



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:03 AM UTC

PDB ID : 3ZEF / pdb_00003zef
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

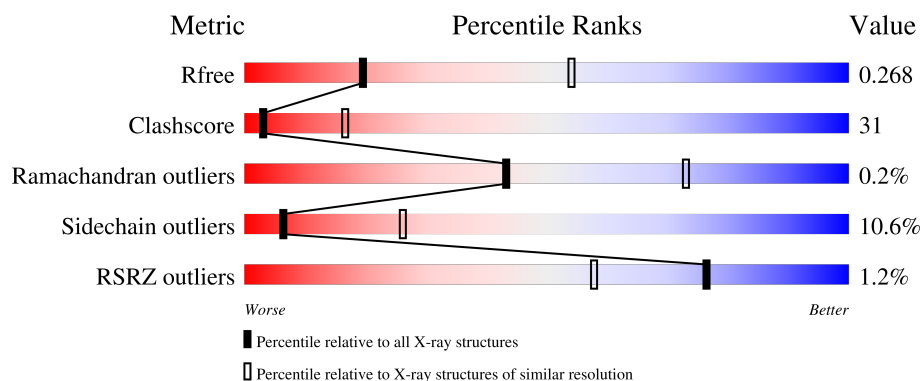
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. 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	 74% 16% • 8%
1	D	355	 67% 18% • • 11%
2	B	1531	 51% 32% 8% • 9%
2	E	1531	 57% 29% 6% • 7%

2 Entry composition

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
1	A	327	Total	C	N	O	S	0	0	0
			2684	1722	438	508	16			
1	D	317	Total	C	N	O	S	0	0	0
			2618	1682	426	493	17			

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

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

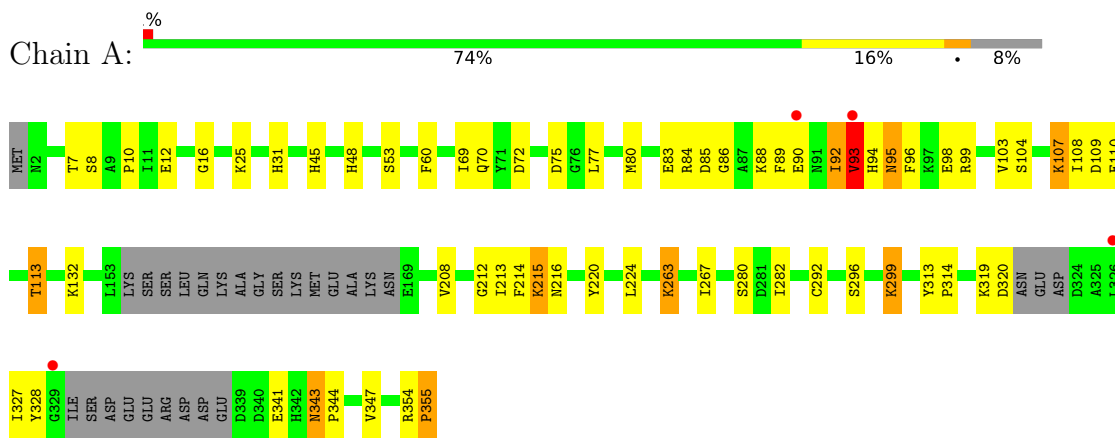
There are 8 discrepancies between the modelled and reference sequences:

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

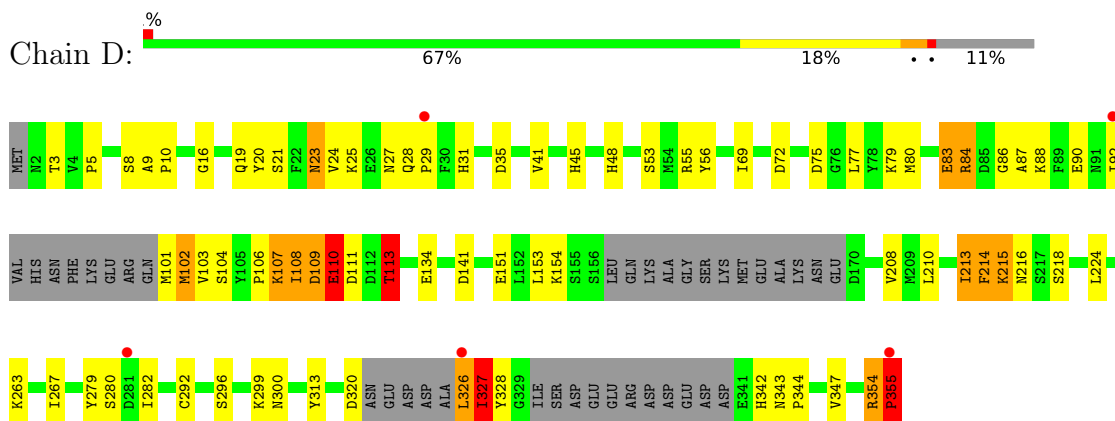
3 Residue-property plots [i](#)

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.

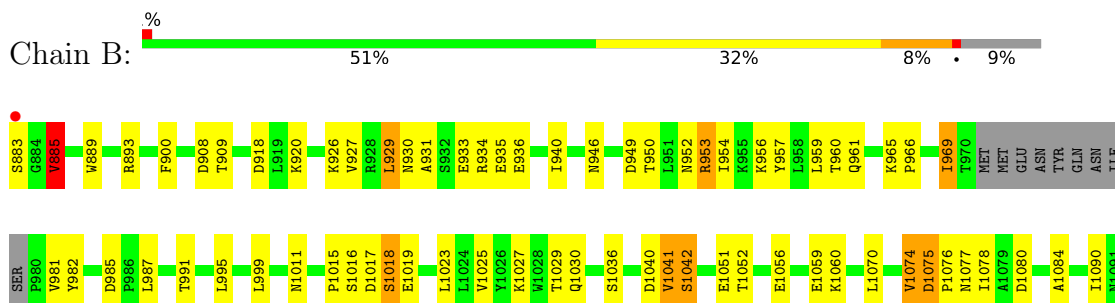
• Molecule 1: A1 CISTRON-SPLICING FACTOR AAR2



• Molecule 1: A1 CISTRON-SPLICING FACTOR AAR2



• Molecule 2: PRE-MRNA-SPLICING FACTOR 8



L2307	D2243	E2179	GLU	L1889	G1822	K1713	PHE	E1467	F1092
T2308	L2244	Q2180	ALA	F1890	L1823	L1717	LYS	E1308	K1093
D2309	G2245	N2181	ALA	L1892	Q1824	H1718	LYS	I1309	D1094
E2310	D2246	V1987	GLY	K1891	T1825	E1719	LEU	K1311	H1097
G2311	L2247	L1988	ALA	I1893	TYR	T1720	THR	R1473	V1098
P2312	E2248	E2052	SER	I1894	GLN	E1721	HIS	R1474	I1104
Q2313	D2249	Q2054	THR	H1895	SER	N1721	ALA	L1475	R1105
W2314	T2250	L1991	VAL	T1896	VAL	D1722	R1594	A1476	L1107
G2315	E2251	Y1992	MET	W1899	GLN	L1727	R1595	F1477	G1106
E2316	D2252	D1993	LYS	GLY	GLU	T1728	G1597	E1478	L1107
E2317	L2253	D1994	THR	GLY	PRO	T1729	L1598	G1324	K1108
N2318	E2254	W1995	LYS	GLN	PHE	N1730	S1599	S1325	M1212
N2322	L2255	L1996	THR	LYS	LEU	K1731	Q1600	I1340	M1213
N2323	L2256	D1997	ILE	R1904	ASN	W1732	I1488	I1340	A1110
G2324	G2257	R1998	ASN	R1905	SER	M1733	R1604	F1343	S1111
V2325	E2262	L1999	ALA	Q1907	SER	W1733	R1605	F1343	I1121
L2326	G2264	S2000	GLY	S1907	ASN	R1739	F1495	E1348	W1228
F2329	Y2067	S2001	GLY	I1908	Y1840	D1742	A1503	E1348	L1124
E2330	N2068	Y2002	GLY	A1909	A1841	D1742	P1612	E1354	L1125
P2331	V2069	T2003	ILE	V1917	E1842	D1747	R1506	P1355	R1233
T2332	N2070	A2004	VAL	S1917	L1843	D1747	R1506	S1237	P1137
F2333	E2263	S2006	VAL	Q1922	F1844	W1750	R1509	L1238	A1138
S2334	Q2202	R2007	VAL	V1921	R1845	R1750	I1510	T1239	N1139
T2335	Q2203	L2008	ALA	R1922	N1846	Y1759	I1511	S1377	N1140
A2204	SER	T2009	SER	S1923	D1847	Y1759	R1512	F1377	F1141
A2205	ALA	L2010	ALA	E1927	I1848	D1762	P1639	F1383	N1142
A2206	ASP	L2011	THR	E1928	K1849	D1762	T1640	E1387	N1145
L2280	TYR	Q2016	GLY	Q1929	L1850	N1764	R1515	F1388	M1145
E2281	L2082	T2017	SER	P1930	F1851	Y1764	R1521	Y1389	S1149
E2282	L2083	T2018	GLN	K1931	Y1852	P1768	W1526	L1394	K1150
L2283	L2084	N2018	THR	Q1932	D1853	Y1768	Y1542	I1405	V1152
A2284	G2085	E2019	PHE	L1941	D1854	Y1768	Y1546	I1405	E1153
E2285	Q2086	E2020	SER	L1941	T1855	G1772	Y1546	L1406	K1154
E2286	N2087	E2020	LYS	L1941	N1856	Y1768	H1559	S1415	A1155
E2287	L2088	K2023	LYS	L1944	Y1857	Y1768	Q1677	Q1273	H1156
E2288	K2089	M2024	LYS	E1945	Y1858	D1785	I1678	R1274	P1157
E2289	A2090	I2025	LYS	E1945	R1859	A1786	E1679	E1275	E1276
E2290	Q2091	L2026	SER	M1948	V1860	Y1786	K1563	E1276	GLU
E2291	VAL	S2028	VAL	R1957	K1864	F1791	K1683	VAL	R1159
E2292	LYS	D2029	LYS	R1957	T1865	F1791	T1430	VAL	T1162
E2293	ARG	P2030	ARG	P1958	F1866	K1795	H1431	VAL	R1163
E2294	GLN	T2031	GLN	T1959	E1867	P1796	E1432	SER	Y1164
E2295	LYS	I2032	LYS	E1960	G1868	L1797	D1433	N1281	L1165
E2296	MET	I2033	MET	E1961	P1869	N1800	E1434	D1282	D1166
E2297	ALA	I2034	ALA	R1962	N1869	S1801	K1435	R1167	R1167
E2298	LEU	K2035	LEU	L1963	V1870	M1802	F1574	W1286	I1168
E2299	GLU	S2036	GLU	M1969	I1875	R1803	W1575	I1437	Y1169
E2300	GLU	Y2037	GLU	M1969	N1876	T1804	GLY	I1444	Y1169
E2301	ALA	H2038	ALA	L1974	F1880	T1805	LYS	I1444	E1176
E2302	ALA	L2039	ALA	S1975	T1881	K1806	ALA	W1447	D1177
E2303	ARG	W2040	ARG	D1976	L1882	M1807	SER	T1293	D1177
E2304	SER	P2041	SER	D1976	L1882	K1807	GLY	K1294	E1180
E2305	GLU	S2042	GLU	V1977	P1883	A1808	PHE	Q1295	E1180
E2306	LYS	F2043	LYS	V1978	P1884	N1809	GLU	R1296	E1181
E2307	GLN	T2044	GLN	M1979	K1885	P1810	ASP	T1463	E1181
E2308	ASN	T2045	ASN	K1980	T1886	E1817	MET	K1464	D1194
E2309	ASP	E2046	ASP	E1983	E1887	E1817	GLN	E1466	E1185
E2310	GLU	Q2047	GLU	E1983	H1888	E1817	GLN	Q1466	Y1186

Chain E: 57% 29% 6% 7%



ALA	D2175	D2249	P2331	
GLU	F2176	T2250	T2332	
GLN	V2177	E2251	F2333	
ILE	E2178	G2252		
ASP	E2179	L2253	Q2338	
VAL	Q2180	E2254	L2339	
PHE	N2181	L2255	L2340	
SER	V2182	L2256	G2347	
	Y2183			
		I2259	I2350	
	L2189	H2260	I2351	
	L2190		P2352	
	K2191	E2264	S2353	
	K2192	E2265	G2354	
	F2193	L2266	N2355	
	I2194	K2267		
	E2195	F2268	V2356	
	I2196	M2269	V2357	
	S2197	A2270	N2358	
	D2198	A2271	Y2359	
	V2199	S2272	T2360	
	K2200	E2273	F2361	
	I2201		M2362	
	Q2202			
	V2203		N2367	
		H2277	Q2368	
	N2210	S2278		
	S2211	K2279		
	A2212	L2280	D2371	
	K2213	F2281	Y2372	
	D2214		N2373	
	H2215	K2284	F2374	
	F2216	K2285		
	K2217	R2286	K2375	
	V2218			
	K2219	I2289	I2378	
	E2220	I2293	P2379	
	I2221	F2294	L2380	
	K2222	S2295	E2381	
	V2223	T2296	F2382	
			Y2383	
		L2302	N2384	
		S2303	E2385	
		A2304	M2386	
		Y2305	H2387	
			R2388	
		P2389		
		V2390		
		H2391		
		G2311	F2392	
			L2393	
		N2318		
			S2396	
		I2321	GLU	
			LEU	
		V2324	ALA	
		L2325	GLY	
		S2326	ASP	
		E2327	GLU	
		G2328	GLU	
		F2329	LEU	
		E2330	GLU	

4 Data and refinement statistics

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 – 3.10 137.45 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (137.45-3.10) 99.8 (137.45-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.30 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.75	0/2754	0.97	3/3725 (0.1%)
1	D	0.77	0/2685	1.03	10/3626 (0.3%)
2	B	0.82	6/11671 (0.1%)	1.07	51/15827 (0.3%)
2	E	0.80	2/11856 (0.0%)	1.03	35/16074 (0.2%)
All	All	0.80	8/28966 (0.0%)	1.04	99/39252 (0.3%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1601	ILE	N-CA	-7.04	1.41	1.46
2	B	1164	TYR	CA-C	-6.62	1.44	1.52
2	B	1559	HIS	C-O	-6.53	1.15	1.24
2	B	1165	LEU	N-CA	-5.75	1.39	1.46
2	B	1559	HIS	CA-C	-5.63	1.44	1.52
2	B	1075	ASP	C-N	5.51	1.39	1.34
2	E	1708	GLU	CD-OE1	5.22	1.35	1.25
2	B	1962	ARG	CA-C	-5.06	1.46	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	THR	N-CA-C	11.08	122.92	111.07
2	E	2029	ASP	CA-C-N	10.65	130.87	119.05
2	E	2029	ASP	C-N-CA	10.65	130.87	119.05
2	B	1704	GLU	N-CA-C	10.05	124.11	109.14
2	B	1905	LEU	N-CA-C	9.76	122.00	111.36
2	B	1427	ALA	N-CA-C	9.54	121.44	111.14
2	B	2257	GLY	N-CA-C	8.84	121.94	110.45
2	B	931	ALA	N-CA-C	8.51	120.17	111.07
2	B	1092	PHE	N-CA-C	-8.33	99.54	110.53
2	B	927	VAL	CB-CA-C	-8.01	101.43	111.92
1	D	41	VAL	N-CA-C	-7.77	96.88	108.85
2	B	2154	LYS	N-CA-C	-7.63	102.96	111.28
2	B	1727	LEU	N-CA-C	7.60	120.72	109.24
2	E	2387	HIS	N-CA-C	-7.59	100.88	111.81
2	E	1762	ASP	N-CA-C	7.52	121.17	109.52
1	D	214	PHE	N-CA-C	-7.47	97.06	109.46
2	E	2084	LEU	N-CA-C	7.42	120.99	110.23
2	B	2185	LEU	CA-C-N	7.38	129.81	120.51
2	B	2185	LEU	C-N-CA	7.38	129.81	120.51
2	B	1075	ASP	CA-C-N	-7.35	112.61	120.47
2	B	1075	ASP	C-N-CA	-7.35	112.61	120.47
2	B	1572	GLY	N-CA-C	7.32	125.42	115.32
2	B	885	VAL	N-CA-C	-7.28	103.37	110.72
2	B	2180	GLN	N-CA-C	-7.17	100.39	110.50
2	E	1712	SER	N-CA-C	7.12	119.94	110.53
1	D	107	LYS	N-CA-C	7.06	118.91	108.60
2	E	1761	THR	N-CA-C	-7.02	101.70	111.81
2	B	1959	THR	N-CA-C	6.83	120.10	109.52
1	A	113	THR	N-CA-C	6.76	118.30	111.07
1	D	355	PRO	CA-N-CD	-6.72	102.59	112.00
2	B	1164	TYR	CA-C-N	6.55	129.06	120.28
2	B	1164	TYR	C-N-CA	6.55	129.06	120.28
2	E	2016	LYS	N-CA-C	-6.45	104.18	111.14
2	B	2342	SER	N-CA-C	6.44	119.67	109.50
1	D	110	GLU	N-CA-C	-6.39	104.67	113.56
2	E	1713	LYS	N-CA-C	-6.36	101.04	110.20
2	E	1711	VAL	N-CA-C	6.29	117.77	108.65
2	E	1346	PHE	N-CA-C	6.28	118.20	111.36
2	B	1713	LYS	N-CA-C	-6.27	99.71	109.87
2	E	1832	GLU	CA-C-N	-6.17	113.60	120.14
2	E	1832	GLU	C-N-CA	-6.17	113.60	120.14
2	E	1601	ILE	CA-C-N	-6.13	113.96	120.03
2	E	1601	ILE	C-N-CA	-6.13	113.96	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	927	VAL	CB-CA-C	-6.09	104.06	112.04
2	B	2311	GLY	N-CA-C	-6.08	105.14	112.49
2	E	2182	VAL	CB-CA-C	-6.07	101.47	110.82
2	B	2187	LYS	N-CA-C	6.05	117.67	111.14
2	B	2374	PHE	N-CA-C	5.99	117.96	108.79
2	E	2051	ILE	N-CA-C	-5.95	104.93	110.53
2	B	2034	ILE	N-CA-C	5.95	116.50	108.17
2	B	2184	VAL	N-CA-CB	-5.95	102.84	111.52
2	E	1836	ASN	N-CA-C	-5.90	100.35	109.14
2	B	2179	GLU	N-CA-C	5.88	117.49	111.14
2	B	1176	GLU	N-CA-C	5.81	118.09	111.11
1	A	355	PRO	CA-N-CD	-5.78	103.91	112.00
2	B	2277	HIS	N-CA-C	5.76	117.64	111.36
2	E	1465	ARG	N-CA-C	-5.75	104.71	110.97
2	B	2160	THR	CB-CA-C	-5.73	101.11	110.85
1	D	327	ILE	CB-CA-C	-5.70	104.55	112.02
2	B	2318	ASN	N-CA-C	5.69	118.18	108.90
2	E	1704	GLU	N-CA-C	5.69	118.75	109.59
2	B	1860	VAL	N-CA-C	5.67	116.87	108.65
2	B	2204	ALA	N-CA-C	5.65	117.55	109.14
2	B	1896	THR	N-CA-C	5.65	119.27	112.38
2	E	2388	ARG	CA-C-N	-5.63	114.12	119.76
2	E	2388	ARG	C-N-CA	-5.63	114.12	119.76
2	B	2155	SER	N-CA-C	-5.61	103.12	110.53
2	E	2085	GLY	N-CA-C	-5.61	102.68	112.55
1	A	93	VAL	N-CA-C	-5.58	99.85	107.99
2	E	2040	TRP	N-CA-C	5.54	114.67	108.25
2	B	1963	LEU	CA-C-N	5.53	126.75	119.84
2	B	1963	LEU	C-N-CA	5.53	126.75	119.84
2	E	2066	LYS	N-CA-C	-5.52	105.17	111.07
2	B	1595	ARG	N-CA-C	5.51	117.37	111.36
2	E	2281	PHE	N-CA-C	5.51	121.42	114.31
2	B	1477	PHE	N-CA-C	-5.49	105.20	111.07
2	B	2007	ARG	N-CA-C	-5.47	105.21	111.07
1	D	218	SER	N-CA-C	5.47	117.32	111.36
1	D	354	ARG	N-CA-C	5.44	119.64	112.35
2	E	1727	LEU	N-CA-C	5.39	117.26	109.07
2	E	931	ALA	N-CA-C	5.37	116.82	111.07
2	E	2378	ILE	N-CA-C	-5.37	101.72	108.05
2	B	1166	ASP	N-CA-C	-5.34	106.78	113.72
2	B	1434	GLU	N-CA-C	-5.33	106.82	113.38
2	B	1164	TYR	N-CA-C	-5.22	100.40	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2157	ILE	N-CA-C	-5.21	105.42	110.42
2	B	2384	ASN	N-CA-C	-5.20	103.17	110.50
2	B	1896	THR	CB-CA-C	-5.19	99.38	110.32
2	B	1163	ARG	N-CA-C	5.17	116.85	108.41
2	B	1923	SER	N-CA-C	5.16	117.80	111.82
2	B	2315	GLY	N-CA-C	-5.15	106.55	112.73
2	B	1867	GLU	N-CA-C	5.12	117.64	111.40
2	B	935	GLU	CB-CA-C	-5.12	102.15	110.85
2	E	1275	MET	N-CA-C	5.07	116.97	107.99
2	E	2351	ILE	N-CA-C	5.07	113.47	107.84
1	D	113	THR	CB-CA-C	-5.05	102.95	110.88
2	E	2391	HIS	N-CA-C	-5.05	101.61	109.24
2	E	1840	TYR	N-CA-C	5.04	117.67	111.82
2	B	1987	VAL	N-CA-C	-5.01	101.26	108.48

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 ⓘ

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	57	0
1	D	2618	0	2494	84	0
2	B	11401	0	11345	904	1
2	E	11582	0	11528	736	1
All	All	28285	0	27897	1765	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 (1765) 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:E:2210:MET:HE1	2:E:2252:GLY:C	1.23	1.50
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:CE	2:E:2252:GLY:C	1.89	1.43
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: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:2024:MET:HE1	2:E:2157:ILE:CG2	1.62	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:E:2210:MET:HE1	2:E:2253:LEU:N	1.49	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:E:2210:MET:HE2	2:E:2253:LEU:CA	1.66	1.22
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:E:2210:MET:CE	2:E:2253:LEU:N	1.99	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:B:1993:ASP:OD2	2:B:2038:HIS:HB3	1.39	1.21
2:B:1993:ASP:CG	2:B:2038:HIS:HB3	1.64	1.21
2:E:2034:ILE:HD12	2:E:2040:TRP:C	1.64	1.21
2:E:2034:ILE:HG23	2:E:2040:TRP:C	1.62	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:B:2210:MET:HE3	2:B:2253:LEU:CA	1.75	1.17
2:E:2024:MET:CE	2:E:2157:ILE:CG2	2.21	1.17
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2052:GLU:O	2:B:2056:ARG:HG3	1.48	1.14
2:E:1763:ASN:C	2:E:1766:MET:CE	2.20	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
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:E:2210:MET:HE2	2:E:2253:LEU:HA	1.19	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: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:E:2024:MET:HE1	2:E:2157:ILE:HG23	1.34	1.09
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: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:E:1727:LEU:C	2:E:1728:ILE:HD13	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:1763:ASN:HA	2:E:1766:MET:HE1	1.40	1.04
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:2034:ILE:CG2	2:E:2040:TRP:C	2.32	1.02
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:1763:ASN:CA	2:E:1766:MET:HE1	1.90	1.02
2:E:1465:ARG:HG2	2:E:1465:ARG:HH11	1.24	1.02
2:E:2034:ILE:CD1	2:E:2041:PRO:HA	1.71	1.02
2:B:2210:MET:CE	2:B:2253:LEU:CA	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:E:2210:MET:HE1	2:E:2252:GLY:CA	1.95	0.95
2:B:1887:GLY:HA3	2:B:1992:TYR:CD2	2.01	0.95
2:E:2024:MET:HE1	2:E:2157:ILE:HG22	1.45	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:2237:GLN:C	2:B:2238:ILE:HD13	1.92	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:E:2011:LEU:HD13	2:E:2040:TRP:CE3	2.03	0.94
2:B:2210:MET:HE3	2:B:2253:LEU:HA	0.96	0.94
2:E:2041:PRO:HB2	2:E:2043:PHE:HE1	1.23	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1252:SER:O	2:B:1274:ARG:NH1	1.99	0.93
1:D:106:PRO:C	1:D:107:LYS:HG2	1.93	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
2:B:2259:ILE:HD12	2:B:2291:ILE:C	1.93	0.93
1:D:19:GLN:HE21	1:D:110:GLU:HG2	1.25	0.93
2:E:1763:ASN:C	2:E:1766:MET:HE1	1.87	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:1763:ASN:C	2:E:1766:MET:HE2	1.97	0.88
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: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
2:B:2256:LEU:C	2:B:2288:CYS:SG	2.58	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:2224:VAL:C	2:B:2349:PHE:CE1	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1992:TYR:OH	2:E:2005:PHE:HB2	1.76	0.86
2:E:2210:MET:HE2	2:E:2253:LEU:N	1.78	0.86
2:B:2044:THR:HG23	2:B:2047:GLN:CD	2.00	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
2:E:2202:GLN:NE2	2:E:2235:SER:C	2.34	0.85
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
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:1961:ASN:CG	2:B:2079:ILE:HD11	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:E:2189:LEU:CD1	2:E:2224:VAL:HG23	2.09	0.82
2:B:2157:ILE:C	2:B:2160:THR:HG1	1.86	0.82
2:B:2279:LYS:HZ3	2:B:2368:GLN:HE22	1.26	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: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:E:2078:GLU:C	2:E:2079:ILE:HD13	2.05	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: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: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:2281:PHE:C	2:B:2286:ARG:HA	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2039:LEU:C	2:E:2040:TRP:CD1	2.59	0.80
2:E:1711:VAL:CG1	2:E:1791:PHE:HB3	2.11	0.80
2:E:2210:MET:SD	2:E:2252:GLY:C	2.57	0.80
2:B:1707:HIS:NE2	2:B:1708:GLU:HB2	1.97	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: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: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:1570:TRP:O	2:E:1571:GLU:CD	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2024:MET:CE	2:E:2157:ILE:HG23	2.01	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:E:2047:GLN:C	2:E:2050:THR:H	1.92	0.78
2:B:2358:ASN:N	2:B:2387:HIS:CE1	2.39	0.78
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:B:2034:ILE:HG12	2:B:2040:TRP:C	2.09	0.78
2:E:1705:SER:OG	2:E:1730:ASN:C	2.27	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: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:2210:MET:CE	2:E:2253:LEU:CA	2.47	0.76
2:E:2201:ILE:HG21	2:E:2382:PHE:HZ	1.49	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
2:E:2178:GLU:C	2:E:2217:LYS:HZ2	1.88	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:PRO:HB3	2:B:1858:TYR:CE1	2.21	0.76
2:B:2279:LYS:HZ3	2:B:2368:GLN:NE2	1.83	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:2080:LYS:HE3	2:E:2083:ILE:HD12	1.68	0.76
1:A:292:CYS:O	1:A:296:SER:OG	2.03	0.75
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
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: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
1:D:292:CYS:O	1:D:296:SER:OG	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1705:SER:HG	2:E:1730:ASN:C	1.93	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
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:2182:VAL:CG1	2:B:2338:GLN:CD	2.62	0.73
2:B:2238:ILE:HD13	2:B:2238:ILE:N	2.03	0.73
2:E:1472:ASN:C	2:E:2325:LEU:HB2	2.09	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: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: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: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:E:2162:LEU:HD13	2:E:2194:ILE:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1961:ASN:CG	2:B:2079:ILE:CD1	2.63	0.71
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: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: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:E:2381:GLU:H	2:E:2381:GLU:CD	1.99	0.70
2:B:2044:THR:OG1	2:B:2047:GLN:CG	2.39	0.70
2:E:1711:VAL:HG12	2:E:1790:TRP:C	2.17	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:B:1704:GLU:HG3	2:B:1730:ASN:O	1.92	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:2087:ASN:C	2:E:2088:ILE:HG12	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2223:THR:HG23	2:B:2348:ASN:O	1.92	0.69
2:B:2259:ILE:CD1	2:B:2291:ILE:C	2.63	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
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: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:2044:THR:H	2:B:2047:GLN:CD	2.01	0.69
2:B:2152:TRP:HA	2:B:2154:LYS:N	2.07	0.69
2:E:2327:GLU:OE1	2:E:2327:GLU:HA	1.93	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: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:E:1867:GLU:CD	2:E:1867:GLU:H	2.01	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:2210:MET:HE2	2:B:2252:GLY:O	1.93	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: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: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:2037:TYR:C	2:B:2038:HIS:HD2	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2044:THR:N	2:B:2047:GLN:OE1	2.27	0.67
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:E:2024:MET:HE3	2:E:2157:ILE:CG2	2.20	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: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
1:A:319:LYS:O	1:A:320:ASP:OD1	2.14	0.65
2:B:1186:TYR:HB2	2:B:1228:TRP:CE3	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1849:LYS:C	2:B:1850:LEU:HD23	2.22	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: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: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:1639:PRO:C	2:E:1640:THR:HG23	2.22	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:2308:THR:HG23	2:B:2333:PHE:C	2.19	0.64
2:E:1763:ASN:ND2	2:E:1763:ASN:H	1.93	0.64
2:B:1747:ASP:CG	2:B:1750:ARG:HG3	2.23	0.64
2:B:2224:VAL:C	2:B:2349:PHE:HE1	2.04	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:2350:ILE:HG23	2:B:2375:LYS:C	2.23	0.63
2:B:2035:LYS:HB3	2:B:2037:TYR:HD1	1.62	0.63
2:B:2256:LEU:C	2:B:2288:CYS:HG	2.07	0.63
2:B:1149:SER:OG	2:B:1152:VAL:HG12	1.97	0.63
2:B:2182:VAL:HG12	2:B:2338:GLN:CD	2.21	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:2039:LEU:C	2:E:2040:TRP:CG	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2339:LEU:C	2:B:2340:LEU:HD12	2.24	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
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
2:E:1763:ASN:O	2:E:1766:MET:HE3	2.00	0.62
2:E:950:THR:O	2:E:954:ILE:HG13	2.00	0.62
2:E:1431:HIS:C	2:E:1433:ASP:H	2.07	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:1639:PRO:C	2:B:1640:THR:HG23	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:2018:ASN:CG	2:E:2058:LEU:HD11	2.20	0.61
2:B:1853:ASP:OD1	2:B:1855:THR:N	2.19	0.61
2:B:2191:LYS:C	2:B:2195:GLU:HG3	2.25	0.61
1:D:109:ASP:O	1:D:110:GLU:HB2	1.99	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: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:2034:ILE:CD1	2:E:2040:TRP:C	2.58	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:1763:ASN:HA	2:E:1766:MET:CE	2.24	0.61
2:B:2210:MET:HE3	2:B:2253:LEU:CB	2.29	0.61
2:B:2315:GLY:C	2:B:2318:ASN:H	2.08	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: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:1598:LEU:C	2:B:1598:LEU:HD13	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:2025:ILE:HG23	2:E:2054:GLN:CD	2.26	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:1706:VAL:HG23	2:E:1706:VAL:O	2.01	0.60
2:E:1998:ARG:HD2	2:E:2045:ASP:CG	2.27	0.60
2:E:2024:MET:CE	2:E:2157:ILE:HG22	2.11	0.60
2:B:2034:ILE:HG12	2:B:2041:PRO:N	2.18	0.59
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
1:A:314:PRO:HB2	1:A:319:LYS:HB2	1.84	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:2002:TYR:C	2:B:2002:TYR:CD1	2.80	0.59
2:B:2258:TRP:H	2:B:2258:TRP:CD1	2.21	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:B:2037:TYR:C	2:B:2038:HIS:CD2	2.80	0.59
2:B:2309:ASP:O	2:B:2313:GLN:N	2.34	0.59
2:E:2074:LEU:C	2:E:2075:THR:HG1	2.07	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:1598:LEU:C	2:E:1598:LEU:HD22	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1840:TYR:HH	2:B:2005:PHE:HD2	1.51	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
2:B:2007:ARG:HG2	2:B:2052:GLU:CD	2.28	0.58
2:B:2183:TYR:HD2	2:B:2289:ILE:HD13	1.67	0.58
2:B:2296:THR:O	2:B:2297:PRO:C	2.44	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:2307:LEU:HD12	2:B:2307:LEU:C	2.28	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:B:2339:LEU:HD12	2:B:2339:LEU:C	2.26	0.57
2:E:1324:GLY:CA	2:E:1325:SER:CB	2.76	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:1624:LEU:C	2:B:1624:LEU:HD23	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1599:SER:C	2:B:1600:GLN:HG2	2.29	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
2:E:1721:ASN:OD1	2:E:1722:ASP:N	2.38	0.57
2:E:2267:LYS:C	2:E:2305:TYR:HH	2.03	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: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: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:E:2024:MET:HE3	2:E:2157:ILE:HG21	1.84	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
1:D:3:THR:CG2	1:D:102:MET:HE3	2.36	0.56
2:E:1599:SER:C	2:E:1600:GLN:HG2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2152:TRP:HA	2:B:2153:ARG:C	2.29	0.56
2:B:2182:VAL:HG13	2:B:2338:GLN:CD	2.23	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: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: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
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:H	2:B:2258:TRP:HD1	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
2:E:1472:ASN:C	2:E:2325:LEU:CB	2.75	0.55
1:A:31:HIS:HB3	1:A:96:PHE:CD2	2.41	0.55
2:B:1993:ASP:CG	2:B:2038:HIS:CB	2.58	0.55
2:E:1293:THR:O	2:E:1295:GLN:N	2.39	0.55
2:E:2025:ILE:CG2	2:E:2054:GLN:CD	2.79	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:1764:VAL:N	2:E:1766:MET:HE2	2.21	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
1:D:153:LEU:HD23	1:D:153:LEU:C	2.32	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:2061:THR:O	2:B:2064:GLY:N	2.41	0.54
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:1604:ARG:HH22	2:B:1822:GLY:C	2.14	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:2064:GLY:C	2:E:2067:TYR:H	2.11	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:B:2223:THR:OG1	2:B:2348:ASN:OD1	2.08	0.54
1:D:77:LEU:C	1:D:77:LEU:HD12	2.33	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
2:B:2208:TYR:C	2:B:2253:LEU:HD21	2.33	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:1766:MET:C	2:E:1767:TYR:HD1	2.16	0.54
2:E:1825:ILE:O	2:E:1826:TYR:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2188:ASN:ND2	2:B:2346:THR:HB	2.20	0.53
2:B:2278:SER:HB3	2:B:2316:GLU:CG	2.38	0.53
2:B:2381:GLU:H	2:B:2381:GLU:CD	2.00	0.53
2:B:1190:ASN:N	2:B:1191:PRO:HD3	2.22	0.53
2:B:1808:ALA:O	2:B:1809:ASN:C	2.51	0.53
2:B:1866:PHE:N	2:B:1866:PHE:CD1	2.76	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
1:A:48:HIS:CG	1:A:53:SER:HG	2.25	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:2379:PRO:C	2:B:2380:LEU:HD23	2.33	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:E:1761:THR:O	2:E:1761:THR:OG1	2.21	0.53
2:E:2384:ASN:HD22	2:E:2384:ASN:C	2.16	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: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:B:2269:MET:HE3	2:B:2273:GLU:HB3	1.89	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
2:B:2284:LYS:C	2:B:2284:LYS:HE3	2.34	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:B:2044:THR:CG2	2:B:2047:GLN:CD	2.80	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:LEU:HD23	1:D:224:LEU:C	2.33	0.53
2:E:2003:THR:O	2:E:2006:SER:N	2.42	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:2210:MET:CE	2:B:2252:GLY:C	2.82	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:1762:ASP:CG	2:E:1763:ASN:N	2.66	0.53
2:E:2384:ASN:ND2	2:E:2385:GLU:N	2.57	0.53
1:A:77:LEU:C	1:A:77:LEU:HD12	2.33	0.52
2:B:1259:LEU:CD2	2:B:1268:ARG:HG3	2.39	0.52
2:B:2353:SER:O	2:B:2375:LYS:NZ	2.30	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:E:2037:TYR:C	2:E:2038:HIS:CD2	2.88	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
2:B:1721:ASN:CB	2:E:1463:THR:HB	2.39	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:E:2268:PHE:CD1	2:E:2268:PHE:C	2.87	0.52
2:B:1104:ILE:CG2	2:B:1107:LEU:HD13	2.39	0.52
2:B:2058:LEU:O	2:B:2059:ILE:C	2.52	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:B:1189:GLU:C	2:B:1191:PRO:HD3	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2060:LEU:O	2:B:2063:TYR:CB	2.53	0.52
2:B:2192:LYS:C	2:B:2195:GLU:HB2	2.35	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
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:1791:PHE:CD1	2:E:1791:PHE:C	2.87	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:2044:THR:H	2:E:2047:GLN:CD	2.18	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:B:1791:PHE:CD1	2:B:1791:PHE:C	2.87	0.51
2:E:2011:LEU:O	2:E:2014:ALA:HB3	2.09	0.51
2:E:2037:TYR:C	2:E:2038:HIS:HD2	2.17	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: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
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:1966:SER:HG	2:E:2016:LYS:HE3	1.72	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:1760:THR:C	2:E:1762:ASP:H	2.19	0.51
2:E:1899:TRP:HA	2:E:1899:TRP:HE3	1.75	0.51
2:B:1570:TRP:C	2:B:1571:GLU:HG3	2.36	0.51
2:B:959:LEU:HD12	2:B:1077:ASN:OD1	2.11	0.51
2:E:1767:TYR:HD1	2:E:1767:TYR:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2198:ASP:CG	2:B:2199:VAL:N	2.68	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:E:1895:HIS:CD2	2:E:1982:THR:C	2.89	0.51
2:E:2050:THR:HA	2:E:2053:SER:HB3	1.93	0.51
2:E:2081:ASP:CG	2:E:2082:ILE:HG23	2.37	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:1679:GLU:HB3	2:B:1704:GLU:C	2.36	0.50
2:B:2081:ASP:CG	2:B:2082:ILE:HG23	2.36	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
1:D:106:PRO:C	1:D:107:LYS:CG	2.72	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:2264:GLU:C	2:E:2294:PHE:CD1	2.89	0.50
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:E:2002:TYR:C	2:E:2002:TYR:CD1	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1727:LEU:C	2:B:1728:ILE:HG12	2.36	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:280:SER:HB2	1:D:313:TYR:CE1	2.47	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
2:E:1763:ASN:O	2:E:1766:MET:HE1	2.05	0.50
2:B:2044:THR:N	2:B:2047:GLN:CD	2.70	0.49
2:B:2210:MET:HE2	2:B:2253:LEU:HA	1.81	0.49
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: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:2083:ILE:HG22	2:E:2084:LEU:N	2.27	0.49
1:A:280:SER:HB2	1:A:313:TYR:CE1	2.48	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:E:2084:LEU:HD22	2:E:2084:LEU:C	2.37	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
2:E:988:GLU:O	2:E:991:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1711:VAL:CA	2:E:1790:TRP:O	2.60	0.49
2:E:2028:SER:C	2:E:2030:PRO:HD3	2.37	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:2247:LEU:CD1	2:B:2375:LYS:HA	2.42	0.49
2:B:2278:SER:HG	2:B:2316:GLU:HG3	1.76	0.49
2:E:1394:LEU:HD23	2:E:1570:TRP:CZ2	2.47	0.49
2:E:1684:GLU:CD	2:E:1702:THR:OG1	2.52	0.49
2:E:2163:TYR:CE1	2:E:2164:LEU:CD2	2.96	0.49
1:A:224:LEU:HD23	1:A:224:LEU:C	2.37	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
2:B:2240:ASN:O	2:B:2241:ILE:C	2.56	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
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
2:E:1431:HIS:C	2:E:1433:ASP:N	2.71	0.49
2:E:2087:ASN:ND2	2:E:2088:ILE:N	2.61	0.49
2:E:2174:ASP:CG	2:E:2175:ASP:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:2163:TYR:CD1	2:E:2164:LEU:N	2.81	0.48
2:E:2248:PRO:C	2:E:2249:ASP:OD1	2.56	0.48
2:B:2210:MET:HE1	2:B:2253:LEU:CA	2.37	0.48
2:B:2282:ALA:O	2:B:2286:ARG:HG2	2.14	0.48
2:B:2301:SER:C	2:B:2302:LEU:HD12	2.39	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:2182:VAL:HG23	2:B:2182:VAL:O	2.11	0.48
2:B:2208:TYR:OH	2:B:2244:ILE:HG23	2.13	0.48
2:E:1209:LYS:HG2	2:E:1212:ARG:NH2	2.27	0.48
2:E:1884:PRO:O	2:E:1992:TYR:OH	2.30	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: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:E:1343:PHE:HB3	2:E:1444:ILE:HD13	1.96	0.48
2:E:2271:ALA:HA	2:E:2329:PHE:CE1	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2358:ASN:CB	2:B:2387:HIS:HE1	2.04	0.48
2:E:946:ASN:O	2:E:950:THR:OG1	2.31	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:B:2329:PHE:C	2:B:2330:GLU:HG2	2.39	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: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:1707:HIS:CE1	2:B:1708:GLU:CD	2.92	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
1:D:292:CYS:C	1:D:296:SER:HG	2.20	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:2053:SER:OG	2:E:2054:GLN:N	2.48	0.47
2:B:1075:ASP:CB	2:B:1078:ILE:HD12	2.45	0.47
2:B:1097:HIS:ND1	2:B:1097:HIS:C	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1604:ARG:HH22	2:E:1822:GLY:C	2.23	0.47
2:E:1687:HIS:ND1	2:E:1688:PRO:CD	2.78	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:B:2166:LEU:O	2:B:2167:LYS:C	2.56	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: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:2178:GLU:HB3	2:B:2217:LYS:HZ2	1.80	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
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
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: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:1763:ASN:CA	2:E:1766:MET:CE	2.68	0.46
2:E:1834:PHE:HD2	2:E:1960:GLU:CG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2210:MET:HE2	2:B:2252:GLY:C	2.40	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: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:E:1849:LYS:C	2:E:1850:LEU:HD23	2.40	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:1853:ASP:CG	2:B:1855:THR:OG1	2.57	0.46
2:E:1027:LYS:O	2:E:1145:MET:HE1	2.15	0.46
2:E:1679:GLU:HB3	2:E:1704:GLU:O	2.16	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
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:1762:ASP:CG	2:E:1763:ASN:H	2.23	0.46
2:E:1763:ASN:N	2:E:1763:ASN:HD22	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1137:PRO:O	2:B:1140:ASN:C	2.59	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:2189:LEU:HD21	2:E:2347:GLY:C	2.41	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
1:A:89:PHE:CD1	1:A:89:PHE:C	2.94	0.45
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:965:LYS:HE3	2:E:985:ASP:CG	2.41	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:2157:ILE:C	2:B:2160:THR:OG1	2.44	0.45
1:D:84:ARG:HH11	1:D:84:ARG:CG	2.27	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
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:2062:GLU:CD	2:E:2065:ARG:HH21	2.23	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:1415:SER:O	2:B:1563:LYS:NZ	2.50	0.45
2:E:1766:MET:C	2:E:1767:TYR:CD1	2.94	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:2210:MET:HE1	2:B:2253:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2247:LEU:HD23	2:B:2374:PHE:HB2	1.99	0.45
2:B:2282:ALA:C	2:B:2286:ARG:HG2	2.42	0.45
1:D:72:ASP:OD2	1:D:75:ASP:HB2	2.17	0.45
2:E:930:ASN:ND2	2:E:933:GLU:CD	2.74	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:1477:PHE:CD1	2:E:1477:PHE:C	2.94	0.45
2:E:2070:ASN:O	2:E:2071:ILE:HG23	2.16	0.45
2:B:2178:GLU:C	2:B:2217:LYS:HZ3	2.24	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
1:D:141:ASP:C	1:D:141:ASP:OD1	2.60	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: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
2:B:2386:MET:O	2:B:2387:HIS:C	2.60	0.45
1:D:108:ILE:H	1:D:108:ILE:CD1	2.30	0.45
2:E:1837:SER:O	2:E:1840:TYR:HB2	2.17	0.45
2:E:1867:GLU:CD	2:E:1867:GLU:N	2.73	0.45
2:E:2183:TYR:CE1	2:E:2289:ILE:HD13	2.52	0.45
2:E:2386:MET:C	2:E:2388:ARG:N	2.74	0.45
1:A:263:LYS:HD2	1:A:263:LYS:HA	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1843:LEU:C	2:B:1849:LYS:HE3	2.41	0.45
2:B:1927:GLU:H	2:B:1927:GLU:CD	2.23	0.45
2:B:2185:LEU:HA	2:B:2186:PRO:HD3	1.57	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:1747:ASP:CG	2:B:1750:ARG:CG	2.90	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:1834:PHE:C	2:E:1957:ARG:HH21	2.26	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
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:1826:TYR:CG	2:E:1826:TYR:O	2.70	0.44
2:E:2039:LEU:CA	2:E:2040:TRP:CD1	3.00	0.44
2:B:1868:GLY:C	2:B:1870:VAL:HG23	2.42	0.44
2:B:1999:LEU:HD21	2:B:2003:THR:CB	2.48	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:B:2386:MET:HE2	2:B:2387:HIS:CD2	2.52	0.44
2:E:1347:ARG:NH1	2:E:1445:THR:O	2.38	0.44
2:E:2190:LEU:O	2:E:2190:LEU:HG	2.17	0.44
2:B:2048:TRP:HA	2:B:2048:TRP:CE3	2.53	0.44
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:1558:GLU:O	2:E:1558:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1731:LYS:HZ3	2:E:1768:PRO:CB	2.30	0.44
2:E:2046:GLU:O	2:E:2049:ILE:HG23	2.04	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:2178:GLU:C	2:B:2217:LYS:NZ	2.76	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:2181:ASN:C	2:B:2338:GLN:HB2	2.43	0.44
2:B:2192:LYS:O	2:B:2193:PHE:C	2.60	0.44
2:E:1104:ILE:CG2	2:E:1107:LEU:CD1	2.96	0.44
2:E:2021:SER:C	2:E:2024:MET:H	2.22	0.44
2:E:2043:PHE:HD2	2:E:2051:ILE:CG1	2.21	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:E:1598:LEU:C	2:E:1598:LEU:CD2	2.91	0.44
2:E:1727:LEU:C	2:E:1728:ILE:CD1	2.71	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:2386:MET:HE3	2:B:2387:HIS:N	2.33	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
1:A:60:PHE:CD1	1:A:80:MET:HE1	2.53	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:1526:TRP:CD1	2:B:1526:TRP:H	2.35	0.43
2:B:1886:THR:HG1	2:B:1888:HIS:CE1	2.32	0.43
2:B:2024:MET:SD	2:B:2157:ILE:HG21	2.58	0.43
2:B:2192:LYS:C	2:B:2195:GLU:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:ARG:HH11	2:B:953:ARG:CG	2.31	0.43
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:2309:ASP:C	2:B:2312:TYR:HB2	2.43	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: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:2210:MET:CE	2:B:2253:LEU:CB	2.93	0.43
2:B:2270:ALA:HB1	2:B:2324:VAL:HA	2.00	0.43
2:E:953:ARG:HG3	2:E:953:ARG:HH11	1.83	0.43
2:E:1081:TYR:CD1	2:E:1081:TYR:C	2.97	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:1321:MET:HA	2:B:1321:MET:HE3	2.01	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:1841:ALA:O	2:B:1842:GLU:C	2.61	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:2231:GLY:O	2:B:2232:HIS:CD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1027:LYS:O	2:B:1145:MET:HE1	2.18	0.43
2:B:2029:ASP:CG	2:B:2032:ILE:HG22	2.44	0.43
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:E:2353:SER:C	2:E:2375:LYS:NZ	2.71	0.43
1:A:109:ASP:OD1	1:A:109:ASP:C	2.60	0.43
2:B:1704:GLU:CG	2:B:1705:SER:N	2.81	0.43
1:D:327:ILE:HG21	1:D:328:TYR:HE1	1.84	0.43
2:B:2182:VAL:HA	2:B:2338:GLN:C	2.44	0.42
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:B:2386:MET:HE2	2:B:2387:HIS:H	1.84	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
1:A:48:HIS:CE1	1:A:53:SER:HG	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: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:1639:PRO:C	2:E:1640:THR:CG2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:2372:TYR:C	2:E:2373:ASN:ND2	2.77	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:1674:ASP:OD1	2:E:1674:ASP:N	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
1:D:8:SER:C	1:D:10:PRO:HD3	2.44	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
2:B:2268:PHE:C	2:B:2268:PHE:CD1	2.98	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:965:LYS:HE3	2:B:985:ASP:CG	2.45	0.41
2:B:2035:LYS:C	2:B:2037:TYR:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1464:LYS:O	2:E:1465:ARG:C	2.61	0.41
2:E:1611:SER:N	2:E:1612:PRO:CD	2.83	0.41
2:E:1624:LEU:C	2:E:1624:LEU:CD2	2.93	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:2158:ALA:C	2:E:2160:THR:N	2.77	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: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
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:1694:MET:HE1	2:E:1738:LEU:O	2.19	0.41
2:E:2070:ASN:O	2:E:2071:ILE:CG2	2.69	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: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:48:HIS:HD1	1:A:53:SER:HG	1.58	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:1763:ASN:C	2:E:1763:ASN:HD22	2.29	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:1760:THR:C	2:E:1762:ASP:N	2.78	0.41
2:E:1996:LEU:HD21	2:E:2001:SER:HA	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2386:MET:CE	2:B:2387:HIS:CD2	3.03	0.41
1:D:109:ASP:OD1	1:D:109:ASP:C	2.64	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
1:A:7:THR:HG21	1:A:70:GLN:OE1	2.21	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:B:2264:GLU:CD	2:B:2266:LEU:HD21	2.46	0.41
2:E:1279:VAL:HG12	2:E:1280:SER:N	2.36	0.41
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:2030:PRO:CG	2:E:2153:ARG:NE	2.77	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:1594:GLN:CD	2:B:1596:THR:H	2.28	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: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
2:B:2386:MET:HE2	2:B:2387:HIS:N	2.35	0.40
1:D:107:LYS:HA	1:D:108:ILE:HA	1.87	0.40
2:E:969:ILE:HG22	2:E:982:TYR:CD2	2.57	0.40
2:E:1624:LEU:HD21	2:E:1633:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1845:ASN:OD1	2:E:1845:ASN:C	2.65	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
2:E:1383:PHE:CE2	2:E:1387:VAL:HG21	2.55	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:2017:THR:HG23	2:B:2062:GLU:CD	2.46	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: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%)	36	67
2	B	1384/1531 (90%)	1345 (97%)	38 (3%)	1 (0%)	48	78
2	E	1406/1531 (92%)	1360 (97%)	42 (3%)	4 (0%)	36	67
All	All	3416/3772 (91%)	3313 (97%)	97 (3%)	6 (0%)	43	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	2088	ILE
2	E	2286	ARG
2	B	2088	ILE
1	D	29	PRO
2	E	1726	GLY
2	E	2215	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/326 (90%)	280 (96%)	13 (4%)	25	56
1	D	289/326 (89%)	268 (93%)	21 (7%)	13	40
2	B	1256/1373 (92%)	1100 (88%)	156 (12%)	4	19
2	E	1278/1373 (93%)	1138 (89%)	140 (11%)	6	24
All	All	3116/3398 (92%)	2786 (89%)	330 (11%)	6	26

All (330) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	92	ILE
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	267	ILE
1	A	299	LYS
1	A	341	GLU
1	A	343	ASN
2	B	883	SER
2	B	885	VAL
2	B	908	ASP

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Mol	Chain	Res	Type
2	B	926	LYS
2	B	929	LEU
2	B	952	ASN
2	B	953	ARG
2	B	956	LYS
2	B	960	THR
2	B	969	ILE
2	B	987	LEU
2	B	1018	SER
2	B	1041	VAL
2	B	1042	SER
2	B	1052	THR
2	B	1074	VAL
2	B	1097	HIS
2	B	1105	ARG
2	B	1139	ASN
2	B	1152	VAL
2	B	1163	ARG
2	B	1165	LEU
2	B	1177	ASP
2	B	1214	ARG
2	B	1218	GLN
2	B	1237	SER
2	B	1239	THR
2	B	1273	GLN
2	B	1282	ASP
2	B	1294	LYS
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	1463	THR
2	B	1465	ARG
2	B	1466	GLN
2	B	1467	GLU
2	B	1478	GLU
2	B	1488	ILE
2	B	1510	ILE
2	B	1512	ARG
2	B	1521	ARG

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Mol	Chain	Res	Type
2	B	1569	SER
2	B	1571	GLU
2	B	1573	LEU
2	B	1595	ARG
2	B	1598	LEU
2	B	1679	GLU
2	B	1691	SER
2	B	1706	VAL
2	B	1710	GLU
2	B	1713	LYS
2	B	1727	LEU
2	B	1728	ILE
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	1842	GLU
2	B	1845	ASN
2	B	1848	ILE
2	B	1849	LYS
2	B	1859	ARG
2	B	1864	LYS
2	B	1867	GLU
2	B	1882	LEU
2	B	1893	ILE
2	B	1894	ILE
2	B	1896	THR
2	B	1927	GLU
2	B	1932	GLN
2	B	1979	MET
2	B	1980	LYS
2	B	1988	LEU
2	B	1991	ILE
2	B	1994	ASP
2	B	1997	ASP
2	B	2001	SER
2	B	2002	TYR
2	B	2006	SER
2	B	2016	LYS

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Mol	Chain	Res	Type
2	B	2017	THR
2	B	2018	ASN
2	B	2026	LEU
2	B	2032	ILE
2	B	2035	LYS
2	B	2038	HIS
2	B	2039	LEU
2	B	2044	THR
2	B	2045	ASP
2	B	2047	GLN
2	B	2050	THR
2	B	2051	ILE
2	B	2053	SER
2	B	2054	GLN
2	B	2055	MET
2	B	2057	ASP
2	B	2080	LYS
2	B	2153	ARG
2	B	2155	SER
2	B	2160	THR
2	B	2163	TYR
2	B	2165	ARG
2	B	2177	VAL
2	B	2185	LEU
2	B	2187	LYS
2	B	2199	VAL
2	B	2202	GLN
2	B	2210	MET
2	B	2222	LYS
2	B	2236	VAL
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	2265	GLU
2	B	2266	LEU

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Mol	Chain	Res	Type
2	B	2267	LYS
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
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	2345	ILE
2	B	2349	PHE
2	B	2367	ASN
2	B	2380	LEU
2	B	2381	GLU
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	101	MET
1	D	102	MET
1	D	108	ILE
1	D	109	ASP
1	D	110	GLU
1	D	113	THR
1	D	213	ILE
1	D	215	LYS
1	D	216	ASN

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Mol	Chain	Res	Type
1	D	267	ILE
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	926	LYS
2	E	930	ASN
2	E	942	GLU
2	E	953	ARG
2	E	956	LYS
2	E	969	ILE
2	E	987	LEU
2	E	990	ILE
2	E	1052	THR
2	E	1093	LYS
2	E	1095	MET
2	E	1152	VAL
2	E	1163	ARG
2	E	1165	LEU
2	E	1166	ASP
2	E	1189	GLU
2	E	1214	ARG
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	1294	LYS
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	1488	ILE

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Mol	Chain	Res	Type
2	E	1510	ILE
2	E	1530	SER
2	E	1568	ASN
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	1708	GLU
2	E	1713	LYS
2	E	1715	SER
2	E	1723	SER
2	E	1727	LEU
2	E	1728	ILE
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	1837	SER
2	E	1842	GLU
2	E	1859	ARG
2	E	1862	VAL
2	E	1882	LEU
2	E	1893	ILE
2	E	1897	SER
2	E	1927	GLU
2	E	1962	ARG
2	E	1972	ASP
2	E	1985	GLN
2	E	1991	ILE

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Mol	Chain	Res	Type
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	2079	ILE
2	E	2080	LYS
2	E	2084	LEU
2	E	2086	GLN
2	E	2087	ASN
2	E	2088	ILE
2	E	2095	ARG
2	E	2157	ILE
2	E	2163	TYR
2	E	2172	SER
2	E	2177	VAL
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	2199	VAL
2	E	2201	ILE
2	E	2203	VAL
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

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Mol	Chain	Res	Type
2	E	2284	LYS
2	E	2296	THR
2	E	2326	SER
2	E	2327	GLU
2	E	2332	THR
2	E	2338	GLN
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	2386	MET
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 (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	343	ASN
2	B	907	ASN
2	B	961	GLN
2	B	1030	GLN
2	B	1087	ASN
2	B	1139	ASN
2	B	1254	ASN
2	B	1470	GLN
2	B	1471	GLN
2	B	1500	HIS
2	B	1652	HIS
2	B	1863	HIS
2	B	1869	ASN
2	B	1895	HIS
2	B	1947	HIS
2	B	1985	GLN
2	B	2038	HIS

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Mol	Chain	Res	Type
2	B	2054	GLN
2	B	2070	ASN
2	B	2087	ASN
2	B	2232	HIS
2	B	2368	GLN
2	B	2373	ASN
2	B	2384	ASN
2	B	2387	HIS
1	D	31	HIS
1	D	45	HIS
1	D	48	HIS
1	D	216	ASN
1	D	219	ASN
1	D	244	HIS
2	E	930	ASN
2	E	961	GLN
2	E	1091	ASN
2	E	1097	HIS
2	E	1140	ASN
2	E	1218	GLN
2	E	1245	ASN
2	E	1254	ASN
2	E	1281	ASN
2	E	1404	HIS
2	E	1470	GLN
2	E	1508	HIS
2	E	1516	GLN
2	E	1600	GLN
2	E	1655	GLN
2	E	1763	ASN
2	E	1863	HIS
2	E	1883	ASN
2	E	1947	HIS
2	E	1985	GLN
2	E	2018	ASN
2	E	2054	GLN
2	E	2070	ASN
2	E	2087	ASN
2	E	2159	ASN
2	E	2202	GLN
2	E	2232	HIS
2	E	2237	GLN

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Mol	Chain	Res	Type
2	E	2260	HIS
2	E	2306	ASN
2	E	2336	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 oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	327/355 (92%)	-0.25	4 (1%) 76 58	40, 75, 133, 168	1 (0%)
1	D	317/355 (89%)	-0.24	5 (1%) 70 49	38, 73, 131, 170	0
2	B	1398/1531 (91%)	0.02	18 (1%) 75 56	38, 103, 176, 253	0
2	E	1420/1531 (92%)	-0.11	14 (0%) 79 61	37, 90, 160, 245	0
All	All	3462/3772 (91%)	-0.08	41 (1%) 76 58	37, 92, 165, 253	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	GLU	4.8
2	B	2059	ILE	4.6
2	B	1433	ASP	4.2
1	D	281	ASP	3.8
1	D	92	ILE	3.6
2	E	1707	HIS	3.5
2	B	2058	LEU	3.5
1	A	329	GLY	3.5
2	B	1276	GLU	3.4
2	B	2221	ILE	3.2
2	B	2027	LEU	3.1
2	B	883	SER	3.0
2	E	1708	GLU	2.9
2	E	1596	THR	2.8
2	E	1703	MET	2.7
1	D	355	PRO	2.6
2	B	2379	PRO	2.6
2	E	2074	LEU	2.6
2	B	2060	LEU	2.5
1	A	93	VAL	2.5
1	A	326	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	2176	PHE	2.4
2	B	2304	ALA	2.3
2	E	1283	GLU	2.3
2	E	1191	PRO	2.3
2	E	2385	GLU	2.2
2	E	2059	ILE	2.2
2	B	1893	ILE	2.2
1	D	326	LEU	2.2
1	D	29	PRO	2.2
2	E	1920	LEU	2.1
2	E	1924	LEU	2.1
2	B	2236	VAL	2.1
2	E	1565	THR	2.1
2	B	2071	ILE	2.1
2	B	2209	GLY	2.1
2	B	1810	PRO	2.1
2	E	1769	SER	2.1
2	E	2088	ILE	2.1
2	B	1596	THR	2.1
2	B	2289	ILE	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 oligosaccharides 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.