:HG21	2.51	0.46
2:E:1961:ASN:OD1	2:E:2079:ILE:CD1	2.63	0.46
1:A:103:VAL:HG22	1:A:104:SER:N	2.30	0.46
1:A:327:ILE:HG21	1:A:328:TYR:CE2	2.51	0.46
2:B:2208:TYR:N	2:B:2223:THR:O	2.40	0.46
2:B:2282:ALA:HA	2:B:2286:ARG:HG2	1.98	0.46
2:E:936:GLU:O	2:E:940:ILE:HD13	2.16	0.46
2:E:1425:PHE:CD1	2:E:1425:PHE:N	2.84	0.46
2:E:1887:GLY:CA	2:E:1992:TYR:CD2	2.98	0.46
2:E:2014:ALA:N	2:E:2059:ILE:HD11	2.31	0.46
2:E:2211:SER:HA	2:E:2219:LYS:HA	1.97	0.46
2:E:2212:ALA:HB3	2:E:2218:VAL:HB	1.97	0.46
2:B:1121:ILE:HD13	2:B:1239:THR:CG2	2.46	0.45
2:B:1121:ILE:HD13	2:B:1239:THR:HG21	1.96	0.45
2:B:1177:ASP:O	2:B:1181:GLU:HB2	2.16	0.45
2:E:1597:GLY:CA	2:E:1599:SER:N	2.78	0.45
1:A:86:GLY:O	1:A:90:GLU:N	2.43	0.45
1:A:280:SER:CB	1:A:313:TYR:CE1	2.98	0.45
2:B:1976:ASP:OD1	2:B:1980:LYS:HD2	2.16	0.45
2:B:1996:LEU:HD21	2:B:2001:SER:HA	1.99	0.45
2:B:2041:PRO:CG	2:B:2043:PHE:CD1	2.99	0.45
2:B:2178:GLU:C	2:B:2217:LYS:HZ3	2.18	0.45
2:B:2308:THR:HG23	2:B:2333:PHE:C	2.19	0.45
1:D:84:ARG:HH11	1:D:84:ARG:CG	2.27	0.45
2:E:2002:TYR:C	2:E:2002:TYR:CD1	2.89	0.45
2:B:1727:LEU:C	2:B:1728:ILE:HG12	2.36	0.45
2:B:2070:ASN:O	2:B:2071:ILE:HG23	2.16	0.45
2:B:2176:PHE:CA	2:B:2338:GLN:NE2	2.73	0.45
2:B:2182:VAL:HA	2:B:2338:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2339:LEU:HD12	2:B:2340:LEU:CA	2.41	0.45
2:E:1459:ALA:O	2:E:1463:THR:HG23	2.17	0.45
2:E:1999:LEU:CD1	2:E:2004:ALA:HB2	2.45	0.45
2:E:2264:GLU:C	2:E:2294:PHE:CD1	2.89	0.45
2:E:2277:HIS:ND1	2:E:2281:PHE:HD2	2.07	0.45
2:B:957:TYR:HD2	2:B:991:THR:HG21	1.80	0.45
2:B:1238:LEU:O	2:B:1239:THR:HG22	2.16	0.45
2:B:1090:ILE:HD11	2:B:1104:ILE:HD11	1.99	0.45
2:B:1707:HIS:NE2	2:B:1708:GLU:OE1	2.50	0.45
2:B:1843:LEU:HD21	2:B:1851:PHE:HE2	1.82	0.45
2:B:2247:LEU:HD23	2:B:2374:PHE:HB2	1.99	0.45
1:D:72:ASP:OD2	1:D:75:ASP:HB2	2.17	0.45
2:E:2047:GLN:HA	2:E:2050:THR:HB	1.97	0.45
2:E:2061:THR:CG2	2:E:2062:GLU:N	2.79	0.45
1:A:354:ARG:CB	1:A:355:PRO:HD3	2.44	0.45
2:B:1097:HIS:CE1	2:B:1098:VAL:O	2.70	0.45
2:B:1844:PHE:CD1	2:B:1844:PHE:N	2.84	0.45
2:B:1977:VAL:CG1	2:B:1978:VAL:N	2.78	0.45
2:B:2177:VAL:N	2:B:2338:GLN:HE22	2.13	0.45
2:B:2208:TYR:CG	2:B:2253:LEU:CD1	3.00	0.45
2:B:2208:TYR:OH	2:B:2244:ILE:CG2	2.65	0.45
2:B:2286:ARG:HD3	2:B:2312:TYR:CD1	2.52	0.45
2:E:1059:GLU:OE1	2:E:1059:GLU:N	2.49	0.45
2:E:2070:ASN:O	2:E:2071:ILE:HG23	2.16	0.45
2:B:2210:MET:SD	2:B:2222:LYS:HD2	2.47	0.45
2:B:2215:HIS:HB3	2:B:2218:VAL:CG2	2.46	0.45
2:B:2386:MET:H	2:B:2386:MET:HG3	1.63	0.45
2:B:1104:ILE:CG2	2:B:1107:LEU:CD1	2.95	0.45
2:B:1472:ASN:HB3	2:B:2325:LEU:O	2.17	0.45
2:B:1886:THR:HG1	2:B:1888:HIS:CE1	2.31	0.45
2:B:2081:ASP:OD1	2:B:2082:ILE:HG23	2.16	0.45
2:B:2208:TYR:CZ	2:B:2244:ILE:HG21	2.52	0.45
2:B:2260:HIS:NE2	2:B:2273:GLU:OE2	2.50	0.45
2:B:2343:ASP:CB	2:B:2344:ARG:NH2	2.79	0.45
1:D:103:VAL:HG22	1:D:104:SER:N	2.31	0.45
2:E:1881:THR:O	2:E:1889:LEU:HD12	2.16	0.45
2:E:1987:VAL:HB	2:E:1989:PHE:HE1	1.81	0.45
2:E:2223:THR:HG21	2:E:2350:ILE:HG12	1.99	0.45
2:B:2159:ASN:HD21	2:B:2198:ASP:HA	1.77	0.45
2:B:2192:LYS:HA	2:B:2195:GLU:HG3	1.99	0.45
1:D:108:ILE:H	1:D:108:ILE:CD1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1763:ASN:ND2	2:E:1763:ASN:N	2.61	0.45
2:E:1826:TYR:CG	2:E:1826:TYR:O	2.70	0.45
2:E:1837:SER:O	2:E:1840:TYR:HB2	2.17	0.45
2:E:2183:TYR:CE1	2:E:2289:ILE:HD13	2.52	0.45
1:A:263:LYS:HD2	1:A:263:LYS:HA	1.60	0.45
2:B:2185:LEU:HA	2:B:2186:PRO:HD3	1.57	0.45
2:B:2192:LYS:C	2:B:2195:GLU:HB2	2.35	0.45
2:B:2278:SER:HG	2:B:2316:GLU:HG3	1.80	0.45
2:E:1156:HIS:ND1	2:E:1157:PRO:HD2	2.32	0.45
2:E:2081:ASP:OD1	2:E:2082:ILE:HG23	2.17	0.45
1:A:343:ASN:HD22	1:A:343:ASN:HA	1.64	0.44
2:B:2264:GLU:HG2	2:B:2265:GLU:O	2.16	0.44
2:E:1195:PHE:CD1	2:E:1217:ARG:HD2	2.52	0.44
2:E:1684:GLU:CD	2:E:1702:THR:OG1	2.52	0.44
2:E:1996:LEU:CD2	2:E:2001:SER:HA	2.47	0.44
2:E:2037:TYR:CE1	2:E:2038:HIS:CD2	3.01	0.44
2:E:2089:LYS:HA	2:E:2090:ALA:HA	1.66	0.44
1:A:224:LEU:HD23	1:A:224:LEU:C	2.37	0.44
2:B:2240:ASN:O	2:B:2241:ILE:C	2.56	0.44
2:B:2354:GLY:O	2:B:2355:ASN:HB2	2.17	0.44
2:E:1093:LYS:HD3	2:E:1094:ASP:HA	2.00	0.44
2:E:1370:ARG:CG	2:E:1370:ARG:NH1	2.79	0.44
2:E:1710:GLU:HA	2:E:1727:LEU:O	2.17	0.44
2:E:2039:LEU:CA	2:E:2040:TRP:CD1	3.00	0.44
2:B:1999:LEU:HD21	2:B:2003:THR:CB	2.48	0.44
2:B:2210:MET:HE1	2:B:2253:LEU:N	2.31	0.44
2:B:2305:TYR:HB3	2:B:2334:SER:CB	2.47	0.44
2:E:958:LEU:HA	2:E:1081:TYR:CD2	2.52	0.44
2:B:2277:HIS:CE1	2:B:2288:CYS:O	2.70	0.44
2:E:1347:ARG:HD3	2:E:1445:THR:O	2.17	0.44
2:E:1825:ILE:O	2:E:1825:ILE:HG22	2.16	0.44
2:E:2003:THR:O	2:E:2007:ARG:N	2.50	0.44
2:E:2227:VAL:HG12	2:E:2239:SER:OG	2.14	0.44
2:B:2043:PHE:CZ	2:B:2051:ILE:CD1	2.78	0.44
2:B:2178:GLU:O	2:B:2217:LYS:HG2	2.17	0.44
2:B:2277:HIS:ND1	2:B:2307:LEU:HD23	2.32	0.44
2:B:2284:LYS:CE	2:B:2285:LYS:HA	2.47	0.44
2:E:1347:ARG:NH1	2:E:1445:THR:O	2.38	0.44
2:E:1763:ASN:CA	2:E:1766:MET:HE1	2.46	0.44
2:E:2190:LEU:HG	2:E:2190:LEU:O	2.17	0.44
2:B:2048:TRP:HA	2:B:2048:TRP:CE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2232:HIS:HB2	2:B:2235:SER:O	2.17	0.44
2:B:2262:GLN:HG2	2:B:2293:ILE:O	2.18	0.44
1:D:263:LYS:HD2	1:D:263:LYS:HA	1.80	0.44
2:E:1362:LYS:O	2:E:1366:ARG:HG3	2.17	0.44
2:E:1431:HIS:C	2:E:1433:ASP:N	2.71	0.44
2:E:1558:GLU:O	2:E:1558:GLU:HG3	2.18	0.44
2:E:2046:GLU:O	2:E:2049:ILE:HG23	2.04	0.44
2:E:2174:ASP:CG	2:E:2175:ASP:H	2.14	0.44
2:E:2248:PRO:C	2:E:2249:ASP:OD1	2.56	0.44
2:E:2357:TRP:H	2:E:2387:HIS:HE1	1.64	0.44
2:B:1343:PHE:HB3	2:B:1444:ILE:CD1	2.48	0.44
2:B:2163:TYR:CE1	2:B:2164:LEU:HD23	2.53	0.44
2:B:2183:TYR:CD1	2:B:2219:LYS:CD	2.90	0.44
2:E:2191:LYS:HE2	2:E:2195:GLU:OE2	2.17	0.44
2:E:2202:GLN:HE22	2:E:2235:SER:N	2.10	0.44
1:A:109:ASP:O	1:A:109:ASP:OD1	2.35	0.44
2:B:965:LYS:HB3	2:B:966:PRO:HD2	1.98	0.44
2:B:1887:GLY:HA2	2:B:1992:TYR:CD2	2.44	0.44
2:B:2301:SER:C	2:B:2302:LEU:HD12	2.39	0.44
2:E:1104:ILE:CG2	2:E:1107:LEU:CD1	2.96	0.44
2:E:2043:PHE:HD2	2:E:2051:ILE:CG1	2.21	0.44
1:A:48:HIS:CG	1:A:53:SER:HG	2.32	0.44
2:B:2067:TYR:N	2:B:2067:TYR:CD1	2.86	0.44
2:E:1090:ILE:HD11	2:E:1104:ILE:HD11	1.99	0.44
2:E:1431:HIS:O	2:E:1433:ASP:N	2.51	0.44
2:B:1784:TYR:CD1	2:B:1806:MET:HG3	2.53	0.43
2:B:2011:LEU:HB3	2:B:2040:TRP:CZ3	2.53	0.43
2:B:2040:TRP:CD1	2:B:2040:TRP:N	2.86	0.43
2:B:2044:THR:CG2	2:B:2047:GLN:CD	2.80	0.43
2:E:908:ASP:OD1	2:E:994:TYR:OH	2.25	0.43
2:E:1059:GLU:OE2	2:E:1105:ARG:NH2	2.51	0.43
2:E:1093:LYS:HD3	2:E:1093:LYS:HA	1.79	0.43
2:E:1624:LEU:HD21	2:E:1633:PHE:HB3	2.00	0.43
2:E:1992:TYR:O	2:E:1993:ASP:HB2	2.18	0.43
2:E:2029:ASP:OD2	2:E:2032:ILE:CD1	2.65	0.43
2:B:1305:SER:O	2:B:1309:ILE:HG13	2.18	0.43
2:B:1354:GLU:N	2:B:1355:PRO:CD	2.81	0.43
2:B:2024:MET:SD	2:B:2157:ILE:HG21	2.58	0.43
2:E:2066:LYS:CB	2:E:2067:TYR:CD1	2.97	0.43
2:E:2242:PRO:CB	2:E:2374:PHE:CE2	3.01	0.43
2:B:953:ARG:HH11	2:B:953:ARG:CG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1842:GLU:O	2:B:1844:PHE:N	2.51	0.43
2:B:1894:ILE:HD13	2:B:1894:ILE:HA	1.86	0.43
2:B:2045:ASP:O	2:B:2048:TRP:HB2	2.18	0.43
2:B:2179:GLU:HA	2:B:2217:LYS:HE2	2.01	0.43
1:D:20:TYR:CE2	1:D:106:PRO:HG2	2.53	0.43
2:E:1292:ARG:NH1	2:E:1293:THR:HG22	2.33	0.43
2:E:2083:ILE:CG2	2:E:2084:LEU:H	2.32	0.43
2:E:2223:THR:HG21	2:E:2350:ILE:CG1	2.48	0.43
2:B:2017:THR:HG21	2:B:2062:GLU:HG3	1.99	0.43
2:B:2020:GLU:HG3	2:B:2164:LEU:HD12	2.00	0.43
2:B:2054:GLN:HE21	2:B:2054:GLN:HB3	1.64	0.43
2:B:2342:SER:OG	2:B:2344:ARG:N	2.37	0.43
2:B:2358:ASN:CB	2:B:2387:HIS:HD1	2.18	0.43
1:D:25:LYS:O	1:D:28:GLN:CB	2.66	0.43
2:E:930:ASN:ND2	2:E:933:GLU:HB2	2.32	0.43
2:B:1906:SER:O	2:B:1909:ALA:HB3	2.19	0.43
2:B:2087:ASN:CB	2:B:2089:LYS:HG3	2.46	0.43
2:B:2166:LEU:O	2:B:2167:LYS:C	2.56	0.43
2:E:1354:GLU:N	2:E:1355:PRO:CD	2.81	0.43
2:E:1788:GLY:O	2:E:1790:TRP:CD1	2.71	0.43
2:E:2181:ASN:O	2:E:2338:GLN:HG3	2.18	0.43
2:B:1853:ASP:OD1	2:B:1854:ASP:N	2.51	0.43
2:B:2270:ALA:HB1	2:B:2324:VAL:HA	2.00	0.43
1:D:35:ASP:O	1:D:107:LYS:NZ	2.34	0.43
2:E:953:ARG:HG3	2:E:953:ARG:HH11	1.83	0.43
2:E:1784:TYR:CD1	2:E:1806:MET:HG3	2.53	0.43
2:E:2063:TYR:O	2:E:2067:TYR:CD1	2.71	0.43
2:E:2154:LYS:O	2:E:2157:ILE:HB	2.18	0.43
2:B:1542:TYR:CE2	2:B:1546:VAL:HG21	2.53	0.43
2:B:1864:LYS:NZ	2:B:1865:THR:O	2.44	0.43
2:B:2281:PHE:HB3	2:B:2286:ARG:O	2.19	0.43
2:E:2253:LEU:HA	2:E:2253:LEU:HD23	1.90	0.43
2:E:2384:ASN:HB3	2:E:2387:HIS:HD2	1.83	0.43
2:B:1187:LEU:O	2:B:1191:PRO:CG	2.66	0.43
2:B:2085:GLY:HA3	2:B:2086:GLN:HA	1.79	0.43
2:B:2153:ARG:HH11	2:B:2153:ARG:HG3	1.82	0.43
2:B:2178:GLU:HB3	2:B:2217:LYS:HZ2	1.84	0.43
2:B:2231:GLY:O	2:B:2232:HIS:CD2	2.71	0.43
2:B:2329:PHE:C	2:B:2330:GLU:HG2	2.39	0.43
2:B:2357:TRP:CZ3	2:B:2382:PHE:CE1	3.04	0.43
1:D:9:ALA:N	1:D:10:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2185:LEU:HG	2:B:2186:PRO:HD2	2.00	0.43
2:E:1091:ASN:HB3	2:E:1093:LYS:HE2	2.00	0.43
2:E:2318:ASN:HB3	2:E:2321:ILE:HD11	2.01	0.43
2:B:1704:GLU:CG	2:B:1705:SER:N	2.81	0.43
2:B:1707:HIS:CE1	2:B:1708:GLU:CD	2.92	0.43
1:D:327:ILE:HG21	1:D:328:TYR:HE1	1.84	0.43
2:E:1835:LEU:HB3	2:E:1959:THR:HB	2.00	0.42
2:E:2065:ARG:HB3	2:E:2065:ARG:HH11	1.81	0.42
2:E:2302:LEU:N	2:E:2302:LEU:CD1	2.82	0.42
2:B:1051:GLU:HG3	2:B:1169:TYR:CE2	2.54	0.42
2:B:1383:PHE:CE2	2:B:1387:VAL:HG21	2.54	0.42
2:B:1721:ASN:HB3	2:E:1463:THR:HB	2.00	0.42
2:B:1961:ASN:HA	2:B:2079:ILE:CD1	2.49	0.42
2:B:2076:GLN:OE1	2:B:2076:GLN:HA	2.19	0.42
2:B:2230:LEU:CB	2:B:2237:GLN:HG3	2.47	0.42
2:E:2086:GLN:O	2:E:2088:ILE:HG12	2.20	0.42
2:E:2155:SER:HB3	2:E:2383:TYR:CE2	2.53	0.42
2:B:1847:ASP:O	2:B:1849:LYS:HD2	2.19	0.42
2:B:1917:VAL:O	2:B:1921:VAL:HG23	2.19	0.42
2:B:2189:LEU:HD21	2:B:2347:GLY:HA3	2.01	0.42
2:E:958:LEU:HD23	2:E:1081:TYR:CD2	2.55	0.42
2:E:1596:THR:O	2:E:1598:LEU:HB3	2.19	0.42
2:E:1763:ASN:HD22	2:E:1764:VAL:N	2.17	0.42
2:E:2061:THR:HG22	2:E:2062:GLU:N	2.34	0.42
2:B:1321:MET:HA	2:B:1321:MET:CE	2.49	0.42
2:B:2064:GLY:O	2:B:2068:ASN:HA	2.19	0.42
2:B:2373:ASN:O	2:B:2374:PHE:CG	2.72	0.42
2:E:1567:PHE:CE2	2:E:1820:ARG:NH1	2.84	0.42
2:E:1837:SER:O	2:E:1840:TYR:CB	2.68	0.42
2:E:2087:ASN:O	2:E:2088:ILE:HG12	2.19	0.42
2:B:1097:HIS:ND1	2:B:1097:HIS:C	2.73	0.42
2:B:2063:TYR:CE1	2:B:2081:ASP:O	2.73	0.42
2:E:1435:LYS:HD3	2:E:1549:ALA:O	2.19	0.42
2:E:2075:THR:HG22	2:E:2076:GLN:N	2.34	0.42
2:E:2086:GLN:O	2:E:2086:GLN:HG2	2.19	0.42
2:B:957:TYR:O	2:B:961:GLN:N	2.48	0.42
2:B:1848:ILE:HD11	2:B:1928:GLU:O	2.14	0.42
2:B:1894:ILE:O	2:B:1894:ILE:HG22	2.18	0.42
2:E:1234:VAL:HG11	2:E:1239:THR:CG2	2.49	0.42
2:E:1596:THR:O	2:E:1598:LEU:CB	2.67	0.42
2:E:1604:ARG:HH22	2:E:1822:GLY:C	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1674:ASP:N	2:E:1674:ASP:OD1	2.52	0.42
2:E:1717:LEU:HB2	2:E:1786:ALA:HB3	2.02	0.42
2:E:1964:PRO:HG3	2:E:2013:ARG:CZ	2.49	0.42
2:E:2020:GLU:HG3	2:E:2164:LEU:HD12	2.02	0.42
2:E:2259:ILE:HD11	2:E:2293:ILE:HD11	2.01	0.42
2:B:1015:PRO:HD2	2:B:1165:LEU:CD2	2.36	0.42
2:B:1661:ILE:HG12	2:B:1805:ILE:CD1	2.50	0.42
2:B:2035:LYS:O	2:B:2037:TYR:N	2.53	0.42
1:D:23:ASN:N	1:D:23:ASN:ND2	2.68	0.42
2:B:1800:ASN:OD1	2:B:1803:ARG:NH1	2.53	0.42
2:B:1854:ASP:CA	2:B:1857:VAL:HG23	2.49	0.42
2:B:1944:LEU:O	2:B:1948:MET:HG2	2.20	0.42
2:B:2208:TYR:HB3	2:B:2253:LEU:CG	2.45	0.42
2:B:2232:HIS:HE1	2:B:2237:GLN:HE21	1.68	0.42
1:D:3:THR:HG22	1:D:5:PRO:HD3	2.01	0.42
2:B:969:ILE:HG22	2:B:982:TYR:CD2	2.55	0.42
2:B:2063:TYR:HE1	2:B:2081:ASP:O	2.02	0.42
2:E:1484:TRP:CH2	2:E:1495:PHE:HB2	2.55	0.42
2:E:2388:ARG:HD3	2:E:2389:PRO:HD2	2.02	0.42
1:A:214:PHE:CD1	1:A:220:TYR:HA	2.55	0.42
2:B:1904:ARG:HD3	2:B:1907:GLN:OE1	2.20	0.42
2:B:2229:GLN:NE2	2:B:2357:TRP:CE3	2.88	0.42
1:D:282:ILE:HD13	2:E:1604:ARG:HD2	2.02	0.42
2:E:2021:SER:O	2:E:2024:MET:HB3	2.20	0.42
2:B:1893:ILE:CG2	2:B:1978:VAL:HG13	2.50	0.41
2:B:2010:LEU:HD12	2:B:2010:LEU:HA	1.82	0.41
2:B:2230:LEU:HD12	2:B:2230:LEU:HA	1.84	0.41
1:D:48:HIS:HE1	1:D:56:TYR:OH	2.03	0.41
2:E:1370:ARG:NH1	2:E:1370:ARG:HG2	2.36	0.41
2:E:1611:SER:N	2:E:1612:PRO:CD	2.83	0.41
2:E:1712:SER:OG	2:E:1713:LYS:N	2.51	0.41
2:E:2078:GLU:O	2:E:2079:ILE:HD13	2.20	0.41
2:B:1717:LEU:HB2	2:B:1786:ALA:HB3	2.02	0.41
2:B:2082:ILE:O	2:B:2083:ILE:CG1	2.69	0.41
2:B:2309:ASP:O	2:B:2312:TYR:N	2.53	0.41
2:E:1849:LYS:C	2:E:1850:LEU:HD23	2.40	0.41
2:B:1674:ASP:OD1	2:B:1674:ASP:N	2.53	0.41
2:B:1843:LEU:HD11	2:B:1884:PRO:HG3	1.94	0.41
2:B:1853:ASP:CG	2:B:1855:THR:OG1	2.57	0.41
2:B:1990:ASN:OD1	2:B:1992:TYR:N	2.52	0.41
2:B:2183:TYR:CD1	2:B:2219:LYS:CB	3.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2309:ASP:N	2:B:2310:GLU:OE1	2.54	0.41
2:B:2351:ILE:HG21	2:B:2379:PRO:HA	2.02	0.41
2:E:2070:ASN:O	2:E:2071:ILE:CG2	2.69	0.41
2:E:2386:MET:C	2:E:2388:ARG:N	2.74	0.41
2:B:2258:TRP:CD1	2:B:2258:TRP:N	2.82	0.41
2:B:2278:SER:OG	2:B:2312:TYR:O	2.38	0.41
2:B:2318:ASN:ND2	2:B:2318:ASN:N	2.68	0.41
1:D:84:ARG:CG	1:D:84:ARG:NH1	2.84	0.41
1:D:328:TYR:CD2	2:E:1543:ARG:NH1	2.89	0.41
2:E:965:LYS:HE3	2:E:985:ASP:CG	2.41	0.41
2:E:995:LEU:O	2:E:999:LEU:HG	2.21	0.41
2:E:2304:ALA:HB3	2:E:2339:LEU:HD23	1.98	0.41
1:A:282:ILE:HD13	2:B:1604:ARG:HD2	2.03	0.41
2:E:986:PRO:O	2:E:990:ILE:HD12	2.20	0.41
2:E:1705:SER:HB3	2:E:1709:TRP:CE3	2.55	0.41
2:E:1762:ASP:CG	2:E:1763:ASN:H	2.23	0.41
2:E:2084:LEU:HD22	2:E:2084:LEU:C	2.37	0.41
2:E:2182:VAL:HG12	2:E:2338:GLN:HB3	2.02	0.41
2:E:2280:LEU:HB2	2:E:2281:PHE:CD2	2.56	0.41
1:A:16:GLY:HA3	1:A:45:HIS:CE1	2.54	0.41
2:B:1435:LYS:NZ	2:E:1351:VAL:HG13	2.36	0.41
2:B:1673:LEU:HA	2:B:1678:ILE:HB	2.03	0.41
2:B:1686:VAL:HG12	2:B:1687:HIS:N	2.36	0.41
2:B:1963:LEU:HD23	2:B:1963:LEU:HA	1.95	0.41
2:E:1624:LEU:CD2	2:E:1625:VAL:N	2.83	0.41
2:E:1996:LEU:HD21	2:E:2001:SER:HA	2.02	0.41
2:B:1137:PRO:O	2:B:1140:ASN:C	2.59	0.41
2:B:1889:LEU:HD23	2:B:1891:LEU:HB2	2.03	0.41
2:B:2307:LEU:HD12	2:B:2308:THR:O	2.21	0.41
2:B:2386:MET:CE	2:B:2387:HIS:CD2	3.03	0.41
2:E:1763:ASN:O	2:E:1766:MET:HE3	2.18	0.41
2:E:2014:ALA:CA	2:E:2059:ILE:CD1	2.72	0.41
2:E:2157:ILE:HD12	2:E:2157:ILE:HA	1.74	0.41
2:E:2189:LEU:HD21	2:E:2347:GLY:C	2.41	0.41
1:A:7:THR:HG21	1:A:70:GLN:OE1	2.21	0.41
1:A:89:PHE:CD1	1:A:89:PHE:C	2.94	0.41
2:B:1080:ASP:O	2:B:1084:ALA:HB2	2.21	0.41
2:B:1150:LYS:HD2	2:B:1292:ARG:HH22	1.84	0.41
2:B:1405:ILE:HB	2:B:1437:ILE:HB	2.02	0.41
2:B:2017:THR:HG23	2:B:2062:GLU:HG3	2.03	0.41
2:E:1279:VAL:HG12	2:E:1280:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1826:TYR:CA	2:E:1827:GLN:HB2	2.50	0.41
2:E:1865:THR:OG1	2:E:1869:ASN:HB2	2.20	0.41
2:E:2028:SER:C	2:E:2030:PRO:HD3	2.37	0.41
2:E:2030:PRO:CG	2:E:2153:ARG:NE	2.77	0.41
2:E:2267:LYS:C	2:E:2305:TYR:OH	2.58	0.41
2:B:2157:ILE:C	2:B:2160:THR:OG1	2.44	0.41
2:B:2386:MET:HE1	2:B:2387:HIS:CD2	2.56	0.41
2:E:1826:TYR:CA	2:E:1827:GLN:CB	2.99	0.41
2:E:2067:TYR:N	2:E:2067:TYR:CD1	2.89	0.41
2:B:995:LEU:O	2:B:999:LEU:HG	2.21	0.40
2:B:2247:LEU:HD23	2:B:2374:PHE:CB	2.51	0.40
1:D:16:GLY:HA3	1:D:45:HIS:CE1	2.56	0.40
2:E:1466:GLN:O	2:E:1469:ILE:CA	2.69	0.40
2:E:1766:MET:C	2:E:1767:TYR:CD1	2.94	0.40
2:E:2057:ASP:O	2:E:2061:THR:HB	2.22	0.40
2:E:2230:LEU:HD23	2:E:2237:GLN:NE2	2.36	0.40
2:B:2070:ASN:O	2:B:2071:ILE:CG2	2.69	0.40
2:B:2082:ILE:O	2:B:2083:ILE:HG13	2.21	0.40
2:B:2089:LYS:HA	2:B:2090:ALA:HA	1.74	0.40
2:B:2184:VAL:O	2:B:2221:ILE:CG1	2.69	0.40
2:B:2191:LYS:O	2:B:2195:GLU:CG	2.44	0.40
2:E:946:ASN:HB3	2:E:949:ASP:OD2	2.21	0.40
2:E:1168:ILE:O	2:E:1168:ILE:HG13	2.21	0.40
2:E:1889:LEU:HD12	2:E:1889:LEU:HA	1.86	0.40
2:E:1995:TRP:HZ3	2:E:2007:ARG:HG2	1.58	0.40
2:B:1107:LEU:HD23	2:B:1109:PHE:CZ	2.56	0.40
2:B:1153:GLU:O	2:B:1159:ARG:HD3	2.21	0.40
2:B:1168:ILE:O	2:B:1168:ILE:HG13	2.21	0.40
2:B:1324:GLY:HA2	2:B:1325:SER:HB3	2.03	0.40
2:B:2207:ILE:CG1	2:B:2257:GLY:O	2.70	0.40
1:D:107:LYS:HA	1:D:108:ILE:HA	1.87	0.40
2:E:930:ASN:ND2	2:E:933:GLU:CD	2.74	0.40
2:E:969:ILE:HG22	2:E:982:TYR:CD2	2.57	0.40
2:E:1477:PHE:CD1	2:E:1477:PHE:C	2.94	0.40
2:E:1624:LEU:HD21	2:E:1633:PHE:CD1	2.57	0.40
2:E:1894:ILE:O	2:E:1894:ILE:HG22	2.21	0.40
2:E:2029:ASP:OD2	2:E:2032:ILE:HD11	2.21	0.40
2:B:1187:LEU:HD23	2:B:1187:LEU:HA	1.85	0.40
2:B:2153:ARG:NH1	2:B:2153:ARG:HG2	2.36	0.40
1:D:141:ASP:OD1	1:D:141:ASP:C	2.60	0.40
2:E:1383:PHE:CE2	2:E:1387:VAL:HG21	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1727:LEU:C	2:E:1728:ILE:CD1	2.71	0.40
2:E:2203:VAL:HG22	2:E:2357:TRP:CZ3	2.57	0.40
2:B:1762:ASP:OD1	2:B:1764:VAL:HG22	2.22	0.40
2:B:1893:ILE:HG23	2:B:1978:VAL:HG13	2.02	0.40
2:B:2060:LEU:O	2:B:2063:TYR:CA	2.70	0.40
2:B:2162:LEU:HD23	2:B:2165:ARG:HE	1.86	0.40
2:B:2224:VAL:CA	2:B:2349:PHE:CE1	3.04	0.40
2:E:2177:VAL:HG23	2:E:2177:VAL:O	2.21	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)
2:B:1685:THR:OG1	2:E:2309:ASP:OD2[4_545]	1.96	0.24

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	319/355 (90%)	310 (97%)	9 (3%)	0	100	100
1	D	307/355 (86%)	298 (97%)	8 (3%)	1 (0%)	41	73
2	B	1384/1531 (90%)	1345 (97%)	38 (3%)	1 (0%)	51	83
2	E	1406/1531 (92%)	1360 (97%)	42 (3%)	4 (0%)	41	73
All	All	3416/3772 (91%)	3313 (97%)	97 (3%)	6 (0%)	47	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	2088	ILE
2	E	2286	ARG

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Mol	Chain	Res	Type
2	B	2088	ILE
1	D	29	PRO
2	E	1726	GLY
2	E	2215	HIS

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	293/326 (90%)	284 (97%)	9 (3%)	40	70
1	D	289/326 (89%)	269 (93%)	20 (7%)	15	45
2	B	1256/1373 (92%)	1108 (88%)	148 (12%)	5	21
2	E	1278/1373 (93%)	1151 (90%)	127 (10%)	8	29
All	All	3116/3398 (92%)	2812 (90%)	304 (10%)	8	29

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	A	95	ASN
1	A	107	LYS
1	A	110	GLU
1	A	132	LYS
1	A	215	LYS
1	A	263	LYS
1	A	299	LYS
1	A	343	ASN
2	B	883	SER
2	B	885	VAL
2	B	908	ASP
2	B	929	LEU
2	B	952	ASN
2	B	953	ARG
2	B	956	LYS
2	B	960	THR

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Mol	Chain	Res	Type
2	B	969	ILE
2	B	987	LEU
2	B	1018	SER
2	B	1019	GLU
2	B	1042	SER
2	B	1074	VAL
2	B	1096	SER
2	B	1097	HIS
2	B	1105	ARG
2	B	1139	ASN
2	B	1165	LEU
2	B	1177	ASP
2	B	1213	MET
2	B	1218	GLN
2	B	1237	SER
2	B	1239	THR
2	B	1273	GLN
2	B	1282	ASP
2	B	1305	SER
2	B	1321	MET
2	B	1348	GLU
2	B	1377	SER
2	B	1406	LEU
2	B	1430	THR
2	B	1465	ARG
2	B	1466	GLN
2	B	1467	GLU
2	B	1478	GLU
2	B	1510	ILE
2	B	1512	ARG
2	B	1521	ARG
2	B	1569	SER
2	B	1571	GLU
2	B	1573	LEU
2	B	1594	GLN
2	B	1595	ARG
2	B	1598	LEU
2	B	1679	GLU
2	B	1691	SER
2	B	1703	MET
2	B	1706	VAL
2	B	1710	GLU

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Mol	Chain	Res	Type
2	B	1713	LYS
2	B	1727	LEU
2	B	1739	ARG
2	B	1742	ASP
2	B	1750	ARG
2	B	1802	MET
2	B	1804	THR
2	B	1805	ILE
2	B	1817	GLU
2	B	1821	LYS
2	B	1842	GLU
2	B	1845	ASN
2	B	1848	ILE
2	B	1849	LYS
2	B	1858	TYR
2	B	1859	ARG
2	B	1864	LYS
2	B	1867	GLU
2	B	1869	ASN
2	B	1882	LEU
2	B	1896	THR
2	B	1897	SER
2	B	1904	ARG
2	B	1926	LYS
2	B	1927	GLU
2	B	1932	GLN
2	B	1962	ARG
2	B	1972	ASP
2	B	1979	MET
2	B	1980	LYS
2	B	1988	LEU
2	B	1997	ASP
2	B	2001	SER
2	B	2002	TYR
2	B	2006	SER
2	B	2016	LYS
2	B	2018	ASN
2	B	2026	LEU
2	B	2032	ILE
2	B	2038	HIS
2	B	2039	LEU
2	B	2044	THR

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Mol	Chain	Res	Type
2	B	2045	ASP
2	B	2047	GLN
2	B	2048	TRP
2	B	2050	THR
2	B	2053	SER
2	B	2054	GLN
2	B	2057	ASP
2	B	2153	ARG
2	B	2155	SER
2	B	2160	THR
2	B	2163	TYR
2	B	2165	ARG
2	B	2187	LYS
2	B	2199	VAL
2	B	2202	GLN
2	B	2210	MET
2	B	2222	LYS
2	B	2237	GLN
2	B	2238	ILE
2	B	2239	SER
2	B	2243	ASP
2	B	2246	ASP
2	B	2247	LEU
2	B	2250	THR
2	B	2253	LEU
2	B	2254	GLU
2	B	2256	LEU
2	B	2258	TRP
2	B	2265	GLU
2	B	2268	PHE
2	B	2277	HIS
2	B	2280	LEU
2	B	2283	ASP
2	B	2284	LYS
2	B	2286	ARG
2	B	2295	SER
2	B	2301	SER
2	B	2303	SER
2	B	2306	ASN
2	B	2307	LEU
2	B	2309	ASP
2	B	2318	ASN

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Mol	Chain	Res	Type
2	B	2332	THR
2	B	2334	SER
2	B	2336	HIS
2	B	2339	LEU
2	B	2341	LEU
2	B	2343	ASP
2	B	2344	ARG
2	B	2345	ILE
2	B	2349	PHE
2	B	2362	MET
2	B	2367	ASN
2	B	2382	PHE
2	B	2384	ASN
2	B	2386	MET
1	D	21	SER
1	D	23	ASN
1	D	24	VAL
1	D	27	ASN
1	D	83	GLU
1	D	84	ARG
1	D	85	ASP
1	D	101	MET
1	D	102	MET
1	D	104	SER
1	D	108	ILE
1	D	109	ASP
1	D	113	THR
1	D	215	LYS
1	D	216	ASN
1	D	299	LYS
1	D	300	ASN
1	D	326	LEU
1	D	327	ILE
1	D	355	PRO
2	E	885	VAL
2	E	908	ASP
2	E	909	THR
2	E	930	ASN
2	E	942	GLU
2	E	945	ASP
2	E	953	ARG
2	E	956	LYS

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Mol	Chain	Res	Type
2	E	969	ILE
2	E	987	LEU
2	E	1093	LYS
2	E	1095	MET
2	E	1096	SER
2	E	1165	LEU
2	E	1166	ASP
2	E	1189	GLU
2	E	1213	MET
2	E	1272	ARG
2	E	1273	GLN
2	E	1275	MET
2	E	1281	ASN
2	E	1282	ASP
2	E	1292	ARG
2	E	1321	MET
2	E	1348	GLU
2	E	1370	ARG
2	E	1377	SER
2	E	1382	ARG
2	E	1426	ARG
2	E	1432	GLU
2	E	1465	ARG
2	E	1477	PHE
2	E	1510	ILE
2	E	1512	ARG
2	E	1530	SER
2	E	1568	ASN
2	E	1574	PHE
2	E	1596	THR
2	E	1598	LEU
2	E	1600	GLN
2	E	1624	LEU
2	E	1679	GLU
2	E	1691	SER
2	E	1693	LYS
2	E	1694	MET
2	E	1702	THR
2	E	1704	GLU
2	E	1707	HIS
2	E	1710	GLU
2	E	1713	LYS

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Mol	Chain	Res	Type
2	E	1715	SER
2	E	1722	ASP
2	E	1723	SER
2	E	1727	LEU
2	E	1729	THR
2	E	1730	ASN
2	E	1732	MET
2	E	1761	THR
2	E	1763	ASN
2	E	1765	SER
2	E	1767	TYR
2	E	1769	SER
2	E	1817	GLU
2	E	1821	LYS
2	E	1842	GLU
2	E	1859	ARG
2	E	1862	VAL
2	E	1882	LEU
2	E	1897	SER
2	E	1927	GLU
2	E	1962	ARG
2	E	1972	ASP
2	E	1985	GLN
2	E	2001	SER
2	E	2002	TYR
2	E	2007	ARG
2	E	2018	ASN
2	E	2020	GLU
2	E	2021	SER
2	E	2033	THR
2	E	2034	ILE
2	E	2035	LYS
2	E	2047	GLN
2	E	2048	TRP
2	E	2059	ILE
2	E	2061	THR
2	E	2065	ARG
2	E	2077	THR
2	E	2080	LYS
2	E	2084	LEU
2	E	2086	GLN
2	E	2087	ASN

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Mol	Chain	Res	Type
2	E	2095	ARG
2	E	2163	TYR
2	E	2172	SER
2	E	2178	GLU
2	E	2179	GLU
2	E	2182	VAL
2	E	2183	TYR
2	E	2189	LEU
2	E	2197	SER
2	E	2201	ILE
2	E	2214	ASP
2	E	2215	HIS
2	E	2222	LYS
2	E	2249	ASP
2	E	2264	GLU
2	E	2266	LEU
2	E	2267	LYS
2	E	2277	HIS
2	E	2296	THR
2	E	2326	SER
2	E	2327	GLU
2	E	2332	THR
2	E	2339	LEU
2	E	2340	LEU
2	E	2360	THR
2	E	2362	MET
2	E	2367	ASN
2	E	2368	GLN
2	E	2371	ASP
2	E	2375	LYS
2	E	2380	LEU
2	E	2384	ASN
2	E	2388	ARG
2	E	2393	LEU
2	E	2396	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	343	ASN
2	B	1030	GLN

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Mol	Chain	Res	Type
2	B	1087	ASN
2	B	1139	ASN
2	B	1470	GLN
2	B	1471	GLN
2	B	1863	HIS
2	B	1869	ASN
2	B	1895	HIS
2	B	1985	GLN
2	B	2038	HIS
2	B	2054	GLN
2	B	2087	ASN
2	B	2202	GLN
2	B	2237	GLN
2	B	2318	ASN
2	B	2338	GLN
2	B	2368	GLN
2	B	2373	ASN
2	B	2384	ASN
2	B	2387	HIS
1	D	48	HIS
1	D	219	ASN
1	D	244	HIS
2	E	930	ASN
2	E	1087	ASN
2	E	1091	ASN
2	E	1097	HIS
2	E	1140	ASN
2	E	1218	GLN
2	E	1281	ASN
2	E	1470	GLN
2	E	1540	ASN
2	E	1600	GLN
2	E	1655	GLN
2	E	1763	ASN
2	E	1863	HIS
2	E	1985	GLN
2	E	2018	ASN
2	E	2054	GLN
2	E	2087	ASN
2	E	2159	ASN
2	E	2202	GLN
2	E	2232	HIS

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Mol	Chain	Res	Type
2	E	2237	GLN
2	E	2260	HIS
2	E	2358	ASN
2	E	2373	ASN
2	E	2384	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å^2)	Q<0.9
1	A	327/355 (92%)	-0.32	4 (1%) 79 61	40, 75, 133, 168	1 (0%)
1	D	317/355 (89%)	-0.37	0 100 100	38, 73, 131, 170	0
2	B	1398/1531 (91%)	-0.10	35 (2%) 57 34	38, 103, 176, 253	0
2	E	1420/1531 (92%)	-0.15	26 (1%) 68 47	37, 90, 160, 245	0
All	All	3462/3772 (91%)	-0.17	65 (1%) 66 46	37, 92, 165, 253	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2096	GLN	15.9
2	E	2093	VAL	6.8
2	E	2323	ASN	6.5
2	B	2385	GLU	5.8
2	E	2321	ILE	5.4
2	B	2174	ASP	5.3
2	B	2268	PHE	5.2
2	E	2326	SER	5.1
2	B	2059	ILE	5.1
2	E	2325	LEU	5.0
2	B	2361	PHE	4.7
2	E	2322	MET	4.5
2	B	2221	ILE	3.9
2	B	2251	GLU	3.7
2	B	2322	MET	3.6
2	E	2059	ILE	3.6
2	E	2095	ARG	3.5
2	B	1433	ASP	3.5
2	B	2060	LEU	3.5
2	E	2361	PHE	3.5
1	A	329	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	1324	GLY	3.4
2	E	2081	ASP	3.2
2	E	1680	SER	3.1
2	E	2082	ILE	3.1
2	B	2320	ASP	3.1
2	E	2057	ASP	3.1
2	E	2324	VAL	3.0
2	B	2052	GLU	2.9
2	B	2072	SER	2.9
2	E	2214	ASP	2.9
2	E	2094	LYS	2.8
2	B	1292	ARG	2.8
2	E	2072	SER	2.8
2	E	2071	ILE	2.7
2	E	2385	GLU	2.7
2	B	1899	TRP	2.7
2	B	2275	ALA	2.6
2	E	2092	SER	2.6
2	B	2262	GLN	2.5
2	B	2384	ASN	2.5
2	B	1238	LEU	2.4
2	B	2288	CYS	2.4
2	B	2179	GLU	2.4
2	B	2091	PRO	2.4
1	A	110	GLU	2.3
2	E	1323	SER	2.3
2	E	2382	PHE	2.3
2	B	2087	ASN	2.3
2	E	1681	VAL	2.3
2	E	2320	ASP	2.2
2	B	1894	ILE	2.2
2	B	2289	ILE	2.2
1	A	40	HIS	2.2
2	B	2183	TYR	2.2
2	B	2264	GLU	2.2
2	B	1674	ASP	2.2
1	A	169	GLU	2.2
2	B	2286	ARG	2.1
2	B	2214	ASP	2.1
2	B	2311	GLY	2.1
2	B	2333	PHE	2.0
2	B	2317	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	2060	LEU	2.0
2	B	2210	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.