



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:38 AM UTC

PDB ID : 1IWO / pdb_00001iwo
Title : Crystal structure of the SR Ca²⁺-ATPase in the absence of Ca²⁺
Authors : Toyoshima, C.; Nomura, H.
Deposited on : 2002-05-26
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

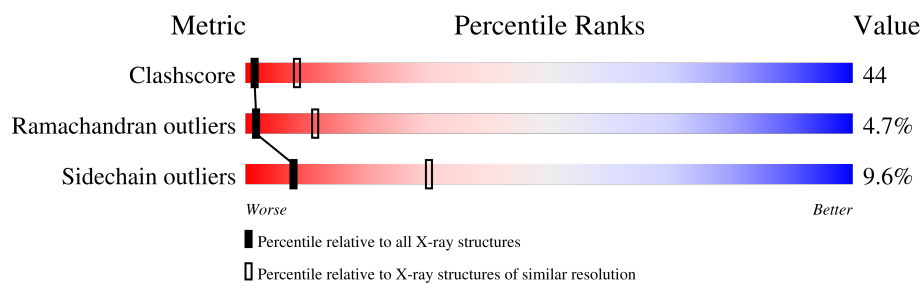
1 Overall quality at a glance

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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	994	35% 54% 10% .
1	B	994	35% 55% 9% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15434 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.

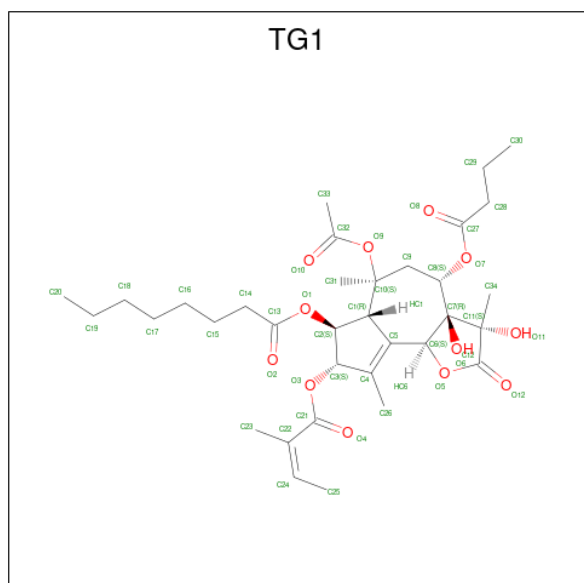
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	B	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	ASP	SEE REMARK 999	UNP P04191
B	994	GLY	ASP	SEE REMARK 999	UNP P04191

- Molecule 2 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (CCD ID: TG1) (formula: C₃₄H₅₀O₁₂).



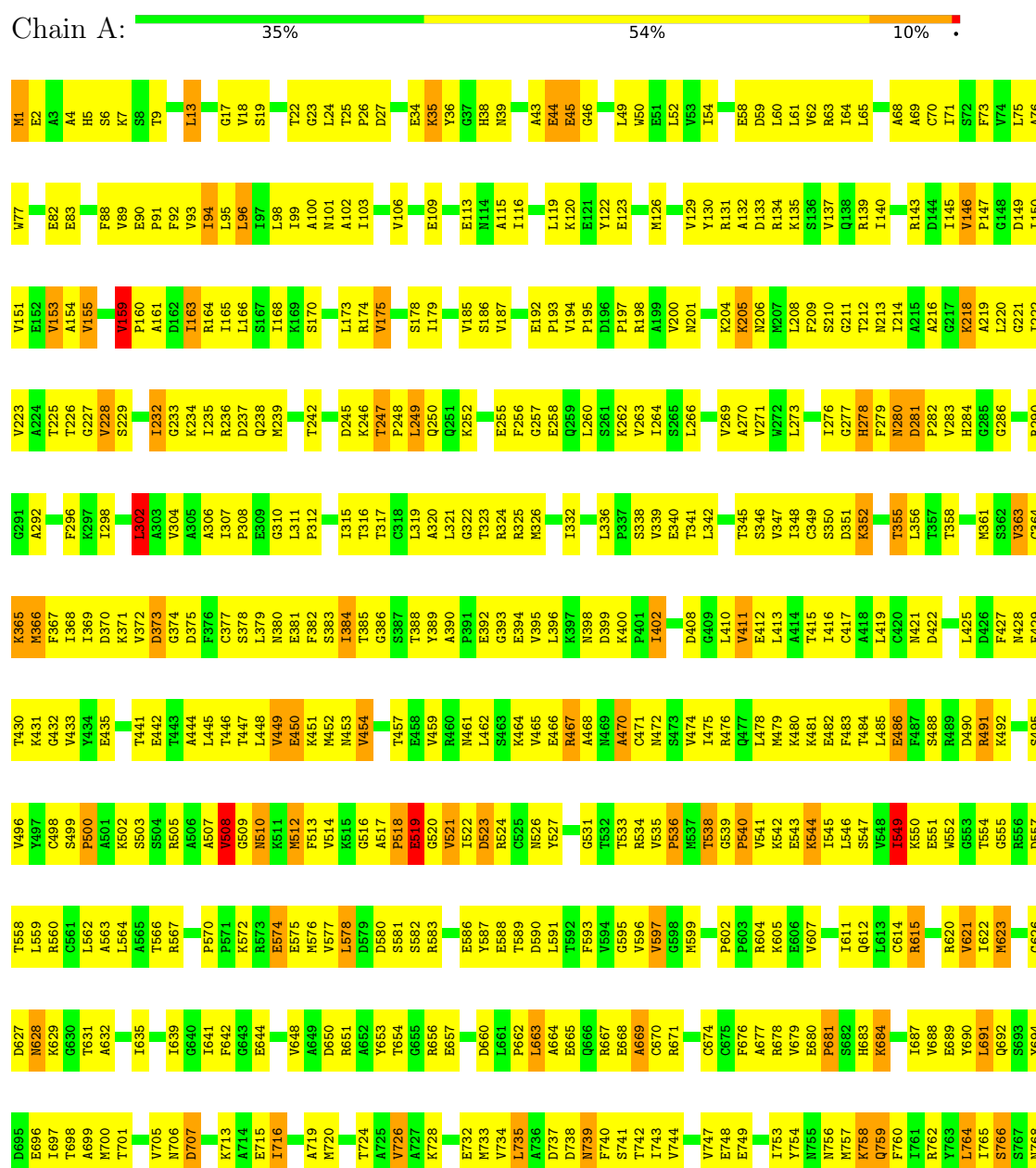
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			46	34	12		
2	B	1	Total	C	O	0	0
			46	34	12		

3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



1983	1916	1984	1943	1985	1944	1986	1945	1987	1946	1988	1947	1989	1948	1990	1949	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050	2051	2052	2053	2054	2055	2056	2057	2058	2059	2060	2061	2062	2063	2064	2065	2066	2067	2068	2069	2070	2071	2072	2073	2074	2075	2076	2077	2078	2079	2080	2081	2082	2083	2084	2085	2086	2087	2088	2089	2090	2091	2092	2093	2094	2095	2096	2097	2098	2099	2100	2101	2102	2103	2104	2105	2106	2107	2108	2109	2110	2111	2112	2113	2114	2115	2116	2117	2118	2119	2120	2121	2122	2123	2124	2125	2126	2127	2128	2129	2130	2131	2132	2133	2134	2135	2136	2137	2138	2139	2140	2141	2142	2143	2144	2145	2146	2147	2148	2149	2150	2151	2152	2153	2154	2155	2156	2157	2158	2159	2160	2161	2162	2163	2164	2165	2166	2167	2168	2169	2170	2171	2172	2173	2174	2175	2176	2177	2178	2179	2180	2181	2182	2183	2184	2185	2186	2187	2188	2189	2190	2191	2192	2193	2194	2195	2196	2197	2198	2199	2200	2201	2202	2203	2204	2205	2206	2207	2208	2209	2210	2211	2212	2213	2214	2215	2216	2217	2218	2219	2220	2221	2222	2223	2224	2225	2226	2227	2228	2229	2230	2231	2232	2233	2234	2235	2236	2237	2238	2239	2240	2241	2242	2243	2244	2245	2246	2247	2248	2249	2250	2251	2252	2253	2254	2255	2256	2257	2258	2259	2260	2261	2262	2263	2264	2265	2266	2267	2268	2269	2270	2271	2272	2273	2274	2275	2276	2277	2278	2279	2280	2281	2282	2283	2284	2285	2286	2287	2288	2289	2290	2291	2292	2293	2294	2295	2296	2297	2298	2299	2300	2301	2302	2303	2304	2305	2306	2307	2308	2309	2310	2311	2312	2313	2314	2315	2316	2317	2318	2319	2320	2321	2322	2323	2324	2325	2326	2327	2328	2329	2330	2331	2332	2333	2334	2335	2336	2337	2338	2339	2340	2341	2342	2343	2344	2345	2346	2347	2348	2349	2350	2351	2352	2353	2354	2355	2356	2357	2358	2359	2360	2361	2362	2363	2364	2365	2366	2367	2368	2369	2370	2371	2372	2373	2374	2375	2376	2377	2378	2379	2380	2381	2382	2383	2384	2385	2386	2387	2388	2389	2390	2391	2392	2393	2394	2395	2396	2397	2398	2399	2400	2401	2402	2403	2404	2405	2406	2407	2408	2409	2410	2411	2412	2413	2414	2415	2416	2417	2418	2419	2420	2421	2422	2423	2424	2425	2426	2427	2428	2429
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	71.74Å 71.74Å 590.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.10	Depositor
% Data completeness (in resolution range)	95.7 (15.00-3.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15434	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TG1

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	0.53	0/7812	1.00	35/10592 (0.3%)
1	B	0.54	0/7812	1.00	35/10592 (0.3%)
All	All	0.54	0/15624	1.00	70/21184 (0.3%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	874	MET	N-CA-C	-9.38	99.75	112.03
1	A	874	MET	N-CA-C	-9.37	99.76	112.03
1	A	5	HIS	N-CA-C	-7.73	103.57	113.16
1	B	5	HIS	N-CA-C	-7.73	103.57	113.16
1	A	159	VAL	CA-C-N	7.42	127.05	119.56
1	A	159	VAL	C-N-CA	7.42	127.05	119.56
1	B	159	VAL	CA-C-N	7.42	127.05	119.56
1	B	159	VAL	C-N-CA	7.42	127.05	119.56
1	A	877	THR	N-CA-C	-7.36	103.28	111.82
1	B	877	THR	N-CA-C	-7.36	103.28	111.82
1	B	924	ARG	N-CA-C	-6.88	105.16	113.97
1	A	924	ARG	N-CA-C	-6.85	105.20	113.97
1	B	684	LYS	N-CA-C	-6.67	104.03	111.71
1	A	684	LYS	N-CA-C	-6.66	104.05	111.71
1	A	873	PHE	N-CA-C	6.64	118.23	108.14
1	B	873	PHE	N-CA-C	6.64	118.23	108.14
1	A	302	LEU	N-CA-C	-6.34	106.08	113.88
1	B	302	LEU	N-CA-C	-6.34	106.08	113.88
1	A	508	VAL	CB-CA-C	-6.34	101.76	111.08
1	B	508	VAL	CB-CA-C	-6.34	101.76	111.08
1	A	163	ILE	N-CA-C	6.29	116.94	107.75
1	B	163	ILE	N-CA-C	6.29	116.93	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ALA	N-CA-C	6.08	121.13	108.53
1	B	4	ALA	N-CA-C	6.08	121.13	108.53
1	A	310	GLY	N-CA-C	-6.08	107.45	114.69
1	B	310	GLY	N-CA-C	-6.07	107.47	114.69
1	A	164	ARG	N-CA-C	-5.95	100.31	109.76
1	B	164	ARG	N-CA-C	-5.95	100.31	109.76
1	B	508	VAL	O-C-N	5.92	128.71	122.62
1	A	508	VAL	O-C-N	5.88	128.68	122.62
1	B	123	GLU	CA-C-N	5.80	127.08	119.84
1	B	123	GLU	C-N-CA	5.80	127.08	119.84
1	A	123	GLU	CA-C-N	5.77	127.06	119.84
1	A	123	GLU	C-N-CA	5.77	127.06	119.84
1	A	503	SER	O-C-N	5.61	130.49	123.19
1	B	503	SER	O-C-N	5.61	130.49	123.19
1	A	13	LEU	N-CA-C	-5.56	105.59	112.38
1	A	355	THR	N-CA-C	-5.56	104.67	112.12
1	B	355	THR	N-CA-C	-5.56	104.67	112.12
1	B	13	LEU	N-CA-C	-5.55	105.61	112.38
1	A	969	MET	N-CA-C	-5.48	105.21	111.07
1	B	969	MET	N-CA-C	-5.47	105.21	111.07
1	A	77	TRP	N-CA-C	-5.35	107.12	113.97
1	B	77	TRP	N-CA-C	-5.35	107.12	113.97
1	A	526	ASN	N-CA-C	-5.29	106.85	113.72
1	B	526	ASN	N-CA-C	-5.29	106.85	113.72
1	B	549	ILE	N-CA-C	-5.29	105.23	110.62
1	B	912	ALA	N-CA-C	-5.28	106.79	113.18
1	A	549	ILE	N-CA-C	-5.28	105.24	110.62
1	A	363	VAL	CB-CA-C	-5.27	104.91	111.08
1	B	363	VAL	CB-CA-C	-5.27	104.91	111.08
1	A	912	ALA	N-CA-C	-5.27	106.81	113.18
1	A	505	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	826	GLU	CA-C-N	5.25	125.46	120.31
1	A	826	GLU	C-N-CA	5.25	125.46	120.31
1	B	826	GLU	CA-C-N	5.25	125.46	120.31
1	B	826	GLU	C-N-CA	5.25	125.46	120.31
1	A	929	VAL	N-CA-C	-5.24	104.41	111.44
1	B	929	VAL	N-CA-C	-5.23	104.43	111.44
1	B	505	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	A	777	LEU	N-CA-C	-5.19	105.27	111.03
1	B	777	LEU	N-CA-C	-5.19	105.27	111.03
1	A	615	ARG	N-CA-C	-5.13	105.77	111.36
1	B	615	ARG	N-CA-C	-5.13	105.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	LEU	N-CA-C	-5.11	105.40	110.97
1	B	249	LEU	N-CA-C	-5.11	105.40	110.97
1	A	784	PRO	N-CA-C	-5.03	103.21	111.21
1	B	784	PRO	N-CA-C	-5.03	103.22	111.21
1	A	852	ALA	N-CA-C	-5.02	107.23	113.55
1	B	852	ALA	N-CA-C	-5.02	107.23	113.55

There are no chirality outliers.

There are no planarity outliers.

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	7671	0	7764	680	0
1	B	7671	0	7764	677	0
2	A	46	0	50	5	0
2	B	46	0	50	5	0
All	All	15434	0	15628	1354	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (1354) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:LYS:HE3	1:A:958:LYS:HA	1.20	1.11
1:B:958:LYS:HA	1:B:958:LYS:HE3	1.20	1.09
1:B:201:ASN:HA	1:B:204:LYS:HD2	1.38	1.04
1:A:201:ASN:HA	1:A:204:LYS:HD2	1.38	1.02
1:B:411:VAL:HG13	1:B:454:VAL:HB	1.42	1.01
1:A:758:LYS:O	1:A:762:ARG:HG3	1.63	0.98
1:A:411:VAL:HG13	1:A:454:VAL:HB	1.42	0.97
1:B:538:THR:HB	1:B:540:PRO:HD2	1.45	0.96
1:A:538:THR:HB	1:A:540:PRO:HD2	1.45	0.96
1:B:758:LYS:O	1:B:762:ARG:HG3	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:THR:HG22	1:B:250:GLN:H	1.29	0.95
1:A:247:THR:HG22	1:A:250:GLN:H	1.29	0.94
1:B:368:ILE:HD13	1:B:410:LEU:HD23	1.51	0.93
1:B:788:ILE:HG22	1:B:789:PRO:HD2	1.51	0.91
1:A:788:ILE:HG22	1:A:789:PRO:HD2	1.51	0.90
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.51	0.90
1:B:583:ARG:O	1:B:586:GLU:HG2	1.72	0.89
1:A:583:ARG:O	1:A:586:GLU:HG2	1.72	0.89
1:A:383:SER:C	1:A:384:ILE:HD13	1.99	0.88
1:B:481:LYS:HA	1:B:498:CYS:HB3	1.54	0.88
1:A:481:LYS:HA	1:A:498:CYS:HB3	1.54	0.88
1:B:232:ILE:H	1:B:232:ILE:HD12	1.38	0.88
1:B:383:SER:C	1:B:384:ILE:HD13	1.99	0.88
1:B:366:MET:HE2	1:B:448:LEU:HD21	1.54	0.88
1:A:232:ILE:HD12	1:A:232:ILE:H	1.38	0.88
1:B:174:ARG:HB2	1:B:216:ALA:HB3	1.56	0.87
1:A:366:MET:HE2	1:A:448:LEU:HD21	1.55	0.87
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.56	0.86
1:B:1:MET:HG2	1:B:225:THR:HG22	1.57	0.86
1:B:262:LYS:NZ	1:B:266:LEU:HD21	1.91	0.85
1:A:604:ARG:HB3	1:A:607:VAL:HG13	1.57	0.85
1:A:100:ALA:HA	1:A:103:ILE:HD12	1.58	0.85
1:B:100:ALA:HA	1:B:103:ILE:HD12	1.58	0.85
1:A:984:LEU:O	1:A:987:ILE:HG22	1.77	0.85
1:A:739:ASN:C	1:A:739:ASN:HD22	1.83	0.84
1:B:604:ARG:HB3	1:B:607:VAL:HG13	1.57	0.84
1:B:984:LEU:O	1:B:987:ILE:HG22	1.77	0.84
1:A:1:MET:HG2	1:A:225:THR:HG22	1.57	0.84
1:B:739:ASN:C	1:B:739:ASN:HD22	1.83	0.84
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.60	0.84
1:A:13:LEU:HD23	1:A:222:ILE:HD12	1.58	0.84
1:A:89:VAL:O	1:A:93:VAL:HG23	1.77	0.84
1:A:262:LYS:NZ	1:A:266:LEU:HD21	1.91	0.84
1:B:147:PRO:HA	1:B:223:VAL:HG12	1.60	0.84
1:A:558:THR:HG21	1:A:635:ILE:HG12	1.61	0.83
1:B:89:VAL:O	1:B:93:VAL:HG23	1.77	0.83
1:B:13:LEU:HD23	1:B:222:ILE:HD12	1.58	0.83
1:B:558:THR:HG21	1:B:635:ILE:HG12	1.61	0.83
1:B:491:ARG:HH11	1:B:491:ARG:HG3	1.45	0.82
1:A:739:ASN:O	1:A:742:THR:HG22	1.80	0.82
1:A:873:PHE:HB2	1:A:875:GLN:HG3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.45	0.82
1:B:873:PHE:HB2	1:B:875:GLN:HG3	1.62	0.82
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.60	0.81
1:A:563:ALA:O	1:A:564:LEU:HD23	1.80	0.81
1:B:739:ASN:O	1:B:742:THR:HG22	1.80	0.81
1:A:447:THR:HG22	1:A:451:LYS:HE3	1.63	0.81
1:B:447:THR:HG22	1:B:451:LYS:HE3	1.63	0.81
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.46	0.81
1:A:628:ASN:HD21	1:A:631:THR:H	1.28	0.81
1:A:890:ILE:HD12	1:A:890:ILE:H	1.46	0.81
1:B:260:LEU:HD11	1:B:306:ALA:HB1	1.60	0.81
1:B:563:ALA:O	1:B:564:LEU:HD23	1.80	0.80
1:A:961:ALA:HB1	1:A:966:GLN:HG2	1.64	0.80
1:A:557:ASP:O	1:A:559:LEU:HG	1.82	0.80
1:B:281:ASP:HB2	1:B:282:PRO:HD3	1.65	0.79
1:B:724:THR:O	1:B:728:LYS:HG3	1.82	0.79
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.64	0.79
1:B:890:ILE:HD12	1:B:890:ILE:H	1.46	0.79
1:B:557:ASP:O	1:B:559:LEU:HG	1.82	0.79
1:A:724:THR:O	1:A:728:LYS:HG3	1.82	0.78
1:B:129:VAL:HG12	1:B:151:VAL:HG12	1.65	0.78
1:B:680:GLU:HB3	1:B:681:PRO:HD2	1.64	0.78
1:B:961:ALA:HB1	1:B:966:GLN:HG2	1.64	0.78
1:B:911:ASN:HA	1:B:914:ASN:HD22	1.46	0.78
1:B:628:ASN:HD21	1:B:631:THR:H	1.28	0.78
1:B:632:ALA:HA	1:B:635:ILE:HD12	1.66	0.78
1:B:153:VAL:HB	1:B:214:ILE:HG13	1.65	0.78
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.65	0.78
1:A:281:ASP:HB2	1:A:282:PRO:HD3	1.65	0.78
1:B:9:THR:HG23	1:B:166:LEU:HD22	1.67	0.77
1:B:52:LEU:HD23	1:B:106:VAL:HG13	1.67	0.77
1:A:153:VAL:HB	1:A:214:ILE:HG13	1.65	0.76
1:A:9:THR:HG23	1:A:166:LEU:HD22	1.67	0.76
1:A:52:LEU:HD23	1:A:106:VAL:HG13	1.67	0.75
1:A:632:ALA:HA	1:A:635:ILE:HD12	1.66	0.75
1:B:705:VAL:HG13	1:B:726:VAL:HG21	1.69	0.75
1:B:720:MET:HE3	1:B:738:ASP:HB3	1.69	0.75
1:A:802:LEU:HB3	1:A:936:SER:HB2	1.69	0.75
1:B:758:LYS:HG3	1:B:828:LEU:HD22	1.69	0.75
1:B:958:LYS:HE3	1:B:958:LYS:CA	2.11	0.75
1:A:720:MET:HE3	1:A:738:ASP:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:VAL:CG1	1:B:726:VAL:HG21	2.17	0.74
1:A:758:LYS:HG3	1:A:828:LEU:HD22	1.69	0.74
1:B:411:VAL:HG13	1:B:454:VAL:CB	2.18	0.74
1:B:947:ILE:HG22	1:B:953:LEU:HD13	1.69	0.74
1:A:851:ALA:HB1	1:A:903:VAL:HG21	1.70	0.74
1:B:326:MET:HE1	1:B:339:VAL:HG12	1.70	0.74
1:B:491:ARG:HH12	1:B:588:GLU:CD	1.96	0.74
1:B:802:LEU:HB3	1:B:936:SER:HB2	1.69	0.74
1:B:874:MET:HG2	1:B:891:PHE:CD2	2.23	0.74
1:B:350:SER:HA	1:B:701:THR:HG21	1.70	0.74
1:A:319:LEU:HG	1:A:339:VAL:HG21	1.69	0.73
1:A:705:VAL:CG1	1:A:726:VAL:HG21	2.17	0.73
1:A:705:VAL:HG13	1:A:726:VAL:HG21	1.69	0.73
1:B:232:ILE:HD12	1:B:232:ILE:N	2.03	0.73
1:B:260:LEU:O	1:B:264:ILE:HG13	1.89	0.73
1:A:52:LEU:HG	1:A:106:VAL:HG22	1.70	0.73
1:A:260:LEU:O	1:A:264:ILE:HG13	1.89	0.73
1:A:232:ILE:HD12	1:A:232:ILE:N	2.03	0.73
1:A:350:SER:HA	1:A:701:THR:HG21	1.70	0.73
1:A:563:ALA:C	1:A:564:LEU:HD23	2.14	0.73
1:A:947:ILE:HG22	1:A:953:LEU:HD13	1.69	0.73
1:B:851:ALA:HB1	1:B:903:VAL:HG21	1.70	0.73
1:A:491:ARG:HH12	1:A:588:GLU:CD	1.96	0.73
1:A:326:MET:HE1	1:A:339:VAL:HG12	1.70	0.73
1:A:605:LYS:HD2	1:A:605:LYS:N	2.04	0.73
1:B:788:ILE:HG13	1:B:791:GLN:CD	2.14	0.72
1:B:319:LEU:HG	1:B:339:VAL:HG21	1.69	0.72
1:B:262:LYS:HZ2	1:B:266:LEU:HD21	1.54	0.72
1:B:52:LEU:HG	1:B:106:VAL:HG22	1.70	0.72
1:B:567:ARG:HH11	1:B:570:PRO:HA	1.55	0.72
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.54	0.72
1:B:683:HIS:O	1:B:687:ILE:HG13	1.88	0.72
1:B:605:LYS:HD2	1:B:605:LYS:N	2.04	0.72
1:B:563:ALA:C	1:B:564:LEU:HD23	2.14	0.72
1:B:628:ASN:ND2	1:B:631:THR:H	1.88	0.72
1:A:683:HIS:O	1:A:687:ILE:HG13	1.88	0.72
1:B:131:ARG:HH11	1:B:131:ARG:HG3	1.54	0.72
1:B:324:ARG:HD2	1:B:324:ARG:C	2.15	0.72
1:A:324:ARG:HD2	1:A:324:ARG:C	2.15	0.72
1:A:874:MET:HG2	1:A:891:PHE:CD2	2.23	0.72
1:A:979:GLY:O	1:A:983:ILE:HG12	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.72	0.71
1:A:628:ASN:ND2	1:A:631:THR:H	1.88	0.71
1:A:788:ILE:HG13	1:A:791:GLN:CD	2.14	0.71
1:A:921:SER:HG	1:A:986:PHE:HD1	1.36	0.71
1:A:311:LEU:N	1:A:312:PRO:HD2	2.05	0.71
1:B:921:SER:HG	1:B:986:PHE:HD1	1.37	0.71
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.72	0.71
1:B:756:ASN:OD1	1:B:810:ASN:HB2	1.91	0.71
1:B:865:VAL:HB	1:B:868:HIS:HB2	1.72	0.71
1:A:411:VAL:HG13	1:A:454:VAL:CB	2.18	0.71
1:A:958:LYS:HE3	1:A:958:LYS:CA	2.11	0.71
1:B:130:TYR:HB2	1:B:150:ILE:HG13	1.72	0.71
1:B:350:SER:HA	1:B:701:THR:CG2	2.21	0.71
1:A:567:ARG:HH11	1:A:570:PRO:HA	1.55	0.70
1:B:411:VAL:HA	1:B:454:VAL:HG11	1.72	0.70
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.27	0.70
1:A:130:TYR:HB2	1:A:150:ILE:HG13	1.72	0.70
1:A:967:TRP:O	1:A:970:VAL:HB	1.91	0.70
1:B:967:TRP:O	1:B:970:VAL:HB	1.91	0.70
1:B:50:TRP:CH2	1:B:54:ILE:HD11	2.27	0.70
1:A:350:SER:HA	1:A:701:THR:CG2	2.21	0.70
1:A:756:ASN:OD1	1:A:810:ASN:HB2	1.91	0.70
1:B:311:LEU:N	1:B:312:PRO:HD2	2.05	0.70
1:A:567:ARG:NH1	1:A:570:PRO:HA	2.07	0.70
1:B:476:ARG:HG3	1:B:476:ARG:HH11	1.56	0.70
1:A:535:VAL:HB	1:A:536:PRO:HD2	1.74	0.70
1:B:535:VAL:HB	1:B:536:PRO:HD2	1.74	0.70
1:B:370:ASP:HB3	1:B:378:SER:OG	1.92	0.70
1:B:351:ASP:H	1:B:701:THR:HG21	1.56	0.69
1:B:979:GLY:O	1:B:983:ILE:HG12	1.90	0.69
1:B:499:SER:HB2	1:B:500:PRO:HD2	1.74	0.69
1:B:567:ARG:NH1	1:B:570:PRO:HA	2.07	0.69
1:A:956:ILE:HG13	1:A:957:PHE:N	2.08	0.69
1:A:370:ASP:HB3	1:A:378:SER:OG	1.92	0.69
1:A:476:ARG:HG3	1:A:476:ARG:HH11	1.56	0.69
1:B:449:VAL:HG21	1:B:472:ASN:OD1	1.93	0.69
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.23	0.69
1:A:351:ASP:H	1:A:701:THR:HG21	1.56	0.68
1:A:851:ALA:CB	1:A:903:VAL:HG21	2.24	0.68
1:A:499:SER:HB2	1:A:500:PRO:HD2	1.74	0.68
1:A:324:ARG:HD2	1:A:325:ARG:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:GLU:OE1	1:B:450:GLU:HA	1.94	0.68
1:A:631:THR:O	1:A:635:ILE:HG13	1.93	0.68
1:B:324:ARG:HD2	1:B:325:ARG:N	2.08	0.68
1:A:449:VAL:HG21	1:A:472:ASN:OD1	1.93	0.68
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.76	0.68
1:A:367:PHE:CD2	1:A:379:LEU:HD13	2.29	0.68
1:A:26:PRO:HD3	1:A:133:ASP:HB3	1.76	0.68
1:A:232:ILE:H	1:A:232:ILE:CD1	2.07	0.68
1:A:262:LYS:HZ3	1:A:266:LEU:HD21	1.58	0.68
1:B:9:THR:HG23	1:B:166:LEU:CD2	2.24	0.68
1:A:450:GLU:HA	1:A:450:GLU:OE1	1.94	0.67
1:B:358:THR:OG1	1:B:602:PRO:HG2	1.94	0.67
1:A:352:LYS:HE2	1:A:635:ILE:HG21	1.75	0.67
1:B:922:LEU:HD23	1:B:927:PRO:HG3	1.77	0.67
1:B:499:SER:HB3	1:B:510:ASN:HD21	1.60	0.67
1:A:499:SER:HB3	1:A:510:ASN:ND2	2.10	0.67
1:A:720:MET:HB3	1:A:738:ASP:OD1	1.95	0.67
1:B:315:ILE:HD12	1:B:316:THR:N	2.09	0.67
1:B:631:THR:O	1:B:635:ILE:HG13	1.93	0.67
1:A:358:THR:OG1	1:A:602:PRO:HG2	1.94	0.67
1:B:781:LEU:O	1:B:783:LEU:N	2.28	0.67
1:B:967:TRP:CZ3	1:B:970:VAL:HG11	2.30	0.67
1:A:967:TRP:CZ3	1:A:970:VAL:HG11	2.30	0.67
1:B:352:LYS:HE2	1:B:635:ILE:HG21	1.75	0.67
1:B:368:ILE:HD13	1:B:410:LEU:CD2	2.23	0.67
1:B:956:ILE:HG13	1:B:957:PHE:N	2.08	0.67
1:A:319:LEU:HB3	1:A:336:LEU:HD12	1.76	0.67
1:A:9:THR:HG23	1:A:166:LEU:CD2	2.24	0.67
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.76	0.67
1:A:315:ILE:HD12	1:A:316:THR:N	2.09	0.66
1:A:781:LEU:O	1:A:783:LEU:N	2.28	0.66
1:B:367:PHE:CD2	1:B:379:LEU:HD13	2.29	0.66
1:A:944:HIS:O	1:A:947:ILE:HG13	1.95	0.66
1:B:26:PRO:HD3	1:B:133:ASP:HB3	1.76	0.66
1:B:851:ALA:CB	1:B:903:VAL:HG21	2.24	0.66
1:A:130:TYR:HE2	1:A:137:VAL:HA	1.61	0.66
1:A:684:LYS:HB3	1:A:700:MET:HE3	1.76	0.66
1:A:499:SER:HB3	1:A:510:ASN:HD21	1.60	0.66
1:B:944:HIS:O	1:B:947:ILE:HG13	1.96	0.66
1:A:19:SER:HB3	1:A:22:THR:OG1	1.95	0.66
1:A:140:ILE:HD11	1:A:145:ILE:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ILE:HG23	1:A:674:CYS:HA	1.77	0.66
1:B:499:SER:HB3	1:B:510:ASN:ND2	2.10	0.66
1:B:863:PRO:HG2	1:B:890:ILE:HG21	1.76	0.66
1:B:278:HIS:HA	1:B:282:PRO:HD2	1.78	0.66
1:B:684:LYS:HB3	1:B:700:MET:HE3	1.76	0.66
1:A:338:SER:HA	1:A:341:THR:HG22	1.78	0.66
1:A:447:THR:CG2	1:A:451:LYS:HE3	2.25	0.66
1:A:922:LEU:HD23	1:A:927:PRO:HG3	1.77	0.66
1:A:491:ARG:NH1	1:A:588:GLU:OE2	2.29	0.66
1:B:622:ILE:HG23	1:B:674:CYS:HA	1.77	0.66
1:B:642:PHE:CZ	1:B:648:VAL:HB	2.31	0.66
1:A:642:PHE:CZ	1:A:648:VAL:HB	2.31	0.66
1:A:863:PRO:HG2	1:A:890:ILE:HG21	1.76	0.66
1:B:140:ILE:HD11	1:B:145:ILE:HG12	1.77	0.66
1:B:232:ILE:H	1:B:232:ILE:CD1	2.07	0.66
1:A:262:LYS:HZ2	1:A:266:LEU:HD21	1.58	0.65
1:B:447:THR:CG2	1:B:451:LYS:HE3	2.26	0.65
1:A:366:MET:HE1	1:A:452:MET:SD	2.36	0.65
1:B:19:SER:HB3	1:B:22:THR:OG1	1.95	0.65
1:B:319:LEU:HB3	1:B:336:LEU:HD12	1.76	0.65
1:B:517:ALA:HB1	1:B:519:GLU:OE1	1.97	0.65
1:A:370:ASP:HB3	1:A:378:SER:HG	1.61	0.65
1:A:373:ASP:O	1:A:375:ASP:N	2.30	0.65
1:B:366:MET:HE1	1:B:452:MET:SD	2.36	0.65
1:B:720:MET:HB3	1:B:738:ASP:OD1	1.95	0.65
1:A:874:MET:HG2	1:A:891:PHE:HD2	1.61	0.65
1:B:342:LEU:HA	1:B:716:ILE:CD1	2.27	0.65
1:B:373:ASP:O	1:B:375:ASP:N	2.30	0.65
1:B:396:LEU:HD12	1:B:396:LEU:O	1.97	0.65
1:A:278:HIS:HA	1:A:282:PRO:HD2	1.78	0.65
1:B:367:PHE:HZ	1:B:545:ILE:HG23	1.62	0.65
1:A:396:LEU:HD12	1:A:396:LEU:O	1.97	0.65
1:A:483:PHE:HE2	1:A:485:LEU:HD21	1.62	0.65
1:A:863:PRO:O	1:A:865:VAL:N	2.30	0.65
1:B:130:TYR:HE2	1:B:137:VAL:HA	1.61	0.65
1:B:491:ARG:NH1	1:B:588:GLU:OE2	2.29	0.65
1:B:863:PRO:O	1:B:865:VAL:N	2.30	0.65
1:A:342:LEU:HA	1:A:716:ILE:CD1	2.27	0.65
1:B:338:SER:HA	1:B:341:THR:HG22	1.78	0.64
1:B:312:PRO:O	1:B:315:ILE:HG13	1.97	0.64
1:A:278:HIS:O	1:B:49:LEU:HB3	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:THR:HA	1:A:968:LEU:HD13	1.79	0.64
1:B:364:CYS:HA	1:B:384:ILE:HG12	1.79	0.64
1:A:663:LEU:HD12	1:A:663:LEU:H	1.63	0.64
1:B:663:LEU:HD12	1:B:663:LEU:H	1.63	0.64
1:B:483:PHE:HE2	1:B:485:LEU:HD21	1.62	0.64
1:B:572:LYS:HB3	1:B:574:GLU:OE2	1.98	0.64
1:A:312:PRO:O	1:A:315:ILE:HG13	1.97	0.64
1:A:367:PHE:HZ	1:A:545:ILE:HG23	1.62	0.64
1:B:874:MET:HG2	1:B:891:PHE:HD2	1.61	0.64
1:A:115:ALA:HB3	1:A:239:MET:HE1	1.80	0.64
1:A:517:ALA:HB1	1:A:519:GLU:OE1	1.96	0.64
1:A:519:GLU:CD	1:A:519:GLU:H	2.05	0.64
1:B:262:LYS:HZ3	1:B:266:LEU:HD21	1.63	0.64
1:A:408:ASP:O	1:A:411:VAL:HG23	1.99	0.63
1:B:519:GLU:H	1:B:519:GLU:CD	2.05	0.63
1:B:965:THR:HA	1:B:968:LEU:HD13	1.79	0.63
1:B:366:MET:HG3	1:B:382:PHE:HB2	1.79	0.63
1:A:572:LYS:HB3	1:A:574:GLU:OE2	1.98	0.63
1:A:668:GLU:O	1:A:671:ARG:HG2	1.98	0.63
1:A:844:VAL:CG1	1:A:907:ILE:HG21	2.29	0.63
1:A:364:CYS:HA	1:A:384:ILE:HG12	1.79	0.63
1:B:396:LEU:HD13	1:B:399:ASP:HA	1.81	0.63
1:B:739:ASN:HD22	1:B:740:PHE:N	1.96	0.63
1:B:895:GLU:N	1:B:896:PRO:HD2	2.14	0.63
1:A:396:LEU:HD13	1:A:399:ASP:HA	1.81	0.62
1:A:873:PHE:HD1	1:A:875:GLN:H	1.46	0.62
1:B:668:GLU:O	1:B:671:ARG:HG2	1.98	0.62
1:A:366:MET:HG3	1:A:382:PHE:HB2	1.79	0.62
1:A:896:PRO:O	1:A:899:MET:HB2	1.99	0.62
1:B:873:PHE:HD1	1:B:875:GLN:H	1.46	0.62
1:A:377:CYS:HB3	1:A:541:VAL:HG22	1.81	0.62
1:B:377:CYS:HB3	1:B:541:VAL:HG22	1.81	0.62
1:B:402:ILE:HD13	1:B:402:ILE:H	1.65	0.62
1:A:739:ASN:HD22	1:A:740:PHE:N	1.96	0.62
1:B:408:ASP:O	1:B:411:VAL:HG23	1.99	0.62
1:B:737:ASP:OD2	1:B:739:ASN:HB3	1.99	0.62
1:B:39:ASN:OD1	1:B:226:THR:HB	2.00	0.62
1:B:355:THR:HG22	1:B:740:PHE:HB2	1.82	0.62
1:B:662:PRO:HD2	1:B:665:GLU:OE2	1.99	0.62
1:B:896:PRO:O	1:B:899:MET:HB2	1.98	0.62
1:A:59:ASP:O	1:A:62:VAL:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:PRO:HD2	1:A:665:GLU:OE2	1.99	0.62
1:A:737:ASP:OD2	1:A:739:ASN:HB3	2.00	0.62
1:B:814:LEU:CD2	1:B:815:ASP:H	2.13	0.62
1:A:342:LEU:HD12	1:A:716:ILE:HD13	1.82	0.62
1:B:951:ASP:HB2	1:B:952:PRO:HD3	1.80	0.62
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.80	0.62
1:B:115:ALA:HB3	1:B:239:MET:HE1	1.80	0.62
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.82	0.61
1:B:342:LEU:HD12	1:B:716:ILE:HD13	1.82	0.61
1:A:39:ASN:OD1	1:A:226:THR:HB	2.00	0.61
1:A:765:ILE:HD11	1:A:829:ILE:HD12	1.83	0.61
1:A:895:GLU:N	1:A:896:PRO:HD2	2.14	0.61
1:B:50:TRP:CZ3	1:B:54:ILE:HD11	2.35	0.61
1:A:542:LYS:HE3	1:A:546:LEU:HD11	1.82	0.61
1:B:765:ILE:HD11	1:B:829:ILE:HD12	1.83	0.61
1:A:950:VAL:O	1:A:954:PRO:HD2	2.01	0.61
1:B:950:VAL:O	1:B:954:PRO:HD2	2.01	0.61
1:B:263:VAL:O	1:B:266:LEU:HB2	2.01	0.61
1:B:264:ILE:HG23	1:B:302:LEU:HD12	1.82	0.61
1:B:844:VAL:CG1	1:B:907:ILE:HG21	2.29	0.61
1:A:50:TRP:CZ3	1:A:54:ILE:HD11	2.36	0.60
1:B:491:ARG:HG3	1:B:491:ARG:NH1	2.16	0.60
1:A:298:ILE:O	1:A:302:LEU:HB2	2.01	0.60
1:A:457:THR:O	1:A:459:VAL:HG13	2.01	0.60
1:A:792:LEU:O	1:A:795:VAL:HB	2.02	0.60
1:B:298:ILE:O	1:B:302:LEU:HB2	2.01	0.60
1:B:792:LEU:O	1:B:795:VAL:HB	2.01	0.60
1:A:402:ILE:HD13	1:A:402:ILE:H	1.65	0.60
1:A:814:LEU:CD2	1:A:815:ASP:H	2.13	0.60
1:A:947:ILE:O	1:A:947:ILE:HD12	2.02	0.60
1:A:130:TYR:CE2	1:A:137:VAL:HA	2.36	0.60
1:A:366:MET:HG3	1:A:366:MET:O	2.01	0.60
1:B:59:ASP:O	1:B:62:VAL:HG22	2.00	0.60
1:B:457:THR:O	1:B:459:VAL:HG13	2.01	0.60
1:B:947:ILE:HD12	1:B:947:ILE:O	2.02	0.60
1:A:264:ILE:HG23	1:A:302:LEU:HD12	1.82	0.60
1:B:298:ILE:HD12	1:B:298:ILE:C	2.27	0.60
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.17	0.59
1:A:298:ILE:C	1:A:298:ILE:HD12	2.27	0.59
1:A:355:THR:HA	1:A:738:ASP:O	2.02	0.59
1:B:384:ILE:HD13	1:B:384:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:LYS:HE3	1:B:546:LEU:HD11	1.82	0.59
1:A:263:VAL:O	1:A:266:LEU:HB2	2.01	0.59
1:B:130:TYR:CE2	1:B:137:VAL:HA	2.36	0.59
1:A:384:ILE:HD13	1:A:384:ILE:N	2.17	0.59
1:A:502:LYS:HG3	1:A:502:LYS:O	2.02	0.59
1:B:319:LEU:HG	1:B:339:VAL:CG2	2.32	0.59
1:B:417:CYS:O	1:B:421:ASN:HB2	2.03	0.59
1:B:968:LEU:HD12	1:B:968:LEU:H	1.67	0.59
1:A:916:LEU:HB2	1:A:925:MET:SD	2.42	0.59
1:B:52:LEU:CD2	1:B:106:VAL:HG13	2.33	0.59
1:A:735:LEU:HD13	1:A:742:THR:CG2	2.33	0.59
1:A:968:LEU:HD12	1:A:968:LEU:H	1.67	0.59
1:B:441:THR:HG21	1:B:560:ARG:NH1	2.18	0.59
1:B:628:ASN:HD21	1:B:631:THR:N	1.99	0.59
1:B:863:PRO:CG	1:B:890:ILE:HG21	2.32	0.59
1:B:975:LEU:H	1:B:975:LEU:HD22	1.67	0.59
1:A:441:THR:HG21	1:A:560:ARG:NH1	2.18	0.59
1:A:605:LYS:HD2	1:A:605:LYS:H	1.68	0.59
1:A:880:HIS:N	1:A:881:PRO:HD2	2.18	0.59
1:A:970:VAL:O	1:A:973:ILE:HG22	2.03	0.59
1:B:880:HIS:N	1:B:881:PRO:HD2	2.18	0.59
1:A:417:CYS:O	1:A:421:ASN:HB2	2.03	0.59
1:A:863:PRO:CG	1:A:890:ILE:HG21	2.32	0.59
1:B:351:ASP:N	1:B:701:THR:HG21	2.18	0.59
1:A:499:SER:CB	1:A:510:ASN:ND2	2.66	0.58
1:B:367:PHE:CE2	1:B:379:LEU:HD13	2.38	0.58
1:B:413:LEU:HD22	1:B:564:LEU:HD12	1.85	0.58
1:B:735:LEU:HD13	1:B:742:THR:CG2	2.33	0.58
1:A:541:VAL:O	1:A:545:ILE:HG13	2.03	0.58
1:A:975:LEU:HD22	1:A:975:LEU:H	1.67	0.58
1:B:126:MET:SD	1:B:139:ARG:HD3	2.43	0.58
1:B:355:THR:HA	1:B:738:ASP:O	2.02	0.58
1:B:366:MET:HG3	1:B:366:MET:O	2.01	0.58
1:B:482:GLU:HG2	1:B:498:CYS:HA	1.86	0.58
1:A:482:GLU:HG2	1:A:498:CYS:HA	1.86	0.58
1:A:801:GLY:O	1:A:804:ALA:HB3	2.04	0.58
1:B:502:LYS:O	1:B:502:LYS:HG3	2.02	0.58
1:B:844:VAL:HG12	1:B:907:ILE:HG21	1.86	0.58
1:A:315:ILE:HD12	1:A:315:ILE:C	2.29	0.58
1:A:356:LEU:CD2	1:A:623:MET:HG3	2.33	0.58
1:B:958:LYS:HA	1:B:958:LYS:CE	2.09	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:HE2	1:A:137:VAL:CA	2.16	0.58
1:B:247:THR:HG23	1:B:340:GLU:OE1	2.04	0.58
1:B:366:MET:HB3	1:B:597:VAL:HG12	1.84	0.58
1:A:757:MET:HA	1:A:760:PHE:CE2	2.39	0.58
1:B:499:SER:CB	1:B:510:ASN:ND2	2.66	0.58
1:A:52:LEU:CD2	1:A:106:VAL:HG13	2.33	0.58
1:A:247:THR:HG23	1:A:340:GLU:OE1	2.04	0.58
1:A:248:PRO:O	1:A:252:LYS:HG2	2.04	0.58
1:A:319:LEU:HG	1:A:339:VAL:CG2	2.32	0.58
1:B:18:VAL:HG12	1:B:19:SER:N	2.19	0.58
1:A:126:MET:SD	1:A:139:ARG:HD3	2.43	0.58
1:A:351:ASP:N	1:A:701:THR:HG21	2.18	0.58
1:A:367:PHE:CE2	1:A:379:LEU:HD13	2.38	0.58
1:A:527:TYR:HB3	1:A:534:ARG:HD3	1.85	0.58
1:B:541:VAL:O	1:B:545:ILE:HG13	2.03	0.58
1:B:916:LEU:HB2	1:B:925:MET:SD	2.42	0.58
1:A:628:ASN:HD21	1:A:631:THR:N	1.99	0.57
1:A:947:ILE:O	1:A:948:LEU:HD12	2.04	0.57
1:B:970:VAL:O	1:B:973:ILE:HG22	2.03	0.57
1:A:366:MET:HB3	1:A:597:VAL:HG12	1.84	0.57
1:A:810:ASN:HD21	1:A:916:LEU:HA	1.69	0.57
1:B:342:LEU:HA	1:B:716:ILE:HD13	1.85	0.57
1:B:757:MET:HA	1:B:760:PHE:CE2	2.39	0.57
1:A:336:LEU:O	1:A:339:VAL:HG22	2.04	0.57
1:A:491:ARG:HG3	1:A:491:ARG:NH1	2.16	0.57
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.45	0.57
1:A:894:PRO:HB2	1:A:959:LEU:H	1.69	0.57
1:B:130:TYR:HE2	1:B:137:VAL:CA	2.16	0.57
1:B:527:TYR:HB3	1:B:534:ARG:HD3	1.85	0.57
1:A:346:SER:OG	1:A:696:GLU:HG2	2.04	0.57
1:A:576:MET:HE3	1:A:587:TYR:CG	2.39	0.57
1:A:676:PHE:CE1	1:A:687:ILE:HD13	2.40	0.57
1:A:705:VAL:C	1:A:707:ASP:H	2.13	0.57
1:A:765:ILE:O	1:A:769:VAL:HG23	2.05	0.57
1:B:209:PHE:O	1:B:212:THR:HB	2.05	0.57
1:B:346:SER:OG	1:B:696:GLU:HG2	2.04	0.57
1:B:615:ARG:NH1	1:B:620:ARG:HA	2.20	0.57
1:B:676:PHE:CE1	1:B:687:ILE:HD13	2.40	0.57
1:A:276:ILE:HG22	1:A:279:PHE:HB3	1.86	0.57
1:B:629:LYS:HB2	1:B:654:THR:HG22	1.86	0.57
1:B:911:ASN:HA	1:B:914:ASN:ND2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:PRO:O	1:B:252:LYS:HG2	2.04	0.57
1:B:758:LYS:HZ1	1:B:822:ARG:HE	1.52	0.57
1:B:801:GLY:O	1:B:804:ALA:HB3	2.04	0.57
1:B:947:ILE:O	1:B:948:LEU:HD12	2.04	0.57
1:A:212:THR:CG2	1:A:213:ASN:N	2.68	0.57
1:B:356:LEU:CD2	1:B:623:MET:HG3	2.33	0.57
1:B:576:MET:HE3	1:B:587:TYR:CG	2.39	0.57
1:A:629:LYS:HB2	1:A:654:THR:HG22	1.86	0.57
1:A:844:VAL:HG12	1:A:907:ILE:HG21	1.86	0.57
1:B:315:ILE:HD12	1:B:315:ILE:C	2.29	0.57
1:B:833:LEU:HG	1:B:837:TYR:CE2	2.40	0.57
1:B:967:TRP:CE3	1:B:970:VAL:HG11	2.40	0.57
1:A:13:LEU:CD2	1:A:222:ILE:HD12	2.33	0.57
1:A:342:LEU:HA	1:A:716:ILE:HD13	1.85	0.57
1:B:276:ILE:HG22	1:B:279:PHE:HB3	1.86	0.57
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.85	0.56
1:A:18:VAL:HG12	1:A:19:SER:N	2.19	0.56
1:A:161:ALA:HA	1:A:210:SER:HB2	1.88	0.56
1:A:539:GLY:O	1:A:543:GLU:HG2	2.05	0.56
1:A:833:LEU:HG	1:A:837:TYR:HE2	1.70	0.56
1:A:924:ARG:C	1:A:926:PRO:HD3	2.30	0.56
1:B:212:THR:CG2	1:B:213:ASN:N	2.68	0.56
1:B:803:PRO:HG2	1:B:909:MET:HE1	1.87	0.56
1:A:209:PHE:O	1:A:212:THR:HB	2.05	0.56
1:A:814:LEU:HD22	1:A:815:ASP:H	1.70	0.56
1:B:161:ALA:HA	1:B:210:SER:HB2	1.88	0.56
1:B:336:LEU:O	1:B:339:VAL:HG22	2.04	0.56
1:B:605:LYS:HD2	1:B:605:LYS:H	1.68	0.56
1:B:914:ASN:HB3	1:B:981:ASP:OD2	2.05	0.56
1:B:924:ARG:C	1:B:926:PRO:HD3	2.30	0.56
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.70	0.56
1:A:205:LYS:NZ	1:A:205:LYS:HB3	2.20	0.56
1:A:512:MET:HE1	1:A:587:TYR:C	2.31	0.56
1:B:367:PHE:CZ	1:B:545:ILE:HG23	2.41	0.56
1:B:715:GLU:C	1:B:716:ILE:HG13	2.30	0.56
1:B:894:PRO:HB2	1:B:959:LEU:H	1.69	0.56
1:A:833:LEU:HG	1:A:837:TYR:CE2	2.40	0.56
1:A:901:LEU:O	1:A:905:VAL:HG23	2.06	0.56
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.70	0.56
1:B:791:GLN:O	1:B:795:VAL:HG23	2.06	0.56
1:B:833:LEU:HG	1:B:837:TYR:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ILE:HD11	1:A:566:THR:HG23	1.87	0.56
1:A:615:ARG:NH1	1:A:620:ARG:HA	2.20	0.56
1:A:748:GLU:HB2	1:A:817:MET:HE2	1.87	0.56
1:A:791:GLN:O	1:A:795:VAL:HG23	2.06	0.56
1:B:76:ALA:O	1:B:88:PHE:HE2	1.89	0.56
1:B:355:THR:OG1	1:B:720:MET:HE1	2.06	0.56
1:B:748:GLU:HB2	1:B:817:MET:HE2	1.87	0.56
1:B:765:ILE:O	1:B:769:VAL:HG23	2.05	0.56
1:B:774:CYS:SG	1:B:787:LEU:HD12	2.45	0.56
1:A:715:GLU:C	1:A:716:ILE:HG13	2.30	0.56
1:A:760:PHE:CD1	1:A:760:PHE:C	2.84	0.56
1:A:803:PRO:HG2	1:A:909:MET:HE1	1.87	0.56
1:B:13:LEU:CD2	1:B:222:ILE:HD12	2.33	0.56
1:B:810:ASN:HD21	1:B:916:LEU:HA	1.70	0.56
1:A:466:GLU:C	1:A:468:ALA:H	2.14	0.56
1:A:967:TRP:CE3	1:A:970:VAL:HG11	2.40	0.56
1:B:760:PHE:CD1	1:B:760:PHE:C	2.84	0.56
1:B:466:GLU:C	1:B:468:ALA:H	2.14	0.55
1:A:355:THR:OG1	1:A:720:MET:HE1	2.06	0.55
1:A:749:GLU:O	1:A:753:ILE:HG12	2.06	0.55
1:A:794:TRP:HH2	1:A:943:LEU:HB3	1.72	0.55
1:B:18:VAL:HG13	1:B:24:LEU:HD23	1.87	0.55
1:B:205:LYS:NZ	1:B:205:LYS:HB3	2.20	0.55
1:A:76:ALA:O	1:A:88:PHE:HE2	1.89	0.55
1:A:844:VAL:HG12	1:A:907:ILE:HD13	1.89	0.55
1:B:416:ILE:HD11	1:B:566:THR:HG23	1.87	0.55
1:A:147:PRO:HA	1:A:223:VAL:CG1	2.35	0.55
1:A:367:PHE:CZ	1:A:545:ILE:HG23	2.41	0.55
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.05	0.55
1:B:539:GLY:O	1:B:543:GLU:HG2	2.05	0.55
1:A:921:SER:OG	1:A:986:PHE:HD1	1.89	0.55
1:B:705:VAL:C	1:B:707:ASP:H	2.13	0.55
1:B:322:GLY:O	1:B:325:ARG:HB3	2.07	0.55
1:B:844:VAL:HG12	1:B:907:ILE:HD13	1.89	0.55
1:B:901:LEU:O	1:B:905:VAL:HG23	2.06	0.55
1:A:18:VAL:HG13	1:A:24:LEU:HD23	1.87	0.55
1:A:836:ARG:O	1:A:840:ILE:HG12	2.07	0.55
1:B:512:MET:HE1	1:B:587:TYR:C	2.31	0.55
1:A:322:GLY:O	1:A:325:ARG:HB3	2.07	0.55
1:B:363:VAL:HB	1:B:448:LEU:HD13	1.89	0.55
1:B:749:GLU:O	1:B:753:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HE2	1:A:7:LYS:HA	1.89	0.55
1:B:586:GLU:O	1:B:589:THR:HG22	2.07	0.55
1:A:284:HIS:CE1	1:B:45:GLU:HB3	2.42	0.55
1:B:836:ARG:O	1:B:840:ILE:HG12	2.07	0.55
1:A:325:ARG:NH1	1:A:753:ILE:HD11	2.22	0.54
1:A:735:LEU:HD22	1:A:742:THR:HG23	1.89	0.54
1:B:814:LEU:HD22	1:B:815:ASP:H	1.70	0.54
1:A:586:GLU:O	1:A:589:THR:HG22	2.07	0.54
1:A:911:ASN:HA	1:A:914:ASN:ND2	2.18	0.54
1:B:131:ARG:HG3	1:B:131:ARG:NH1	2.17	0.54
1:B:325:ARG:NH1	1:B:753:ILE:HD11	2.22	0.54
1:B:668:GLU:OE1	1:B:671:ARG:HD3	2.07	0.54
1:B:773:VAL:HB	1:B:845:GLY:HA3	1.88	0.54
1:A:428:ASN:HB2	1:A:435:GLU:CG	2.38	0.54
1:A:739:ASN:C	1:A:739:ASN:ND2	2.54	0.54
1:A:773:VAL:HB	1:A:845:GLY:HA3	1.88	0.54
1:B:192:GLU:HG3	1:B:193:PRO:HD2	1.90	0.54
1:B:428:ASN:HB2	1:B:435:GLU:CG	2.38	0.54
1:B:899:MET:O	1:B:903:VAL:HG23	2.07	0.54
1:A:315:ILE:O	1:A:319:LEU:HD13	2.08	0.54
1:B:70:CYS:O	1:B:71:ILE:C	2.51	0.54
1:B:364:CYS:O	1:B:383:SER:HA	2.07	0.54
1:A:748:GLU:HG3	1:A:817:MET:SD	2.47	0.54
1:B:739:ASN:C	1:B:739:ASN:ND2	2.54	0.54
1:B:748:GLU:HG3	1:B:817:MET:SD	2.47	0.54
1:A:260:LEU:HD13	2:A:1001:TG1:H252	1.89	0.54
1:A:342:LEU:O	1:A:345:THR:OG1	2.24	0.54
1:A:476:ARG:HG3	1:A:476:ARG:NH1	2.23	0.54
1:A:894:PRO:O	1:A:898:THR:HG22	2.08	0.54
1:A:1:MET:HG2	1:A:225:THR:CG2	2.34	0.54
1:A:668:GLU:OE1	1:A:671:ARG:HD3	2.07	0.54
1:B:315:ILE:O	1:B:319:LEU:HD13	2.08	0.54
1:B:794:TRP:HH2	1:B:943:LEU:HB3	1.72	0.54
1:B:977:VAL:HG13	1:B:978:ILE:N	2.23	0.54
1:A:363:VAL:HB	1:A:448:LEU:HD13	1.89	0.53
1:A:967:TRP:HZ3	1:A:970:VAL:HG11	1.73	0.53
1:B:735:LEU:HD22	1:B:742:THR:HG23	1.89	0.53
1:B:894:PRO:O	1:B:898:THR:HG22	2.08	0.53
1:A:192:GLU:HG3	1:A:193:PRO:HD2	1.90	0.53
1:B:50:TRP:O	1:B:54:ILE:HG12	2.08	0.53
1:B:921:SER:OG	1:B:986:PHE:HD1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:962:LEU:O	1:B:966:GLN:HB3	2.08	0.53
1:A:364:CYS:O	1:A:383:SER:HA	2.07	0.53
1:A:962:LEU:O	1:A:966:GLN:HB3	2.08	0.53
1:B:762:ARG:O	1:B:766:SER:HB3	2.08	0.53
1:A:70:CYS:O	1:A:71:ILE:C	2.51	0.53
1:A:366:MET:CE	1:A:448:LEU:HD21	2.34	0.53
1:A:622:ILE:HG23	1:A:674:CYS:CA	2.39	0.53
1:A:899:MET:O	1:A:903:VAL:HG23	2.07	0.53
1:B:1:MET:HG2	1:B:225:THR:CG2	2.34	0.53
1:B:116:ILE:HA	1:B:119:LEU:HD23	1.91	0.53
1:A:50:TRP:O	1:A:54:ILE:HG12	2.08	0.53
1:A:762:ARG:O	1:A:766:SER:HB3	2.08	0.53
1:B:476:ARG:HG3	1:B:476:ARG:NH1	2.23	0.53
1:B:622:ILE:HG23	1:B:674:CYS:CA	2.39	0.53
1:A:558:THR:HG22	1:A:558:THR:O	2.08	0.53
1:A:863:PRO:O	1:A:865:VAL:HG13	2.09	0.53
1:B:558:THR:O	1:B:558:THR:HG22	2.08	0.53
1:B:688:VAL:HG23	1:B:700:MET:HE2	1.91	0.53
1:B:1:MET:HA	1:B:225:THR:HG22	1.91	0.53
1:B:49:LEU:C	1:B:49:LEU:HD23	2.34	0.53
1:A:868:HIS:O	1:A:869:GLN:HB2	2.09	0.53
1:A:977:VAL:HG13	1:A:978:ILE:N	2.24	0.53
1:B:7:LYS:HE2	1:B:7:LYS:HA	1.89	0.53
1:B:593:PHE:CD1	1:B:593:PHE:C	2.87	0.53
1:B:868:HIS:O	1:B:869:GLN:HB2	2.09	0.53
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.39	0.53
1:B:260:LEU:HD13	2:B:1002:TG1:H252	1.89	0.53
1:A:1:MET:HA	1:A:225:THR:HG22	1.91	0.52
1:A:903:VAL:O	1:A:907:ILE:HG13	2.09	0.52
1:A:915:SER:C	1:A:917:SER:H	2.17	0.52
1:A:924:ARG:HA	1:A:924:ARG:NE	2.24	0.52
1:B:777:LEU:O	1:B:780:ALA:N	2.41	0.52
1:B:915:SER:C	1:B:917:SER:H	2.17	0.52
1:A:382:PHE:CZ	1:A:410:LEU:HD11	2.45	0.52
1:B:412:GLU:HA	1:B:415:THR:OG1	2.10	0.52
1:B:671:ARG:HD2	1:B:694:TYR:CZ	2.45	0.52
1:B:924:ARG:HA	1:B:924:ARG:NE	2.24	0.52
1:A:462:LEU:HD22	1:A:466:GLU:OE1	2.10	0.52
1:A:627:ASP:O	1:A:677:ALA:HB1	2.10	0.52
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.45	0.52
1:A:769:VAL:HA	2:A:1001:TG1:H231	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:MET:CE	1:B:448:LEU:HD21	2.34	0.52
1:B:495:SER:CB	1:B:588:GLU:OE1	2.58	0.52
1:B:627:ASP:O	1:B:677:ALA:HB1	2.10	0.52
1:B:628:ASN:HD21	1:B:631:THR:CB	2.23	0.52
1:B:705:VAL:HG12	1:B:726:VAL:HG21	1.92	0.52
1:B:758:LYS:NZ	1:B:822:ARG:HE	2.07	0.52
1:B:863:PRO:O	1:B:865:VAL:HG13	2.09	0.52
1:A:758:LYS:NZ	1:A:822:ARG:HE	2.07	0.52
1:A:857:MET:SD	1:A:867:TYR:HA	2.50	0.52
1:B:596:VAL:HG12	1:B:597:VAL:N	2.24	0.52
1:B:611:ILE:HD12	1:B:641:ILE:HD11	1.92	0.52
1:B:769:VAL:HA	2:B:1002:TG1:H231	1.91	0.52
1:B:903:VAL:O	1:B:907:ILE:HG13	2.09	0.52
1:A:49:LEU:HD23	1:A:49:LEU:O	2.10	0.52
1:A:355:THR:OG1	1:A:720:MET:CE	2.58	0.52
1:A:495:SER:CB	1:A:588:GLU:OE1	2.58	0.52
1:B:24:LEU:HG	1:B:149:ASP:HA	1.92	0.52
1:B:671:ARG:HB3	1:B:694:TYR:CE1	2.45	0.52
1:B:770:GLY:HA3	1:B:844:VAL:CG2	2.39	0.52
1:A:412:GLU:HA	1:A:415:THR:OG1	2.10	0.52
1:B:235:ILE:HD11	1:B:706:ASN:HA	1.92	0.52
1:B:705:VAL:HG12	1:B:726:VAL:HG11	1.91	0.52
1:B:865:VAL:HB	1:B:868:HIS:CB	2.39	0.52
1:A:18:VAL:HG12	1:A:19:SER:H	1.74	0.52
1:A:49:LEU:HD23	1:A:49:LEU:C	2.34	0.52
1:A:173:LEU:HD12	1:A:216:ALA:O	2.10	0.52
1:A:235:ILE:HD11	1:A:706:ASN:HA	1.92	0.52
1:A:444:ALA:HB3	1:A:599:MET:HE1	1.92	0.52
1:A:628:ASN:HD21	1:A:631:THR:CB	2.23	0.52
1:A:688:VAL:HG23	1:A:700:MET:HE2	1.91	0.52
1:A:705:VAL:HG12	1:A:726:VAL:HG11	1.91	0.52
1:B:18:VAL:HG12	1:B:19:SER:H	1.74	0.52
1:B:382:PHE:CZ	1:B:410:LEU:HD11	2.45	0.52
1:A:596:VAL:HG12	1:A:597:VAL:N	2.24	0.52
1:A:958:LYS:HA	1:A:958:LYS:CE	2.09	0.51
1:B:495:SER:HB3	1:B:588:GLU:OE1	2.11	0.51
1:A:116:ILE:HA	1:A:119:LEU:HD23	1.91	0.51
1:A:593:PHE:CD1	1:A:593:PHE:C	2.87	0.51
1:A:810:ASN:HA	1:A:930:ASN:HD22	1.76	0.51
1:B:49:LEU:HD23	1:B:49:LEU:O	2.10	0.51
1:A:247:THR:HG23	1:A:249:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:MET:HG2	1:A:441:THR:HA	1.92	0.51
1:A:671:ARG:HB3	1:A:694:TYR:CE1	2.45	0.51
1:A:865:VAL:HB	1:A:868:HIS:CB	2.39	0.51
1:B:155:VAL:HA	1:B:214:ILE:O	2.10	0.51
1:B:247:THR:HG23	1:B:249:LEU:H	1.75	0.51
1:B:621:VAL:HG13	1:B:641:ILE:HD12	1.93	0.51
1:A:198:ARG:HG2	1:A:198:ARG:HH11	1.76	0.51
1:A:611:ILE:HD12	1:A:641:ILE:HD11	1.92	0.51
1:B:338:SER:C	1:B:340:GLU:N	2.67	0.51
1:B:512:MET:HE1	1:B:587:TYR:O	2.10	0.51
1:A:24:LEU:HG	1:A:149:ASP:HA	1.92	0.51
1:B:71:ILE:HG22	1:B:75:LEU:HD13	1.92	0.51
1:A:35:LYS:HD3	1:A:35:LYS:C	2.36	0.51
1:A:155:VAL:HA	1:A:214:ILE:O	2.10	0.51
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.38	0.51
1:B:173:LEU:HD12	1:B:216:ALA:O	2.10	0.51
1:B:462:LEU:HD22	1:B:466:GLU:OE1	2.10	0.51
1:B:614:CYS:SG	1:B:744:VAL:HG22	2.51	0.51
1:B:857:MET:SD	1:B:867:TYR:HA	2.50	0.51
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.93	0.51
1:A:179:ILE:O	1:A:705:VAL:HG22	2.11	0.51
1:B:179:ILE:O	1:B:705:VAL:HG22	2.11	0.51
1:B:444:ALA:HB3	1:B:599:MET:HE1	1.92	0.51
1:A:512:MET:HE1	1:A:587:TYR:O	2.10	0.51
1:A:794:TRP:CH2	1:A:943:LEU:HB3	2.46	0.51
1:B:24:LEU:HD12	1:B:149:ASP:HB3	1.93	0.51
1:B:133:ASP:O	1:B:134:ARG:HG3	2.11	0.51
1:B:355:THR:OG1	1:B:720:MET:CE	2.58	0.51
1:A:133:ASP:O	1:A:134:ARG:HG3	2.11	0.51
1:A:614:CYS:SG	1:A:744:VAL:HG22	2.51	0.51
1:A:621:VAL:HG13	1:A:641:ILE:HD12	1.93	0.51
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.46	0.51
1:B:198:ARG:HG2	1:B:198:ARG:HH11	1.76	0.51
1:B:969:MET:O	1:B:973:ILE:HB	2.11	0.51
1:A:61:LEU:HD22	1:A:307:ILE:CD1	2.41	0.51
1:A:342:LEU:HA	1:A:716:ILE:HD11	1.92	0.51
1:A:705:VAL:HG12	1:A:726:VAL:HG21	1.92	0.51
1:A:917:SER:N	1:A:925:MET:HE2	2.26	0.51
1:B:370:ASP:HB2	1:B:379:LEU:O	2.11	0.51
1:B:550:LYS:O	1:B:551:GLU:C	2.54	0.51
1:B:794:TRP:CH2	1:B:943:LEU:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:HB3	1:A:209:PHE:CZ	2.46	0.50
1:A:754:TYR:CD1	1:A:754:TYR:O	2.64	0.50
1:A:836:ARG:HG2	1:A:836:ARG:HH11	1.77	0.50
1:A:987:ILE:HG12	1:A:987:ILE:O	2.12	0.50
1:B:290:ARG:C	1:B:292:ALA:H	2.20	0.50
1:A:25:THR:O	1:A:27:ASP:N	2.44	0.50
1:A:278:HIS:O	1:B:49:LEU:CB	2.59	0.50
1:A:577:VAL:HG11	1:A:580:ASP:OD2	2.11	0.50
1:B:228:VAL:HA	1:B:233:GLY:HA3	1.93	0.50
1:B:361:MET:HG2	1:B:441:THR:HA	1.92	0.50
1:B:957:PHE:O	1:B:958:LYS:NZ	2.42	0.50
1:A:338:SER:C	1:A:340:GLU:N	2.67	0.50
1:B:44:GLU:O	1:B:45:GLU:HG3	2.12	0.50
1:B:754:TYR:O	1:B:754:TYR:CD1	2.65	0.50
1:B:810:ASN:HA	1:B:930:ASN:HD22	1.75	0.50
1:B:987:ILE:HG12	1:B:987:ILE:O	2.12	0.50
1:A:777:LEU:O	1:A:780:ALA:N	2.41	0.50
1:A:957:PHE:O	1:A:958:LYS:NZ	2.42	0.50
1:B:61:LEU:HD22	1:B:307:ILE:CD1	2.41	0.50
1:B:69:ALA:O	1:B:73:PHE:HB2	2.12	0.50
1:B:281:ASP:HB2	1:B:282:PRO:CD	2.35	0.50
1:A:71:ILE:HG22	1:A:75:LEU:HD13	1.92	0.50
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.76	0.50
1:A:550:LYS:O	1:A:551:GLU:C	2.54	0.50
1:A:863:PRO:HG2	1:A:890:ILE:CG2	2.42	0.50
1:B:65:LEU:O	1:B:68:ALA:HB3	2.12	0.50
1:B:201:ASN:HB3	1:B:209:PHE:CZ	2.46	0.50
1:B:235:ILE:CD1	1:B:706:ASN:HA	2.42	0.50
1:B:342:LEU:HA	1:B:716:ILE:HD11	1.92	0.50
1:B:593:PHE:HZ	1:B:596:VAL:HG23	1.77	0.50
1:B:795:VAL:HA	1:B:799:THR:OG1	2.12	0.50
1:A:69:ALA:O	1:A:73:PHE:HB2	2.12	0.50
1:A:680:GLU:HB3	1:A:681:PRO:CD	2.39	0.50
1:A:969:MET:O	1:A:973:ILE:HB	2.11	0.50
1:B:25:THR:O	1:B:27:ASP:N	2.44	0.50
1:B:35:LYS:HD3	1:B:35:LYS:C	2.36	0.50
1:A:44:GLU:O	1:A:45:GLU:HG3	2.12	0.50
1:A:235:ILE:CD1	1:A:706:ASN:HA	2.42	0.50
1:A:546:LEU:O	1:A:549:ILE:N	2.45	0.50
1:A:758:LYS:HZ1	1:A:822:ARG:HE	1.59	0.50
1:A:857:MET:C	1:A:859:ALA:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ALA:O	1:B:474:VAL:HG23	2.12	0.50
1:B:546:LEU:O	1:B:549:ILE:N	2.45	0.50
1:B:758:LYS:HG3	1:B:828:LEU:CD2	2.41	0.50
1:B:857:MET:C	1:B:859:ALA:H	2.20	0.50
1:A:320:ALA:O	1:A:323:THR:HB	2.12	0.50
1:A:412:GLU:O	1:A:415:THR:N	2.45	0.50
1:A:500:PRO:HD3	1:A:509:GLY:O	2.12	0.50
1:A:639:ILE:HG13	1:A:641:ILE:HG12	1.93	0.50
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.27	0.50
1:B:320:ALA:O	1:B:323:THR:HB	2.12	0.50
1:B:639:ILE:HG13	1:B:641:ILE:HG12	1.93	0.50
1:B:771:GLU:O	1:B:774:CYS:HB3	2.12	0.50
1:B:791:GLN:O	1:B:792:LEU:C	2.55	0.50
1:B:917:SER:N	1:B:925:MET:HE2	2.27	0.50
1:B:950:VAL:O	1:B:952:PRO:HD2	2.12	0.50
1:A:495:SER:HB3	1:A:588:GLU:OE1	2.10	0.49
1:A:795:VAL:HA	1:A:799:THR:OG1	2.11	0.49
1:B:500:PRO:HD3	1:B:509:GLY:O	2.12	0.49
1:B:874:MET:HG2	1:B:891:PHE:CE2	2.47	0.49
1:B:967:TRP:HZ3	1:B:970:VAL:HG11	1.73	0.49
1:A:278:HIS:HA	1:A:282:PRO:CD	2.42	0.49
1:A:281:ASP:HB2	1:A:282:PRO:CD	2.35	0.49
1:A:442:GLU:O	1:A:445:LEU:N	2.46	0.49
1:A:470:ALA:O	1:A:474:VAL:HG23	2.12	0.49
1:A:518:PRO:HA	1:A:563:ALA:HB2	1.94	0.49
1:A:631:THR:HG22	1:A:635:ILE:HD11	1.93	0.49
1:B:278:HIS:HA	1:B:282:PRO:CD	2.42	0.49
1:B:442:GLU:O	1:B:445:LEU:N	2.46	0.49
1:B:513:PHE:HD1	1:B:566:THR:HG22	1.76	0.49
1:B:631:THR:HG22	1:B:635:ILE:HD11	1.93	0.49
1:B:769:VAL:HG21	2:B:1002:TG1:H332	1.95	0.49
1:A:228:VAL:HA	1:A:233:GLY:HA3	1.93	0.49
1:A:771:GLU:O	1:A:774:CYS:HB3	2.12	0.49
1:A:874:MET:HG2	1:A:891:PHE:CE2	2.47	0.49
1:B:577:VAL:HG11	1:B:580:ASP:OD2	2.11	0.49
1:A:370:ASP:HB2	1:A:379:LEU:O	2.11	0.49
1:A:416:ILE:O	1:A:417:CYS:C	2.56	0.49
1:A:734:VAL:HG12	1:A:734:VAL:O	2.13	0.49
1:B:926:PRO:HB3	1:B:928:TRP:CE2	2.46	0.49
1:A:25:THR:C	1:A:27:ASP:N	2.70	0.49
1:A:95:LEU:O	1:A:99:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:O	1:A:549:ILE:HB	2.13	0.49
1:B:82:GLU:CD	1:B:82:GLU:H	2.20	0.49
1:B:147:PRO:HA	1:B:223:VAL:CG1	2.35	0.49
1:B:159:VAL:HG23	1:B:212:THR:O	2.12	0.49
1:B:552:TRP:HB3	1:B:559:LEU:HD12	1.94	0.49
1:A:65:LEU:O	1:A:68:ALA:HB3	2.12	0.49
1:A:527:TYR:HD1	1:A:536:PRO:HA	1.77	0.49
1:A:593:PHE:HZ	1:A:596:VAL:HG23	1.77	0.49
1:B:836:ARG:HG2	1:B:836:ARG:HH11	1.77	0.49
1:A:154:ALA:CB	1:A:218:LYS:HB2	2.43	0.49
1:A:159:VAL:HG23	1:A:212:THR:O	2.12	0.49
1:A:444:ALA:HB3	1:A:599:MET:CE	2.43	0.49
1:A:680:GLU:HB2	1:A:683:HIS:CE1	2.48	0.49
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.95	0.49
1:B:653:TYR:O	1:B:676:PHE:HA	2.13	0.49
1:A:324:ARG:C	1:A:324:ARG:CD	2.85	0.49
1:A:690:TYR:C	1:A:692:GLN:H	2.21	0.49
1:A:952:PRO:O	1:A:955:MET:HB3	2.13	0.49
1:B:680:GLU:HB2	1:B:683:HIS:CE1	2.48	0.49
1:B:690:TYR:C	1:B:692:GLN:N	2.69	0.49
1:B:863:PRO:HG2	1:B:890:ILE:CG2	2.42	0.49
1:B:974:SER:C	1:B:976:PRO:HD2	2.38	0.49
1:A:82:GLU:H	1:A:82:GLU:CD	2.20	0.49
1:B:869:GLN:HB3	1:B:872:HIS:CD2	2.48	0.49
1:B:129:VAL:HG21	1:B:140:ILE:HD13	1.94	0.49
1:B:416:ILE:O	1:B:417:CYS:C	2.56	0.49
1:A:290:ARG:C	1:A:292:ALA:H	2.20	0.48
1:A:791:GLN:O	1:A:792:LEU:C	2.55	0.48
1:B:154:ALA:CB	1:B:218:LYS:HB2	2.43	0.48
1:B:444:ALA:HB3	1:B:599:MET:CE	2.43	0.48
1:B:527:TYR:HD1	1:B:536:PRO:HA	1.77	0.48
1:B:546:LEU:O	1:B:549:ILE:HB	2.13	0.48
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.27	0.48
1:A:232:ILE:N	1:A:232:ILE:CD1	2.72	0.48
1:A:366:MET:CE	1:A:448:LEU:HD11	2.43	0.48
1:A:765:ILE:HD13	2:A:1001:TG1:H292	1.95	0.48
1:B:317:THR:O	1:B:321:LEU:HG	2.13	0.48
1:B:518:PRO:HA	1:B:563:ALA:HB2	1.94	0.48
1:A:950:VAL:O	1:A:952:PRO:HD2	2.12	0.48
1:B:23:GLY:O	1:B:132:ALA:HB2	2.14	0.48
1:B:95:LEU:O	1:B:99:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:HB3	1:B:356:LEU:HD11	1.96	0.48
1:B:412:GLU:O	1:B:415:THR:N	2.45	0.48
1:B:777:LEU:O	1:B:778:THR:C	2.56	0.48
1:B:952:PRO:O	1:B:955:MET:HB3	2.12	0.48
1:A:433:VAL:HG13	1:A:435:GLU:OE2	2.14	0.48
1:A:774:CYS:HA	1:A:845:GLY:O	2.13	0.48
1:B:628:ASN:ND2	1:B:631:THR:N	2.60	0.48
1:B:775:ILE:O	1:B:775:ILE:HG22	2.13	0.48
1:B:777:LEU:HB2	1:B:849:VAL:HG21	1.95	0.48
1:A:317:THR:O	1:A:321:LEU:HG	2.13	0.48
1:A:481:LYS:HE2	1:A:496:VAL:HG21	1.96	0.48
1:A:836:ARG:HG2	1:A:836:ARG:NH1	2.29	0.48
1:A:959:LEU:HG	1:A:960:LYS:N	2.28	0.48
1:B:342:LEU:O	1:B:345:THR:OG1	2.24	0.48
1:A:311:LEU:N	1:A:312:PRO:CD	2.76	0.48
1:A:552:TRP:HB3	1:A:559:LEU:HD12	1.94	0.48
1:A:653:TYR:O	1:A:676:PHE:HA	2.13	0.48
1:A:769:VAL:HG21	2:A:1001:TG1:H332	1.95	0.48
1:A:974:SER:C	1:A:976:PRO:HD2	2.38	0.48
1:B:25:THR:C	1:B:27:ASP:N	2.70	0.48
1:B:366:MET:CE	1:B:448:LEU:HD11	2.43	0.48
1:B:690:TYR:C	1:B:692:GLN:H	2.21	0.48
1:B:959:LEU:HG	1:B:960:LYS:N	2.28	0.48
1:A:129:VAL:HG21	1:A:140:ILE:HD13	1.94	0.48
1:B:137:VAL:HG13	1:B:137:VAL:O	2.13	0.48
1:B:499:SER:CB	1:B:510:ASN:HD21	2.27	0.48
1:A:137:VAL:HG13	1:A:137:VAL:O	2.13	0.48
1:B:93:VAL:O	1:B:94:ILE:C	2.57	0.48
1:B:372:VAL:HG12	1:B:373:ASP:N	2.29	0.48
1:B:433:VAL:HG13	1:B:435:GLU:OE2	2.14	0.48
1:B:481:LYS:HE2	1:B:496:VAL:HG21	1.96	0.48
1:B:774:CYS:HA	1:B:845:GLY:O	2.13	0.48
1:B:925:MET:HE1	1:B:985:LYS:NZ	2.29	0.48
1:A:544:LYS:HE2	1:A:544:LYS:HA	1.96	0.47
1:A:698:THR:HG22	1:A:699:ALA:N	2.29	0.47
1:A:775:ILE:HG22	1:A:775:ILE:O	2.13	0.47
1:A:897:MET:SD	1:A:958:LYS:HD3	2.54	0.47
1:A:427:PHE:HB3	1:A:465:VAL:HG22	1.96	0.47
1:A:925:MET:HE1	1:A:985:LYS:NZ	2.29	0.47
1:B:304:VAL:HG21	1:B:789:PRO:HA	1.96	0.47
1:B:680:GLU:HB3	1:B:681:PRO:CD	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:915:SER:C	1:B:917:SER:N	2.72	0.47
1:A:1:MET:N	1:A:36:TYR:CZ	2.83	0.47
1:A:968:LEU:HD12	1:A:968:LEU:N	2.29	0.47
1:A:427:PHE:CD2	1:A:464:LYS:HB3	2.49	0.47
1:A:777:LEU:C	1:A:779:ALA:N	2.72	0.47
1:A:869:GLN:HB3	1:A:872:HIS:CD2	2.48	0.47
1:A:966:GLN:HA	1:A:966:GLN:NE2	2.29	0.47
1:B:844:VAL:HG11	1:B:907:ILE:HG21	1.96	0.47
1:A:304:VAL:HG21	1:A:789:PRO:HA	1.96	0.47
1:A:350:SER:HB3	1:A:356:LEU:HD11	1.96	0.47
1:A:626:GLY:O	1:A:678:ARG:NE	2.45	0.47
1:A:777:LEU:O	1:A:779:ALA:N	2.48	0.47
1:A:844:VAL:HG11	1:A:907:ILE:HG21	1.96	0.47
1:B:1:MET:N	1:B:36:TYR:CZ	2.83	0.47
1:B:269:VAL:O	1:B:273:LEU:HG	2.14	0.47
1:B:430:THR:HB	1:B:431:LYS:HD2	1.97	0.47
1:B:734:VAL:HG12	1:B:734:VAL:O	2.13	0.47
1:A:206:ASN:OD1	1:A:206:ASN:C	2.58	0.47
1:A:869:GLN:HB3	1:A:872:HIS:HD2	1.80	0.47
1:A:953:LEU:C	1:A:955:MET:H	2.23	0.47
1:B:166:LEU:HG	1:B:221:GLY:HA2	1.97	0.47
1:B:255:GLU:O	1:B:258:GLU:HB2	2.15	0.47
1:B:427:PHE:CD2	1:B:464:LYS:HB3	2.49	0.47
1:B:604:ARG:O	1:B:607:VAL:HG22	2.15	0.47
1:B:836:ARG:HG2	1:B:836:ARG:NH1	2.29	0.47
1:B:946:LEU:O	1:B:953:LEU:HD12	2.15	0.47
1:A:98:LEU:O	1:A:101:ASN:HB3	2.14	0.47
1:A:269:VAL:O	1:A:273:LEU:HG	2.14	0.47
1:A:277:GLY:O	1:A:280:ASN:N	2.48	0.47
1:A:312:PRO:HA	1:A:315:ILE:HG13	1.96	0.47
1:A:428:ASN:O	1:A:432:GLY:HA2	2.15	0.47
1:A:628:ASN:ND2	1:A:631:THR:N	2.60	0.47
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.97	0.47
1:A:956:ILE:HD11	1:A:957:PHE:CZ	2.50	0.47
1:B:427:PHE:HB3	1:B:465:VAL:HG22	1.96	0.47
1:B:544:LYS:HA	1:B:544:LYS:HE2	1.96	0.47
1:B:765:ILE:HD13	2:B:1002:TG1:H292	1.95	0.47
1:B:966:GLN:HA	1:B:966:GLN:NE2	2.29	0.47
1:A:255:GLU:O	1:A:258:GLU:HB2	2.15	0.47
1:A:365:LYS:HB2	1:A:552:TRP:CZ3	2.50	0.47
1:A:372:VAL:HG12	1:A:373:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PHE:O	1:A:96:LEU:HB2	2.15	0.47
1:A:915:SER:C	1:A:917:SER:N	2.72	0.47
1:B:98:LEU:O	1:B:101:ASN:HB3	2.14	0.47
1:B:192:GLU:CG	1:B:193:PRO:HD2	2.45	0.47
1:B:278:HIS:HA	1:B:282:PRO:CG	2.44	0.47
1:B:311:LEU:N	1:B:312:PRO:CD	2.77	0.47
1:B:347:VAL:HG12	1:B:348:ILE:N	2.30	0.47
1:B:719:ALA:O	1:B:734:VAL:HA	2.15	0.47
1:B:968:LEU:HD12	1:B:968:LEU:N	2.29	0.47
1:A:23:GLY:O	1:A:132:ALA:HB2	2.14	0.47
1:A:946:LEU:O	1:A:953:LEU:HD12	2.15	0.47
1:B:92:PHE:O	1:B:96:LEU:HB2	2.15	0.47
1:B:365:LYS:HB2	1:B:552:TRP:CZ3	2.50	0.47
1:B:620:ARG:HH22	1:B:671:ARG:HA	1.80	0.47
1:B:628:ASN:N	1:B:628:ASN:HD22	2.13	0.47
1:B:835:PHE:O	1:B:838:MET:HB3	2.15	0.47
1:A:93:VAL:O	1:A:94:ILE:C	2.57	0.46
1:A:308:PRO:HA	1:A:768:ASN:HD21	1.80	0.46
1:A:499:SER:CB	1:A:510:ASN:HD21	2.27	0.46
1:A:620:ARG:HH22	1:A:671:ARG:HA	1.80	0.46
1:A:869:GLN:O	1:A:872:HIS:HB2	2.15	0.46
1:B:130:TYR:HB2	1:B:150:ILE:CG1	2.44	0.46
1:B:308:PRO:HA	1:B:768:ASN:HD21	1.80	0.46
1:B:338:SER:C	1:B:340:GLU:H	2.23	0.46
1:B:428:ASN:O	1:B:432:GLY:HA2	2.15	0.46
1:B:777:LEU:O	1:B:779:ALA:N	2.48	0.46
1:B:897:MET:SD	1:B:958:LYS:HD3	2.54	0.46
1:B:925:MET:SD	1:B:925:MET:O	2.73	0.46
1:B:956:ILE:HD11	1:B:957:PHE:CZ	2.50	0.46
1:A:352:LYS:HE3	1:A:635:ILE:HD13	1.97	0.46
1:A:604:ARG:O	1:A:607:VAL:HG22	2.15	0.46
1:A:737:ASP:C	1:A:739:ASN:N	2.73	0.46
1:A:835:PHE:O	1:A:838:MET:HB3	2.15	0.46
1:B:312:PRO:HA	1:B:315:ILE:HG13	1.96	0.46
1:B:324:ARG:C	1:B:324:ARG:CD	2.85	0.46
1:B:425:LEU:HD13	1:B:446:THR:HG21	1.96	0.46
1:A:119:LEU:HD12	1:A:232:ILE:CG2	2.46	0.46
1:A:514:VAL:HG21	1:A:591:LEU:HD22	1.97	0.46
1:A:868:HIS:O	1:A:869:GLN:CB	2.64	0.46
1:B:508:VAL:HG12	1:B:509:GLY:N	2.30	0.46
1:B:462:LEU:HB3	1:B:466:GLU:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:GLN:HB3	1:B:872:HIS:HD2	1.80	0.46
1:B:895:GLU:N	1:B:896:PRO:CD	2.78	0.46
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.97	0.46
1:A:168:ILE:HA	1:A:219:ALA:CB	2.46	0.46
1:A:192:GLU:CG	1:A:193:PRO:HD2	2.45	0.46
1:A:278:HIS:HA	1:A:282:PRO:CG	2.44	0.46
1:A:462:LEU:HB3	1:A:466:GLU:CB	2.46	0.46
1:A:508:VAL:HG12	1:A:509:GLY:N	2.30	0.46
1:A:925:MET:SD	1:A:925:MET:O	2.73	0.46
1:B:119:LEU:HD12	1:B:232:ILE:CG2	2.46	0.46
1:B:206:ASN:OD1	1:B:206:ASN:C	2.58	0.46
1:B:626:GLY:O	1:B:678:ARG:NE	2.45	0.46
1:A:719:ALA:O	1:A:734:VAL:HA	2.15	0.46
1:A:810:ASN:ND2	1:A:916:LEU:HA	2.30	0.46
1:B:154:ALA:O	1:B:214:ILE:HB	2.16	0.46
1:B:168:ILE:HA	1:B:219:ALA:CB	2.46	0.46
1:B:499:SER:CB	1:B:500:PRO:HD2	2.44	0.46
1:B:580:ASP:O	1:B:583:ARG:N	2.45	0.46
1:A:408:ASP:HB2	1:A:531:GLY:HA2	1.97	0.46
1:A:425:LEU:HD13	1:A:446:THR:HG21	1.96	0.46
1:A:628:ASN:N	1:A:628:ASN:HD22	2.13	0.46
1:A:924:ARG:O	1:A:926:PRO:HD3	2.16	0.46
1:B:90:GLU:OE1	1:B:789:PRO:HG3	2.16	0.46
1:B:810:ASN:ND2	1:B:916:LEU:HA	2.30	0.46
1:A:154:ALA:O	1:A:214:ILE:HB	2.16	0.46
1:A:166:LEU:HG	1:A:221:GLY:HA2	1.97	0.46
1:A:430:THR:HB	1:A:431:LYS:HD2	1.97	0.46
1:B:234:LYS:O	1:B:238:GLN:HG3	2.16	0.46
1:B:408:ASP:HB2	1:B:531:GLY:HA2	1.97	0.46
1:B:441:THR:O	1:B:441:THR:HG22	2.16	0.46
1:B:754:TYR:OH	1:B:828:LEU:HD21	2.16	0.46
1:B:957:PHE:O	1:B:958:LYS:CE	2.64	0.46
1:A:234:LYS:O	1:A:238:GLN:HG3	2.16	0.46
1:A:338:SER:C	1:A:340:GLU:H	2.23	0.46
1:A:777:LEU:O	1:A:778:THR:C	2.56	0.46
1:A:453:ASN:CG	1:A:471:CYS:SG	2.99	0.46
1:A:227:GLY:C	1:A:229:SER:H	2.24	0.45
1:A:654:THR:HA	1:A:677:ALA:O	2.17	0.45
1:B:43:ALA:HB2	1:B:120:LYS:NZ	2.31	0.45
1:B:347:VAL:HG13	1:B:620:ARG:HB3	1.98	0.45
1:B:514:VAL:HG21	1:B:591:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:LEU:C	1:B:955:MET:H	2.23	0.45
1:A:174:ARG:HD3	1:A:186:SER:OG	2.16	0.45
1:A:347:VAL:HG12	1:A:348:ILE:N	2.30	0.45
1:B:212:THR:HG22	1:B:213:ASN:N	2.31	0.45
1:B:277:GLY:O	1:B:280:ASN:N	2.48	0.45
1:B:278:HIS:CA	1:B:282:PRO:HD2	2.45	0.45
1:B:698:THR:HG22	1:B:699:ALA:N	2.29	0.45
1:B:720:MET:HE3	1:B:738:ASP:CB	2.43	0.45
1:B:777:LEU:C	1:B:779:ALA:N	2.72	0.45
1:A:100:ALA:HA	1:A:103:ILE:CD1	2.40	0.45
1:A:146:VAL:HG23	1:A:147:PRO:O	2.17	0.45
1:A:441:THR:O	1:A:441:THR:HG22	2.16	0.45
1:A:690:TYR:C	1:A:692:GLN:N	2.69	0.45
1:A:754:TYR:OH	1:A:828:LEU:HD21	2.16	0.45
1:B:175:VAL:HG12	1:B:213:ASN:O	2.16	0.45
1:B:516:GLY:O	1:B:563:ALA:N	2.49	0.45
1:B:533:THR:HG22	1:B:534:ARG:N	2.31	0.45
1:B:737:ASP:C	1:B:739:ASN:N	2.73	0.45
1:B:816:ILE:CG2	1:B:817:MET:N	2.79	0.45
1:B:868:HIS:O	1:B:869:GLN:CB	2.64	0.45
1:B:869:GLN:O	1:B:872:HIS:HB2	2.15	0.45
1:B:924:ARG:O	1:B:926:PRO:HD3	2.16	0.45
1:A:43:ALA:HB2	1:A:120:LYS:NZ	2.31	0.45
1:A:459:VAL:C	1:A:461:ASN:H	2.24	0.45
1:A:890:ILE:H	1:A:890:ILE:CD1	2.24	0.45
1:B:146:VAL:HG23	1:B:147:PRO:O	2.17	0.45
1:B:174:ARG:HD3	1:B:186:SER:OG	2.16	0.45
1:B:246:LYS:O	1:B:247:THR:C	2.60	0.45
1:B:393:GLY:O	1:B:394:GLU:HG3	2.17	0.45
1:B:628:ASN:ND2	1:B:628:ASN:O	2.49	0.45
1:A:533:THR:HG22	1:A:534:ARG:N	2.31	0.45
1:A:551:GLU:O	1:A:555:GLY:N	2.44	0.45
1:A:697:ILE:HA	1:A:715:GLU:HG2	1.99	0.45
1:A:957:PHE:O	1:A:958:LYS:CE	2.64	0.45
1:A:968:LEU:H	1:A:968:LEU:CD1	2.29	0.45
1:B:281:ASP:O	1:B:282:PRO:C	2.60	0.45
1:B:679:VAL:HG13	1:B:679:VAL:O	2.16	0.45
1:A:347:VAL:HG13	1:A:620:ARG:HB3	1.98	0.45
1:A:628:ASN:ND2	1:A:628:ASN:O	2.49	0.45
1:A:873:PHE:HD1	1:A:875:GLN:N	2.12	0.45
1:B:475:ILE:HA	1:B:478:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ASP:O	1:B:582:SER:N	2.50	0.45
1:B:697:ILE:HA	1:B:715:GLU:HG2	1.99	0.45
1:B:968:LEU:H	1:B:968:LEU:CD1	2.29	0.45
1:A:175:VAL:HG12	1:A:213:ASN:O	2.16	0.45
1:A:428:ASN:HB2	1:A:435:GLU:HG3	1.99	0.45
1:A:580:ASP:O	1:A:582:SER:N	2.50	0.45
1:A:737:ASP:C	1:A:739:ASN:H	2.25	0.45
1:A:25:THR:O	1:A:26:PRO:C	2.60	0.45
1:A:90:GLU:OE1	1:A:789:PRO:HG3	2.16	0.45
1:A:246:LYS:HB3	1:A:250:GLN:HE21	1.82	0.45
1:A:816:ILE:CG2	1:A:817:MET:N	2.80	0.45
1:B:352:LYS:HE3	1:B:635:ILE:HD13	1.97	0.45
1:B:447:THR:O	1:B:451:LYS:HG3	2.17	0.45
1:B:654:THR:HA	1:B:677:ALA:O	2.17	0.45
1:A:212:THR:HG22	1:A:213:ASN:N	2.31	0.45
1:A:246:LYS:O	1:A:247:THR:C	2.60	0.45
1:A:393:GLY:O	1:A:394:GLU:HG3	2.17	0.45
1:A:419:LEU:CD1	1:A:479:MET:HB2	2.46	0.45
1:A:576:MET:HE3	1:A:587:TYR:HB3	1.99	0.45
1:A:679:VAL:O	1:A:679:VAL:HG13	2.16	0.45
1:A:791:GLN:HE22	1:A:897:MET:HB3	1.82	0.45
1:B:419:LEU:CD1	1:B:479:MET:HB2	2.46	0.45
1:B:453:ASN:CG	1:B:471:CYS:SG	2.99	0.45
1:A:179:ILE:HD13	1:A:211:GLY:O	2.18	0.45
1:A:380:ASN:OD1	1:A:382:PHE:CE1	2.69	0.45
1:B:52:LEU:HD11	1:B:109:GLU:HG3	1.99	0.45
1:B:61:LEU:HD22	1:B:307:ILE:HD12	1.99	0.45
1:B:227:GLY:C	1:B:229:SER:H	2.24	0.45
1:B:236:ARG:NH1	1:B:237:ASP:OD2	2.50	0.45
1:B:380:ASN:OD1	1:B:382:PHE:CE1	2.69	0.45
1:B:408:ASP:HB2	1:B:531:GLY:CA	2.47	0.45
1:B:791:GLN:HE22	1:B:897:MET:HB3	1.82	0.45
1:A:178:SER:O	1:A:179:ILE:C	2.59	0.44
1:A:369:ILE:HD13	1:A:379:LEU:HD22	1.98	0.44
1:A:419:LEU:HD11	1:A:479:MET:HB2	1.98	0.44
1:A:546:LEU:O	1:A:547:SER:C	2.59	0.44
1:B:419:LEU:HD11	1:B:479:MET:HB2	1.98	0.44
1:B:546:LEU:O	1:B:547:SER:C	2.59	0.44
1:A:168:ILE:HA	1:A:219:ALA:HB2	1.99	0.44
1:A:281:ASP:O	1:A:282:PRO:C	2.60	0.44
1:A:447:THR:O	1:A:451:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:SER:O	1:B:179:ILE:C	2.59	0.44
1:B:428:ASN:HB2	1:B:435:GLU:HG3	1.99	0.44
1:B:488:SER:C	1:B:490:ASP:N	2.74	0.44
1:A:421:ASN:HD21	1:A:442:GLU:HB3	1.82	0.44
1:A:499:SER:CB	1:A:500:PRO:HD2	2.44	0.44
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.53	0.44
1:A:925:MET:HE1	1:A:985:LYS:HZ1	1.81	0.44
1:A:475:ILE:HA	1:A:478:LEU:HD13	1.99	0.44
1:A:691:LEU:O	1:A:696:GLU:HB2	2.17	0.44
1:A:948:LEU:C	1:A:954:PRO:HB3	2.42	0.44
1:B:576:MET:HE3	1:B:587:TYR:HB3	1.99	0.44
1:B:628:ASN:HD21	1:B:631:THR:HB	1.83	0.44
1:B:671:ARG:HD2	1:B:694:TYR:CE1	2.53	0.44
1:B:737:ASP:C	1:B:739:ASN:H	2.25	0.44
1:B:833:LEU:CG	1:B:837:TYR:HE2	2.30	0.44
1:A:61:LEU:HD21	1:A:257:GLY:HA2	1.99	0.44
1:A:981:ASP:O	1:A:984:LEU:N	2.51	0.44
1:B:667:ARG:HB2	1:B:690:TYR:CE1	2.53	0.44
1:A:134:ARG:HB3	1:A:135:LYS:H	1.72	0.44
1:B:451:LYS:O	1:B:452:MET:C	2.61	0.44
1:B:926:PRO:HA	1:B:927:PRO:HD3	1.93	0.44
1:A:332:ILE:O	1:A:733:MET:HA	2.18	0.44
1:A:413:LEU:HD13	1:A:413:LEU:C	2.43	0.44
1:A:516:GLY:O	1:A:563:ALA:N	2.49	0.44
1:A:865:VAL:O	1:A:868:HIS:CB	2.66	0.44
1:A:895:GLU:N	1:A:896:PRO:CD	2.78	0.44
1:B:179:ILE:HD13	1:B:211:GLY:O	2.17	0.44
1:B:246:LYS:HB3	1:B:250:GLN:HE21	1.82	0.44
1:B:670:CYS:O	1:B:691:LEU:HD11	2.18	0.44
1:B:865:VAL:O	1:B:868:HIS:CB	2.66	0.44
1:A:52:LEU:HD11	1:A:109:GLU:HG3	1.99	0.44
1:A:260:LEU:CD1	2:A:1001:TG1:H252	2.47	0.44
1:A:488:SER:C	1:A:490:ASP:H	2.26	0.44
1:A:650:ASP:OD2	1:A:651:ARG:HG2	2.18	0.44
1:A:833:LEU:CG	1:A:837:TYR:HE2	2.30	0.44
1:B:6:SER:OG	1:B:197:PRO:HA	2.18	0.44
1:B:948:LEU:C	1:B:954:PRO:HB3	2.42	0.44
1:B:39:ASN:CG	1:B:226:THR:HB	2.43	0.44
1:B:739:ASN:O	1:B:740:PHE:C	2.61	0.44
1:A:629:LYS:HB2	1:A:654:THR:CG2	2.48	0.43
1:B:260:LEU:CD1	2:B:1002:TG1:H252	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ILE:HD11	1:B:410:LEU:HG	2.00	0.43
1:B:459:VAL:C	1:B:461:ASN:H	2.24	0.43
1:B:524:ARG:HB2	1:B:591:LEU:HD12	2.00	0.43
1:B:551:GLU:O	1:B:555:GLY:N	2.44	0.43
1:A:6:SER:OG	1:A:197:PRO:HA	2.18	0.43
1:A:165:ILE:HD11	1:A:208:LEU:HD21	2.00	0.43
1:A:408:ASP:HB2	1:A:531:GLY:CA	2.47	0.43
1:B:421:ASN:HD21	1:B:442:GLU:HB3	1.82	0.43
1:A:122:TYR:HE1	1:A:726:VAL:HG13	1.83	0.43
1:A:758:LYS:HG3	1:A:828:LEU:CD2	2.41	0.43
1:B:165:ILE:HD11	1:B:208:LEU:HD21	2.00	0.43
1:B:873:PHE:HD1	1:B:875:GLN:N	2.12	0.43
1:A:235:ILE:HD13	1:A:705:VAL:O	2.19	0.43
1:A:935:GLY:O	1:A:936:SER:C	2.62	0.43
1:B:413:LEU:HD13	1:B:413:LEU:C	2.43	0.43
1:B:953:LEU:C	1:B:955:MET:N	2.75	0.43
1:B:981:ASP:O	1:B:982:GLU:C	2.61	0.43
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.99	0.43
1:A:689:GLU:CD	1:A:713:LYS:HZ3	2.26	0.43
1:A:981:ASP:O	1:A:982:GLU:C	2.61	0.43
1:B:168:ILE:HA	1:B:219:ALA:HB2	1.99	0.43
1:B:342:LEU:CD1	1:B:716:ILE:HD13	2.48	0.43
1:B:791:GLN:H	1:B:791:GLN:HG3	1.61	0.43
1:B:915:SER:O	1:B:917:SER:N	2.51	0.43
1:A:382:PHE:HD2	1:A:395:VAL:HG12	1.83	0.43
1:A:743:ILE:O	1:A:747:VAL:HG23	2.19	0.43
1:B:38:HIS:CE1	1:B:143:ARG:HH12	2.37	0.43
1:B:61:LEU:HD21	1:B:257:GLY:HA2	1.99	0.43
1:B:369:ILE:HD13	1:B:379:LEU:HD22	1.98	0.43
1:B:691:LEU:O	1:B:696:GLU:HB2	2.17	0.43
1:A:38:HIS:CD2	1:A:143:ARG:NH2	2.87	0.43
1:A:247:THR:HG22	1:A:250:GLN:N	2.13	0.43
1:A:368:ILE:HD11	1:A:410:LEU:HG	2.00	0.43
1:A:596:VAL:CG1	1:A:597:VAL:N	2.82	0.43
1:A:628:ASN:HD21	1:A:631:THR:HB	1.83	0.43
1:A:667:ARG:HB2	1:A:690:TYR:CE1	2.53	0.43
1:A:670:CYS:O	1:A:691:LEU:HD11	2.18	0.43
1:B:25:THR:O	1:B:26:PRO:C	2.60	0.43
1:B:928:TRP:HA	1:B:934:LEU:HD12	2.00	0.43
1:B:981:ASP:O	1:B:984:LEU:N	2.51	0.43
1:A:510:ASN:HD22	1:A:510:ASN:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ASN:O	1:A:740:PHE:C	2.61	0.43
1:A:913:LEU:HD21	1:A:937:ILE:CD1	2.49	0.43
1:A:915:SER:O	1:A:917:SER:N	2.51	0.43
1:B:2:GLU:O	1:B:2:GLU:HG2	2.18	0.43
1:B:806:ALA:HA	1:B:809:PHE:CD2	2.54	0.43
1:A:39:ASN:CG	1:A:226:THR:HB	2.43	0.43
1:A:338:SER:O	1:A:340:GLU:N	2.52	0.43
1:A:486:GLU:H	1:A:486:GLU:HG3	1.55	0.43
1:A:488:SER:C	1:A:490:ASP:N	2.74	0.43
1:A:948:LEU:O	1:A:954:PRO:HB3	2.19	0.43
1:B:380:ASN:O	1:B:382:PHE:CD1	2.72	0.43
1:A:390:ALA:C	1:A:392:GLU:H	2.27	0.43
1:B:6:SER:HA	1:B:194:VAL:O	2.19	0.43
1:B:263:VAL:O	1:B:266:LEU:N	2.50	0.43
1:B:332:ILE:O	1:B:733:MET:HA	2.18	0.43
1:B:519:GLU:O	1:B:523:ASP:HB2	2.19	0.43
1:A:58:GLU:HG2	1:A:63:ARG:NH2	2.34	0.42
1:A:519:GLU:O	1:A:523:ASP:HB2	2.19	0.42
1:A:524:ARG:HB2	1:A:591:LEU:HD12	2.01	0.42
1:A:547:SER:O	1:A:550:LYS:N	2.52	0.42
1:B:122:TYR:HE1	1:B:726:VAL:HG13	1.83	0.42
1:B:390:ALA:C	1:B:392:GLU:H	2.27	0.42
1:B:398:ASN:C	1:B:400:LYS:H	2.27	0.42
1:B:959:LEU:HG	1:B:960:LYS:H	1.84	0.42
1:A:757:MET:HA	1:A:760:PHE:CD2	2.54	0.42
1:B:38:HIS:CD2	1:B:143:ARG:NH2	2.86	0.42
1:B:39:ASN:CB	1:B:226:THR:HB	2.50	0.42
1:B:58:GLU:HG2	1:B:63:ARG:NH2	2.34	0.42
1:B:450:GLU:OE2	1:B:467:ARG:O	2.37	0.42
1:B:562:LEU:HD12	1:B:562:LEU:HA	1.88	0.42
1:B:948:LEU:O	1:B:954:PRO:HB3	2.19	0.42
1:A:170:SER:HB3	1:A:218:LYS:H	1.84	0.42
1:A:290:ARG:C	1:A:292:ALA:N	2.77	0.42
1:A:788:ILE:O	1:A:789:PRO:C	2.62	0.42
1:B:165:ILE:HD11	1:B:208:LEU:CD2	2.49	0.42
1:B:382:PHE:HD2	1:B:395:VAL:HG12	1.83	0.42
1:B:547:SER:O	1:B:550:LYS:N	2.52	0.42
1:B:650:ASP:OD2	1:B:651:ARG:HG2	2.18	0.42
1:B:691:LEU:HD12	1:B:691:LEU:HA	1.79	0.42
1:A:165:ILE:HD11	1:A:208:LEU:CD2	2.49	0.42
1:A:256:PHE:HE2	1:A:308:PRO:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:LEU:C	1:A:783:LEU:H	2.28	0.42
1:B:102:ALA:O	1:B:103:ILE:C	2.63	0.42
1:B:495:SER:OG	1:B:588:GLU:OE1	2.37	0.42
1:B:657:GLU:HA	1:B:660:ASP:OD2	2.20	0.42
1:B:687:ILE:HG22	1:B:691:LEU:HD22	2.00	0.42
1:A:6:SER:HA	1:A:194:VAL:O	2.19	0.42
1:A:38:HIS:CE1	1:A:143:ARG:HH12	2.37	0.42
1:A:312:PRO:HA	1:A:315:ILE:CG1	2.50	0.42
1:A:483:PHE:CE2	1:A:485:LEU:HD21	2.48	0.42
1:A:535:VAL:CB	1:A:536:PRO:HD2	2.47	0.42
1:A:900:ALA:O	1:A:903:VAL:HB	2.20	0.42
1:A:959:LEU:HG	1:A:960:LYS:H	1.84	0.42
1:B:44:GLU:CD	1:B:46:GLY:H	2.27	0.42
1:B:900:ALA:O	1:B:903:VAL:HB	2.20	0.42
1:A:380:ASN:O	1:A:382:PHE:CD1	2.72	0.42
1:A:450:GLU:OE2	1:A:467:ARG:O	2.37	0.42
1:A:491:ARG:O	1:A:492:LYS:C	2.62	0.42
1:A:547:SER:O	1:A:550:LYS:HB3	2.20	0.42
1:A:735:LEU:HB3	1:A:742:THR:HG21	2.02	0.42
1:A:806:ALA:HA	1:A:809:PHE:CD2	2.54	0.42
1:B:235:ILE:HD13	1:B:705:VAL:O	2.19	0.42
1:B:256:PHE:HE2	1:B:308:PRO:HG3	1.84	0.42
1:B:290:ARG:C	1:B:292:ALA:N	2.77	0.42
1:B:312:PRO:HA	1:B:315:ILE:CG1	2.50	0.42
1:B:488:SER:C	1:B:490:ASP:H	2.26	0.42
1:B:544:LYS:O	1:B:544:LYS:HD3	2.19	0.42
1:B:580:ASP:C	1:B:582:SER:N	2.78	0.42
1:B:653:TYR:CZ	1:B:669:ALA:HB1	2.55	0.42
1:B:743:ILE:O	1:B:747:VAL:HG23	2.19	0.42
1:B:875:GLN:C	1:B:877:THR:H	2.28	0.42
1:A:39:ASN:CB	1:A:226:THR:HB	2.50	0.42
1:A:519:GLU:HG2	1:A:520:GLY:H	1.84	0.42
1:A:928:TRP:HA	1:A:934:LEU:HD12	2.00	0.42
1:B:385:THR:O	1:B:393:GLY:HA3	2.20	0.42
1:B:491:ARG:O	1:B:492:LYS:C	2.62	0.42
1:B:596:VAL:CG1	1:B:597:VAL:N	2.82	0.42
1:B:705:VAL:HG23	1:B:706:ASN:N	2.35	0.42
1:B:874:MET:HE3	1:B:891:PHE:HD2	1.85	0.42
1:B:966:GLN:HA	1:B:966:GLN:HE21	1.85	0.42
1:A:44:GLU:CD	1:A:46:GLY:H	2.27	0.42
1:A:159:VAL:CG1	1:A:163:ILE:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LYS:O	1:A:575:GLU:HB2	2.20	0.42
1:A:653:TYR:CZ	1:A:669:ALA:HB1	2.55	0.42
1:A:705:VAL:HG23	1:A:706:ASN:N	2.35	0.42
1:A:865:VAL:O	1:A:868:HIS:HB2	2.19	0.42
1:A:977:VAL:CG1	1:A:978:ILE:N	2.83	0.42
1:A:981:ASP:HB3	1:A:982:GLU:H	1.72	0.42
1:B:735:LEU:HB3	1:B:742:THR:HG21	2.02	0.42
1:B:802:LEU:N	1:B:802:LEU:HD22	2.35	0.42
1:B:913:LEU:HD21	1:B:937:ILE:CD1	2.49	0.42
1:B:925:MET:HE1	1:B:985:LYS:HZ1	1.84	0.42
1:B:935:GLY:O	1:B:936:SER:C	2.62	0.42
1:A:278:HIS:CA	1:A:282:PRO:HD2	2.45	0.42
1:A:657:GLU:HA	1:A:660:ASP:OD2	2.20	0.42
1:B:170:SER:HB3	1:B:218:LYS:H	1.84	0.42
1:B:270:ALA:O	1:B:271:VAL:C	2.63	0.42
1:B:382:PHE:CD2	1:B:395:VAL:HG12	2.55	0.42
1:B:629:LYS:HB2	1:B:654:THR:CG2	2.48	0.42
1:B:757:MET:C	1:B:759:GLN:N	2.77	0.42
1:B:894:PRO:HA	1:B:897:MET:HE3	2.02	0.42
1:A:451:LYS:O	1:A:452:MET:C	2.61	0.42
1:A:580:ASP:C	1:A:582:SER:N	2.78	0.42
1:A:593:PHE:CZ	1:A:596:VAL:HG23	2.54	0.42
1:A:802:LEU:N	1:A:802:LEU:HD22	2.35	0.42
1:A:966:GLN:HA	1:A:966:GLN:HE21	1.85	0.42
1:B:589:THR:O	1:B:590:ASP:C	2.62	0.42
1:B:593:PHE:CE1	1:B:595:GLY:N	2.88	0.42
1:A:59:ASP:OD2	1:A:61:LEU:HB2	2.20	0.41
1:A:102:ALA:O	1:A:103:ILE:C	2.63	0.41
1:A:687:ILE:HG22	1:A:691:LEU:HD22	2.00	0.41
1:A:880:HIS:C	1:A:882:HIS:N	2.78	0.41
1:A:544:LYS:O	1:A:544:LYS:HD3	2.19	0.41
1:A:875:GLN:C	1:A:877:THR:H	2.28	0.41
1:B:321:LEU:O	1:B:324:ARG:HG3	2.21	0.41
1:B:757:MET:HA	1:B:760:PHE:CD2	2.54	0.41
1:B:865:VAL:O	1:B:868:HIS:HB2	2.20	0.41
1:B:977:VAL:CG1	1:B:978:ILE:N	2.83	0.41
1:A:130:TYR:HB2	1:A:150:ILE:CG1	2.44	0.41
1:A:270:ALA:O	1:A:271:VAL:C	2.63	0.41
1:A:368:ILE:CD1	1:A:410:LEU:CD2	2.96	0.41
1:A:385:THR:O	1:A:393:GLY:HA3	2.20	0.41
1:A:496:VAL:HG12	1:A:513:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASP:O	1:A:583:ARG:N	2.45	0.41
1:A:874:MET:HE3	1:A:891:PHE:HD2	1.85	0.41
1:A:888:CYS:C	1:A:890:ILE:H	2.28	0.41
1:A:962:LEU:C	1:A:964:LEU:N	2.75	0.41
1:B:59:ASP:OD2	1:B:61:LEU:HB2	2.20	0.41
1:B:496:VAL:HG12	1:B:513:PHE:HB2	2.02	0.41
1:B:746:ALA:O	1:B:747:VAL:C	2.63	0.41
1:A:2:GLU:O	1:A:2:GLU:HG2	2.18	0.41
1:A:382:PHE:CD2	1:A:395:VAL:HG12	2.55	0.41
1:A:388:THR:OG1	1:A:389:TYR:N	2.53	0.41
1:A:628:ASN:ND2	1:A:631:THR:HB	2.35	0.41
1:B:71:ILE:HG23	1:B:296:PHE:HD2	1.85	0.41
1:B:338:SER:O	1:B:340:GLU:N	2.52	0.41
1:B:371:LYS:HE3	1:B:371:LYS:HB2	1.97	0.41
1:B:519:GLU:HG2	1:B:520:GLY:H	1.84	0.41
1:B:880:HIS:N	1:B:881:PRO:CD	2.83	0.41
1:B:916:LEU:C	1:B:925:MET:HE2	2.45	0.41
1:B:336:LEU:HB2	1:B:337:PRO:HD3	2.03	0.41
1:B:499:SER:HB2	1:B:500:PRO:CD	2.48	0.41
1:B:684:LYS:CB	1:B:700:MET:HE3	2.46	0.41
1:B:878:GLU:C	1:B:880:HIS:H	2.28	0.41
1:A:236:ARG:NH1	1:A:237:ASP:OD2	2.50	0.41
1:A:604:ARG:HB3	1:A:607:VAL:CG1	2.40	0.41
1:B:159:VAL:CG1	1:B:163:ILE:HD12	2.50	0.41
1:B:547:SER:O	1:B:550:LYS:HB3	2.20	0.41
1:B:662:PRO:O	1:B:664:ALA:N	2.54	0.41
1:B:981:ASP:OD2	1:B:985:LYS:HD2	2.21	0.41
1:A:349:CYS:HA	1:A:622:ILE:O	2.21	0.41
1:A:593:PHE:CE1	1:A:595:GLY:N	2.88	0.41
1:A:662:PRO:O	1:A:664:ALA:N	2.54	0.41
1:A:894:PRO:HA	1:A:897:MET:HE3	2.02	0.41
1:B:59:ASP:O	1:B:60:LEU:C	2.63	0.41
1:B:174:ARG:HA	1:B:187:VAL:O	2.21	0.41
1:B:396:LEU:HA	1:B:402:ILE:HD12	2.03	0.41
1:B:419:LEU:CD1	1:B:513:PHE:HE2	2.34	0.41
1:B:678:ARG:HH11	1:B:678:ARG:HG3	1.86	0.41
1:B:764:LEU:HA	1:B:764:LEU:HD12	1.75	0.41
1:B:840:ILE:HD13	1:B:980:LEU:CD2	2.51	0.41
1:A:222:ILE:O	1:A:222:ILE:HG23	2.21	0.41
1:A:772:VAL:O	1:A:773:VAL:C	2.63	0.41
1:A:873:PHE:CB	1:A:875:GLN:HE21	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:LEU:C	1:A:955:MET:N	2.75	0.41
1:B:222:ILE:O	1:B:222:ILE:HG23	2.21	0.41
1:B:740:PHE:O	1:B:741:SER:C	2.64	0.41
1:B:880:HIS:C	1:B:882:HIS:N	2.78	0.41
1:A:71:ILE:HG23	1:A:296:PHE:HD2	1.85	0.41
1:A:342:LEU:CD1	1:A:716:ILE:HD13	2.48	0.41
1:A:398:ASN:C	1:A:400:LYS:H	2.27	0.41
1:A:421:ASN:HD21	1:A:442:GLU:C	2.29	0.41
1:A:520:GLY:O	1:A:521:VAL:C	2.64	0.41
1:A:759:GLN:O	1:A:762:ARG:N	2.54	0.41
1:A:816:ILE:HG23	1:A:817:MET:HG2	2.03	0.41
1:A:867:TYR:N	1:A:867:TYR:CD1	2.89	0.41
1:A:950:VAL:O	1:A:952:PRO:CD	2.69	0.41
1:B:65:LEU:O	1:B:69:ALA:N	2.54	0.41
1:B:380:ASN:O	1:B:382:PHE:HD1	2.04	0.41
1:B:400:LYS:HA	1:B:401:PRO:HD2	1.93	0.41
1:B:511:LYS:HA	1:B:511:LYS:HD3	1.97	0.41
1:B:593:PHE:CZ	1:B:596:VAL:HG23	2.55	0.41
1:B:628:ASN:ND2	1:B:631:THR:HB	2.35	0.41
1:B:867:TYR:CD1	1:B:867:TYR:N	2.89	0.41
1:B:888:CYS:C	1:B:890:ILE:H	2.28	0.41
1:B:912:ALA:O	1:B:933:LEU:HD21	2.21	0.41
1:A:480:LYS:O	1:A:498:CYS:HB2	2.21	0.41
1:A:521:VAL:O	1:A:522:ILE:C	2.64	0.41
1:A:562:LEU:HD12	1:A:562:LEU:HA	1.88	0.41
1:A:589:THR:O	1:A:590:ASP:C	2.62	0.41
1:A:916:LEU:C	1:A:925:MET:HE2	2.45	0.41
1:B:154:ALA:HB2	1:B:218:LYS:HG3	2.03	0.41
1:B:349:CYS:HA	1:B:622:ILE:O	2.21	0.41
1:B:453:ASN:ND2	1:B:471:CYS:SG	2.94	0.41
1:B:781:LEU:C	1:B:783:LEU:H	2.28	0.41
1:B:950:VAL:O	1:B:952:PRO:CD	2.69	0.41
1:B:962:LEU:C	1:B:964:LEU:N	2.75	0.41
1:A:91:PRO:HG2	1:A:92:PHE:H	1.86	0.40
1:A:154:ALA:HB2	1:A:218:LYS:HG3	2.03	0.40
1:A:678:ARG:HG3	1:A:678:ARG:HH11	1.86	0.40
1:A:793:LEU:C	1:A:795:VAL:N	2.78	0.40
1:B:873:PHE:CB	1:B:875:GLN:HE21	2.34	0.40
1:A:59:ASP:O	1:A:60:LEU:C	2.63	0.40
1:A:174:ARG:HA	1:A:187:VAL:O	2.21	0.40
1:A:453:ASN:ND2	1:A:471:CYS:SG	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:PHE:O	1:A:741:SER:C	2.64	0.40
1:A:788:ILE:CG2	1:A:789:PRO:HD2	2.38	0.40
1:A:981:ASP:OD2	1:A:985:LYS:HD2	2.21	0.40
1:B:25:THR:C	1:B:27:ASP:H	2.30	0.40
1:B:180:LEU:O	1:B:706:ASN:CG	2.64	0.40
1:B:513:PHE:CD1	1:B:566:THR:HG22	2.56	0.40
1:B:572:LYS:O	1:B:575:GLU:HB2	2.20	0.40
1:A:60:LEU:O	1:A:64:ILE:HG12	2.22	0.40
1:A:875:GLN:C	1:A:877:THR:N	2.78	0.40
1:B:368:ILE:CD1	1:B:410:LEU:CD2	2.96	0.40
1:A:65:LEU:O	1:A:69:ALA:N	2.54	0.40
1:A:350:SER:HA	1:A:701:THR:HG22	2.01	0.40
1:A:350:SER:CA	1:A:701:THR:HG21	2.48	0.40
1:A:428:ASN:HB2	1:A:435:GLU:HG2	2.03	0.40
1:A:622:ILE:CD1	1:A:691:LEU:HD21	2.52	0.40
1:B:303:ALA:C	1:B:305:ALA:N	2.78	0.40
1:B:622:ILE:HG23	1:B:674:CYS:C	2.47	0.40
1:B:737:ASP:O	1:B:739:ASN:N	2.55	0.40
1:A:352:LYS:HA	1:A:356:LEU:HB2	2.04	0.40
1:A:499:SER:HB2	1:A:500:PRO:CD	2.48	0.40
1:A:684:LYS:CB	1:A:700:MET:HE3	2.46	0.40
1:A:764:LEU:HD12	1:A:764:LEU:HA	1.75	0.40
1:A:802:LEU:HD22	1:A:802:LEU:H	1.85	0.40
1:A:840:ILE:HD13	1:A:980:LEU:CD2	2.51	0.40
1:A:893:ALA:C	1:A:896:PRO:HD2	2.46	0.40
1:B:60:LEU:O	1:B:64:ILE:HG12	2.22	0.40
1:B:250:GLN:O	1:B:254:ASP:OD2	2.40	0.40
1:B:273:LEU:HA	1:B:276:ILE:HD11	2.03	0.40
1:B:480:LYS:O	1:B:498:CYS:HB2	2.21	0.40
1:B:635:ILE:HG13	1:B:635:ILE:H	1.70	0.40
1:B:698:THR:CG2	1:B:699:ALA:N	2.85	0.40
1:B:857:MET:O	1:B:859:ALA:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	992/994 (100%)	760 (77%)	185 (19%)	47 (5%)	2	11
1	B	992/994 (100%)	760 (77%)	185 (19%)	47 (5%)	2	11
All	All	1984/1988 (100%)	1520 (77%)	370 (19%)	94 (5%)	2	11

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	782	GLY
1	A	864	GLY
1	A	951	ASP
1	A	965	THR
1	B	782	GLY
1	B	864	GLY
1	B	951	ASP
1	B	965	THR
1	A	94	ILE
1	A	374	GLY
1	A	581	SER
1	A	857	MET
1	A	858	TYR
1	A	883	PHE
1	A	964	LEU
1	A	981	ASP
1	B	94	ILE
1	B	374	GLY
1	B	581	SER
1	B	857	MET
1	B	858	TYR
1	B	883	PHE
1	B	964	LEU
1	B	981	ASP
1	A	280	ASN
1	A	281	ASP
1	A	454	VAL
1	A	467	ARG
1	A	470	ALA
1	A	500	PRO
1	A	519	GLU

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Mol	Chain	Res	Type
1	A	521	VAL
1	A	536	PRO
1	A	540	PRO
1	A	644	GLU
1	A	663	LEU
1	A	795	VAL
1	B	280	ASN
1	B	281	ASP
1	B	454	VAL
1	B	467	ARG
1	B	470	ALA
1	B	500	PRO
1	B	519	GLU
1	B	521	VAL
1	B	536	PRO
1	B	540	PRO
1	B	644	GLU
1	B	663	LEU
1	B	795	VAL
1	A	286	GLY
1	A	507	ALA
1	A	735	LEU
1	A	758	LYS
1	A	916	LEU
1	A	982	GLU
1	B	286	GLY
1	B	507	ALA
1	B	735	LEU
1	B	758	LYS
1	B	916	LEU
1	B	982	GLU
1	A	283	VAL
1	A	352	LYS
1	A	578	LEU
1	A	681	PRO
1	A	869	GLN
1	B	283	VAL
1	B	352	LYS
1	B	578	LEU
1	B	681	PRO
1	B	869	GLN
1	A	669	ALA

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Mol	Chain	Res	Type
1	A	716	ILE
1	A	975	LEU
1	B	669	ALA
1	B	716	ILE
1	B	975	LEU
1	A	17	GLY
1	A	228	VAL
1	A	386	GLY
1	A	952	PRO
1	B	17	GLY
1	B	228	VAL
1	B	386	GLY
1	B	952	PRO
1	A	865	VAL
1	A	950	VAL
1	B	865	VAL
1	B	950	VAL
1	A	185	VAL
1	B	185	VAL
1	A	195	PRO
1	B	195	PRO

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	840/840 (100%)	759 (90%)	81 (10%)	8	30
1	B	840/840 (100%)	759 (90%)	81 (10%)	8	30
All	All	1680/1680 (100%)	1518 (90%)	162 (10%)	8	30

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	34	GLU

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Mol	Chain	Res	Type
1	A	35	LYS
1	A	44	GLU
1	A	45	GLU
1	A	83	GLU
1	A	96	LEU
1	A	113	GLU
1	A	146	VAL
1	A	153	VAL
1	A	155	VAL
1	A	159	VAL
1	A	160	PRO
1	A	175	VAL
1	A	200	VAL
1	A	205	LYS
1	A	218	LYS
1	A	220	LEU
1	A	232	ILE
1	A	242	THR
1	A	245	ASP
1	A	247	THR
1	A	278	HIS
1	A	302	LEU
1	A	365	LYS
1	A	366	MET
1	A	371	LYS
1	A	373	ASP
1	A	381	GLU
1	A	384	ILE
1	A	402	ILE
1	A	411	VAL
1	A	422	ASP
1	A	429	GLU
1	A	449	VAL
1	A	450	GLU
1	A	484	THR
1	A	486	GLU
1	A	491	ARG
1	A	508	VAL
1	A	510	ASN
1	A	512	MET
1	A	518	PRO
1	A	519	GLU

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Mol	Chain	Res	Type
1	A	523	ASP
1	A	538	THR
1	A	544	LYS
1	A	549	ILE
1	A	554	THR
1	A	574	GLU
1	A	578	LEU
1	A	597	VAL
1	A	612	GLN
1	A	621	VAL
1	A	623	MET
1	A	628	ASN
1	A	656	ARG
1	A	691	LEU
1	A	707	ASP
1	A	726	VAL
1	A	732	GLU
1	A	739	ASN
1	A	759	GLN
1	A	764	LEU
1	A	766	SER
1	A	785	GLU
1	A	788	ILE
1	A	793	LEU
1	A	796	ASN
1	A	797	LEU
1	A	814	LEU
1	A	815	ASP
1	A	816	ILE
1	A	857	MET
1	A	883	PHE
1	A	956	ILE
1	A	958	LYS
1	A	972	LYS
1	A	973	ILE
1	A	982	GLU
1	A	986	PHE
1	B	1	MET
1	B	34	GLU
1	B	35	LYS
1	B	44	GLU
1	B	45	GLU

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Mol	Chain	Res	Type
1	B	83	GLU
1	B	96	LEU
1	B	113	GLU
1	B	146	VAL
1	B	153	VAL
1	B	155	VAL
1	B	159	VAL
1	B	160	PRO
1	B	175	VAL
1	B	200	VAL
1	B	205	LYS
1	B	218	LYS
1	B	220	LEU
1	B	232	ILE
1	B	242	THR
1	B	245	ASP
1	B	247	THR
1	B	278	HIS
1	B	302	LEU
1	B	365	LYS
1	B	366	MET
1	B	371	LYS
1	B	373	ASP
1	B	381	GLU
1	B	384	ILE
1	B	402	ILE
1	B	411	VAL
1	B	422	ASP
1	B	429	GLU
1	B	449	VAL
1	B	450	GLU
1	B	484	THR
1	B	486	GLU
1	B	491	ARG
1	B	508	VAL
1	B	510	ASN
1	B	512	MET
1	B	518	PRO
1	B	519	GLU
1	B	523	ASP
1	B	538	THR
1	B	544	LYS

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Mol	Chain	Res	Type
1	B	549	ILE
1	B	554	THR
1	B	574	GLU
1	B	578	LEU
1	B	597	VAL
1	B	612	GLN
1	B	621	VAL
1	B	623	MET
1	B	628	ASN
1	B	656	ARG
1	B	691	LEU
1	B	707	ASP
1	B	726	VAL
1	B	732	GLU
1	B	739	ASN
1	B	759	GLN
1	B	764	LEU
1	B	766	SER
1	B	785	GLU
1	B	788	ILE
1	B	793	LEU
1	B	796	ASN
1	B	797	LEU
1	B	814	LEU
1	B	815	ASP
1	B	816	ILE
1	B	857	MET
1	B	883	PHE
1	B	956	ILE
1	B	958	LYS
1	B	972	LYS
1	B	973	ILE
1	B	982	GLU
1	B	986	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	250	GLN
1	A	275	ASN
1	A	380	ASN

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Mol	Chain	Res	Type
1	A	461	ASN
1	A	510	ASN
1	A	628	ASN
1	A	739	ASN
1	A	768	ASN
1	A	872	HIS
1	A	875	GLN
1	A	914	ASN
1	A	919	ASN
1	A	966	GLN
1	B	38	HIS
1	B	250	GLN
1	B	275	ASN
1	B	380	ASN
1	B	461	ASN
1	B	510	ASN
1	B	628	ASN
1	B	739	ASN
1	B	768	ASN
1	B	872	HIS
1	B	875	GLN
1	B	914	ASN
1	B	919	ASN
1	B	966	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TG1	B	1002	-	44,48,48	1.81	14 (31%)	47,72,72	1.98	11 (23%)
2	TG1	A	1001	-	44,48,48	1.80	14 (31%)	47,72,72	1.98	11 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TG1	B	1002	-	-	9/33/99/99	0/3/3/3
2	TG1	A	1001	-	-	9/33/99/99	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	TG1	O4-C21	5.77	1.33	1.21
2	A	1001	TG1	O4-C21	5.73	1.33	1.21
2	A	1001	TG1	O3-C3	3.36	1.51	1.44
2	B	1002	TG1	O3-C3	3.36	1.51	1.44
2	A	1001	TG1	O6-C7	3.25	1.48	1.43
2	B	1002	TG1	O6-C7	3.25	1.48	1.43
2	A	1001	TG1	O1-C13	3.24	1.43	1.34
2	B	1002	TG1	O1-C13	3.24	1.43	1.34
2	A	1001	TG1	C34-C11	3.22	1.57	1.53
2	B	1002	TG1	C34-C11	3.22	1.57	1.53
2	A	1001	TG1	C11-C7	3.08	1.59	1.55
2	B	1002	TG1	C11-C7	3.08	1.59	1.55
2	A	1001	TG1	O7-C27	2.82	1.42	1.34
2	B	1002	TG1	O7-C27	2.82	1.42	1.34
2	A	1001	TG1	C9-C10	2.55	1.58	1.54
2	B	1002	TG1	C9-C10	2.55	1.58	1.54
2	A	1001	TG1	C21-C22	2.53	1.58	1.50
2	B	1002	TG1	C21-C22	2.53	1.58	1.50
2	A	1001	TG1	C31-C10	2.40	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	TG1	C31-C10	2.40	1.57	1.52
2	B	1002	TG1	C1-C2	2.26	1.58	1.54
2	A	1001	TG1	C1-C2	2.25	1.58	1.54
2	A	1001	TG1	O11-C11	2.21	1.46	1.42
2	B	1002	TG1	O11-C11	2.21	1.46	1.42
2	B	1002	TG1	C9-C8	2.09	1.55	1.52
2	A	1001	TG1	C9-C8	2.09	1.55	1.52
2	A	1001	TG1	C3-C4	2.07	1.53	1.50
2	B	1002	TG1	C3-C4	2.04	1.53	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	TG1	C10-O9-C32	5.77	134.87	121.36
2	B	1002	TG1	C10-O9-C32	5.77	134.87	121.36
2	B	1002	TG1	O12-C12-C11	-4.18	124.05	128.28
2	A	1001	TG1	O12-C12-C11	-4.15	124.08	128.28
2	B	1002	TG1	O7-C8-C9	4.09	113.95	106.63
2	A	1001	TG1	O7-C8-C9	4.08	113.92	106.63
2	A	1001	TG1	O1-C2-C3	-3.89	102.83	110.18
2	B	1002	TG1	O1-C2-C3	-3.89	102.83	110.18
2	A	1001	TG1	C7-C6-C5	3.83	125.46	115.41
2	B	1002	TG1	C7-C6-C5	3.83	125.46	115.41
2	B	1002	TG1	O5-C12-O12	3.40	126.01	121.60
2	A	1001	TG1	O5-C12-O12	3.40	126.00	121.60
2	A	1001	TG1	C24-C22-C21	3.18	132.74	120.79
2	B	1002	TG1	C24-C22-C21	3.18	132.74	120.79
2	B	1002	TG1	C6-O5-C12	-2.98	106.66	110.80
2	A	1001	TG1	C6-O5-C12	-2.97	106.68	110.80
2	A	1001	TG1	C23-C22-C21	-2.66	109.29	116.12
2	B	1002	TG1	C23-C22-C21	-2.66	109.29	116.12
2	A	1001	TG1	C2-O1-C13	-2.49	113.54	117.59
2	B	1002	TG1	C2-O1-C13	-2.49	113.54	117.59
2	A	1001	TG1	O7-C27-O8	2.06	128.53	123.70
2	B	1002	TG1	O7-C27-O8	2.06	128.53	123.70

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	TG1	O3-C21-C22-C23
2	A	1001	TG1	O3-C21-C22-C24

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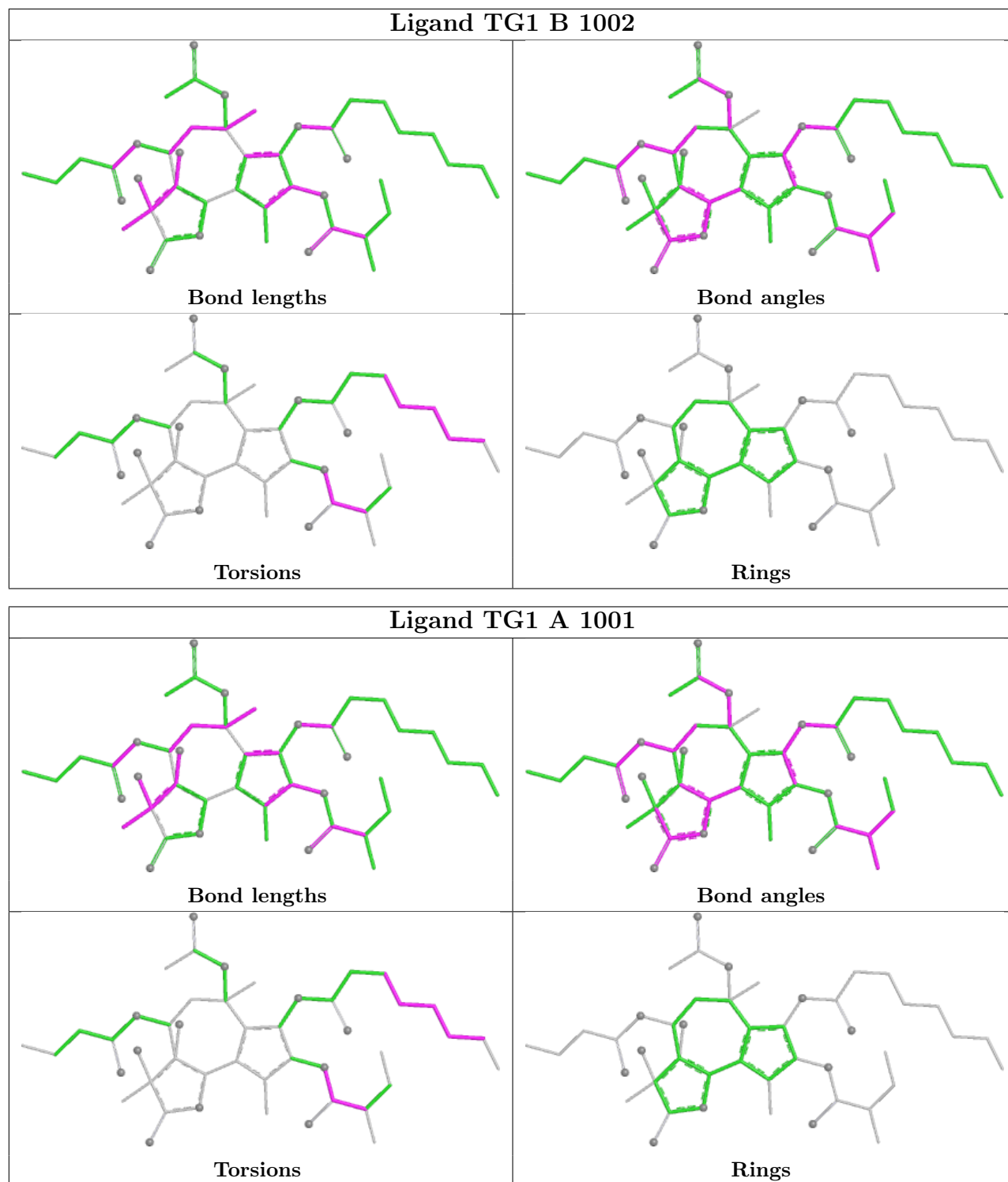
Mol	Chain	Res	Type	Atoms
2	A	1001	TG1	O4-C21-C22-C23
2	B	1002	TG1	O3-C21-C22-C23
2	B	1002	TG1	O3-C21-C22-C24
2	B	1002	TG1	O4-C21-C22-C23
2	A	1001	TG1	O4-C21-C22-C24
2	B	1002	TG1	O4-C21-C22-C24
2	A	1001	TG1	C22-C21-O3-C3
2	B	1002	TG1	C22-C21-O3-C3
2	A	1001	TG1	C15-C16-C17-C18
2	B	1002	TG1	C15-C16-C17-C18
2	A	1001	TG1	C16-C17-C18-C19
2	B	1002	TG1	C16-C17-C18-C19
2	A	1001	TG1	C14-C15-C16-C17
2	B	1002	TG1	C14-C15-C16-C17
2	A	1001	TG1	C17-C18-C19-C20
2	B	1002	TG1	C17-C18-C19-C20

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	TG1	5	0
2	A	1001	TG1	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.