



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 29, 2020 – 10:10 PM EST

PDB ID : 7K17  
Title : Re-refined crystal structure of DNA-dependent protein kinase catalytic subunit complexed with Ku80 C-terminal helix  
Authors : Chen, X.; Gellert, M.; Yang, W.  
Deposited on : 2020-09-07  
Resolution : 4.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.16  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.16

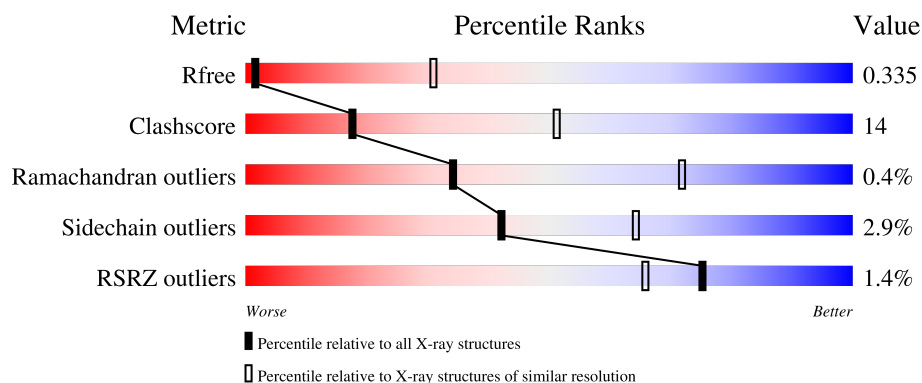
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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  $\geq 3$ , 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	3986	<div> <div></div> <div>62%</div> <div>28%</div> <div>9%</div> </div>
1	B	3986	<div> <div></div> <div>62%</div> <div>28%</div> <div>9%</div> </div>
2	C	192	<div> <div></div> <div>95%</div> </div>
2	D	192	<div> <div></div> <div>95%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 56895 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	3629	Total	C	N	O	S	0	0	0
			28238	18117	4751	5184	186			
1	B	3645	Total	C	N	O	S	0	0	0
			28521	18300	4815	5221	185			

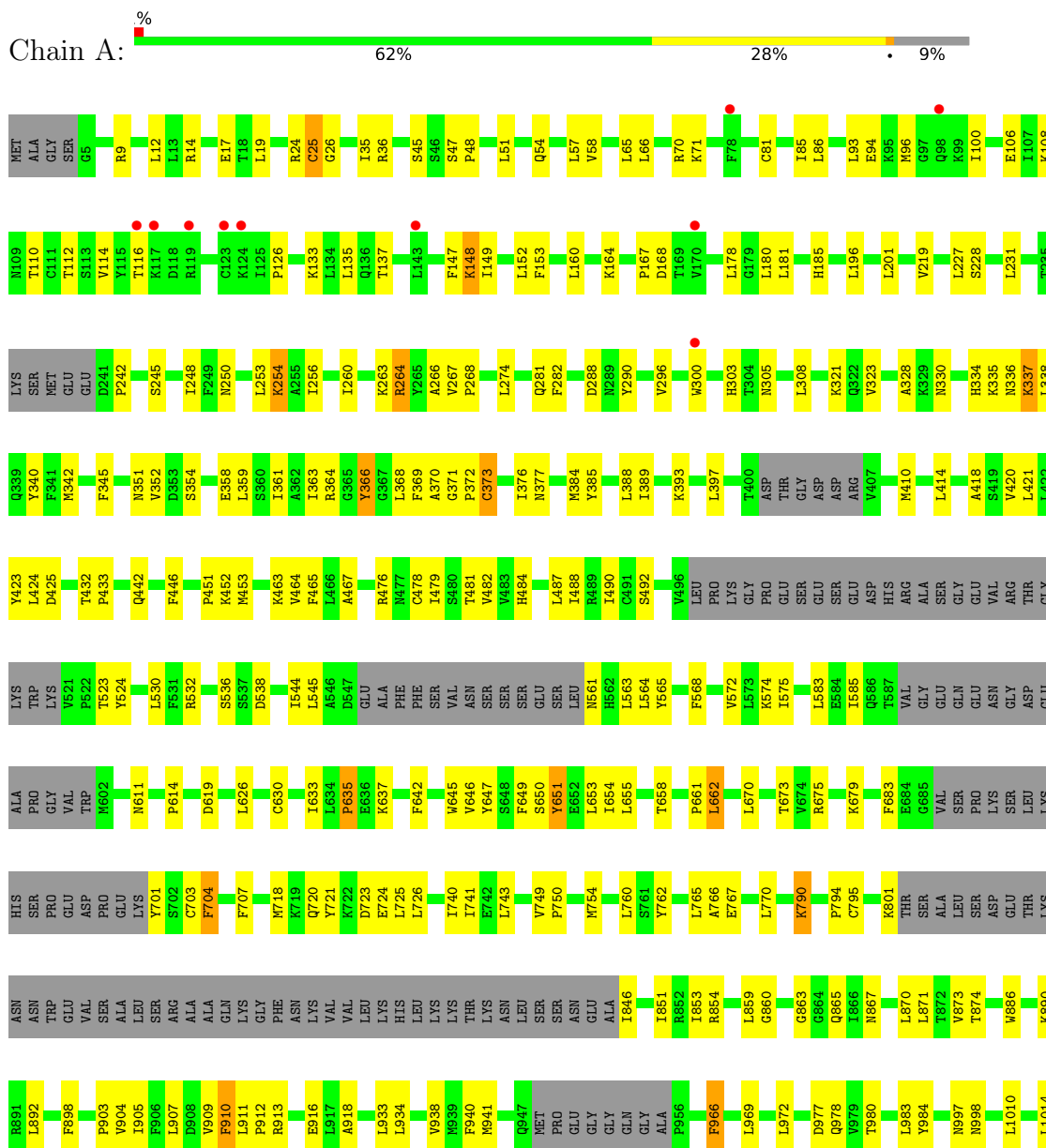
- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	9	Total	C	N	O	S	0	0	0
			68	43	9	15	1			
2	C	9	Total	C	N	O	S	0	0	0
			68	43	9	15	1			

### 3 Residue-property plots

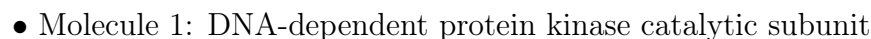
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA-dependent protein kinase catalytic subunit



L2237	R2143	THR	G1789	L1702	H1800	Q1509	L1406	CYS	PRO	G1122	V1018
L2241	L2144	GLY	S1790	T1703	L1601	L1510	L1406	PHE	SER	T1123	V1018
K2246	K2148	ARG	T1793	L1707	D1602	L1514	Y1411	THR	GLY	I1124	S1023
C2248	E1993	ARG	Q1794	L1707	S1604	L1515	L1415	GLY	ALA	Q1125	R1026
L2249	V1994	ARG	L1797	R1712	K1612	F1519	E1416	ALA	ALA	L1134	C1029
S2250	E1995	PRO	V1801	V1713	H1613	A1520	R1420	GLY	PRO	I1137	C1029
L2251	E2155	GLU	Y1802	Q1716	K1617	L1528	K1422	ASN	THR	I1138	C1032
P2252	E2155	ASP	Y1802	L1717	L1618	L1528	K1422	ARG	LEU	E1139	C1032
R2254	V2156	PRO	V1820	I1718	T1621	L1533	A1425	LEU	LEU	K1140	L1037
L2255	L2165	THR	A1822	H1721	T1625	L1534	A1425	THR	TVR	K1141	L1037
L2256	L2168	HIS	S1823	P1722	H1625	P1535	Q1426	ARG	LEU	H1142	K1038
F2257	L2168	ASP	S1823	P1722	T1641	A1536	S1427	GLY	ARG	V1143	V1039
F2260	N2177	ASP	L1825	M1724	W1633	V1537	E1429	PRO	PRO	N1146	I1041
D2269	C2178	VAL	L1825	Q1725	W1633	LEU	E1430	SER	PHE	K1147	K1042
D2269	C2178	LEU	W1829	P1730	D1636	THR	L1431	LEU	SER	R1151	S1052
I2274	E2180	ARG	H1830	P1730	E1640	ALA	A1432	M1342	LEU	Q1251	S1052
Q2275	G2181	LYS	C1831	T1733	E1640	SER	A1433	E1343	P1154	P1154	N1055
L2276	L2182	GLU	S1832	P1733	T1641	LEU	V1434	F1344	R1155	R1155	T1056
L2277	H2183	ALA	L1833	P1733	K1642	GLY	N1435	T1345	G1156	G1156	K1057
W2185	Y2184	ARG	D1834	R1735	L1646	SER	L1436	T1346	F1157	F1157	A1067
V2186	W2185	GLU	A1835	F1736	L1646	SER	F1439	T1347	C1164	C1164	A1067
V2187	V2186	ALA	L1836	F1736	L1653	GLN	D1440	L1348	L1165	L1165	N1071
E2188	E2091	ASN	R1837	Y1739	L1653	GLY	D1440	L1349	L1166	L1166	A1072
L2189	R2092	GLY	F1840	M1743	S1657	SER	V1443	S1352	G1167	G1167	F1073
V2190	C2093	ASP	F1840	M1743	S1657	ILE	V1443	VAL	A1263	A1263	R1074
A2191	L2100	SER	V1843	L1747	VAL	ILE	V1443	SER	A1263	A1263	R1074
L2192	V2101	ASP	V1843	L1747	VAL	ILE	V1443	SER	A1263	A1263	R1074
L2193	L2192	GLY	V1845	L1750	PHE	PHE	L1448	E1354	C1266	C1266	R1075
D2288	L2194	PRO	V1845	L1750	PHE	PHE	L1448	E1354	C1266	C1266	R1075
Q2290	S2195	SER	I1848	S1753	THR	HIS	H1459	W1356	G1077	G1077	G1077
Q2291	S2195	TVR	D1849	Q1754	THR	HIS	H1459	W1356	G1077	G1077	G1077
C2292	T2197	MET	V1850	S1755	SER	G1556	L1463	L1357	C1183	C1183	A1078
G2293	G2198	SER	L1851	S1755	SER	G1556	L1463	L1357	C1183	C1183	A1078
L2294	L2199	SER	K1852	L1758	G1666	S1657	D1474	L1361	L1192	L1192	F1089
Q2295	A2200	GLN	S1853	L1758	G1666	S1657	D1474	D1362	K1193	K1193	R1090
S2296	T2203	GLY	T1856	E1760	P1669	N1568	V1479	N1365	V1195	V1195	P1196
V2304	D2208	GLU	K1857	E1764	T1674	L1572	L1483	H1367	L1197	L1197	V1096
N2305	N2306	ASP	L1858	V1765	Y1675	K1573	L1483	H1367	S1203	S1203	F1099
F2309	L2219	SER	S1861	L1766	I1676	N1574	V1487	L1368	P1204	P1204	V1100
Y2312	M2220	VAL	T1865	C1767	L1679	D1576	G1494	V1371	F1296	F1296	F1101
V2315	V2223	GLN	T1865	C1767	L1679	D1576	G1494	L1372	F1297	F1297	E1102
V2315	H2225	SER	T1865	C1767	L1679	D1576	G1494	V1372	L1298	L1298	A1103
A2318	P2226	TVR	Y1873	M1774	T1682	L1580	GLN	V1373	L1212	L1212	L1104
A2318	K2227	SER	Y1873	M1774	K1683	L1580	GLN	V1373	K1213	K1213	V1105
E2321	V2230	GLN	D1878	F1778	L1686	E1581	CYS	V1389	L1220	L1220	Y1107
V2322	F2231	ASP	Y1881	Q1779	A1592	M1583	P1501	ASP	F1224	F1224	A1114
V2138	V2138	PRO	L1981	Q1779	A1592	M1583	P1501	ASP	I1E	I1E	D1117
P2139	P2139	ARG	L1981	Q1779	A1592	M1583	P1501	ASP	ALA	ALA	E1118
L2326	N2234	ALA	H1890	R1783	L1695	V1593	D1504	L1385	G1228	G1228	D1117
L2327	L2327	ALA	H1891	R1787	L1695	V1593	D1504	P1396	G1230	G1230	E1118
			K1892	R1788	F1698	G1599	K1508	L1402	LYS	GLN	L1121

M3846	G3707	I3606	L3506	L3416	Y3315	Y3316	SER	L3121	A3006	GLU	K2549	C2435	R2398
M3858	R3708	E3607	A3511	D3418	L3316	L3317	ASP	H3122	E3007	LEU	T2550	L2436	Y2329
Y3859	I3719	G3618	G3527	F3419	N3319	N3320	ARG	S3123	I3019	ALA	E2551	D2437	E2338
K3860	T3727	D3619	V3514	G3420	R3324	R3325	VAL	K3128	D3020	LYS	S2556	I2439	L2341
A3862	R3733	A3622	G3515	Q3422	D3326	D3327	GLN	L3129	P3024	VAL	F2561	L2446	C2342
T3867	R3737	P3623	H3516	Q3423	I3329	I3330	GLN	V3132	N3028	ARG	T2562	K2447	E2343
Y3868	R3737	P3623	S3517	R3425	L3329	L3330	GLU	Q3133	I3030	LYS	L2563	P2448	L2344
R3872	I3740	R3629	T3522	E3428	L3330	L3331	D3226	E3137	W3031	ALA	Y2572	K2350	K2351
K3877	R3759	R3630	Q3527	F3429	T3333	T3334	I3243	I3138	T3039	ARG	P2573	L2451	Q2351
D3881	Q3760	F3632	P3532	ALA	R3335	R3336	D3244	F3144	Y3043	PRO	K2823	V2458	T2385
R3885	D3761	I3634	I3534	VAL	N3339	N3340	R3247	R3157	Y3043	PRO	K2824	V2459	F2357
R3885	V3764	F3636	I3535	ASP	D3354	D3355	Q3249	P3156	L3049	PRO	T2825	H2464	D2358
V3888	N3772	F3640	F3542	SER	D3354	D3355	K3257	L3157	L3053	PRO	F2826	P2465	K2359
S3891	L3775	K3642	D3544	LEU	I3359	I3360	L3258	K3158	A3057	PRO	F2576	H2464	K2359
E3895	D3778	H3643	S3546	Q3440	L3362	L3363	K3260	R3159	Q3059	PRO	E2578	P2465	K2359
A3896	S3779	L3651	H3549	A3441	SER	SER	E3261	K3164	R3068	PRO	E2588	C2469	K2366
L3900	A3780	R3652	R3550	Y3442	GLY	GLY	T3268	R3167	S3060	PRO	Y2589	L2476	V2367
R3901	C3781	K3653	K3551	V3447	SER	SER	R3269	R3167	L3061	PRO	T2590	L2477	P2372
R3901	R3784	M3654	K3552	K3449	SER	SER	D3270	D3170	F3063	PRO	T2591	M2473	P2373
L3910	A3785	L3656	F3554	K3450	GLU	GLU	I3273	A3171	F3064	PRO	E2577	Q2472	A2375
L3918	L3786	S3657	V3555	L3451	D3369	D3370	V3274	D3174	I3065	PRO	E2578	S2489	F2378
G3919	R3789	D3658	I3558	R3462	H3384	H3385	S3275	D3181	E3072	PRO	E2594	D2492	M2379
I3920	T3790	N3659	K3559	L3463	L3385	L3386	V3276	L3186	I3077	PRO	X2743	S2495	L2393
L3925	P3795	D3661	L3562	K3464	S3386	S3387	Q3278	R3186	L3078	PRO	X2743	I2498	K2394
H3924	R3795	I3662	L3562	R3467	V3389	V3390	S3279	F3189	H3081	PRO	X2753	V2505	T2396
L3925	S3798	M3665	V3567	L3468	Q3390	Q3391	H3285	K3192	Y3082	PRO	X2757	L2506	C2397
V3930	R3799	L3666	D3570	I3471	ALA	ALA	Q3291	K3196	E3085	PRO	P2781	N2514	L2398
V3937	C3801	L3667	L3575	P3476	GLU	GLU	G3292	L3197	L3088	PRO	D2782	L2402	L2403
I3938	L3802	K3669	D3577	Q3476	GLU	GLU	G3292	T3198	L3091	PRO	Q2784	L2517	R2404
F3946	T3811	M3670	Q3577	L3480	ALA	ALA	E3295	PRD	D2973	PRO	L2785	R2522	M2408
G3947	L3812	S3674	F3585	S3481	GLN	GLN	L3298	LEU	D3094	PRO	K2886	H2527	T2409
S3948	D3814	P3676	K3586	L3482	PRO	PRO	L3298	PRD	D3094	PRO	P2887	E2528	E2410
A3949	D3814	P3676	D3587	I3487	SER	SER	L3301	GLU	D3095	PRO	V2888	T2529	L2411
V3955	M3820	F3690	W3588	S3488	TRP	TRP	L3301	ASP	R3098	PRO	L2790	P2530	P2530
F3956	E3924	E3693	S3889	S3489	SER	SER	V3304	ASN	R3098	PRO	T2791	L2531	L2415
E3957	E3924	F3694	N3590	V3490	CYS	CYS	L3307	MET	Q3108	PRO	T2792	L2531	L2415
R3962	R3833	L3695	L3593	Q3494	GLY	GLY	D3308	ASN	S3109	PRO	L2793	R2538	D2419
A3963	A3834	R3696	R3593	Q3494	PRD	PRD	F3110	VAL	F3110	PRO	L2794	F2420	F2420
K3975	P3835	N3697	L3596	S3497	ASP	ASP	N3310	ASP	E2885	PRO	Q2795	A2541	V2421
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T3977	Y3839	L3699	P3600	K3502	V3312	V3313	V3312	GLY	D3118	PRO	A2796	L2542	Q2422
I3983	W3842	I3701	V3601	V3503	S3314	S3315	S3314	PRD	V3119	PRO	Z2798	Y2546	S2547
												P2548	V2434



T2240	L2241	W2245	K2246	D2247	C2248	L2249	S2250	P2251	L2251	L2252	ARG	ARG	ARG	GLU	GLN	ARG	ASP	PRO	THR	THR	VAL	LEU	E2082	L2083	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	A2212	L2219	V2223	F2224	H2225	P2226	K2227	V2230	F2231	Y2316	A2320	E2321	I2326	T2327	I2328	K2329																																	
VAL	PRO	GLU	GLU	R2000	K2001	K2002	K2003	Y2004	L2007	HIS	ASP	ASP	VAL	LEU	ALA	ASN	GLY	ASP	SER	ASP	GLY	PRO	ALA	ASN	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	VAL	GLN	SER	TYR	SER	TYR	GLN	ASP	PRO	ARG	PRO	ALA	THR	GLY	ARG	PHE																																		
C1904	T1905	T1906	L1910	E1910	L1915	L1918	F1923	S1941	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900	C1904	T1905	T1906	L1910	E1910	L1915	L1918	F1923	S1941	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900			
T1733	N1737	Y1739	M1743	L1747	L1750	E1751	L1752	S1753	Q1754	L1758	M1762	V1765	L1766	C1767	R1768	V1773	F1778	Q1779	S1780	S1781	F1782	R1786	A1786	R1787	R1788	G1789	S1790	T1793	L1797	V1801	Y1802	L1695	P1697	F1698	L1702	H1721	R1727	P1730	L1828	L1613	Q1614	G1615	K1616	L1618	A1619	T1620	T1621	L1622	L1623	W1626	K1627	K1628	W1633	L1648	I1652	Q1653	I1655	S1658	F1661	S1667	S1668	F1671	F1672	T1673	T1674	L1684	D1685	H1687	L1688	K1689	G1690	V1693	T1694	L1696	P1697	F1698	L1702	H1721	R1727	P1730	L1828													
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VAL	PRO	GLU	GLU	R2000	K2001	K2002	K2003	Y2004	L2007	HIS	ASP	ASP	VAL	LEU	ALA	ASN	GLY	ASP	SER	ASP	GLY	PRO	ALA	ASN	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	VAL	GLN	SER	TYR	SER	TYR	GLN	ASP	PRO	ARG	PRO	ALA	THR	GLY	ARG	PHE																																		
W2152	T2153	E2154	E2155	V2156	F2157	H2163	W2164	L2168	L2169	A2172	G2178	L2083	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	VAL	GLN	SER	TYR	SER	TYR	GLN	ASP	PRO	ARG	PRO	ALA	THR	GLY	ARG	PHE																																														
T2240	L2241	W2245	K2246	D2247	C2248	L2249	S2250	P2251	L2251	L2252	ARG	ARG	ARG	GLU	GLN	ARG	ASP	PRO	THR	THR	VAL	LEU	E2082	L2083	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	A2212	L2219	V2223	F2224	H2225	P2226	K2227	V2230	F2231	Y2316	A2320	E2321	I2326	T2327	I2328	K2329																																		
VAL	PRO	GLU	GLU	R2000	K2001	K2002	K2003	Y2004	L2007	HIS	ASP	ASP	VAL	LEU	ALA	ASN	GLY	ASP	SER	ASP	GLY	PRO	ALA	ASN	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	VAL	GLN	SER	TYR	SER	TYR	GLN	ASP	PRO	ARG	PRO	ALA	THR	GLY	ARG	PHE																																		
C1904	T1905	T1906	L1910	E1910	L1915	L1918	F1923	S1941	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900	C1904	T1905	T1906	L1910	E1910	L1915	L1918	F1923	S1941	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900			
T1733	N1737	Y1739	M1743	L1747	L1750	E1751	L1752	S1753	Q1754	L1758	M1762	V1765	L1766	C1767	R1768	V1773	F1778	Q1779	S1780	S1781	F1782	R1786	A1786	R1787	R1788	G1789	S1790	T1793	L1797	V1801	Y1802	L1695	P1697	F1698	L1702	H1721	R1727	P1730	L1828	L1613	Q1614	G1615	K1616	L1618	A1619	T1620	T1621	L1622	L1623	W1626	K1627	K1628	W1633	L1648	I1652	Q1653	I1655	S1658	F1661	S1667	S1668	F1671	F1672	T1673	T1674	L1684	D1685	H1687	L1688	K1689	G1690	V1693	T1694	L1696	P1697	F1698	L1702	H1721	R1727	P1730	L1828													
W1829	H1830	C1831	L1832	S1833	L1834	A1835	R1837	L1838	F1839	F1840	S1841	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900	C1904	T1905	T1906	L1910	E1910	L1915	L1918	F1923	S1841	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900
VAL	PRO	GLU	GLU	R2000	K2001	K2002	K2003	Y2004	L2007	HIS	ASP	ASP	VAL	LEU	ALA	ASN	GLY	ASP	SER	ASP	GLY	PRO	ALA	ASN	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	VAL	GLN	SER	TYR	SER	TYR	GLN	ASP	PRO	ARG	PRO	ALA	THR	GLY	ARG	PHE																																		
W2152	T2153	E2154	E2155	V2156	F2157	H2163	W2164	L2168	L2169	A2172	G2178	L2083	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	VAL	GLN	SER	TYR	SER	TYR	GLN	ASP	PRO	ARG	PRO	ALA	THR	GLY	ARG	PHE																																														
T2240	L2241	W2245	K2246	D2247	C2248	L2249	S2250	P2251	L2251	L2252	ARG	ARG	ARG	GLU	GLN	ARG	ASP	PRO	THR	THR	VAL	LEU	E2082	L2083	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	A2212	L2219	V2223	F2224	H2225	P2226	K2227	V2230	F2231	Y2316	A2320	E2321	I2326	T2327	I2328	K2329																																		
VAL	PRO	GLU	GLU	R2000	K2001	K2002	K2003	Y2004	L2007	HIS	ASP	ASP	VAL	LEU	ALA	ASN	GLY	ASP	SER	ASP	GLY	PRO	ALA	ASN	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	VAL	GLN	SER	TYR	SER	TYR	GLN	ASP	PRO	ARG	PRO	ALA	THR	GLY	ARG	PHE																																		
C1904	T1905	T1906	L1910	E1910	L1915	L1918	F1923	S1941	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900	C1904	T1905	T1906	L1910	E1910	L1915	L1918	F1923	S1941	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900			
T1733	N1737	Y1739	M1743	L1747	L1750	E1751	L1752	S1753	Q1754	L1758	M1762	V1765	L1766	C1767	R1768	V1773	F1778	Q1779	S1780	S1781	F1782	R1786	A1786	R1787	R1788	G1789	S1790	T1793	L1797	V1801	Y1802	L1695	P1697	F1698	L1702	H1721	R1727	P1730	L1828	L1613	Q1614	G1615	K1616	L1618	A1619	T1620	T1621	L1622	L1623	W1626	K1627	K1628	W1633	L1648	I1652	Q1653	I1655	S1658	F1661	S1667	S1668	F1671	F1672	T1673	T1674	L1684	D1685	H1687	L1688	K1689	G1690	V1693	T1694	L1696	P1697	F1698	L1702	H1721	R1727	P1730	L1828													
W1829	H1830	C1831	L1832	S1833	L1834	A1835	R1837	L1838	F1839	F1840	S1841	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900	C1904	T1905	T1906	L1910	E1910	L1915	L1918	F1923	S1841	T1842	I1843	V1844	V1845	L1848	L1851	R1854	L1858	N1859	E1860	S1861	T1862	F1863	V1865	L1866	K1870	M1871	G1872	K1875	L1876	L1877	D1878	M1879	V1880	Y1881	L1882	R1883	L1884	P1885	V1889	K1892	E1893	S1894	K1895	L1896	M1897	F1900
VAL	PRO	GLU	GLU	R2000	K2001	K2002	K2003	Y2004	L2007	HIS	ASP	ASP	VAL	LEU	ALA	ASN	GLY	ASP	SER	ASP	GLY	PRO	ALA	ASN	E2084	M2085	N2089	R2090	K2091	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	PRO	GLN	GLY	GLU	ASP	VAL	GLN	SER	TYR	SER	TYR	GLN	ASP	PRO	ARG	PRO	ALA	THR	GLY	ARG	PHE																																		
W2152	T2153	E2154	E2155	V2156	F2157	H2163	W2164	L2168	L2169																																																																																					



R3992	P3879	I3740	R3630	Q3494	L3298	L3157	ARG	D2821	P2548	V2458	Y2329
L3997	A3880	R3741	K3631	Q3497	T3299	S3047	LEU	K2822	K2549	V2459	K2339
F4005	D3881	G3742	F3632	S5437	V3300	K3048	PRO	K2823	E2550	F2461	K2334
E4008	L3882	H3743	I3633	M3503	T3303	L3049	PRO	T2825	E2551	F2462	E2460
F4009	R3885	D3744	F3636	V3502	L3307	K3050	D2919	K2829	F2554	Q2472	L2341
F4010	V3888	K3753	D3641	M3503	L3307	L3051	V2920	K2835	L2555	M2473	C2342
F4011	S3891	G3755	K3642	L3506	N3319	L3052	L2921	E2925	S2556	L2476	E2343
F4012	T3892	L3758	G3645	D3507	F3323	L3053	R2922	E2925	N2560	L2477	L2344
F4013	R3893	R3759	G3646	Q3510	R3324	A3057	E2925	N2841	M2565	L2476	K2359
F4014	L3898	Q3760	G3647	V3512	D3325	Q3059	D2937	N2841	K2566	L2477	K2366
N4015	L3898	D3761	G3648	A3513	Q3326	L3061	R2940	N2845	M2568	L2477	V2367
F4016	G3764	R3765	L3651	V3514	R3327	GLU	R2940	T2846	K2568	L2477	K2366
L4031	V3764	L3775	L3652	L3506	R3327	ASP	R2940	T2846	K2568	L2477	K2366
E4035	N3772	L3775	L3653	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
A4047	L3910	L3775	L3654	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
K4050	L3913	L3775	L3655	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
A4054	L3917	D3778	L3656	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
I4055	L3918	S3779	L3657	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
A4058	G3919	R3784	L3658	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
I4059	L3920	A3785	L3659	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
A4064	H3924	L3786	L3660	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
H4068	N3926	L3786	L3661	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
Y4077	V3937	L3786	L3662	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
R4082	L3938	S3798	L3663	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
H4087	H3944	R3799	L3664	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
A4090	A3945	L3800	L3665	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
E4095	F3946	G3801	L3666	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
S4096	G3947	L3802	L3667	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
E4101	S3948	T3811	L3668	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
T4102	A3949	M3820	L3669	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
Q4103	V3955	E3824	L3670	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
D4113	P3956	L3829	L3671	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
T4116	E3957	R3833	L3672	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
L4117	L3958	V3842	L3673	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
R4119	N3969	G3861	L3674	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
T4120	E3976	A3862	L3675	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
W4121	L3979	T3867	L3676	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
E4125	L3983	R3872	L3677	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
P4126	M3984	E3875	L3678	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
	L3988	S3876	L3679	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
	L3988	R3733	L3680	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
		V3878	L3681	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3682	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3683	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3684	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3685	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3686	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3687	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3688	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3689	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3690	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3691	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3692	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3693	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3694	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3695	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3696	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3697	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3698	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3699	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3700	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3701	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3702	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3703	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3704	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3705	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3706	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3707	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3708	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3709	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3710	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3711	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3712	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3713	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3714	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3715	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3716	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3717	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3718	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3719	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3720	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3721	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3722	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3723	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3724	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3725	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3726	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3727	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3728	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3729	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3730	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3731	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3732	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3733	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3734	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3735	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3736	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3737	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3738	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3739	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3740	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3741	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3742	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3743	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3744	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3745	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3746	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3747	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3748	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3749	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3750	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3751	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3752	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3753	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3754	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3755	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3756	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3757	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3758	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3759	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3760	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3761	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3762	D3507	R3327	ASP	R2940	T2846	K2568	L2477	K2366
			L3763	D3507	R3327	ASP	R2				



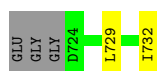
- Molecule 2: X-ray repair cross-complementing protein 5

Chain D:  95%

[illegible]

- Molecule 2: X-ray repair cross-complementing protein 5

Chain C:  95%

[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.12Å 132.64Å 296.59Å 90.00° 105.53° 90.00°	Depositor
Resolution (Å)	49.92 – 4.30 49.92 – 4.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.92-4.30) 97.6 (49.92-4.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.286 , 0.335 0.286 , 0.335	Depositor DCC
$R_{free}$ test set	2009 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	184.6	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 157.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	56895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.29	0/28603	0.52	5/38757 (0.0%)
1	B	0.29	0/28898	0.51	8/39125 (0.0%)
2	C	0.25	0/67	0.43	0/90
2	D	0.28	0/67	0.50	0/90
All	All	0.29	0/57635	0.52	13/78062 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3652	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	A	2781	PRO	N-CA-CB	6.49	111.08	103.30
1	B	1858	LEU	CB-CG-CD1	-6.17	100.51	111.00
1	B	1752	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	B	1752	LEU	CB-CG-CD2	5.72	120.72	111.00
1	A	2100	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	1825	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	B	907	LEU	CB-CG-CD2	5.43	120.22	111.00
1	B	261	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	57	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	2208	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	3259	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	1752	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1994	VAL	Peptide
1	A	2120	ARG	Peptide
1	B	1202	ARG	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	28238	0	27963	774	0
1	B	28521	0	28367	774	0
2	C	68	0	64	1	0
2	D	68	0	64	1	0
All	All	56895	0	56458	1550	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 14.

All (1550) 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:260:ILE:HG22	1:A:300:TRP:CZ2	1.96	1.00
1:B:3701:ILE:HD12	1:B:3740:ILE:HD11	1.50	0.94
1:A:645:TRP:O	1:A:649:PHE:HB2	1.71	0.91
1:A:1406:LEU:HB3	1:A:1415:LEU:HD11	1.51	0.89
1:B:2459:VAL:HB	1:B:2505:VAL:HG21	1.55	0.88
1:A:3028:ASN:HA	1:A:3031:TRP:HD1	1.39	0.86
1:A:385:TYR:CE2	1:A:389:ILE:HD11	2.10	0.86
1:A:354:SER:HB3	1:A:358:GLU:HB2	1.62	0.82
1:B:1608:ARG:HA	1:B:1612:LYS:HB3	1.62	0.81
1:A:1676:ILE:O	1:A:1680:ALA:HB2	1.81	0.79
1:A:3545:THR:HG22	1:A:3546:SER:H	1.47	0.79
1:B:1615:GLY:HA3	1:B:1655:ILE:HG21	1.61	0.79
1:B:3325:ASP:HA	1:B:3328:ILE:HD12	1.65	0.79
1:B:3700:GLU:HA	1:B:3718:ARG:HA	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HG22	1:A:300:TRP:CH2	2.19	0.78
1:A:1204:PRO:HB2	1:A:1275:THR:HG22	1.65	0.78
1:B:1579:VAL:HG21	1:B:1621:THR:HG21	1.66	0.78
1:B:583:LEU:HA	1:B:614:PRO:HA	1.66	0.78
1:A:873:VAL:HG13	1:A:874:THR:H	1.48	0.77
1:B:135:LEU:HD12	1:B:177:LEU:HD11	1.67	0.77
1:B:1686:LEU:HD11	1:B:1721:HIS:HB3	1.66	0.76
1:A:3930:VAL:HG12	1:A:3937:VAL:HG12	1.67	0.76
1:A:1787:ARG:HB3	1:A:1831:CYS:HB3	1.66	0.76
1:B:873:VAL:HG13	1:B:874:THR:H	1.50	0.76
1:A:801:LYS:HA	1:A:3115:SER:HB2	1.68	0.76
1:A:2825:THR:HG22	1:A:2826:LEU:H	1.51	0.76
1:B:3700:GLU:HG3	1:B:3718:ARG:HG2	1.66	0.75
1:A:1178:ARG:NH1	1:A:1183:CYS:SG	2.59	0.75
1:B:1068:LEU:HD11	1:B:1106:ILE:HG13	1.68	0.75
1:B:1076:LEU:HB2	1:B:1123:THR:HG22	1.68	0.75
1:B:1832:SER:H	1:B:1883:ARG:HH22	1.34	0.75
1:B:2851:PHE:HB3	1:B:2854:PHE:HB3	1.69	0.75
1:A:363:ILE:HG23	1:A:388:LEU:HD11	1.69	0.74
1:A:770:LEU:HD23	1:A:854:ARG:HD3	1.68	0.74
1:B:1090:ARG:HB2	1:B:1137:ILE:HG12	1.68	0.74
1:B:1406:LEU:HB3	1:B:1415:LEU:HD11	1.70	0.74
1:B:1727:ARG:HD2	1:B:1773:VAL:HG23	1.69	0.74
1:A:66:LEU:HD21	1:A:106:GLU:HB3	1.69	0.74
1:A:1082:PHE:HZ	1:A:1134:LEU:HG	1.53	0.73
1:B:1955:VAL:HG13	1:B:1956:PHE:H	1.52	0.73
1:A:14:ARG:HA	1:A:17:GLU:HG2	1.70	0.73
1:B:2965:TYR:HA	1:B:2968:ALA:HB3	1.70	0.73
1:A:3503:VAL:HG21	1:A:3532:PRO:HB2	1.71	0.73
1:A:35:ILE:HD12	1:A:81:CYS:HB2	1.70	0.73
1:A:300:TRP:CE3	1:A:308:LEU:HD21	2.24	0.73
1:B:2451:LEU:HD23	1:B:2484:TYR:HE2	1.54	0.73
1:A:1697:PRO:HB3	1:A:1753:SER:HB3	1.71	0.73
1:B:200:PHE:HD1	1:B:223:CYS:HG	1.35	0.72
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.22	0.72
1:B:4011:PHE:HA	1:B:4015:ASN:HB2	1.70	0.72
1:A:3144:PHE:O	1:A:3150:ASN:ND2	2.22	0.72
1:B:1825:LEU:HD22	1:B:1879:VAL:HG21	1.70	0.72
1:A:1090:ARG:HB2	1:A:1137:ILE:HG12	1.70	0.72
1:A:2837:LEU:O	1:A:2841:ASN:ND2	2.21	0.72
1:A:260:ILE:HA	1:A:300:TRP:CH2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1991:PRO:HG2	1:B:2000:ARG:HH22	1.55	0.72
1:B:2823:PHE:HD1	1:B:2824:LYS:HG2	1.53	0.72
1:A:4011:PHE:HA	1:A:4015:ASN:HB2	1.71	0.72
1:A:4042:GLN:NE2	1:A:4046:TYR:CE2	2.57	0.71
1:B:3137:GLU:OE1	1:B:3164:TRP:NE1	2.22	0.71
1:B:424:LEU:O	1:B:471:LYS:NZ	2.22	0.71
1:A:228:SER:HA	1:A:274:LEU:HD13	1.71	0.71
1:B:1892:LYS:HD2	1:B:1892:LYS:H	1.55	0.71
1:A:1845:VAL:HA	1:A:1848:ILE:HG22	1.72	0.71
1:A:3695:LEU:HD12	1:A:3698:GLU:HG2	1.71	0.71
1:B:394:GLN:HB3	1:B:1687:HIS:HB2	1.72	0.71
1:B:1817:GLN:NE2	1:B:1871:MET:SD	2.64	0.71
1:B:19:LEU:HD22	1:B:71:LYS:HG3	1.73	0.71
1:B:3833:ARG:HB3	1:B:3877:LYS:HE2	1.73	0.71
1:A:1373:VAL:HG11	1:A:1422:LYS:HE3	1.74	0.70
1:B:2148:LYS:O	1:B:2152:ASN:ND2	2.23	0.70
1:A:1955:VAL:HG23	1:A:1957:ASN:H	1.56	0.70
1:B:1257:LEU:HD22	1:B:1337:VAL:HG11	1.73	0.70
1:A:1406:LEU:HD13	1:A:1415:LEU:HD21	1.74	0.70
1:B:3549:HIS:HA	1:B:3552:LYS:HE2	1.72	0.70
1:A:3772:ASN:HA	1:A:3775:LEU:HB2	1.73	0.69
1:A:762:TYR:HB3	1:A:765:LEU:HD22	1.72	0.69
1:B:1766:LEU:HG	1:B:1778:PHE:HD2	1.56	0.69
1:B:990:GLN:HG2	1:B:2780:LEU:O	1.90	0.69
1:B:228:SER:HA	1:B:274:LEU:HD13	1.74	0.69
1:B:54:GLN:HA	1:B:57:LEU:HB3	1.73	0.69
1:B:2880:CYS:HB3	1:B:2886:GLN:HA	1.73	0.69
1:A:2887:PRO:HG2	1:A:3895:GLU:HG2	1.75	0.69
1:A:1257:LEU:HD22	1:A:1337:VAL:HG11	1.73	0.69
1:B:859:LEU:HG	1:B:867:ASN:HD21	1.56	0.69
1:A:148:LYS:H	1:A:148:LYS:HD3	1.57	0.69
1:A:4037:ASN:ND2	1:A:4066:LEU:O	2.25	0.69
1:A:1082:PHE:CZ	1:A:1134:LEU:HG	2.29	0.68
1:A:160:LEU:HD21	1:A:178:LEU:HD12	1.76	0.68
1:B:72:SER:O	1:B:82:ARG:NH1	2.26	0.68
1:B:323:VAL:HG13	1:B:369:PHE:HZ	1.59	0.68
1:B:992:ILE:O	1:B:996:THR:HG22	1.94	0.68
1:A:2290:PRO:HD3	1:A:2296:SER:HB3	1.76	0.68
1:B:2387:PRO:HG3	1:B:2418:LYS:HB3	1.74	0.68
1:A:1930:GLU:OE1	1:A:1937:ARG:NH2	2.26	0.68
1:A:2952:ILE:HD13	1:A:2975:ALA:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3949:ALA:HB1	1:B:3957:GLU:HG3	1.75	0.68
1:A:2140:LEU:HD21	1:A:2178:GLY:HA2	1.76	0.68
1:B:1896:ILE:HD13	1:B:1906:THR:HB	1.74	0.68
1:A:3545:THR:HG22	1:A:3546:SER:N	2.09	0.67
1:B:2290:PRO:HD3	1:B:2296:SER:HB3	1.76	0.67
1:A:330:ASN:HB2	1:A:334:HIS:CD2	2.29	0.67
1:A:3577:GLN:HG3	1:A:3630:ARG:HD3	1.76	0.67
1:B:1406:LEU:HD13	1:B:1415:LEU:HD21	1.76	0.67
1:B:339:GLN:NE2	1:B:343:GLU:OE2	2.28	0.67
1:B:1147:LYS:O	1:B:1151:ARG:NH2	2.27	0.67
1:B:1398:VAL:HA	1:B:1401:ASN:HB2	1.75	0.67
1:A:1686:LEU:HD13	1:A:1721:HIS:HB3	1.77	0.67
1:A:1560:TYR:OH	1:A:1568:ASN:ND2	2.27	0.67
1:B:1440:ASP:HB2	1:B:1443:VAL:HG22	1.76	0.67
1:A:3775:LEU:HD11	1:A:3910:LEU:HD11	1.77	0.67
1:B:1828:LEU:O	1:B:1883:ARG:NH2	2.20	0.66
1:B:1483:LEU:HD22	1:B:1514:LEU:HD11	1.76	0.66
1:B:3775:LEU:HD11	1:B:3910:LEU:HD11	1.77	0.66
1:A:3462:ARG:NH1	1:A:3497:SER:OG	2.29	0.66
1:B:2194:LEU:HD11	1:B:2241:LEU:HD13	1.77	0.66
1:B:3503:VAL:HG21	1:B:3532:PRO:HB2	1.77	0.66
1:B:3585:PHE:HD2	1:B:3667:LEU:HD13	1.60	0.66
1:B:3758:LEU:HD12	1:B:3801:GLY:HA3	1.77	0.66
1:A:2148:LYS:O	1:A:2152:ASN:ND2	2.26	0.66
1:A:2312:TYR:HB3	1:A:2315:VAL:HG12	1.78	0.66
1:B:1626:TRP:CD1	1:B:1671:VAL:HG12	2.31	0.66
1:A:3339:ASN:ND2	1:A:3422:GLN:OE1	2.29	0.66
1:B:1984:LEU:HD11	1:B:2139:PRO:HG2	1.77	0.66
1:B:1361:LYS:HA	1:B:1364:CYS:HB2	1.78	0.65
1:B:272:LEU:HB3	1:B:315:ALA:HB2	1.77	0.65
1:A:1850:VAL:O	1:A:1870:LYS:NZ	2.25	0.65
1:A:903:PRO:HG3	1:A:2816:ILE:HG12	1.77	0.65
1:A:4083:GLY:HA3	1:A:4091:ALA:HB2	1.77	0.65
1:A:1052:SER:HB2	1:A:1055:ASN:HB2	1.77	0.65
1:A:328:ALA:HA	1:A:372:PRO:HB3	1.79	0.65
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.76	0.65
1:B:1038:LYS:NZ	1:B:1088:GLU:OE2	2.30	0.65
1:B:1750:LEU:HD13	1:B:1758:LEU:HB2	1.79	0.65
1:B:3946:PHE:O	1:B:3948:SER:N	2.27	0.65
1:B:1345:THR:HG21	1:B:1368:LEU:HD21	1.78	0.65
1:B:1750:LEU:HG	1:B:1785:ILE:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2448:PRO:HB3	1:A:2498:ILE:HD13	1.79	0.64
1:B:1612:LYS:O	1:B:1614:GLN:N	2.29	0.64
1:A:178:LEU:HB3	1:A:196:LEU:HD11	1.79	0.64
1:A:2286:PRO:HB3	1:A:2329:TYR:CE2	2.32	0.64
1:A:2458:VAL:HG11	1:A:2476:ILE:HD11	1.78	0.64
1:A:2856:SER:HA	1:A:2888:VAL:HG11	1.79	0.64
1:B:1108:MET:HG3	1:B:1131:ILE:HG21	1.80	0.64
1:B:363:ILE:HG23	1:B:388:LEU:HD11	1.79	0.64
1:B:1969:GLU:HB3	1:B:1977:ILE:HG13	1.79	0.64
1:A:2181:GLY:O	1:A:2183:HIS:N	2.30	0.64
1:A:2409:THR:O	1:A:2411:LEU:N	2.31	0.64
1:B:2952:ILE:HD13	1:B:2975:ALA:HB2	1.80	0.64
1:B:3880:ALA:HB1	1:B:3969:ASN:HD22	1.62	0.64
1:A:160:LEU:O	1:A:164:LYS:NZ	2.22	0.64
1:B:2011:ALA:HA	1:B:2195:SER:HA	1.80	0.64
1:B:572:VAL:HG23	1:B:626:LEU:HD11	1.79	0.64
1:B:66:LEU:HD11	1:B:110:THR:HG21	1.79	0.64
1:B:704:PHE:CE1	1:B:741:ILE:HG12	2.33	0.64
1:A:2148:LYS:HA	1:A:2151:ILE:HD12	1.80	0.63
1:B:3005:LEU:HA	1:B:3254:LEU:HD13	1.80	0.63
1:B:373:CYS:SG	1:B:376:ILE:HG21	2.37	0.63
1:B:35:ILE:HD13	1:B:85:ILE:HG13	1.79	0.63
1:B:3468:LEU:HA	1:B:3471:ILE:HG22	1.79	0.63
1:A:3137:GLU:OE1	1:A:3164:TRP:NE1	2.32	0.63
1:B:1845:VAL:HA	1:B:1848:ILE:HG22	1.81	0.63
1:B:1877:LEU:O	1:B:1881:TYR:HB2	1.99	0.63
1:B:2133:LEU:HB2	1:B:2146:LEU:HD23	1.81	0.63
1:A:3587:ASP:OD2	1:A:3733:ARG:NH1	2.32	0.63
1:B:1623:LEU:HD22	1:B:1671:VAL:HG11	1.81	0.63
1:B:2148:LYS:HA	1:B:2151:ILE:HD12	1.80	0.63
1:B:3328:ILE:HD11	1:B:3412:ALA:HB2	1.81	0.63
1:B:359:LEU:O	1:B:363:ILE:HG12	1.99	0.63
1:A:93:LEU:HD12	1:A:100:ILE:HD13	1.81	0.62
1:B:1525:CYS:SG	1:B:1574:ASN:ND2	2.70	0.62
1:A:1825:LEU:O	1:A:1829:TRP:HB2	1.98	0.62
1:B:3027:LEU:HG	1:B:3067:LYS:HD2	1.81	0.62
1:A:3813:LYS:HB2	1:A:3925:LEU:HB3	1.81	0.62
1:B:3879:PRO:O	1:B:3966:GLN:NE2	2.31	0.62
1:A:3468:LEU:HA	1:A:3471:ILE:HG22	1.80	0.62
1:B:148:LYS:HB3	1:B:151:GLU:HB2	1.80	0.62
1:A:1582:LEU:HG	1:A:1593:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1992:VAL:HG12	1:B:2183:HIS:CD2	2.35	0.62
1:A:1346:THR:HG22	1:A:1402:LEU:HA	1.82	0.62
1:A:2375:ALA:HB3	1:A:2404:ARG:HG2	1.82	0.62
1:B:1658:SER:HB3	1:B:1661:PHE:HE1	1.64	0.62
1:B:2085:MET:HA	1:B:2089:ASN:HB2	1.82	0.62
1:B:1612:LYS:C	1:B:1614:GLN:H	2.02	0.62
1:B:4117:LEU:HB3	1:B:4126:PRO:HB2	1.80	0.62
1:B:451:PRO:O	1:B:452:LYS:HG2	1.99	0.62
1:B:704:PHE:HE1	1:B:741:ILE:HG12	1.64	0.62
1:B:2458:VAL:HG11	1:B:2476:ILE:HD11	1.81	0.61
1:B:1820:VAL:O	1:B:1825:LEU:HG	2.00	0.61
1:A:1833:LEU:HG	1:A:1835:ALA:H	1.65	0.61
1:B:2538:ARG:NE	1:B:2565:MET:SD	2.73	0.61
1:A:1181:THR:HG22	1:A:1184:ARG:HH12	1.66	0.61
1:B:16:GLN:NE2	1:B:62:ASP:O	2.33	0.61
1:A:1166:LEU:HD12	1:A:1166:LEU:H	1.65	0.61
1:A:1106:ILE:HD11	1:A:1155:ARG:H	1.65	0.61
1:B:1992:VAL:HG23	1:B:1993:GLU:H	1.65	0.61
1:B:3630:ARG:O	1:B:3633:ILE:HG12	2.01	0.61
1:B:1121:LEU:HD22	1:B:1123:THR:HG23	1.81	0.61
1:B:333:MET:SD	1:B:333:MET:N	2.72	0.61
1:A:1448:LEU:HD23	1:A:1510:LEU:HD21	1.81	0.61
1:B:1143:VAL:HA	1:B:1197:LEU:HD21	1.82	0.61
1:B:770:LEU:HD23	1:B:854:ARG:HD2	1.82	0.61
1:A:3174:ASP:O	1:A:3249:GLN:NE2	2.30	0.61
1:A:4064:LEU:O	1:A:4068:HIS:HB2	2.01	0.61
1:A:1533:LEU:HD22	1:A:1589:ASN:HB2	1.83	0.60
1:B:376:ILE:HG13	1:B:377:ASN:H	1.65	0.60
1:A:1733:THR:HB	1:A:1736:PHE:H	1.66	0.60
1:A:2588:GLU:HG3	1:A:2785:ILE:HD11	1.83	0.60
1:A:2940:ARG:HG3	1:A:2957:LEU:HD22	1.81	0.60
1:B:864:GLY:HA2	1:B:867:ASN:HB2	1.83	0.60
1:A:1579:VAL:HG21	1:A:1621:THR:HG21	1.82	0.60
1:B:12:LEU:HD23	1:B:64:GLY:HA2	1.83	0.60
1:B:2178:GLY:O	1:B:2182:ILE:HB	2.00	0.60
1:B:358:GLU:O	1:B:361:ILE:HG12	2.01	0.60
1:A:3955:VAL:HG11	1:A:4121:TRP:CE3	2.37	0.60
1:B:1425:ALA:O	1:B:1429:GLU:HG2	2.01	0.60
1:B:3031:TRP:HZ2	1:B:3068:ALA:HB1	1.66	0.60
1:B:394:GLN:HE22	1:B:1688:LEU:HD23	1.67	0.60
1:A:704:PHE:CE1	1:A:741:ILE:HG12	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1212:LEU:HD13	1:B:1220:LEU:HD22	1.84	0.60
1:B:2234:ASN:HA	1:B:2237:ILE:HD12	1.83	0.60
1:A:300:TRP:HE3	1:A:308:LEU:HD21	1.67	0.60
1:A:2546:TYR:CE2	1:A:2548:PRO:HB3	2.36	0.60
1:A:2575:PRO:HB3	1:A:2787:HIS:NE2	2.17	0.60
1:A:2841:ASN:O	1:A:2845:ASN:ND2	2.29	0.60
1:A:647:TYR:HD1	1:A:703:CYS:HB3	1.67	0.60
1:B:4058:VAL:HG21	1:B:4095:GLU:HB3	1.84	0.60
1:A:1574:ASN:HB3	1:A:1577:LEU:HD21	1.83	0.59
1:A:321:LYS:HA	1:A:368:LEU:HD21	1.83	0.59
1:B:3079:GLU:HB2	1:B:3102:TYR:HE1	1.67	0.59
1:B:3842:TRP:HH2	1:B:3867:THR:HG22	1.66	0.59
1:A:1892:LYS:HD3	1:A:1892:LYS:H	1.67	0.59
1:A:54:GLN:HA	1:A:57:LEU:HB3	1.85	0.59
1:B:3733:ARG:NH2	1:B:3755:GLY:O	2.35	0.59
1:B:3028:ASN:HA	1:B:3031:TRP:HD1	1.66	0.59
1:A:1255:CYS:SG	1:A:3695:LEU:HD23	2.42	0.59
1:A:1676:ILE:O	1:A:1680:ALA:CB	2.50	0.59
1:A:3309:GLU:HG2	1:A:3310:ASN:H	1.66	0.59
1:A:3789:ARG:HG2	1:A:3938:ILE:HD12	1.82	0.59
1:B:1302:ALA:HA	1:B:1382:ILE:HA	1.83	0.59
1:B:1828:LEU:HB3	1:B:1879:VAL:HG11	1.84	0.59
1:B:903:PRO:HG3	1:B:2816:ILE:HG12	1.84	0.59
1:B:3484:THR:HG22	1:B:3513:ALA:HA	1.83	0.59
1:A:3696:ARG:HD2	1:A:3697:ASN:H	1.67	0.59
1:A:487:LEU:HD21	1:A:568:PHE:HE1	1.68	0.59
1:B:156:PHE:HA	1:B:159:GLU:HB2	1.85	0.59
1:B:473:PRO:HA	1:B:476:ARG:HG2	1.83	0.59
1:A:2373:PRO:HA	1:A:2404:ARG:HE	1.67	0.59
1:A:366:TYR:CE2	1:A:384:MET:HG2	2.37	0.59
1:B:1612:LYS:HG3	1:B:1613:HIS:H	1.68	0.59
1:B:166:ILE:HG22	1:B:168:ASP:H	1.68	0.59
1:A:1686:LEU:HD23	1:A:1686:LEU:H	1.68	0.59
1:A:3795:PRO:HA	1:A:3801:GLY:HA2	1.85	0.59
1:A:572:VAL:HG23	1:A:626:LEU:HD21	1.83	0.59
1:A:1743:MET:HG3	1:A:1774:MET:HE1	1.85	0.58
1:A:260:ILE:CG2	1:A:300:TRP:CZ2	2.81	0.58
1:B:1138:ILE:HG21	1:B:1194:PHE:CE1	2.39	0.58
1:B:1881:TYR:CE1	1:B:1889:VAL:HG21	2.38	0.58
1:B:3130:GLN:HB3	1:B:3178:ILE:HG12	1.84	0.58
1:A:1483:LEU:HD22	1:A:1514:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3110:PHE:HD1	1:A:3128:LYS:HD2	1.68	0.58
1:B:1362:ASP:O	1:B:1367:HIS:ND1	2.21	0.58
1:A:1783:ARG:HB3	1:A:1830:HIS:CD2	2.38	0.58
1:B:1427:SER:HA	1:B:1430:GLU:HG2	1.84	0.58
1:B:1582:LEU:HG	1:B:1593:VAL:HG23	1.86	0.58
1:A:1675:TYR:O	1:A:1679:LEU:HD23	2.04	0.58
1:A:2249:LEU:O	1:A:2251:ILE:N	2.36	0.58
1:A:3121:LEU:O	1:A:3124:SER:OG	2.21	0.58
1:A:3962:ARG:NH1	1:A:4128:MET:O	2.35	0.58
1:B:3514:VAL:HG23	1:B:3517:SER:HB2	1.85	0.58
1:A:2522:ARG:HG3	1:A:2561:PHE:HE1	1.68	0.58
1:A:260:ILE:HG22	1:A:300:TRP:CE2	2.39	0.58
1:A:3630:ARG:O	1:A:3633:ILE:HG12	2.02	0.58
1:A:670:LEU:HA	1:A:673:THR:HG22	1.85	0.58
1:B:1801:VAL:HB	1:B:1824:LEU:HD12	1.86	0.58
1:A:4005:PHE:O	1:A:4011:PHE:HZ	1.86	0.58
1:A:3587:ASP:HB3	1:A:4022:LYS:HE2	1.85	0.58
1:A:4042:GLN:HE21	1:A:4046:TYR:HE2	1.50	0.58
1:B:1831:CYS:HA	1:B:1883:ARG:HH12	1.69	0.58
1:B:2490:GLU:OE1	1:B:2496:GLN:NE2	2.37	0.58
1:B:3421:ASP:OD1	1:B:3467:ARG:NE	2.37	0.58
1:B:859:LEU:O	1:B:867:ASN:ND2	2.36	0.58
1:A:2234:ASN:HA	1:A:2237:ILE:HD12	1.86	0.58
1:A:260:ILE:HA	1:A:300:TRP:HH2	1.67	0.58
1:B:2201:THR:HB	1:B:2205:VAL:H	1.68	0.58
1:B:3407:ALA:HA	1:B:3410:ILE:HG12	1.86	0.58
1:B:4055:ASN:HB2	1:B:4095:GLU:HA	1.86	0.58
1:A:3696:ARG:HD2	1:A:3697:ASN:N	2.18	0.57
1:B:2459:VAL:HG21	1:B:2501:LEU:HD11	1.86	0.57
1:B:3462:ARG:HG3	1:B:3494:GLN:HB3	1.85	0.57
1:A:2255:LEU:HD23	1:A:2256:ILE:H	1.69	0.57
1:B:2150:VAL:HG13	1:B:2157:PHE:CD2	2.39	0.57
1:B:1279:LEU:H	1:B:1279:LEU:HD23	1.69	0.57
1:B:1930:GLU:HB3	1:B:1937:ARG:HH12	1.68	0.57
1:A:1023:SER:HA	1:A:1026:ARG:HE	1.69	0.57
1:A:1976:LEU:HD22	1:A:1979:GLU:HG3	1.87	0.57
1:A:25:CYS:SG	1:A:26:GLY:N	2.77	0.57
1:A:3549:HIS:HA	1:A:3552:LYS:HE2	1.85	0.57
1:A:724:GLU:HG2	1:A:725:LEU:N	2.18	0.57
1:B:1605:PHE:CE1	1:B:1608:ARG:HD3	2.40	0.57
1:A:1103:ALA:HB1	1:A:1106:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2294:ILE:HG22	1:A:2295:GLN:H	1.70	0.57
1:A:3946:PHE:O	1:A:3948:SER:N	2.30	0.57
1:B:1619:ALA:HB1	1:B:1652:ILE:HG23	1.85	0.57
1:A:892:LEU:HB3	1:A:940:PHE:HE2	1.70	0.57
1:B:2119:PRO:N	1:B:2163:HIS:HE2	2.02	0.57
1:B:3789:ARG:HG2	1:B:3938:ILE:HD12	1.85	0.57
1:A:2084:GLU:O	1:A:2089:ASN:ND2	2.38	0.57
1:A:2610:UNK:O	1:A:2614:UNK:CB	2.52	0.57
1:A:2894:GLU:OE2	1:A:3901:ARG:NH2	2.37	0.57
1:A:760:LEU:O	1:A:760:LEU:HD13	2.05	0.57
1:B:1298:LEU:HB3	1:B:1367:HIS:HB3	1.86	0.57
1:B:1837:ARG:HH11	1:B:1884:LEU:HD21	1.69	0.57
1:B:3698:GLU:HG3	1:B:3718:ARG:HD2	1.87	0.57
1:A:1212:LEU:HD13	1:A:1220:LEU:HD22	1.86	0.57
1:B:583:LEU:HD12	1:B:611:ASN:ND2	2.20	0.57
1:A:3640:PHE:CZ	1:A:3670:MET:HG3	2.39	0.57
1:A:108:LYS:HE3	1:A:152:LEU:HD22	1.87	0.57
1:A:2591:ILE:HD13	1:A:2796:ALA:HB2	1.86	0.57
1:B:2528:GLU:O	1:B:2529:THR:HG22	2.05	0.57
1:B:3577:GLN:HG3	1:B:3630:ARG:HD3	1.85	0.57
1:A:1990:PHE:CZ	1:A:2144:LEU:HD21	2.40	0.56
1:A:3590:ASN:HA	1:A:3593:ARG:HG2	1.87	0.56
1:A:3820:MET:HB3	1:A:3824:GLU:HG3	1.86	0.56
1:A:662:LEU:HD23	1:A:662:LEU:H	1.70	0.56
1:B:3008:TRP:HB2	1:B:3051:LEU:HD13	1.87	0.56
1:B:3842:TRP:CH2	1:B:3867:THR:HG22	2.40	0.56
1:A:3244:ASP:OD1	1:A:3247:ARG:NH1	2.37	0.56
1:A:3327:ASN:HB3	1:A:3384:HIS:O	2.06	0.56
1:B:2359:LYS:H	1:B:2359:LYS:HD2	1.71	0.56
1:B:2797:VAL:HG13	1:B:2804:ILE:HG21	1.87	0.56
1:B:2877:SER:HB2	1:B:2925:GLU:HB3	1.86	0.56
1:B:3617:LEU:HD13	1:B:3636:PHE:CD2	2.41	0.56
1:B:414:LEU:HD12	1:B:464:VAL:HG21	1.86	0.56
1:A:1076:LEU:HB2	1:A:1123:THR:HG22	1.88	0.56
1:A:2251:ILE:HD11	1:A:2288:TYR:CZ	2.40	0.56
1:A:2591:ILE:HD11	1:A:2792:THR:HB	1.88	0.56
1:A:3662:ILE:HA	1:A:3665:MET:HE2	1.86	0.56
1:B:3480:LEU:HD11	1:B:3510:GLN:OE1	2.05	0.56
1:B:3630:ARG:HG2	1:B:3632:PHE:H	1.70	0.56
1:A:2528:GLU:O	1:A:2529:THR:HG22	2.06	0.56
1:A:2826:LEU:HA	1:A:2829:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2923:TRP:CE3	1:A:2946:GLU:HG3	2.41	0.56
1:B:3588:TRP:HH2	1:B:3651:LEU:HD21	1.70	0.56
1:B:3631:LYS:HD3	1:B:3682:GLU:HB3	1.87	0.56
1:A:2083:LEU:H	1:A:2083:LEU:HD12	1.70	0.56
1:A:3514:VAL:HG23	1:A:3517:SER:HB2	1.85	0.56
1:A:3918:LEU:O	1:A:3920:ILE:HG13	2.05	0.56
1:B:181:LEU:HB3	1:B:189:MET:HE1	1.88	0.56
1:B:2409:THR:HG23	1:B:2410:GLU:H	1.71	0.56
1:A:1504:ASP:HB3	1:A:1507:CYS:HB3	1.87	0.56
1:B:2225:HIS:O	1:B:2227:LYS:N	2.39	0.56
1:B:2940:ARG:HG3	1:B:2957:LEU:HD22	1.86	0.56
1:B:3918:LEU:O	1:B:3920:ILE:HG13	2.06	0.56
1:A:724:GLU:HG3	1:A:2743:UNK:O	2.06	0.56
1:A:2137:ILE:HG13	1:A:2138:VAL:H	1.71	0.56
1:A:354:SER:CB	1:A:358:GLU:HB2	2.36	0.56
1:A:2446:LEU:O	1:A:2451:LEU:HB2	2.06	0.56
1:A:3278:GLN:HG2	1:A:3329:LEU:HD21	1.87	0.56
1:A:385:TYR:CZ	1:A:389:ILE:HD11	2.41	0.56
1:A:704:PHE:HE1	1:A:741:ILE:HG12	1.71	0.56
1:A:2131:GLY:O	1:A:2135:ASN:ND2	2.38	0.55
1:A:242:PRO:HA	1:A:245:SER:HB3	1.88	0.55
1:B:996:THR:OG1	1:B:1040:SER:HA	2.06	0.55
1:B:1686:LEU:HD11	1:B:1721:HIS:CB	2.36	0.55
1:B:2824:LYS:O	1:B:2829:LYS:HG3	2.05	0.55
1:B:3297:VAL:HA	1:B:3300:VAL:HG22	1.87	0.55
1:B:1155:ARG:HH21	1:B:3689:ASP:HB3	1.70	0.55
1:A:3138:ILE:HG12	1:A:3189:PHE:HZ	1.71	0.55
1:A:3285:HIS:NE2	1:A:3333:THR:OG1	2.35	0.55
1:A:3463:LEU:HD13	1:A:3498:TRP:HZ2	1.71	0.55
1:B:1271:ILE:HD13	1:B:1348:LEU:HD13	1.89	0.55
1:B:1993:GLU:OE2	1:B:2230:VAL:HB	2.06	0.55
1:B:2480:ILE:O	1:B:2484:TYR:HB2	2.06	0.55
1:B:864:GLY:HA2	1:B:867:ASN:CB	2.36	0.55
1:A:4006:VAL:HG21	1:A:4044:ILE:HG12	1.88	0.55
1:B:1096:VAL:HB	1:B:1101:PHE:HE2	1.69	0.55
1:B:1563:PHE:HB2	1:B:1567:ILE:HG13	1.88	0.55
1:B:2519:LEU:HD22	1:B:2606:UNK:O	2.07	0.55
1:A:1750:LEU:HD13	1:A:1758:LEU:HB2	1.87	0.55
1:A:305:ASN:HB2	1:A:308:LEU:HB3	1.87	0.55
1:B:1752:LEU:HD12	1:B:1753:SER:N	2.21	0.55
1:A:2088:LEU:HD11	1:A:2144:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2547:SER:O	1:B:2549:LYS:N	2.40	0.55
1:B:3244:ASP:OD1	1:B:3247:ARG:NH1	2.39	0.55
1:A:1037:LEU:O	1:A:1040:SER:OG	2.21	0.55
1:A:2823:PHE:HD1	1:A:2824:LYS:HG2	1.71	0.55
1:A:2978:LYS:HG3	1:A:2981:TRP:CD2	2.41	0.55
1:A:478:CYS:HA	1:A:481:THR:HG22	1.88	0.55
1:B:446:PHE:CZ	1:B:454:GLN:HG2	2.41	0.55
1:A:3727:THR:OG1	1:A:3737:ARG:HB3	2.07	0.55
1:B:2949:THR:OG1	1:B:2990:GLU:OE2	2.23	0.55
1:B:78:PHE:O	1:B:82:ARG:NH1	2.39	0.55
1:A:1769:GLU:O	1:A:1822:ARG:NH1	2.40	0.55
1:B:483:VAL:HG23	1:B:571:SER:HB2	1.89	0.55
1:A:35:ILE:HD13	1:A:85:ILE:HG13	1.89	0.55
1:B:1040:SER:O	1:B:1049:GLN:NE2	2.39	0.55
1:A:2246:LYS:NZ	1:A:2284:ASP:OD2	2.38	0.55
1:A:2590:THR:HG22	1:A:2591:ILE:H	1.72	0.55
1:A:3888:VAL:HA	1:A:3891:SER:HB2	1.88	0.55
1:B:1538:LEU:O	1:B:1553:PHE:N	2.40	0.55
1:B:1802:TYR:CZ	1:B:1843:ILE:HD11	2.42	0.55
1:B:2856:SER:HA	1:B:2888:VAL:HG11	1.89	0.55
1:B:3121:LEU:O	1:B:3124:SER:OG	2.25	0.55
1:B:801:LYS:HA	1:B:3115:SER:HB2	1.88	0.55
1:A:1298:LEU:HB3	1:A:1367:HIS:HB3	1.88	0.54
1:A:1668:PHE:HZ	1:A:1702:LEU:HD22	1.72	0.54
1:B:2133:LEU:HD13	1:B:2146:LEU:HB3	1.88	0.54
1:A:1881:TYR:CE1	1:A:1951:VAL:HG23	2.42	0.54
1:A:351:ASN:OD1	1:A:352:VAL:N	2.39	0.54
1:A:3522:THR:HG23	1:A:3562:LEU:HD13	1.89	0.54
1:B:1090:ARG:HH11	1:B:1137:ILE:HD13	1.71	0.54
1:B:2255:LEU:HD23	1:B:2256:ILE:H	1.71	0.54
1:A:3527:GLN:HG2	1:A:3700:GLU:HB3	1.89	0.54
1:A:3760:GLN:OE1	1:A:4019:LYS:NZ	2.27	0.54
1:B:201:LEU:HD21	1:B:248:ILE:HG12	1.88	0.54
1:B:583:LEU:HD12	1:B:611:ASN:HD22	1.72	0.54
1:A:1147:LYS:O	1:A:1151:ARG:NH2	2.41	0.54
1:A:359:LEU:O	1:A:363:ILE:HG12	2.08	0.54
1:A:3811:THR:OG1	1:A:3814:ASP:OD1	2.25	0.54
1:B:1104:LEU:HD12	1:B:1134:LEU:HD23	1.89	0.54
1:B:1368:LEU:HA	1:B:1371:VAL:HG22	1.88	0.54
1:B:3692:VAL:HA	1:B:3696:ARG:NH1	2.22	0.54
1:A:2931:ARG:NH2	1:A:3043:TYR:OH	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:TYR:CE1	1:A:655:LEU:HD21	2.43	0.54
1:B:1367:HIS:O	1:B:1371:VAL:HG13	2.08	0.54
1:B:25:CYS:SG	1:B:26:GLY:N	2.81	0.54
1:B:2584:CYS:SG	1:B:2783:ILE:HG12	2.48	0.54
1:B:2560:ASN:ND2	1:B:2799:GLN:OE1	2.35	0.54
1:A:1228:GLY:HA3	1:A:1259:LEU:HD13	1.89	0.54
1:A:2614:UNK:HA	1:A:2795:GLN:OE1	2.08	0.54
1:A:3422:GLN:HE22	1:A:3423:GLN:HE21	1.55	0.54
1:A:4117:LEU:HB3	1:A:4126:PRO:HB2	1.90	0.54
1:B:1206:LEU:O	1:B:1210:ASP:HB2	2.08	0.54
1:B:2140:LEU:HD21	1:B:2178:GLY:HA2	1.90	0.54
1:B:334:HIS:HB3	1:B:337:LYS:HD2	1.89	0.54
1:B:522:PRO:HB3	1:B:526:ASP:CG	2.28	0.54
1:A:12:LEU:HD21	1:A:58:VAL:HG12	1.89	0.54
1:A:1760:GLU:O	1:A:1764:GLU:HG2	2.07	0.54
1:A:1896:ILE:HG22	1:A:1911:LEU:H	1.71	0.54
1:B:1967:PHE:CE1	1:B:2129:LEU:HD11	2.41	0.54
1:B:2409:THR:O	1:B:2411:LEU:N	2.40	0.54
1:B:3443:PRO:HA	1:B:3471:ILE:HD11	1.89	0.54
1:B:346:TYR:HA	1:B:349:ILE:HG22	1.89	0.54
1:A:1101:PHE:CE1	1:A:1138:ILE:HG12	2.43	0.54
1:A:201:LEU:HD21	1:A:248:ILE:HG12	1.88	0.54
1:B:1802:TYR:CE1	1:B:1843:ILE:HD11	2.43	0.54
1:B:2582:SER:HB2	1:B:2781:PRO:HD2	1.90	0.54
1:A:3949:ALA:HB1	1:A:3957:GLU:HG3	1.89	0.54
1:B:1504:ASP:HB3	1:B:1507:CYS:HB3	1.89	0.54
1:B:1881:TYR:CE1	1:B:1951:VAL:HG23	2.43	0.54
1:B:860:GLY:HA3	1:B:3136:THR:OG1	2.08	0.54
1:A:2165:LEU:HD21	1:A:2208:ASP:OD2	2.08	0.54
1:B:204:LEU:O	1:B:208:MET:HB2	2.08	0.54
1:B:662:LEU:HD23	1:B:662:LEU:H	1.73	0.54
1:A:2091:HIS:O	1:A:2092:GLU:HG2	2.08	0.53
1:A:2188:GLU:O	1:A:2192:THR:HG22	2.08	0.53
1:A:860:GLY:HA2	1:A:3132:VAL:HG23	1.89	0.53
1:B:645:TRP:O	1:B:649:PHE:HB2	2.08	0.53
1:A:2996:LEU:HD13	1:A:3039:THR:HB	1.90	0.53
1:B:1575:LEU:HD23	1:B:1617:LYS:HG2	1.91	0.53
1:B:1758:LEU:O	1:B:1762:MET:HB2	2.08	0.53
1:B:2546:TYR:CE2	1:B:2548:PRO:HB3	2.43	0.53
1:B:3133:GLN:O	1:B:3137:GLU:HG2	2.08	0.53
1:A:1090:ARG:HH11	1:A:1137:ILE:HD13	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1633:TRP:CZ2	1:A:1674:THR:HG22	2.44	0.53
1:A:2464:HIS:ND1	1:A:2465:PRO:O	2.41	0.53
1:A:3057:ALA:C	1:A:3059:GLN:H	2.12	0.53
1:B:1825:LEU:HD11	1:B:1875:LYS:HB3	1.90	0.53
1:B:2190:VAL:HA	1:B:2193:ILE:HG22	1.90	0.53
1:B:2234:ASN:O	1:B:2238:ILE:HG13	2.08	0.53
1:B:464:VAL:O	1:B:468:LEU:HD23	2.09	0.53
1:A:1089:PHE:CE1	1:A:1096:VAL:HA	2.44	0.53
1:A:3243:ILE:HD13	1:A:3259:LEU:HD13	1.91	0.53
1:A:3328:ILE:HD11	1:A:3412:ALA:HB2	1.91	0.53
1:B:1153:LEU:HD12	1:B:1154:PRO:HD2	1.90	0.53
1:B:1291:LEU:H	1:B:1291:LEU:HD12	1.74	0.53
1:B:1503:LEU:HD12	1:B:1508:LYS:HE2	1.89	0.53
1:B:2894:GLU:OE2	1:B:3901:ARG:NH2	2.31	0.53
1:B:859:LEU:HD21	1:B:870:LEU:HD13	1.91	0.53
1:A:1718:ILE:HG23	1:A:1722:PHE:CD2	2.44	0.53
1:A:2877:SER:HB2	1:A:2925:GLU:HB3	1.91	0.53
1:A:3411:ASP:OD1	1:A:3411:ASP:N	2.41	0.53
1:A:544:ILE:HG13	1:A:545:LEU:HG	1.90	0.53
1:B:1195:VAL:HG23	1:B:1196:PRO:HD3	1.89	0.53
1:B:1854:ARG:O	1:B:1866:GLN:NE2	2.41	0.53
1:B:8:VAL:HG12	1:B:9:ARG:H	1.73	0.53
1:A:451:PRO:O	1:A:452:LYS:HG2	2.09	0.53
1:A:418:ALA:HB2	1:A:464:VAL:HG23	1.91	0.53
1:A:654:ILE:O	1:A:658:THR:OG1	2.26	0.53
1:A:1195:VAL:HG23	1:A:1196:PRO:HD3	1.91	0.53
1:A:1297:PHE:CZ	1:A:1301:ILE:HD13	2.44	0.53
1:B:279:ALA:HB1	1:B:322:GLN:HG3	1.90	0.53
1:A:1463:LEU:HG	1:A:1466:ASN:HB2	1.90	0.53
1:A:2492:ASP:HB3	1:A:2495:SER:H	1.74	0.53
1:A:966:PHE:CE1	1:A:969:LEU:HD12	2.43	0.53
1:B:2182:ILE:HD11	1:B:2185:MET:HB3	1.90	0.53
1:A:410:MET:HG2	1:A:442:GLN:HB2	1.90	0.53
1:B:1884:LEU:HD23	1:B:1885:PRO:HD2	1.91	0.53
1:A:1368:LEU:HA	1:A:1371:VAL:HG22	1.91	0.52
1:A:3975:LYS:HB2	1:A:3977:THR:HG22	1.91	0.52
1:A:2304:VAL:HG11	1:A:2344:LEU:HG	1.90	0.52
1:A:3325:ASP:HA	1:A:3328:ILE:HD12	1.91	0.52
1:A:342:MET:HE3	1:A:345:PHE:HD2	1.74	0.52
1:B:157:TYR:OH	1:B:195:ASN:HB3	2.09	0.52
1:A:1955:VAL:O	1:A:1957:ASN:ND2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3786:LEU:HD21	1:A:3983:ILE:HD12	1.92	0.52
1:B:1346:THR:HG23	1:B:1405:ALA:HB2	1.91	0.52
1:B:2532:PRO:HB2	1:B:2537:ASP:HB2	1.90	0.52
1:B:3360:LEU:HG	1:B:3373:VAL:HG21	1.91	0.52
1:B:531:PHE:HA	1:B:534:LEU:HD12	1.90	0.52
1:A:1104:LEU:HD12	1:A:1134:LEU:HB3	1.92	0.52
1:A:1134:LEU:O	1:A:1138:ILE:HG13	2.10	0.52
1:A:1990:PHE:HE2	1:A:2144:LEU:HD11	1.74	0.52
1:A:3535:ILE:HD12	1:A:3759:ARG:CZ	2.40	0.52
1:B:1297:PHE:CZ	1:B:1301:ILE:HD13	2.45	0.52
1:B:3319:ASN:O	1:B:3323:PHE:HB2	2.10	0.52
1:A:1279:LEU:HD23	1:A:1279:LEU:H	1.74	0.52
1:A:2546:TYR:HH	1:A:2854:PHE:HE2	1.58	0.52
1:A:765:LEU:HD23	1:A:766:ALA:H	1.73	0.52
1:B:1962:TYR:O	1:B:1967:PHE:HD2	1.92	0.52
1:B:2188:GLU:O	1:B:2191:ALA:HB3	2.08	0.52
1:B:113:SER:O	1:B:117:LYS:HG2	2.10	0.52
1:B:3341:LEU:HD13	1:B:3374:ILE:HG12	1.92	0.52
1:A:3330:LEU:HD13	1:A:3384:HIS:CE1	2.44	0.52
1:A:3654:MET:HG2	1:A:3656:LEU:HB2	1.92	0.52
1:A:3667:LEU:HA	1:A:3670:MET:HE3	1.91	0.52
1:A:9:ARG:HB2	1:A:57:LEU:HD11	1.92	0.52
1:A:3761:ASP:HA	1:A:3764:VAL:HG22	1.92	0.52
1:A:655:LEU:HD22	1:A:1389:VAL:HG12	1.91	0.52
1:A:96:MET:SD	1:A:96:MET:N	2.83	0.52
1:B:1765:VAL:HA	1:B:1768:ARG:HB2	1.91	0.52
1:B:1481:THR:HG22	1:B:1524:LEU:HD11	1.91	0.52
1:B:1948:ALA:O	1:B:1952:ILE:HG13	2.10	0.52
1:B:2402:LEU:O	1:B:2405:VAL:HG23	2.10	0.52
1:B:3913:ILE:HB	1:B:3984:MET:HG2	1.91	0.52
1:A:3028:ASN:HA	1:A:3031:TRP:CD1	2.31	0.52
1:A:3617:LEU:HD22	1:A:3636:PHE:CE2	2.45	0.52
1:A:19:LEU:CD2	1:A:71:LYS:HG3	2.39	0.52
1:A:749:VAL:N	1:A:750:PRO:HD2	2.25	0.52
1:A:794:PRO:CG	1:A:873:VAL:HB	2.41	0.52
1:B:3786:LEU:HD21	1:B:3983:ILE:HD12	1.91	0.52
1:A:1283:GLY:HA2	1:A:1358:LEU:CD1	2.40	0.51
1:A:1572:LEU:HD11	1:A:1604:SER:HB3	1.92	0.51
1:A:3567:VAL:HG11	1:A:3697:ASN:HB3	1.90	0.51
1:A:3588:TRP:HH2	1:A:3651:LEU:HD21	1.74	0.51
1:A:898:PHE:HD2	1:A:903:PRO:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3586:LYS:HD3	1:B:3667:LEU:HD21	1.91	0.51
1:B:738:HIS:NE2	1:B:745:VAL:HG23	2.24	0.51
1:A:1071:ASN:HD21	1:A:1073:PHE:HB2	1.75	0.51
1:A:86:LEU:HB2	1:A:126:PRO:HB2	1.92	0.51
1:B:1142:HIS:CE1	1:B:1146:ASN:HA	2.45	0.51
1:A:1427:SER:HA	1:A:1430:GLU:HG2	1.92	0.51
1:B:496:VAL:HG12	1:B:497:LEU:H	1.75	0.51
1:B:683:PHE:O	1:B:740:ILE:HG12	2.10	0.51
1:B:996:THR:HA	1:B:1001:PHE:HD1	1.74	0.51
1:A:1724:MET:SD	1:A:1724:MET:N	2.81	0.51
1:A:1783:ARG:HD2	1:A:1830:HIS:ND1	2.24	0.51
1:A:1896:ILE:HD13	1:A:1906:THR:O	2.11	0.51
1:A:3144:PHE:HE1	1:A:3156:PRO:HB2	1.75	0.51
1:A:323:VAL:HG13	1:A:369:PHE:HZ	1.75	0.51
1:A:414:LEU:HG	1:A:464:VAL:HG21	1.92	0.51
1:A:890:LYS:HD3	1:A:909:VAL:HG13	1.93	0.51
1:B:178:LEU:HD23	1:B:181:LEU:HD12	1.92	0.51
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.93	0.51
1:B:1142:HIS:ND1	1:B:1145:LEU:O	2.44	0.51
1:B:1633:TRP:CZ2	1:B:1674:THR:HG22	2.46	0.51
1:B:2461:PHE:HB2	1:B:2473:MET:HG3	1.92	0.51
1:B:3506:LEU:HA	1:B:3511:ALA:HB1	1.91	0.51
1:A:2251:ILE:HD12	1:A:2253:TYR:CE2	2.46	0.51
1:B:1851:LEU:O	1:B:1870:LYS:NZ	2.38	0.51
1:A:1686:LEU:HD22	1:A:1721:HIS:CD2	2.46	0.51
1:A:2886:GLN:N	1:A:2887:PRO:HD3	2.25	0.51
1:A:3258:LEU:HA	1:A:3261:GLU:HG2	1.91	0.51
1:B:1020:PRO:HA	1:B:1073:PHE:CE1	2.45	0.51
1:B:1102:GLU:O	1:B:1154:PRO:HB3	2.11	0.51
1:B:1575:LEU:HG	1:B:1576:ASP:H	1.76	0.51
1:A:2223:VAL:HG23	1:A:2234:ASN:HB3	1.93	0.51
1:A:2575:PRO:HB3	1:A:2787:HIS:CE1	2.46	0.51
1:B:1055:ASN:O	1:B:1058:SER:OG	2.22	0.51
1:B:2101:VAL:HG12	1:B:2156:VAL:HG21	1.92	0.51
1:B:3718:ARG:H	1:B:3743:HIS:CE1	2.28	0.51
1:B:1947:CYS:O	1:B:1951:VAL:HG12	2.11	0.51
1:B:354:SER:HB2	1:B:359:LEU:CB	2.41	0.51
1:B:4008:GLU:O	1:B:4010:SER:N	2.44	0.51
1:A:2288:TYR:HD1	1:A:2291:GLN:HB2	1.76	0.51
1:A:3545:THR:CG2	1:A:3546:SER:H	2.22	0.51
1:A:3506:LEU:HD22	1:A:3555:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3585:PHE:HD2	1:A:3667:LEU:HD13	1.75	0.51
1:A:661:PRO:HD2	1:A:662:LEU:HD23	1.93	0.51
1:A:718:MET:HA	1:A:721:TYR:CD2	2.46	0.51
1:B:3958:LEU:HB2	1:B:4116:ILE:HG23	1.93	0.51
1:B:532:ARG:O	1:B:536:SER:HB3	2.10	0.51
1:A:1766:LEU:HG	1:A:1778:PHE:HD2	1.76	0.50
1:A:3842:TRP:CZ2	1:A:3867:THR:HG22	2.46	0.50
1:B:1027:ASP:OD1	1:B:1027:ASP:N	2.43	0.50
1:B:3271:ASP:HA	1:B:3274:VAL:HG12	1.93	0.50
1:B:60:SER:HB2	1:B:63:PHE:O	2.11	0.50
1:B:782:ARG:O	1:B:786:GLN:HG3	2.11	0.50
1:A:2472:GLN:O	1:A:2476:ILE:HG23	2.12	0.50
1:A:3354:ASP:O	1:A:3358:ARG:HG2	2.11	0.50
1:B:1766:LEU:HG	1:B:1778:PHE:CD2	2.44	0.50
1:B:3717:VAL:HA	1:B:3743:HIS:HE1	1.76	0.50
1:A:1038:LYS:HD3	1:A:1042:LYS:HE3	1.94	0.50
1:A:3630:ARG:HG2	1:A:3632:PHE:H	1.76	0.50
1:B:2004:TYR:CZ	1:B:2187:VAL:HG11	2.46	0.50
1:B:2249:LEU:HG	1:B:2285:LEU:HD13	1.94	0.50
1:B:3542:PHE:CG	1:B:3552:LYS:HG2	2.47	0.50
1:B:495:VAL:HG12	1:B:496:VAL:H	1.76	0.50
1:A:1104:LEU:HD13	1:A:1138:ILE:HD11	1.92	0.50
1:A:1653:LEU:HB3	1:A:1698:PHE:CD1	2.47	0.50
1:A:2409:THR:O	1:A:2411:LEU:HB2	2.11	0.50
1:A:3619:ASP:HB2	1:A:3622:ALA:HB2	1.93	0.50
1:B:1693:VAL:O	1:B:1696:LEU:HD23	2.12	0.50
1:B:2887:PRO:HB3	1:B:3898:LEU:HD22	1.94	0.50
1:B:3065:ILE:HG23	1:B:3078:LEU:HD21	1.94	0.50
1:B:3648:GLY:O	1:B:3652:LEU:HD12	2.11	0.50
1:A:1848:ILE:O	1:A:1852:LYS:HB2	2.12	0.50
1:A:1861:SER:O	1:A:1865:THR:OG1	2.24	0.50
1:A:2138:VAL:HG12	1:A:2143:ARG:HB2	1.92	0.50
1:A:487:LEU:HA	1:A:490:ILE:HG12	1.94	0.50
1:B:2419:ASP:HB2	1:B:2422:GLN:HB2	1.94	0.50
1:B:479:ILE:HA	1:B:482:VAL:HG12	1.93	0.50
1:B:487:LEU:HD21	1:B:568:PHE:HE1	1.77	0.50
1:B:780:ILE:HG21	1:B:785:MET:SD	2.52	0.50
1:B:786:GLN:HA	1:B:789:TYR:CD2	2.46	0.50
1:A:2375:ALA:O	1:A:2379:MET:N	2.44	0.50
1:A:3772:ASN:HD21	1:A:3790:THR:HG23	1.76	0.50
1:A:3992:ARG:HD3	1:A:4100:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1554:SER:OG	1:B:1557:GLU:HB2	2.12	0.50
1:B:1934:LEU:H	1:B:1934:LEU:HD23	1.75	0.50
1:B:2263:LYS:HA	1:B:2309:PHE:CE2	2.46	0.50
1:B:3674:SER:O	1:B:3676:PRO:HD3	2.12	0.50
1:B:897:PRO:HA	1:B:902:LYS:HG3	1.93	0.50
1:B:898:PHE:HD2	1:B:903:PRO:HD2	1.75	0.50
1:A:1681:ASP:O	1:A:1683:LYS:N	2.37	0.50
1:A:2281:MET:SD	1:A:2287:PRO:HD3	2.51	0.50
1:A:2402:LEU:HD13	1:A:2434:VAL:HG23	1.94	0.50
1:A:3533:PHE:HE2	1:A:3559:LYS:HD3	1.76	0.50
1:B:1335:CYS:HB3	1:B:1384:PHE:CE1	2.47	0.50
1:B:1566:THR:O	1:B:1570:GLU:HG2	2.12	0.50
1:B:1602:ASP:HA	1:B:2045:PHE:HE2	1.77	0.50
1:B:3462:ARG:NH1	1:B:3497:SER:OG	2.45	0.50
1:B:3881:ASP:N	1:B:3881:ASP:OD1	2.43	0.50
1:A:1154:PRO:HG2	1:A:1157:PHE:HB2	1.93	0.50
1:A:1579:VAL:O	1:A:1583:MET:HG2	2.12	0.50
1:A:94:GLU:OE1	1:A:133:LYS:HD2	2.11	0.50
1:B:1837:ARG:HG3	1:B:1884:LEU:HD11	1.94	0.50
1:B:3992:ARG:NH1	1:B:4103:GLN:OE1	2.44	0.50
1:B:388:LEU:HD23	1:B:420:VAL:HG11	1.93	0.50
1:A:2182:ILE:HG23	1:A:2186:VAL:HG21	1.93	0.50
1:A:2359:LYS:H	1:A:2359:LYS:HD2	1.77	0.50
1:A:865:GLN:HG2	1:A:3170:ASP:HB3	1.94	0.50
1:A:385:TYR:CZ	1:A:389:ILE:CD1	2.95	0.50
1:B:108:LYS:HG2	1:B:131:LEU:HD11	1.94	0.50
1:B:1833:LEU:HG	1:B:1835:ALA:H	1.77	0.50
1:B:3586:LYS:HG2	1:B:3667:LEU:HD11	1.94	0.50
1:B:670:LEU:HA	1:B:673:THR:HG22	1.93	0.50
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.45	0.49
1:A:997:ASN:OD1	1:A:998:ASN:N	2.44	0.49
1:B:1082:PHE:HA	1:B:1085:ILE:HG12	1.92	0.49
1:B:200:PHE:HD1	1:B:223:CYS:SG	2.34	0.49
1:B:933:LEU:HB2	1:B:2793:PRO:HB2	1.94	0.49
1:B:3532:PRO:HA	1:B:3535:ILE:HG12	1.93	0.49
1:A:2393:LEU:HA	1:A:2396:LEU:HD12	1.94	0.49
1:A:3422:GLN:HE21	1:A:3423:GLN:HG2	1.77	0.49
1:B:1923:PHE:HA	1:B:1941:HIS:CG	2.46	0.49
1:B:898:PHE:CD2	1:B:903:PRO:HD2	2.47	0.49
1:A:3421:ASP:OD1	1:A:3467:ARG:NE	2.45	0.49
1:A:393:LYS:HA	1:A:397:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1099:PHE:CZ	1:B:1152:ARG:HD2	2.47	0.49
1:B:1611:GLN:HG2	1:B:1611:GLN:O	2.12	0.49
1:A:3049:LEU:HD22	1:A:3085:GLU:HG3	1.94	0.49
1:A:3259:LEU:HD12	1:A:3276:TRP:NE1	2.27	0.49
1:B:1612:LYS:C	1:B:1614:GLN:N	2.65	0.49
1:B:3798:SER:O	1:B:3799:ARG:HG2	2.12	0.49
1:A:1783:ARG:HB3	1:A:1830:HIS:CG	2.47	0.49
1:A:683:PHE:HB3	1:A:740:ILE:HG13	1.93	0.49
1:A:863:GLY:O	1:A:867:ASN:HB2	2.13	0.49
1:B:1406:LEU:CB	1:B:1415:LEU:HD11	2.41	0.49
1:B:3867:THR:HG21	1:B:4119:ARG:CZ	2.43	0.49
1:A:1342:MET:O	1:A:1346:THR:HG23	2.11	0.49
1:A:476:ARG:NH2	1:A:1503:LEU:HD22	2.28	0.49
1:A:1612:LYS:O	1:A:1613:HIS:ND1	2.45	0.49
1:A:3065:ILE:HG23	1:A:3078:LEU:HD21	1.94	0.49
1:A:538:ASP:OD2	1:A:561:ASN:N	2.45	0.49
1:A:767:GLU:HG2	1:A:851:ILE:HD11	1.94	0.49
1:B:2310:VAL:HG12	1:B:2316:TYR:CG	2.47	0.49
1:B:305:ASN:OD1	1:B:306:VAL:N	2.46	0.49
1:A:476:ARG:HH22	1:A:1503:LEU:HD22	1.78	0.49
1:A:3082:TYR:HB3	1:A:3085:GLU:OE1	2.13	0.49
1:A:619:ASP:OD2	1:A:2035:THR:HB	2.13	0.49
1:B:1206:LEU:O	1:B:1210:ASP:CB	2.59	0.49
1:A:1895:LYS:O	1:A:1899:VAL:HG23	2.12	0.49
1:A:2250:SER:O	1:A:2252:PRO:HD3	2.13	0.49
1:A:3095:ASP:OD1	1:A:3098:ARG:HB2	2.13	0.49
1:A:532:ARG:HG2	1:A:637:LYS:HE2	1.94	0.49
1:B:1334:LYS:O	1:B:1337:VAL:HG22	2.12	0.49
1:B:1747:LEU:HD12	1:B:1781:SER:HB2	1.95	0.49
1:B:1900:PHE:HB3	1:B:1904:CYS:SG	2.53	0.49
1:B:631:ARG:HH21	1:B:668:LYS:HD3	1.78	0.49
1:B:997:ASN:OD1	1:B:998:ASN:N	2.45	0.49
1:A:110:THR:O	1:A:114:VAL:HG23	2.13	0.49
1:A:1425:ALA:HA	1:A:1428:ILE:HD12	1.95	0.49
1:A:2219:LEU:O	1:A:2223:VAL:HB	2.13	0.49
1:A:2459:VAL:HB	1:A:2505:VAL:HG21	1.95	0.49
1:B:339:GLN:O	1:B:343:GLU:HG2	2.12	0.49
1:B:4054:ALA:HA	1:B:4096:SER:HA	1.95	0.49
1:A:370:ALA:HB1	1:A:420:VAL:HG23	1.94	0.48
1:A:2887:PRO:CG	1:A:3895:GLU:HG2	2.42	0.48
1:A:3120:LEU:HD11	1:A:3896:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3937:VAL:C	1:A:3938:ILE:HD13	2.32	0.48
1:A:938:VAL:HA	1:A:941:MET:HG2	1.95	0.48
1:B:1204:PRO:HG2	1:B:1205:ASN:ND2	2.28	0.48
1:B:1730:PRO:HG2	1:B:1733:THR:HG21	1.95	0.48
1:B:3444:ALA:HA	1:B:3479:THR:HG21	1.95	0.48
1:A:1096:VAL:HB	1:A:1101:PHE:HE2	1.78	0.48
1:A:264:ARG:O	1:A:266:ALA:N	2.46	0.48
1:A:3778:ASP:OD1	1:A:3779:SER:N	2.46	0.48
1:A:538:ASP:HB2	1:A:561:ASN:OD1	2.14	0.48
1:A:718:MET:HE2	1:A:726:LEU:HG	1.96	0.48
1:B:1606:ARG:HG2	1:B:2042:GLN:OE1	2.12	0.48
1:B:1668:PHE:O	1:B:1671:VAL:HG22	2.13	0.48
1:B:2249:LEU:O	1:B:2251:ILE:N	2.46	0.48
2:D:728:LEU:O	2:D:731:MET:HB2	2.12	0.48
1:A:479:ILE:HA	1:A:482:VAL:HG12	1.96	0.48
1:B:1739:TYR:O	1:B:1743:MET:HG2	2.14	0.48
1:B:2294:ILE:HG22	1:B:2295:GLN:H	1.77	0.48
1:B:267:VAL:HG23	1:B:268:PRO:HD3	1.94	0.48
1:B:3937:VAL:C	1:B:3938:ILE:HD13	2.33	0.48
1:A:1853:SER:OG	1:A:1870:LYS:NZ	2.42	0.48
1:A:1984:LEU:HD11	1:A:2139:PRO:HG2	1.95	0.48
1:A:1992:VAL:HG23	1:A:1993:GLU:H	1.77	0.48
1:A:2182:ILE:HG12	1:A:2186:VAL:HG23	1.94	0.48
1:A:2411:LEU:HG	1:A:2415:LEU:HD13	1.94	0.48
1:A:2885:GLN:C	1:A:2887:PRO:HD3	2.33	0.48
1:B:1103:ALA:HB1	1:B:1106:ILE:HB	1.94	0.48
1:B:620:PHE:O	1:B:624:ILE:HG12	2.14	0.48
1:B:972:LEU:HD13	1:B:984:TYR:CE2	2.49	0.48
1:A:720:GLN:OE1	1:A:1026:ARG:NH2	2.47	0.48
1:A:1071:ASN:OD1	1:A:1072:ALA:N	2.47	0.48
1:A:1459:HIS:CG	1:A:1520:ALA:HB1	2.48	0.48
1:A:2085:MET:HA	1:A:2089:ASN:HB2	1.95	0.48
1:A:3050:LYS:NZ	1:A:3181:ASP:OD1	2.34	0.48
1:A:3448:GLU:HG2	1:A:3482:LEU:HD11	1.95	0.48
1:A:3760:GLN:O	1:A:3764:VAL:HG13	2.14	0.48
1:B:1328:GLU:OE1	1:B:1328:GLU:N	2.45	0.48
1:B:2301:GLN:HA	1:B:2344:LEU:HD21	1.95	0.48
1:B:256:ILE:HB	1:B:300:TRP:HZ3	1.77	0.48
1:B:3413:TYR:CD1	1:B:3449:LYS:HG3	2.49	0.48
1:A:1753:SER:O	1:A:1755:SER:N	2.46	0.48
1:A:3307:LEU:HD22	1:A:3330:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:HB3	1:A:467:ALA:HB1	1.95	0.48
1:A:421:LEU:HD22	1:A:424:LEU:HD23	1.96	0.48
1:B:1626:TRP:CE3	1:B:1674:THR:HG21	2.48	0.48
1:B:2245:TRP:O	1:B:2247:ASP:N	2.46	0.48
1:B:570:LYS:O	1:B:574:LYS:HB2	2.12	0.48
1:A:108:LYS:NZ	1:A:147:PHE:HB3	2.28	0.48
1:A:2257:PHE:HA	1:A:2260:PHE:CE2	2.49	0.48
1:B:1124:ILE:H	1:B:1124:ILE:HD12	1.79	0.48
1:B:272:LEU:HD13	1:B:312:ALA:HA	1.94	0.48
1:A:135:LEU:HB2	1:A:180:LEU:HD21	1.95	0.48
1:A:2852:PRO:HG2	1:A:2853:PRO:HD3	1.96	0.48
1:A:3701:ILE:HD12	1:A:3740:ILE:HD11	1.96	0.48
1:A:572:VAL:HA	1:A:575:ILE:HD12	1.96	0.48
1:B:1926:ASN:HB3	1:B:1974:ASN:O	2.14	0.48
1:B:1956:PHE:HB2	1:B:1961:PHE:HE2	1.79	0.48
1:B:3069:MET:SD	1:B:3075:LYS:HG3	2.54	0.48
1:A:2934:GLY:HA2	1:A:2936:TYR:CE2	2.49	0.48
1:A:3778:ASP:HB3	1:A:3781:CYS:HB2	1.95	0.48
1:B:3300:VAL:HG11	1:B:3336:ILE:HG21	1.96	0.48
1:A:2168:LEU:HB3	1:A:2189:ILE:HG23	1.95	0.48
1:A:2277:LEU:HA	1:A:2280:VAL:HG12	1.96	0.48
1:A:296:VAL:O	1:A:300:TRP:HD1	1.97	0.48
1:A:726:LEU:HD21	1:A:754:MET:HG2	1.95	0.48
1:B:2320:ALA:O	1:B:2367:VAL:HG22	2.14	0.48
1:B:3407:ALA:H	1:B:3410:ILE:HG23	1.78	0.48
1:A:2251:ILE:HD12	1:A:2253:TYR:HE2	1.79	0.47
1:A:3171:ALA:HB1	1:A:3248:LYS:HD2	1.96	0.47
1:A:3413:TYR:CE1	1:A:3449:LYS:HG3	2.48	0.47
1:A:366:TYR:CZ	1:A:384:MET:HG2	2.49	0.47
1:A:977:ASP:OD1	1:A:978:GLN:N	2.47	0.47
1:B:1029:CYS:O	1:B:1032:CYS:HB2	2.14	0.47
1:B:1875:LYS:O	1:B:1878:ASP:HB2	2.14	0.47
1:B:3596:LEU:HD22	1:B:3606:ILE:HD12	1.96	0.47
1:A:2190:VAL:HA	1:A:2193:ILE:HG22	1.95	0.47
1:B:1586:SER:OG	1:B:1628:LYS:O	2.29	0.47
1:B:215:PRO:O	1:B:216:LYS:HG2	2.14	0.47
1:B:2572:TYR:N	1:B:2573:PRO:HD3	2.29	0.47
1:B:3772:ASN:HD21	1:B:3790:THR:HG23	1.78	0.47
1:B:2937:ASP:OD1	1:B:3784:ARG:NH2	2.47	0.47
1:A:1102:GLU:O	1:A:1105:VAL:HG22	2.14	0.47
1:A:1203:SER:HB3	1:A:1204:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PHE:HE1	1:A:196:LEU:HD13	1.79	0.47
1:A:1977:ILE:O	1:A:1981:LEU:HB2	2.15	0.47
1:A:565:TYR:HE1	1:A:642:PHE:HD1	1.61	0.47
1:B:3083:SER:HA	1:B:3086:LEU:HD12	1.96	0.47
1:A:1361:LYS:O	1:A:1365:ASN:HB2	2.15	0.47
1:A:2393:LEU:H	1:A:2393:LEU:HD12	1.78	0.47
1:A:3599:THR:HG23	1:A:3601:VAL:HG12	1.96	0.47
1:B:2004:TYR:HB3	1:B:2233:HIS:CE1	2.49	0.47
1:B:3307:LEU:HA	1:B:3307:LEU:HD12	1.68	0.47
1:B:3487:ILE:HG23	1:B:3516:HIS:NE2	2.29	0.47
1:B:446:PHE:CE1	1:B:454:GLN:HG2	2.49	0.47
1:A:3049:LEU:HD21	1:A:3088:LEU:HD12	1.97	0.47
1:A:790:LYS:HD3	1:A:790:LYS:H	1.79	0.47
1:B:995:PHE:HB3	1:B:1006:THR:HG22	1.97	0.47
1:B:2106:ARG:NH2	1:B:2155:GLU:OE1	2.47	0.47
1:B:2873:PRO:HB3	1:B:2922:ARG:HA	1.97	0.47
1:A:1519:PHE:CZ	1:A:1528:LEU:HD22	2.49	0.47
1:A:1787:ARG:HG2	1:A:1787:ARG:O	2.15	0.47
1:A:3659:PHE:CE2	1:A:3661:ASP:HB3	2.50	0.47
1:A:646:VAL:O	1:A:650:SER:OG	2.28	0.47
1:B:1658:SER:HB3	1:B:1661:PHE:CE1	2.47	0.47
1:B:2574:ASN:C	1:B:2576:MET:H	2.16	0.47
1:B:606:SER:OG	1:B:1023:SER:HB2	2.15	0.47
1:A:1124:ILE:HD12	1:A:1124:ILE:H	1.79	0.47
1:A:1725:GLN:O	1:A:1772:HIS:ND1	2.45	0.47
1:A:3544:ASP:OD1	1:A:3549:HIS:NE2	2.47	0.47
1:A:3693:GLU:HG2	1:A:3694:PHE:H	1.80	0.47
1:A:373:CYS:HA	1:A:376:ILE:CG2	2.45	0.47
1:A:3860:LYS:HB3	1:A:4076:ASP:OD2	2.14	0.47
1:A:425:ASP:N	1:A:425:ASP:OD1	2.48	0.47
1:B:1202:ARG:O	1:B:1207:TRP:HB2	2.15	0.47
1:B:125:ILE:HB	1:B:126:PRO:HD3	1.96	0.47
1:B:786:GLN:HA	1:B:789:TYR:HD2	1.79	0.47
1:A:1359:LEU:HB3	1:A:1363:LEU:HD11	1.96	0.47
1:A:1433:ALA:HB3	1:A:1436:LEU:HG	1.97	0.47
1:B:1426:GLN:HG2	1:B:1427:SER:N	2.30	0.47
1:B:3955:VAL:HG11	1:B:4121:TRP:CE3	2.50	0.47
1:B:859:LEU:HG	1:B:867:ASN:ND2	2.25	0.47
1:B:986:PRO:O	1:B:990:GLN:HG3	2.14	0.47
1:A:1448:LEU:HG	1:A:1510:LEU:HD11	1.97	0.47
1:A:1765:VAL:HG23	1:A:1768:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2036:LEU:HD23	1:A:2036:LEU:HA	1.67	0.47
1:A:1949:ILE:HG12	1:A:2100:LEU:HD23	1.97	0.47
1:A:305:ASN:HB2	1:A:308:LEU:CB	2.45	0.47
1:B:1265:GLU:OE2	1:B:1340:ARG:HD2	2.15	0.47
1:B:1400:VAL:HG13	1:B:1461:ALA:HB2	1.96	0.47
1:B:1372:LEU:HD12	1:B:1402:LEU:HD23	1.97	0.47
1:B:14:ARG:HH12	1:B:34:LEU:HD21	1.80	0.47
1:B:2286:PRO:HB3	1:B:2329:TYR:CE2	2.50	0.47
1:B:3528:ALA:HB2	1:B:3705:TYR:CG	2.50	0.47
1:B:620:PHE:HZ	1:B:663:ILE:HD12	1.80	0.47
1:A:2184:TYR:H	1:A:2187:VAL:HG23	1.80	0.47
1:A:2556:SER:HB2	1:A:2799:GLN:HA	1.97	0.47
1:B:1992:VAL:HG23	1:B:1994:VAL:HG23	1.97	0.47
1:B:3479:THR:HB	1:B:3482:LEU:HD23	1.97	0.47
1:B:4126:PRO:HD2	1:B:4127:TRP:CE3	2.50	0.47
1:B:923:ASP:OD2	1:B:925:GLN:HB2	2.15	0.47
1:B:996:THR:HA	1:B:1001:PHE:CD1	2.49	0.47
1:A:1934:LEU:HD23	1:A:1934:LEU:H	1.80	0.47
1:A:2893:LEU:HD13	1:A:2926:LEU:HB2	1.97	0.47
1:A:3418:ASP:OD2	1:A:3464:LYS:NZ	2.38	0.47
1:B:1135:CYS:O	1:B:1138:ILE:HG22	2.15	0.47
1:B:2556:SER:HB2	1:B:2799:GLN:HG2	1.97	0.47
1:B:256:ILE:O	1:B:296:VAL:HG21	2.15	0.47
1:B:3130:GLN:NE2	1:B:3174:ASP:OD1	2.48	0.47
1:B:3885:ARG:HA	1:B:3888:VAL:HG12	1.97	0.47
1:B:465:PHE:HE1	1:B:482:VAL:HG11	1.80	0.47
1:A:1121:LEU:HD22	1:A:1123:THR:HG23	1.97	0.46
1:A:1146:ASN:OD1	1:A:1164:CYS:HB3	2.14	0.46
1:A:2753:UNK:O	1:A:2757:UNK:CB	2.63	0.46
1:A:2967:GLU:O	1:A:2971:GLN:HG2	2.15	0.46
1:A:358:GLU:O	1:A:361:ILE:HG12	2.15	0.46
1:B:2409:THR:O	1:B:2411:LEU:HB2	2.14	0.46
1:B:2472:GLN:O	1:B:2476:ILE:HG23	2.14	0.46
1:B:2973:ASP:O	1:B:2977:ASN:ND2	2.48	0.46
1:B:487:LEU:HD21	1:B:568:PHE:CE1	2.49	0.46
1:A:2194:LEU:HD11	1:A:2241:LEU:HD13	1.96	0.46
1:A:933:LEU:HD22	1:A:2797:VAL:HG11	1.96	0.46
1:A:2563:LEU:HD21	1:A:2812:LEU:HD11	1.97	0.46
1:A:3085:GLU:OE1	1:A:3085:GLU:N	2.34	0.46
1:A:4042:GLN:NE2	1:A:4046:TYR:HE2	2.08	0.46
1:B:1653:LEU:HB3	1:B:1698:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2458:VAL:HG13	1:B:2473:MET:HG2	1.96	0.46
1:B:253:LEU:HD11	1:B:257:ARG:HD2	1.97	0.46
1:B:852:ARG:HD3	1:B:3111:MET:SD	2.55	0.46
1:B:3120:LEU:HD23	1:B:3120:LEU:H	1.79	0.46
1:B:3129:LEU:O	1:B:3132:VAL:HG22	2.16	0.46
1:B:3389:VAL:HG21	1:B:3449:LYS:HE2	1.96	0.46
1:A:1890:HIS:ND1	1:A:1912:THR:HG21	2.30	0.46
1:B:1783:ARG:HD2	1:B:1830:HIS:ND1	2.30	0.46
1:B:3701:ILE:HD12	1:B:3740:ILE:CD1	2.34	0.46
1:A:2105:HIS:ND1	1:A:2156:VAL:HG13	2.30	0.46
1:B:2971:GLN:HA	1:B:2974:GLU:HB2	1.96	0.46
1:B:3913:ILE:O	1:B:3917:ILE:HG12	2.16	0.46
1:A:1416:GLU:O	1:A:1420:ARG:HG3	2.16	0.46
1:A:335:LYS:HB2	1:A:376:ILE:HD11	1.98	0.46
1:B:1562:LEU:HA	1:B:1562:LEU:HD23	1.75	0.46
1:B:2169:LEU:HD11	1:B:2212:ALA:HA	1.98	0.46
1:B:256:ILE:C	1:B:258:PRO:HD3	2.36	0.46
1:B:2591:ILE:HD11	1:B:2792:THR:CB	2.45	0.46
1:B:767:GLU:HG2	1:B:851:ILE:HD11	1.97	0.46
1:A:133:LYS:O	1:A:137:THR:HG22	2.15	0.46
1:A:3324:ARG:O	1:A:3328:ILE:HG13	2.16	0.46
1:B:1224:PHE:HD1	1:B:1266:CYS:SG	2.39	0.46
1:B:2482:ASP:OD2	1:B:2530:ARG:NH1	2.49	0.46
1:B:2950:LYS:HD3	1:B:2950:LYS:HA	1.64	0.46
1:B:3554:PHE:CE2	1:B:3558:ILE:HD11	2.51	0.46
1:B:3879:PRO:HG2	1:B:3882:LEU:HD22	1.98	0.46
1:B:4054:ALA:H	1:B:4103:GLN:NE2	2.14	0.46
1:B:425:ASP:OD1	1:B:425:ASP:N	2.46	0.46
1:B:677:ALA:HB1	1:B:683:PHE:HE2	1.80	0.46
1:A:2921:LEU:HD23	1:A:2921:LEU:H	1.81	0.46
1:A:3487:ILE:HG23	1:A:3516:HIS:NE2	2.31	0.46
1:A:3545:THR:CG2	1:A:3546:SER:N	2.78	0.46
1:A:418:ALA:HB1	1:A:463:LYS:HG3	1.96	0.46
1:B:1601:LEU:HD22	1:B:1618:LEU:HD21	1.96	0.46
1:B:2288:TYR:CD2	1:B:2291:GLN:HB2	2.51	0.46
1:B:2412:TYR:OH	1:B:2453:GLU:HG2	2.16	0.46
1:B:451:PRO:C	1:B:453:MET:H	2.19	0.46
1:B:749:VAL:N	1:B:750:PRO:HD2	2.30	0.46
1:A:1343:GLU:O	1:A:1346:THR:OG1	2.26	0.46
1:A:1713:VAL:O	1:A:1716:GLN:HB2	2.14	0.46
1:B:1166:LEU:HD12	1:B:1166:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1697:PRO:HG2	1:B:1752:LEU:HD11	1.98	0.46
1:B:131:LEU:HD22	1:B:177:LEU:HD21	1.97	0.46
1:B:2402:LEU:HD13	1:B:2434:VAL:HG23	1.97	0.46
1:B:2591:ILE:HD12	1:B:2591:ILE:H	1.81	0.46
1:B:3303:THR:OG1	1:B:3303:THR:O	2.32	0.46
1:B:3502:MET:SD	1:B:3514:VAL:HG21	2.56	0.46
1:A:3419:PHE:O	1:A:3422:GLN:HG3	2.16	0.46
1:B:1733:THR:O	1:B:1737:ASN:HB2	2.16	0.46
1:B:2393:LEU:H	1:B:2393:LEU:HD12	1.81	0.46
1:B:323:VAL:HG13	1:B:369:PHE:CZ	2.46	0.46
1:B:364:ARG:HH21	1:B:368:LEU:HB2	1.80	0.46
1:A:1075:ARG:NH2	1:A:1117:ASP:OD1	2.49	0.46
1:A:1100:VAL:HG12	1:A:1134:LEU:HD11	1.98	0.46
1:A:1139:GLU:OE1	1:A:1193:LYS:HE2	2.16	0.46
1:A:1352:SER:O	1:A:1354:GLU:N	2.42	0.46
1:A:1640:GLU:C	1:A:1642:LYS:H	2.19	0.46
1:A:1754:GLN:HB2	1:A:1797:LEU:HD11	1.96	0.46
1:A:1981:LEU:O	1:A:1981:LEU:HD23	2.16	0.46
1:A:2551:GLU:HG3	1:A:2849:SER:HB2	1.99	0.46
1:A:338:LEU:HD21	1:A:376:ILE:HG21	1.98	0.46
1:A:647:TYR:O	1:A:651:TYR:HB2	2.16	0.46
1:B:1797:LEU:O	1:B:1801:VAL:HG23	2.16	0.46
1:B:762:TYR:CE1	1:B:764:PRO:HD2	2.51	0.46
1:B:96:MET:N	1:B:96:MET:SD	2.89	0.46
1:A:1425:ALA:O	1:A:1429:GLU:HG2	2.16	0.45
1:A:2165:LEU:HD12	1:A:2200:ALA:HB1	1.97	0.45
1:A:3295:GLU:HA	1:A:3298:LEU:HD12	1.99	0.45
1:A:3607:GLU:OE2	1:A:3655:LYS:NZ	2.48	0.45
1:A:3694:PHE:O	1:A:3696:ARG:N	2.47	0.45
1:A:977:ASP:HB3	1:A:980:THR:HG22	1.98	0.45
1:B:1479:VAL:O	1:B:1483:LEU:HG	2.16	0.45
1:B:1684:LEU:HA	1:B:1684:LEU:HD23	1.77	0.45
1:B:2224:PHE:CE2	1:B:2226:PRO:HG3	2.51	0.45
1:B:4090:ARG:NH1	1:B:4113:ASP:OD2	2.39	0.45
1:A:2394:LYS:O	1:A:2398:LEU:HG	2.16	0.45
1:A:3658:ASP:OD1	1:A:3659:PHE:N	2.49	0.45
1:A:918:ALA:O	1:A:972:LEU:HD21	2.16	0.45
1:B:1779:GLN:NE2	1:B:1822:ARG:O	2.47	0.45
1:B:216:LYS:O	1:B:220:LEU:HD13	2.16	0.45
1:B:3082:TYR:C	1:B:3084:GLN:H	2.19	0.45
1:B:397:LEU:HD11	1:B:438:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1881:TYR:CD1	1:A:1951:VAL:HG23	2.51	0.45
1:A:2281:MET:HE1	1:A:2326:ILE:HG23	1.97	0.45
1:A:3133:GLN:O	1:A:3137:GLU:HG2	2.17	0.45
1:A:4006:VAL:HB	1:A:4040:PRO:HB3	1.99	0.45
1:A:4008:GLU:O	1:A:4010:SER:N	2.48	0.45
1:A:651:TYR:O	1:A:655:LEU:HG	2.17	0.45
1:A:907:LEU:HA	1:A:910:PHE:CZ	2.51	0.45
1:B:1423:ILE:HD12	1:B:1458:LEU:HD11	1.99	0.45
1:B:1529:VAL:HA	1:B:1532:LEU:HD12	1.97	0.45
1:B:1840:PHE:O	1:B:1843:ILE:HG22	2.16	0.45
1:B:2524:PHE:O	1:B:2530:ARG:HG2	2.16	0.45
1:B:2841:ASN:O	1:B:2845:ASN:ND2	2.37	0.45
1:B:3694:PHE:O	1:B:3696:ARG:HG3	2.15	0.45
2:C:729:LEU:O	2:C:732:ILE:HB	2.16	0.45
1:A:1224:PHE:HD1	1:A:1266:CYS:SG	2.39	0.45
1:A:3575:LEU:HB3	1:A:3800:LEU:HD21	1.98	0.45
1:A:574:LYS:HA	1:A:574:LYS:HD2	1.71	0.45
1:B:2486:ASP:O	1:B:2488:GLU:N	2.50	0.45
1:B:3659:PHE:HD2	1:B:3662:ILE:HG12	1.80	0.45
1:B:4013:TRP:HA	1:B:4016:PHE:HB3	1.98	0.45
1:B:907:LEU:CD2	1:B:940:PHE:CD2	2.99	0.45
1:A:2973:ASP:O	1:A:2977:ASN:ND2	2.47	0.45
1:A:3335:ARG:NH1	1:A:3422:GLN:HG2	2.31	0.45
1:A:743:LEU:HD12	1:A:743:LEU:O	2.16	0.45
1:B:148:LYS:O	1:B:152:LEU:HB2	2.16	0.45
1:B:1832:SER:OG	1:B:1833:LEU:N	2.50	0.45
1:B:3288:SER:HB2	1:B:3296:GLN:HG3	1.99	0.45
1:B:3354:ASP:N	1:B:3354:ASP:OD1	2.46	0.45
1:B:3862:ALA:HB3	1:B:4119:ARG:HH12	1.81	0.45
1:B:4047:ALA:HA	1:B:4050:LYS:HG2	1.98	0.45
1:A:1920:TYR:HA	1:A:1923:PHE:CZ	2.52	0.45
1:A:2787:HIS:O	1:A:2790:LEU:HG	2.17	0.45
1:A:3506:LEU:HA	1:A:3511:ALA:HB1	1.98	0.45
1:B:3455:LYS:HE2	1:B:3489:SER:O	2.17	0.45
1:A:1427:SER:O	1:A:1431:LEU:HG	2.16	0.45
1:A:1646:LEU:HD13	1:A:1692:ALA:HB2	1.98	0.45
1:A:19:LEU:O	1:A:24:ARG:NH1	2.50	0.45
1:A:253:LEU:HA	1:A:256:ILE:HG12	1.98	0.45
1:B:2004:TYR:O	1:B:2007:ILE:HB	2.17	0.45
1:A:1181:THR:HG22	1:A:1184:ARG:NH1	2.30	0.45
1:A:1580:LEU:HG	1:A:1625:HIS:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2538:ARG:O	1:A:2542:LEU:HG	2.17	0.45
1:A:3120:LEU:HD23	1:A:3120:LEU:H	1.81	0.45
1:A:376:ILE:HG23	1:A:377:ASN:H	1.82	0.45
1:A:3885:ARG:HA	1:A:3888:VAL:HG12	1.99	0.45
1:B:3061:LEU:O	1:B:3065:ILE:HG12	2.16	0.45
1:A:1143:VAL:HG23	1:A:1197:LEU:HD22	1.98	0.45
1:A:288:ASP:N	1:A:288:ASP:OD1	2.50	0.45
1:A:371:GLY:HA2	1:A:423:TYR:CD2	2.52	0.45
1:A:3948:SER:HB3	1:A:4016:PHE:HZ	1.82	0.45
1:B:1205:ASN:HA	1:B:1275:THR:HA	1.99	0.45
1:B:1941:HIS:HB3	1:B:1981:LEU:HD23	1.98	0.45
1:B:2277:LEU:HD21	1:B:2326:ILE:HD11	1.99	0.45
1:B:3493:TRP:CE3	1:B:3494:GLN:HG3	2.52	0.45
1:B:3563:ASP:CG	1:B:3568:ILE:H	2.21	0.45
1:B:3988:LEU:O	1:B:3992:ARG:HG2	2.17	0.45
1:A:2420:PHE:HE1	1:A:2435:CYS:HB2	1.82	0.45
1:A:2572:TYR:HA	1:A:2787:HIS:CD2	2.52	0.45
1:A:3476:PRO:HA	1:A:3480:LEU:HD13	1.99	0.45
1:A:583:LEU:HA	1:A:614:PRO:HA	1.99	0.45
1:B:12:LEU:HD21	1:B:58:VAL:HA	1.99	0.45
1:B:1362:ASP:OD1	1:B:1362:ASP:N	2.50	0.45
1:B:1872:GLY:O	1:B:1876:ILE:HG13	2.17	0.45
1:B:1906:THR:HG22	1:B:1906:THR:O	2.16	0.45
1:B:1877:LEU:HD13	1:B:1915:LEU:HD11	1.98	0.45
1:B:2172:ALA:HB2	1:B:2189:ILE:HG21	1.99	0.45
1:B:4005:PHE:O	1:B:4011:PHE:HZ	1.99	0.45
1:A:3813:LYS:HB2	1:A:3925:LEU:CB	2.47	0.44
1:B:1006:THR:OG1	1:B:1054:VAL:HG21	2.17	0.44
1:B:1190:LEU:HD23	1:B:1190:LEU:HA	1.80	0.44
1:B:3082:TYR:HB3	1:B:3085:GLU:OE1	2.17	0.44
1:B:3962:ARG:NH1	1:B:4125:GLU:O	2.29	0.44
1:B:487:LEU:HA	1:B:490:ILE:HG12	2.00	0.44
1:A:1878:ASP:OD2	1:A:1946:ASN:HB3	2.17	0.44
1:A:2249:LEU:O	1:A:2251:ILE:HG23	2.17	0.44
1:A:3091:LEU:O	1:A:3192:LYS:HE2	2.16	0.44
1:A:3257:LYS:HG3	1:A:3258:LEU:N	2.31	0.44
1:B:1072:ALA:HA	1:B:1075:ARG:NH2	2.32	0.44
1:B:1508:LYS:HZ2	1:B:1562:LEU:HD22	1.82	0.44
1:B:1727:ARG:HH21	1:B:1773:VAL:HG23	1.83	0.44
1:B:3113:ASN:O	1:B:3117:ILE:HG13	2.17	0.44
1:B:3450:MET:HB3	1:B:3468:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3733:ARG:HD3	1:B:3753:LYS:HG2	1.98	0.44
1:B:3811:THR:HG21	1:B:3926:ASN:ND2	2.32	0.44
1:B:4064:LEU:HD13	1:B:4077:TYR:HB3	1.98	0.44
1:B:569:VAL:HG12	1:B:573:LEU:HD23	1.99	0.44
1:A:1633:TRP:CD1	1:A:1633:TRP:N	2.85	0.44
1:B:1143:VAL:HG23	1:B:1197:LEU:HG	1.99	0.44
1:B:2168:LEU:HB2	1:B:2193:ILE:HD12	1.99	0.44
1:B:2436:LEU:HD23	1:B:2472:GLN:HB3	1.99	0.44
1:B:303:HIS:O	1:B:305:ASN:N	2.44	0.44
1:B:3295:GLU:HA	1:B:3298:LEU:HD12	1.99	0.44
1:A:1730:PRO:HG2	1:A:1733:THR:OG1	2.16	0.44
1:A:2531:LEU:HD22	1:A:2541:ALA:HB1	2.00	0.44
1:A:2801:ASP:HB3	1:A:2804:ILE:HG22	1.99	0.44
1:A:3385:LEU:HD22	1:A:3416:LEU:HB2	2.00	0.44
1:A:635:PRO:O	1:A:679:LYS:NZ	2.44	0.44
1:A:19:LEU:HD21	1:A:71:LYS:HG3	1.98	0.44
1:A:870:LEU:HB3	1:A:3129:LEU:HD11	1.99	0.44
1:B:1298:LEU:CB	1:B:1367:HIS:HB3	2.47	0.44
1:B:2894:GLU:O	1:B:2896:ALA:N	2.44	0.44
1:B:3659:PHE:CE2	1:B:3662:ILE:HG23	2.53	0.44
1:B:377:ASN:HB3	1:B:380:ASP:H	1.83	0.44
1:A:2473:MET:O	1:A:2476:ILE:HG12	2.17	0.44
1:A:2813:PHE:CD2	1:A:2861:ILE:HB	2.53	0.44
1:A:2870:SER:HB2	1:A:2922:ARG:HH22	1.81	0.44
1:B:1690:GLY:O	1:B:1693:VAL:HG12	2.18	0.44
1:B:3057:ALA:C	1:B:3059:GLN:H	2.19	0.44
1:B:720:GLN:OE1	1:B:1026:ARG:NH2	2.50	0.44
1:A:2389:PHE:CE1	1:A:2393:LEU:HD22	2.53	0.44
1:A:267:VAL:HG23	1:A:268:PRO:HD3	2.00	0.44
1:A:3833:ARG:HB3	1:A:3877:LYS:HE2	2.00	0.44
1:A:859:LEU:HD21	1:A:870:LEU:HD13	1.99	0.44
1:B:1070:PRO:HA	1:B:1113:LEU:HD21	1.99	0.44
1:B:1900:PHE:CE2	1:B:1906:THR:OG1	2.71	0.44
1:B:2404:ARG:HD2	1:B:2404:ARG:HA	1.64	0.44
1:B:605:THR:OG1	1:B:1027:ASP:HB3	2.18	0.44
1:A:1010:LEU:O	1:A:1014:LEU:HD13	2.18	0.44
1:A:2122:LEU:HD23	1:A:2122:LEU:HA	1.66	0.44
1:A:2572:TYR:N	1:A:2573:PRO:HD3	2.32	0.44
1:A:359:LEU:HD23	1:A:359:LEU:H	1.81	0.44
1:A:563:LEU:HD13	1:A:563:LEU:HA	1.84	0.44
1:B:1041:ILE:HG22	1:B:1049:GLN:HE22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2972:TYR:HB3	1:B:2998:SER:OG	2.17	0.44
1:B:3326:GLN:O	1:B:3329:LEU:HG	2.16	0.44
1:B:364:ARG:HH22	1:B:368:LEU:HD13	1.81	0.44
1:A:1633:TRP:CH2	1:A:1674:THR:HG22	2.53	0.44
1:A:1951:VAL:O	1:A:1955:VAL:HG13	2.18	0.44
1:A:1990:PHE:HZ	1:A:2144:LEU:HD21	1.83	0.44
1:A:250:ASN:O	1:A:254:LYS:HE2	2.17	0.44
1:A:2785:ILE:HG12	1:A:2786:LYS:HB2	1.99	0.44
1:A:3094:ASP:OD1	1:A:3196:LYS:NZ	2.43	0.44
1:A:336:ASN:OD1	1:A:337:LYS:HD2	2.18	0.44
1:A:3846:MET:HG2	1:A:3862:ALA:HB2	2.00	0.44
1:B:1089:PHE:CE1	1:B:1096:VAL:HA	2.53	0.44
1:B:1787:ARG:HB3	1:B:1831:CYS:HB3	1.98	0.44
1:B:263:LYS:HA	1:B:263:LYS:HD3	1.82	0.44
1:B:3629:ARG:HD2	1:B:3633:ILE:HD11	2.00	0.44
1:B:3666:LEU:HA	1:B:3669:LYS:HG2	2.00	0.44
1:A:1483:LEU:O	1:A:1487:VAL:HG23	2.18	0.44
1:A:1712:ARG:O	1:A:1716:GLN:HG2	2.18	0.44
1:A:3422:GLN:HE22	1:A:3423:GLN:NE2	2.15	0.44
1:B:1563:PHE:C	1:B:1565:GLU:H	2.21	0.44
1:B:1813:SER:HB3	1:B:1936:ARG:NH2	2.32	0.44
1:B:1861:SER:O	1:B:1865:THR:OG1	2.25	0.44
1:B:2870:SER:HB2	1:B:2922:ARG:HH22	1.83	0.44
1:B:3085:GLU:N	1:B:3085:GLU:OE1	2.40	0.44
1:B:3307:LEU:HD21	1:B:3326:GLN:OE1	2.17	0.44
1:A:1948:ALA:O	1:A:1952:ILE:HG13	2.18	0.43
1:A:2572:TYR:CD2	1:A:2787:HIS:HB2	2.53	0.43
1:A:2863:CYS:HB2	1:A:2892:LEU:HD13	1.99	0.43
1:A:388:LEU:HA	1:A:388:LEU:HD12	1.86	0.43
1:A:642:PHE:HE2	1:A:673:THR:HG1	1.66	0.43
1:A:765:LEU:HD23	1:A:766:ALA:N	2.32	0.43
1:B:1563:PHE:HD1	1:B:1567:ILE:HD11	1.83	0.43
1:B:16:GLN:NE2	1:B:63:PHE:HA	2.33	0.43
1:B:2146:LEU:HD12	1:B:2146:LEU:HA	1.87	0.43
1:B:2538:ARG:O	1:B:2542:LEU:HG	2.17	0.43
1:A:1029:CYS:O	1:A:1032:CYS:HB2	2.18	0.43
1:A:1067:ALA:O	1:A:1075:ARG:HB2	2.18	0.43
1:A:1075:ARG:NE	1:A:1114:ALA:HB2	2.34	0.43
1:A:1282:LEU:HD13	1:A:1291:LEU:HD21	1.99	0.43
1:A:1361:LYS:HA	1:A:1364:CYS:HB2	2.00	0.43
1:A:1802:TYR:CZ	1:A:1843:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3662:ILE:HA	1:A:3665:MET:CE	2.48	0.43
1:A:3835:PRO:O	1:A:3839:TYR:HB2	2.17	0.43
1:B:1787:ARG:HG2	1:B:1787:ARG:O	2.18	0.43
1:B:2084:GLU:O	1:B:2089:ASN:ND2	2.49	0.43
1:B:2264:ASP:O	1:B:2266:ASN:N	2.49	0.43
1:B:2239:LYS:HG3	1:B:2279:ILE:HG23	2.00	0.43
1:B:713:GLU:O	1:B:716:VAL:HG12	2.19	0.43
1:A:1723:PRO:HD2	1:A:1739:TYR:CD1	2.53	0.43
1:A:1790:SER:O	1:A:1793:THR:HG22	2.18	0.43
1:B:1672:PHE:HE2	1:B:1702:LEU:HD21	1.84	0.43
1:B:1848:ILE:HD12	1:B:1848:ILE:HA	1.85	0.43
1:B:2958:LEU:HG	1:B:4101:GLU:HG2	2.00	0.43
1:B:3386:SER:O	1:B:3389:VAL:HG22	2.18	0.43
1:B:3778:ASP:OD1	1:B:3779:SER:N	2.50	0.43
1:A:4099:SER:O	1:A:4103:GLN:HB2	2.18	0.43
1:A:583:LEU:HD23	1:A:583:LEU:H	1.83	0.43
1:A:585:ILE:HA	1:A:611:ASN:OD1	2.18	0.43
1:B:1186:LYS:HD3	1:B:1186:LYS:HA	1.82	0.43
1:B:1463:LEU:HG	1:B:1466:ASN:HB2	2.00	0.43
1:B:2372:PRO:HG2	1:B:2373:PRO:HD3	2.01	0.43
1:B:3659:PHE:CE2	1:B:3661:ASP:HB3	2.53	0.43
1:B:3910:LEU:HA	1:B:3910:LEU:HD12	1.84	0.43
1:B:414:LEU:HA	1:B:414:LEU:HD13	1.87	0.43
1:A:1294:VAL:O	1:A:1298:LEU:HD13	2.18	0.43
1:A:1479:VAL:O	1:A:1483:LEU:HG	2.17	0.43
1:A:1666:GLY:C	1:A:1669:PRO:HD2	2.39	0.43
1:A:2091:HIS:O	1:A:2093:CYS:N	2.52	0.43
1:A:227:LEU:O	1:A:231:LEU:HB2	2.18	0.43
1:A:2281:MET:HG2	1:A:2326:ILE:HG12	2.01	0.43
1:A:3623:PRO:HG2	1:A:3633:ILE:HD12	2.00	0.43
1:A:432:THR:N	1:A:433:PRO:HD2	2.33	0.43
1:A:561:ASN:HA	1:A:564:LEU:HD12	2.00	0.43
1:B:1017:ILE:HG23	1:B:1018:VAL:HG13	2.01	0.43
1:B:1023:SER:HA	1:B:1026:ARG:HE	1.83	0.43
1:B:1747:LEU:HD12	1:B:1781:SER:CB	2.48	0.43
1:B:1790:SER:O	1:B:1793:THR:HG22	2.18	0.43
1:B:1832:SER:N	1:B:1883:ARG:HH22	2.11	0.43
1:B:2375:ALA:O	1:B:2379:MET:N	2.51	0.43
1:B:2439:ILE:O	1:B:2443:MET:HG3	2.19	0.43
1:B:2950:LYS:HE3	1:B:2981:TRP:CE3	2.54	0.43
1:B:3068:ALA:O	1:B:3074:GLN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3979:LEU:O	1:B:3983:ILE:HG12	2.19	0.43
1:A:1208:LEU:HA	1:A:1208:LEU:HD12	1.81	0.43
1:A:1575:LEU:HD23	1:A:1617:LYS:HG2	2.00	0.43
1:A:3077:ILE:HG23	1:A:3081:HIS:CE1	2.52	0.43
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.51	0.43
1:A:3999:THR:HA	1:A:4002:MET:CE	2.49	0.43
1:B:1361:LYS:HD2	1:B:1361:LYS:HA	1.88	0.43
1:B:1626:TRP:CZ3	1:B:1674:THR:HG21	2.54	0.43
1:B:2398:LEU:O	1:B:2401:VAL:HG12	2.19	0.43
1:B:765:LEU:HA	1:B:768:VAL:HG12	2.01	0.43
1:A:1718:ILE:HG12	1:A:1722:PHE:CE2	2.54	0.43
1:A:2327:LEU:HD13	1:A:2371:PHE:CD2	2.54	0.43
1:A:2419:ASP:HB2	1:A:2422:GLN:HB2	2.00	0.43
1:A:3268:THR:HG23	1:A:3269:ARG:H	1.84	0.43
1:B:1839:PHE:HA	1:B:1842:THR:HG22	2.00	0.43
1:B:2551:GLU:HA	1:B:2554:PHE:HB2	2.00	0.43
1:B:3829:LEU:HA	1:B:3829:LEU:HD23	1.87	0.43
1:B:3988:LEU:HD21	1:B:4103:GLN:OE1	2.19	0.43
1:B:4126:PRO:HD2	1:B:4127:TRP:CZ3	2.53	0.43
1:B:418:ALA:CB	1:B:463:LYS:HG3	2.49	0.43
1:B:977:ASP:O	1:B:980:THR:HG22	2.18	0.43
1:A:3596:LEU:HD22	1:A:3606:ILE:HD12	2.01	0.43
1:A:3670:MET:HB2	1:A:3670:MET:HE2	1.78	0.43
1:A:3798:SER:O	1:A:3799:ARG:HG2	2.19	0.43
1:A:3867:THR:HG21	1:A:4119:ARG:CZ	2.49	0.43
1:B:2511:ILE:HG12	1:B:2550:ILE:HG22	2.01	0.43
1:B:2548:PRO:HG3	1:B:2846:THR:HB	2.01	0.43
1:B:3418:ASP:OD2	1:B:3464:LYS:NZ	2.31	0.43
1:B:484:HIS:CE1	1:B:575:ILE:HG13	2.53	0.43
1:A:3019:ILE:HG21	1:A:3029:LYS:HB3	2.01	0.43
1:A:3301:LEU:HD11	1:A:3359:ILE:HD11	2.01	0.43
1:A:3669:LYS:HE2	1:A:3669:LYS:HB2	1.92	0.43
1:A:647:TYR:CD1	1:A:703:CYS:HB3	2.51	0.43
1:A:873:VAL:HG13	1:A:874:THR:N	2.26	0.43
1:B:1346:THR:HG23	1:B:1405:ALA:CB	2.49	0.43
1:B:2451:LEU:HA	1:B:2451:LEU:HD12	1.78	0.43
1:B:2492:ASP:HB3	1:B:2495:SER:H	1.84	0.43
1:B:276:ALA:HA	1:B:318:SER:CB	2.49	0.43
1:B:3411:ASP:N	1:B:3411:ASP:OD1	2.46	0.43
1:B:3742:GLY:C	1:B:3744:ASP:H	2.22	0.43
1:A:1122:GLY:HA2	1:A:1125:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:O	1:A:116:THR:OG1	2.32	0.43
1:A:149:ILE:HB	1:A:185:HIS:ND1	2.34	0.43
1:A:1962:TYR:O	1:A:1967:PHE:HD2	2.02	0.43
1:A:2225:HIS:CE1	1:A:2230:VAL:HG21	2.54	0.43
1:A:3489:SER:O	1:A:3490:VAL:HG23	2.19	0.43
1:A:4044:ILE:HA	1:A:4044:ILE:HD13	1.72	0.43
1:A:4054:ALA:H	1:A:4103:GLN:NE2	2.16	0.43
1:A:633:ILE:C	1:A:635:PRO:HD3	2.39	0.43
1:A:723:ASP:N	1:A:723:ASP:OD1	2.52	0.43
1:A:912:PRO:O	1:A:916:GLU:HB2	2.19	0.43
1:B:1001:PHE:CE1	1:B:1044:ILE:HD11	2.54	0.43
1:B:1859:ASN:HB3	1:B:1862:THR:HG22	2.01	0.43
1:B:3820:MET:HB3	1:B:3824:GLU:HG3	2.00	0.43
1:A:1348:LEU:HG	1:A:1359:LEU:HD21	2.01	0.42
1:A:1411:TYR:O	1:A:1415:LEU:HG	2.19	0.42
1:A:1440:ASP:OD1	1:A:1440:ASP:N	2.52	0.42
1:A:1858:LEU:HA	1:A:1858:LEU:HD23	1.88	0.42
1:A:3661:ASP:O	1:A:3665:MET:HG3	2.18	0.42
1:B:2219:LEU:O	1:B:2223:VAL:HB	2.19	0.42
1:B:3324:ARG:O	1:B:3328:ILE:HG13	2.18	0.42
1:B:3872:ARG:HA	1:B:3875:GLU:HG2	2.01	0.42
1:B:487:LEU:HD22	1:B:571:SER:OG	2.19	0.42
1:B:523:THR:OG1	1:B:524:TYR:N	2.52	0.42
1:A:1057:LYS:HE3	1:A:1099:PHE:HB2	2.01	0.42
1:A:1134:LEU:HA	1:A:1134:LEU:HD23	1.83	0.42
1:A:1263:ALA:HA	1:A:1266:CYS:HG	1.84	0.42
1:A:2896:ALA:O	1:A:2899:ARG:NE	2.47	0.42
1:A:465:PHE:HE1	1:A:482:VAL:HG11	1.84	0.42
1:A:969:LEU:HD23	1:A:969:LEU:HA	1.79	0.42
1:B:1579:VAL:O	1:B:1583:MET:HG2	2.19	0.42
1:B:1648:LEU:O	1:B:1652:ILE:HG12	2.20	0.42
1:B:1984:LEU:O	1:B:1984:LEU:HD23	2.19	0.42
1:B:3114:TYR:CE2	1:B:3125:ARG:HB3	2.54	0.42
1:B:527:TYR:O	1:B:531:PHE:HD1	2.02	0.42
1:B:961:LEU:O	1:B:965:THR:OG1	2.21	0.42
1:A:168:ASP:OD1	1:A:219:VAL:HG23	2.19	0.42
1:A:1801:VAL:HB	1:A:1824:LEU:HD12	2.01	0.42
1:A:1856:THR:HG22	1:A:1858:LEU:HB2	2.00	0.42
1:A:2477:LEU:HB3	1:A:2506:LEU:HG	2.02	0.42
1:A:2881:LEU:HD23	1:A:2886:GLN:HE21	1.84	0.42
1:A:3118:ASP:OD2	1:A:3895:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4027:TRP:O	1:A:4028:ILE:HG23	2.18	0.42
1:A:4085:LYS:H	1:A:4091:ALA:HB3	1.84	0.42
1:A:767:GLU:OE1	1:A:854:ARG:NH1	2.52	0.42
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.86	0.42
1:A:1333:SER:O	1:A:1336:THR:HG22	2.20	0.42
1:A:1342:MET:HA	1:A:1345:THR:HG22	2.02	0.42
1:A:1515:LEU:HD21	1:A:1519:PHE:CE2	2.54	0.42
1:A:1820:VAL:O	1:A:1825:LEU:HG	2.19	0.42
1:A:1851:LEU:HB3	1:A:1918:LEU:HD13	2.01	0.42
1:A:2225:HIS:O	1:A:2227:LYS:N	2.52	0.42
1:A:2288:TYR:CD1	1:A:2291:GLN:HB2	2.54	0.42
1:A:2368:THR:HA	1:A:2371:PHE:O	2.20	0.42
1:A:3020:ASP:O	1:A:3024:PRO:HB3	2.18	0.42
1:A:3274:VAL:O	1:A:3278:GLN:HG3	2.19	0.42
1:A:4055:ASN:HB3	1:A:4058:VAL:HG23	2.00	0.42
1:B:101:ALA:HB1	1:B:143:LEU:HD11	2.02	0.42
1:B:104:SER:HB3	1:B:134:LEU:HD11	2.01	0.42
1:B:1927:MET:HE3	1:B:1927:MET:HB2	1.90	0.42
1:B:302:ALA:HB2	1:B:358:GLU:OE2	2.20	0.42
1:B:51:LEU:HD11	1:B:95:LYS:HD3	2.01	0.42
1:B:651:TYR:CE1	1:B:655:LEU:HD11	2.53	0.42
1:A:1873:TYR:HA	1:A:1873:TYR:HD1	1.78	0.42
1:A:1990:PHE:HB2	1:A:2179:GLY:HA3	2.01	0.42
1:A:2350:LYS:HG2	1:A:2378:PHE:HE1	1.84	0.42
1:A:3535:ILE:HD12	1:A:3759:ARG:NH1	2.33	0.42
1:A:767:GLU:HG3	1:A:846:ILE:HD13	2.01	0.42
1:A:983:LEU:O	1:A:984:TYR:HB2	2.19	0.42
1:B:3049:LEU:O	1:B:3053:LEU:HG	2.18	0.42
1:B:354:SER:HA	1:B:358:GLU:HB2	2.00	0.42
1:B:3654:MET:HG2	1:B:3656:LEU:HB2	2.02	0.42
1:B:3891:SER:C	1:B:3893:SER:H	2.22	0.42
1:A:1788:ARG:H	1:A:1794:GLN:HE21	1.67	0.42
1:A:1840:PHE:O	1:A:1843:ILE:HG22	2.19	0.42
1:A:2193:ILE:O	1:A:2196:TRP:NE1	2.52	0.42
1:A:2514:ASN:O	1:A:2517:LEU:HB3	2.18	0.42
1:A:3450:MET:HB2	1:A:3450:MET:HE2	1.92	0.42
1:A:3998:LEU:O	1:A:4002:MET:HG3	2.19	0.42
1:B:1254:LEU:H	1:B:1254:LEU:HD22	1.84	0.42
1:B:1264:LEU:HD21	1:B:1341:ILE:HG13	2.01	0.42
1:B:2556:SER:HB2	1:B:2799:GLN:HA	2.01	0.42
1:B:3558:ILE:O	1:B:3562:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:PHE:O	1:B:417:VAL:HG23	2.19	0.42
1:A:1909:ASN:HB2	1:A:1913:LYS:HB2	2.01	0.42
1:A:2101:VAL:HG12	1:A:2156:VAL:HG21	2.01	0.42
1:A:2436:LEU:O	1:A:2439:ILE:HG22	2.19	0.42
1:A:3144:PHE:CE2	1:A:3157:LEU:HD13	2.55	0.42
1:A:71:LYS:HD3	1:A:71:LYS:O	2.20	0.42
1:B:1010:LEU:O	1:B:1014:LEU:HD13	2.20	0.42
1:B:1519:PHE:CE2	1:B:1528:LEU:HD22	2.54	0.42
1:B:2312:TYR:O	1:B:2315:VAL:HG12	2.19	0.42
1:B:2921:LEU:O	1:B:2925:GLU:HG2	2.20	0.42
1:A:1395:LEU:HB3	1:A:1396:PRO:HD3	2.02	0.42
1:A:1703:THR:O	1:A:1707:LEU:HB2	2.19	0.42
1:A:178:LEU:HD23	1:A:181:LEU:HD12	2.01	0.42
1:A:2105:HIS:CG	1:A:2156:VAL:HG13	2.55	0.42
1:A:3502:MET:SD	1:A:3514:VAL:HG21	2.59	0.42
1:B:93:LEU:HD21	1:B:134:LEU:HD12	2.01	0.42
1:B:2288:TYR:HD2	1:B:2291:GLN:HB2	1.85	0.42
1:B:2586:PHE:N	1:B:2783:ILE:HD11	2.34	0.42
1:B:3006:ALA:O	1:B:3257:LYS:HE3	2.20	0.42
1:B:3760:GLN:O	1:B:3764:VAL:HG13	2.20	0.42
1:B:528:VAL:HA	1:B:633:ILE:HD11	2.02	0.42
1:A:1601:LEU:HD22	1:A:1618:LEU:HD21	2.02	0.42
1:A:1952:ILE:O	1:A:1955:VAL:HG22	2.20	0.42
1:A:2255:LEU:HD23	1:A:2256:ILE:HG13	2.01	0.42
1:A:268:PRO:HB2	1:A:308:LEU:HD11	2.01	0.42
1:A:484:HIS:CE1	1:A:488:ILE:HD11	2.55	0.42
1:B:2128:PHE:CZ	1:B:2132:LYS:HD2	2.55	0.42
1:B:2251:ILE:HD12	1:B:2253:TYR:CE2	2.55	0.42
1:B:3464:LYS:HE3	1:B:3997:LEU:HD23	2.01	0.42
1:B:736:LEU:HD22	1:B:741:ILE:HD12	2.01	0.42
1:A:1018:VAL:CG1	1:A:1074:LYS:HA	2.50	0.42
1:A:1283:GLY:HA2	1:A:1358:LEU:HD11	2.02	0.42
1:A:1991:PRO:O	1:A:2184:TYR:HB2	2.20	0.42
1:A:3110:PHE:CD1	1:A:3128:LYS:HD2	2.52	0.42
1:A:3511:ALA:HB3	1:A:3551:ASN:ND2	2.34	0.42
1:A:3554:PHE:CE2	1:A:3558:ILE:HD11	2.54	0.42
1:A:3629:ARG:NH2	1:A:3634:GLN:HB2	2.35	0.42
1:A:3868:VAL:O	1:A:3872:ARG:HG2	2.19	0.42
1:A:465:PHE:CE1	1:A:482:VAL:HG11	2.55	0.42
1:A:966:PHE:HE1	1:A:969:LEU:HD12	1.83	0.42
1:B:2255:LEU:HD23	1:B:2256:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2334:LYS:HE3	1:B:2334:LYS:HB2	1.90	0.42
1:B:2304:VAL:HG21	1:B:2344:LEU:HG	2.02	0.42
1:B:2458:VAL:CG1	1:B:2476:ILE:HD11	2.50	0.42
1:B:2855:VAL:HA	1:B:2858:ILE:HG12	2.02	0.42
1:B:3654:MET:HE2	1:B:3656:LEU:HB2	2.02	0.42
1:B:573:LEU:HA	1:B:576:VAL:HG12	2.01	0.42
1:B:631:ARG:HG3	1:B:672:ILE:HD11	2.01	0.42
1:A:1982:ILE:HG22	1:A:1983:ASP:H	1.85	0.41
1:A:227:LEU:HD21	1:A:248:ILE:HD13	2.01	0.41
1:A:2801:ASP:O	1:A:2804:ILE:HG22	2.20	0.41
1:A:3326:GLN:O	1:A:3329:LEU:HG	2.20	0.41
1:B:1455:CYS:HA	1:B:1458:LEU:HD12	2.01	0.41
1:B:1623:LEU:HA	1:B:1623:LEU:HD23	1.87	0.41
1:B:1828:LEU:HA	1:B:1828:LEU:HD23	1.90	0.41
1:B:3144:PHE:CZ	1:B:3157:LEU:HD13	2.55	0.41
1:B:4055:ASN:HB3	1:B:4058:VAL:HG23	2.02	0.41
1:B:4082:ARG:HH12	1:B:4091:ALA:HA	1.85	0.41
1:A:1916:ILE:HA	1:A:1916:ILE:HD13	1.91	0.41
1:A:1947:CYS:O	1:A:1951:VAL:HG12	2.20	0.41
1:A:2389:PHE:HB3	1:A:2393:LEU:HB2	2.02	0.41
1:A:934:LEU:HB3	1:A:984:TYR:OH	2.20	0.41
1:B:1083:ASN:OD1	1:B:1126:GLN:HG3	2.19	0.41
1:B:1361:LYS:O	1:B:1365:ASN:HB2	2.20	0.41
1:B:132:ILE:HD12	1:B:173:LYS:HD2	2.01	0.41
1:B:1837:ARG:N	1:B:1837:ARG:HD3	2.34	0.41
1:B:1956:PHE:O	1:B:1958:GLU:HG3	2.20	0.41
1:B:2151:ILE:HD13	1:B:2188:GLU:HB3	2.01	0.41
1:B:217:LEU:HB3	1:B:218:PRO:HD3	2.02	0.41
1:B:3268:THR:HG23	1:B:3269:ARG:H	1.85	0.41
1:B:3339:ASN:OD1	1:B:3426:LYS:NZ	2.37	0.41
1:B:3413:TYR:HB3	1:B:3449:LYS:O	2.21	0.41
1:B:3761:ASP:HA	1:B:3764:VAL:HG22	2.02	0.41
1:B:69:VAL:HG22	1:B:82:ARG:HG3	2.02	0.41
1:B:873:VAL:HG13	1:B:874:THR:N	2.28	0.41
1:A:1579:VAL:HG22	1:A:1579:VAL:H	1.66	0.41
1:A:2220:MET:HG2	1:A:2276:LEU:HD11	2.02	0.41
1:A:2274:ILE:HD12	1:A:2318:ALA:HB3	2.02	0.41
1:A:2402:LEU:CD1	1:A:2437:ASP:HB3	2.50	0.41
1:A:2887:PRO:HD2	1:A:2888:VAL:H	1.84	0.41
1:A:2923:TRP:CD2	1:A:2946:GLU:HG3	2.55	0.41
1:A:303:HIS:ND1	1:A:305:ASN:OD1	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1225:GLU:OE2	1:B:1288:SER:OG	2.38	0.41
1:B:2003:LYS:HD3	1:B:2184:TYR:HE1	1.85	0.41
1:B:2528:GLU:OE2	1:B:2533:SER:HB3	2.21	0.41
1:B:2519:LEU:HD13	1:B:2610:UNK:CA	2.50	0.41
1:A:1096:VAL:HB	1:A:1101:PHE:CE2	2.55	0.41
1:A:1599:GLY:HA2	1:A:1602:ASP:OD1	2.21	0.41
1:A:2338:GLU:HA	1:A:2341:LEU:HD21	2.02	0.41
1:A:3463:LEU:HD13	1:A:3498:TRP:CZ2	2.52	0.41
1:A:3652:LEU:HB3	1:A:3653:ARG:HE	1.86	0.41
1:A:3708:ARG:HD2	1:A:3708:ARG:HA	1.85	0.41
1:B:1096:VAL:HB	1:B:1101:PHE:CE2	2.53	0.41
1:B:1261:LEU:HD21	1:B:1337:VAL:HA	2.02	0.41
1:B:1825:LEU:O	1:B:1829:TRP:HB2	2.21	0.41
1:B:2590:THR:OG1	1:B:2591:ILE:N	2.53	0.41
1:B:3701:ILE:HB	1:B:3719:ILE:HB	2.02	0.41
1:B:3924:HIS:H	1:B:3924:HIS:CD2	2.37	0.41
1:A:1141:LYS:HD2	1:A:1141:LYS:HA	1.80	0.41
1:A:1389:VAL:O	1:A:1393:ALA:HB3	2.21	0.41
1:A:1440:ASP:HB2	1:A:1443:VAL:HG22	2.02	0.41
1:A:1474:ASP:OD1	1:A:1474:ASP:N	2.54	0.41
1:A:1646:LEU:HD23	1:A:1646:LEU:HA	1.87	0.41
1:A:263:LYS:O	1:A:264:ARG:HG2	2.21	0.41
1:B:170:VAL:O	1:B:174:VAL:HG23	2.19	0.41
1:B:2379:MET:HG3	1:B:2383:PHE:CE2	2.55	0.41
1:B:3562:LEU:HD12	1:B:3562:LEU:HA	1.88	0.41
1:B:3652:LEU:HB3	1:B:3653:ARG:HE	1.86	0.41
1:B:3802:LEU:HA	1:B:3802:LEU:HD12	1.96	0.41
1:B:3944:HIS:HB3	1:B:3948:SER:HB2	2.02	0.41
1:A:1117:ASP:O	1:A:1118:GLU:HG2	2.20	0.41
1:A:1747:LEU:HD21	1:A:1778:PHE:CE1	2.55	0.41
1:A:3881:ASP:N	1:A:3881:ASP:OD1	2.48	0.41
1:A:653:LEU:HD13	1:A:670:LEU:HG	2.03	0.41
1:A:983:LEU:HD12	1:A:983:LEU:HA	1.90	0.41
1:B:1448:LEU:HD23	1:B:1510:LEU:HD11	2.02	0.41
1:B:1949:ILE:HD11	1:B:2097:LEU:HD23	2.02	0.41
1:B:2477:LEU:HB3	1:B:2506:LEU:HG	2.02	0.41
1:B:2507:ILE:HG22	1:B:2550:ILE:HD11	2.02	0.41
1:B:3082:TYR:O	1:B:3084:GLN:N	2.54	0.41
1:B:3554:PHE:O	1:B:3558:ILE:HG13	2.20	0.41
1:B:3647:GLY:O	1:B:3651:LEU:HB3	2.20	0.41
1:B:569:VAL:HA	1:B:572:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:ASP:OD2	1:A:1123:THR:OG1	2.25	0.41
1:A:1349:LEU:HD21	1:A:1356:TRP:HA	2.02	0.41
1:A:1717:LEU:O	1:A:1721:HIS:HB2	2.20	0.41
1:A:2289:ASP:O	1:A:2291:GLN:N	2.53	0.41
1:A:2436:LEU:HD22	1:A:2469:CYS:SG	2.61	0.41
1:A:3167:ARG:O	1:A:3186:ARG:NH2	2.52	0.41
1:A:3462:ARG:NH1	1:A:3707:GLY:HA3	2.35	0.41
1:A:3802:LEU:HA	1:A:3802:LEU:HD12	1.86	0.41
1:A:385:TYR:CD2	1:A:389:ILE:HD11	2.50	0.41
1:A:446:PHE:CD1	1:A:530:LEU:HD22	2.55	0.41
1:A:871:LEU:HD23	1:A:871:LEU:H	1.84	0.41
1:A:913:ARG:HD2	1:A:913:ARG:HA	1.88	0.41
1:B:1052:SER:HB3	1:B:1055:ASN:HB2	2.02	0.41
1:B:1601:LEU:HA	1:B:1601:LEU:HD13	1.95	0.41
1:B:2256:ILE:H	1:B:2256:ILE:HG13	1.56	0.41
1:B:2366:LYS:HD3	1:B:2366:LYS:HA	1.84	0.41
1:B:2591:ILE:HD11	1:B:2792:THR:OG1	2.21	0.41
1:B:3465:PHE:HB3	1:B:3466:PRO:HD3	2.03	0.41
1:B:3598:LYS:NZ	1:B:4031:ILE:HD13	2.36	0.41
1:A:1134:LEU:O	1:A:1137:ILE:HG22	2.19	0.41
1:A:1334:LYS:O	1:A:1337:VAL:HG22	2.21	0.41
1:A:1969:GLU:HB3	1:A:1977:ILE:HG13	2.03	0.41
1:A:3061:LEU:HA	1:A:3061:LEU:HD12	1.88	0.41
1:A:414:LEU:HG	1:A:464:VAL:CG2	2.51	0.41
1:A:451:PRO:C	1:A:453:MET:H	2.24	0.41
1:B:1586:SER:HA	1:B:1593:VAL:HG11	2.01	0.41
1:B:1969:GLU:HB2	1:B:1975:LEU:O	2.21	0.41
1:B:2825:THR:O	1:B:2829:LYS:N	2.40	0.41
1:B:3641:ASP:O	1:B:3645:GLY:N	2.53	0.41
1:B:738:HIS:ND1	1:B:741:ILE:O	2.54	0.41
1:A:1534:ASN:HA	1:A:1535:PRO:HD3	1.87	0.41
1:A:1733:THR:HG22	1:A:1735:ARG:H	1.84	0.41
1:A:1832:SER:OG	1:A:1833:LEU:N	2.52	0.41
1:A:1982:ILE:HG22	1:A:1983:ASP:N	2.36	0.41
1:A:1990:PHE:CE2	1:A:2144:LEU:HD11	2.55	0.41
1:A:2203:THR:OG1	1:A:2247:ASP:HB2	2.21	0.41
1:A:2284:ASP:HB3	1:A:2285:LEU:HG	2.03	0.41
1:A:2322:VAL:O	1:A:2326:ILE:HG13	2.20	0.41
1:A:2792:THR:N	1:A:2793:PRO:HD2	2.36	0.41
1:B:1696:LEU:N	1:B:1697:PRO:CD	2.84	0.41
1:B:1848:ILE:HD11	1:B:1918:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:VAL:HG22	1:B:213:ARG:H	1.86	0.41
1:B:2586:PHE:H	1:B:2783:ILE:HD11	1.85	0.41
1:B:354:SER:CB	1:B:359:LEU:H	2.33	0.41
1:B:612:LEU:HD23	1:B:612:LEU:HA	1.82	0.41
1:A:1779:GLN:O	1:A:1783:ARG:HG3	2.20	0.41
1:A:2447:LYS:O	1:A:2449:VAL:N	2.50	0.41
1:A:3542:PHE:HZ	1:A:3555:VAL:HG21	1.86	0.41
1:A:385:TYR:O	1:A:389:ILE:HG13	2.21	0.41
1:A:3924:HIS:H	1:A:3924:HIS:CD2	2.39	0.41
1:A:904:VAL:O	1:A:905:ILE:HD13	2.21	0.41
1:B:1433:ALA:O	1:B:1436:LEU:HD23	2.21	0.41
1:B:1617:LYS:HE3	1:B:1617:LYS:HB2	1.89	0.41
1:B:1930:GLU:HB3	1:B:1937:ARG:NH1	2.36	0.41
1:B:2268:LYS:HD3	1:B:2314:GLU:OE2	2.21	0.41
1:B:2814:SER:HA	1:B:2865:HIS:NE2	2.36	0.41
1:B:3577:GLN:HA	1:B:3630:ARG:HH11	1.85	0.41
1:B:393:LYS:HA	1:B:397:LEU:HD13	2.03	0.41
1:B:4064:LEU:O	1:B:4068:HIS:HB2	2.21	0.41
1:B:683:PHE:HB3	1:B:740:ILE:HD13	2.03	0.41
1:B:776:TRP:O	1:B:780:ILE:HG22	2.20	0.41
1:A:1564:SER:O	1:A:1603:GLN:HG3	2.21	0.41
1:A:1914:THR:O	1:A:1918:LEU:HG	2.20	0.41
1:A:1978:PHE:O	1:A:1982:ILE:HG12	2.21	0.41
1:A:2351:GLN:O	1:A:2355:THR:HG22	2.21	0.41
1:A:2942:ILE:H	1:A:2942:ILE:HG12	1.75	0.41
1:A:3386:SER:O	1:A:3389:VAL:HG22	2.21	0.41
1:A:290:TYR:HE2	1:A:340:TYR:CD2	2.39	0.41
1:A:3988:LEU:O	1:A:3992:ARG:HG2	2.21	0.41
1:A:4031:ILE:HG13	1:A:4035:GLU:HB2	2.03	0.41
1:A:655:LEU:HD22	1:A:1389:VAL:CG1	2.51	0.41
1:A:873:VAL:CG1	1:A:874:THR:H	2.27	0.41
1:B:1267:TYR:HB3	1:B:1344:PHE:CE1	2.56	0.41
1:B:1419:LEU:HD13	1:B:1467:ILE:HD11	2.03	0.41
1:B:2091:HIS:O	1:B:2093:CYS:N	2.54	0.41
1:B:2140:LEU:HD21	1:B:2179:GLY:H	1.84	0.41
1:B:3480:LEU:HD12	1:B:3480:LEU:HA	1.86	0.41
1:A:1938:ARG:HH21	1:A:1983:ASP:HA	1.86	0.40
1:A:2366:LYS:HA	1:A:2366:LYS:HD3	1.86	0.40
1:A:3666:LEU:HA	1:A:3669:LYS:HG2	2.03	0.40
1:A:3719:ILE:HD12	1:A:3740:ILE:HD12	2.02	0.40
1:A:523:THR:OG1	1:A:524:TYR:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:HA	1:A:12:LEU:HD13	2.04	0.40
1:B:1197:LEU:O	1:B:1197:LEU:HD23	2.21	0.40
1:B:1334:LYS:NZ	1:B:1383:GLY:HA3	2.35	0.40
1:B:1344:PHE:O	1:B:1347:THR:HG22	2.21	0.40
1:B:1372:LEU:O	1:B:1375:THR:OG1	2.32	0.40
1:B:2097:LEU:HB3	1:B:2149:LEU:HD11	2.03	0.40
1:B:2164:TRP:O	1:B:2196:TRP:HZ3	2.04	0.40
1:B:2263:LYS:HA	1:B:2309:PHE:HE2	1.86	0.40
1:B:3129:LEU:HD23	1:B:3129:LEU:HA	1.92	0.40
1:B:620:PHE:CZ	1:B:663:ILE:HD12	2.56	0.40
1:A:1372:LEU:HD12	1:A:1402:LEU:HD23	2.02	0.40
1:A:2253:TYR:HD2	1:A:2292:CYS:HB2	1.87	0.40
1:A:2306:ASN:O	1:A:2309:PHE:HB2	2.21	0.40
1:B:1263:ALA:HA	1:B:1266:CYS:SG	2.62	0.40
1:B:1627:LYS:HB2	1:B:1627:LYS:HE2	1.80	0.40
1:B:1832:SER:H	1:B:1883:ARG:NH2	2.10	0.40
1:B:1894:SER:HA	1:B:1897:ASN:HB2	2.03	0.40
1:B:2514:ASN:O	1:B:2517:LEU:HB3	2.21	0.40
1:B:2884:LEU:HD23	1:B:2884:LEU:HA	1.97	0.40
1:A:1178:ARG:HG2	1:A:1180:GLN:H	1.86	0.40
1:A:2294:ILE:HG22	1:A:2295:GLN:N	2.35	0.40
1:A:2551:GLU:HG3	1:A:2849:SER:CB	2.50	0.40
1:A:3053:LEU:HD11	1:A:3088:LEU:HD13	2.03	0.40
1:A:853:ILE:HD11	1:A:3108:GLN:OE1	2.21	0.40
1:A:3674:SER:O	1:A:3676:PRO:HD3	2.21	0.40
1:B:1101:PHE:CE1	1:B:1138:ILE:HD13	2.56	0.40
1:B:1423:ILE:HD11	1:B:1467:ILE:HD13	2.03	0.40
1:B:1831:CYS:HA	1:B:1883:ARG:NH1	2.36	0.40
1:B:179:GLY:HA3	1:B:226:GLY:HA2	2.04	0.40
1:B:2956:ALA:HB1	1:B:2972:TYR:CZ	2.56	0.40
1:B:3011:LEU:HD23	1:B:3047:SER:HB3	2.03	0.40
1:B:3389:VAL:HB	1:B:3413:TYR:HE1	1.85	0.40
1:B:357:LYS:O	1:B:360:SER:HB3	2.21	0.40
1:B:681:LYS:O	1:B:683:PHE:N	2.54	0.40
1:B:738:HIS:HE1	1:B:748:TYR:CE1	2.39	0.40
1:B:765:LEU:HD23	1:B:766:ALA:H	1.85	0.40
1:A:1503:LEU:HD12	1:A:1508:LYS:HE2	2.03	0.40
1:A:1515:LEU:CD2	1:A:1519:PHE:CE2	3.04	0.40
1:A:3059:GLN:HE21	1:A:3063:THR:HG23	1.86	0.40
1:A:3896:ALA:O	1:A:3900:LEU:HD13	2.22	0.40
1:A:47:SER:N	1:A:48:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1436:LEU:HD13	1:B:1444:ASP:HB3	2.03	0.40
1:B:1832:SER:O	1:B:1833:LEU:HB2	2.21	0.40
1:B:3530:VAL:HA	1:B:3562:LEU:HD21	2.04	0.40
1:B:384:MET:C	1:B:386:VAL:H	2.24	0.40
1:A:1078:ALA:O	1:A:1107:TYR:OH	2.38	0.40
1:A:1261:LEU:HD21	1:A:1337:VAL:HG12	2.03	0.40
1:A:2549:LYS:HD3	1:A:2549:LYS:HA	1.96	0.40
1:A:3462:ARG:HG3	1:A:3494:GLN:HB3	2.02	0.40
1:A:3858:MET:HB3	1:A:3858:MET:HE2	1.92	0.40
1:A:45:SER:HB3	1:A:51:LEU:HD22	2.04	0.40
1:A:886:TRP:CZ3	1:A:911:LEU:HG	2.56	0.40
1:B:9:ARG:HA	1:B:12:LEU:HD13	2.03	0.40
1:B:1333:SER:O	1:B:1337:VAL:HG13	2.21	0.40
1:B:172:GLU:HB2	1:B:218:PRO:O	2.21	0.40
1:B:1754:GLN:HB2	1:B:1797:LEU:HD11	2.03	0.40
1:B:1982:ILE:HG22	1:B:1983:ASP:N	2.36	0.40
1:B:2310:VAL:HG12	1:B:2316:TYR:CD2	2.56	0.40
1:B:476:ARG:NH2	1:B:1503:LEU:HD22	2.36	0.40
1:B:76:ILE:O	1:B:79:ARG:NH1	2.54	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	3544/3986 (89%)	3047 (86%)	482 (14%)	15 (0%)	34	72
1	B	3559/3986 (89%)	3069 (86%)	475 (13%)	15 (0%)	34	72
2	C	7/192 (4%)	7 (100%)	0	0	100	100
2	D	7/192 (4%)	7 (100%)	0	0	100	100
All	All	7117/8356 (85%)	6130 (86%)	957 (13%)	30 (0%)	34	72

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2182	ILE
1	A	2250	SER
1	A	2410	GLU
1	A	2781	PRO
1	B	1613	HIS
1	B	2250	SER
1	B	2410	GLU
1	A	1681	ASP
1	B	2246	LYS
1	B	3059	GLN
1	B	2206	PRO
1	B	2406	GLU
1	B	2407	GLY
1	A	167	PRO
1	A	2577	PHE
1	A	3059	GLN
1	A	1682	THR
1	A	1956	PHE
1	A	2886	GLN
1	A	2121	ASP
1	A	2177	ASN
1	B	304	THR
1	B	682	TYR
1	B	2577	PHE
1	A	635	PRO
1	A	2783	ILE
1	B	1992	VAL
1	B	2226	PRO
1	B	2573	PRO
1	B	2781	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3046/3515 (87%)	2953 (97%)	93 (3%)	40	63
1	B	3093/3515 (88%)	3005 (97%)	88 (3%)	43	65
2	C	8/165 (5%)	8 (100%)	0	100	100
2	D	8/165 (5%)	8 (100%)	0	100	100
All	All	6155/7360 (84%)	5974 (97%)	181 (3%)	42	64

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	CYS
1	A	36	ARG
1	A	65	LEU
1	A	70	ARG
1	A	148	LYS
1	A	254	LYS
1	A	264	ARG
1	A	281	GLN
1	A	282	PHE
1	A	337	LYS
1	A	364	ARG
1	A	366	TYR
1	A	373	CYS
1	A	492	SER
1	A	536	SER
1	A	630	CYS
1	A	651	TYR
1	A	662	LEU
1	A	675	ARG
1	A	701	TYR
1	A	704	PHE
1	A	707	PHE
1	A	790	LYS
1	A	795	CYS
1	A	910	PHE
1	A	966	PHE
1	A	1099	PHE
1	A	1107	TYR
1	A	1192	TYR
1	A	1213	LYS

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Mol	Chain	Res	Type
1	A	1229	CYS
1	A	1296	PHE
1	A	1507	CYS
1	A	1613	HIS
1	A	1633	TRP
1	A	1636	ASP
1	A	1679	LEU
1	A	1695	LEU
1	A	1787	ARG
1	A	1829	TRP
1	A	1837	ARG
1	A	1881	TYR
1	A	1910	GLU
1	A	1931	ASN
1	A	1979	GLU
1	A	1987	ARG
1	A	2029	SER
1	A	2154	GLU
1	A	2184	TYR
1	A	2196	TRP
1	A	2231	PHE
1	A	2248	CYS
1	A	2254	ARG
1	A	2269	ASP
1	A	2275	GLN
1	A	2306	ASN
1	A	2312	TYR
1	A	2321	GLU
1	A	2341	LEU
1	A	2342	CYS
1	A	2357	GLU
1	A	2389	PHE
1	A	2408	MET
1	A	2425	ARG
1	A	2489	SER
1	A	2527	HIS
1	A	2574	ASN
1	A	2577	PHE
1	A	2579	HIS
1	A	2809	PHE
1	A	2821	ASP
1	A	2851	PHE

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Mol	Chain	Res	Type
1	A	2931	ARG
1	A	2978	LYS
1	A	3005	LEU
1	A	3120	LEU
1	A	3122	HIS
1	A	3159	ARG
1	A	3244	ASP
1	A	3425	ARG
1	A	3428	GLU
1	A	3442	TYR
1	A	3570	ASP
1	A	3629	ARG
1	A	3632	PHE
1	A	3642	LYS
1	A	3659	PHE
1	A	3690	PHE
1	A	3694	PHE
1	A	3696	ARG
1	A	3775	LEU
1	A	3784	ARG
1	A	4087	HIS
1	B	25	CYS
1	B	45	SER
1	B	108	LYS
1	B	262	LEU
1	B	282	PHE
1	B	351	ASN
1	B	379	LYS
1	B	468	LEU
1	B	492	SER
1	B	583	LEU
1	B	630	CYS
1	B	662	LEU
1	B	704	PHE
1	B	707	PHE
1	B	795	CYS
1	B	886	TRP
1	B	910	PHE
1	B	1099	PHE
1	B	1107	TYR
1	B	1127	CYS
1	B	1167	ASP

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Mol	Chain	Res	Type
1	B	1205	ASN
1	B	1213	LYS
1	B	1229	CYS
1	B	1279	LEU
1	B	1370	ARG
1	B	1409	SER
1	B	1507	CYS
1	B	1558	TYR
1	B	1588	ASP
1	B	1667	SER
1	B	1695	LEU
1	B	1727	ARG
1	B	1762	MET
1	B	1787	ARG
1	B	1788	ARG
1	B	1813	SER
1	B	1829	TRP
1	B	1837	ARG
1	B	1864	ASP
1	B	1881	TYR
1	B	1910	GLU
1	B	1990	PHE
1	B	2083	LEU
1	B	2085	MET
1	B	2154	GLU
1	B	2184	TYR
1	B	2195	SER
1	B	2231	PHE
1	B	2233	HIS
1	B	2269	ASP
1	B	2306	ASN
1	B	2321	GLU
1	B	2334	LYS
1	B	2341	LEU
1	B	2342	CYS
1	B	2389	PHE
1	B	2404	ARG
1	B	2489	SER
1	B	2492	ASP
1	B	2527	HIS
1	B	2568	MET
1	B	2577	PHE

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Mol	Chain	Res	Type
1	B	2585	GLU
1	B	2800	ARG
1	B	2809	PHE
1	B	2821	ASP
1	B	2835	LYS
1	B	2851	PHE
1	B	2978	LYS
1	B	3005	LEU
1	B	3014	CYS
1	B	3120	LEU
1	B	3168	TYR
1	B	3244	ASP
1	B	3323	PHE
1	B	3378	TYR
1	B	3422	GLN
1	B	3428	GLU
1	B	3507	ASP
1	B	3570	ASP
1	B	3629	ARG
1	B	3642	LYS
1	B	3689	ASP
1	B	3694	PHE
1	B	3696	ARG
1	B	3716	HIS
1	B	4087	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	GLN
1	A	1721	HIS
1	A	3059	GLN
1	A	3423	GLN
1	A	3924	HIS
1	A	4015	ASN
1	B	484	HIS
1	B	1048	GLN
1	B	1049	GLN
1	B	3130	GLN
1	B	3278	GLN
1	B	3743	HIS
1	B	3969	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2614:UNK	C	2740:UNK	N	43.02
1	A	2614:UNK	C	2739:UNK	N	37.67
1	B	2765:UNK	C	2779:ASP	N	14.02
1	A	2765:UNK	C	2779:ASP	N	13.16

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	3590/3986 (90%)	-0.14	46 (1%) 77 68	144, 217, 281, 339	0
1	B	3607/3986 (90%)	-0.11	55 (1%) 73 64	148, 210, 309, 413	0
2	C	9/192 (4%)	-0.39	0 100 100	217, 221, 227, 228	0
2	D	9/192 (4%)	-0.53	0 100 100	160, 169, 180, 182	0
All	All	7215/8356 (86%)	-0.13	101 (1%) 75 66	144, 213, 288, 413	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	SER	5.7
1	B	46	SER	5.2
1	A	3310	ASN	5.0
1	B	55	THR	4.6
1	B	1994	VAL	4.3
1	A	3316	LEU	4.2
1	B	100	ILE	4.2
1	A	2986	PRO	4.0
1	B	11	SER	4.0
1	A	1993	GLU	4.0
1	B	30	ALA	3.8
1	A	1435	ASN	3.7
1	A	3311	ASN	3.7
1	B	3025	PRO	3.6
1	A	2985	GLU	3.6
1	B	1993	GLU	3.5
1	B	143	LEU	3.4
1	B	74	ASN	3.3
1	B	99	LYS	3.3
1	A	123	CYS	3.2
1	B	45	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	4026	SER	3.1
1	B	546	ALA	3.1
1	B	10	CYS	3.1
1	B	56	SER	3.0
1	B	142	ARG	2.9
1	A	3312	VAL	2.9
1	B	3502	MET	2.9
1	B	119	ARG	2.9
1	A	3642	LYS	2.9
1	A	3007	GLU	2.9
1	B	93	LEU	2.8
1	A	170	VAL	2.8
1	B	23	ASP	2.8
1	B	28	ALA	2.8
1	A	116	THR	2.8
1	A	3277	VAL	2.8
1	B	1047	GLN	2.7
1	A	3270	ASP	2.7
1	A	1439	PRO	2.6
1	A	3292	GLY	2.6
1	B	24	ARG	2.6
1	B	2983	ASP	2.6
1	B	3506	LEU	2.6
1	B	138	PHE	2.6
1	B	356	ASN	2.6
1	B	67	VAL	2.6
1	A	3449	LYS	2.5
1	B	42	CYS	2.4
1	B	3861	GLY	2.4
1	A	3319	ASN	2.4
1	A	2919	ASP	2.4
1	A	3643	HIS	2.3
1	B	3026	ASP	2.3
1	A	3280	TYR	2.3
1	A	300	TRP	2.3
1	A	1292	LYS	2.3
1	A	3447	VAL	2.3
1	A	119	ARG	2.3
1	A	3301	LEU	2.3
1	A	3304	VAL	2.3
1	A	2895	GLU	2.3
1	B	144	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	4035	GLU	2.3
1	B	89	LEU	2.3
1	B	14	ARG	2.3
1	B	181	LEU	2.2
1	B	1271	ILE	2.2
1	B	3028	ASN	2.2
1	A	78	PHE	2.2
1	B	2002	LYS	2.2
1	A	143	LEU	2.2
1	A	3451	LEU	2.2
1	B	2010	GLU	2.2
1	B	107	ILE	2.2
1	A	2484	TYR	2.2
1	A	2984	GLY	2.2
1	A	3291	GLN	2.2
1	B	101	ALA	2.2
1	B	178	LEU	2.2
1	A	2489	SER	2.1
1	B	123	CYS	2.1
1	A	3139	GLN	2.1
1	A	124	LYS	2.1
1	A	3314	SER	2.1
1	B	1287	GLN	2.1
1	B	48	PRO	2.1
1	B	3440	GLN	2.1
1	A	2198	GLY	2.1
1	A	3072	GLU	2.1
1	B	34	LEU	2.1
1	A	3273	LEU	2.1
1	A	98	GLN	2.0
1	A	117	LYS	2.0
1	B	1284	THR	2.0
1	B	4128	MET	2.0
1	B	137	THR	2.0
1	B	104	SER	2.0
1	B	135	LEU	2.0
1	B	3976	GLU	2.0
1	A	1382	ILE	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.