



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 10:19 PM EST

PDB ID : 6EEC  
EMDB ID : EMD-9041  
Title : Mycobacterium tuberculosis RNAP promoter unwinding intermediate complex  
with RbpA/CarD and AP3 promoter captured by Coralopyronin  
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.  
Deposited on : 2018-08-13  
Resolution : 3.55 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

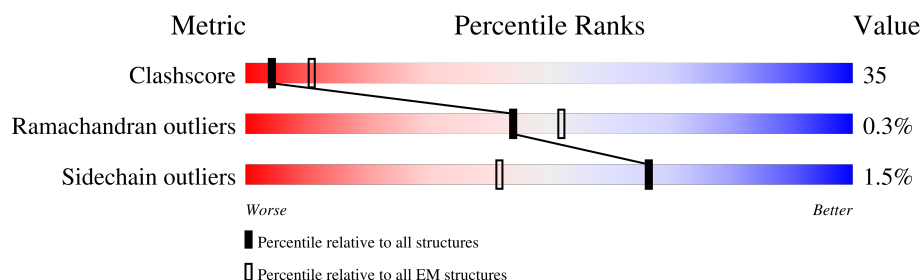
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.55 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
2	C	1179	
3	D	1326	
4	E	110	
5	F	531	
6	J	111	
7	O	90	

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Mol	Chain	Length	Quality of chain
8	P	90	 12% 58% 30%
9	M	162	 43% 55% ..

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 29936 atoms, of which 40 are hydrogens and 0 are deuteriums.

In the tables below, 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1759	1112	298	346	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8593	5381	1507	1666	39		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1266	Total	C	N	O	S	0	0
			9873	6184	1794	1853	42		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A5U053
D	0	ALA	-	expression tag	UNP A5U053

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A5U053
D	1318	HIS	-	expression tag	UNP A5U053
D	1319	HIS	-	expression tag	UNP A5U053
D	1320	HIS	-	expression tag	UNP A5U053
D	1321	HIS	-	expression tag	UNP A5U053
D	1322	HIS	-	expression tag	UNP A5U053
D	1323	HIS	-	expression tag	UNP A5U053
D	1324	HIS	-	expression tag	UNP A5U053

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	319	Total	C	N	O	S	0	0
			2518	1571	456	482	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P9WGI0
F	-1	PRO	-	expression tag	UNP P9WGI0
F	0	HIS	-	expression tag	UNP P9WGI0

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	108	Total	C	N	O	S	0	0
			881	543	168	167	3		

- Molecule 7 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	65	Total	C	N	O	P	0	0
			1336	633	243	395	65		

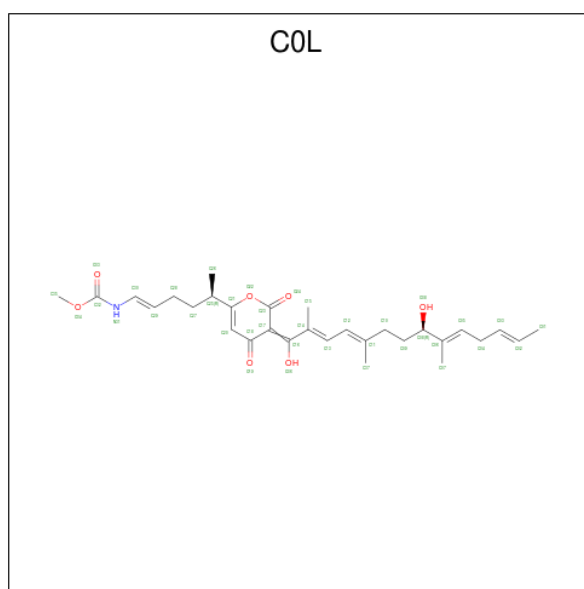
- Molecule 8 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	63	Total	C	N	O	P	0	0
			1289	610	242	374	63		

- Molecule 9 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	159	Total	C	N	O	S	0	0
			1241	777	224	239	1		

- Molecule 10 is methyl [(1E,5R)-5-[(3E)-3-[(2E,4E,8R,9E,12E)-1,8-dihydroxy-2,5,9-trimethyltetradeca-2,4,9,12-tetraen-1-ylidene]-2,4-dioxo-3,4-dihydro-2H-pyran-6-yl}hex-1-en-1-yl]carbamate (three-letter code: C0L) (formula: C<sub>30</sub>H<sub>41</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	H	N	O	0
			78	30	40	1	7	

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	D	1	Total	Mg	0
			1	1	



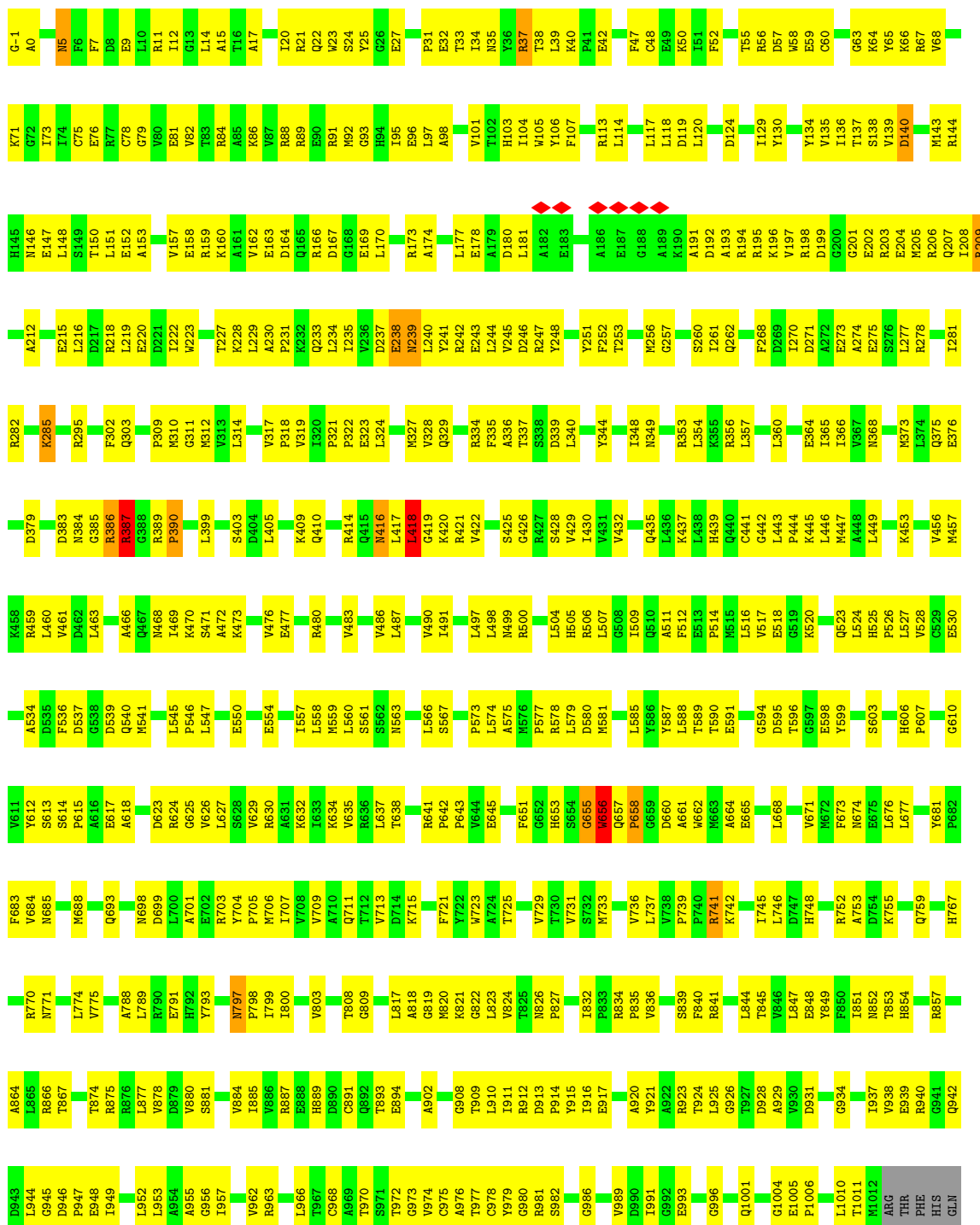


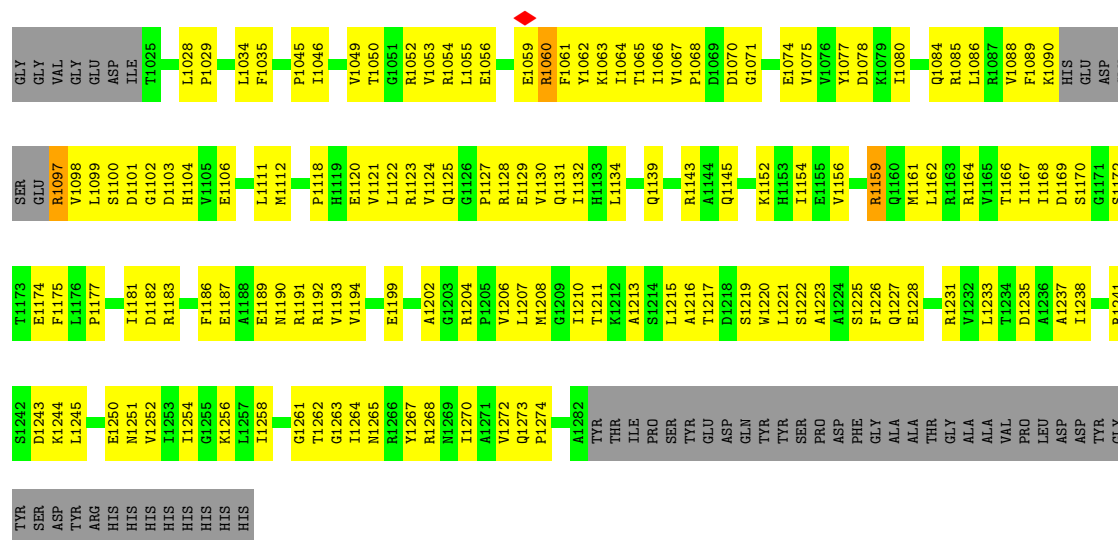
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:  44% 49% 6%

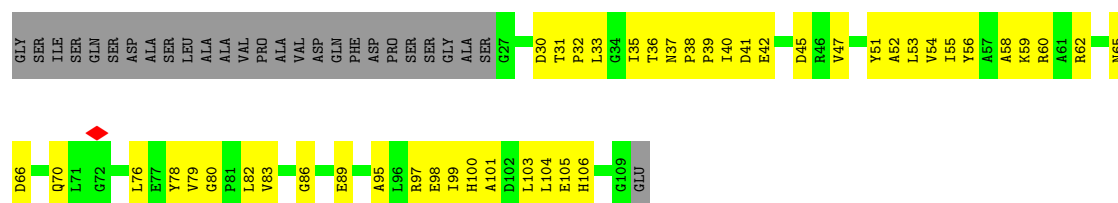
Y1027	Y1028	Y1029	M1030	M1031	K1032	L1033	H1034	H1035	L1036	V1037	D1038	D1039	K1040	I1041	H1042	A1043	R1044	L1045	S1046	P1047	P1048	Y1049	S1050	M1051	I1052	P1056	L1057	G1058	Q1062	F1063	Q1066	R1067	E1070	W1074	A1075	M1076	Q1077	A1078	Y1079	G1080	A1081	A1082	Y1083	T1084	E1087	L1088	I1091	K1092	S1093	D1094	R1927	L1928	Q1930	E1933	T1934	H1935	L1936	G1943	Y1946	W1955	A1956	G1963	V1966	W1969	A1974	R1977	K1978	L1979	G1981	G1982	K1983	L1984	A1985	G1986	R1987	R1988	Y1972	T1974	P1975	Y1976	A1980	Q1981	E1982	L1983	E1984	G1987	L1988	L1989	L1993	P1994	R1995	R1996	D1997	G1998	D1999	L1001	G1006	L11010	R11014	M1926	Y1922	P1923	S1924	R1925	R1926	R1927	R1928	R1929	R1930	R1931	R1932	R1933	R1934	R1935	R1936	R1937	R1938	R1939	R1940	R1941	R1942	R1943	R1944	R1945	R1946	R1947	R1948	R1949	R1950	R1951	R1952	R1953	R1954	R1955	R1956	R1957	R1958	R1959	R1960	R1961	R1962	R1963	R1964	R1965	R1966	R1967	R1968	R1969	R1970	R1971	R1972	R1973	R1974	R1975	R1976	R1977	R1978	R1979	R1980	R1981	R1982	R1983	R1984	R1985	R1986	R1987	R1988	R1989	R1990	R1991	R1992	R1993	R1994	R1995	R1996	R1997	R1998	R1999	R2000	R2001	R2002	R2003	R2004	R2005	R2006	R2007	R2008	R2009	R2010	R2011	R2012	R2013	R2014	R2015	R2016	R2017	R2018	R2019	R2020	R2021	R2022	R2023	R2024	R2025	R2026	R2027	R2028	R2029	R2030	R2031	R2032	R2033	R2034	R2035	R2036	R2037	R2038	R2039	R2040	R2041	R2042	R2043	R2044	R2045	R2046	R2047	R2048	R2049	R2050	R2051	R2052	R2053	R2054	R2055	R2056	R2057	R2058	R2059	R2060	R2061	R2062	R2063	R2064	R2065	R2066	R2067	R2068	R2069	R2070	R2071	R2072	R2073	R2074	R2075	R2076	R2077	R2078	R2079	R2080	R2081	R2082	R2083	R2084	R2085	R2086	R2087	R2088	R2089	R2090	R2091	R2092	R2093	R2094	R2095	R2096	R2097	R2098	R2099	R2100	R2101	R2102	R2103	R2104	R2105	R2106	R2107	R2108	R2109	R2110	R2111	R2112	R2113	R2114	R2115	R2116	R2117	R2118	R2119	R2120	R2121	R2122	R2123	R2124	R2125	R2126	R2127	R2128	R2129	R2130	R2131	R2132	R2133	R2134	R2135	R2136	R2137	R2138	R2139	R2140	R2141	R2142	R2143	R2144	R2145	R2146	R2147	R2148	R2149	R2150	R2151	R2152	R2153	R2154	R2155	R2156	R2157	R2158	R2159	R2160	R2161	R2162	R2163	R2164	R2165	R2166	R2167	R2168	R2169	R2170	R2171	R2172	R2173	R2174	R2175	R2176	R2177	R2178	R2179	R2180	R2181	R2182	R2183	R2184	R2185	R2186	R2187	R2188	R2189	R2190	R2191	R2192	R2193	R2194	R2195	R2196	R2197	R2198	R2199	R2200	R2201	R2202	R2203	R2204	R2205	R2206	R2207	R2208	R2209	R2210	R2211	R2212	R2213	R2214	R2215	R2216	R2217	R2218	R2219	R2220	R2221	R2222	R2223	R2224	R2225	R2226	R2227	R2228	R2229	R2230	R2231	R2232	R2233	R2234	R2235	R2236	R2237	R2238	R2239	R2240	R2241	R2242	R2243	R2244	R2245	R2246	R2247	R2248	R2249	R2250	R2251	R2252	R2253	R2254	R2255	R2256	R2257	R2258	R2259	R2260	R2261	R2262	R2263	R2264	R2265	R2266	R2267	R2268	R2269	R2270	R2271	R2272	R2273	R2274	R2275	R2276	R2277	R2278	R2279	R2280	R2281	R2282	R2283	R2284	R2285	R2286	R2287	R2288	R2289	R2290	R2291	R2292	R2293	R2294	R2295	R2296	R2297	R2298	R2299	R2300	R2301	R2302	R2303	R2304	R2305	R2306	R2307	R2308	R2309	R2310	R2311	R2312	R2313	R2314	R2315	R2316	R2317	R2318	R2319	R2320	R2321	R2322	R2323	R2324	R2325	R2326	R2327	R2328	R2329	R2330	R2331	R2332	R2333	R2334	R2335	R2336	R2337	R2338	R2339	R2340	R2341	R2342	R2343	R2344	R2345	R2346	R2347	R2348	R2349	R2350	R2351	R2352	R2353	R2354	R2355	R2356	R2357	R2358	R2359	R2360	R2361	R2362	R2363	R2364	R2365	R2366	R2367	R2368	R2369	R2370	R2371	R2372	R2373	R2374	R2375	R2376	R2377	R2378	R2379	R2380	R2381	R2382	R2383	R2384	R2385	R2386	R2387	R2388	R2389	R2390	R2391	R2392	R2393	R2394	R2395	R2396	R2397	R2398	R2399	R2400	R2401	R2402	R2403	R2404	R2405	R2406	R2407	R2408	R2409	R2410	R2411	R2412	R2413	R2414	R2415	R2416	R2417	R2418	R2419	R2420	R2421	R2422	R2423	R2424	R2425	R2426	R2427	R2428	R2429	R2430	R2431	R2432	R2433	R2434	R2435	R2436	R2437	R2438	R2439	R2440	R2441	R2442	R2443	R2444	R2445	R2446	R2447	R2448	R2449	R2450	R2451	R2452	R2453	R2454	R2455	R2456	R2457	R2458	R2459	R2460	R2461	R2462	R2463	R2464	R2465	R2466	R2467	R2468	R2469	R2470	R2471	R2472	R2473	R2474	R2475	R2476	R2477	R2478	R2479	R2480	R2481	R2482	R2483	R2484	R2485	R2486	R2487	R2488	R2489	R2490	R2491	R2492	R2493	R2494	R2495	R2496	R2497	R2498	R2499	R2500	R2501	R2502	R2503	R2504	R2505	R2506	R2507	R2508	R2509	R2510	R2511	R2512	R2513	R2514	R2515	R2516	R2517	R2518	R2519	R2520	R2521	R2522	R2523	R2524	R2525	R2526	R2527	R2528	R2529	R2530	R2531	R2532	R2533	R2534	R2535	R2536	R2537	R2538	R2539	R2540	R2541	R2542	R2543	R2544	R2545	R2546	R2547	R2548	R2549	R2550	R2551	R2552	R2553	R2554	R2555	R2556	R2557	R2558	R2559	R2560	R2561	R2562	R2563	R2564	R2565	R2566	R2567	R2568	R2569	R2570	R2571	R2572	R2573	R2574	R2575	R2576	R2577	R2578	R2579	R2580	R2581	R2582	R2583	R2584	R2585	R2586	R2587	R2588	R2589	R2590	R2591	R2592	R2593	R2594	R2595	R2596	R2597	R2598	R2599	R2600	R2601	R2602	R2603	R2604	R2605	R2606	R2607	R2608	R2609	R2610	R2611	R2612	R2613	R2614	R2615	R2616	R2617	R2618	R2619	R2620	R2621	R2622	R2623	R2624	R2625	R2626	R2627	R2628	R2629	R2630	R2631	R2632	R2633	R2634	R2635	R2636	R2637	R2638	R2639	R2640	R2641	R2642	R2643	R2644	R2645	R2646	R2647	R2648	R2649	R2650	R2651	R2652	R2653	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- Molecule 3: DNA-directed RNA polymerase subunit beta'

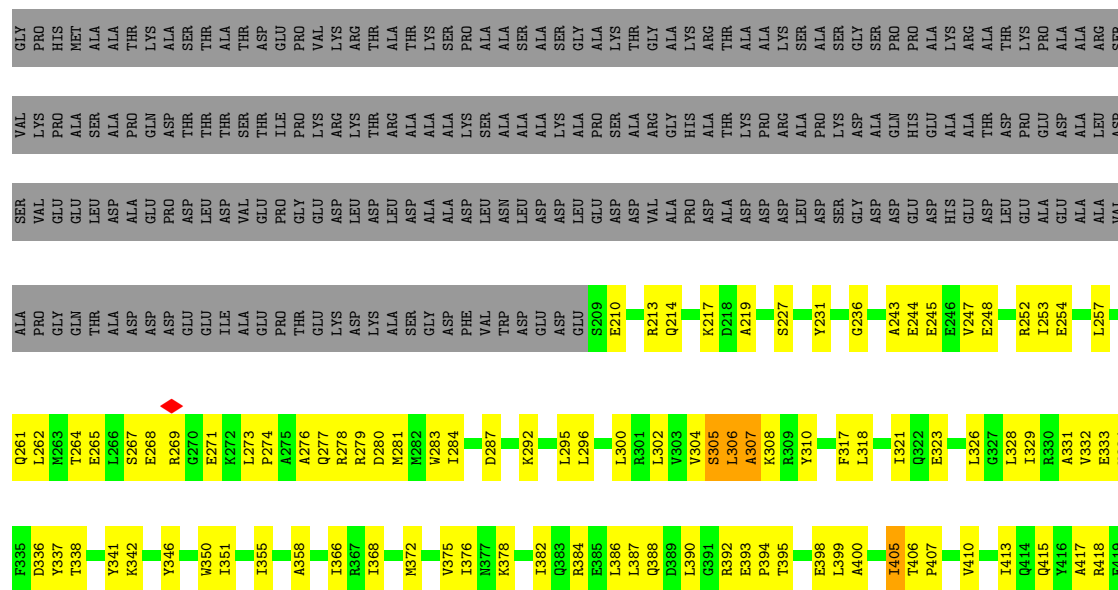
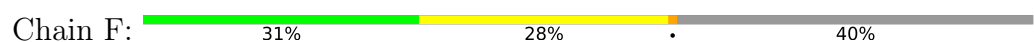




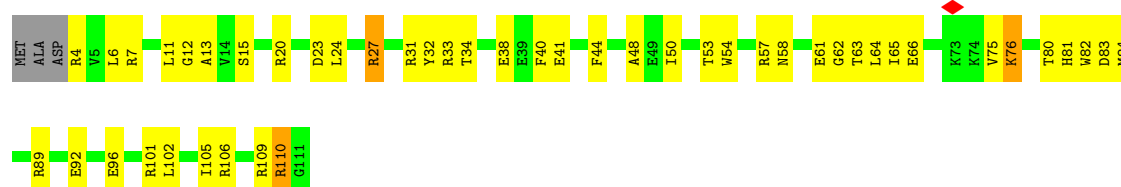
• Molecule 4: DNA-directed RNA polymerase subunit omega



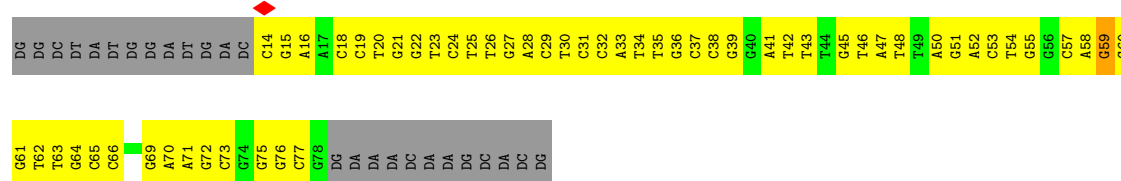
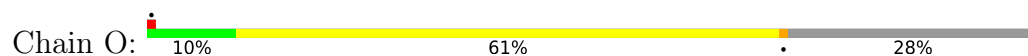
• Molecule 5: RNA polymerase sigma factor SigA



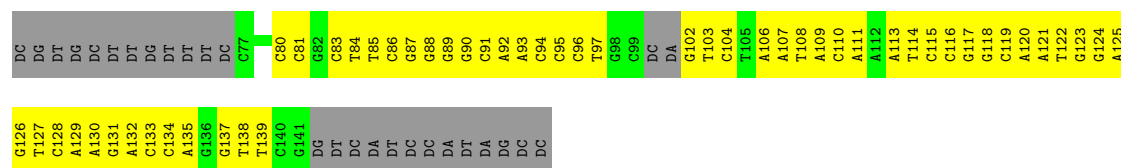
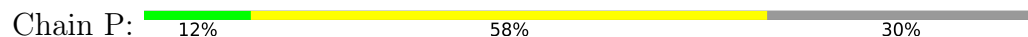
- Molecule 6: RNA polymerase-binding protein RbpA



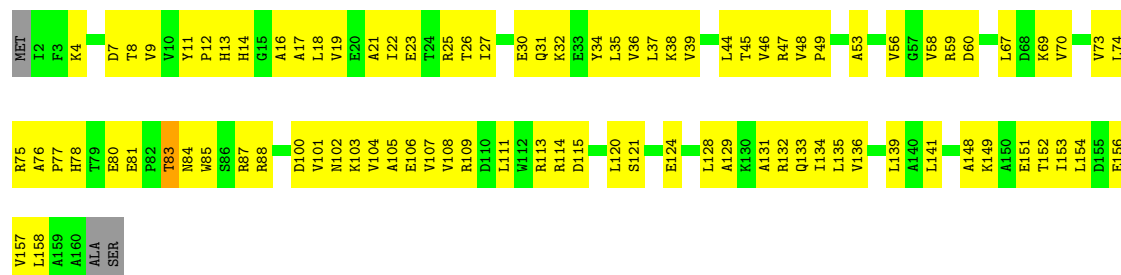
- Molecule 7: DNA (65-MER)



- Molecule 8: DNA (63-MER)



- Molecule 9: RNA polymerase-binding transcription factor CarD



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	246409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	69.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.111	Depositor
Minimum map value	-1.642	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	325.0, 325.0, 325.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, C0L, ZN

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	0.47	0/1742	0.55	0/2370
1	B	0.43	0/1786	0.53	0/2435
2	C	0.55	0/8751	0.61	5/11869 (0.0%)
3	D	0.56	1/10037 (0.0%)	0.59	6/13570 (0.0%)
4	E	0.44	0/662	0.52	0/901
5	F	0.46	0/2549	0.55	3/3438 (0.1%)
6	J	0.38	0/897	0.55	1/1210 (0.1%)
7	O	0.80	0/1497	0.97	2/2310 (0.1%)
8	P	0.76	0/1445	0.91	0/2224
9	M	0.36	0/1257	0.49	0/1700
All	All	0.55	1/30623 (0.0%)	0.63	17/42027 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	656	TRP	CB-CG	-7.29	1.37	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	306	LEU	C-N-CA	-7.20	103.71	121.70
3	D	419	GLY	N-CA-C	7.08	130.80	113.10
3	D	655	GLY	N-CA-C	-6.73	96.27	113.10
2	C	275	LEU	CA-CB-CG	-6.63	100.04	115.30
2	C	288	THR	N-CA-C	-6.59	93.21	111.00
2	C	686	GLN	C-N-CA	-6.46	105.55	121.70
3	D	387	ARG	NE-CZ-NH2	-6.14	117.23	120.30
5	F	306	LEU	CB-CG-CD2	-6.05	100.72	111.00
6	J	75	VAL	C-N-CA	6.02	136.76	121.70
5	F	405	ILE	C-N-CA	-5.98	106.76	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	282	ARG	C-N-CD	5.74	140.46	128.40
3	D	390	PRO	CA-N-CD	-5.46	103.85	111.50
7	O	59	DG	C1'-O4'-C4'	-5.37	104.73	110.10
7	O	59	DG	O4'-C1'-N9	5.08	111.56	108.00
3	D	387	ARG	CG-CD-NE	5.05	122.40	111.80
3	D	656	TRP	N-CA-C	-5.01	97.47	111.00
2	C	285	GLU	C-N-CD	5.00	138.91	128.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1716	0	1756	121	0
1	B	1759	0	1783	145	0
2	C	8593	0	8517	695	0
3	D	9873	0	9938	738	0
4	E	649	0	645	54	0
5	F	2518	0	2540	182	0
6	J	881	0	861	62	0
7	O	1336	0	732	116	0
8	P	1289	0	706	88	0
9	M	1241	0	1259	111	0
10	C	38	40	0	1	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
All	All	29896	40	28737	2075	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 35.

All (2075) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:LEU:CD2	2:C:295:LEU:HD21	1.62	1.30
2:C:271:ASP:O	2:C:275:LEU:HD12	1.25	1.27
2:C:1067:ARG:CZ	3:D:418:LEU:CD2	2.13	1.25
2:C:278:TYR:CE1	2:C:292:ALA:HB2	1.73	1.23
2:C:1067:ARG:NH1	3:D:418:LEU:CD2	2.04	1.21
2:C:278:TYR:CD1	2:C:292:ALA:CB	2.25	1.19
2:C:275:LEU:HD21	2:C:289:LYS:CB	1.72	1.19
2:C:275:LEU:CD2	2:C:289:LYS:HB3	1.73	1.18
5:F:334:LYS:HE2	7:O:48:DT:OP1	1.41	1.17
2:C:271:ASP:O	2:C:275:LEU:CD1	1.91	1.17
2:C:278:TYR:CE1	2:C:292:ALA:CB	2.29	1.15
2:C:463:LEU:HD13	2:C:468:ALA:HB2	1.30	1.12
2:C:273:ALA:O	2:C:276:ASP:N	1.83	1.12
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.27	1.10
2:C:1067:ARG:NH1	3:D:418:LEU:HD22	1.66	1.08
3:D:383:ASP:OD2	3:D:386:ARG:NE	1.86	1.08
9:M:104:VAL:HG11	9:M:134:ILE:HD11	1.35	1.08
2:C:278:TYR:CD1	2:C:292:ALA:HB1	1.89	1.07
2:C:466:GLU:OE1	2:C:466:GLU:N	1.87	1.07
4:E:47:VAL:HG21	4:E:53:LEU:HB2	1.37	1.06
6:J:31:ARG:HG2	6:J:41:GLU:HG2	1.37	1.06
3:D:952:LEU:HD22	3:D:957:ILE:HD11	1.37	1.04
2:C:1067:ARG:NH1	3:D:418:LEU:HD23	1.72	1.03
2:C:278:TYR:O	2:C:281:LEU:N	1.93	1.01
2:C:281:LEU:HD22	2:C:295:LEU:HD21	1.44	0.99
2:C:281:LEU:CD2	2:C:295:LEU:CD2	2.41	0.98
3:D:641:ARG:CA	3:D:657:GLN:HG3	1.93	0.98
2:C:273:ALA:O	2:C:275:LEU:N	1.97	0.97
3:D:389:ARG:NH1	7:O:58:DA:C8	2.31	0.97
2:C:659:THR:HG22	2:C:669:THR:HG22	1.45	0.97
7:O:29:DC:H2''	7:O:30:DT:H5'	1.44	0.97
9:M:26:THR:HB	9:M:31:GLN:HG3	1.46	0.97
1:A:40:ARG:HH12	2:C:903:ASP:HB3	1.31	0.96
1:B:101:GLY:HA2	1:B:131:LYS:HA	1.48	0.96
9:M:74:LEU:HD21	9:M:158:LEU:HD23	1.46	0.95
2:C:278:TYR:HE1	2:C:292:ALA:HB2	1.21	0.94
2:C:1052:ILE:HD11	5:F:423:LEU:HD13	1.49	0.94
3:D:1090:LYS:HD2	3:D:1097:ARG:HE	1.32	0.94
3:D:33:THR:HG21	3:D:327:MET:HE1	1.48	0.93
5:F:305:SER:OG	7:O:54:DT:H4'	1.68	0.93
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	1.51	0.92
3:D:641:ARG:HA	3:D:657:GLN:CG	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1107:VAL:HG11	3:D:469:ILE:HD12	1.50	0.92
3:D:1010:LEU:HD12	3:D:1145:GLN:HG3	1.50	0.92
2:C:278:TYR:HD1	2:C:292:ALA:CB	1.73	0.92
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.51	0.92
6:J:106:ARG:HG3	6:J:110:ARG:HD3	1.53	0.91
2:C:148:LYS:HB3	2:C:414:PRO:HD3	1.52	0.90
3:D:880:VAL:HG21	3:D:1210:ILE:HB	1.52	0.90
3:D:1062:TYR:HB2	3:D:1080:ILE:HG21	1.53	0.90
3:D:181:LEU:HD21	3:D:198:ARG:HD2	1.54	0.90
6:J:64:LEU:HD23	6:J:66:GLU:H	1.37	0.89
2:C:275:LEU:HD21	2:C:289:LYS:HB3	0.91	0.89
2:C:288:THR:CG2	2:C:291:SER:HB3	2.02	0.89
7:O:42:DT:H1'	7:O:43:DT:H5'	1.53	0.89
2:C:1092:LYS:NZ	3:D:545:LEU:O	2.05	0.89
5:F:328:LEU:HD23	5:F:351:ILE:HD11	1.51	0.89
3:D:1190:ASN:HA	3:D:1193:VAL:HG12	1.54	0.89
9:M:115:ASP:HB3	9:M:120:LEU:HD13	1.51	0.89
2:C:294:THR:O	2:C:298:ASN:OD1	1.91	0.88
8:P:107:DA:H2'	8:P:108:DT:H71	1.55	0.88
9:M:111:LEU:HB2	9:M:128:LEU:HD13	1.54	0.88
3:D:676:LEU:HD12	3:D:715:LYS:HB3	1.55	0.87
2:C:515:PRO:HB2	2:C:581:VAL:HG11	1.56	0.87
2:C:273:ALA:O	2:C:274:LEU:C	2.09	0.87
2:C:267:THR:CG2	2:C:272:GLU:HG3	2.04	0.86
2:C:1052:ILE:HD12	5:F:436:GLY:HA3	1.55	0.86
2:C:222:VAL:HG21	2:C:234:VAL:HG22	1.57	0.86
3:D:910:LEU:HD21	3:D:956:GLY:HA2	1.56	0.86
2:C:1067:ARG:CZ	3:D:418:LEU:HD23	2.00	0.86
1:A:98:ARG:HG3	1:A:135:GLU:HG2	1.57	0.85
2:C:1067:ARG:CZ	3:D:418:LEU:HD22	1.96	0.85
5:F:306:LEU:O	5:F:307:ALA:C	2.05	0.85
2:C:270:THR:O	2:C:274:LEU:HD23	1.76	0.85
3:D:1068:PRO:HD2	3:D:1074:GLU:HG2	1.58	0.85
3:D:797:ASN:HB3	3:D:800:ILE:HG22	1.56	0.85
3:D:1066:ILE:HD12	3:D:1075:VAL:HB	1.59	0.85
2:C:281:LEU:HD21	2:C:295:LEU:HD21	1.57	0.84
2:C:288:THR:HG21	2:C:291:SER:HB3	1.57	0.84
2:C:463:LEU:CD1	2:C:468:ALA:HB2	2.07	0.84
7:O:21:DG:H2'	7:O:22:DG:H1'	1.59	0.84
3:D:1217:THR:HG22	3:D:1223:ALA:HB2	1.60	0.84
3:D:417:LEU:O	3:D:418:LEU:O	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD12	1:A:225:LEU:HD22	1.61	0.83
1:B:191:LYS:HE3	1:B:193:ILE:HD11	1.60	0.83
3:D:441:CYS:HB3	3:D:512:PHE:HD2	1.44	0.83
1:A:218:LEU:HD12	1:B:234:ILE:HD11	1.60	0.83
3:D:177:LEU:HD11	3:D:198:ARG:HA	1.60	0.82
2:C:269:GLY:O	2:C:272:GLU:HB3	1.79	0.82
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.61	0.82
5:F:492:ILE:HG22	5:F:503:ILE:HD12	1.61	0.82
7:O:25:DT:H1'	7:O:26:DT:H5'	1.61	0.82
5:F:390:LEU:HD21	5:F:392:ARG:HE	1.45	0.82
2:C:334:THR:HG23	2:C:337:ASP:H	1.46	0.81
2:C:597:LEU:HB3	2:C:976:VAL:HG13	1.60	0.81
9:M:8:THR:HG22	9:M:18:LEU:HD21	1.62	0.81
3:D:1053:VAL:HG12	3:D:1103:ASP:H	1.44	0.81
5:F:470:ARG:NH1	7:O:24:DC:OP2	2.13	0.81
2:C:885:LEU:HD23	2:C:1030:ILE:HD12	1.62	0.81
3:D:1124:VAL:HG12	3:D:1125:GLN:HG3	1.59	0.81
1:B:60:LEU:HD21	1:B:159:ILE:HD13	1.63	0.81
1:A:40:ARG:HE	1:B:33:THR:HG22	1.47	0.80
5:F:470:ARG:HD3	5:F:506:ILE:HD13	1.61	0.80
8:P:117:DG:H1'	8:P:118:DG:H5'	1.63	0.80
2:C:278:TYR:CE1	2:C:292:ALA:HB1	2.09	0.80
5:F:306:LEU:O	5:F:308:LYS:N	2.14	0.80
3:D:444:PRO:HG2	3:D:447:MET:HB3	1.63	0.80
2:C:821:LEU:HB3	5:F:527:LEU:HD11	1.64	0.80
2:C:284:GLY:HA2	5:F:219:ALA:HB1	1.64	0.79
2:C:233:PRO:HG2	2:C:236:VAL:HG23	1.64	0.79
2:C:1067:ARG:HH12	3:D:418:LEU:HD22	1.45	0.79
7:O:61:DG:H2''	7:O:62:DT:H5'	1.62	0.79
1:B:183:VAL:HA	1:B:188:ASP:H	1.48	0.79
2:C:1067:ARG:CZ	3:D:418:LEU:HD21	2.12	0.79
3:D:1167:ILE:HD11	3:D:1181:ILE:HD11	1.65	0.78
2:C:50:VAL:HG22	2:C:503:TYR:HE1	1.48	0.78
3:D:737:LEU:HB2	3:D:793:TYR:HE1	1.48	0.78
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.17	0.78
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.14	0.78
1:B:172:LEU:HD13	1:B:199:LYS:H	1.49	0.77
3:D:923:ARG:HB3	3:D:962:VAL:HG21	1.64	0.77
9:M:75:ARG:HE	9:M:157:VAL:HG13	1.49	0.77
1:B:38:LEU:HD23	1:B:194:LEU:HD11	1.65	0.77
1:A:95:MET:HA	1:A:113:PRO:HD3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:ARG:HD3	2:C:973:SER:HB3	1.64	0.77
3:D:820:MET:HG2	3:D:822:GLY:H	1.48	0.77
1:B:71:GLU:HB3	1:B:75:GLU:HB3	1.67	0.77
2:C:909:ASP:OD2	2:C:995:ASN:ND2	2.16	0.77
3:D:277:LEU:HD11	3:D:295:ARG:HH12	1.48	0.77
1:B:97:LEU:HB3	1:B:136:VAL:HB	1.66	0.77
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.67	0.77
3:D:356:ARG:HE	5:F:326:LEU:HD11	1.49	0.77
2:C:487:GLU:OE2	2:C:613:ARG:NH2	2.18	0.76
3:D:93:GLY:O	3:D:319:VAL:N	2.16	0.76
3:D:706:MET:N	4:E:41:ASP:OD2	2.18	0.76
8:P:93:DA:H1'	8:P:94:DC:H5''	1.67	0.76
2:C:322:LEU:HD23	2:C:357:VAL:HG11	1.67	0.76
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.66	0.76
2:C:767:GLU:HG2	2:C:807:THR:HG22	1.67	0.76
2:C:285:GLU:OE1	2:C:286:PRO:HD2	1.86	0.75
2:C:1032:LYS:HE2	2:C:1036:LEU:HD21	1.69	0.75
3:D:173:ARG:NH1	3:D:204:GLU:OE1	2.17	0.75
7:O:21:DG:H2'	7:O:22:DG:C1'	2.16	0.75
2:C:139:PHE:HB3	2:C:148:LYS:HB2	1.68	0.75
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.68	0.75
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.19	0.75
3:D:101:VAL:O	3:D:314:LEU:N	2.19	0.75
3:D:136:ILE:HG13	3:D:229:LEU:HD11	1.69	0.75
1:B:55:ARG:HG2	1:B:137:GLU:HB2	1.69	0.75
2:C:147:ILE:HG12	9:M:47:ARG:HG2	1.66	0.75
2:C:253:GLY:O	2:C:259:ARG:NH1	2.20	0.75
2:C:278:TYR:CD1	2:C:292:ALA:HB2	2.08	0.75
5:F:493:GLY:O	5:F:497:GLY:N	2.20	0.75
2:C:463:LEU:HD13	2:C:468:ALA:CB	2.15	0.75
3:D:891:CYS:HB3	3:D:970:THR:HG23	1.69	0.74
5:F:334:LYS:HE2	7:O:48:DT:P	2.26	0.74
2:C:307:ASP:O	2:C:308:LEU:C	2.23	0.74
2:C:1066:GLN:OE1	3:D:425:SER:OG	2.04	0.74
2:C:1044:ARG:NH1	2:C:1056:PRO:HB3	2.01	0.74
2:C:1091:ILE:HG23	2:C:1115:PRO:HB3	1.70	0.74
3:D:389:ARG:NH1	7:O:59:DG:C8	2.55	0.74
8:P:86:DC:H1'	8:P:87:DG:H5'	1.68	0.74
3:D:701:ALA:HA	3:D:709:VAL:HG21	1.70	0.74
8:P:133:DC:H2'	8:P:134:DC:H1'	1.70	0.74
1:B:102:PRO:HD3	1:B:131:LYS:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:LEU:HD23	2:C:295:LEU:CD2	2.18	0.74
2:C:288:THR:OG1	2:C:291:SER:HB3	1.87	0.74
3:D:618:ALA:HB1	3:D:668:LEU:HD12	1.69	0.74
3:D:981:ARG:HD3	3:D:986:GLY:HA2	1.68	0.74
2:C:252:PHE:HB3	2:C:255:SER:HB2	1.70	0.73
2:C:278:TYR:HE1	2:C:292:ALA:CB	1.84	0.73
3:D:443:LEU:HD12	3:D:444:PRO:HD2	1.70	0.73
2:C:412:ILE:HD13	2:C:417:LEU:HD11	1.70	0.73
3:D:191:ALA:HA	3:D:194:ARG:HE	1.52	0.73
2:C:267:THR:HG22	2:C:272:GLU:HG3	1.69	0.73
5:F:333:GLU:OE1	6:J:84:MET:HE3	1.89	0.73
2:C:571:VAL:HG21	2:C:575:GLU:HB2	1.71	0.73
3:D:22:GLN:O	6:J:57:ARG:NH2	2.21	0.73
2:C:604:ARG:NH1	2:C:607:MET:SD	2.62	0.73
5:F:302:LEU:O	5:F:305:SER:HB2	1.88	0.73
2:C:348:LEU:HD21	2:C:367:THR:HG22	1.70	0.73
2:C:413:THR:HG22	2:C:416:THR:HG23	1.69	0.73
2:C:442:GLN:O	2:C:678:SER:OG	2.07	0.73
2:C:90:LEU:HD23	2:C:107:PHE:HB3	1.71	0.73
3:D:657:GLN:HA	3:D:657:GLN:NE2	2.01	0.73
3:D:1089:PHE:O	3:D:1097:ARG:N	2.22	0.73
2:C:255:SER:HB3	2:C:258:MET:HB2	1.70	0.72
3:D:449:LEU:HD11	3:D:476:VAL:HG13	1.70	0.72
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.21	0.72
3:D:160:LYS:NZ	3:D:164:ASP:OD1	2.22	0.72
2:C:353:THR:HG23	2:C:354:THR:HG22	1.72	0.72
2:C:1136:GLU:OE2	3:D:11:ARG:NH2	2.19	0.72
3:D:970:THR:OG1	3:D:973:GLY:O	2.06	0.72
3:D:1120:GLU:OE2	3:D:1123:ARG:NH2	2.21	0.72
2:C:101:GLY:O	2:C:142:ASN:ND2	2.23	0.72
2:C:905:PRO:HD2	2:C:916:ILE:HD11	1.71	0.72
3:D:177:LEU:HD13	3:D:201:GLY:HA3	1.71	0.72
1:A:142:ARG:NH2	1:B:230:GLU:OE1	2.22	0.72
2:C:150:GLN:HG2	9:M:44:LEU:HB3	1.70	0.72
3:D:699:ASP:OD1	3:D:703:ARG:NH1	2.23	0.71
2:C:780:VAL:HG23	2:C:781:LEU:HD12	1.72	0.71
2:C:157:PHE:HE1	2:C:389:ILE:HD11	1.55	0.71
2:C:758:ASP:O	2:C:805:LYS:NZ	2.23	0.71
9:M:85:TRP:HA	9:M:88:ARG:HG2	1.71	0.71
2:C:313:ARG:HG3	2:C:331:SER:HA	1.73	0.71
7:O:72:DG:H2''	7:O:73:DC:H2'	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:77:PRO:O	9:M:109:ARG:NH2	2.23	0.71
2:C:532:THR:HG22	2:C:535:GLU:HG2	1.72	0.71
3:D:235:ILE:HG21	3:D:241:TYR:HB2	1.72	0.71
2:C:1057:LEU:HD23	2:C:1062:GLN:HG2	1.73	0.71
3:D:926:GLY:O	3:D:940:ARG:NH2	2.24	0.71
3:D:1274:PRO:HA	4:E:104:LEU:HD23	1.73	0.71
1:A:41:THR:OG1	1:A:215:LEU:HD21	1.90	0.71
2:C:273:ALA:C	2:C:275:LEU:N	2.44	0.71
9:M:23:GLU:OE1	9:M:25:ARG:NH2	2.24	0.71
1:B:18:ARG:NH2	1:B:195:ASP:OD2	2.24	0.70
8:P:135:DA:OP2	8:P:135:DA:H2'	1.90	0.70
3:D:1189:GLU:OE2	3:D:1192:ARG:NH2	2.24	0.70
2:C:892:LYS:HE3	3:D:537:ASP:HB2	1.74	0.70
3:D:1088:VAL:HA	3:D:1098:VAL:HA	1.73	0.70
7:O:58:DA:H2''	7:O:59:DG:H3'	1.73	0.70
2:C:442:GLN:NE2	2:C:679:ASN:OD1	2.24	0.70
2:C:540:VAL:HG22	2:C:561:VAL:CG2	2.20	0.70
2:C:229:LYS:HE3	2:C:281:LEU:O	1.92	0.70
3:D:1172:SER:H	3:D:1199:GLU:HG3	1.56	0.70
2:C:150:GLN:NE2	2:C:413:THR:OG1	2.25	0.70
2:C:737:LEU:HD23	2:C:915:ILE:HG22	1.72	0.70
3:D:594:GLY:N	3:D:598:GLU:OE2	2.24	0.70
3:D:615:PRO:HD3	3:D:637:LEU:HD23	1.74	0.70
2:C:215:ASP:N	2:C:223:GLY:O	2.23	0.70
2:C:584:ARG:HH22	2:C:975:PRO:HB2	1.57	0.70
2:C:801:ILE:HD13	2:C:838:LYS:HG2	1.73	0.70
2:C:1067:ARG:NH2	3:D:418:LEU:CD2	2.55	0.69
3:D:651:PHE:CD2	3:D:655:GLY:HA3	2.26	0.69
2:C:102:SER:O	2:C:142:ASN:N	2.21	0.69
2:C:1074:TRP:HB3	3:D:1001:GLN:HE21	1.58	0.69
5:F:248:GLU:OE2	6:J:101:ARG:NH2	2.25	0.69
1:A:170:PRO:HB3	1:A:202:ILE:HG12	1.73	0.69
3:D:885:ILE:HD11	3:D:887:ARG:HE	1.57	0.69
3:D:144:ARG:O	3:D:148:LEU:HB2	1.93	0.69
1:B:171:VAL:HG12	1:B:198:THR:HG22	1.75	0.69
2:C:435:GLN:HE21	2:C:460:PRO:HD3	1.57	0.69
3:D:981:ARG:O	3:D:1152:LYS:NZ	2.25	0.69
2:C:738:SER:HA	2:C:904:MET:HE3	1.74	0.68
7:O:22:DG:H2''	7:O:23:DT:H5'	1.73	0.68
3:D:410:GLN:NE2	3:D:1225:SER:O	2.22	0.68
7:O:58:DA:H2''	7:O:59:DG:C3'	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD22	1:B:7:PRO:HG2	1.75	0.68
8:P:121:DA:H2'	8:P:122:DT:C1'	2.23	0.68
1:A:7:PRO:HG2	1:B:221:LEU:HD11	1.75	0.68
2:C:192:ASP:O	2:C:196:ASP:N	2.27	0.68
2:C:761:ASP:OD1	2:C:866:ASN:ND2	2.26	0.68
3:D:913:ASP:HB3	3:D:916:ILE:HG13	1.76	0.68
3:D:1228:GLU:OE1	3:D:1231:ARG:NE	2.19	0.68
5:F:296:LEU:HD23	5:F:328:LEU:HD12	1.74	0.68
2:C:438:GLN:OE1	2:C:451:HIS:NE2	2.26	0.68
2:C:278:TYR:O	2:C:280:LYS:N	2.27	0.68
3:D:545:LEU:HD12	3:D:546:PRO:HD2	1.76	0.68
3:D:968:CYS:SG	3:D:975:CYS:N	2.63	0.68
2:C:224:VAL:HB	2:C:232:GLN:HB2	1.75	0.68
2:C:563:ARG:HG3	2:C:564:LYS:H	1.58	0.67
2:C:96:ILE:HD12	2:C:397:GLU:HG3	1.75	0.67
3:D:1162:LEU:HD21	3:D:1207:LEU:HD23	1.77	0.67
5:F:317:PHE:CE2	5:F:321:ILE:HD11	2.29	0.67
9:M:4:LYS:N	9:M:7:ASP:OD2	2.20	0.67
1:B:40:ARG:HH12	3:D:623:ASP:HB3	1.60	0.67
2:C:1094:ASP:HB3	2:C:1119:GLU:H	1.58	0.67
3:D:270:ILE:HD12	3:D:303:GLN:HA	1.74	0.67
3:D:1056:GLU:HB3	3:D:1063:LYS:HB3	1.76	0.67
2:C:288:THR:HG21	2:C:291:SER:CB	2.24	0.67
5:F:405:ILE:HD11	5:F:410:VAL:HG22	1.76	0.67
2:C:463:LEU:HD12	2:C:463:LEU:C	2.14	0.67
3:D:191:ALA:HB2	3:D:194:ARG:HH21	1.59	0.66
3:D:844:LEU:HD23	3:D:848:GLU:HB3	1.75	0.66
3:D:915:TYR:CZ	3:D:1143:ARG:HD3	2.30	0.66
8:P:121:DA:H2'	8:P:122:DT:H1'	1.76	0.66
2:C:203:LYS:HG2	2:C:213:GLU:HG3	1.77	0.66
5:F:283:TRP:CE3	6:J:105:ILE:HD12	2.30	0.66
7:O:50:DA:OP1	9:M:87:ARG:NH2	2.26	0.66
8:P:133:DC:H2'	8:P:134:DC:C1'	2.25	0.66
1:B:108:GLY:N	1:B:121:PRO:O	2.28	0.66
2:C:175:VAL:HG11	2:C:381:VAL:HG23	1.76	0.66
3:D:7:PHE:O	3:D:1256:LYS:NZ	2.28	0.66
3:D:512:PHE:CE1	3:D:561:SER:HB2	2.30	0.66
2:C:308:LEU:O	2:C:331:SER:HB2	1.95	0.66
2:C:584:ARG:HH12	2:C:975:PRO:HB3	1.59	0.66
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.78	0.66
2:C:463:LEU:HD12	2:C:463:LEU:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:518:LYS:O	2:C:525:SER:OG	2.11	0.66
3:D:56:ARG:NE	3:D:59:GLU:OE1	2.22	0.66
2:C:717:LYS:HB2	2:C:719:LEU:HD11	1.77	0.66
2:C:41:PHE:CD2	2:C:980:ALA:HB2	2.31	0.66
3:D:1068:PRO:CD	3:D:1074:GLU:HG2	2.26	0.66
5:F:305:SER:O	5:F:308:LYS:HG2	1.96	0.66
2:C:146:GLU:HG3	9:M:48:VAL:HG22	1.77	0.66
2:C:465:ARG:HB2	2:C:466:GLU:OE1	1.96	0.66
2:C:762:THR:HG23	2:C:765:GLY:H	1.60	0.66
3:D:797:ASN:HD22	3:D:798:PRO:HD2	1.60	0.66
4:E:60:ARG:HH22	4:E:80:GLY:HA3	1.60	0.66
3:D:417:LEU:C	3:D:418:LEU:O	2.32	0.65
3:D:334:ARG:HH11	5:F:418:ARG:HB3	1.61	0.65
3:D:517:VAL:HG12	3:D:518:GLU:O	1.96	0.65
3:D:676:LEU:CD1	3:D:715:LYS:HB3	2.26	0.65
2:C:267:THR:HG23	2:C:272:GLU:HG3	1.77	0.65
2:C:1076:MET:HE1	2:C:1084:THR:HG22	1.79	0.65
3:D:441:CYS:HB3	3:D:512:PHE:CD2	2.30	0.65
3:D:916:ILE:HG23	3:D:920:ALA:HB3	1.78	0.65
5:F:252:ARG:NH2	5:F:287:ASP:OD1	2.28	0.65
2:C:453:ARG:NH2	2:C:501:SER:O	2.30	0.65
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.77	0.65
3:D:550:GLU:HG3	4:E:58:ALA:HB1	1.78	0.65
3:D:1052:ARG:O	3:D:1067:VAL:HB	1.97	0.65
3:D:151:LEU:HD22	3:D:248:TYR:HE1	1.61	0.65
1:A:157:ALA:HB1	1:A:161:ARG:HG3	1.78	0.65
2:C:277:ILE:O	2:C:278:TYR:O	2.15	0.65
2:C:1133:LEU:HD11	3:D:105:TRP:HZ3	1.60	0.65
3:D:39:LEU:HB3	6:J:11:LEU:HD13	1.77	0.65
1:B:43:LEU:HD11	1:B:174:VAL:HB	1.79	0.65
2:C:736:ILE:HD11	2:C:916:ILE:HD12	1.78	0.65
3:D:767:HIS:O	3:D:770:ARG:HG3	1.96	0.65
5:F:390:LEU:HG	5:F:392:ARG:HG2	1.79	0.65
1:B:95:MET:HG2	1:B:113:PRO:HD2	1.77	0.64
3:D:638:THR:HG22	3:D:660:ASP:O	1.96	0.64
3:D:181:LEU:HD21	3:D:198:ARG:CD	2.26	0.64
5:F:210:GLU:OE1	5:F:213:ARG:HG3	1.97	0.64
2:C:277:ILE:O	2:C:278:TYR:C	2.33	0.64
3:D:389:ARG:HD3	3:D:390:PRO:HD2	1.79	0.64
6:J:106:ARG:O	6:J:110:ARG:HD2	1.97	0.64
1:A:93:VAL:HG21	1:A:116:VAL:HG11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:THR:HG23	2:C:272:GLU:CG	2.28	0.64
2:C:848:ILE:HD11	2:C:874:ALA:HB2	1.79	0.64
3:D:35:ASN:HB3	3:D:38:THR:HG22	1.79	0.64
3:D:963:ARG:NH1	3:D:977:THR:OG1	2.30	0.64
3:D:1273:GLN:NE2	4:E:105:GLU:OE2	2.28	0.64
1:B:183:VAL:HA	1:B:188:ASP:N	2.12	0.64
2:C:737:LEU:HD22	2:C:741:LEU:HD12	1.79	0.64
3:D:257:GLY:O	3:D:260:SER:OG	2.09	0.64
5:F:502:ARG:NH2	7:O:24:DC:OP2	2.30	0.64
9:M:26:THR:HA	9:M:31:GLN:HA	1.78	0.64
2:C:220:ASP:OD2	2:C:257:ILE:HG12	1.98	0.64
2:C:540:VAL:HG22	2:C:561:VAL:HG21	1.79	0.64
2:C:922:VAL:HG22	2:C:930:GLN:NE2	2.13	0.64
2:C:239:LYS:NZ	2:C:267:THR:O	2.29	0.64
2:C:306:TYR:HE2	2:C:333:LEU:HG	1.63	0.64
3:D:847:LEU:O	3:D:851:ILE:HG12	1.98	0.64
2:C:202:VAL:HG11	2:C:214:PHE:HB2	1.80	0.64
2:C:646:GLU:HB3	2:C:662:HIS:CE1	2.33	0.64
3:D:118:LEU:HB3	3:D:120:LEU:HD13	1.81	0.64
3:D:63:GLY:O	3:D:66:LYS:NZ	2.31	0.63
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.23	0.63
1:B:107:ALA:O	1:B:110:ILE:HG22	1.98	0.63
3:D:37:ARG:HG3	3:D:38:THR:N	2.13	0.63
3:D:1046:ILE:HD11	3:D:1124:VAL:HG21	1.80	0.63
8:P:132:DA:H2''	8:P:133:DC:H5'	1.79	0.63
2:C:178:GLN:O	2:C:378:LEU:HD12	1.98	0.63
7:O:22:DG:H2'	7:O:23:DT:C6	2.34	0.63
2:C:409:VAL:HG23	2:C:410:GLU:OE1	1.98	0.63
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.79	0.63
8:P:138:DT:H2''	8:P:139:DT:OP2	1.97	0.63
9:M:17:ALA:HB3	9:M:37:LEU:HD21	1.81	0.63
9:M:78:HIS:HA	9:M:113:ARG:HH12	1.63	0.63
9:M:81:GLU:OE2	9:M:88:ARG:HD3	1.99	0.63
1:A:215:LEU:HD12	1:A:219:PHE:CE2	2.33	0.63
2:C:515:PRO:HB3	2:C:530:TYR:HE1	1.63	0.63
3:D:180:ASP:HB3	3:D:197:VAL:CG1	2.29	0.63
3:D:662:TRP:CZ3	3:D:664:ALA:HB2	2.34	0.63
3:D:1139:GLN:HE21	3:D:1154:ILE:HD12	1.61	0.63
7:O:52:DA:H2''	7:O:53:DC:H5'	1.80	0.63
5:F:296:LEU:O	5:F:300:LEU:HG	1.98	0.63
1:B:171:VAL:HA	1:B:198:THR:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:923:ARG:HB3	3:D:962:VAL:CG2	2.29	0.63
3:D:1217:THR:CG2	3:D:1223:ALA:HB2	2.28	0.63
9:M:76:ALA:HB1	9:M:77:PRO:HD2	1.80	0.63
1:A:151:GLN:NE2	2:C:795:GLU:OE2	2.24	0.63
3:D:902:ALA:HA	3:D:913:ASP:H	1.62	0.63
3:D:1118:PRO:HA	3:D:1121:VAL:HG12	1.81	0.63
2:C:296:LEU:O	2:C:296:LEU:HD13	1.99	0.63
3:D:887:ARG:HD2	3:D:972:THR:O	1.99	0.63
9:M:120:LEU:HD23	9:M:124:GLU:HB3	1.80	0.63
2:C:243:TRP:HE3	2:C:247:GLN:HB3	1.64	0.62
2:C:464:SER:OG	2:C:465:ARG:N	2.32	0.62
1:B:118:VAL:HG12	1:B:120:ASN:H	1.64	0.62
3:D:1274:PRO:HG2	4:E:79:VAL:CG1	2.28	0.62
7:O:76:DG:H1'	7:O:77:DC:H5'	1.80	0.62
2:C:642:VAL:O	2:C:702:ILE:HG22	1.99	0.62
2:C:1094:ASP:OD2	3:D:420:LYS:NZ	2.18	0.62
3:D:993:GLU:OE2	4:E:51:TYR:OH	2.16	0.62
3:D:1086:LEU:HB3	3:D:1099:LEU:HB3	1.81	0.62
7:O:59:DG:H4'	7:O:60:DG:H5'	1.80	0.62
2:C:725:PRO:O	3:D:725:THR:HG22	2.00	0.62
7:O:35:DT:H1'	7:O:36:DG:H5'	1.80	0.62
4:E:32:PRO:HB2	4:E:36:THR:HG23	1.80	0.62
8:P:129:DA:H2''	8:P:130:DA:OP2	1.99	0.62
2:C:206:PRO:HG3	2:C:306:TYR:CE1	2.34	0.62
3:D:33:THR:HG23	3:D:47:PHE:CE2	2.34	0.62
3:D:360:LEU:HD21	5:F:329:ILE:HG21	1.80	0.62
7:O:19:DC:H2''	7:O:20:DT:OP2	1.99	0.62
2:C:240:ALA:HA	2:C:274:LEU:CD2	2.29	0.62
2:C:736:ILE:CG1	2:C:916:ILE:HB	2.29	0.62
2:C:915:ILE:HD13	2:C:1030:ILE:HD13	1.82	0.62
5:F:501:GLU:OE1	5:F:504:ARG:HD3	2.00	0.62
2:C:185:VAL:HG12	2:C:204:VAL:HG22	1.82	0.62
2:C:1087:GLU:OE1	2:C:1091:ILE:HD11	2.00	0.62
3:D:834:ARG:HB3	3:D:835:PRO:HA	1.81	0.62
3:D:913:ASP:HB3	3:D:916:ILE:CG1	2.30	0.62
9:M:38:LYS:HB3	9:M:45:THR:HG22	1.81	0.62
2:C:157:PHE:CE1	2:C:389:ILE:HD11	2.33	0.61
2:C:1057:LEU:CD2	2:C:1062:GLN:HG2	2.29	0.61
2:C:230:ARG:O	2:C:231:ARG:NE	2.28	0.61
2:C:715:LEU:N	2:C:1029:TYR:OH	2.33	0.61
3:D:130:TYR:CZ	3:D:387:ARG:NE	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:304:VAL:O	5:F:304:VAL:HG12	2.01	0.61
2:C:505:ARG:NH2	2:C:513:GLU:OE1	2.33	0.61
3:D:1162:LEU:CD2	3:D:1207:LEU:HD23	2.30	0.61
7:O:29:DC:H2'	7:O:30:DT:C7	2.31	0.61
7:O:72:DG:H1'	7:O:73:DC:H5'	1.82	0.61
2:C:1067:ARG:HD2	3:D:421:ARG:HG2	1.82	0.61
5:F:334:LYS:CE	7:O:48:DT:OP1	2.33	0.61
8:P:120:DA:H2'	8:P:120:DA:OP2	1.99	0.61
3:D:147:GLU:OE2	3:D:150:THR:OG1	2.15	0.61
3:D:657:GLN:N	3:D:658:PRO:HD2	2.15	0.61
3:D:1049:VAL:HG11	3:D:1068:PRO:HB3	1.83	0.61
5:F:264:THR:HA	5:F:267:SER:HB3	1.83	0.61
1:A:170:PRO:O	1:A:199:LYS:HG2	2.01	0.61
2:C:1128:LEU:HD21	3:D:1233:LEU:HD21	1.82	0.61
3:D:505:HIS:CE1	3:D:507:LEU:HB2	2.36	0.61
3:D:558:LEU:CD1	4:E:54:VAL:HG21	2.31	0.61
3:D:595:ASP:N	3:D:598:GLU:OE2	2.27	0.61
3:D:823:LEU:HD23	3:D:835:PRO:HB3	1.82	0.61
1:B:52:THR:O	1:B:164:VAL:HG22	2.00	0.61
3:D:1166:THR:HG22	3:D:1204:ARG:HB2	1.82	0.61
5:F:305:SER:O	5:F:308:LYS:CD	2.48	0.61
2:C:252:PHE:HB3	2:C:255:SER:CB	2.30	0.61
2:C:507:ASN:N	2:C:511:PHE:O	2.31	0.61
2:C:807:THR:O	2:C:833:ARG:N	2.32	0.61
2:C:1067:ARG:NH2	3:D:418:LEU:HD22	2.15	0.61
3:D:173:ARG:HD3	3:D:204:GLU:HB2	1.82	0.61
3:D:239:ASN:HD21	3:D:242:ARG:HH21	1.48	0.61
3:D:1056:GLU:O	3:D:1063:LYS:N	2.34	0.61
3:D:976:ALA:O	3:D:979:TYR:N	2.33	0.60
3:D:498:LEU:HB3	3:D:541:MET:CE	2.30	0.60
3:D:820:MET:HG2	3:D:822:GLY:N	2.16	0.60
1:A:46:ILE:HD12	1:A:210:SER:OG	2.01	0.60
1:B:54:ILE:O	1:B:162:ILE:HG13	2.00	0.60
1:B:71:GLU:HG2	1:B:75:GLU:HG2	1.82	0.60
1:B:182:ARG:HG3	1:B:186:ARG:H	1.66	0.60
2:C:288:THR:HG23	2:C:288:THR:O	2.01	0.60
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.82	0.60
3:D:473:LYS:HD2	5:F:448:VAL:HG21	1.83	0.60
3:D:1035:PHE:O	3:D:1161:MET:HE2	2.01	0.60
6:J:53:THR:HB	6:J:61:GLU:OE2	2.02	0.60
2:C:446:LEU:HB2	2:C:713:MET:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:797:ARG:N	2:C:800:ASP:OD2	2.30	0.60
5:F:445:VAL:HG12	5:F:447:ALA:H	1.67	0.60
2:C:268:VAL:O	2:C:272:GLU:CB	2.50	0.60
2:C:482:ARG:NH1	2:C:532:THR:O	2.33	0.60
2:C:1057:LEU:HD11	5:F:438:PHE:HA	1.83	0.60
2:C:431:PHE:O	2:C:437:SER:OG	2.14	0.60
3:D:84:ARG:HD3	3:D:86:LYS:HE3	1.84	0.60
3:D:206:ARG:O	3:D:209:ARG:HG3	2.02	0.60
3:D:130:TYR:CG	3:D:387:ARG:NH2	2.68	0.60
3:D:557:ILE:HD13	4:E:53:LEU:CD1	2.31	0.60
1:A:182:ARG:HA	1:A:188:ASP:OD1	2.01	0.60
2:C:189:GLU:OE1	2:C:367:THR:HG21	2.02	0.60
2:C:270:THR:C	2:C:274:LEU:HD23	2.22	0.60
3:D:683:PHE:CE2	3:D:685:ASN:HB2	2.37	0.60
3:D:1166:THR:CG2	3:D:1204:ARG:HB2	2.32	0.60
2:C:716:GLY:N	2:C:1029:TYR:OH	2.35	0.60
2:C:997:ASP:HB2	2:C:999:ASP:OD2	2.01	0.60
2:C:955:TRP:CD1	2:C:987:GLY:HA3	2.37	0.60
6:J:92:GLU:O	6:J:96:GLU:HG2	2.02	0.60
9:M:120:LEU:HB3	9:M:124:GLU:HB2	1.84	0.59
1:B:55:ARG:HD3	1:B:137:GLU:OE1	2.02	0.59
2:C:150:GLN:OE1	2:C:415:GLN:HB2	2.02	0.59
7:O:58:DA:H2''	7:O:59:DG:C2'	2.32	0.59
2:C:147:ILE:CG1	9:M:47:ARG:HG2	2.32	0.59
2:C:536:GLU:OE2	2:C:562:ARG:NH1	2.30	0.59
2:C:790:VAL:HG13	2:C:802:LEU:O	2.01	0.59
3:D:101:VAL:HG13	3:D:375:GLN:OE1	2.02	0.59
1:B:95:MET:HG2	1:B:113:PRO:CD	2.32	0.59
2:C:195:THR:HG22	2:C:197:LYS:HG3	1.83	0.59
3:D:466:ALA:HB1	3:D:471:SER:OG	2.01	0.59
3:D:1086:LEU:HD23	3:D:1099:LEU:HB3	1.83	0.59
3:D:241:TYR:O	3:D:245:VAL:HG23	2.03	0.59
3:D:944:LEU:HA	3:D:948:GLU:CG	2.33	0.59
2:C:767:GLU:HG2	2:C:807:THR:CG2	2.32	0.59
2:C:1083:TYR:O	2:C:1087:GLU:HG2	2.02	0.59
3:D:1011:THR:OG1	3:D:1145:GLN:NE2	2.36	0.59
6:J:40:PHE:CZ	6:J:58:ASN:HB2	2.37	0.59
9:M:78:HIS:HA	9:M:113:ARG:NH1	2.18	0.59
2:C:105:LEU:HD12	2:C:138:GLU:O	2.03	0.59
5:F:261:GLN:O	5:F:265:GLU:HG2	2.02	0.59
5:F:387:LEU:HD13	5:F:393:GLU:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:173:ARG:HG2	3:D:205:MET:HB2	1.85	0.59
5:F:257:LEU:HD21	6:J:81:HIS:CG	2.38	0.59
2:C:413:THR:OG1	2:C:414:PRO:HD2	2.02	0.59
2:C:727:GLU:H	3:D:725:THR:CG2	2.16	0.59
3:D:614:SER:HB2	3:D:615:PRO:HD2	1.85	0.59
3:D:634:LYS:HG2	3:D:665:GLU:HB3	1.84	0.59
8:P:128:DC:H2''	8:P:129:DA:OP2	2.02	0.59
1:B:68:GLY:O	1:B:129:ASN:N	2.27	0.59
2:C:224:VAL:HG21	2:C:234:VAL:N	2.17	0.59
2:C:922:VAL:HB	2:C:923:PRO:HD3	1.85	0.59
2:C:1077:GLN:NE2	3:D:1252:VAL:HG21	2.18	0.59
2:C:1137:VAL:O	3:D:-1:GLY:HA2	2.03	0.59
3:D:1054:ARG:HB2	3:D:1067:VAL:HG23	1.84	0.59
3:D:1223:ALA:HA	3:D:1226:PHE:CD2	2.38	0.59
8:P:119:DC:H2''	8:P:120:DA:OP2	2.03	0.59
2:C:1111:ASN:ND2	4:E:66:ASP:OD1	2.35	0.58
3:D:887:ARG:HH11	3:D:972:THR:HB	1.67	0.58
7:O:58:DA:H2''	7:O:59:DG:H2'	1.85	0.58
8:P:84:DT:H2''	8:P:85:DT:H71	1.85	0.58
2:C:96:ILE:HB	2:C:105:LEU:HB3	1.84	0.58
3:D:742:LYS:NZ	3:D:819:GLY:O	2.31	0.58
3:D:840:PHE:CD1	3:D:844:LEU:HD11	2.38	0.58
5:F:262:LEU:O	5:F:265:GLU:HB2	2.03	0.58
5:F:467:LEU:HB3	5:F:471:GLU:OE1	2.02	0.58
1:A:55:ARG:NE	1:A:137:GLU:OE2	2.37	0.58
1:B:84:VAL:HG12	1:B:120:ASN:ND2	2.18	0.58
2:C:224:VAL:HB	2:C:232:GLN:CB	2.33	0.58
2:C:270:THR:O	2:C:274:LEU:CD2	2.49	0.58
3:D:511:ALA:O	3:D:560:LEU:HD12	2.03	0.58
3:D:849:TYR:O	3:D:853:THR:HG23	2.02	0.58
2:C:736:ILE:HD11	2:C:916:ILE:HB	1.85	0.58
2:C:926:MET:HE1	3:D:817:LEU:N	2.18	0.58
3:D:75:CYS:HB3	3:D:78:CYS:SG	2.44	0.58
5:F:378:LYS:O	5:F:382:ILE:HG12	2.02	0.58
5:F:460:LEU:HD13	5:F:464:LEU:HD13	1.85	0.58
2:C:485:PRO:O	3:D:857:ARG:NH2	2.35	0.58
3:D:134:TYR:CD1	3:D:256:MET:HB2	2.38	0.58
3:D:656:TRP:HB2	3:D:658:PRO:HG2	1.86	0.58
3:D:1170:SER:OG	3:D:1175:PHE:O	2.09	0.58
5:F:386:LEU:HD12	5:F:399:LEU:HD23	1.85	0.58
2:C:62:GLU:OE1	2:C:69:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:943:GLY:O	2:C:993:LEU:HG	2.04	0.58
3:D:9:GLU:HG2	3:D:1244:LYS:HD2	1.84	0.58
3:D:928:ASP:OD1	3:D:940:ARG:N	2.37	0.58
3:D:1190:ASN:O	3:D:1194:VAL:HG13	2.03	0.58
9:M:111:LEU:HD13	9:M:128:LEU:HB2	1.85	0.58
1:A:215:LEU:HD12	1:A:219:PHE:HE2	1.69	0.58
2:C:515:PRO:HB3	2:C:530:TYR:CE1	2.39	0.58
2:C:737:LEU:HD22	2:C:741:LEU:CD1	2.34	0.58
3:D:81:GLU:OE1	3:D:91:ARG:NH2	2.33	0.58
3:D:147:GLU:HG3	3:D:151:LEU:HG	1.85	0.58
1:B:24:GLU:HB3	1:B:191:LYS:HG3	1.86	0.58
2:C:152:VAL:HG21	2:C:418:ILE:HD12	1.86	0.58
2:C:268:VAL:O	2:C:272:GLU:HG2	2.04	0.58
2:C:395:ARG:NH1	8:P:102:DG:OP2	2.36	0.58
3:D:169:GLU:OE1	3:D:208:ILE:HG23	2.04	0.58
3:D:417:LEU:O	3:D:418:LEU:CB	2.51	0.58
3:D:851:ILE:HA	3:D:854:HIS:HD2	1.69	0.58
5:F:306:LEU:C	5:F:308:LYS:N	2.52	0.58
5:F:342:LYS:CB	7:O:52:DA:H5''	2.34	0.58
6:J:20:ARG:NH1	6:J:23:ASP:HB3	2.18	0.58
7:O:29:DC:H2'	7:O:30:DT:H72	1.86	0.58
8:P:134:DC:H2'	8:P:135:DA:C8	2.38	0.58
2:C:192:ASP:OD1	2:C:194:SER:OG	2.16	0.58
3:D:25:TYR:HD2	3:D:91:ARG:HD3	1.69	0.58
3:D:491:ILE:CD1	3:D:516:LEU:HD21	2.34	0.58
3:D:1219:SER:OG	3:D:1243:ASP:OD2	2.19	0.58
5:F:305:SER:HG	7:O:54:DT:H4'	1.69	0.58
2:C:182:SER:O	2:C:186:TYR:OH	2.12	0.58
2:C:290:GLU:OE1	2:C:290:GLU:HA	2.04	0.58
2:C:884:LYS:O	2:C:1033:LEU:HB2	2.04	0.58
3:D:444:PRO:HG2	3:D:447:MET:CB	2.34	0.58
3:D:915:TYR:CE1	3:D:1143:ARG:HD3	2.39	0.58
3:D:963:ARG:HD3	3:D:978:CYS:SG	2.44	0.58
5:F:491:GLU:O	5:F:494:GLN:HG3	2.04	0.58
7:O:22:DG:H2'	7:O:23:DT:C5	2.39	0.58
1:B:32:TYR:CE1	2:C:1014:ARG:HD3	2.38	0.57
2:C:446:LEU:HB2	2:C:713:MET:CE	2.34	0.57
2:C:756:GLU:HG3	2:C:870:ARG:HG2	1.85	0.57
2:C:1088:LEU:HD23	2:C:1092:LYS:HD2	1.86	0.57
2:C:222:VAL:HG21	2:C:234:VAL:CG2	2.32	0.57
2:C:559:VAL:HG12	2:C:560:LEU:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:HG3	1:A:138:LEU:HB2	1.85	0.57
2:C:650:ILE:HD13	2:C:660:VAL:HG12	1.85	0.57
2:C:803:VAL:O	2:C:836:SER:OG	2.20	0.57
3:D:192:ASP:OD2	3:D:196:LYS:HE3	2.03	0.57
3:D:446:LEU:HD23	3:D:446:LEU:O	2.04	0.57
8:P:106:DA:H2'	8:P:107:DA:O4'	2.05	0.57
8:P:131:DG:H2''	8:P:132:DA:C8	2.39	0.57
1:B:164:VAL:HG23	1:B:165:ASP:O	2.03	0.57
2:C:584:ARG:O	2:C:587:VAL:HG12	2.03	0.57
2:C:591:THR:HG22	2:C:597:LEU:HD22	1.86	0.57
2:C:641:VAL:CG1	2:C:701:VAL:HG13	2.35	0.57
3:D:736:VAL:HG22	3:D:799:ILE:CD1	2.34	0.57
5:F:462:SER:O	5:F:466:THR:HG23	2.04	0.57
7:O:58:DA:H4'	7:O:59:DG:OP1	2.01	0.57
9:M:21:ALA:O	9:M:36:VAL:HG12	2.04	0.57
1:A:2:LEU:HB3	1:B:143:GLY:HA2	1.85	0.57
1:B:30:PHE:HA	1:B:33:THR:CG2	2.34	0.57
2:C:482:ARG:NH1	2:C:533:ALA:HA	2.20	0.57
3:D:512:PHE:HE1	3:D:561:SER:HB2	1.68	0.57
3:D:677:LEU:HD23	3:D:681:TYR:CD2	2.39	0.57
8:P:124:DG:H2''	8:P:125:DA:C8	2.39	0.57
1:B:89:GLU:OE2	1:B:115:GLY:HA3	2.05	0.57
1:B:181:THR:HG21	1:B:191:LYS:HD3	1.86	0.57
2:C:104:SER:N	2:C:140:ILE:O	2.30	0.57
2:C:809:LYS:HB2	2:C:833:ARG:HB2	1.85	0.57
3:D:218:ARG:HD2	3:D:243:GLU:OE2	2.04	0.57
3:D:1264:ILE:HD11	3:D:1267:TYR:CE2	2.40	0.57
5:F:463:VAL:O	5:F:466:THR:OG1	2.12	0.57
7:O:30:DT:OP2	7:O:30:DT:H2'	2.03	0.57
8:P:116:DC:H4'	8:P:117:DG:OP1	2.03	0.57
1:B:183:VAL:HG12	1:B:188:ASP:HA	1.86	0.57
3:D:195:ARG:HD3	3:D:198:ARG:HD3	1.86	0.57
5:F:236:GLY:HA3	7:O:55:DG:N2	2.19	0.57
1:A:15:THR:OG1	1:A:18:ARG:HG3	2.05	0.57
2:C:518:LYS:HD3	2:C:527:GLU:OE1	2.04	0.57
3:D:737:LEU:HB2	3:D:793:TYR:CE1	2.35	0.57
1:A:54:ILE:HD11	1:A:77:ILE:CD1	2.35	0.57
1:A:89:GLU:OE1	1:A:89:GLU:N	2.37	0.57
5:F:253:ILE:HD11	5:F:292:LYS:HA	1.87	0.57
1:B:3:ILE:HB	1:B:234:ILE:HA	1.85	0.57
1:B:40:ARG:NH1	3:D:623:ASP:HB3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:THR:HG23	2:C:146:GLU:OE1	2.05	0.57
2:C:313:ARG:CG	2:C:331:SER:HA	2.35	0.57
3:D:113:ARG:HH21	3:D:1235:ASP:HB3	1.70	0.57
5:F:231:TYR:HE2	5:F:321:ILE:HG21	1.69	0.57
5:F:261:GLN:HG2	6:J:82:TRP:CZ2	2.40	0.57
7:O:23:DT:H2'	7:O:23:DT:OP2	2.05	0.57
9:M:81:GLU:CD	9:M:88:ARG:HB3	2.25	0.57
1:A:153:ARG:HH21	2:C:797:ARG:HD3	1.70	0.56
2:C:470:LEU:O	2:C:470:LEU:HD13	2.05	0.56
3:D:707:ILE:HD13	4:E:39:PRO:HB3	1.86	0.56
3:D:817:LEU:O	3:D:839:SER:HB2	2.05	0.56
3:D:1066:ILE:HD12	3:D:1075:VAL:CB	2.33	0.56
1:B:175:THR:HG22	1:B:195:ASP:HB3	1.87	0.56
3:D:615:PRO:HB3	3:D:671:VAL:HG11	1.87	0.56
1:A:66:VAL:HB	1:A:69:VAL:CG2	2.35	0.56
1:A:182:ARG:HH12	3:D:625:GLY:H	1.53	0.56
1:B:30:PHE:HA	1:B:33:THR:HG23	1.85	0.56
2:C:202:VAL:HG13	2:C:214:PHE:H	1.70	0.56
2:C:240:ALA:HA	2:C:274:LEU:HD22	1.85	0.56
2:C:285:GLU:CD	2:C:286:PRO:HD2	2.25	0.56
2:C:483:MET:CE	2:C:498:GLY:HA3	2.36	0.56
2:C:934:THR:CG2	2:C:1026:GLY:HA3	2.35	0.56
3:D:134:TYR:HD1	3:D:256:MET:HB2	1.70	0.56
3:D:136:ILE:HG13	3:D:229:LEU:CD1	2.36	0.56
3:D:223:TRP:O	3:D:227:THR:HG23	2.05	0.56
3:D:1010:LEU:HD23	3:D:1028:LEU:HB2	1.85	0.56
4:E:47:VAL:HG11	4:E:53:LEU:HD23	1.87	0.56
5:F:280:ASP:O	5:F:284:ILE:HG12	2.04	0.56
5:F:295:LEU:HD23	5:F:332:VAL:HG23	1.86	0.56
7:O:75:DG:H2''	7:O:76:DG:C8	2.41	0.56
1:A:56:ILE:HB	1:A:59:VAL:CG2	2.36	0.56
1:B:92:PRO:HG3	1:B:141:GLU:OE1	2.05	0.56
2:C:278:TYR:O	2:C:279:ARG:C	2.42	0.56
2:C:399:VAL:O	2:C:403:ARG:HG2	2.06	0.56
3:D:235:ILE:CG2	3:D:241:TYR:HB2	2.35	0.56
3:D:339:ASP:OD1	3:D:399:LEU:HD22	2.05	0.56
3:D:840:PHE:CE1	3:D:844:LEU:HD11	2.40	0.56
4:E:56:TYR:HE2	4:E:99:ILE:HG23	1.69	0.56
5:F:384:ARG:O	5:F:388:GLN:NE2	2.38	0.56
5:F:493:GLY:HA2	5:F:503:ILE:HD11	1.87	0.56
9:M:8:THR:HA	9:M:18:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:THR:O	1:B:65:THR:OG1	2.21	0.56
1:B:106:THR:N	1:B:109:ASP:OD2	2.32	0.56
2:C:284:GLY:CA	5:F:219:ALA:HB1	2.34	0.56
3:D:1100:SER:N	3:D:1103:ASP:OD2	2.30	0.56
4:E:56:TYR:CE1	4:E:106:HIS:HB3	2.41	0.56
6:J:33:ARG:HG2	6:J:34:THR:O	2.05	0.56
2:C:522:GLY:O	2:C:553:ARG:HA	2.06	0.56
2:C:771:ARG:O	2:C:773:ILE:HG12	2.05	0.56
3:D:1052:ARG:HA	3:D:1104:HIS:HA	1.87	0.56
3:D:1054:ARG:CG	3:D:1065:THR:HB	2.35	0.56
7:O:32:DC:H2''	7:O:33:DA:C8	2.40	0.56
8:P:106:DA:H2'	8:P:107:DA:C1'	2.36	0.56
1:A:95:MET:HE3	1:A:140:VAL:HG21	1.87	0.56
2:C:288:THR:CB	2:C:291:SER:HB3	2.35	0.56
3:D:329:GLN:HB3	3:D:335:PHE:CE1	2.40	0.56
3:D:527:LEU:HD22	3:D:575:ALA:O	2.06	0.56
3:D:866:ARG:HH11	3:D:1011:THR:HA	1.71	0.56
3:D:1080:ILE:HD11	3:D:1112:MET:HG3	1.88	0.56
2:C:147:ILE:CD1	9:M:47:ARG:HG2	2.36	0.56
2:C:189:GLU:OE1	2:C:189:GLU:N	2.39	0.56
2:C:262:LEU:HD12	2:C:265:ASP:OD2	2.06	0.56
2:C:275:LEU:HD21	2:C:289:LYS:CA	2.34	0.56
3:D:60:CYS:SG	3:D:64:LYS:N	2.79	0.56
3:D:449:LEU:O	3:D:449:LEU:HD13	2.05	0.56
3:D:704:TYR:HB3	3:D:705:PRO:HD2	1.87	0.56
3:D:823:LEU:HD23	3:D:835:PRO:CB	2.36	0.56
9:M:17:ALA:CB	9:M:39:VAL:HA	2.35	0.56
2:C:202:VAL:CG1	2:C:214:PHE:HB2	2.34	0.56
2:C:378:LEU:N	2:C:510:GLY:O	2.39	0.56
2:C:502:VAL:HG23	2:C:587:VAL:O	2.06	0.56
2:C:771:ARG:HD2	2:C:785:ASP:O	2.04	0.56
3:D:334:ARG:NH1	5:F:418:ARG:HB3	2.20	0.56
3:D:437:LYS:NZ	4:E:33:LEU:HD21	2.21	0.56
2:C:222:VAL:CG2	2:C:234:VAL:HG13	2.36	0.56
2:C:1040:LYS:HD2	3:D:540:GLN:HE22	1.71	0.56
3:D:212:ALA:O	3:D:215:GLU:HG2	2.06	0.56
3:D:580:ASP:HB2	3:D:721:PHE:HE1	1.71	0.56
3:D:797:ASN:HD22	3:D:798:PRO:CD	2.19	0.56
3:D:1055:LEU:HB3	3:D:1101:ASP:CB	2.36	0.56
6:J:33:ARG:O	6:J:63:THR:HG22	2.06	0.56
7:O:72:DG:H2''	7:O:73:DC:C2'	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:222:VAL:HG21	2:C:234:VAL:HG13	1.89	0.55
2:C:820:LEU:HD13	5:F:479:PHE:CD2	2.41	0.55
3:D:195:ARG:HD2	3:D:198:ARG:HH11	1.70	0.55
5:F:499:THR:HG21	7:O:26:DT:C7	2.36	0.55
7:O:59:DG:H1'	7:O:60:DG:O4'	2.06	0.55
1:A:42:LEU:HD23	1:A:211:ALA:HB2	1.88	0.55
2:C:817:GLU:HG3	5:F:481:LEU:HD22	1.87	0.55
1:A:93:VAL:HG23	1:A:140:VAL:HB	1.87	0.55
2:C:650:ILE:HD11	2:C:702:ILE:HD11	1.88	0.55
3:D:364:GLU:HG3	3:D:368:ASN:OD1	2.06	0.55
3:D:866:ARG:NH1	3:D:1011:THR:HA	2.20	0.55
7:O:42:DT:H2'	7:O:43:DT:C7	2.36	0.55
2:C:41:PHE:CD2	2:C:974:THR:HG22	2.41	0.55
3:D:159:ARG:O	3:D:162:VAL:HB	2.06	0.55
3:D:222:ILE:HD13	3:D:247:ARG:NH2	2.21	0.55
3:D:498:LEU:HB3	3:D:541:MET:HE1	1.88	0.55
7:O:42:DT:H2'	7:O:43:DT:H72	1.89	0.55
8:P:92:DA:H2''	8:P:93:DA:H5'	1.88	0.55
2:C:104:SER:OG	2:C:140:ILE:HB	2.05	0.55
2:C:322:LEU:CD2	2:C:357:VAL:HG11	2.36	0.55
2:C:677:ARG:HG2	2:C:678:SER:O	2.06	0.55
2:C:848:ILE:CD1	2:C:874:ALA:HB2	2.36	0.55
2:C:961:ASP:O	2:C:962:GLU:HG3	2.05	0.55
3:D:146:ASN:OD1	3:D:147:GLU:N	2.40	0.55
3:D:167:ASP:HA	3:D:170:LEU:HD12	1.89	0.55
3:D:473:LYS:HE3	5:F:448:VAL:HG11	1.88	0.55
6:J:34:THR:OG1	6:J:38:GLU:HB2	2.07	0.55
1:A:98:ARG:HG3	1:A:135:GLU:CG	2.35	0.55
2:C:243:TRP:CE3	2:C:247:GLN:HB3	2.41	0.55
3:D:147:GLU:O	3:D:151:LEU:HG	2.06	0.55
3:D:337:THR:HG23	5:F:420:PRO:HB2	1.87	0.55
4:E:82:LEU:HB3	4:E:103:LEU:HD23	1.87	0.55
5:F:421:ILE:HD11	5:F:425:GLN:HE22	1.71	0.55
6:J:32:TYR:CD1	6:J:64:LEU:HA	2.42	0.55
6:J:40:PHE:CE2	6:J:58:ASN:HB2	2.41	0.55
6:J:76:LYS:H	6:J:76:LYS:HD3	1.72	0.55
6:J:106:ARG:CG	6:J:110:ARG:HD3	2.33	0.55
2:C:139:PHE:CZ	2:C:412:ILE:HD11	2.42	0.55
2:C:204:VAL:HB	2:C:212:LEU:HD21	1.88	0.55
3:D:1251:ASN:ND2	3:D:1256:LYS:HD2	2.22	0.55
5:F:262:LEU:HA	5:F:265:GLU:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:504:ARG:NH2	8:P:128:DC:OP2	2.40	0.55
1:A:194:LEU:HD23	1:A:195:ASP:N	2.22	0.55
2:C:1080:GLY:O	3:D:1261:GLY:HA3	2.06	0.55
3:D:1054:ARG:HB2	3:D:1067:VAL:CG2	2.36	0.55
5:F:400:ALA:HB3	5:F:407:PRO:HG3	1.89	0.55
6:J:31:ARG:O	6:J:65:ILE:HB	2.06	0.55
7:O:58:DA:H1'	7:O:59:DG:O5'	2.07	0.55
2:C:41:PHE:HD2	2:C:980:ALA:HB2	1.71	0.55
2:C:347:ARG:HB3	2:C:352:GLN:HG3	1.87	0.55
3:D:106:TYR:HB3	3:D:312:MET:CE	2.35	0.55
3:D:151:LEU:HD22	3:D:248:TYR:CE1	2.41	0.55
3:D:206:ARG:HA	3:D:209:ARG:HG3	1.89	0.55
3:D:912:ARG:HG3	3:D:916:ILE:HD12	1.89	0.55
7:O:22:DG:C2'	7:O:23:DT:H5'	2.37	0.55
9:M:38:LYS:HA	9:M:45:THR:HA	1.88	0.55
2:C:150:GLN:HG2	9:M:44:LEU:CB	2.35	0.55
2:C:296:LEU:C	2:C:298:ASN:H	2.09	0.55
3:D:376:GLU:OE2	5:F:227:SER:HB2	2.07	0.55
3:D:946:ASP:HB2	3:D:947:PRO:HD3	1.89	0.55
8:P:80:DC:H2''	8:P:81:DC:C6	2.41	0.55
2:C:204:VAL:HB	2:C:212:LEU:CD2	2.36	0.54
3:D:390:PRO:O	3:D:390:PRO:HG2	2.06	0.54
5:F:328:LEU:CD2	5:F:351:ILE:HD11	2.32	0.54
7:O:42:DT:H4'	7:O:43:DT:OP1	2.06	0.54
1:B:9:LEU:HD12	1:B:22:VAL:O	2.06	0.54
2:C:245:SER:O	2:C:249:VAL:HG23	2.07	0.54
2:C:421:ARG:HA	2:C:424:VAL:HG12	1.88	0.54
3:D:1169:ASP:HB2	3:D:1202:ALA:HB3	1.87	0.54
5:F:451:VAL:O	5:F:455:LEU:HD23	2.08	0.54
2:C:160:MET:SD	2:C:164:GLY:HA2	2.46	0.54
3:D:37:ARG:CG	3:D:38:THR:N	2.69	0.54
3:D:113:ARG:HG2	3:D:1238:ILE:CD1	2.37	0.54
3:D:138:SER:HB3	3:D:253:THR:OG1	2.08	0.54
5:F:492:ILE:HA	5:F:495:VAL:HG12	1.90	0.54
7:O:76:DG:H1'	7:O:77:DC:C5'	2.37	0.54
9:M:17:ALA:HB2	9:M:39:VAL:HG12	1.89	0.54
1:A:73:VAL:O	1:A:77:ILE:HG12	2.08	0.54
1:B:25:PRO:HB2	1:B:189:PHE:HB3	1.90	0.54
1:B:107:ALA:HB2	1:B:123:MET:HB3	1.89	0.54
2:C:488:THR:O	2:C:610:ASN:ND2	2.30	0.54
2:C:936:LEU:HD11	2:C:972:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:880:VAL:CG2	3:D:1210:ILE:HB	2.33	0.54
3:D:908:GLY:O	3:D:909:THR:HG23	2.07	0.54
3:D:1168:ILE:HG13	3:D:1202:ALA:HB3	1.89	0.54
1:B:6:ARG:NH2	1:B:237:SER:HA	2.22	0.54
1:B:183:VAL:HA	1:B:188:ASP:HA	1.89	0.54
2:C:72:GLU:O	2:C:76:GLU:HG2	2.07	0.54
2:C:441:ASP:OD2	2:C:447:SER:OG	2.26	0.54
3:D:37:ARG:HG3	3:D:38:THR:H	1.72	0.54
3:D:71:LYS:HG2	6:J:24:LEU:CD1	2.37	0.54
3:D:215:GLU:O	3:D:219:LEU:HD23	2.08	0.54
3:D:277:LEU:HD11	3:D:295:ARG:NH1	2.18	0.54
3:D:366:ILE:HD11	5:F:300:LEU:HD21	1.90	0.54
3:D:445:LYS:NZ	3:D:518:GLU:OE2	2.31	0.54
3:D:606:HIS:HB2	3:D:607:PRO:HD2	1.90	0.54
3:D:674:ASN:HD21	3:D:684:VAL:H	1.56	0.54
4:E:70:GLN:HE22	4:E:76:LEU:HD22	1.72	0.54
5:F:500:ARG:NH1	8:P:127:DT:O4	2.41	0.54
7:O:22:DG:H2'	7:O:23:DT:C7	2.38	0.54
7:O:52:DA:H2''	7:O:53:DC:C5'	2.37	0.54
7:O:59:DG:H4'	7:O:60:DG:C5'	2.38	0.54
1:A:57:ASP:OD1	1:A:58:GLY:N	2.41	0.54
1:A:107:ALA:HA	1:A:125:ILE:HD11	1.88	0.54
1:B:172:LEU:HD13	1:B:199:LYS:N	2.20	0.54
3:D:851:ILE:HA	3:D:854:HIS:CD2	2.43	0.54
3:D:1060:ARG:HG2	3:D:1061:PHE:HD1	1.71	0.54
3:D:1243:ASP:OD1	3:D:1244:LYS:N	2.39	0.54
7:O:42:DT:C6	7:O:43:DT:H72	2.42	0.54
9:M:129:ALA:O	9:M:133:GLN:HG3	2.07	0.54
1:A:61:HIS:HA	1:A:162:ILE:HD11	1.89	0.54
2:C:255:SER:CB	2:C:258:MET:HB2	2.37	0.54
3:D:612:TYR:CE2	3:D:627:LEU:HD11	2.43	0.54
3:D:1125:GLN:OE1	3:D:1129:GLU:HG2	2.07	0.54
9:M:131:ALA:O	9:M:134:ILE:HG13	2.08	0.54
1:A:112:PRO:HB2	1:A:116:VAL:HG23	1.89	0.54
2:C:824:ILE:HA	5:F:511:MET:CE	2.38	0.54
2:C:1037:VAL:HG11	3:D:520:LYS:HB2	1.89	0.54
3:D:166:ARG:O	3:D:170:LEU:HG	2.08	0.54
3:D:222:ILE:HD11	3:D:244:LEU:HA	1.89	0.54
3:D:1128:ARG:O	3:D:1132:ILE:HG12	2.07	0.54
7:O:70:DA:H2''	7:O:71:DA:C8	2.43	0.54
8:P:96:DC:H4'	8:P:97:DT:OP1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:102:DG:H1'	8:P:103:DT:OP1	2.08	0.54
8:P:107:DA:C2'	8:P:108:DT:H71	2.35	0.54
9:M:106:GLU:O	9:M:109:ARG:HG2	2.07	0.54
1:A:65:THR:OG1	2:C:655:ALA:HB3	2.08	0.54
3:D:237:ASP:O	3:D:238:GLU:HG3	2.07	0.54
3:D:910:LEU:CD2	3:D:956:GLY:HA2	2.33	0.54
9:M:16:ALA:CB	9:M:141:LEU:HD12	2.38	0.54
1:A:66:VAL:HB	1:A:69:VAL:HG21	1.89	0.54
2:C:780:VAL:HG23	2:C:781:LEU:CD1	2.38	0.54
3:D:27:GLU:OE2	3:D:96:GLU:HB2	2.08	0.54
1:B:145:GLY:HA2	1:B:169:SER:OG	2.09	0.53
1:B:171:VAL:HG12	1:B:198:THR:CG2	2.38	0.53
2:C:774:PRO:HG2	2:C:834:ASP:HB2	1.90	0.53
3:D:73:ILE:O	3:D:82:VAL:HG12	2.08	0.53
3:D:821:LYS:HB3	3:D:836:VAL:CG1	2.39	0.53
3:D:1054:ARG:HB3	3:D:1065:THR:HB	1.89	0.53
3:D:1258:ILE:O	3:D:1263:GLY:HA3	2.08	0.53
7:O:71:DA:H1'	7:O:72:DG:C8	2.44	0.53
2:C:982:GLU:OE1	3:D:841:ARG:NH2	2.41	0.53
3:D:158:GLU:O	3:D:162:VAL:HG23	2.08	0.53
3:D:353:ARG:NE	5:F:323:GLU:OE2	2.38	0.53
3:D:487:LEU:HA	3:D:490:VAL:HG22	1.89	0.53
3:D:845:THR:N	3:D:848:GLU:OE1	2.38	0.53
7:O:14:DC:H2''	7:O:15:DG:OP2	2.08	0.53
8:P:102:DG:H2''	8:P:103:DT:O5'	2.07	0.53
2:C:344:TYR:OH	2:C:365:VAL:HA	2.08	0.53
2:C:412:ILE:HD13	2:C:417:LEU:CD1	2.37	0.53
2:C:631:GLU:O	2:C:713:MET:N	2.29	0.53
2:C:946:VAL:N	2:C:964:LEU:O	2.34	0.53
2:C:989:LEU:HD21	2:C:1006:GLY:CA	2.38	0.53
3:D:52:PHE:HB3	3:D:322:PRO:HG3	1.90	0.53
3:D:78:CYS:SG	3:D:79:GLY:N	2.82	0.53
3:D:148:LEU:O	3:D:152:GLU:HG2	2.09	0.53
3:D:344:TYR:O	3:D:348:ILE:HG12	2.09	0.53
3:D:577:PRO:HB3	3:D:581:MET:HG3	1.88	0.53
3:D:924:THR:HA	3:D:942:GLN:O	2.08	0.53
7:O:71:DA:H2'	7:O:71:DA:OP2	2.08	0.53
2:C:742:VAL:HG22	2:C:879:ILE:HG22	1.90	0.53
3:D:118:LEU:CB	3:D:120:LEU:HD13	2.39	0.53
9:M:9:VAL:CG1	9:M:37:LEU:HD11	2.38	0.53
9:M:17:ALA:CB	9:M:37:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASN:HD21	1:B:205:ARG:HA	1.72	0.53
1:B:8:THR:O	1:B:23:ILE:HA	2.08	0.53
2:C:77:ARG:HG2	2:C:77:ARG:O	2.08	0.53
2:C:278:TYR:HD1	2:C:292:ALA:HB1	1.43	0.53
2:C:281:LEU:CD2	2:C:295:LEU:HD11	2.39	0.53
2:C:463:LEU:HD12	2:C:464:SER:O	2.09	0.53
2:C:622:GLU:O	2:C:714:ALA:HB1	2.07	0.53
2:C:1051:MET:CE	5:F:441:ASP:HA	2.38	0.53
3:D:271:ASP:O	3:D:275:GLU:HG2	2.08	0.53
3:D:425:SER:OG	3:D:426:GLY:N	2.41	0.53
1:A:93:VAL:CG2	1:A:140:VAL:HB	2.38	0.53
2:C:267:THR:CG2	2:C:272:GLU:CG	2.82	0.53
3:D:240:LEU:O	3:D:244:LEU:HB2	2.07	0.53
3:D:1167:ILE:HD11	3:D:1181:ILE:CD1	2.37	0.53
5:F:262:LEU:HA	5:F:265:GLU:HG3	1.91	0.53
7:O:22:DG:H2''	7:O:23:DT:C5'	2.37	0.53
2:C:374:GLY:HA3	2:C:534:ASP:OD1	2.08	0.53
2:C:885:LEU:CD1	2:C:895:ILE:HD11	2.39	0.53
2:C:956:ALA:CB	2:C:959:LEU:HD12	2.39	0.53
2:C:1117:ILE:HG23	2:C:1118:PRO:HD2	1.89	0.53
3:D:327:MET:HE3	3:D:337:THR:HG22	1.90	0.53
9:M:106:GLU:HA	9:M:109:ARG:HG2	1.90	0.53
1:B:172:LEU:HD11	1:B:199:LYS:HE2	1.91	0.53
2:C:214:PHE:CE1	2:C:224:VAL:HG13	2.43	0.53
2:C:507:ASN:OD1	2:C:508:PRO:HD2	2.08	0.53
3:D:527:LEU:HD13	3:D:713:VAL:HG12	1.90	0.53
3:D:881:SER:O	3:D:996:GLY:HA3	2.09	0.53
3:D:931:ASP:O	3:D:934:GLY:N	2.39	0.53
2:C:357:VAL:CG2	2:C:358:PRO:HD2	2.39	0.53
2:C:611:MET:CE	2:C:890:GLY:HA2	2.38	0.53
2:C:631:GLU:OE1	2:C:631:GLU:N	2.39	0.53
2:C:995:ASN:OD1	2:C:996:ARG:N	2.38	0.53
2:C:1074:TRP:CE2	3:D:878:VAL:HG11	2.44	0.53
3:D:910:LEU:HD22	3:D:953:LEU:O	2.09	0.53
5:F:368:ILE:CG2	5:F:372:MET:HB3	2.38	0.53
7:O:24:DC:H2'	7:O:25:DT:C7	2.38	0.53
9:M:59:ARG:HG2	9:M:60:ASP:O	2.09	0.53
9:M:136:VAL:HG21	9:M:151:GLU:HG2	1.90	0.53
9:M:149:LYS:O	9:M:153:ILE:HG12	2.09	0.53
1:A:66:VAL:O	1:A:69:VAL:HG22	2.09	0.53
1:B:32:TYR:CZ	2:C:1014:ARG:HD3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TYR:O	3:D:624:ARG:NH2	2.42	0.53
2:C:139:PHE:O	2:C:147:ILE:HA	2.09	0.53
2:C:413:THR:CG2	2:C:416:THR:HG23	2.38	0.53
2:C:583:PRO:O	2:C:584:ARG:HD2	2.08	0.53
2:C:735:ILE:O	2:C:896:GLY:N	2.28	0.53
3:D:460:LEU:HD11	3:D:472:ALA:HB1	1.91	0.53
3:D:1220:TRP:HB3	3:D:1241:ARG:HH21	1.74	0.53
5:F:296:LEU:HD23	5:F:328:LEU:CD1	2.39	0.53
8:P:121:DA:H2'	8:P:122:DT:O4'	2.08	0.53
3:D:50:LYS:HG3	3:D:79:GLY:O	2.09	0.52
3:D:1011:THR:H	3:D:1145:GLN:NE2	2.07	0.52
7:O:33:DA:H4'	7:O:34:DT:OP1	2.08	0.52
9:M:53:ALA:O	9:M:58:VAL:HG12	2.09	0.52
1:A:65:THR:HG21	2:C:656:ASP:OD2	2.10	0.52
2:C:296:LEU:HD13	2:C:296:LEU:C	2.30	0.52
3:D:124:ASP:O	3:D:234:LEU:HD21	2.09	0.52
3:D:566:LEU:HD23	3:D:573:PRO:HA	1.91	0.52
6:J:20:ARG:NH1	6:J:23:ASP:O	2.39	0.52
6:J:31:ARG:NE	6:J:41:GLU:OE2	2.41	0.52
9:M:19:VAL:HG12	9:M:37:LEU:HD12	1.90	0.52
2:C:281:LEU:HD22	2:C:295:LEU:CD2	2.24	0.52
2:C:540:VAL:HG22	2:C:561:VAL:HG22	1.90	0.52
3:D:1139:GLN:O	3:D:1143:ARG:HG3	2.08	0.52
1:B:41:THR:O	1:B:45:SER:HB3	2.10	0.52
2:C:189:GLU:O	2:C:189:GLU:HG2	2.09	0.52
2:C:232:GLN:HE22	2:C:236:VAL:HG11	1.75	0.52
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.92	0.52
2:C:1077:GLN:O	2:C:1080:GLY:N	2.41	0.52
3:D:624:ARG:HG2	3:D:625:GLY:H	1.74	0.52
8:P:107:DA:H2'	8:P:108:DT:C6	2.44	0.52
1:B:90:ASP:OD1	1:B:142:ARG:HD3	2.09	0.52
2:C:294:THR:O	2:C:298:ASN:CG	2.46	0.52
3:D:683:PHE:HE2	3:D:685:ASN:HB2	1.74	0.52
3:D:1005:GLU:HB3	3:D:1006:PRO:HD3	1.91	0.52
5:F:415:GLN:HG2	5:F:418:ARG:HH22	1.73	0.52
5:F:506:ILE:O	5:F:510:THR:HG23	2.10	0.52
7:O:38:DC:H2''	7:O:39:DG:OP2	2.09	0.52
3:D:893:THR:OG1	3:D:894:GLU:N	2.43	0.52
4:E:32:PRO:CB	4:E:36:THR:HG23	2.39	0.52
7:O:27:DG:H2''	7:O:28:DA:OP2	2.10	0.52
2:C:206:PRO:HB3	2:C:308:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:306:TYR:CE2	2:C:333:LEU:HG	2.43	0.52
2:C:705:GLY:N	2:C:708:THR:OG1	2.32	0.52
3:D:206:ARG:HA	3:D:209:ARG:CG	2.39	0.52
3:D:216:LEU:O	3:D:220:GLU:HG2	2.09	0.52
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.92	0.52
8:P:107:DA:H2'	8:P:108:DT:C7	2.35	0.52
2:C:233:PRO:HG2	2:C:236:VAL:CG2	2.38	0.52
2:C:281:LEU:HD21	2:C:295:LEU:HD11	1.92	0.52
2:C:641:VAL:O	2:C:643:VAL:HG23	2.09	0.52
3:D:71:LYS:HG2	6:J:24:LEU:HD12	1.91	0.52
3:D:389:ARG:CZ	7:O:59:DG:C8	2.92	0.52
3:D:524:LEU:HD22	3:D:541:MET:SD	2.50	0.52
3:D:884:VAL:HG11	3:D:1156:VAL:HG13	1.92	0.52
3:D:939:GLU:OE1	3:D:939:GLU:N	2.37	0.52
3:D:1084:GLN:C	3:D:1085:ARG:HD2	2.31	0.52
3:D:1274:PRO:HG2	4:E:79:VAL:HG13	1.90	0.52
6:J:80:THR:OG1	6:J:83:ASP:N	2.40	0.52
7:O:25:DT:C6	7:O:26:DT:H72	2.44	0.52
2:C:200:HIS:CD2	2:C:348:LEU:HG	2.45	0.52
2:C:737:LEU:CD2	2:C:915:ILE:HG22	2.39	0.52
2:C:1044:ARG:CZ	2:C:1056:PRO:HB3	2.39	0.52
3:D:24:SER:OG	3:D:93:GLY:HA2	2.10	0.52
3:D:38:THR:HG23	3:D:40:LYS:H	1.74	0.52
3:D:340:LEU:HD11	3:D:405:LEU:CD1	2.39	0.52
3:D:595:ASP:O	3:D:598:GLU:HG3	2.09	0.52
3:D:1060:ARG:HG2	3:D:1061:PHE:CD1	2.44	0.52
5:F:261:GLN:HG2	6:J:82:TRP:CH2	2.44	0.52
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.92	0.52
2:C:736:ILE:CD1	2:C:916:ILE:HD12	2.39	0.52
2:C:737:LEU:HD11	2:C:895:ILE:HD13	1.91	0.52
3:D:222:ILE:HA	3:D:240:LEU:HD11	1.92	0.52
3:D:923:ARG:CB	3:D:962:VAL:HG21	2.37	0.52
9:M:11:TYR:O	9:M:14:HIS:N	2.42	0.52
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.92	0.51
2:C:224:VAL:HG21	2:C:234:VAL:CA	2.40	0.51
2:C:315:LYS:NZ	2:C:375:ASN:OD1	2.19	0.51
2:C:927:ASN:O	2:C:930:GLN:HG2	2.09	0.51
3:D:34:ILE:CG2	3:D:39:LEU:HA	2.39	0.51
1:A:191:LYS:NZ	1:A:193:ILE:HD11	2.25	0.51
1:B:172:LEU:HD11	1:B:199:LYS:CE	2.40	0.51
4:E:47:VAL:HG11	4:E:53:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:372:MET:HA	5:F:375:VAL:HG22	1.92	0.51
8:P:110:DC:H1'	8:P:111:DA:H5'	1.90	0.51
8:P:120:DA:H2''	8:P:121:DA:OP2	2.09	0.51
9:M:35:LEU:HD12	9:M:35:LEU:O	2.10	0.51
2:C:421:ARG:NH2	8:P:103:DT:OP2	2.42	0.51
2:C:879:ILE:HD12	2:C:1032:LYS:HE3	1.91	0.51
2:C:1070:GLU:OE2	3:D:414:ARG:NH2	2.43	0.51
2:C:1107:VAL:CG1	3:D:469:ILE:HD12	2.31	0.51
3:D:113:ARG:NH2	3:D:1235:ASP:HB3	2.25	0.51
3:D:203:ARG:HA	3:D:206:ARG:HG2	1.92	0.51
3:D:274:ALA:O	3:D:278:ARG:HG2	2.10	0.51
3:D:459:ARG:NH1	3:D:463:LEU:HG	2.26	0.51
3:D:1220:TRP:CB	3:D:1241:ARG:HH21	2.24	0.51
2:C:60:SER:O	2:C:63:TRP:HB3	2.09	0.51
2:C:69:ARG:O	2:C:72:GLU:HG3	2.11	0.51
3:D:327:MET:CE	3:D:337:THR:HG22	2.40	0.51
3:D:929:ALA:O	3:D:937:ILE:HG22	2.11	0.51
5:F:406:THR:O	5:F:410:VAL:HG23	2.10	0.51
1:A:40:ARG:NE	1:B:33:THR:HG22	2.21	0.51
1:A:217:GLU:HB3	1:B:234:ILE:HD12	1.93	0.51
1:B:51:VAL:CG2	1:B:138:LEU:HD23	2.41	0.51
2:C:189:GLU:HB3	2:C:200:HIS:CD2	2.46	0.51
2:C:773:ILE:HG23	2:C:834:ASP:OD1	2.10	0.51
2:C:883:ASP:O	2:C:894:VAL:HA	2.11	0.51
2:C:907:LEU:HD23	2:C:1010:LEU:HD23	1.91	0.51
3:D:441:CYS:SG	3:D:514:PRO:HA	2.50	0.51
2:C:647:SER:HB3	2:C:698:ALA:H	1.75	0.51
3:D:588:LEU:O	3:D:588:LEU:HD22	2.09	0.51
5:F:305:SER:O	5:F:308:LYS:CG	2.59	0.51
9:M:104:VAL:HG11	9:M:134:ILE:CD1	2.25	0.51
1:B:3:ILE:O	1:B:4:SER:OG	2.24	0.51
2:C:133:LEU:HB2	2:C:154:MET:HB3	1.91	0.51
2:C:139:PHE:CE2	2:C:412:ILE:HD11	2.45	0.51
2:C:595:PRO:HG3	2:C:888:ARG:NH2	2.26	0.51
2:C:1133:LEU:HD11	3:D:105:TRP:CZ3	2.44	0.51
3:D:573:PRO:O	3:D:574:LEU:HD12	2.11	0.51
7:O:18:DC:H2''	7:O:19:DC:OP2	2.10	0.51
1:B:136:VAL:HG12	1:B:138:LEU:HD12	1.92	0.51
1:B:149:ALA:HA	1:B:164:VAL:O	2.11	0.51
2:C:86:LEU:HD21	2:C:389:ILE:HD13	1.93	0.51
2:C:891:ASN:HD21	2:C:1028:MET:CE	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:32:GLU:HB3	3:D:42:GLU:HG3	1.93	0.51
3:D:139:VAL:HA	3:D:252:PHE:HA	1.92	0.51
3:D:921:TYR:CE1	3:D:949:ILE:HG13	2.46	0.51
3:D:1070:ASP:N	3:D:1071:GLY:HA2	2.25	0.51
7:O:34:DT:H4'	7:O:35:DT:OP1	2.10	0.51
1:A:191:LYS:HZ2	1:A:193:ILE:HD11	1.76	0.51
1:B:159:ILE:HD12	1:B:160:GLY:N	2.25	0.51
2:C:455:LEU:HD11	2:C:500:LEU:CD2	2.41	0.51
3:D:384:ASN:OD1	3:D:385:GLY:N	2.43	0.51
3:D:1139:GLN:HB3	3:D:1143:ARG:CZ	2.41	0.51
5:F:295:LEU:HD23	5:F:332:VAL:CG2	2.41	0.51
9:M:132:ARG:O	9:M:136:VAL:HG23	2.11	0.51
2:C:519:VAL:HG23	2:C:524:VAL:HA	1.93	0.51
2:C:776:ILE:HD11	2:C:780:VAL:HG21	1.93	0.51
2:C:808:PRO:HA	2:C:832:VAL:HA	1.92	0.51
3:D:135:VAL:HG23	3:D:233:GLN:O	2.11	0.51
3:D:491:ILE:HD13	3:D:516:LEU:HD21	1.93	0.51
5:F:273:LEU:HD11	5:F:281:MET:SD	2.51	0.51
5:F:296:LEU:CD2	5:F:328:LEU:HD12	2.41	0.51
8:P:113:DA:C8	8:P:114:DT:H72	2.45	0.51
1:A:33:THR:HG21	1:B:37:SER:HA	1.93	0.50
1:B:43:LEU:O	1:B:169:SER:OG	2.16	0.50
2:C:224:VAL:HG21	2:C:234:VAL:HA	1.93	0.50
2:C:311:VAL:HG22	2:C:509:PHE:HB3	1.93	0.50
2:C:507:ASN:HB3	2:C:511:PHE:H	1.76	0.50
2:C:934:THR:HG22	2:C:1026:GLY:HA3	1.94	0.50
2:C:1091:ILE:HD12	2:C:1102:VAL:CG2	2.34	0.50
3:D:596:THR:HG22	3:D:626:VAL:O	2.11	0.50
3:D:913:ASP:OD1	3:D:914:PRO:HD2	2.11	0.50
5:F:504:ARG:O	5:F:507:GLU:HG3	2.12	0.50
2:C:490:GLU:OE1	2:C:607:MET:HG2	2.12	0.50
2:C:568:VAL:CG2	3:D:847:LEU:HD23	2.41	0.50
2:C:1070:GLU:HB2	3:D:417:LEU:HB2	1.93	0.50
3:D:117:LEU:O	3:D:117:LEU:HD13	2.10	0.50
3:D:913:ASP:HB3	3:D:916:ILE:CD1	2.42	0.50
5:F:501:GLU:HA	5:F:504:ARG:HG2	1.92	0.50
1:B:38:LEU:O	1:B:42:LEU:HD13	2.11	0.50
2:C:119:VAL:HG13	2:C:167:ILE:CD1	2.41	0.50
2:C:158:PRO:HG2	2:C:431:PHE:CE2	2.46	0.50
2:C:626:VAL:HG21	2:C:936:LEU:HD12	1.94	0.50
2:C:658:ILE:O	2:C:669:THR:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:806:VAL:HG22	2:C:832:VAL:HB	1.93	0.50
2:C:860:GLU:C	2:C:861:LEU:HD12	2.32	0.50
3:D:1172:SER:N	3:D:1199:GLU:HG3	2.25	0.50
3:D:1190:ASN:HA	3:D:1193:VAL:CG1	2.34	0.50
4:E:30:ASP:OD1	4:E:31:THR:N	2.43	0.50
3:D:262:GLN:HG3	3:D:310:MET:HE1	1.92	0.50
3:D:558:LEU:HD13	4:E:54:VAL:HG21	1.94	0.50
3:D:803:VAL:HG13	3:D:809:GLY:O	2.11	0.50
3:D:1182:ASP:OD1	3:D:1183:ARG:N	2.45	0.50
7:O:35:DT:H2''	7:O:36:DG:H5'	1.93	0.50
7:O:63:DT:H2''	7:O:64:DG:C8	2.46	0.50
1:A:167:ILE:O	1:A:167:ILE:HG13	2.11	0.50
2:C:189:GLU:HA	2:C:199:LEU:O	2.11	0.50
2:C:737:LEU:HD11	2:C:895:ILE:CD1	2.42	0.50
3:D:5:ASN:O	3:D:5:ASN:ND2	2.44	0.50
3:D:1270:ILE:O	4:E:59:LYS:NZ	2.21	0.50
5:F:387:LEU:HD13	5:F:393:GLU:CG	2.41	0.50
1:A:6:ARG:HB2	1:A:7:PRO:HD2	1.92	0.50
1:A:169:SER:O	1:A:199:LYS:HD3	2.12	0.50
1:A:226:ASN:OD1	1:B:205:ARG:HG3	2.12	0.50
2:C:624:PRO:HA	2:C:718:ASN:HD21	1.77	0.50
2:C:738:SER:CA	2:C:904:MET:HE3	2.41	0.50
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.47	0.50
3:D:23:TRP:HB3	3:D:92:MET:HE3	1.94	0.50
3:D:966:LEU:HD13	3:D:1131:GLN:OE1	2.10	0.50
9:M:38:LYS:CB	9:M:45:THR:HG22	2.41	0.50
9:M:148:ALA:O	9:M:152:THR:HG23	2.12	0.50
3:D:563:ASN:OD1	4:E:40:ILE:HG12	2.12	0.50
3:D:573:PRO:HD3	3:D:698:ASN:OD1	2.12	0.50
3:D:902:ALA:HA	3:D:913:ASP:N	2.26	0.50
3:D:945:GLY:N	3:D:948:GLU:OE2	2.29	0.50
7:O:41:DA:H5'	7:O:41:DA:H8	1.77	0.50
7:O:73:DC:H3'	7:O:73:DC:OP2	2.11	0.50
2:C:1131:LEU:HD13	3:D:105:TRP:CH2	2.47	0.50
3:D:181:LEU:HD21	3:D:198:ARG:CG	2.42	0.50
3:D:525:HIS:CG	3:D:526:PRO:HD2	2.47	0.50
3:D:1034:LEU:HD21	3:D:1134:LEU:HD22	1.93	0.50
3:D:1167:ILE:O	3:D:1177:PRO:HA	2.11	0.50
7:O:57:DC:H4'	7:O:58:DA:OP1	2.11	0.50
7:O:72:DG:C2'	7:O:73:DC:H5'	2.42	0.50
8:P:91:DC:H2''	8:P:92:DA:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:80:GLU:N	9:M:80:GLU:OE1	2.45	0.50
1:B:162:ILE:HD12	1:B:162:ILE:O	2.12	0.50
2:C:388:GLN:HA	2:C:391:VAL:HG12	1.92	0.50
2:C:926:MET:SD	3:D:817:LEU:HG	2.52	0.50
2:C:1045:SER:O	2:C:1046:THR:OG1	2.28	0.50
3:D:336:ALA:HB1	5:F:423:LEU:HG	1.94	0.50
3:D:428:SER:OG	3:D:429:VAL:N	2.44	0.50
3:D:911:ILE:HD12	3:D:911:ILE:O	2.12	0.50
3:D:1187:GLU:O	3:D:1191:ARG:HG2	2.12	0.50
8:P:83:DC:C6	8:P:83:DC:H5'	2.46	0.50
8:P:137:DG:C8	8:P:138:DT:H72	2.47	0.50
2:C:97:GLU:CG	2:C:101:GLY:HA2	2.42	0.49
3:D:95:ILE:CD1	3:D:348:ILE:HD11	2.42	0.49
3:D:1080:ILE:HD11	3:D:1112:MET:HE2	1.93	0.49
9:M:88:ARG:HE	9:M:114:ARG:NH1	2.10	0.49
1:A:137:GLU:OE2	1:A:161:ARG:NH1	2.44	0.49
1:A:152:ASN:OD1	1:A:157:ALA:HB3	2.12	0.49
1:B:6:ARG:NH1	1:B:234:ILE:HG22	2.26	0.49
1:B:80:LEU:HD21	1:B:125:ILE:HD11	1.94	0.49
3:D:337:THR:HG23	5:F:420:PRO:CB	2.42	0.49
3:D:480:ARG:O	3:D:483:VAL:HG12	2.12	0.49
3:D:944:LEU:HA	3:D:948:GLU:HG3	1.94	0.49
5:F:243:ALA:O	5:F:247:VAL:HG23	2.12	0.49
9:M:67:LEU:HA	9:M:70:VAL:HG22	1.94	0.49
1:A:45:SER:HG	1:B:30:PHE:HZ	1.59	0.49
1:B:172:LEU:HD11	1:B:199:LYS:HB3	1.95	0.49
2:C:484:CYS:CB	2:C:588:SER:HB3	2.42	0.49
2:C:601:ASP:OD1	2:C:602:ALA:N	2.45	0.49
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.47	0.49
3:D:64:LYS:HE3	3:D:75:CYS:SG	2.53	0.49
3:D:668:LEU:HD23	3:D:668:LEU:O	2.13	0.49
5:F:492:ILE:CG2	5:F:503:ILE:HD12	2.38	0.49
3:D:241:TYR:CE2	3:D:245:VAL:HG21	2.47	0.49
5:F:366:ILE:O	5:F:366:ILE:HG13	2.12	0.49
6:J:109:ARG:HH11	6:J:110:ARG:HH21	1.59	0.49
1:A:68:GLY:HA3	1:A:132:GLY:HA2	1.95	0.49
2:C:132:PRO:HB3	2:C:153:PHE:HE1	1.77	0.49
2:C:736:ILE:HD11	2:C:916:ILE:CD1	2.41	0.49
2:C:790:VAL:CG1	2:C:802:LEU:HA	2.42	0.49
2:C:883:ASP:HB2	2:C:895:ILE:HD12	1.93	0.49
5:F:386:LEU:HD12	5:F:399:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:19:DC:H2'	7:O:20:DT:H72	1.94	0.49
1:B:30:PHE:HD1	1:B:33:THR:HG21	1.77	0.49
2:C:436:LEU:HD13	2:C:460:PRO:HD2	1.94	0.49
4:E:47:VAL:CG1	4:E:53:LEU:HD23	2.42	0.49
4:E:56:TYR:CD1	4:E:106:HIS:HB3	2.48	0.49
7:O:28:DA:H2''	7:O:29:DC:O4'	2.12	0.49
7:O:35:DT:C2'	7:O:36:DG:H5'	2.43	0.49
8:P:133:DC:H2'	8:P:134:DC:C4'	2.41	0.49
1:A:54:ILE:HG22	1:A:138:LEU:HA	1.93	0.49
1:A:95:MET:CE	1:A:140:VAL:HG21	2.42	0.49
2:C:98:ASP:OD1	2:C:101:GLY:N	2.45	0.49
3:D:33:THR:HG22	3:D:34:ILE:HG13	1.94	0.49
3:D:57:ASP:HB2	6:J:15:SER:H	1.77	0.49
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.94	0.49
9:M:100:ASP:O	9:M:104:VAL:HG23	2.13	0.49
1:B:54:ILE:HD11	1:B:77:ILE:HG12	1.94	0.49
2:C:236:VAL:HG13	2:C:273:ALA:HB1	1.95	0.49
2:C:255:SER:HB3	2:C:258:MET:CB	2.40	0.49
2:C:658:ILE:HD11	2:C:688:PRO:CB	2.43	0.49
2:C:1067:ARG:NH2	3:D:418:LEU:HD21	2.25	0.49
3:D:166:ARG:HG3	3:D:212:ALA:HB2	1.95	0.49
3:D:660:ASP:OD2	3:D:660:ASP:N	2.45	0.49
1:B:107:ALA:HB3	1:B:121:PRO:O	2.13	0.49
2:C:205:ILE:HG22	2:C:211:TRP:CE2	2.48	0.49
2:C:326:GLU:HB2	2:C:327:PRO:HD2	1.95	0.49
3:D:365:ILE:H	3:D:365:ILE:HD12	1.77	0.49
3:D:459:ARG:HH12	3:D:463:LEU:HG	1.76	0.49
3:D:736:VAL:HB	3:D:841:ARG:HD2	1.94	0.49
3:D:917:GLU:HA	3:D:921:TYR:CD2	2.47	0.49
4:E:60:ARG:HG2	4:E:104:LEU:HD11	1.93	0.49
8:P:103:DT:H2''	8:P:104:DC:O4'	2.13	0.49
1:A:65:THR:HG21	2:C:656:ASP:OD1	2.13	0.49
1:A:172:LEU:O	1:A:172:LEU:HD22	2.13	0.49
2:C:147:ILE:O	9:M:46:VAL:HG13	2.13	0.49
2:C:919:THR:CG2	3:D:731:VAL:HG23	2.39	0.49
3:D:57:ASP:HB3	3:D:58:TRP:CE3	2.48	0.49
3:D:755:LYS:O	3:D:759:GLN:HG3	2.13	0.49
5:F:467:LEU:HG	5:F:519:ARG:HH12	1.77	0.49
7:O:22:DG:H2'	7:O:23:DT:H72	1.95	0.49
7:O:24:DC:H2'	7:O:25:DT:H72	1.94	0.49
7:O:30:DT:H2''	7:O:31:DC:OP2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:69:LYS:O	9:M:73:VAL:HG23	2.13	0.49
1:A:14:LEU:HB2	1:A:18:ARG:HD3	1.95	0.48
2:C:176:VAL:HG12	2:C:177:SER:O	2.13	0.48
2:C:268:VAL:O	2:C:272:GLU:CG	2.61	0.48
2:C:760:ARG:N	2:C:767:GLU:OE1	2.26	0.48
3:D:191:ALA:CB	3:D:194:ARG:HH21	2.26	0.48
3:D:498:LEU:HB3	3:D:541:MET:HE2	1.95	0.48
5:F:470:ARG:HH12	7:O:24:DC:P	2.35	0.48
6:J:102:LEU:HD21	6:J:106:ARG:NH2	2.28	0.48
7:O:69:DG:H2''	7:O:70:DA:C8	2.48	0.48
8:P:107:DA:H2''	9:M:85:TRP:CZ2	2.48	0.48
9:M:48:VAL:HG13	9:M:49:PRO:HD2	1.94	0.48
2:C:435:GLN:NE2	2:C:459:GLY:HA2	2.27	0.48
2:C:486:ILE:HD11	3:D:849:TYR:CE2	2.47	0.48
5:F:302:LEU:HB2	7:O:54:DT:C2	2.47	0.48
8:P:81:DC:OP2	8:P:81:DC:H2'	2.14	0.48
8:P:96:DC:C4'	8:P:97:DT:H73	2.43	0.48
8:P:115:DC:H2''	8:P:116:DC:C6	2.48	0.48
1:B:183:VAL:HA	1:B:188:ASP:CA	2.42	0.48
2:C:514:THR:O	2:C:530:TYR:HA	2.13	0.48
2:C:633:ARG:NH1	2:C:637:ASP:OD2	2.46	0.48
3:D:55:THR:O	6:J:12:GLY:HA3	2.13	0.48
3:D:173:ARG:HH21	3:D:177:LEU:N	2.11	0.48
3:D:442:GLY:N	3:D:523:GLN:O	2.35	0.48
3:D:1086:LEU:HD23	3:D:1099:LEU:CB	2.43	0.48
6:J:6:LEU:HD12	6:J:6:LEU:O	2.13	0.48
7:O:33:DA:H8	7:O:33:DA:OP2	1.95	0.48
9:M:17:ALA:CB	9:M:39:VAL:HG12	2.42	0.48
1:A:18:ARG:HB2	1:A:196:VAL:O	2.14	0.48
2:C:1081:ALA:HB1	3:D:554:GLU:OE1	2.13	0.48
3:D:124:ASP:HB3	3:D:234:LEU:CD2	2.43	0.48
3:D:389:ARG:NH1	7:O:59:DG:N7	2.60	0.48
4:E:82:LEU:N	4:E:98:GLU:OE2	2.40	0.48
6:J:81:HIS:HA	6:J:84:MET:CE	2.43	0.48
8:P:129:DA:OP2	8:P:129:DA:H2'	2.12	0.48
9:M:17:ALA:HB1	9:M:39:VAL:HA	1.95	0.48
9:M:149:LYS:O	9:M:152:THR:OG1	2.29	0.48
1:A:157:ALA:HB1	1:A:161:ARG:CG	2.44	0.48
1:B:28:PRO:HD3	1:B:189:PHE:CD1	2.47	0.48
2:C:1134:ASN:N	3:D:15:ALA:HB2	2.29	0.48
3:D:151:LEU:HD13	3:D:248:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1010:LEU:HD12	3:D:1145:GLN:CG	2.33	0.48
3:D:1054:ARG:O	3:D:1065:THR:N	2.45	0.48
3:D:1127:PRO:HA	3:D:1130:VAL:HG12	1.95	0.48
5:F:459:GLN:O	5:F:462:SER:OG	2.22	0.48
6:J:64:LEU:HD23	6:J:65:ILE:N	2.28	0.48
7:O:41:DA:H5'	7:O:41:DA:C8	2.49	0.48
8:P:122:DT:H2'	8:P:123:DG:C8	2.48	0.48
1:B:113:PRO:O	1:B:116:VAL:HG22	2.13	0.48
2:C:378:LEU:CD1	2:C:455:LEU:HD22	2.44	0.48
2:C:444:ASN:HD22	2:C:715:LEU:HD22	1.79	0.48
2:C:482:ARG:NH2	2:C:536:GLU:OE1	2.39	0.48
2:C:800:ASP:O	2:C:838:LYS:HA	2.13	0.48
3:D:1122:LEU:HD22	3:D:1207:LEU:HB2	1.94	0.48
3:D:1251:ASN:HD22	3:D:1256:LYS:HD2	1.78	0.48
6:J:80:THR:OG1	6:J:82:TRP:HB3	2.14	0.48
7:O:19:DC:C6	7:O:20:DT:H72	2.49	0.48
1:A:11:GLU:OE1	1:A:13:VAL:HG23	2.14	0.48
1:A:70:LYS:O	2:C:655:ALA:HB2	2.14	0.48
2:C:421:ARG:HH12	8:P:103:DT:P	2.36	0.48
2:C:721:VAL:HG12	2:C:1026:GLY:O	2.14	0.48
2:C:894:VAL:HG11	3:D:429:VAL:HG21	1.94	0.48
2:C:1079:TYR:O	3:D:558:LEU:HD23	2.14	0.48
3:D:192:ASP:O	3:D:196:LYS:HG3	2.14	0.48
3:D:504:LEU:HB3	3:D:1005:GLU:HG2	1.96	0.48
3:D:550:GLU:HG3	4:E:58:ALA:CB	2.43	0.48
3:D:662:TRP:HZ3	3:D:664:ALA:HB2	1.79	0.48
5:F:386:LEU:CB	5:F:394:PRO:HG2	2.43	0.48
9:M:22:ILE:HG23	9:M:34:TYR:O	2.13	0.48
2:C:344:TYR:CZ	2:C:365:VAL:HA	2.49	0.48
3:D:160:LYS:HD2	3:D:163:GLU:HB3	1.96	0.48
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.96	0.48
3:D:974:VAL:HG12	3:D:1159:ARG:NH1	2.29	0.48
5:F:305:SER:O	5:F:308:LYS:HD3	2.13	0.48
9:M:19:VAL:CG1	9:M:37:LEU:HD12	2.42	0.48
9:M:26:THR:HB	9:M:31:GLN:CG	2.33	0.48
1:A:71:GLU:HB3	1:A:75:GLU:HB3	1.94	0.48
2:C:626:VAL:CG2	2:C:936:LEU:HD12	2.44	0.48
3:D:587:TYR:O	3:D:630:ARG:HD3	2.13	0.48
3:D:913:ASP:HB3	3:D:916:ILE:HD11	1.94	0.48
3:D:1010:LEU:HD23	3:D:1028:LEU:CB	2.44	0.48
3:D:1223:ALA:HA	3:D:1226:PHE:HD2	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:273:LEU:HD23	5:F:274:PRO:O	2.14	0.48
5:F:283:TRP:CD2	6:J:105:ILE:HD12	2.48	0.48
8:P:134:DC:H2''	8:P:135:DA:H5'	1.95	0.48
1:A:54:ILE:HD11	1:A:77:ILE:HD13	1.94	0.48
2:C:240:ALA:HA	2:C:274:LEU:HD21	1.96	0.48
2:C:243:TRP:HA	2:C:247:GLN:OE1	2.14	0.48
2:C:519:VAL:HG23	2:C:523:VAL:C	2.34	0.48
2:C:542:ALA:HB2	2:C:576:VAL:CG1	2.44	0.48
2:C:641:VAL:CG2	2:C:708:THR:HG21	2.43	0.48
3:D:239:ASN:HD21	3:D:242:ARG:NH2	2.12	0.48
3:D:530:GLU:HB2	3:D:578:ARG:HH11	1.78	0.48
3:D:711:GLN:OE1	4:E:30:ASP:HB3	2.14	0.48
4:E:76:LEU:HD23	4:E:78:TYR:CE2	2.49	0.48
8:P:133:DC:H5'	8:P:133:DC:H6	1.78	0.48
1:A:84:VAL:HG13	1:A:84:VAL:O	2.13	0.47
1:A:212:GLY:O	1:A:216:VAL:HG23	2.14	0.47
1:B:176:TYR:HB3	1:B:194:LEU:HD23	1.96	0.47
2:C:313:ARG:HD3	2:C:331:SER:O	2.14	0.47
2:C:568:VAL:HG21	3:D:847:LEU:HD23	1.95	0.47
3:D:153:ALA:O	3:D:157:VAL:HG23	2.13	0.47
5:F:487:ARG:HD2	5:F:491:GLU:OE2	2.14	0.47
6:J:54:TRP:N	6:J:62:GLY:O	2.47	0.47
1:A:144:ARG:HE	1:B:232:ILE:HD11	1.79	0.47
2:C:240:ALA:CB	2:C:277:ILE:HD11	2.44	0.47
2:C:261:THR:O	2:C:265:ASP:N	2.47	0.47
2:C:356:THR:HB	2:C:362:GLU:HB3	1.96	0.47
2:C:483:MET:HE3	2:C:498:GLY:HA3	1.96	0.47
2:C:1038:ASP:OD1	3:D:520:LYS:HD2	2.14	0.47
3:D:136:ILE:HD11	3:D:235:ILE:CD1	2.44	0.47
3:D:456:VAL:HG22	3:D:460:LEU:HD23	1.95	0.47
6:J:54:TRP:O	6:J:62:GLY:N	2.47	0.47
1:A:93:VAL:HG21	1:A:116:VAL:CG1	2.43	0.47
1:B:50:ALA:O	1:B:140:VAL:HG13	2.14	0.47
1:B:170:PRO:O	1:B:199:LYS:HG2	2.14	0.47
2:C:879:ILE:CD1	2:C:1032:LYS:HE3	2.45	0.47
2:C:956:ALA:HB1	2:C:959:LEU:HD12	1.96	0.47
1:A:194:LEU:CD2	1:A:196:VAL:HG23	2.43	0.47
2:C:214:PHE:CD1	2:C:224:VAL:HG13	2.50	0.47
2:C:225:ARG:HG2	2:C:230:ARG:C	2.34	0.47
2:C:240:ALA:CB	2:C:277:ILE:CD1	2.92	0.47
2:C:273:ALA:C	2:C:276:ASP:H	2.06	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:TYR:HD1	2:C:292:ALA:HB3	1.69	0.47
2:C:377:ARG:HB3	2:C:511:PHE:HE1	1.77	0.47
2:C:657:TYR:HA	2:C:670:TYR:O	2.14	0.47
2:C:885:LEU:HD13	2:C:895:ILE:HD11	1.95	0.47
7:O:31:DC:H2''	7:O:32:DC:C5	2.50	0.47
8:P:107:DA:H1'	9:M:85:TRP:CZ2	2.48	0.47
9:M:26:THR:CA	9:M:31:GLN:HA	2.44	0.47
2:C:134:PHE:HE1	2:C:153:PHE:HD1	1.61	0.47
2:C:455:LEU:HD11	2:C:500:LEU:HD23	1.95	0.47
2:C:889:HIS:NE2	2:C:933:GLU:OE1	2.48	0.47
2:C:1074:TRP:HH2	3:D:875:ARG:HG2	1.80	0.47
3:D:268:PHE:CE2	3:D:270:ILE:HG22	2.50	0.47
3:D:656:TRP:O	3:D:656:TRP:CE3	2.68	0.47
3:D:832:ILE:HG22	3:D:834:ARG:H	1.78	0.47
8:P:107:DA:H1'	9:M:85:TRP:HZ2	1.79	0.47
8:P:119:DC:H2''	8:P:120:DA:C8	2.49	0.47
8:P:130:DA:H2''	8:P:131:DG:C5'	2.44	0.47
3:D:180:ASP:HB3	3:D:197:VAL:HG12	1.95	0.47
3:D:329:GLN:HB3	3:D:335:PHE:HE1	1.79	0.47
7:O:64:DG:H2''	7:O:65:DC:C6	2.50	0.47
9:M:74:LEU:HD21	9:M:158:LEU:CD2	2.32	0.47
1:A:95:MET:SD	1:A:110:ILE:HG21	2.55	0.47
1:A:223:ARG:HD3	1:B:216:VAL:HG11	1.97	0.47
1:B:112:PRO:HB2	1:B:116:VAL:HG23	1.96	0.47
1:B:196:VAL:HG22	1:B:198:THR:HG23	1.97	0.47
2:C:231:ARG:O	2:C:232:GLN:HG2	2.15	0.47
2:C:909:ASP:OD2	2:C:1001:LEU:HD11	2.14	0.47
2:C:1083:TYR:HE2	4:E:55:ILE:HD11	1.80	0.47
3:D:84:ARG:CD	3:D:86:LYS:HE3	2.43	0.47
3:D:736:VAL:HG22	3:D:799:ILE:HD13	1.97	0.47
3:D:797:ASN:HB3	3:D:800:ILE:CG2	2.38	0.47
3:D:885:ILE:HD11	3:D:887:ARG:HH21	1.79	0.47
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.50	0.47
5:F:328:LEU:HD23	5:F:351:ILE:CD1	2.35	0.47
5:F:487:ARG:HD2	5:F:491:GLU:CD	2.34	0.47
5:F:516:HIS:O	5:F:520:SER:HB3	2.14	0.47
7:O:47:DA:H1'	7:O:48:DT:H5'	1.95	0.47
9:M:139:LEU:CD1	9:M:154:LEU:HD21	2.45	0.47
2:C:255:SER:HB3	2:C:258:MET:CG	2.44	0.47
2:C:343:GLU:O	2:C:346:VAL:HG12	2.14	0.47
2:C:514:THR:HG23	2:C:515:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:727:GLU:H	3:D:725:THR:HG21	1.79	0.47
3:D:505:HIS:HE1	3:D:507:LEU:HB2	1.78	0.47
5:F:504:ARG:HA	5:F:507:GLU:CG	2.45	0.47
1:B:51:VAL:HG21	1:B:138:LEU:HD23	1.96	0.47
3:D:150:THR:O	3:D:153:ALA:HB3	2.14	0.47
3:D:246:ASP:OD1	3:D:247:ARG:N	2.48	0.47
3:D:527:LEU:HD13	3:D:713:VAL:CG1	2.44	0.47
3:D:981:ARG:HG2	3:D:982:SER:O	2.14	0.47
5:F:306:LEU:C	5:F:308:LYS:H	2.17	0.47
5:F:333:GLU:HG2	6:J:81:HIS:CD2	2.50	0.47
5:F:442:SER:HB3	6:J:7:ARG:HD3	1.97	0.47
5:F:504:ARG:HA	5:F:507:GLU:HG3	1.97	0.47
7:O:21:DG:H2'	7:O:22:DG:O4'	2.15	0.47
2:C:68:PRO:HA	2:C:71:ARG:HB3	1.97	0.47
2:C:461:GLY:N	8:P:97:DT:OP2	2.32	0.47
2:C:736:ILE:CD1	2:C:916:ILE:HB	2.44	0.47
3:D:624:ARG:HG2	3:D:625:GLY:N	2.30	0.47
3:D:753:ALA:HB1	3:D:774:LEU:CD2	2.45	0.47
3:D:966:LEU:HD22	3:D:1131:GLN:CD	2.36	0.47
3:D:1050:THR:HG22	3:D:1106:GLU:C	2.35	0.47
3:D:1273:GLN:O	4:E:105:GLU:HG2	2.14	0.47
4:E:101:ALA:HB3	4:E:103:LEU:HD13	1.97	0.47
5:F:261:GLN:O	5:F:264:THR:HG22	2.15	0.47
7:O:19:DC:C6	7:O:19:DC:H5'	2.50	0.47
7:O:72:DG:H2''	7:O:73:DC:H5'	1.97	0.47
1:A:108:GLY:HA2	1:A:121:PRO:HB3	1.97	0.46
2:C:408:ASP:OD1	2:C:411:ALA:HB3	2.15	0.46
3:D:137:THR:HG22	3:D:253:THR:O	2.15	0.46
3:D:169:GLU:O	3:D:208:ILE:HD13	2.15	0.46
3:D:916:ILE:HG23	3:D:920:ALA:CB	2.42	0.46
4:E:37:ASN:OD1	4:E:38:PRO:HA	2.15	0.46
2:C:52:GLY:O	2:C:55:ASP:N	2.46	0.46
2:C:584:ARG:O	2:C:584:ARG:HG2	2.14	0.46
2:C:723:ILE:O	2:C:919:THR:OG1	2.33	0.46
2:C:1051:MET:HE2	5:F:441:ASP:HA	1.96	0.46
3:D:230:ALA:HB1	3:D:231:PRO:HD2	1.97	0.46
3:D:278:ARG:O	3:D:281:ILE:HG13	2.15	0.46
3:D:585:LEU:HB2	3:D:693:GLN:HE22	1.80	0.46
3:D:924:THR:HG23	3:D:980:GLY:HA2	1.98	0.46
5:F:341:TYR:CE1	7:O:51:DG:H5''	2.50	0.46
8:P:133:DC:H2'	8:P:134:DC:H4'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HE	1:B:33:THR:CG2	2.23	0.46
1:B:50:ALA:O	1:B:140:VAL:HA	2.15	0.46
1:B:95:MET:O	1:B:137:GLU:HA	2.14	0.46
2:C:244:THR:OG1	2:C:247:GLN:HG3	2.15	0.46
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.50	0.46
2:C:516:TYR:N	2:C:529:VAL:O	2.44	0.46
3:D:219:LEU:O	3:D:222:ILE:HG22	2.15	0.46
3:D:525:HIS:O	3:D:528:VAL:HG22	2.15	0.46
3:D:771:ASN:O	3:D:775:VAL:HG23	2.14	0.46
5:F:231:TYR:CE2	5:F:321:ILE:HG21	2.49	0.46
5:F:276:ALA:O	5:F:279:ARG:HG2	2.16	0.46
9:M:75:ARG:NE	9:M:157:VAL:HG13	2.26	0.46
1:A:144:ARG:HD2	1:B:1:MET:HG3	1.97	0.46
1:B:105:VAL:HG12	1:B:125:ILE:HG21	1.96	0.46
2:C:397:GLU:OE2	2:C:401:ARG:NH2	2.49	0.46
2:C:484:CYS:SG	2:C:587:VAL:HA	2.55	0.46
2:C:531:LEU:HD22	2:C:535:GLU:HG3	1.96	0.46
2:C:820:LEU:HD13	5:F:479:PHE:HD2	1.79	0.46
3:D:25:TYR:CE2	3:D:91:ARG:HG2	2.50	0.46
3:D:198:ARG:O	3:D:202:GLU:HG2	2.15	0.46
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.81	0.46
9:M:111:LEU:CB	9:M:128:LEU:HD13	2.35	0.46
2:C:281:LEU:HD23	2:C:295:LEU:CD1	2.46	0.46
2:C:296:LEU:HD22	2:C:296:LEU:HA	1.68	0.46
2:C:516:TYR:CD2	2:C:531:LEU:HD12	2.50	0.46
2:C:587:VAL:HG22	2:C:591:THR:HB	1.98	0.46
2:C:1121:PHE:CE1	3:D:1254:ILE:HG22	2.50	0.46
3:D:383:ASP:HB2	3:D:403:SER:OG	2.15	0.46
3:D:567:SER:OG	3:D:574:LEU:HD13	2.16	0.46
3:D:937:ILE:HD12	3:D:955:ALA:HB2	1.97	0.46
1:A:110:ILE:O	1:A:112:PRO:HD3	2.16	0.46
1:A:153:ARG:NH2	2:C:797:ARG:HD3	2.30	0.46
1:B:55:ARG:CG	1:B:137:GLU:HB2	2.43	0.46
3:D:143:MET:HB3	3:D:251:TYR:CE1	2.51	0.46
3:D:468:ASN:ND2	3:D:470:LYS:HB3	2.30	0.46
3:D:497:LEU:C	3:D:498:LEU:HD12	2.35	0.46
3:D:1052:ARG:HA	3:D:1103:ASP:C	2.36	0.46
5:F:470:ARG:O	5:F:474:VAL:HG23	2.15	0.46
2:C:961:ASP:OD1	2:C:962:GLU:N	2.44	0.46
3:D:432:VAL:HG23	3:D:526:PRO:HB3	1.97	0.46
3:D:595:ASP:OD1	3:D:596:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:641:ARG:N	3:D:657:GLN:HG3	2.30	0.46
3:D:660:ASP:HB3	3:D:661:ALA:H	1.61	0.46
3:D:931:ASP:CG	3:D:955:ALA:HB1	2.36	0.46
3:D:940:ARG:NH1	3:D:963:ARG:HH21	2.12	0.46
8:P:90:DG:H2''	8:P:91:DC:O5'	2.16	0.46
8:P:124:DG:H2''	8:P:125:DA:H8	1.78	0.46
1:A:172:LEU:HB3	1:A:197:GLU:O	2.15	0.46
2:C:115:VAL:HG11	2:C:129:TYR:CZ	2.51	0.46
2:C:207:SER:H	2:C:308:LEU:HA	1.80	0.46
2:C:296:LEU:C	2:C:296:LEU:CD1	2.84	0.46
2:C:466:GLU:H	2:C:466:GLU:CD	1.91	0.46
2:C:480:TYR:CE1	2:C:586:MET:HB3	2.51	0.46
2:C:733:ASP:O	2:C:893:GLY:HA3	2.16	0.46
3:D:174:ALA:O	3:D:178:GLU:HG3	2.16	0.46
3:D:889:HIS:O	3:D:977:THR:HG23	2.16	0.46
7:O:41:DA:C8	7:O:42:DT:H72	2.51	0.46
8:P:103:DT:H2''	8:P:104:DC:O5'	2.15	0.46
9:M:120:LEU:CD2	9:M:124:GLU:HB3	2.44	0.46
1:B:38:LEU:CD2	1:B:194:LEU:HD11	2.40	0.46
1:B:147:VAL:CG1	1:B:166:SER:HB2	2.45	0.46
2:C:571:VAL:HG22	2:C:572:PRO:O	2.16	0.46
3:D:119:ASP:C	3:D:120:LEU:HD12	2.36	0.46
3:D:577:PRO:HA	3:D:581:MET:SD	2.56	0.46
3:D:1118:PRO:HA	3:D:1121:VAL:CG1	2.44	0.46
4:E:42:GLU:HA	4:E:45:ASP:OD2	2.15	0.46
1:B:166:SER:HB3	1:B:168:TYR:CE1	2.50	0.46
2:C:812:THR:O	2:C:814:LEU:HD22	2.16	0.46
3:D:1088:VAL:HG23	3:D:1098:VAL:N	2.31	0.46
3:D:1169:ASP:HB2	3:D:1202:ALA:CB	2.46	0.46
3:D:1181:ILE:HD11	3:D:1186:PHE:HD1	1.81	0.46
5:F:265:GLU:O	5:F:268:GLU:HG3	2.16	0.46
7:O:65:DC:H2''	7:O:66:DC:C6	2.51	0.46
1:A:182:ARG:HG2	1:A:188:ASP:HB3	1.98	0.45
1:B:147:VAL:HG13	1:B:166:SER:HB2	1.98	0.45
2:C:43:LYS:HZ1	2:C:984:GLU:CD	2.20	0.45
2:C:273:ALA:C	2:C:275:LEU:H	2.19	0.45
2:C:612:GLN:HA	2:C:1031:MET:CE	2.46	0.45
2:C:783:ASP:O	2:C:791:ARG:HG3	2.16	0.45
3:D:866:ARG:HD2	3:D:1010:LEU:O	2.16	0.45
3:D:1190:ASN:CA	3:D:1193:VAL:HG12	2.38	0.45
6:J:76:LYS:H	6:J:76:LYS:CD	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:SER:O	1:A:123:MET:HE1	2.15	0.45
2:C:73:SER:O	2:C:77:ARG:HD3	2.16	0.45
2:C:160:MET:CG	2:C:164:GLY:HA2	2.46	0.45
2:C:285:GLU:OE1	2:C:285:GLU:HA	2.17	0.45
3:D:33:THR:HG21	3:D:327:MET:CE	2.32	0.45
3:D:199:ASP:O	3:D:203:ARG:HG3	2.16	0.45
3:D:788:ALA:O	3:D:791:GLU:HG3	2.15	0.45
3:D:1086:LEU:HD23	3:D:1099:LEU:CG	2.47	0.45
5:F:376:ILE:HD13	5:F:417:ALA:HB2	1.98	0.45
8:P:137:DG:H2'	8:P:138:DT:C7	2.46	0.45
2:C:593:MET:CE	2:C:713:MET:HG3	2.46	0.45
2:C:918:ASN:OD1	2:C:919:THR:N	2.48	0.45
3:D:31:PRO:HG3	3:D:349:ASN:OD1	2.16	0.45
3:D:180:ASP:HB3	3:D:197:VAL:HG11	1.99	0.45
3:D:917:GLU:HG2	3:D:921:TYR:CE2	2.52	0.45
5:F:336:ASP:OD1	5:F:337:TYR:N	2.50	0.45
5:F:491:GLU:HA	5:F:494:GLN:HG3	1.98	0.45
1:A:35:GLY:HA2	1:A:192:LEU:HD21	1.98	0.45
1:A:56:ILE:HG12	1:A:136:VAL:HB	1.99	0.45
2:C:141:ASN:HD22	2:C:142:ASN:N	2.15	0.45
2:C:175:VAL:CG1	2:C:381:VAL:HG23	2.43	0.45
2:C:483:MET:HE2	2:C:498:GLY:HA3	1.97	0.45
3:D:24:SER:HA	3:D:92:MET:O	2.17	0.45
3:D:430:ILE:HG21	3:D:541:MET:HG3	1.98	0.45
3:D:603:SER:HA	3:D:606:HIS:O	2.17	0.45
3:D:1059:GLU:C	3:D:1060:ARG:HD3	2.36	0.45
3:D:1166:THR:HB	3:D:1206:VAL:CG1	2.46	0.45
4:E:56:TYR:CE2	4:E:99:ILE:HG12	2.51	0.45
9:M:26:THR:HA	9:M:30:GLU:O	2.16	0.45
2:C:53:LEU:HD12	2:C:637:ASP:HB2	1.99	0.45
2:C:122:CYS:HA	2:C:127:MET:HB2	1.98	0.45
2:C:146:GLU:CG	9:M:48:VAL:HG22	2.46	0.45
2:C:179:LEU:HD23	2:C:378:LEU:HD13	1.98	0.45
2:C:717:LYS:HG3	2:C:746:VAL:O	2.17	0.45
3:D:356:ARG:HH21	5:F:326:LEU:HD13	1.82	0.45
3:D:373:MET:SD	5:F:318:LEU:HB3	2.57	0.45
3:D:902:ALA:CB	3:D:912:ARG:HA	2.47	0.45
3:D:1010:LEU:HD23	3:D:1028:LEU:CA	2.46	0.45
5:F:466:THR:OG1	5:F:519:ARG:NH1	2.49	0.45
6:J:31:ARG:HG2	6:J:41:GLU:CG	2.27	0.45
2:C:61:PHE:CE2	2:C:65:ILE:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:285:GLU:CD	2:C:286:PRO:CD	2.85	0.45
2:C:611:MET:HB3	2:C:1033:LEU:HD21	1.99	0.45
2:C:611:MET:SD	2:C:892:LYS:HD3	2.56	0.45
2:C:822:ARG:NH1	2:C:828:LYS:O	2.49	0.45
3:D:887:ARG:NH1	3:D:972:THR:HB	2.30	0.45
3:D:921:TYR:HE1	3:D:949:ILE:HG13	1.80	0.45
5:F:342:LYS:HB3	7:O:52:DA:H5'	1.98	0.45
5:F:376:ILE:HG12	5:F:413:ILE:HG23	1.98	0.45
8:P:97:DT:O2	8:P:97:DT:H2'	2.17	0.45
1:A:216:VAL:HG13	1:B:216:VAL:HG23	1.97	0.45
1:B:110:ILE:O	1:B:112:PRO:HD3	2.17	0.45
2:C:167:ILE:O	2:C:168:ILE:HD13	2.16	0.45
3:D:136:ILE:HD11	3:D:235:ILE:HD11	1.97	0.45
5:F:333:GLU:HG2	6:J:81:HIS:CG	2.52	0.45
1:A:18:ARG:HB3	1:A:197:GLU:HA	1.99	0.45
1:A:61:HIS:CD2	1:A:63:PHE:HB2	2.52	0.45
1:B:63:PHE:O	1:B:73:VAL:HB	2.17	0.45
2:C:597:LEU:HB3	2:C:976:VAL:CG1	2.40	0.45
2:C:882:GLY:HA3	2:C:1037:VAL:CG2	2.47	0.45
2:C:894:VAL:HG11	3:D:429:VAL:CG2	2.47	0.45
2:C:1043:ALA:HB2	3:D:447:MET:HG3	1.98	0.45
2:C:1049:TYR:OH	2:C:1099:ARG:HD2	2.16	0.45
3:D:439:HIS:CD2	4:E:35:ILE:HG22	2.52	0.45
3:D:500:ARG:CD	3:D:534:ALA:HB2	2.46	0.45
3:D:575:ALA:HB1	3:D:713:VAL:HG11	1.99	0.45
3:D:821:LYS:HB3	3:D:836:VAL:HG11	1.99	0.45
3:D:826:ASN:OD1	3:D:832:ILE:HD11	2.16	0.45
3:D:1064:ILE:HG21	3:D:1111:LEU:HD23	1.99	0.45
2:C:50:VAL:HG22	2:C:503:TYR:CE1	2.39	0.45
3:D:864:ALA:O	3:D:867:THR:HG22	2.17	0.45
3:D:1053:VAL:HG12	3:D:1103:ASP:N	2.23	0.45
7:O:57:DC:H1'	7:O:58:DA:O5'	2.17	0.45
1:B:183:VAL:CA	1:B:188:ASP:H	2.25	0.45
2:C:218:LYS:HE2	2:C:219:ARG:HH11	1.82	0.45
2:C:886:ALA:HB3	2:C:1033:LEU:CD1	2.47	0.45
2:C:1074:TRP:NE1	3:D:878:VAL:HG11	2.31	0.45
3:D:76:GLU:OE2	6:J:48:ALA:HB1	2.16	0.45
3:D:416:ASN:HD22	3:D:417:LEU:H	1.64	0.45
3:D:1221:LEU:HD23	3:D:1250:GLU:HB3	1.97	0.45
7:O:65:DC:OP2	7:O:65:DC:H6	2.00	0.45
8:P:86:DC:H1'	8:P:87:DG:C5'	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:110:DC:H2''	8:P:111:DA:OP2	2.16	0.45
9:M:74:LEU:HD23	9:M:74:LEU:O	2.17	0.45
1:A:70:LYS:NZ	2:C:690:VAL:O	2.40	0.44
2:C:117:ALA:HB3	2:C:122:CYS:SG	2.57	0.44
2:C:296:LEU:C	2:C:298:ASN:N	2.69	0.44
2:C:792:ILE:HD12	2:C:792:ILE:H	1.81	0.44
2:C:1088:LEU:O	3:D:422:VAL:HG12	2.16	0.44
3:D:17:ALA:O	3:D:21:ARG:HG2	2.17	0.44
3:D:88:ARG:O	3:D:323:GLU:HG2	2.17	0.44
3:D:107:PHE:CE2	3:D:129:ILE:HD11	2.52	0.44
3:D:302:PHE:CE1	3:D:309:PRO:HA	2.52	0.44
3:D:444:PRO:HB3	3:D:520:LYS:HA	1.99	0.44
3:D:612:TYR:CE2	3:D:627:LEU:HD21	2.52	0.44
1:A:65:THR:HG21	2:C:656:ASP:CG	2.37	0.44
1:A:182:ARG:HA	1:A:188:ASP:CG	2.37	0.44
2:C:102:SER:HB2	2:C:143:ASN:ND2	2.32	0.44
2:C:234:VAL:O	2:C:238:LEU:HD23	2.17	0.44
2:C:334:THR:HG23	2:C:337:ASP:N	2.24	0.44
2:C:809:LYS:HB3	2:C:831:GLU:O	2.16	0.44
2:C:820:LEU:HD11	2:C:824:ILE:HD11	1.99	0.44
3:D:656:TRP:O	3:D:656:TRP:CD2	2.70	0.44
3:D:1055:LEU:HB3	3:D:1101:ASP:CG	2.37	0.44
5:F:456:LEU:HA	5:F:526:TYR:CE2	2.52	0.44
7:O:42:DT:H2''	7:O:43:DT:O5'	2.16	0.44
9:M:100:ASP:OD2	9:M:102:ASN:HB2	2.17	0.44
1:A:33:THR:CG2	1:B:37:SER:HA	2.46	0.44
2:C:659:THR:HA	2:C:668:ARG:O	2.17	0.44
3:D:674:ASN:ND2	3:D:684:VAL:H	2.14	0.44
3:D:1222:SER:HB2	3:D:1250:GLU:OE2	2.17	0.44
5:F:386:LEU:HD13	5:F:398:GLU:OE1	2.17	0.44
6:J:23:ASP:C	6:J:24:LEU:HD22	2.38	0.44
7:O:60:DG:H2''	7:O:61:DG:H8	1.82	0.44
8:P:124:DG:H8	8:P:124:DG:OP2	2.00	0.44
1:A:211:ALA:O	1:A:215:LEU:HD23	2.17	0.44
1:B:30:PHE:CD1	1:B:33:THR:HG21	2.53	0.44
1:B:71:GLU:HG2	1:B:75:GLU:CG	2.48	0.44
2:C:133:LEU:CB	2:C:154:MET:HB3	2.47	0.44
2:C:378:LEU:HD11	2:C:455:LEU:HD22	1.97	0.44
3:D:12:ILE:HG23	3:D:1237:ALA:HA	1.98	0.44
3:D:97:LEU:HD11	3:D:317:VAL:HG23	1.97	0.44
3:D:106:TYR:HB3	3:D:312:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:138:SER:O	3:D:252:PHE:HB2	2.17	0.44
3:D:435:GLN:OE1	3:D:435:GLN:N	2.41	0.44
3:D:944:LEU:HD22	3:D:949:ILE:CD1	2.48	0.44
5:F:376:ILE:HG12	5:F:413:ILE:CG2	2.48	0.44
5:F:446:VAL:HB	5:F:449:ASP:CG	2.38	0.44
7:O:25:DT:H2'	7:O:25:DT:OP2	2.18	0.44
9:M:27:ILE:CG2	9:M:32:LYS:HD2	2.47	0.44
2:C:707:CYS:O	2:C:714:ALA:N	2.49	0.44
3:D:58:TRP:CE2	3:D:68:VAL:HG22	2.52	0.44
3:D:89:ARG:HD2	3:D:324:LEU:HD21	1.99	0.44
3:D:676:LEU:HD12	3:D:715:LYS:CB	2.38	0.44
4:E:83:VAL:HG13	4:E:97:ARG:HH21	1.81	0.44
9:M:36:VAL:HG13	9:M:36:VAL:O	2.18	0.44
9:M:105:ALA:HA	9:M:108:VAL:HG22	1.99	0.44
1:A:3:ILE:O	1:A:3:ILE:HG13	2.17	0.44
1:A:221:LEU:O	1:A:225:LEU:HB2	2.18	0.44
2:C:148:LYS:HB3	2:C:414:PRO:CD	2.36	0.44
2:C:377:ARG:NH1	2:C:379:ARG:HG2	2.33	0.44
2:C:1137:VAL:HG11	3:D:0:ALA:O	2.18	0.44
3:D:497:LEU:HD23	3:D:511:ALA:HB2	1.99	0.44
3:D:579:LEU:CD2	3:D:808:THR:HB	2.47	0.44
3:D:736:VAL:HG22	3:D:799:ILE:HD11	1.99	0.44
5:F:346:TYR:HB2	7:O:50:DA:N3	2.33	0.44
5:F:491:GLU:HG3	5:F:494:GLN:HE21	1.83	0.44
7:O:62:DT:H1'	7:O:63:DT:H5'	2.00	0.44
8:P:130:DA:H2''	8:P:131:DG:H5'	1.99	0.44
8:P:132:DA:H2'	8:P:132:DA:OP2	2.18	0.44
1:B:105:VAL:O	1:B:125:ILE:HG22	2.16	0.44
1:B:111:VAL:O	1:B:111:VAL:HG13	2.18	0.44
2:C:516:TYR:CD2	2:C:531:LEU:HB2	2.53	0.44
2:C:541:VAL:HG11	2:C:562:ARG:NH2	2.33	0.44
3:D:989:VAL:HG23	3:D:993:GLU:HG3	1.99	0.44
3:D:1120:GLU:O	3:D:1124:VAL:HG23	2.18	0.44
8:P:133:DC:C2'	8:P:134:DC:H4'	2.48	0.44
9:M:9:VAL:HG11	9:M:37:LEU:HD11	1.98	0.44
1:B:107:ALA:HB3	1:B:121:PRO:C	2.38	0.44
2:C:270:THR:OG1	2:C:271:ASP:N	2.50	0.44
2:C:592:ALA:CB	2:C:630:MET:HG3	2.47	0.44
2:C:1044:ARG:HH21	2:C:1047:GLY:H	1.64	0.44
3:D:37:ARG:CG	3:D:38:THR:H	2.28	0.44
3:D:228:LYS:O	3:D:233:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.99	0.44
3:D:741:ARG:HD3	3:D:745:ILE:HD11	1.99	0.44
3:D:746:LEU:HD23	3:D:746:LEU:HA	1.80	0.44
8:P:109:DA:H1'	8:P:110:DC:H5'	1.99	0.44
9:M:53:ALA:HB1	9:M:58:VAL:CG1	2.47	0.44
9:M:120:LEU:HD23	9:M:124:GLU:C	2.38	0.44
2:C:267:THR:HG23	2:C:272:GLU:OE2	2.17	0.44
2:C:891:ASN:HD21	2:C:1028:MET:HE3	1.82	0.44
3:D:65:TYR:CD2	3:D:75:CYS:HB2	2.53	0.44
3:D:212:ALA:O	3:D:216:LEU:HG	2.18	0.44
3:D:925:LEU:HD12	3:D:938:VAL:HG12	2.00	0.44
6:J:27:ARG:HB2	6:J:44:PHE:O	2.18	0.44
6:J:81:HIS:HA	6:J:84:MET:HE2	1.99	0.44
7:O:72:DG:C2'	7:O:73:DC:H2'	2.44	0.44
8:P:88:DG:H2''	8:P:89:DG:O5'	2.17	0.44
8:P:123:DG:H2''	8:P:124:DG:C8	2.53	0.44
1:A:27:GLU:O	1:A:30:PHE:HB3	2.18	0.43
2:C:122:CYS:HB3	2:C:127:MET:O	2.17	0.43
2:C:275:LEU:HD12	2:C:275:LEU:H	1.82	0.43
2:C:349:HIS:ND1	2:C:349:HIS:O	2.51	0.43
2:C:413:THR:HG22	2:C:416:THR:CG2	2.43	0.43
2:C:460:PRO:HA	8:P:97:DT:OP2	2.18	0.43
2:C:475:VAL:O	2:C:475:VAL:HG23	2.17	0.43
2:C:740:ARG:HH21	2:C:914:ASP:CG	2.20	0.43
3:D:130:TYR:CD1	3:D:387:ARG:NH2	2.85	0.43
3:D:340:LEU:HD11	3:D:405:LEU:HD12	2.00	0.43
3:D:432:VAL:CG2	3:D:526:PRO:HB3	2.48	0.43
3:D:1208:MET:HE1	3:D:1213:ALA:HA	2.00	0.43
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.83	0.43
2:C:862:PRO:HG2	2:C:865:VAL:HG21	2.01	0.43
2:C:1091:ILE:CG2	2:C:1115:PRO:HB3	2.45	0.43
3:D:56:ARG:HG2	6:J:13:ALA:H	1.82	0.43
3:D:124:ASP:HB3	3:D:234:LEU:HD22	2.00	0.43
3:D:453:LYS:HA	3:D:456:VAL:HG12	1.99	0.43
3:D:589:THR:HG21	3:D:688:MET:CG	2.48	0.43
3:D:629:VAL:HG21	3:D:723:TRP:CH2	2.52	0.43
3:D:656:TRP:HE3	3:D:658:PRO:HG2	1.83	0.43
3:D:1028:LEU:HB3	3:D:1029:PRO:HD3	2.00	0.43
3:D:1267:TYR:CD1	4:E:52:ALA:HB2	2.54	0.43
4:E:95:ALA:O	4:E:99:ILE:HG13	2.18	0.43
9:M:70:VAL:HG11	9:M:101:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HA	1:A:171:VAL:HG11	2.00	0.43
1:B:54:ILE:HD13	1:B:80:LEU:HD12	1.99	0.43
2:C:256:GLU:O	2:C:259:ARG:HG2	2.18	0.43
3:D:335:PHE:HB2	5:F:420:PRO:HG3	2.00	0.43
3:D:1054:ARG:CB	3:D:1065:THR:HB	2.48	0.43
3:D:1208:MET:HE3	3:D:1213:ALA:CB	2.49	0.43
5:F:310:TYR:HD2	5:F:355:ILE:CG2	2.32	0.43
2:C:46:GLU:O	2:C:46:GLU:HG2	2.18	0.43
2:C:584:ARG:HH22	2:C:975:PRO:CB	2.29	0.43
2:C:884:LYS:HD3	2:C:1035:HIS:HD2	1.82	0.43
3:D:129:ILE:HG22	3:D:261:ILE:HG13	2.01	0.43
3:D:204:GLU:O	3:D:207:GLN:HB3	2.18	0.43
3:D:541:MET:HE2	3:D:541:MET:HB3	1.88	0.43
3:D:591:GLU:OE2	3:D:632:LYS:HB2	2.18	0.43
3:D:729:VAL:HG23	3:D:729:VAL:O	2.17	0.43
3:D:940:ARG:HH11	3:D:963:ARG:HH21	1.67	0.43
3:D:1262:THR:HG22	4:E:51:TYR:HB3	1.99	0.43
2:C:902:GLU:OE1	2:C:902:GLU:N	2.42	0.43
2:C:1078:ALA:HB3	3:D:506:ARG:HG3	1.99	0.43
3:D:203:ARG:O	3:D:206:ARG:HG2	2.17	0.43
5:F:460:LEU:O	5:F:464:LEU:HD13	2.19	0.43
1:A:61:HIS:CD2	1:A:63:PHE:H	2.35	0.43
2:C:549:ASP:N	2:C:553:ARG:O	2.32	0.43
3:D:642:PRO:HB2	3:D:643:PRO:HD2	2.01	0.43
5:F:477:LEU:O	5:F:487:ARG:HB2	2.19	0.43
7:O:15:DG:H2''	7:O:16:DA:OP2	2.16	0.43
7:O:35:DT:C1'	7:O:36:DG:H5'	2.47	0.43
1:B:117:THR:HG23	1:B:117:THR:O	2.19	0.43
1:B:183:VAL:O	1:B:187:THR:HA	2.19	0.43
2:C:235:THR:O	2:C:239:LYS:HG3	2.18	0.43
2:C:275:LEU:HD21	2:C:289:LYS:HA	2.01	0.43
2:C:600:ASP:OD2	2:C:889:HIS:ND1	2.48	0.43
2:C:881:ASP:OD1	2:C:881:ASP:N	2.51	0.43
2:C:885:LEU:HD13	2:C:895:ILE:CG1	2.48	0.43
2:C:1057:LEU:HD12	2:C:1057:LEU:HA	1.85	0.43
3:D:95:ILE:HD13	3:D:348:ILE:HD11	2.00	0.43
6:J:20:ARG:HH11	6:J:23:ASP:HB3	1.83	0.43
6:J:109:ARG:HH11	6:J:110:ARG:NH2	2.17	0.43
7:O:42:DT:C1'	7:O:43:DT:H5'	2.36	0.43
2:C:41:PHE:CE2	2:C:980:ALA:HB2	2.54	0.43
2:C:61:PHE:HB2	2:C:160:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:VAL:O	2:C:206:PRO:HD3	2.19	0.43
2:C:435:GLN:HE21	2:C:460:PRO:CD	2.28	0.43
2:C:758:ASP:HB3	2:C:868:LEU:CD2	2.42	0.43
2:C:989:LEU:HD21	2:C:1006:GLY:HA2	2.01	0.43
3:D:148:LEU:O	3:D:148:LEU:HD13	2.19	0.43
3:D:195:ARG:HD2	3:D:198:ARG:NH1	2.32	0.43
3:D:877:LEU:HA	3:D:877:LEU:HD23	1.73	0.43
3:D:915:TYR:CE2	3:D:1143:ARG:HD3	2.52	0.43
3:D:925:LEU:CD2	3:D:944:LEU:HD11	2.48	0.43
4:E:83:VAL:HG11	4:E:97:ARG:HE	1.84	0.43
5:F:342:LYS:HG2	7:O:53:DC:OP2	2.18	0.43
5:F:470:ARG:HD3	5:F:506:ILE:CD1	2.41	0.43
2:C:102:SER:O	2:C:141:ASN:ND2	2.50	0.43
2:C:187:PHE:CE1	2:C:202:VAL:HB	2.54	0.43
3:D:566:LEU:HD23	3:D:573:PRO:CA	2.49	0.43
3:D:826:ASN:OD1	3:D:827:PRO:HD2	2.18	0.43
3:D:991:ILE:HG22	3:D:991:ILE:O	2.19	0.43
7:O:26:DT:H2''	7:O:27:DG:O5'	2.18	0.43
8:P:128:DC:H2''	8:P:129:DA:H8	1.83	0.43
9:M:70:VAL:HG11	9:M:101:VAL:HG12	2.01	0.43
9:M:70:VAL:HG12	9:M:102:ASN:ND2	2.34	0.43
1:B:28:PRO:HD3	1:B:189:PHE:HD1	1.84	0.43
1:B:87:SER:OG	1:B:116:VAL:HG12	2.19	0.43
2:C:206:PRO:CB	2:C:308:LEU:HB3	2.49	0.43
2:C:307:ASP:O	2:C:309:ALA:N	2.52	0.43
2:C:388:GLN:HG3	2:C:430:PHE:HB2	2.01	0.43
2:C:822:ARG:O	2:C:826:GLY:N	2.52	0.43
2:C:904:MET:HG2	2:C:913:VAL:O	2.19	0.43
2:C:955:TRP:NE1	2:C:987:GLY:HA3	2.34	0.43
2:C:1044:ARG:NH2	2:C:1048:PRO:O	2.49	0.43
3:D:33:THR:HG23	3:D:47:PHE:HE2	1.80	0.43
3:D:48:CYS:SG	3:D:50:LYS:HB3	2.59	0.43
3:D:52:PHE:CG	3:D:322:PRO:HD3	2.54	0.43
3:D:281:ILE:HD12	3:D:282:ARG:N	2.34	0.43
3:D:491:ILE:HG23	3:D:514:PRO:HG2	2.00	0.43
3:D:673:PHE:O	3:D:676:LEU:HB2	2.18	0.43
3:D:753:ALA:HB1	3:D:774:LEU:HD22	2.00	0.43
3:D:874:THR:OG1	3:D:1004:GLY:HA3	2.19	0.43
5:F:449:ASP:OD1	5:F:450:ALA:N	2.52	0.43
7:O:28:DA:OP2	7:O:28:DA:H3'	2.19	0.43
7:O:36:DG:H1'	7:O:37:DC:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:34:TYR:CE1	9:M:49:PRO:HG3	2.54	0.43
1:B:210:SER:O	1:B:214:THR:HG23	2.19	0.42
2:C:63:TRP:HD1	2:C:70:TRP:CE2	2.37	0.42
2:C:163:LYS:HE3	2:C:639:GLY:O	2.19	0.42
2:C:485:PRO:HD2	2:C:586:MET:O	2.19	0.42
2:C:598:GLU:OE1	2:C:598:GLU:N	2.43	0.42
2:C:738:SER:N	2:C:914:ASP:O	2.40	0.42
2:C:993:LEU:HD12	2:C:993:LEU:O	2.19	0.42
3:D:268:PHE:HE2	3:D:270:ILE:HG22	1.83	0.42
3:D:1066:ILE:HD11	3:D:1077:TYR:HE2	1.84	0.42
3:D:1080:ILE:HD11	3:D:1112:MET:SD	2.59	0.42
5:F:271:GLU:OE2	5:F:274:PRO:HD3	2.18	0.42
9:M:156:GLU:OE2	9:M:157:VAL:HG23	2.18	0.42
1:B:81:LYS:HE3	3:D:613:SER:HB3	2.01	0.42
1:B:203:SER:HB2	1:B:204:PRO:HD2	2.00	0.42
2:C:220:ASP:CG	2:C:257:ILE:HG12	2.40	0.42
2:C:296:LEU:O	2:C:298:ASN:N	2.52	0.42
2:C:886:ALA:HB3	2:C:1033:LEU:HD11	2.00	0.42
2:C:1077:GLN:NE2	10:C:1201:C0L:O33	2.51	0.42
3:D:106:TYR:HB3	3:D:312:MET:HE3	1.99	0.42
3:D:285:LYS:HD3	3:D:285:LYS:H	1.85	0.42
3:D:389:ARG:NH1	7:O:58:DA:N7	2.51	0.42
3:D:635:VAL:HG23	3:D:637:LEU:HG	2.01	0.42
5:F:254:GLU:OE1	6:J:89:ARG:NH1	2.52	0.42
5:F:461:GLN:OE1	5:F:476:ARG:NH2	2.52	0.42
8:P:116:DC:H1'	8:P:117:DG:H5'	2.01	0.42
8:P:138:DT:H1'	8:P:139:DT:O5'	2.18	0.42
1:A:87:SER:OG	1:A:88:GLU:N	2.53	0.42
1:B:102:PRO:HD3	1:B:131:LYS:N	2.29	0.42
2:C:347:ARG:HD3	2:C:355:MET:HG3	2.02	0.42
2:C:413:THR:HG23	2:C:416:THR:H	1.83	0.42
2:C:542:ALA:HB3	2:C:579:MET:HA	2.00	0.42
2:C:681:GLY:O	2:C:751:HIS:HA	2.19	0.42
3:D:460:LEU:HD11	3:D:472:ALA:CB	2.50	0.42
3:D:590:THR:CG2	3:D:630:ARG:HD2	2.50	0.42
3:D:1264:ILE:HD11	3:D:1267:TYR:HE2	1.83	0.42
4:E:33:LEU:HD12	4:E:33:LEU:O	2.19	0.42
5:F:395:THR:OG1	5:F:398:GLU:HB2	2.20	0.42
5:F:516:HIS:O	5:F:520:SER:CB	2.67	0.42
9:M:83:THR:O	9:M:84:ASN:HB2	2.19	0.42
1:B:66:VAL:HB	1:B:69:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:ILE:HG12	9:M:47:ARG:H	1.84	0.42
2:C:516:TYR:CE2	2:C:531:LEU:HB2	2.55	0.42
2:C:541:VAL:HA	2:C:578:TYR:O	2.18	0.42
2:C:1044:ARG:HH12	2:C:1057:LEU:H	1.66	0.42
2:C:1138:LEU:HD11	3:D:11:ARG:CZ	2.48	0.42
3:D:33:THR:HG23	3:D:47:PHE:CD2	2.53	0.42
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.84	0.42
3:D:409:LYS:O	3:D:409:LYS:HD3	2.20	0.42
3:D:500:ARG:HH21	3:D:539:ASP:CG	2.23	0.42
3:D:550:GLU:OE2	4:E:62:ARG:HD2	2.19	0.42
3:D:1054:ARG:HB3	3:D:1065:THR:C	2.40	0.42
2:C:756:GLU:CG	2:C:870:ARG:HG2	2.49	0.42
3:D:25:TYR:CD2	3:D:91:ARG:HD3	2.53	0.42
3:D:82:VAL:O	3:D:82:VAL:HG13	2.19	0.42
3:D:505:HIS:CD2	3:D:1005:GLU:HG3	2.54	0.42
3:D:736:VAL:HG12	3:D:818:ALA:HB2	2.01	0.42
3:D:1191:ARG:O	3:D:1194:VAL:HG22	2.20	0.42
3:D:1267:TYR:O	4:E:55:ILE:HG21	2.18	0.42
5:F:478:ARG:NH2	8:P:126:DG:OP1	2.44	0.42
9:M:88:ARG:HH21	9:M:114:ARG:CZ	2.33	0.42
2:C:357:VAL:CG1	2:C:360:GLY:HA3	2.48	0.42
2:C:737:LEU:CD1	2:C:895:ILE:HD13	2.50	0.42
2:C:879:ILE:HD12	2:C:879:ILE:HA	1.96	0.42
3:D:14:LEU:HD21	3:D:311:GLY:C	2.40	0.42
3:D:39:LEU:HA	3:D:39:LEU:HD23	1.82	0.42
3:D:104:ILE:HD12	3:D:379:ASP:HB3	2.01	0.42
3:D:383:ASP:HA	3:D:403:SER:OG	2.20	0.42
3:D:736:VAL:CG1	3:D:841:ARG:HD2	2.49	0.42
3:D:1052:ARG:HB2	3:D:1102:GLY:C	2.40	0.42
5:F:386:LEU:HB3	5:F:394:PRO:HG2	2.01	0.42
1:A:111:VAL:HG13	1:A:111:VAL:O	2.20	0.42
2:C:205:ILE:HG22	2:C:211:TRP:CD2	2.54	0.42
2:C:259:ARG:O	2:C:263:GLU:HG2	2.20	0.42
2:C:294:THR:O	2:C:298:ASN:CB	2.68	0.42
2:C:646:GLU:HB3	2:C:662:HIS:ND1	2.35	0.42
2:C:719:LEU:HD13	2:C:1030:ILE:HG12	2.01	0.42
2:C:728:GLY:O	2:C:731:TYR:HB2	2.19	0.42
3:D:1122:LEU:HD13	3:D:1130:VAL:HG11	2.02	0.42
5:F:510:THR:O	5:F:514:LEU:HD23	2.19	0.42
9:M:134:ILE:HD12	9:M:135:LEU:N	2.35	0.42
1:B:89:GLU:OE1	1:B:89:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:222:VAL:CG2	2:C:234:VAL:H	2.33	0.42
3:D:173:ARG:CG	3:D:205:MET:HB2	2.49	0.42
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.84	0.42
3:D:963:ARG:HB3	3:D:978:CYS:HA	2.02	0.42
3:D:1056:GLU:N	3:D:1063:LYS:O	2.53	0.42
3:D:1208:MET:CE	3:D:1213:ALA:HA	2.50	0.42
5:F:296:LEU:HD21	5:F:329:ILE:HA	2.00	0.42
9:M:25:ARG:O	9:M:32:LYS:N	2.53	0.42
9:M:141:LEU:HA	9:M:141:LEU:HD23	1.76	0.42
1:A:153:ARG:HH21	2:C:797:ARG:CD	2.33	0.42
1:B:41:THR:OG1	1:B:215:LEU:HD21	2.20	0.42
1:B:84:VAL:HG23	1:B:199:LYS:HD3	2.01	0.42
2:C:230:ARG:O	2:C:231:ARG:HG2	2.20	0.42
2:C:356:THR:HG23	2:C:356:THR:O	2.20	0.42
2:C:593:MET:HE1	2:C:713:MET:HG3	2.00	0.42
3:D:500:ARG:HD2	3:D:534:ALA:HB2	2.02	0.42
5:F:257:LEU:HD21	6:J:81:HIS:ND1	2.35	0.42
5:F:439:ILE:HG12	6:J:6:LEU:CD1	2.50	0.42
8:P:131:DG:H2''	8:P:132:DA:H8	1.83	0.42
9:M:151:GLU:HA	9:M:154:LEU:HD12	2.02	0.42
1:B:85:VAL:O	1:B:85:VAL:HG13	2.19	0.42
1:B:145:GLY:O	1:B:168:TYR:HB2	2.20	0.42
1:B:213:LYS:HA	1:B:216:VAL:HG12	2.01	0.42
2:C:139:PHE:CE1	2:C:412:ILE:HD11	2.55	0.42
2:C:345:LEU:O	2:C:345:LEU:HD22	2.20	0.42
2:C:357:VAL:HG23	2:C:358:PRO:HD2	2.02	0.42
2:C:884:LYS:HD3	2:C:1035:HIS:CD2	2.55	0.42
2:C:1092:LYS:HE2	3:D:547:LEU:CD1	2.50	0.42
3:D:52:PHE:CB	3:D:322:PRO:HG3	2.49	0.42
3:D:199:ASP:HB3	3:D:203:ARG:NH1	2.35	0.42
3:D:1045:PRO:O	3:D:1111:LEU:HD13	2.20	0.42
3:D:1167:ILE:HG21	3:D:1175:PHE:HB3	2.02	0.42
4:E:86:GLY:N	4:E:89:GLU:OE1	2.36	0.42
5:F:400:ALA:HB2	5:F:410:VAL:HG21	2.02	0.42
6:J:50:ILE:HG22	6:J:64:LEU:HD12	2.02	0.42
7:O:72:DG:C1'	7:O:73:DC:H5'	2.48	0.42
9:M:25:ARG:HH12	9:M:47:ARG:HD3	1.85	0.42
1:A:45:SER:HB3	1:B:232:ILE:HD11	2.02	0.41
1:A:175:THR:HB	2:C:910:GLY:N	2.35	0.41
1:B:150:VAL:HG13	1:B:150:VAL:O	2.20	0.41
2:C:213:GLU:OE1	2:C:213:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:TYR:CE1	2:C:365:VAL:HA	2.55	0.41
2:C:452:LYS:O	2:C:453:ARG:HB2	2.20	0.41
2:C:894:VAL:HG22	3:D:536:PHE:O	2.19	0.41
2:C:904:MET:HG3	2:C:913:VAL:HG22	2.01	0.41
3:D:1127:PRO:O	3:D:1130:VAL:HG12	2.20	0.41
3:D:1272:VAL:HG22	4:E:56:TYR:HD1	1.84	0.41
5:F:331:ALA:HB2	5:F:350:TRP:HB2	2.02	0.41
9:M:9:VAL:HG23	9:M:59:ARG:O	2.20	0.41
1:A:2:LEU:HD12	1:A:2:LEU:O	2.21	0.41
1:A:56:ILE:HB	1:A:59:VAL:HG21	2.01	0.41
1:B:43:LEU:HA	1:B:171:VAL:CG2	2.50	0.41
1:B:105:VAL:HA	1:B:109:ASP:OD2	2.21	0.41
2:C:94:SER:HA	2:C:95:PRO:HA	1.77	0.41
2:C:281:LEU:HD12	2:C:281:LEU:HA	1.58	0.41
2:C:294:THR:H	2:C:294:THR:HG23	1.58	0.41
3:D:417:LEU:HD23	3:D:417:LEU:HA	1.91	0.41
3:D:497:LEU:CD2	3:D:511:ALA:HB2	2.50	0.41
3:D:524:LEU:HD12	3:D:524:LEU:HA	1.72	0.41
3:D:591:GLU:OE2	3:D:632:LYS:HD2	2.21	0.41
3:D:683:PHE:CD2	3:D:685:ASN:HB2	2.55	0.41
3:D:844:LEU:HD12	3:D:844:LEU:N	2.35	0.41
3:D:1174:GLU:O	3:D:1174:GLU:HG3	2.19	0.41
3:D:1245:LEU:CD2	3:D:1250:GLU:HB3	2.50	0.41
5:F:310:TYR:HD2	5:F:355:ILE:HG21	1.85	0.41
5:F:382:ILE:HG22	5:F:399:LEU:CD2	2.49	0.41
9:M:136:VAL:HG22	9:M:154:LEU:CD1	2.51	0.41
1:A:183:VAL:HG22	1:A:184:GLU:H	1.86	0.41
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.86	0.41
2:C:165:THR:HG21	2:C:440:MET:SD	2.60	0.41
2:C:201:SER:OG	2:C:202:VAL:N	2.52	0.41
2:C:587:VAL:CG2	2:C:591:THR:HB	2.51	0.41
2:C:980:ALA:HA	2:C:984:GLU:OE1	2.20	0.41
8:P:137:DG:H2'	8:P:138:DT:H72	2.02	0.41
2:C:38:ARG:HH21	2:C:712:GLU:CD	2.24	0.41
2:C:112:PHE:CZ	2:C:133:LEU:HD21	2.55	0.41
2:C:131:ALA:HA	2:C:132:PRO:HD3	1.90	0.41
2:C:135:VAL:HG21	2:C:154:MET:HE3	2.01	0.41
2:C:147:ILE:O	2:C:147:ILE:HG13	2.19	0.41
2:C:148:LYS:O	2:C:414:PRO:HG3	2.20	0.41
2:C:183:PRO:HB2	2:C:206:PRO:HA	2.02	0.41
2:C:234:VAL:HG21	2:C:258:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:288:THR:CG2	2:C:291:SER:CB	2.85	0.41
2:C:507:ASN:HD22	2:C:511:PHE:HB2	1.85	0.41
2:C:1051:MET:HE3	3:D:328:VAL:HG21	2.00	0.41
2:C:1076:MET:HG3	3:D:509:ILE:CD1	2.51	0.41
3:D:329:GLN:O	3:D:329:GLN:HG3	2.21	0.41
3:D:386:ARG:CG	3:D:386:ARG:HH11	2.33	0.41
3:D:557:ILE:HD13	4:E:53:LEU:HD13	2.01	0.41
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.21	0.41
5:F:323:GLU:HG3	5:F:358:ALA:CB	2.50	0.41
5:F:342:LYS:HB2	7:O:52:DA:H5''	2.01	0.41
1:A:71:GLU:HG2	1:A:75:GLU:HG2	2.02	0.41
1:A:83:LEU:HA	1:A:123:MET:HE3	2.01	0.41
1:A:105:VAL:O	1:A:125:ILE:HB	2.20	0.41
1:A:217:GLU:HB3	1:B:234:ILE:CD1	2.50	0.41
1:B:84:VAL:O	1:B:84:VAL:HG13	2.21	0.41
2:C:824:ILE:HA	5:F:511:MET:HE1	2.01	0.41
2:C:1094:ASP:O	2:C:1119:GLU:HB2	2.20	0.41
3:D:827:PRO:HG3	3:D:854:HIS:ND1	2.36	0.41
3:D:937:ILE:CD1	3:D:955:ALA:HB2	2.51	0.41
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.41	0.41
8:P:94:DC:H2''	8:P:95:DC:C6	2.56	0.41
9:M:44:LEU:HD23	9:M:44:LEU:H	1.84	0.41
9:M:88:ARG:HH21	9:M:114:ARG:NH2	2.18	0.41
2:C:41:PHE:HE1	2:C:963:LEU:HD22	1.85	0.41
2:C:271:ASP:O	2:C:275:LEU:HD11	2.05	0.41
2:C:295:LEU:O	2:C:295:LEU:HG	2.18	0.41
2:C:475:VAL:HG23	3:D:854:HIS:ND1	2.35	0.41
2:C:476:HIS:ND1	2:C:477:PRO:HD2	2.36	0.41
2:C:777:SER:OG	2:C:778:ASP:N	2.53	0.41
2:C:1117:ILE:CG2	2:C:1118:PRO:HD2	2.50	0.41
3:D:114:LEU:HG	3:D:312:MET:HE2	2.03	0.41
3:D:140:ASP:O	3:D:143:MET:N	2.53	0.41
3:D:273:GLU:OE2	3:D:295:ARG:NH2	2.39	0.41
3:D:329:GLN:HB3	3:D:335:PHE:CD1	2.56	0.41
3:D:456:VAL:HG23	3:D:486:VAL:HG12	2.03	0.41
3:D:645:GLU:OE1	3:D:645:GLU:N	2.50	0.41
3:D:741:ARG:CD	3:D:745:ILE:HD11	2.50	0.41
5:F:386:LEU:HB2	5:F:394:PRO:HG2	2.02	0.41
8:P:108:DT:H1'	8:P:109:DA:H5'	2.02	0.41
9:M:53:ALA:O	9:M:56:VAL:HG12	2.20	0.41
9:M:153:ILE:O	9:M:157:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:O	1:A:150:VAL:HG13	2.20	0.41
2:C:128:THR:O	2:C:128:THR:HG23	2.20	0.41
2:C:428:LYS:HE2	2:C:428:LYS:HB3	1.92	0.41
3:D:824:VAL:HG11	3:D:852:ASN:HA	2.03	0.41
5:F:338:THR:HG23	6:J:89:ARG:NH2	2.35	0.41
6:J:11:LEU:HD23	6:J:11:LEU:HA	1.85	0.41
9:M:132:ARG:NH2	9:M:151:GLU:HB3	2.36	0.41
9:M:153:ILE:HA	9:M:156:GLU:CG	2.51	0.41
1:A:11:GLU:OE2	1:A:19:SER:HB2	2.21	0.41
1:A:45:SER:HB3	1:B:232:ILE:CD1	2.50	0.41
2:C:400:VAL:O	2:C:404:MET:HB2	2.21	0.41
2:C:617:PRO:HA	2:C:707:CYS:SG	2.60	0.41
2:C:928:ILE:HD11	3:D:841:ARG:HA	2.02	0.41
2:C:928:ILE:HG21	3:D:817:LEU:HD22	2.03	0.41
2:C:967:GLN:HB3	2:C:968:PRO:HD2	2.01	0.41
2:C:1070:GLU:HG2	2:C:1074:TRP:CE2	2.55	0.41
3:D:37:ARG:H	3:D:37:ARG:HG2	1.62	0.41
3:D:748:HIS:CE1	3:D:752:ARG:HD2	2.55	0.41
3:D:1063:LYS:HD2	3:D:1078:ASP:OD1	2.20	0.41
6:J:80:THR:O	6:J:83:ASP:HB2	2.20	0.41
2:C:126:ASP:O	2:C:169:ASN:HA	2.20	0.41
2:C:281:LEU:CD2	2:C:295:LEU:CD1	2.98	0.41
2:C:546:SER:HA	2:C:547:PRO:HD3	1.93	0.41
2:C:568:VAL:HB	3:D:834:ARG:HD2	2.02	0.41
2:C:723:ILE:O	2:C:723:ILE:HG22	2.21	0.41
2:C:848:ILE:HD11	2:C:874:ALA:CB	2.50	0.41
2:C:1051:MET:HE1	5:F:441:ASP:HA	2.03	0.41
3:D:91:ARG:O	3:D:321:PRO:HG3	2.21	0.41
3:D:193:ALA:O	3:D:197:VAL:HG23	2.20	0.41
3:D:357:LEU:HD23	3:D:357:LEU:HA	1.90	0.41
3:D:797:ASN:ND2	3:D:798:PRO:HD2	2.31	0.41
3:D:817:LEU:HD23	3:D:817:LEU:HA	1.92	0.41
3:D:1054:ARG:HB3	3:D:1065:THR:O	2.20	0.41
3:D:1139:GLN:HB3	3:D:1143:ARG:NH1	2.36	0.41
5:F:277:GLN:O	5:F:281:MET:HG2	2.20	0.41
5:F:317:PHE:O	5:F:321:ILE:HG13	2.21	0.41
8:P:120:DA:H2'	8:P:120:DA:P	2.61	0.41
8:P:138:DT:C6	8:P:139:DT:H72	2.55	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.86	0.41
2:C:281:LEU:HD23	2:C:295:LEU:HD22	2.00	0.41
2:C:1057:LEU:HG	2:C:1058:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:822:GLY:O	3:D:835:PRO:HB2	2.21	0.41
3:D:925:LEU:HD21	3:D:944:LEU:HD11	2.03	0.41
3:D:1046:ILE:HD11	3:D:1124:VAL:CG2	2.50	0.41
4:E:60:ARG:HH22	4:E:80:GLY:CA	2.31	0.41
7:O:64:DG:H2''	7:O:65:DC:OP2	2.21	0.41
9:M:53:ALA:C	9:M:58:VAL:HG12	2.42	0.41
1:A:69:VAL:HG23	1:A:71:GLU:O	2.21	0.40
1:B:100:GLN:HA	1:B:132:GLY:O	2.21	0.40
1:B:184:GLU:CB	3:D:445:LYS:HZ3	2.34	0.40
2:C:282:ARG:HE	2:C:282:ARG:HB3	1.54	0.40
2:C:519:VAL:HG12	2:C:577:ASP:C	2.40	0.40
2:C:721:VAL:HG23	2:C:915:ILE:HG13	2.03	0.40
2:C:934:THR:HG23	2:C:1026:GLY:HA3	2.03	0.40
3:D:66:LYS:C	3:D:67:ARG:HD2	2.41	0.40
3:D:270:ILE:CD1	3:D:303:GLN:HA	2.49	0.40
3:D:527:LEU:CD1	3:D:713:VAL:HG12	2.50	0.40
3:D:1055:LEU:HB3	3:D:1101:ASP:HB2	2.02	0.40
3:D:1215:LEU:HD21	3:D:1227:GLN:HB3	2.03	0.40
3:D:1268:ARG:HD2	3:D:1268:ARG:O	2.21	0.40
5:F:244:GLU:HG2	5:F:245:GLU:N	2.36	0.40
5:F:305:SER:OG	7:O:54:DT:C4'	2.54	0.40
8:P:129:DA:H2''	8:P:130:DA:H8	1.86	0.40
2:C:503:TYR:HD2	2:C:581:VAL:HG21	1.86	0.40
3:D:336:ALA:HA	5:F:421:ILE:O	2.21	0.40
3:D:473:LYS:O	3:D:477:GLU:HG2	2.22	0.40
3:D:1005:GLU:HB3	3:D:1006:PRO:CD	2.51	0.40
5:F:273:LEU:HD22	5:F:278:ARG:HB2	2.03	0.40
5:F:478:ARG:NH1	5:F:489:LEU:HG	2.36	0.40
8:P:107:DA:H5'	9:M:121:SER:HB3	2.03	0.40
2:C:532:THR:HG23	2:C:534:ASP:H	1.86	0.40
2:C:720:LEU:HD12	2:C:720:LEU:HA	1.81	0.40
3:D:314:LEU:HA	3:D:314:LEU:HD12	1.80	0.40
3:D:336:ALA:HB1	5:F:423:LEU:CD2	2.50	0.40
3:D:487:LEU:HG	3:D:491:ILE:CD1	2.51	0.40
6:J:38:GLU:HG3	6:J:58:ASN:ND2	2.36	0.40
7:O:45:DG:H2''	7:O:46:DT:O5'	2.22	0.40
8:P:125:DA:H2''	8:P:126:DG:H8	1.86	0.40
1:A:14:LEU:HB2	1:A:18:ARG:CD	2.51	0.40
1:A:172:LEU:HB2	1:A:199:LYS:HB3	2.04	0.40
1:B:60:LEU:CD2	1:B:159:ILE:HD13	2.43	0.40
1:B:168:TYR:O	1:B:170:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:GLN:O	2:C:442:GLN:HG3	2.21	0.40
2:C:624:PRO:HB3	2:C:1029:TYR:CE1	2.57	0.40
3:D:457:MET:O	3:D:461:VAL:HG23	2.22	0.40
5:F:214:GLN:HA	5:F:217:LYS:NZ	2.36	0.40
7:O:23:DT:H2'	7:O:23:DT:H6	1.75	0.40
8:P:108:DT:H4'	9:M:85:TRP:CD1	2.57	0.40
1:A:183:VAL:HG22	1:A:184:GLU:N	2.37	0.40
1:B:112:PRO:HA	1:B:113:PRO:HD2	1.99	0.40
1:B:167:ILE:HD11	3:D:617:GLU:HB2	2.03	0.40
2:C:219:ARG:O	2:C:221:THR:N	2.54	0.40
2:C:284:GLY:HA2	5:F:219:ALA:O	2.21	0.40
2:C:882:GLY:HA3	2:C:1037:VAL:HG21	2.04	0.40
3:D:20:ILE:HG23	3:D:318:PRO:HB3	2.02	0.40
3:D:505:HIS:HB3	3:D:1005:GLU:HG3	2.02	0.40
3:D:819:GLY:N	3:D:839:SER:HB3	2.37	0.40
3:D:1045:PRO:HB3	3:D:1077:TYR:CE1	2.56	0.40
3:D:1210:ILE:HG13	3:D:1211:THR:N	2.37	0.40
4:E:70:GLN:HG2	4:E:70:GLN:O	2.22	0.40
5:F:492:ILE:O	5:F:495:VAL:HG12	2.21	0.40
6:J:64:LEU:CD2	6:J:66:GLU:H	2.20	0.40
8:P:83:DC:C2'	8:P:84:DT:H71	2.51	0.40
9:M:12:PRO:HA	9:M:13:HIS:HA	1.53	0.40
9:M:103:LYS:O	9:M:107:VAL:HG23	2.21	0.40
9:M:139:LEU:HD12	9:M:154:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	223/347 (64%)	197 (88%)	26 (12%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	235/347 (68%)	194 (83%)	41 (17%)	0	100	100
2	C	1109/1179 (94%)	937 (84%)	168 (15%)	4 (0%)	34	71
3	D	1260/1326 (95%)	1141 (91%)	115 (9%)	4 (0%)	41	74
4	E	81/110 (74%)	76 (94%)	5 (6%)	0	100	100
5	F	317/531 (60%)	296 (93%)	20 (6%)	1 (0%)	41	74
6	J	106/111 (96%)	87 (82%)	19 (18%)	0	100	100
9	M	157/162 (97%)	144 (92%)	12 (8%)	1 (1%)	25	64
All	All	3488/4113 (85%)	3072 (88%)	406 (12%)	10 (0%)	44	74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	418	LEU
3	D	658	PRO
2	C	274	LEU
3	D	653	HIS
2	C	53	LEU
2	C	278	TYR
9	M	83	THR
2	C	297	GLU
3	D	238	GLU
5	F	307	ALA

### 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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/297 (65%)	192 (99%)	2 (1%)	76	89
1	B	194/297 (65%)	193 (100%)	1 (0%)	88	95
2	C	935/997 (94%)	918 (98%)	17 (2%)	59	81
3	D	1042/1103 (94%)	1024 (98%)	18 (2%)	60	83
4	E	69/89 (78%)	68 (99%)	1 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	264/429 (62%)	262 (99%)	2 (1%)	81	92
6	J	93/97 (96%)	89 (96%)	4 (4%)	29	63
9	M	129/131 (98%)	129 (100%)	0	100	100
All	All	2920/3440 (85%)	2875 (98%)	45 (2%)	66	84

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	205	ARG
1	B	226	ASN
2	C	77	ARG
2	C	81	ASN
2	C	141	ASN
2	C	181	ARG
2	C	193	LYS
2	C	271	ASP
2	C	279	ARG
2	C	282	ARG
2	C	288	THR
2	C	293	GLN
2	C	295	LEU
2	C	296	LEU
2	C	419	ASN
2	C	466	GLU
2	C	584	ARG
2	C	787	ARG
2	C	958	ARG
3	D	5	ASN
3	D	37	ARG
3	D	140	ASP
3	D	209	ARG
3	D	239	ASN
3	D	285	LYS
3	D	386	ARG
3	D	387	ARG
3	D	416	ASN
3	D	418	LEU
3	D	499	ASN
3	D	656	TRP
3	D	733	MET

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Mol	Chain	Res	Type
3	D	741	ARG
3	D	797	ASN
3	D	1060	ARG
3	D	1097	ARG
3	D	1159	ARG
4	E	65	ASN
5	F	269	ARG
5	F	305	SER
6	J	4	ARG
6	J	27	ARG
6	J	76	LYS
6	J	110	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	124	HIS
1	B	79	ASN
1	B	226	ASN
2	C	81	ASN
2	C	141	ASN
2	C	143	ASN
2	C	150	GLN
2	C	232	GLN
2	C	419	ASN
2	C	435	GLN
2	C	685	ASN
2	C	875	GLN
2	C	891	ASN
2	C	920	HIS
2	C	930	GLN
2	C	1035	HIS
3	D	239	ASN
3	D	307	ASN
3	D	416	ASN
3	D	494	HIS
3	D	505	HIS
3	D	540	GLN
3	D	657	GLN
3	D	687	GLN
3	D	693	GLN

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Mol	Chain	Res	Type
3	D	767	HIS
3	D	797	ASN
3	D	1001	GLN
3	D	1139	GLN
3	D	1145	GLN
3	D	1251	ASN
4	E	65	ASN
5	F	388	GLN
5	F	425	GLN
5	F	494	GLN
5	F	516	HIS
9	M	14	HIS
9	M	102	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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
10	C0L	C	1201	-	36,38,38	2.64	13 (36%)	38,49,49	2.96	12 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	C0L	C	1201	-	-	20/38/57/57	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1201	C0L	O24-C23	8.59	1.39	1.21
10	C	1201	C0L	O19-C18	5.63	1.39	1.24
10	C	1201	C0L	C17-C16	4.61	1.50	1.39
10	C	1201	C0L	O36-C16	-4.53	1.18	1.33
10	C	1201	C0L	C17-C18	-4.06	1.35	1.45
10	C	1201	C0L	C13-C12	3.83	1.56	1.42
10	C	1201	C0L	C32-N31	3.68	1.43	1.37
10	C	1201	C0L	C20-C18	-3.66	1.34	1.44
10	C	1201	C0L	O34-C35	-3.04	1.38	1.45
10	C	1201	C0L	O34-C32	2.53	1.38	1.34
10	C	1201	C0L	C17-C23	-2.51	1.38	1.45
10	C	1201	C0L	O38-C08	-2.24	1.38	1.42
10	C	1201	C0L	O22-C23	-2.09	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	C0L	O34-C32-N31	10.50	120.28	109.16
10	C	1201	C0L	C23-O22-C21	-6.85	118.03	122.22
10	C	1201	C0L	C35-O34-C32	-6.17	108.38	115.66
10	C	1201	C0L	O36-C16-C17	4.90	128.90	119.87
10	C	1201	C0L	C13-C12-C11	-4.73	120.05	127.30
10	C	1201	C0L	O33-C32-N31	-4.37	119.36	125.41
10	C	1201	C0L	C23-C17-C18	4.27	121.98	119.41
10	C	1201	C0L	O34-C32-O33	-2.88	120.35	124.58
10	C	1201	C0L	C28-C27-C25	-2.70	109.25	114.39
10	C	1201	C0L	O19-C18-C17	-2.58	119.33	122.97
10	C	1201	C0L	C10-C09-C08	-2.21	111.44	114.46
10	C	1201	C0L	O22-C23-O24	2.15	119.07	115.20

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1201	C0L	C05-C06-C08-C09
10	C	1201	C0L	C07-C06-C08-C09
10	C	1201	C0L	C13-C14-C16-O36
10	C	1201	C0L	C15-C14-C16-O36
10	C	1201	C0L	C14-C16-C17-C18
10	C	1201	C0L	C14-C16-C17-C23
10	C	1201	C0L	O36-C16-C17-C18
10	C	1201	C0L	O36-C16-C17-C23
10	C	1201	C0L	C20-C21-C25-C26
10	C	1201	C0L	O22-C21-C25-C26
10	C	1201	C0L	O22-C21-C25-C27
10	C	1201	C0L	N31-C32-O34-C35
10	C	1201	C0L	O33-C32-O34-C35
10	C	1201	C0L	O34-C32-N31-C30
10	C	1201	C0L	C07-C06-C08-O38
10	C	1201	C0L	O33-C32-N31-C30
10	C	1201	C0L	C05-C06-C08-O38
10	C	1201	C0L	C02-C03-C04-C05
10	C	1201	C0L	C27-C28-C29-C30
10	C	1201	C0L	C06-C08-C09-C10

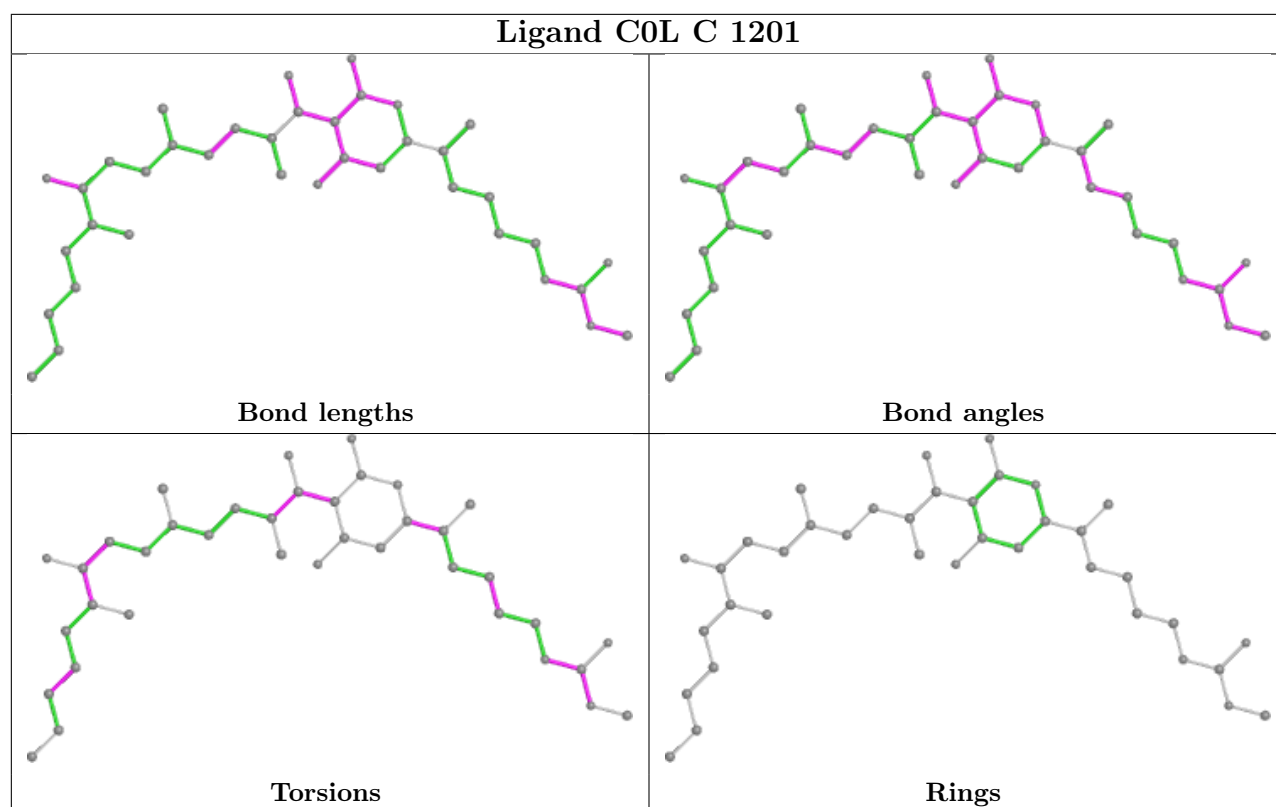
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1201	C0L	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

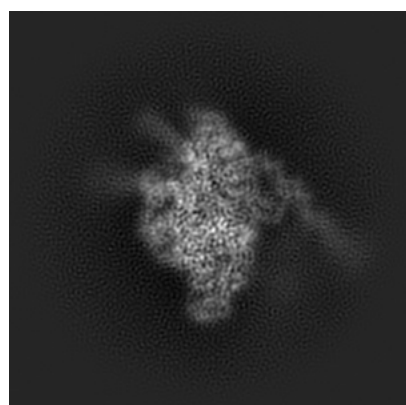
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9041. These allow visual inspection of the internal detail of the map and identification of artifacts.

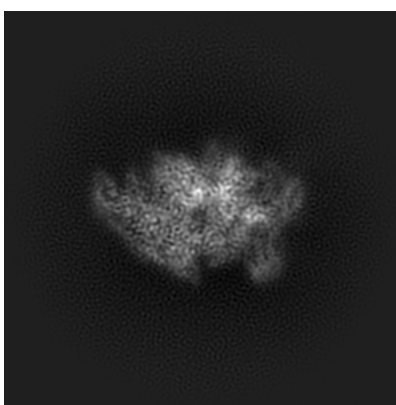
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

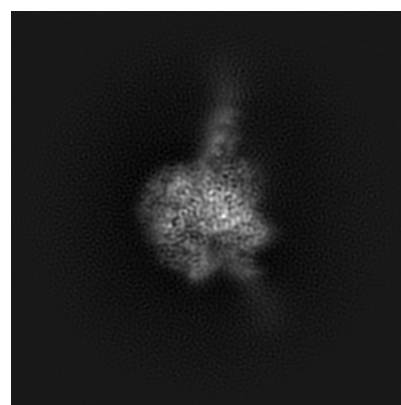
#### 6.1.1 Primary map



X



Y

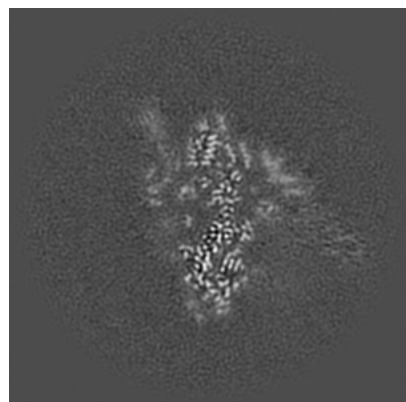


Z

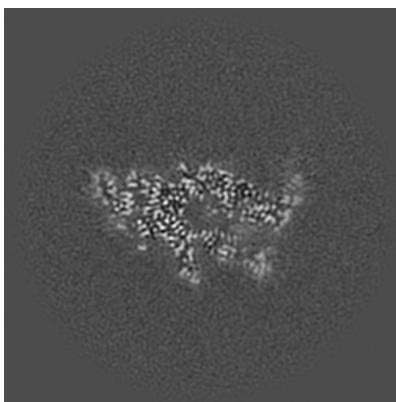
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

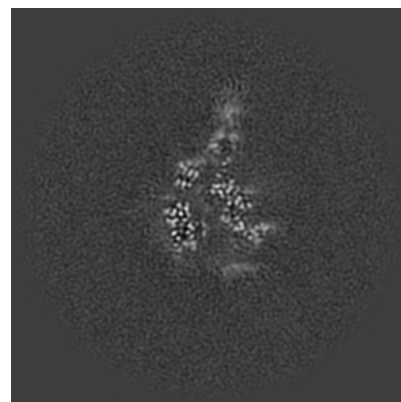
#### 6.2.1 Primary map



X Index: 125



Y Index: 125

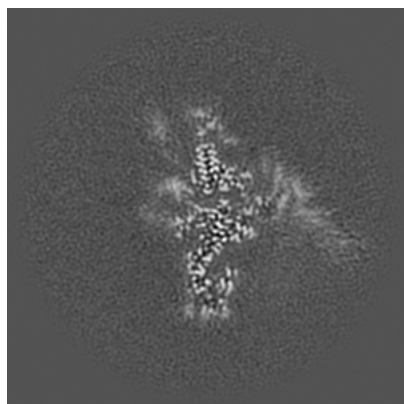


Z Index: 125

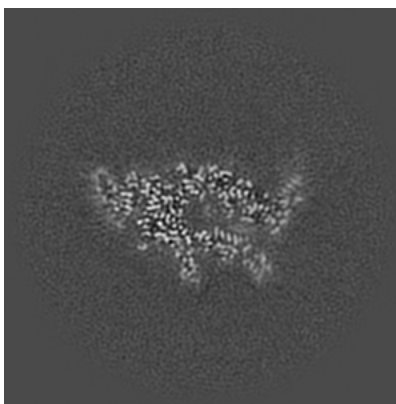
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

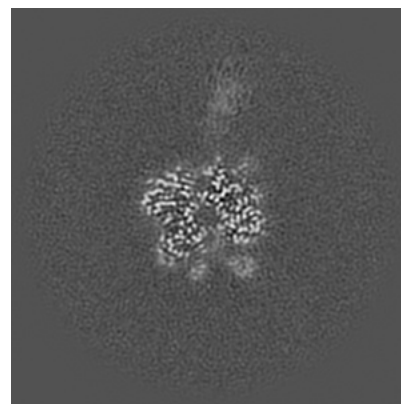
### 6.3.1 Primary map



X Index: 132



Y Index: 124

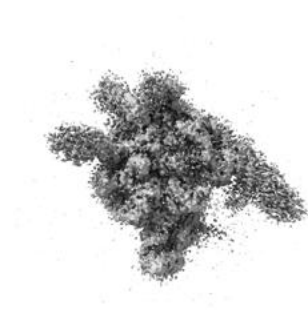


Z Index: 113

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

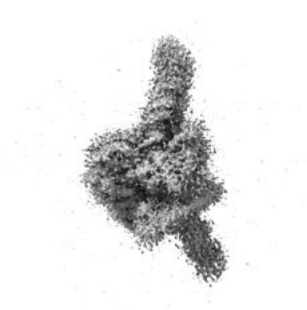
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

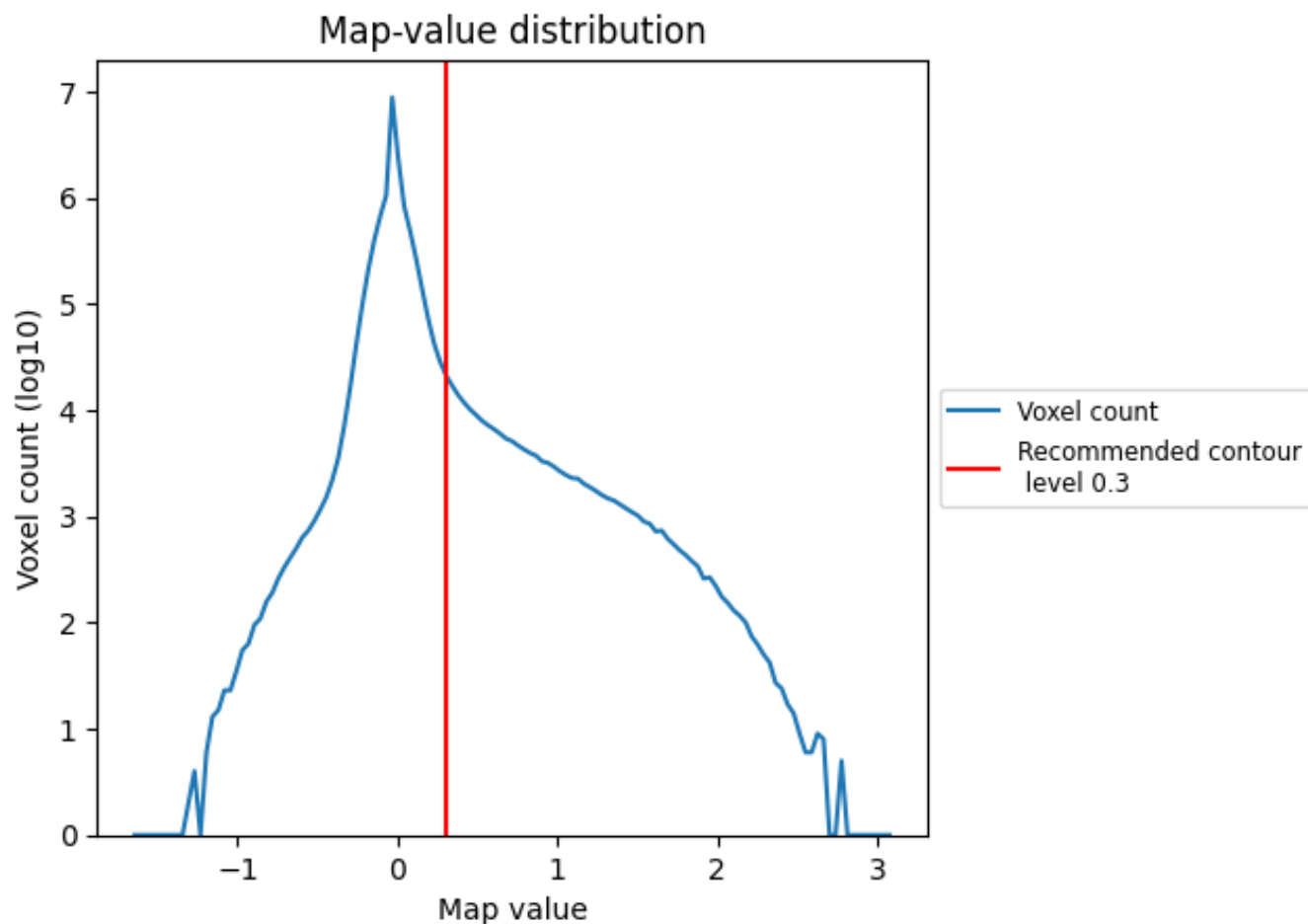
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

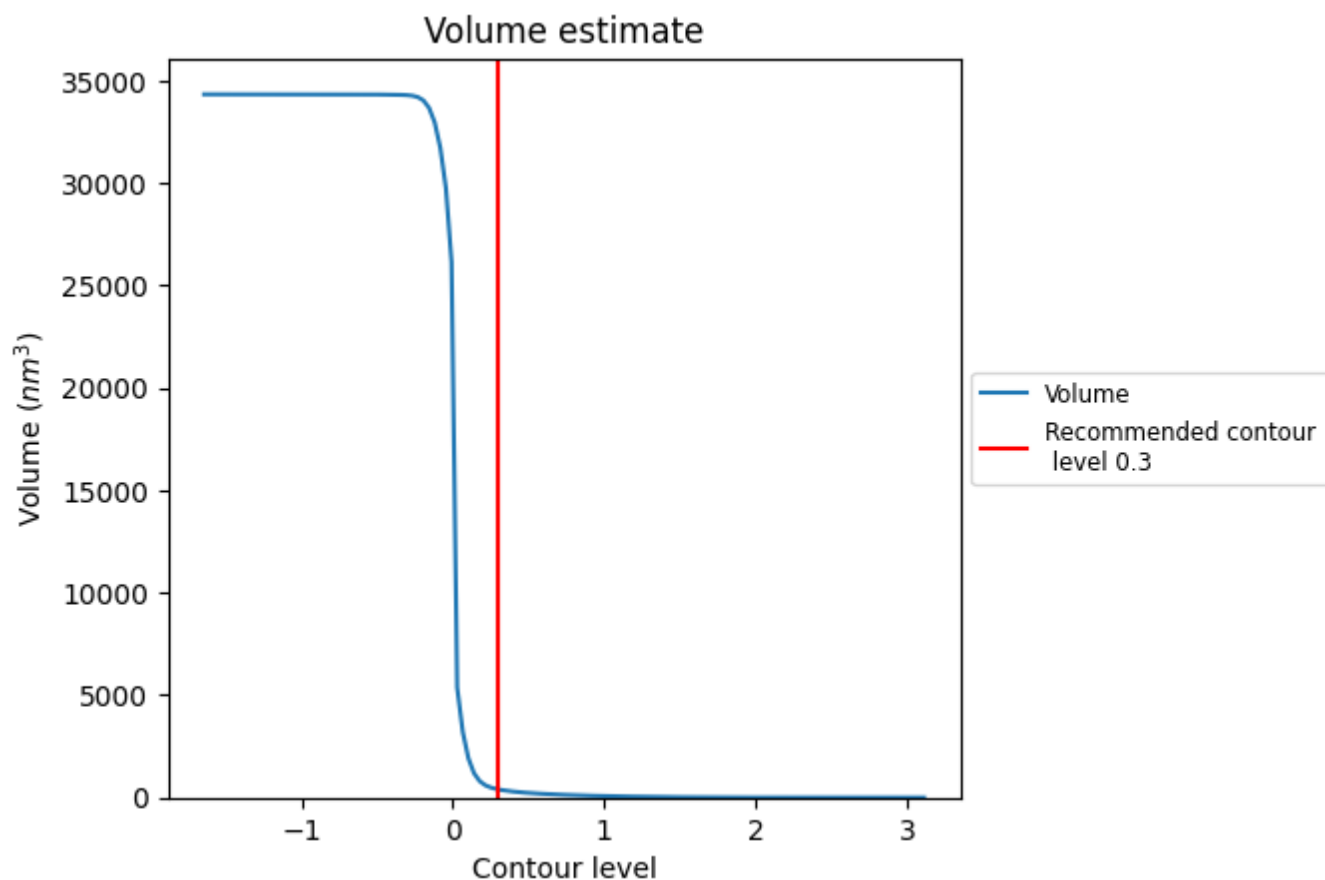
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

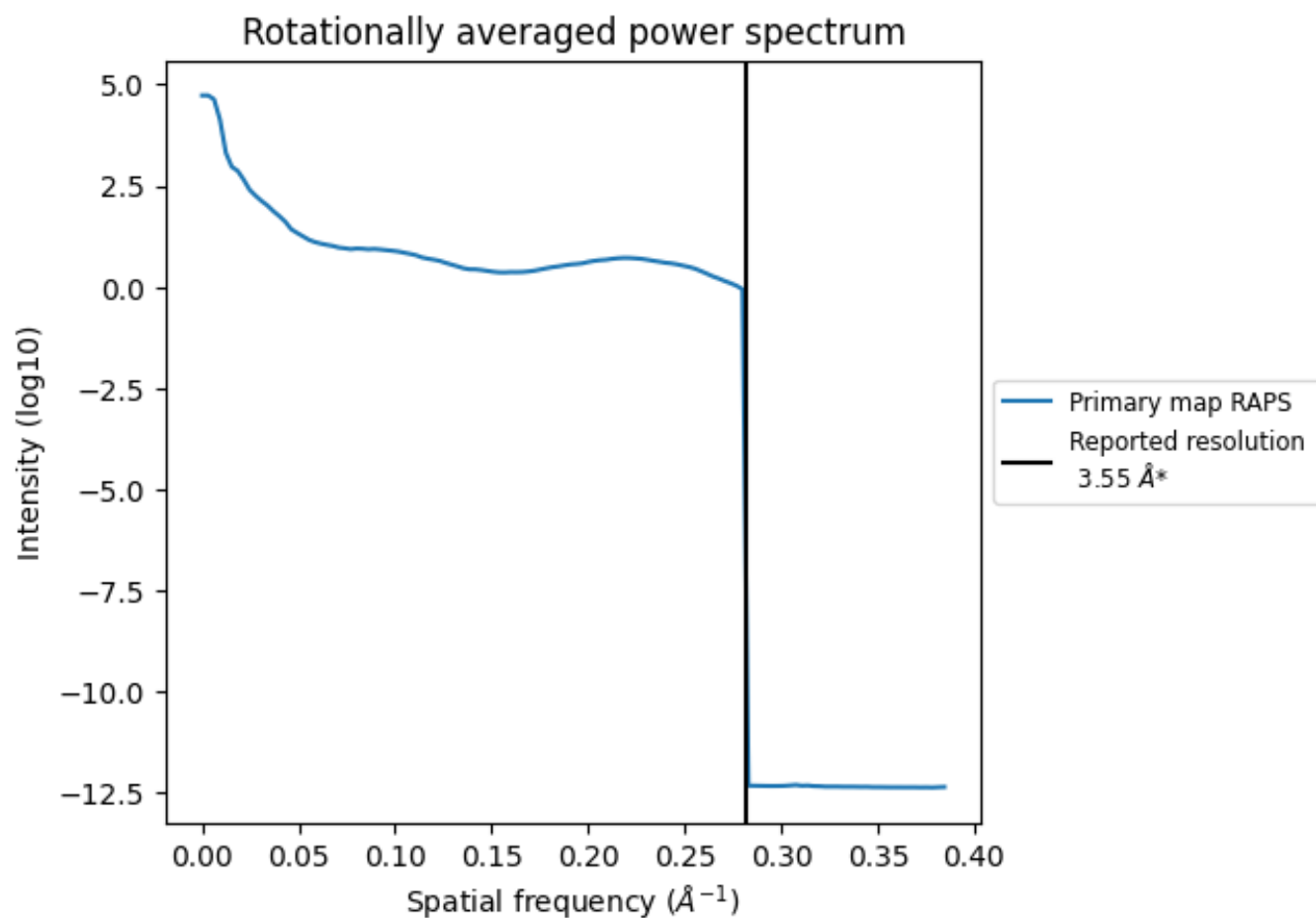
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm<sup>3</sup>; this corresponds to an approximate mass of 362 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.282 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

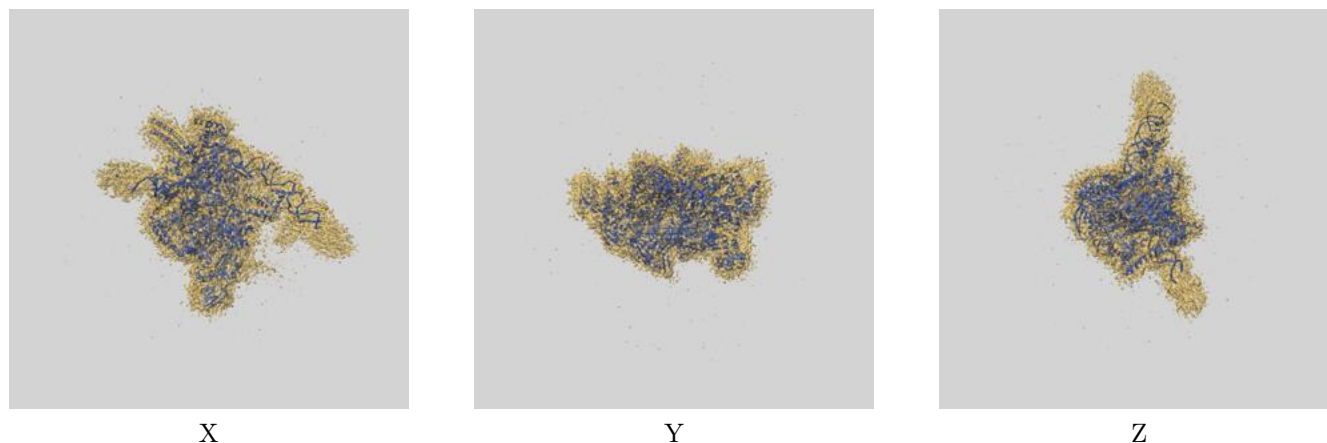
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9041 and PDB model 6EEC. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



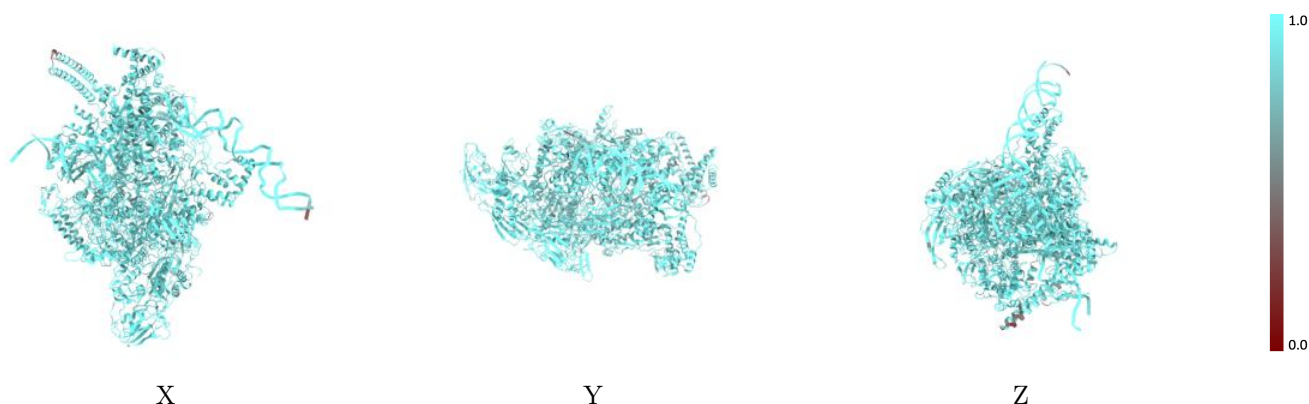
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



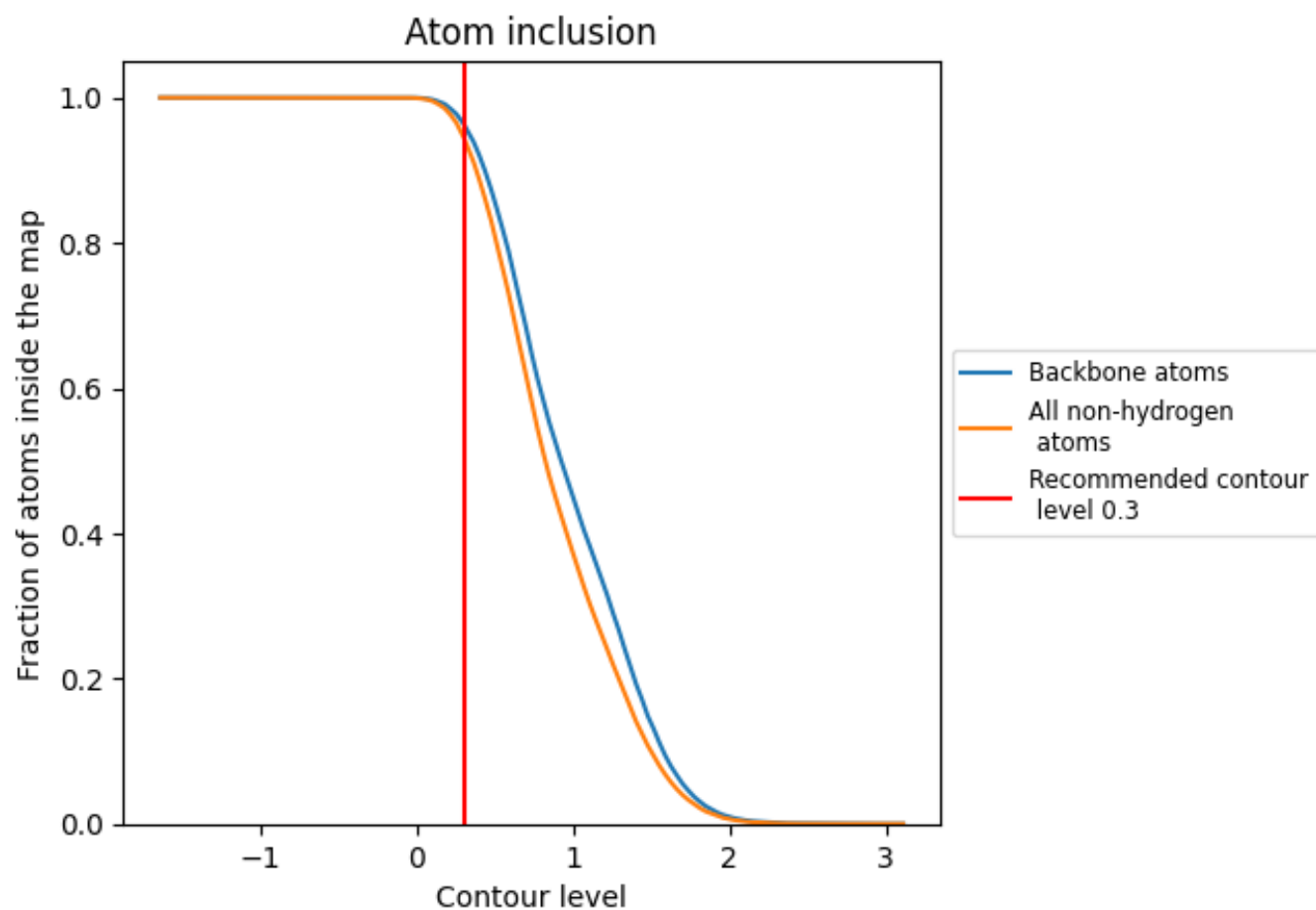
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9447	<div><div></div></div> 0.4480
A	<div><div></div></div> 0.9667	<div><div></div></div> 0.4860
B	<div><div></div></div> 0.9498	<div><div></div></div> 0.4650
C	<div><div></div></div> 0.9519	<div><div></div></div> 0.4860
D	<div><div></div></div> 0.9444	<div><div></div></div> 0.4640
E	<div><div></div></div> 0.9024	<div><div></div></div> 0.4470
F	<div><div></div></div> 0.9309	<div><div></div></div> 0.4170
J	<div><div></div></div> 0.9385	<div><div></div></div> 0.4170
M	<div><div></div></div> 0.9158	<div><div></div></div> 0.3740
O	<div><div></div></div> 0.9506	<div><div></div></div> 0.3070
P	<div><div></div></div> 0.9659	<div><div></div></div> 0.3020

1.0

0.0

<0.0