



Full wwPDB EM Validation Report ⓘ

Aug 28, 2025 – 03:15 PM EDT

PDB ID : 9CI3 / pdb_00009ci3
EMDB ID : EMD-45609
Title : Structure of the LRRK2/14-3-3 complex
Authors : Martinez Fiesco, J.A.; Zhang, P.
Deposited on : 2024-07-02
Resolution : 3.96 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

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>.

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

EMDB validation analysis : 0.0.1.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

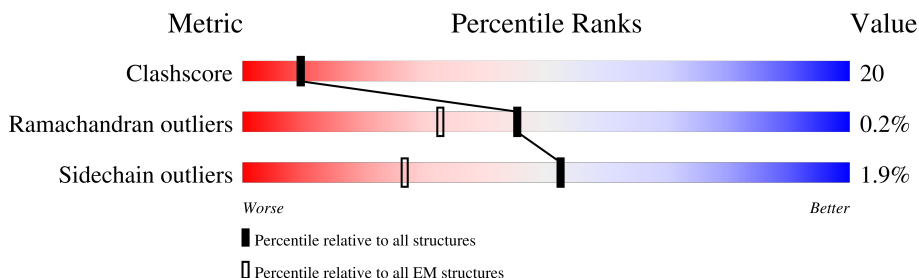
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.96 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	B	265	<div> <div>43%</div> <div>55%</div> <div>35%</div> <div>9%</div> </div>
1	C	265	<div> <div>32%</div> <div>54%</div> <div>34%</div> <div>• 11%</div> </div>
2	A	2562	<div> <div>28%</div> <div>36%</div> <div>23%</div> <div>• 41%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15926 atoms, of which 0 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 14-3-3 protein gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	237	Total	C	N	O	S	0	0
			1909	1190	325	384	10		
1	B	240	Total	C	N	O	S	0	0
			1935	1204	330	391	10		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	initiating methionine	UNP P61981
C	-16	GLY	-	expression tag	UNP P61981
C	-15	SER	-	expression tag	UNP P61981
C	-14	HIS	-	expression tag	UNP P61981
C	-13	HIS	-	expression tag	UNP P61981
C	-12	HIS	-	expression tag	UNP P61981
C	-11	HIS	-	expression tag	UNP P61981
C	-10	HIS	-	expression tag	UNP P61981
C	-9	HIS	-	expression tag	UNP P61981
C	-8	SER	-	expression tag	UNP P61981
C	-7	GLY	-	expression tag	UNP P61981
C	-6	GLU	-	expression tag	UNP P61981
C	-5	ASN	-	expression tag	UNP P61981
C	-4	LEU	-	expression tag	UNP P61981
C	-3	TYR	-	expression tag	UNP P61981
C	-2	PHE	-	expression tag	UNP P61981
C	-1	GLN	-	expression tag	UNP P61981
C	0	GLY	-	expression tag	UNP P61981
B	-17	MET	-	initiating methionine	UNP P61981
B	-16	GLY	-	expression tag	UNP P61981
B	-15	SER	-	expression tag	UNP P61981
B	-14	HIS	-	expression tag	UNP P61981
B	-13	HIS	-	expression tag	UNP P61981
B	-12	HIS	-	expression tag	UNP P61981
B	-11	HIS	-	expression tag	UNP P61981
B	-10	HIS	-	expression tag	UNP P61981

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P61981
B	-8	SER	-	expression tag	UNP P61981
B	-7	GLY	-	expression tag	UNP P61981
B	-6	GLU	-	expression tag	UNP P61981
B	-5	ASN	-	expression tag	UNP P61981
B	-4	LEU	-	expression tag	UNP P61981
B	-3	TYR	-	expression tag	UNP P61981
B	-2	PHE	-	expression tag	UNP P61981
B	-1	GLN	-	expression tag	UNP P61981
B	0	GLY	-	expression tag	UNP P61981

- Molecule 2 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	1521	Total	C	N	O	P	S	0	0
			12054	7711	2074	2197	2	70		

There are 36 discrepancies between the modelled and reference sequences:

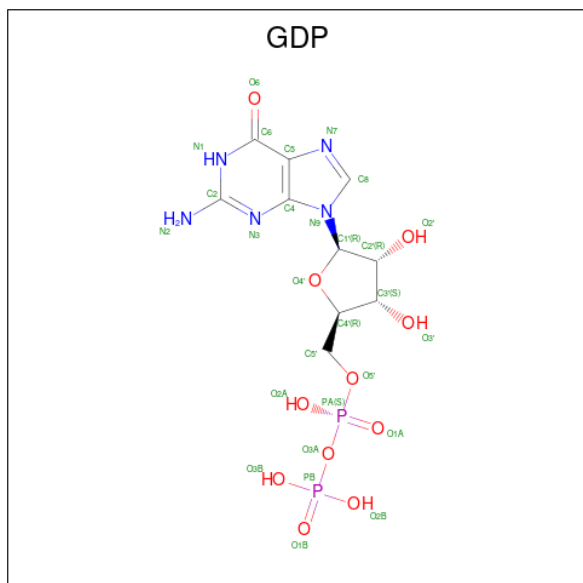
Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP Q5S007
A	-33	GLY	-	expression tag	UNP Q5S007
A	-32	SER	-	expression tag	UNP Q5S007
A	-31	ASP	-	expression tag	UNP Q5S007
A	-30	TYR	-	expression tag	UNP Q5S007
A	-29	LYS	-	expression tag	UNP Q5S007
A	-28	ASP	-	expression tag	UNP Q5S007
A	-27	HIS	-	expression tag	UNP Q5S007
A	-26	ASP	-	expression tag	UNP Q5S007
A	-25	GLY	-	expression tag	UNP Q5S007
A	-24	ASP	-	expression tag	UNP Q5S007
A	-23	TYR	-	expression tag	UNP Q5S007
A	-22	LYS	-	expression tag	UNP Q5S007
A	-21	ASP	-	expression tag	UNP Q5S007
A	-20	HIS	-	expression tag	UNP Q5S007
A	-19	ASP	-	expression tag	UNP Q5S007
A	-18	ILE	-	expression tag	UNP Q5S007
A	-17	ASP	-	expression tag	UNP Q5S007
A	-16	TYR	-	expression tag	UNP Q5S007
A	-15	LYS	-	expression tag	UNP Q5S007
A	-14	ASP	-	expression tag	UNP Q5S007
A	-13	ASP	-	expression tag	UNP Q5S007

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ASP	-	expression tag	UNP Q5S007
A	-11	ASP	-	expression tag	UNP Q5S007
A	-10	LYS	-	expression tag	UNP Q5S007
A	-9	LEU	-	expression tag	UNP Q5S007
A	-8	GLY	-	expression tag	UNP Q5S007
A	-7	LEU	-	expression tag	UNP Q5S007
A	-6	GLU	-	expression tag	UNP Q5S007
A	-5	VAL	-	expression tag	UNP Q5S007
A	-4	LEU	-	expression tag	UNP Q5S007
A	-3	PHE	-	expression tag	UNP Q5S007
A	-2	GLN	-	expression tag	UNP Q5S007
A	-1	GLY	-	expression tag	UNP Q5S007
A	0	PRO	-	expression tag	UNP Q5S007
A	50	HIS	ARG	variant	UNP Q5S007

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



T1912	D1844	L1749	D1675	I1606	S1536	GLN	W1376	F1308	L1243	M1183	N1117	F1050
S1913	H1845	V1750	H1676	M1607	E1537	ARG	P1377	K1309	W1244	K1184	K1118	P1051
L1914	P1846	H1768	R1677	A1608	R1538	K1463	I1378	H1310	S1245	F1185	I1119	S1052
R1915	R1847	L1763	I1680	I1611	K1539	K1468	R1381	I1311	R1246	S1186	G1121	Y1053
L1916		K1764	E1681	V1615	I1543	L1474	D1382	G1312	K1249	I1188	L1122	L1055
R1917		V1767	P1683	E1616	F1544	K1476	K1383	K1313	L1250	P1189	C1123	M1056
R1918		R1771	H1684	G1617	F1545	R1477	R1385	K1314	H1251	A1190		M1057
Q1919		R1772	C1685	C1618	I1548	P1480	D1386	K1316	L1252	E1191		S1058
E1920		I1775	H1686	C1619	D1549	L1481	D1387	K1317	K1257	I1192		C1059
L1921		L1776	R1687	P1619	R1550	I1482	L1388	D1317	L1259	L1193		C1059
V1922		L1777	S1688	K1620	K1551	E1483	V1389	I1319	K1258	N1194		I1060
V1923		E1689	R1552	H1621	R1552	Y1485	V1392	F1320	I1260	L1195		A1061
L1924		R1693	Q1555	P1622	Q1555	V1488	F1395	L1322	I1260	P1196		N1062
C1925		L1694	L1556	K1623	L1556	N1488		Q1323	E1263	H1197		S1066
L1926		I1625	V1557	G1624	V1557	N1489	F1401	Q1324	I1264	L1198		R1067
H1927		E1632	E1558	I1625	E1558	A1490	Y1402	R1325	L1136	S1137		N1068
H1928		K1633	E1559	I1625	E1559	T1491	S1403	L1326	G1205	R1199		
H1929		F1634	M1560	I1625	E1560	E1492	T1404	L1327	C1266	S1200		G1071
P1930		L1635	Q1561	S1636	Q1561	E1493	H1405	K1328	L1267	M1203		P1072
S1931		S1637	Q1563	L1637	Q1563	L1497	H1407	A1329	E1288	D1202		S1073
L1932		LVS	L1574	LVS	L1574	A1498	F1408	V1330	N1269	S1204		V1074
L1933		N1644	F1575	N1644	F1575	K1499	M1409	G1341	L1270	S1205		V1075
S1934		M1645	L1576	M1645	L1576	L1500	Y1415	N1278	L1144	N1206		L1076
L1935		S1647	S1579	S1647	S1579	K1512	Y1416	P1214	S1145	D1207		D1077
G1939		Q1648	V1581	Q1648	V1581	I1513	L1416	K1218	E1146	L1208		P1078
R1940		GLY	L1582	GLY	L1582		A1417	S1219	N1147	Q1209		T1079
P1942		ARG	L1583	ARG	L1583		V1418	M1221	F1148	Y1210		V1080
R1943		ARG	H1584	ARG	H1584			L1222	L1149	L1211		K1081
M1944		ARG	F1585	ARG	F1585			L1225	E1150	G1213		C1082
M1945		ARG	Q1586	ARG	Q1586			L1226	P1153	P1214		P1083
V1946		ARG	Q1586	ARG	Q1586			L1227	L1085	A1215		T1084
M1947		ARG	D1587	ARG	D1587			L1228	K1154	H1216		L1085
L1948		ARG	P1588	ARG	P1588			L1229	V1155	W1217		K1086
E1949		ARG	A1589	ARG	A1589			L1230	E1156	S1157		Q1087
A1950		ARG	L1590	ARG	L1590			L1231	F1158	S1159		F1088
L1955		ARG	Q1591	ARG	Q1591			L1232	S1157	S1159		S1091
D1956		ARG	L1592	ARG	L1592			L1233	A1160	M1161		Y1092
R1957		ARG	L1593	ARG	L1593			L1234	R1161	A1160		M1093
L1958		ARG	D1594	ARG	D1594			L1235	M1162	R1163		Q1094
R1959		ARG	L1595	ARG	L1595			L1236	L1171	L1171		L1095
L1960		ARG	Y1596	ARG	Y1596			L1237	P1172	F1165		S1096
Q1961		ARG	F1597	ARG	F1597			L1238	L1168	P1227		F1097
D1962		ARG	V1598	ARG	V1598			L1239	M1169	L1228		E1100
L1963		ARG	E1599	ARG	E1599			L1240	P1173	H1229		N1101
A1964		ARG	V1602	ARG	V1602			L1241	F1170	Q1231		L1102
S1965		ARG	L1603	ARG	L1603			L1242	M1175	M1230		L1103
L1966		ARG		ARG				L1243	L1177	Q1231		T1103
T1967		ARG		ARG				L1244	L1171	L1232		D1104
R1968		ARG		ARG				L1245	P1172	S1233		V1105
		ARG		ARG				L1246	P1173	I1234		V1106
Q1971		ARG		ARG				L1247	P1173	L1235		E1107
H1972		ARG		ARG				L1248	P1173	D1236		L1108
R1973		ARG		ARG				L1249	P1173	L1237		K1109
T1974		ARG		ARG				L1250	P1173	L1238		L1109
A1975		ARG		ARG				L1251	P1173	L1239		E1110
L1976		ARG		ARG				L1252	P1173	L1240		L1114
H1977		ARG		ARG				L1253	P1173	L1241		E1115

L2493	T2494	V2495	W2496	D2497	L2498	N2499	L2500	P2501	H2502	E2503	V2504	Q2505	N2506	L2507	E2508	K2509	H2510	L2511	E2512	V2513	L2514	K2515	E2516	L2517	A2518	E2519	K2520	H2521	R2522	R2523	T2524	S2525	V2526	E2527																									
H2433	L2434	L2435	L2436	L2437	D2438	L2439	S2440	T2441	R2442	L2443	L2444	L2445	R2446	V2447	L2448	Y2449	N2450	N2453	S2454	V2455	R2456	V2457	L2458	N2459	T2460	A2461	Q2462	L2463	Q2464	S2465	L2466	K2467	N2468	N2469	M2470	L2471	V2472	L2473	G2474	Y2475	N2476	R2477	K2478	ASN	THR	GLU	GLY	THR	GLN	LYS	E2488	L2489	Q2490	S2491	C2492				
Y2364	I2365	A2366	K2367	Q2368	N2369	S2370	W2376	D2377	K2378	K2379	T2380	E2381	L2382	L2383	C2384	G2385	L2386	C2389	V2390	L2393	R2394	E2395	V2396	M2397	VAL	LYS	GLU	ASN	LYS	GLU	SER	HIS	LYS	MET	SER	TYR	S2411	G2412	R2413	V2414	K2415	T2416	L2419	Q2420	THR	GLN	LYS	N2422	T2423	A2424	L2425	W2426	L2427	G2428	T2429	Q2430			
C2302	L2303	S2304	E2305	S2306	T2307	N2308	S2309	T2310	E2311	R2312	N2313	V2314	N2315	W2316	G2317	Q2318	C2319	G2320	T2321	F2324	S2325	F2326	S2327	N2328	D2329	F2330	T2331	L2332	Q2333	K2334	L2335	L2336	E2337	T2338	R2339	T2340	S2341	Q2342	L2343	F2344	S2345	W2346	A2347	A2348	F2349	S2350	D2351	S2352	N2353	T2354	T2355	T2356	W2357	D2360	T2361	A2362	L2363		
K2240	M2241	T2242	D2243	S2244	V2245	T2246	C2247	N2251	S2252	F2253	S2254	K2255	Q2256	S2257	K2258	Q2259	K2260	N2261	F2262	L2263	L2264	V2265	G2266	T2267	A2268	D2269	G2270	K2271	L2272	A2273	L2274	F2275	E2276	D2277	K2278	T2279	V2280	K2281	L2282	K2283	G2284	A2285	A2286	P2287	L2288	K2289	L2290	L2291	N2292	L2293	G2294	N2295	V2296	S2297	T2298	P2299	L2300	M2301	
L2179	L2182	D2183	L2184	N2185	T2186	E2187	G2188	Y2189	T2190	S2191	E2192	E2193	V2194	A2195	D2196	S2197	R2198	T2199	L2200	C2201	L2202	A2203	L2204	V2205	H2206	L2207	P2208	V2209	E2210	K2211	E2212	S2213	W2214	L2215	V2216	S2217	G2218	T2219	Q2220	S2221	G2222	T2223	L2224	L2225	V2226	T2227	N2228	K2229	T2229	E2230	D2231	G2232	K2233	K2234	R2235	H2236	T2237	L2238	E2239
L2115	K2116	E2117	N2118	P2119	Q2120	E2121	R2122	P2123	T2124	S2125	A2126	Q2127	V2128	F2129	D2130	L2131	L2132	N2133	E2136	L2137	V2138	C2139	L2140	T2141	R2142	L2143	L2144	L2145	L2146	P2147	K2148	N2149	V2150	L2151	L2152	E2153	T2158	H2159	H2160	N2161	S2162	R2163	N2164	A2165	S2166	T2167	W2168	L2169	G2170	C2171	G2172	H2173	T2174	R2175	R2176	G2177	Q2178		
V2048	I2049	Y2050	N2051	Q2052	Q2053	A2054	D2055	V2056	Y2057	S2058	F2059	G2060	L2061	L2062	L2067	G2071	R2072	I2073	V2074	E2075	G2076	L2077	K2078	F2079	P2080	N2081	E2082	F2083	D2084	E2085	L2086	E2087	I2088	Q2089	G2090	K2091	L2092	P2093	V2096	K2097	E2098	Y2099	G2100	C2101	A2102	P2105	M2106	V2107	E2108	K2109	L2110	I2111	K2112	Q2113	C2114				
V1978	A1979	D1980	R1983	H1986	S1987	I1991	Y1992	R1993	D1994	L1995	K1996	L2001	L2002	P2007	N2008	A2009	I2010	I2011	I2012	K2013	K2014	L2015	A2016	D2017	V2018	G2019	I2020	A2021	Q2022	Y2023	C2024	C2025	R2026	N2027	GLY	ILE	LYS	T2031	S2032	E2033	G2034	T2035	P2036	G2037	F2038	R2039	A2040	P2041	E2042	V2043	A2044	R2045	G2046	N2047					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.360	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.122	Depositor
Map size (Å)	325.62, 325.62, 325.62	wwPDB
Map dimensions	402, 402, 402	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.17	0/1963	0.46	0/2648
1	C	0.17	0/1937	0.43	0/2613
2	A	0.19	0/12271	0.46	6/16603 (0.0%)
All	All	0.18	0/16171	0.46	6/21864 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	938	PRO	CA-N-CD	-9.96	98.06	112.00
2	A	938	PRO	CB-CA-C	7.04	123.18	111.56
2	A	938	PRO	N-CA-CB	-6.67	96.25	103.25
2	A	2142	ARG	N-CA-C	6.30	116.77	107.88
2	A	2500	LEU	N-CA-C	5.83	122.68	109.81
2	A	1425	GLN	CA-CB-CG	5.14	124.39	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2142	ARG	Sidechain

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	B	1935	0	1898	84	0
1	C	1909	0	1878	82	0
2	A	12054	0	12234	475	0
3	A	28	0	12	0	0
All	All	15926	0	16022	626	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 20.

All (626) 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:A:1240:LYS:HD2	2:A:1243:LEU:HD22	1.54	0.90
1:C:225:LEU:O	1:C:229:ASN:ND2	2.08	0.87
2:A:1437:ASN:HD21	2:A:1702:MET:HE3	1.37	0.86
1:C:57:ARG:NH2	2:A:935:SEP:O2P	2.11	0.84
2:A:2456:ARG:NH1	2:A:2475:TYR:OH	2.11	0.83
2:A:1161:ARG:HH21	2:A:1181:SER:H	1.28	0.81
2:A:2241:MET:HE3	2:A:2243:ASP:H	1.45	0.80
2:A:2460:THR:HA	2:A:2470:MET:HA	1.63	0.79
2:A:1068:ASN:O	2:A:1093:ASN:ND2	2.15	0.79
1:C:227:ARG:NH2	2:A:1728:ARG:O	2.17	0.78
2:A:2146:LEU:HD12	2:A:2147:PRO:HD2	1.63	0.78
2:A:1701:PRO:HG2	2:A:1704:PHE:HB2	1.65	0.76
2:A:1341:GLY:O	2:A:1434:TRP:NE1	2.18	0.76
2:A:1439:LYS:HB2	2:A:1480:PRO:HD3	1.68	0.76
2:A:1767:VAL:HG21	2:A:1777:LEU:HB2	1.67	0.76
1:C:54:GLY:HA2	1:C:57:ARG:HD3	1.68	0.76
2:A:1119:ILE:HB	2:A:1139:ASN:HD21	1.50	0.76
1:C:165:MET:O	1:C:172:ARG:NH1	2.19	0.75
2:A:1115:GLU:HB2	2:A:1137:SER:HB3	1.68	0.75
2:A:1246:ARG:H	2:A:1246:ARG:HD3	1.52	0.75
1:B:161:SER:HA	1:B:165:MET:HG2	1.69	0.74
1:B:132:ARG:NH1	1:B:154:TYR:OH	2.18	0.74
2:A:1858:ASP:HB2	2:A:1918:ARG:HH12	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2499:ASN:C	2:A:2501:PRO:HD2	2.13	0.73
1:B:117:TYR:HB3	1:B:165:MET:HE1	1.69	0.72
1:C:86:ARG:NH2	1:C:90:GLU:OE2	2.21	0.72
1:C:88:LYS:NZ	1:B:22:ASP:OD2	2.22	0.72
2:A:2251:ASN:HD21	2:A:2262:PHE:HB2	1.55	0.71
2:A:1353:GLN:HE22	2:A:1492:GLU:HA	1.56	0.71
2:A:1866:ARG:HA	2:A:1869:MET:HE3	1.73	0.70
2:A:1076:LEU:HD22	2:A:1105:VAL:HG21	1.72	0.70
2:A:1076:LEU:HB3	2:A:1101:ASN:HB2	1.74	0.70
2:A:1437:ASN:ND2	2:A:1702:MET:HE3	2.06	0.70
2:A:2355:ILE:HG22	2:A:2356:THR:HG23	1.74	0.70
1:C:213:GLU:O	1:C:217:LYS:NZ	2.23	0.70
1:B:164:HIS:ND1	1:B:165:MET:SD	2.64	0.69
2:A:1433:PRO:O	2:A:1437:ASN:ND2	2.20	0.69
2:A:2106:MET:HE1	2:A:2137:LEU:HB2	1.75	0.69
1:C:142:LYS:O	1:C:146:VAL:HG23	1.93	0.68
2:A:2271:LYS:HA	2:A:2292:ASN:HA	1.75	0.68
2:A:1610:ILE:HG13	2:A:1611:LEU:HD12	1.75	0.68
1:B:170:PRO:HA	1:B:173:LEU:HD12	1.77	0.67
2:A:1584:HIS:ND1	2:A:1586:GLN:OE1	2.27	0.67
1:B:124:LEU:HD13	1:B:127:LYS:HD3	1.76	0.67
1:B:27:MET:SD	1:B:27:MET:N	2.69	0.66
2:A:2224:LEU:HB2	2:A:2238:LEU:HB2	1.76	0.66
1:B:156:GLU:O	1:B:160:ILE:HG12	1.96	0.66
1:C:217:LYS:HA	1:C:220:THR:HG22	1.78	0.66
2:A:1315:ALA:HA	2:A:1318:ILE:HD12	1.77	0.66
2:A:1703:GLY:O	2:A:1707:ARG:NH1	2.28	0.66
2:A:1222:LEU:H	2:A:1246:ARG:HH21	1.43	0.66
2:A:1243:LEU:O	2:A:1246:ARG:NH1	2.27	0.66
1:C:124:LEU:HD23	1:C:127:LYS:HD3	1.77	0.65
2:A:1386:ARG:HH12	2:A:1519:VAL:HG13	1.61	0.65
2:A:2139:CYS:SG	2:A:2500:LEU:HB3	2.36	0.65
2:A:1137:SER:HA	2:A:1161:ARG:H	1.60	0.65
1:B:221:LEU:HA	1:B:224:GLN:HE22	1.62	0.65
2:A:1270:LEU:HD21	2:A:1273:LEU:HD13	1.79	0.65
1:C:134:LEU:HB2	1:C:146:VAL:HG11	1.78	0.65
1:B:143:ARG:O	1:B:147:VAL:HG12	1.97	0.65
2:A:1338:MET:HE1	2:A:1409:MET:HA	1.77	0.65
2:A:2140:LEU:HB2	2:A:2496:TRP:CE3	2.32	0.64
2:A:1776:LEU:O	2:A:1780:VAL:HG12	1.98	0.64
2:A:1095:LEU:HD23	2:A:1119:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2213:SER:O	2:A:2229:THR:OG1	2.16	0.63
1:B:123:TYR:HA	1:B:126:MET:HE3	1.80	0.63
2:A:2216:VAL:HG12	2:A:2226:VAL:HG22	1.81	0.63
2:A:1316:LYS:NZ	2:A:2045:ARG:O	2.31	0.63
1:B:177:LEU:HD11	1:B:222:ILE:HG23	1.80	0.63
2:A:987:LEU:HD22	2:A:1013:LEU:HD11	1.79	0.63
2:A:1138:LYS:N	2:A:1161:ARG:O	2.26	0.63
2:A:1492:GLU:N	2:A:1492:GLU:OE1	2.31	0.63
2:A:1230:ASN:HD21	2:A:1232:ILE:HD12	1.64	0.63
2:A:2507:LEU:O	2:A:2511:ILE:HG12	1.98	0.63
2:A:1168:MET:HB3	2:A:1171:LEU:HD23	1.78	0.63
2:A:2082:GLU:HA	2:A:2085:GLU:HG2	1.81	0.63
1:C:205:ILE:HA	1:C:208:LEU:HD23	1.80	0.62
2:A:1076:LEU:O	2:A:1101:ASN:ND2	2.19	0.62
2:A:992:ASN:O	2:A:1021:ASN:ND2	2.32	0.62
1:B:216:TYR:O	1:B:220:THR:HG23	1.99	0.62
2:A:1406:PRO:HG2	2:A:1703:GLY:HA3	1.80	0.62
2:A:1449:LEU:HD11	2:A:1482:ILE:HD13	1.82	0.62
2:A:1155:VAL:HB	2:A:1175:MET:HE1	1.82	0.61
2:A:1864:LEU:HD11	2:A:1922:VAL:HA	1.82	0.61
2:A:1876:GLU:HB3	2:A:1897:ALA:HB3	1.81	0.61
2:A:1940:ILE:HG13	2:A:1941:ARG:H	1.65	0.61
2:A:1944:MET:SD	2:A:1944:MET:N	2.73	0.61
2:A:2116:LYS:O	2:A:2122:ARG:NH1	2.30	0.61
2:A:2299:PRO:O	2:A:2320:GLY:N	2.31	0.61
1:C:12:ARG:O	1:C:15:GLU:HG3	2.00	0.61
2:A:1195:LEU:HD12	2:A:1198:LEU:HD12	1.83	0.61
1:B:92:GLU:O	1:B:96:VAL:HG23	2.00	0.61
2:A:1552:ARG:HH12	2:A:1556:LEU:HG	1.65	0.61
2:A:2474:GLY:O	2:A:2492:CYS:N	2.33	0.61
2:A:2177:GLY:HA3	2:A:2195:ALA:HB3	1.82	0.60
1:B:201:PHE:O	1:B:205:ILE:HG12	2.01	0.60
2:A:1693:ARG:HD3	2:A:1777:LEU:HD11	1.83	0.60
2:A:1955:LEU:HG	2:A:1959:LEU:HD23	1.83	0.60
1:B:78:LYS:HA	1:B:81:MET:HE2	1.84	0.60
2:A:990:SER:O	2:A:1021:ASN:ND2	2.34	0.60
2:A:2301:MET:SD	2:A:2301:MET:N	2.74	0.60
2:A:2311:GLU:HG3	2:A:2314:VAL:HG12	1.83	0.60
2:A:1918:ARG:HA	2:A:1921:LEU:HG	1.84	0.60
2:A:1931:SER:HB3	2:A:2514:ARG:HH22	1.66	0.60
2:A:1680:ILE:HD11	2:A:1732:MET:HE1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LYS:O	1:B:81:MET:HG3	2.02	0.60
2:A:1552:ARG:NH1	2:A:1555:GLN:OE1	2.35	0.60
2:A:1879:GLN:HG2	2:A:1894:TYR:HE2	1.67	0.60
2:A:2420:GLN:HG2	2:A:2421:LYS:H	1.67	0.60
2:A:1994:ASP:OD1	2:A:1996:LYS:NZ	2.35	0.59
1:C:143:ARG:O	1:C:147:VAL:HG13	2.02	0.59
2:A:1134:LEU:HB3	2:A:1158:PHE:HD1	1.65	0.59
2:A:1270:LEU:HB3	2:A:1291:LEU:HD11	1.85	0.59
2:A:1434:TRP:O	2:A:1438:ILE:HG12	2.03	0.59
1:C:169:HIS:ND1	1:C:171:ILE:HG12	2.18	0.59
2:A:1739:TYR:HB2	2:A:1749:LEU:HD13	1.83	0.59
1:B:43:ASN:O	1:B:47:VAL:HG12	2.02	0.59
2:A:1188:ILE:HD11	2:A:1212:PRO:HD2	1.84	0.59
2:A:1622:PRO:HG2	2:A:1625:ILE:HD12	1.84	0.59
2:A:1116:GLY:HA2	2:A:1138:LYS:HB2	1.83	0.59
2:A:1659:ALA:HB1	2:A:1669:VAL:HG22	1.83	0.59
2:A:2288:LEU:HB3	2:A:2289:LYS:HD2	1.85	0.59
1:C:50:LYS:NZ	2:A:938:PRO:HG2	2.17	0.59
1:B:152:LYS:NZ	1:B:156:GLU:OE1	2.34	0.58
1:B:70:THR:HB	1:B:78:LYS:HE2	1.85	0.58
2:A:1093:ASN:N	2:A:1117:ASN:OD1	2.31	0.58
2:A:1694:LEU:HB2	2:A:1811:TRP:HB2	1.86	0.58
2:A:1092:TYR:OH	2:A:1138:LYS:NZ	2.30	0.58
1:B:49:TYR:HA	1:B:52:VAL:HG22	1.85	0.58
2:A:1031:CYS:HB2	2:A:1057:MET:HE1	1.84	0.58
2:A:1226:LEU:HD13	2:A:1251:HIS:HB2	1.84	0.58
2:A:2151:ILE:O	2:A:2172:GLY:N	2.35	0.58
2:A:2326:PHE:HA	2:A:2333:GLN:HG2	1.86	0.58
2:A:1224:GLU:HG2	2:A:1249:LYS:HD3	1.86	0.58
2:A:2241:MET:HE3	2:A:2243:ASP:N	2.18	0.58
2:A:1610:ILE:HD13	2:A:1653:LEU:HD21	1.86	0.58
1:B:123:TYR:HD1	1:B:126:MET:HE1	1.69	0.57
1:B:217:LYS:O	1:B:221:LEU:HG	2.04	0.57
2:A:1045:ASN:O	2:A:1068:ASN:ND2	2.36	0.57
2:A:1386:ARG:NH1	2:A:1519:VAL:O	2.36	0.57
2:A:2499:ASN:O	2:A:2501:PRO:HD2	2.04	0.57
1:B:160:ILE:HA	1:B:163:GLU:HG2	1.86	0.57
2:A:1177:ILE:HD11	2:A:1199:ARG:HE	1.70	0.57
1:C:128:GLY:O	1:C:132:ARG:HG2	2.05	0.57
1:B:213:GLU:HA	1:B:216:TYR:HB3	1.86	0.57
2:A:1702:MET:HE2	2:A:1702:MET:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2228:ASN:OD1	2:A:2229:THR:N	2.37	0.57
1:B:191:GLU:O	1:B:195:HIS:ND1	2.30	0.57
2:A:1260:ILE:HG12	2:A:1281:LEU:HD11	1.85	0.57
2:A:1324:GLN:C	2:A:1524:PRO:HB3	2.29	0.57
2:A:1851:PRO:HG2	2:A:1854:GLN:HB2	1.86	0.57
1:B:122:PHE:CD1	1:B:126:MET:HE2	2.40	0.57
1:B:183:TYR:HD1	1:B:187:GLN:HG3	1.70	0.56
2:A:1039:HIS:HA	2:A:1062:ASN:HB3	1.87	0.56
1:B:214:ASP:HA	1:B:217:LYS:HZ3	1.71	0.56
2:A:931:ARG:O	2:A:932:HIS:ND1	2.38	0.56
2:A:2314:VAL:HG13	2:A:2316:TRP:HE1	1.70	0.56
2:A:2473:LEU:HD21	2:A:2491:SER:HB2	1.87	0.56
2:A:1509:LEU:HD23	2:A:1519:VAL:HG21	1.87	0.56
1:B:124:LEU:HA	1:B:127:LYS:HG2	1.86	0.56
2:A:1705:TRP:CE2	2:A:1736:GLN:HB3	2.41	0.56
2:A:1550:ARG:HG3	2:A:1594:ASP:HA	1.87	0.56
2:A:1333:ASN:OD1	2:A:1386:ARG:HD2	2.06	0.56
2:A:1940:ILE:O	2:A:1941:ARG:HG2	2.06	0.56
2:A:2107:VAL:HA	2:A:2110:LEU:HG	1.87	0.56
2:A:2449:TYR:O	2:A:2450:ASN:ND2	2.39	0.56
1:C:223:MET:HA	1:C:226:LEU:HD23	1.87	0.56
2:A:2111:ILE:O	2:A:2115:LEU:N	2.39	0.56
1:C:43:ASN:O	1:C:47:VAL:HG22	2.05	0.56
2:A:2222:GLY:HA3	2:A:2241:MET:O	2.06	0.56
1:C:83:ARG:HA	1:C:86:ARG:HG2	1.88	0.56
2:A:1083:PRO:HB2	2:A:1108:LYS:HG2	1.86	0.56
2:A:1285:PRO:HD2	2:A:1288:MET:HE3	1.88	0.55
1:B:57:ARG:NH1	2:A:910:SEP:O1P	2.31	0.55
2:A:1193:LEU:HD21	2:A:1212:PRO:HG2	1.86	0.55
2:A:1974:ILE:O	2:A:1978:VAL:HG12	2.05	0.55
2:A:1067:ARG:HD3	2:A:1883:PHE:HB2	1.88	0.55
2:A:1651:LYS:O	2:A:1655:LYS:HG3	2.07	0.55
1:C:23:MET:HG3	1:C:48:ALA:HB1	1.88	0.55
1:C:97:CYS:SG	1:C:98:GLN:N	2.79	0.55
2:A:1986:HIS:CE1	2:A:2052:GLN:HB3	2.42	0.55
2:A:2175:ASP:OD1	2:A:2175:ASP:N	2.40	0.55
2:A:2494:THR:HG23	2:A:2496:TRP:HE1	1.71	0.55
2:A:1435:LEU:HD11	2:A:1449:LEU:HD21	1.88	0.55
2:A:1435:LEU:HD12	2:A:1474:LEU:HD11	1.89	0.55
2:A:1771:ARG:O	2:A:1775:ILE:HG13	2.07	0.55
1:C:105:ASP:OD1	1:C:106:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1337:LEU:HD22	2:A:1392:VAL:HG12	1.87	0.55
2:A:2470:MET:SD	2:A:2471:LEU:N	2.80	0.55
1:C:143:ARG:NH1	1:C:147:VAL:HG11	2.22	0.54
1:B:38:SER:N	1:B:41:GLU:OE1	2.36	0.54
2:A:2469:VAL:HA	2:A:2497:ASP:HA	1.89	0.54
2:A:2396:VAL:HG11	2:A:2447:VAL:HG11	1.88	0.54
2:A:1168:MET:HE3	2:A:1192:ILE:HD11	1.89	0.54
2:A:1677:ARG:HB3	2:A:1734:TRP:CE2	2.42	0.54
2:A:1491:THR:OG1	2:A:1492:GLU:OE1	2.12	0.54
2:A:1737:GLY:HA2	2:A:1750:VAL:O	2.07	0.54
2:A:1905:VAL:HG12	2:A:1946:VAL:HG13	1.90	0.54
2:A:1646:MET:SD	2:A:1648:GLN:HB2	2.48	0.54
2:A:1693:ARG:NH2	2:A:1829:ASP:OD2	2.33	0.54
2:A:1799:ASP:OD1	2:A:1799:ASP:N	2.39	0.54
2:A:1530:LEU:HA	2:A:1533:ILE:HG12	1.88	0.54
2:A:1839:LEU:HD12	2:A:1941:ARG:HH22	1.72	0.54
1:C:57:ARG:O	1:C:61:ARG:HG3	2.08	0.54
1:C:108:LEU:HD22	1:C:123:TYR:CZ	2.43	0.54
2:A:1695:TYR:OH	2:A:1781:VAL:HG23	2.08	0.54
1:C:224:GLN:HE21	2:A:1727:LEU:HB2	1.71	0.54
2:A:1342:ASN:OD1	2:A:1402:TYR:OH	2.26	0.54
2:A:1149:LEU:HD23	2:A:1171:LEU:HD13	1.88	0.53
2:A:1227:PHE:O	2:A:1230:ASN:ND2	2.41	0.53
2:A:1257:LEU:HB2	2:A:1278:ASN:ND2	2.23	0.53
2:A:2500:LEU:O	2:A:2504:VAL:N	2.28	0.53
1:B:12:ARG:O	1:B:15:GLU:HG3	2.08	0.53
2:A:1780:VAL:O	2:A:1784:ILE:HG22	2.08	0.53
2:A:2425:LEU:N	2:A:2437:LEU:O	2.33	0.53
1:C:58:SER:O	1:C:62:VAL:HG22	2.08	0.53
1:C:183:TYR:HD1	1:C:187:GLN:HG3	1.73	0.53
1:B:28:LYS:HE3	1:B:28:LYS:HA	1.91	0.53
2:A:998:ASP:OD1	2:A:1001:SER:OG	2.26	0.53
2:A:1512:LYS:HA	2:A:1517:LEU:H	1.73	0.53
2:A:1587:ASP:OD1	2:A:1587:ASP:N	2.40	0.53
2:A:1695:TYR:HB2	2:A:1763:LEU:HB3	1.91	0.53
2:A:1960:GLN:HE22	2:A:2074:VAL:HG23	1.73	0.53
2:A:1564:LEU:H	2:A:1564:LEU:HD23	1.73	0.53
1:B:121:VAL:HG21	1:B:165:MET:HE3	1.91	0.53
2:A:1404:THR:HG22	2:A:1658:ILE:HG12	1.91	0.53
2:A:1576:LEU:HD12	2:A:1581:VAL:HG11	1.91	0.53
1:C:131:TYR:HB3	1:C:150:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1908:PHE:HE2	2:A:1945:LEU:HB2	1.73	0.53
1:C:222:ILE:HG23	1:C:225:LEU:HD12	1.91	0.53
2:A:2140:LEU:HD12	2:A:2495:VAL:O	2.09	0.52
2:A:2178:GLN:HA	2:A:2193:GLU:HA	1.91	0.52
2:A:1214:PRO:HB3	2:A:1243:LEU:HB3	1.90	0.52
2:A:2327:SER:OG	2:A:2329:ASP:OD1	2.20	0.52
1:C:108:LEU:HD22	1:C:123:TYR:CE2	2.44	0.52
2:A:1185:PHE:HB2	2:A:1206:ASN:HD21	1.73	0.52
2:A:1973:ARG:HG2	2:A:2012:ILE:HD12	1.92	0.52
1:B:220:THR:O	1:B:223:MET:N	2.42	0.52
2:A:1863:ASP:OD1	2:A:1863:ASP:N	2.42	0.52
2:A:1235:LEU:HD11	2:A:1257:LEU:HD23	1.92	0.52
2:A:1545:PHE:HZ	2:A:1646:MET:HE3	1.75	0.52
2:A:1086:LYS:HG3	2:A:1087:GLN:HG2	1.91	0.52
2:A:1314:LYS:HD2	2:A:1316:LYS:HE2	1.90	0.52
1:B:87:GLU:O	1:B:91:LYS:HG2	2.10	0.52
2:A:1048:THR:O	2:A:1071:GLY:N	2.42	0.52
2:A:1161:ARG:HH22	2:A:1202:ASP:HB3	1.74	0.52
2:A:1731:ARG:HG3	2:A:1731:ARG:HH11	1.76	0.52
2:A:2034:GLY:HA3	2:A:2039:ARG:HH11	1.74	0.52
2:A:2144:ILE:N	2:A:2493:LEU:O	2.25	0.52
1:C:124:LEU:HA	1:C:127:LYS:HG2	1.92	0.51
1:B:27:MET:HG3	1:B:45:LEU:HA	1.93	0.51
1:B:212:ASN:O	1:B:216:TYR:N	2.40	0.51
2:A:2266:GLY:HA2	2:A:2300:LEU:HD23	1.91	0.51
2:A:2367:LYS:HB2	2:A:2370:SER:HB3	1.92	0.51
1:C:27:MET:HG3	1:C:45:LEU:HA	1.93	0.51
2:A:1870:LEU:HB2	2:A:1939:GLY:HA3	1.92	0.51
1:C:26:ALA:O	1:C:30:VAL:HG12	2.10	0.51
1:C:201:PHE:O	1:C:205:ILE:HG12	2.10	0.51
2:A:1257:LEU:HD12	2:A:1257:LEU:H	1.76	0.51
2:A:1968:ARG:H	2:A:1971:GLN:HE22	1.57	0.51
2:A:2105:PRO:HD2	2:A:2141:THR:O	2.11	0.51
2:A:2146:LEU:HG	2:A:2150:VAL:HG21	1.93	0.51
1:C:83:ARG:NH1	1:C:87:GLU:OE1	2.43	0.51
2:A:1165:LEU:O	2:A:1183:ASN:ND2	2.44	0.51
2:A:2510:HIS:O	2:A:2514:ARG:HB2	2.11	0.51
1:B:57:ARG:NH2	2:A:910:SEP:O3P	2.37	0.51
2:A:2140:LEU:HA	2:A:2496:TRP:HA	1.92	0.51
2:A:2142:ARG:HG2	2:A:2495:VAL:HB	1.91	0.51
2:A:1894:TYR:N	2:A:1905:VAL:O	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2118:ASN:HB3	2:A:2121:GLU:HB2	1.91	0.51
2:A:1278:ASN:HD22	2:A:1281:LEU:HB2	1.76	0.51
2:A:1305:ASN:HA	2:A:1516:GLN:HG3	1.93	0.51
2:A:1637:LYS:HZ2	2:A:1644:ASN:N	2.09	0.51
2:A:1845:GLN:OE1	2:A:1847:ARG:HG2	2.10	0.51
2:A:1973:ARG:NH1	2:A:2007:PRO:O	2.44	0.51
2:A:2420:GLN:NE2	2:A:2501:PRO:HG3	2.26	0.51
1:B:123:TYR:HA	1:B:126:MET:CE	2.41	0.51
2:A:1501:ARG:O	2:A:1505:ILE:HG13	2.11	0.51
2:A:2072:ARG:HG2	2:A:2083:PHE:HE1	1.76	0.51
2:A:2420:GLN:HE22	2:A:2501:PRO:HG3	1.74	0.51
2:A:1925:CYS:O	2:A:1928:HIS:NE2	2.44	0.50
1:C:162:LYS:HG3	1:C:172:ARG:NH2	2.27	0.50
1:B:147:VAL:HG23	1:B:182:PHE:CZ	2.47	0.50
2:A:2093:PRO:HB2	2:A:2098:GLU:HG3	1.92	0.50
2:A:2179:LEU:HB3	2:A:2192:GLU:HG3	1.93	0.50
1:C:130:TYR:HA	1:C:133:TYR:CD2	2.46	0.50
2:A:1418:VAL:O	2:A:1431:MET:HE1	2.12	0.50
1:B:83:ARG:NH1	1:B:87:GLU:OE2	2.44	0.50
2:A:2001:LEU:N	2:A:2014:LYS:O	2.42	0.50
2:A:2433:HIS:C	2:A:2434:ILE:HD13	2.37	0.50
2:A:2132:LEU:HA	2:A:2137:LEU:HD22	1.93	0.50
2:A:2293:ILE:HD12	2:A:2332:ILE:HD11	1.93	0.50
2:A:2471:LEU:HD11	2:A:2493:LEU:HG	1.93	0.50
2:A:1877:PHE:CZ	2:A:1879:GLN:HB2	2.46	0.50
2:A:2106:MET:CE	2:A:2137:LEU:HB2	2.41	0.50
2:A:2241:MET:SD	2:A:2242:THR:N	2.85	0.50
1:C:27:MET:HE3	1:C:27:MET:HA	1.94	0.50
1:C:222:ILE:HA	1:C:225:LEU:HG	1.93	0.50
2:A:1533:ILE:HD13	2:A:1562:LEU:HD11	1.92	0.50
2:A:1575:PHE:HD2	2:A:1576:LEU:HD22	1.77	0.50
2:A:2251:ASN:HB2	2:A:2315:MET:HE1	1.94	0.50
2:A:1971:GLN:H	2:A:1971:GLN:CD	2.20	0.49
2:A:1017:GLU:HB3	2:A:1019:HIS:CE1	2.47	0.49
2:A:1353:GLN:NE2	2:A:1491:THR:O	2.46	0.49
2:A:1395:PHE:CD1	2:A:1405:HIS:HD2	2.29	0.49
1:C:20:TYR:HA	1:C:23:MET:SD	2.52	0.49
2:A:1862:ALA:HB1	2:A:1866:ARG:HH12	1.77	0.49
1:C:82:VAL:HG22	1:B:13:LEU:HD21	1.95	0.49
2:A:2462:GLN:HB2	2:A:2467:LYS:HA	1.95	0.49
2:A:2516:GLU:O	2:A:2520:LYS:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1973:ARG:HD3	2:A:1976:LEU:HD12	1.93	0.49
1:B:147:VAL:HG23	1:B:182:PHE:HZ	1.76	0.49
2:A:2295:ASN:H	2:A:2298:THR:HG1	1.60	0.49
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.78	0.49
2:A:1047:PHE:H	2:A:1068:ASN:HD21	1.61	0.49
2:A:1369:VAL:HG23	2:A:1401:PHE:HE2	1.78	0.48
2:A:1501:ARG:O	2:A:1504:ILE:HG22	2.12	0.48
2:A:1122:ILE:HD11	2:A:1145:SER:N	2.28	0.48
2:A:2176:ARG:HH21	2:A:2195:ALA:N	2.09	0.48
2:A:2246:THR:OG1	2:A:2300:LEU:O	2.25	0.48
2:A:2267:THR:HG22	2:A:2268:ALA:H	1.77	0.48
1:C:131:TYR:HD1	1:C:146:VAL:HG13	1.78	0.48
2:A:1043:HIS:HB3	2:A:1066:SER:H	1.77	0.48
2:A:1287:GLU:O	2:A:1290:LYS:NZ	2.45	0.48
2:A:1610:ILE:HG21	2:A:1653:LEU:HD21	1.94	0.48
1:B:46:SER:OG	2:A:914:GLY:HA3	2.13	0.48
2:A:2025:CYS:SG	2:A:2026:ARG:N	2.86	0.48
2:A:2090:GLY:HA2	2:A:2115:LEU:HD11	1.95	0.48
2:A:2470:MET:CB	2:A:2498:ILE:HG22	2.43	0.48
1:B:130:TYR:HA	1:B:133:TYR:CD2	2.49	0.48
1:B:221:LEU:HB2	2:A:916:PHE:CE2	2.48	0.48
2:A:2039:ARG:HE	2:A:2040:ALA:H	1.61	0.48
2:A:1134:LEU:HB3	2:A:1158:PHE:CD1	2.47	0.48
2:A:1355:MET:HE1	2:A:1374:LYS:HD2	1.95	0.48
2:A:1415:TYR:CD2	2:A:1438:ILE:HD12	2.49	0.48
2:A:1545:PHE:CZ	2:A:1646:MET:HE3	2.48	0.48
2:A:2107:VAL:HG23	2:A:2110:LEU:HD12	1.94	0.48
1:B:12:ARG:O	1:B:16:GLN:HG3	2.13	0.48
2:A:2245:VAL:HA	2:A:2267:THR:HG23	1.94	0.48
2:A:1361:ASP:N	2:A:1361:ASP:OD1	2.47	0.48
2:A:2517:LEU:HA	2:A:2520:LYS:HB3	1.96	0.48
2:A:1538:ARG:HG3	2:A:1599:GLU:HB3	1.96	0.47
1:B:129:ASP:CG	1:B:178:ASN:HD22	2.22	0.47
2:A:1252:LEU:HB3	2:A:1257:LEU:HD21	1.96	0.47
2:A:1296:ASP:OD1	2:A:1296:ASP:N	2.47	0.47
2:A:1407:HIS:CE1	2:A:1791:TRP:HH2	2.32	0.47
2:A:1912:THR:O	2:A:1943:ARG:NH1	2.47	0.47
2:A:2270:GLY:HA3	2:A:2294:GLY:H	1.78	0.47
2:A:2321:THR:HG21	2:A:2339:ARG:HG3	1.96	0.47
2:A:2434:ILE:HD11	2:A:2455:VAL:HG21	1.96	0.47
2:A:1334:ARG:HA	2:A:1389:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1073:SER:OG	2:A:1075:VAL:HG13	2.14	0.47
2:A:1448:ILE:HD11	2:A:1507:GLU:HG3	1.97	0.47
2:A:2299:PRO:HG2	2:A:2301:MET:HE1	1.96	0.47
1:B:221:LEU:HA	1:B:224:GLN:NE2	2.27	0.47
2:A:1050:PHE:HB2	2:A:1074:VAL:HG23	1.97	0.47
1:B:10:LYS:HB3	1:B:10:LYS:HE2	1.75	0.47
2:A:1907:ILE:HD13	2:A:1944:MET:HB3	1.95	0.47
2:A:1966:LEU:HB3	2:A:1971:GLN:NE2	2.29	0.47
1:B:118:GLU:HG2	1:B:119:SER:N	2.28	0.47
2:A:1338:MET:HE3	2:A:1415:TYR:CE2	2.50	0.47
2:A:1709:ILE:HG12	2:A:1738:ILE:HD11	1.97	0.47
2:A:1717:PRO:HG3	2:A:1776:LEU:HD21	1.97	0.47
2:A:2182:LEU:HD13	2:A:2189:TYR:HB2	1.96	0.47
1:C:63:ILE:HD11	1:C:85:TYR:HB3	1.97	0.47
2:A:1160:ALA:O	2:A:1180:LEU:HA	2.14	0.47
2:A:1176:THR:HG22	2:A:1177:ILE:HG12	1.96	0.47
1:C:66:ILE:HA	1:C:69:LYS:HG2	1.97	0.47
2:A:1230:ASN:OD1	2:A:1231:GLN:N	2.48	0.47
2:A:1646:MET:SD	2:A:1648:GLN:N	2.88	0.47
2:A:2251:ASN:CB	2:A:2315:MET:HE1	2.45	0.47
2:A:1134:LEU:HD22	2:A:1158:PHE:CE1	2.50	0.47
2:A:1995:LEU:HG	2:A:2062:LEU:HD11	1.96	0.47
2:A:2009:ALA:O	2:A:2510:HIS:NE2	2.46	0.47
2:A:2105:PRO:HG2	2:A:2142:ARG:HB2	1.96	0.47
2:A:2196:ASP:OD1	2:A:2196:ASP:N	2.47	0.47
1:C:97:CYS:HB2	1:C:134:LEU:HD21	1.98	0.46
2:A:1165:LEU:C	2:A:1183:ASN:HD21	2.22	0.46
1:C:5:GLU:HA	1:C:8:VAL:HG22	1.96	0.46
2:A:1282:ARG:NH1	2:A:1303:HIS:H	2.13	0.46
2:A:2467:LYS:H	2:A:2467:LYS:HD2	1.80	0.46
2:A:1548:ILE:HD12	2:A:1598:VAL:HG21	1.97	0.46
2:A:1996:LYS:NZ	2:A:2035:THR:H	2.12	0.46
2:A:2272:LEU:HB2	2:A:2291:LEU:HB2	1.96	0.46
1:B:221:LEU:HB2	2:A:916:PHE:HE2	1.80	0.46
2:A:936:LEU:O	2:A:938:PRO:HD2	2.15	0.46
2:A:1051:PRO:C	2:A:1053:TYR:H	2.24	0.46
2:A:1908:PHE:CE2	2:A:1945:LEU:HB2	2.51	0.46
1:B:104:LEU:O	1:B:109:ILE:HG12	2.14	0.46
2:A:939:ILE:O	2:A:940:PHE:C	2.59	0.46
2:A:1334:ARG:HD2	2:A:1389:VAL:HG23	1.98	0.46
2:A:1942:PRO:HD2	2:A:1944:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2207:LEU:HD21	2:A:2278:LYS:HA	1.96	0.46
2:A:1168:MET:HG3	2:A:1192:ILE:HG12	1.97	0.46
2:A:2106:MET:SD	2:A:2140:LEU:HD23	2.56	0.46
1:C:225:LEU:HD22	2:A:934:ASN:HD21	1.80	0.46
1:B:173:LEU:O	1:B:177:LEU:HG	2.16	0.46
2:A:1340:VAL:O	2:A:1417:ALA:HA	2.16	0.46
2:A:1371:ILE:HG13	2:A:1373:VAL:HG23	1.96	0.46
1:C:129:ASP:O	1:C:132:ARG:HG3	2.15	0.46
1:B:28:LYS:HE3	1:B:103:LEU:HD22	1.98	0.46
1:C:78:LYS:HD2	1:C:78:LYS:HA	1.75	0.45
2:A:1205:SER:O	2:A:1205:SER:OG	2.19	0.45
2:A:1694:LEU:HD21	2:A:1764:LYS:HE2	1.98	0.45
2:A:2522:ARG:O	2:A:2525:SER:OG	2.32	0.45
1:C:222:ILE:O	1:C:226:LEU:HD22	2.16	0.45
2:A:2105:PRO:HD2	2:A:2142:ARG:HB3	1.98	0.45
2:A:1202:ASP:HA	2:A:1226:LEU:HB2	1.97	0.45
2:A:2413:ARG:O	2:A:2430:GLY:N	2.40	0.45
1:B:204:ALA:HB3	1:B:223:MET:HE1	1.98	0.45
2:A:1838:ASP:OD1	2:A:1838:ASP:N	2.49	0.45
1:C:94:GLU:HA	1:C:97:CYS:SG	2.56	0.45
2:A:1061:ALA:HB1	2:A:1086:LYS:HG2	1.97	0.45
2:A:1120:SER:HA	2:A:1140:HIS:O	2.16	0.45
2:A:1814:TYR:OH	2:A:1827:LEU:HD22	2.17	0.45
2:A:2047:ASN:OD1	2:A:2047:ASN:N	2.50	0.45
2:A:2183:ASP:OD1	2:A:2184:LEU:N	2.49	0.45
2:A:1168:MET:HE1	2:A:1185:PHE:HZ	1.82	0.45
2:A:1579:SER:O	2:A:1579:SER:OG	2.32	0.45
2:A:1739:TYR:HD2	2:A:1749:LEU:HD13	1.81	0.45
1:C:124:LEU:HB3	1:C:157:ALA:HB2	1.99	0.45
2:A:1958:LEU:HD22	2:A:2002:LEU:HD12	1.99	0.45
2:A:2137:LEU:HG	2:A:2138:VAL:N	2.31	0.45
2:A:2251:ASN:ND2	2:A:2262:PHE:HB2	2.27	0.45
1:C:20:TYR:O	1:C:23:MET:HG2	2.16	0.45
2:A:998:ASP:O	2:A:1001:SER:OG	2.35	0.45
2:A:1146:GLU:HA	2:A:1169:PRO:HB2	1.98	0.45
2:A:1995:LEU:N	2:A:1996:LYS:HE3	2.32	0.45
2:A:2176:ARG:NE	2:A:2195:ALA:O	2.50	0.45
2:A:2241:MET:HE2	2:A:2267:THR:HG21	1.98	0.45
2:A:2291:LEU:HD11	2:A:2330:PHE:HB3	1.99	0.45
1:C:97:CYS:HA	1:C:100:VAL:HG22	1.98	0.44
2:A:1584:HIS:CE1	2:A:1586:GLN:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1995:LEU:H	2:A:1996:LYS:HE3	1.82	0.44
2:A:2148:LYS:HA	2:A:2148:LYS:HD2	1.79	0.44
2:A:2225:LEU:HD11	2:A:2235:ARG:HE	1.81	0.44
2:A:2461:ALA:N	2:A:2469:VAL:O	2.50	0.44
1:B:127:LYS:HB2	1:B:127:LYS:HE3	1.79	0.44
2:A:939:ILE:H	2:A:939:ILE:HG12	1.54	0.44
2:A:1172:PRO:HD2	2:A:1175:MET:HE3	1.99	0.44
2:A:2446:ARG:NH2	2:A:2508:GLU:HG3	2.32	0.44
1:C:50:LYS:HZ2	2:A:938:PRO:HG2	1.81	0.44
2:A:1811:TRP:CE3	2:A:1826:LEU:HB3	2.51	0.44
2:A:2129:PHE:O	2:A:2133:ASN:N	2.49	0.44
2:A:2434:ILE:O	2:A:2448:ILE:HD12	2.17	0.44
1:C:104:LEU:HD23	1:C:127:LYS:HB3	1.99	0.44
2:A:1729:PRO:HB3	2:A:1742:TRP:CE2	2.53	0.44
1:C:49:TYR:HA	1:C:52:VAL:HG12	1.99	0.44
1:C:158:HIS:CE1	1:C:162:LYS:HD3	2.53	0.44
2:A:1123:CYS:HB2	2:A:1148:PHE:CZ	2.53	0.44
2:A:2470:MET:HB2	2:A:2498:ILE:HG22	1.98	0.44
1:B:236:ASP:OD1	1:B:236:ASP:N	2.50	0.44
2:A:1024:THR:HA	2:A:1047:PHE:CD1	2.53	0.44
2:A:1840:LEU:HD12	2:A:1841:VAL:N	2.33	0.44
2:A:1879:GLN:HG2	2:A:1894:TYR:CE2	2.49	0.44
2:A:2319:CYS:HB2	2:A:2324:PHE:CE1	2.53	0.44
2:A:2366:ALA:HB1	2:A:2414:VAL:HG11	2.00	0.44
1:C:40:GLU:HA	1:C:43:ASN:HD21	1.83	0.44
1:C:224:GLN:NE2	2:A:1728:ARG:HG2	2.32	0.44
1:C:226:LEU:HA	1:C:229:ASN:HD21	1.83	0.44
2:A:1310:HIS:HB3	2:A:1574:HIS:CE1	2.53	0.44
2:A:1529:GLU:O	2:A:1533:ILE:HG23	2.18	0.44
2:A:1932:LEU:HD12	2:A:2015:ILE:HG13	1.99	0.44
1:C:88:LYS:O	1:C:91:LYS:HG2	2.18	0.44
1:B:49:TYR:HB3	1:B:130:TYR:OH	2.18	0.44
2:A:1864:LEU:HD11	2:A:1922:VAL:HG23	1.99	0.44
2:A:1940:ILE:HG23	2:A:1941:ARG:HE	1.82	0.44
1:C:179:TYR:OH	1:C:183:TYR:OH	2.27	0.44
1:B:28:LYS:HD3	1:B:49:TYR:OH	2.18	0.44
2:A:1537:GLU:CD	2:A:1548:ILE:HD11	2.43	0.44
2:A:1673:LEU:HD21	2:A:1733:TYR:HB3	2.00	0.44
2:A:1932:LEU:HD12	2:A:2015:ILE:O	2.17	0.44
2:A:2287:PRO:HG2	2:A:2290:ILE:HD11	2.00	0.44
1:B:4:ARG:O	1:B:8:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1533:ILE:HG13	2:A:1534:ILE:N	2.32	0.43
2:A:2197:SER:HB2	2:A:2220:GLN:HG2	2.00	0.43
1:C:63:ILE:HD12	1:C:85:TYR:HD2	1.84	0.43
1:B:57:ARG:O	1:B:61:ARG:HG3	2.19	0.43
1:B:65:SER:O	1:B:69:LYS:HG2	2.18	0.43
2:A:2233:LYS:HE2	2:A:2233:LYS:HB3	1.84	0.43
2:A:1107:GLU:HG3	2:A:1129:LYS:HE3	1.98	0.43
2:A:1161:ARG:NH2	2:A:1181:SER:H	2.07	0.43
2:A:1606:ILE:HA	2:A:1609:GLN:HG3	2.01	0.43
2:A:1019:HIS:CB	2:A:1043:HIS:H	2.31	0.43
2:A:1320:ARG:NH2	2:A:1567:ASN:O	2.52	0.43
2:A:1734:TRP:CE3	2:A:1737:GLY:HA3	2.53	0.43
2:A:1931:SER:HB3	2:A:2514:ARG:NH2	2.31	0.43
2:A:2148:LYS:HZ2	2:A:2490:GLN:HG2	1.82	0.43
2:A:2171:CYS:SG	2:A:2178:GLN:N	2.91	0.43
2:A:2329:ASP:OD2	2:A:2331:THR:OG1	2.33	0.43
2:A:2446:ARG:CZ	2:A:2508:GLU:HG3	2.48	0.43
2:A:1930:PRO:HD3	2:A:2522:ARG:HH12	1.83	0.43
1:B:165:MET:SD	1:B:165:MET:N	2.92	0.43
2:A:2166:SER:OG	2:A:2182:LEU:O	2.32	0.43
1:C:63:ILE:HA	1:C:66:ILE:HG12	1.99	0.43
1:C:124:LEU:CB	1:C:157:ALA:HB2	2.49	0.43
2:A:1321:PHE:HE1	2:A:1527:TYR:HE2	1.67	0.43
2:A:1550:ARG:HG2	2:A:1596:TYR:HE1	1.83	0.43
2:A:2459:MET:SD	2:A:2460:THR:N	2.85	0.43
1:B:124:LEU:O	1:B:127:LYS:HG2	2.19	0.43
2:A:1207:ASP:OD1	2:A:1207:ASP:N	2.49	0.43
2:A:1521:GLN:OE1	2:A:1523:ILE:HG23	2.19	0.43
2:A:2152:VAL:HG21	2:A:2169:LEU:HD23	2.01	0.43
2:A:2172:GLY:HA2	2:A:2198:ARG:HD3	2.00	0.43
2:A:1356:LYS:HB2	2:A:1356:LYS:NZ	2.34	0.43
2:A:1652:LEU:HA	2:A:1655:LYS:HG3	2.01	0.43
2:A:2500:LEU:O	2:A:2503:GLU:N	2.51	0.43
1:C:23:MET:HG3	1:C:48:ALA:CB	2.49	0.43
2:A:1211:LEU:HD23	2:A:1211:LEU:HA	1.92	0.43
2:A:1425:GLN:OE1	2:A:1425:GLN:O	2.37	0.43
2:A:2128:VAL:HA	2:A:2131:ILE:HG22	2.01	0.43
2:A:1003:LYS:HA	2:A:1003:LYS:HD3	1.82	0.42
2:A:1175:MET:HB2	2:A:1195:LEU:HD13	1.99	0.42
2:A:1550:ARG:HG2	2:A:1596:TYR:CE1	2.54	0.42
2:A:1651:LYS:HG3	2:A:1655:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1978:VAL:HG13	2:A:2059:PHE:HE1	1.83	0.42
2:A:2255:LYS:HD2	2:A:2328:ASN:HB3	2.01	0.42
2:A:2300:LEU:HA	2:A:2319:CYS:HA	2.01	0.42
1:B:162:LYS:HA	1:B:162:LYS:HD3	1.69	0.42
2:A:1027:PRO:HG2	2:A:1030:LEU:HB2	2.01	0.42
2:A:1395:PHE:CD1	2:A:1405:HIS:CD2	3.07	0.42
2:A:1502:LYS:HA	2:A:1502:LYS:HD3	1.85	0.42
2:A:1771:ARG:HD3	2:A:1866:ARG:HE	1.84	0.42
1:C:229:ASN:HB2	1:C:233:TRP:CZ2	2.54	0.42
2:A:1055:LEU:HD22	2:A:1085:LEU:HD21	2.01	0.42
2:A:2146:LEU:HD12	2:A:2147:PRO:CD	2.42	0.42
2:A:1584:HIS:NE2	2:A:1593:SER:O	2.53	0.42
2:A:2200:LEU:HD13	2:A:2245:VAL:O	2.20	0.42
1:B:69:LYS:HA	1:B:69:LYS:HD3	1.93	0.42
2:A:1214:PRO:HG3	2:A:1244:TRP:CZ3	2.55	0.42
2:A:1378:ILE:HD13	2:A:1378:ILE:HA	1.91	0.42
2:A:2215:ILE:HB	2:A:2227:ILE:HG23	2.02	0.42
2:A:2438:ASP:HB3	2:A:2442:ARG:O	2.20	0.42
1:C:108:LEU:HD23	1:C:108:LEU:HA	1.90	0.42
1:C:178:ASN:HA	1:C:181:VAL:HG22	2.02	0.42
1:C:184:TYR:CD2	1:C:184:TYR:C	2.97	0.42
2:A:1145:SER:O	2:A:1148:PHE:HB2	2.18	0.42
2:A:1402:TYR:HA	2:A:1405:HIS:HD1	1.84	0.42
2:A:1893:VAL:HA	2:A:1906:LYS:HA	2.02	0.42
1:B:197:ALA:HB3	1:B:230:LEU:HD21	2.00	0.42
2:A:1244:TRP:HA	2:A:1246:ARG:NH1	2.34	0.42
2:A:1973:ARG:HD3	2:A:1973:ARG:HA	1.89	0.42
2:A:1994:ASP:CG	2:A:1996:LYS:HZ2	2.27	0.42
2:A:2216:VAL:HG21	2:A:2263:LEU:HD11	2.01	0.42
1:C:129:ASP:OD1	1:C:178:ASN:ND2	2.53	0.42
1:B:57:ARG:HH12	2:A:910:SEP:P	2.39	0.42
2:A:1190:GLU:HA	2:A:1193:LEU:HB2	2.02	0.42
2:A:1873:ASP:OD1	2:A:1873:ASP:N	2.52	0.42
2:A:2316:TRP:CE3	2:A:2363:LEU:HD21	2.55	0.42
2:A:2476:ASN:O	2:A:2478:LYS:HE2	2.19	0.42
2:A:1317:ASP:N	2:A:1317:ASP:OD1	2.53	0.42
2:A:1376:TRP:CZ3	2:A:1378:ILE:HD11	2.55	0.42
2:A:1603:LEU:O	2:A:1607:MET:HG2	2.20	0.42
1:C:39:ASN:O	1:C:43:ASN:ND2	2.52	0.42
2:A:1369:VAL:HG23	2:A:1401:PHE:CE2	2.55	0.42
2:A:1409:MET:HG2	2:A:1415:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1476:LYS:HD2	2:A:1476:LYS:HA	1.67	0.42
2:A:2152:VAL:HG21	2:A:2169:LEU:HB3	2.01	0.42
2:A:1449:LEU:O	2:A:1485:TYR:HA	2.20	0.41
2:A:2081:ASN:OD1	2:A:2081:ASN:N	2.53	0.41
2:A:2300:LEU:HD12	2:A:2318:GLY:O	2.20	0.41
2:A:2509:LYS:HA	2:A:2512:GLU:HG3	2.02	0.41
1:C:168:THR:HG21	1:C:211:LEU:HD11	2.01	0.41
2:A:1504:ILE:HD12	2:A:1504:ILE:HA	1.86	0.41
2:A:1959:LEU:HD12	2:A:1960:GLN:HG2	2.01	0.41
2:A:2143:ARG:HA	2:A:2494:THR:HA	2.02	0.41
2:A:2246:THR:N	2:A:2266:GLY:O	2.45	0.41
1:B:21:ASP:OD1	1:B:22:ASP:N	2.51	0.41
1:B:96:VAL:O	1:B:100:VAL:HG23	2.19	0.41
2:A:1602:TRP:CE2	2:A:1606:ILE:HG13	2.55	0.41
2:A:2146:LEU:HD23	2:A:2491:SER:OG	2.20	0.41
2:A:1351:LEU:HD11	2:A:1392:VAL:HG11	2.01	0.41
2:A:1926:HIS:HA	2:A:1928:HIS:CD2	2.54	0.41
2:A:1996:LYS:HZ1	2:A:2035:THR:H	1.67	0.41
2:A:1129:LYS:HD2	2:A:1130:GLU:HB2	2.03	0.41
1:B:169:HIS:O	1:B:173:LEU:HG	2.21	0.41
2:A:1092:TYR:CD2	2:A:1116:GLY:HA3	2.55	0.41
2:A:1777:LEU:O	2:A:1781:VAL:HG12	2.20	0.41
2:A:2247:CYS:O	2:A:2266:GLY:N	2.43	0.41
2:A:2427:ILE:HD11	2:A:2435:LEU:HB2	2.02	0.41
2:A:2434:ILE:CD1	2:A:2455:VAL:HG21	2.51	0.41
1:B:41:GLU:H	1:B:41:GLU:HG3	1.67	0.41
2:A:1712:LEU:O	2:A:1714:GLU:N	2.53	0.41
2:A:1956:ASP:OD1	2:A:1956:ASP:N	2.52	0.41
2:A:1230:ASN:OD1	2:A:1232:ILE:HG13	2.21	0.41
2:A:2390:VAL:HA	2:A:2393:LEU:HB2	2.01	0.41
1:B:60:TRP:CE2	1:B:137:VAL:HG12	2.56	0.41
1:B:158:HIS:NE2	1:B:162:LYS:HE2	2.35	0.41
2:A:983:TYR:HB3	2:A:1009:HIS:CE1	2.56	0.41
2:A:1016:LEU:CD2	2:A:1040:LEU:HA	2.51	0.41
2:A:1359:LYS:HG3	2:A:1360:SER:H	1.85	0.41
2:A:1488:VAL:HG21	2:A:1497:LEU:HD13	2.02	0.41
2:A:1914:LEU:O	2:A:1917:LEU:HG	2.21	0.41
2:A:1932:LEU:HD11	2:A:2017:ASP:HB3	2.02	0.41
2:A:2236:HIS:NE2	2:A:2280:VAL:O	2.45	0.41
2:A:2467:LYS:HD2	2:A:2467:LYS:N	2.35	0.41
1:C:27:MET:HB3	1:C:45:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1269:ASN:O	2:A:1269:ASN:ND2	2.42	0.41
2:A:1877:PHE:HZ	2:A:1879:GLN:HB2	1.86	0.41
2:A:1956:ASP:O	2:A:1960:GLN:HG2	2.21	0.41
2:A:1019:HIS:HB3	2:A:1043:HIS:H	1.86	0.40
2:A:1311:ILE:HD13	2:A:1586:GLN:HE21	1.86	0.40
1:B:58:SER:HA	1:B:61:ARG:CZ	2.51	0.40
2:A:1335:MET:HE3	2:A:1336:LYS:H	1.86	0.40
2:A:1346:GLY:O	2:A:1418:VAL:HG11	2.21	0.40
2:A:1592:LEU:HD13	2:A:1648:GLN:HB3	2.04	0.40
2:A:1657:GLN:HG2	2:A:1710:ASN:CG	2.47	0.40
1:C:140:GLY:O	1:C:143:ARG:HB3	2.21	0.40
1:C:158:HIS:ND1	1:C:158:HIS:C	2.79	0.40
2:A:1933:ILE:O	2:A:1933:ILE:HG13	2.22	0.40
1:B:124:LEU:HB3	1:B:157:ALA:HB2	2.02	0.40
2:A:1305:ASN:HB2	2:A:1516:GLN:HE21	1.86	0.40
2:A:1395:PHE:HD1	2:A:1405:HIS:CD2	2.39	0.40
2:A:2049:ILE:HD12	2:A:2049:ILE:HA	1.95	0.40
1:C:4:ARG:HH21	1:C:41:GLU:CD	2.26	0.40
1:C:104:LEU:O	1:C:109:ILE:HG13	2.21	0.40
1:B:58:SER:HA	1:B:61:ARG:NH2	2.37	0.40
1:B:108:LEU:HD12	1:B:123:TYR:CZ	2.56	0.40
1:B:183:TYR:CD1	1:B:187:GLN:HG3	2.54	0.40
2:A:1279:LEU:O	2:A:1282:ARG:NH2	2.55	0.40
2:A:1499:LYS:HD2	2:A:1499:LYS:HA	1.86	0.40
2:A:1677:ARG:HB3	2:A:1734:TRP:CZ2	2.56	0.40
2:A:1718:TYR:CE2	2:A:1865:PRO:HG3	2.56	0.40
2:A:1739:TYR:CD2	2:A:1749:LEU:HD13	2.56	0.40
2:A:2212:GLU:OE2	2:A:2214:TRP:NE1	2.55	0.40
2:A:2472:VAL:HB	2:A:2494:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	B	238/265 (90%)	236 (99%)	2 (1%)	0	100	100
1	C	235/265 (89%)	231 (98%)	4 (2%)	0	100	100
2	A	1499/2562 (58%)	1356 (90%)	140 (9%)	3 (0%)	44	76
All	All	1972/3092 (64%)	1823 (92%)	146 (7%)	3 (0%)	45	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	938	PRO
2	A	940	PHE
2	A	1713	LEU

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	B	211/231 (91%)	209 (99%)	2 (1%)	75	83
1	C	208/231 (90%)	203 (98%)	5 (2%)	44	62
2	A	1346/2310 (58%)	1320 (98%)	26 (2%)	52	69
All	All	1765/2772 (64%)	1732 (98%)	33 (2%)	52	69

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	87	GLU
1	C	134	LEU
1	C	158	HIS
1	C	175	LEU
1	C	195	HIS
1	B	62	VAL
1	B	224	GLN
2	A	938	PRO
2	A	939	ILE
2	A	1076	LEU

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Mol	Chain	Res	Type
2	A	1114	LEU
2	A	1175	MET
2	A	1192	ILE
2	A	1203	MET
2	A	1291	LEU
2	A	1330	VAL
2	A	1388	LEU
2	A	1392	VAL
2	A	1513	ILE
2	A	1519	VAL
2	A	1582	LEU
2	A	1603	LEU
2	A	1758	HIS
2	A	2137	LEU
2	A	2138	VAL
2	A	2139	CYS
2	A	2141	THR
2	A	2267	THR
2	A	2397	MET
2	A	2436	LEU
2	A	2457	VAL
2	A	2498	ILE
2	A	2500	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	9	GLN
1	C	164	HIS
1	C	178	ASN
1	C	224	GLN
1	C	229	ASN
1	B	106	ASN
1	B	178	ASN
2	A	1021	ASN
2	A	1068	ASN
2	A	1251	HIS
2	A	1278	ASN
2	A	1353	GLN
2	A	1407	HIS
2	A	1779	GLN
2	A	1854	GLN

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Mol	Chain	Res	Type
2	A	1960	GLN
2	A	1986	HIS
2	A	2420	GLN
2	A	2506	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SEP	A	910	2	8,9,10	1.60	1 (12%)	7,12,14	1.30	1 (14%)
2	SEP	A	935	2	8,9,10	1.57	1 (12%)	7,12,14	1.52	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	A	910	2	-	1/6/8/10	-
2	SEP	A	935	2	-	5/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	935	SEP	P-O1P	3.47	1.61	1.50
2	A	910	SEP	P-O1P	3.47	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	935	SEP	OG-CB-CA	3.57	111.62	108.14
2	A	910	SEP	OG-CB-CA	2.88	110.94	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	935	SEP	N-CA-CB-OG
2	A	935	SEP	C-CA-CB-OG
2	A	935	SEP	CB-OG-P-O1P
2	A	935	SEP	CB-OG-P-O2P
2	A	935	SEP	CB-OG-P-O3P
2	A	910	SEP	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	910	SEP	3	0
2	A	935	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GDP	A	2601	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	3 (10%)

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
3	GDP	A	2601	-	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	GDP	C6-N1	-2.20	1.34	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	GDP	C8-N7-C5	2.96	107.58	102.55
3	A	2601	GDP	O4'-C1'-N9	2.34	111.84	108.75
3	A	2601	GDP	C5-C6-N1	2.08	118.03	114.07

There are no chirality outliers.

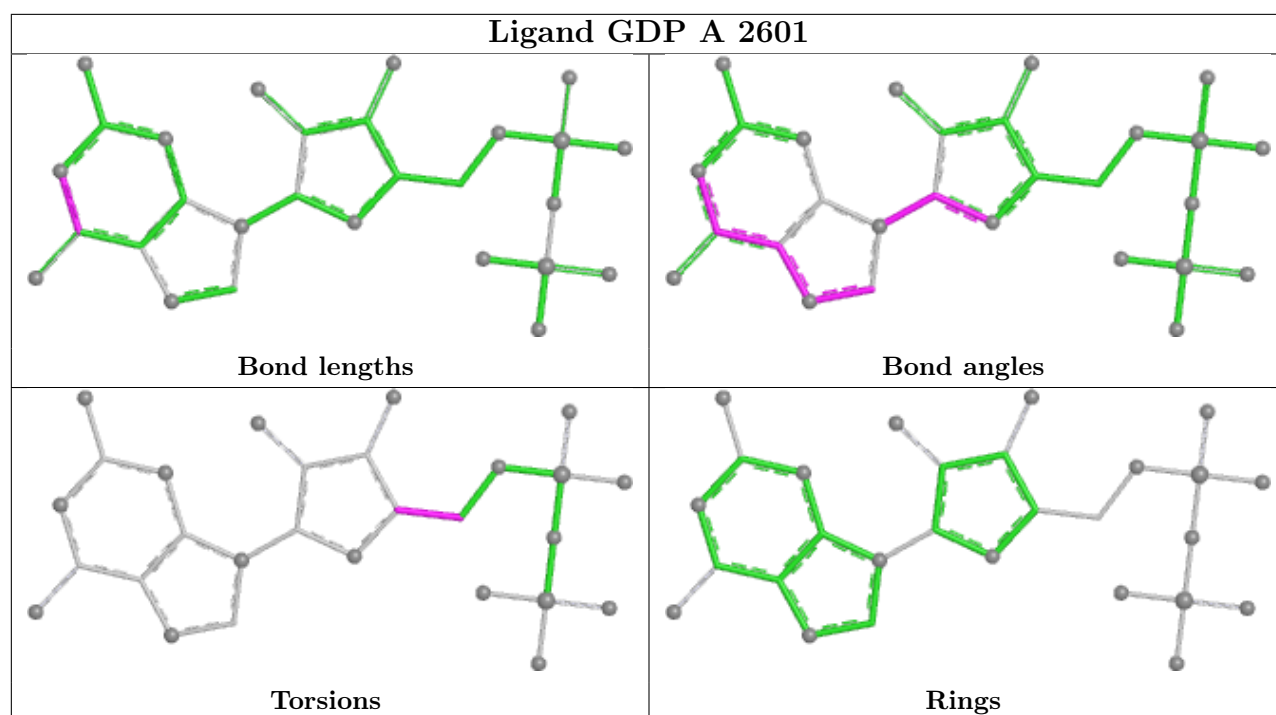
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	GDP	O4'-C4'-C5'-O5'
3	A	2601	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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.

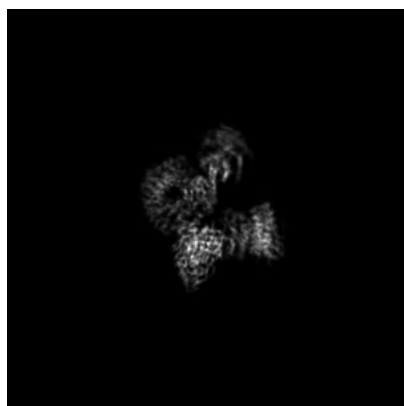
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45609. These allow visual inspection of the internal detail of the map and identification of artifacts.

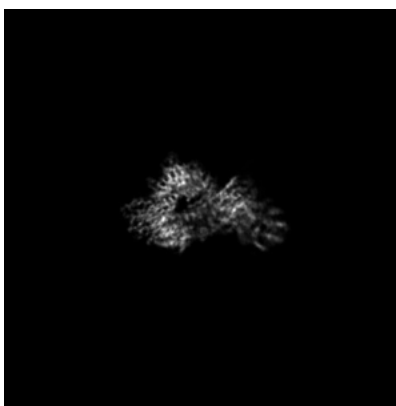
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

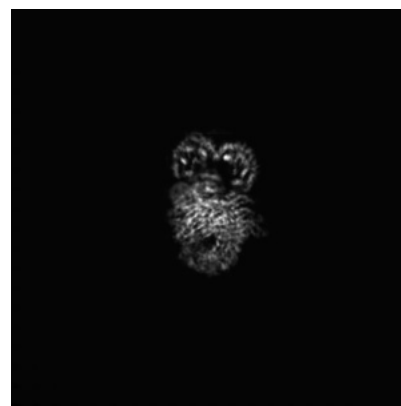
6.1.1 Primary map



X

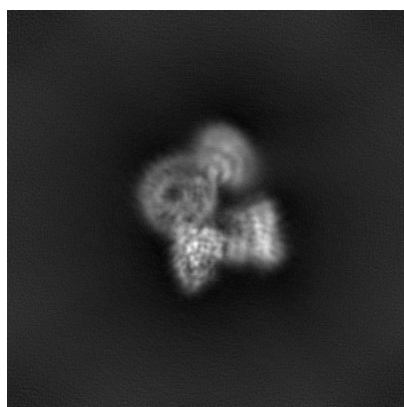


Y

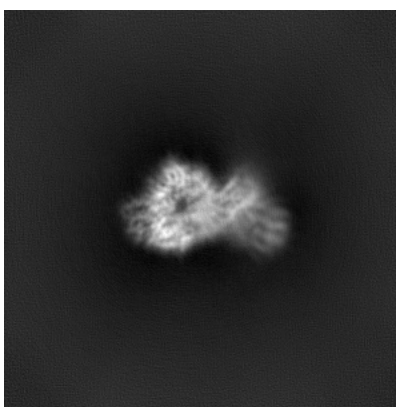


Z

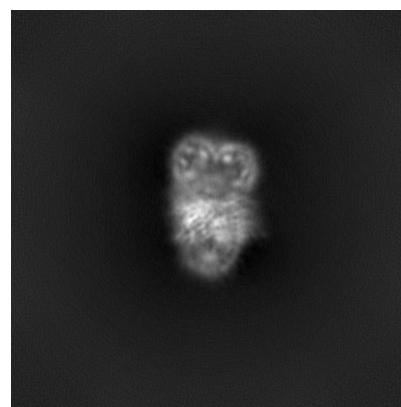
6.1.2 Raw map



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: 201

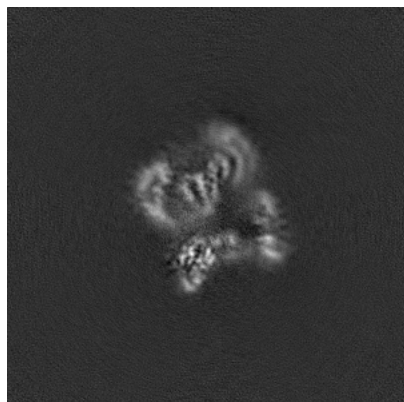


Y Index: 201

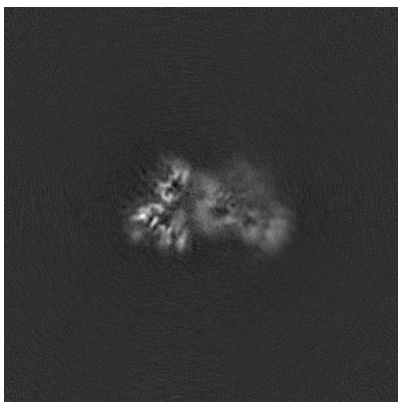


Z Index: 201

6.2.2 Raw map



X Index: 201



Y Index: 201



Z Index: 201

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: 193

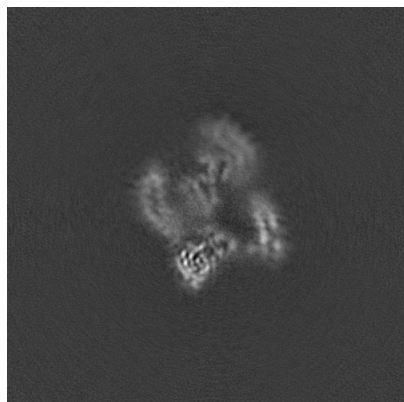


Y Index: 189

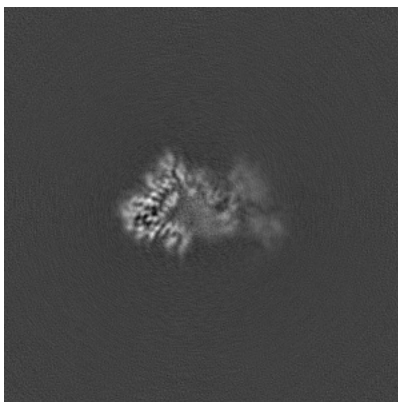


Z Index: 167

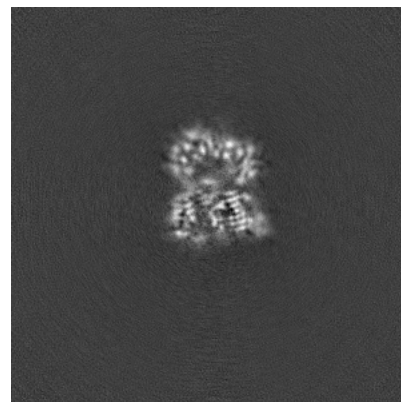
6.3.2 Raw map



X Index: 193



Y Index: 189

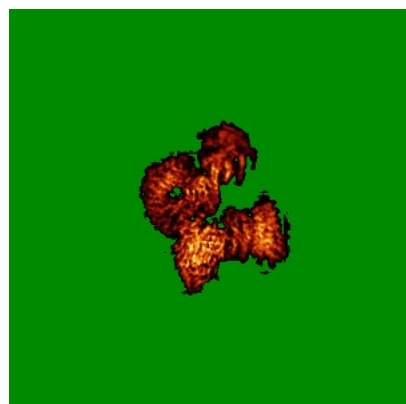


Z Index: 166

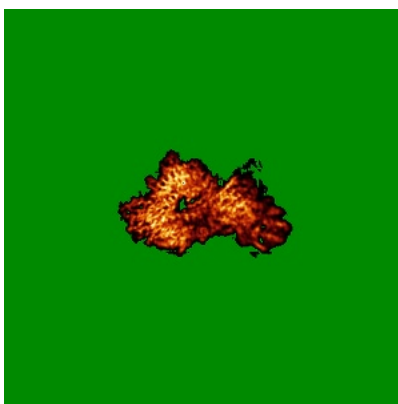
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

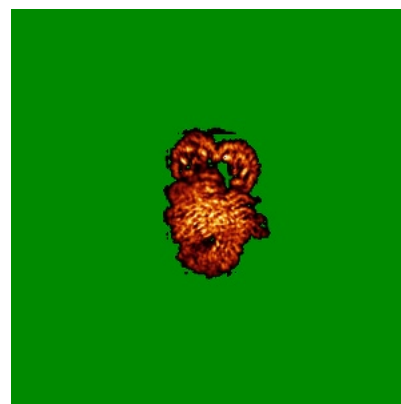
6.4.1 Primary map



X

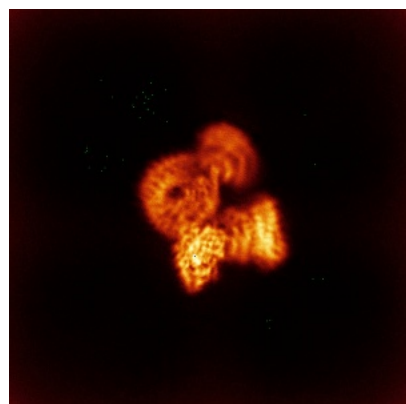


Y

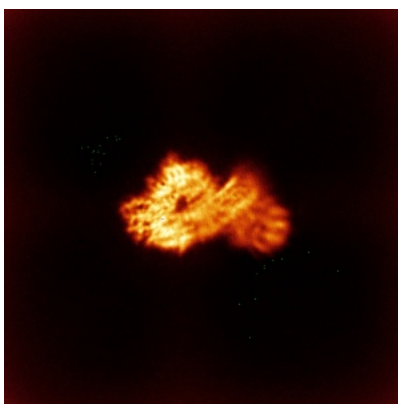


Z

6.4.2 Raw map



X



Y

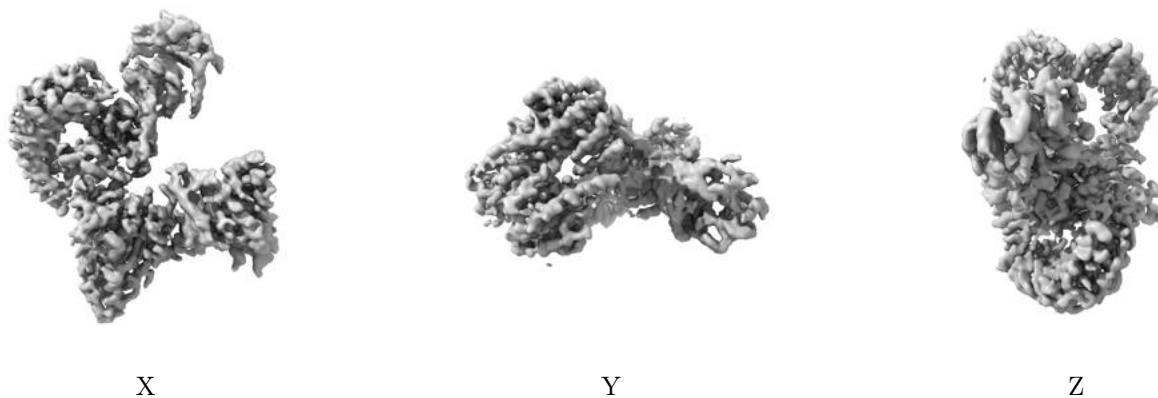


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

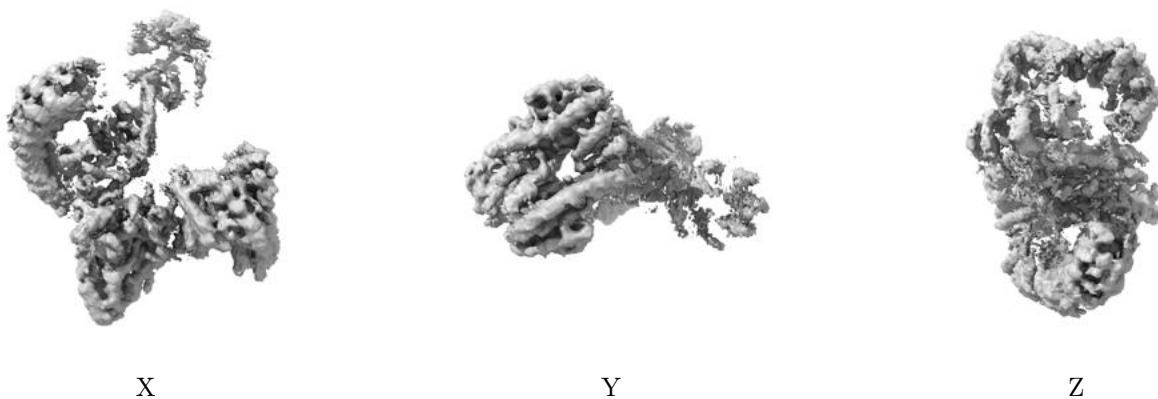
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.122. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

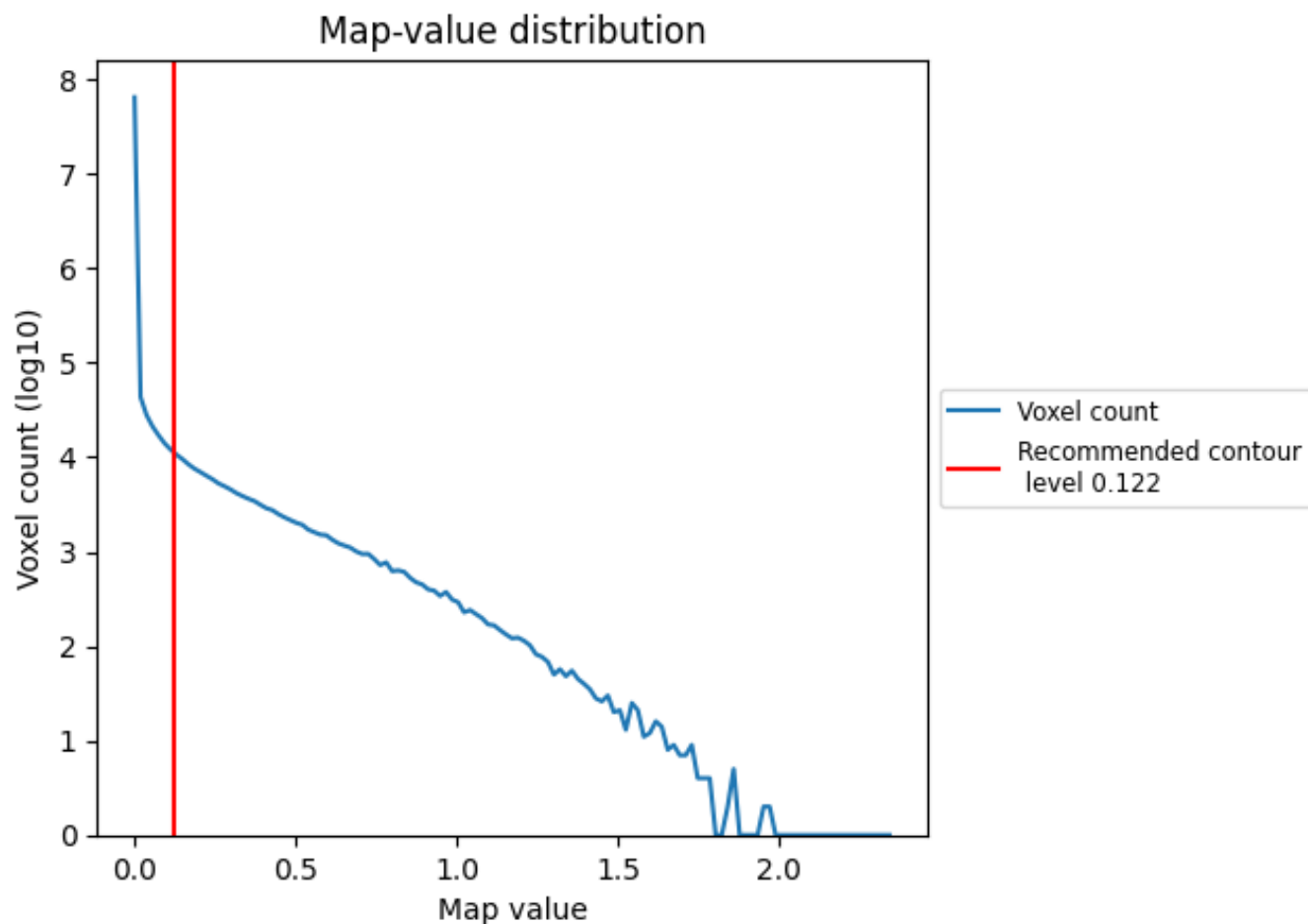
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

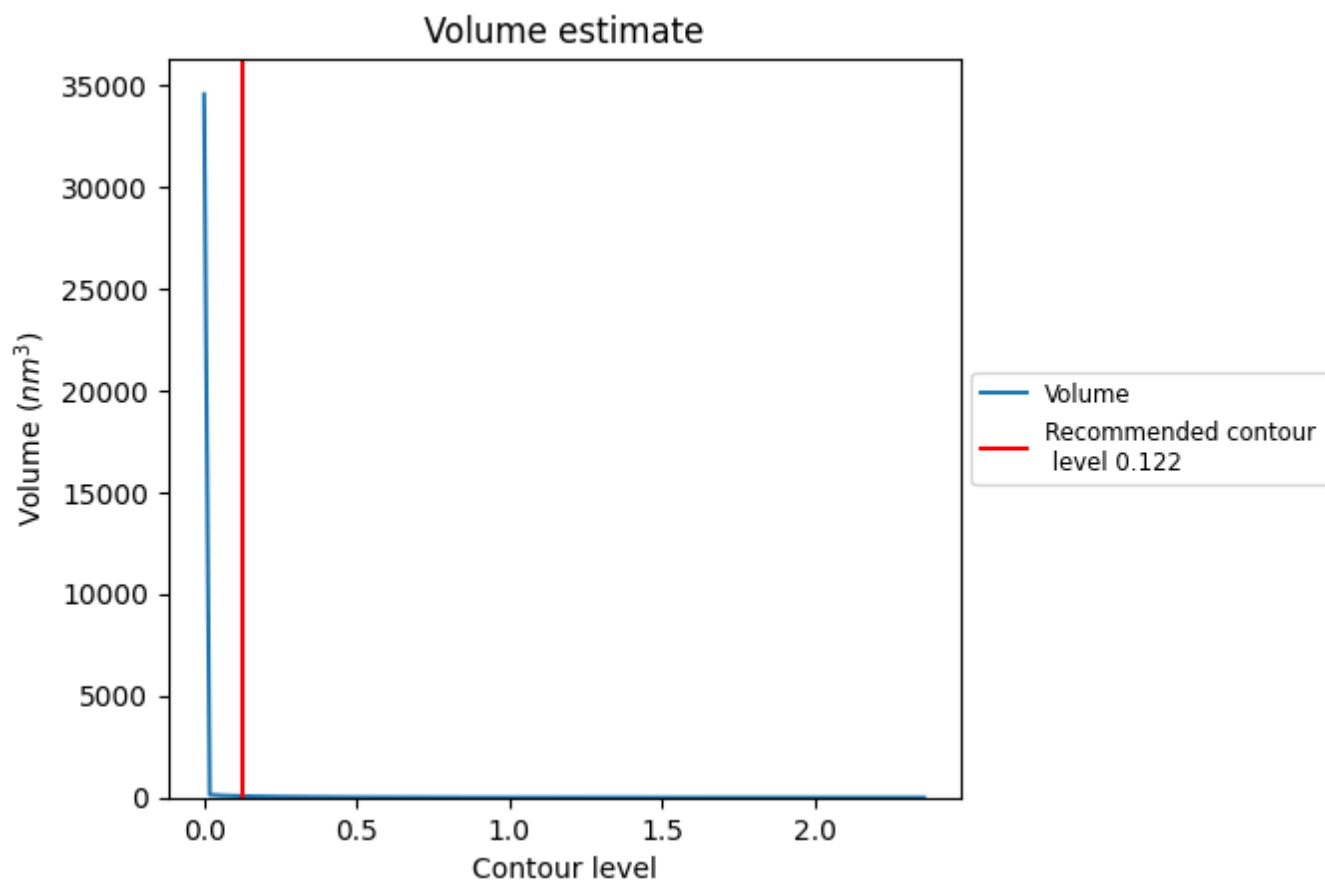
This section contains the results of statistical analysis of the map.

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.

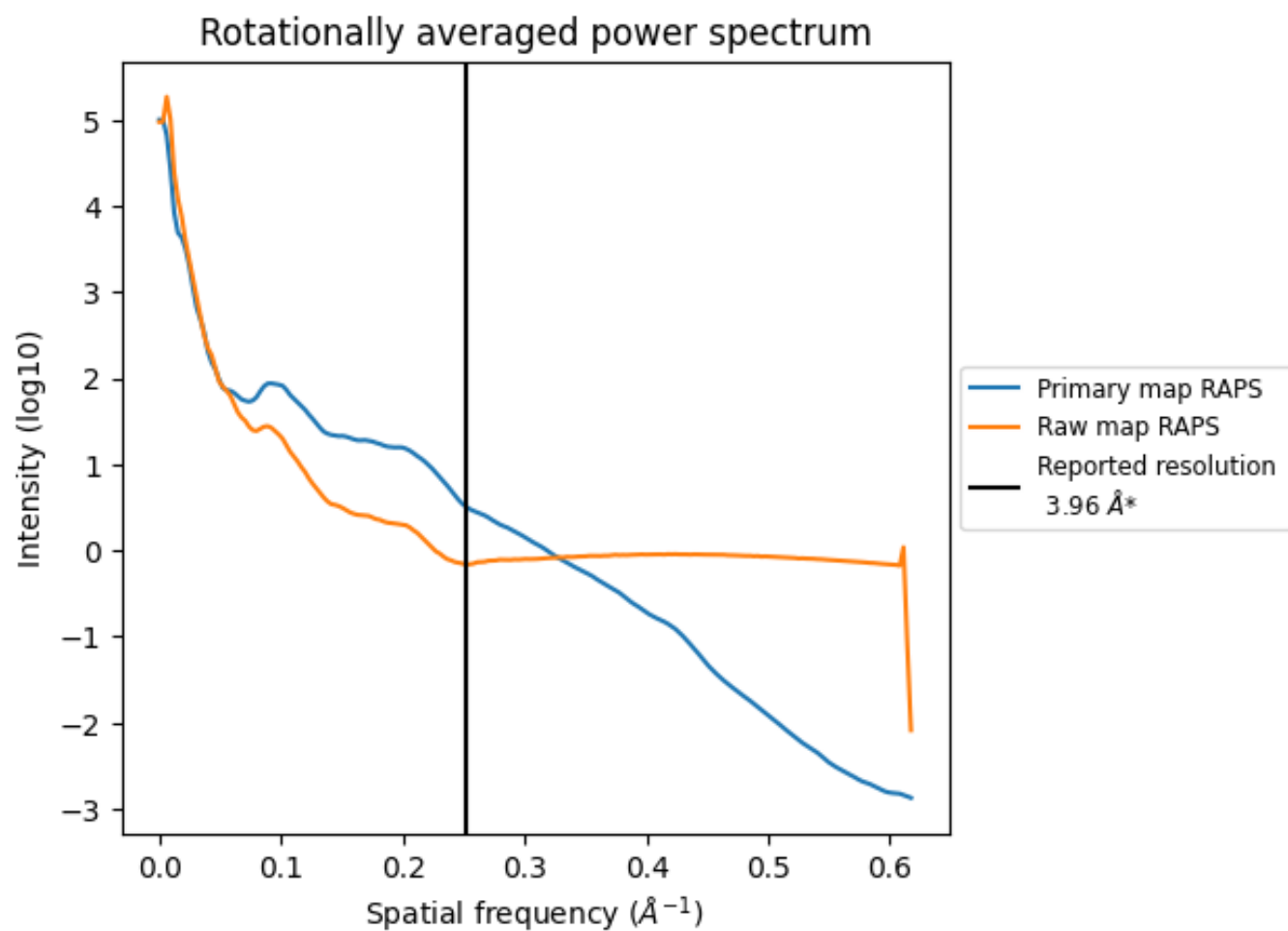
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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 ⓘ

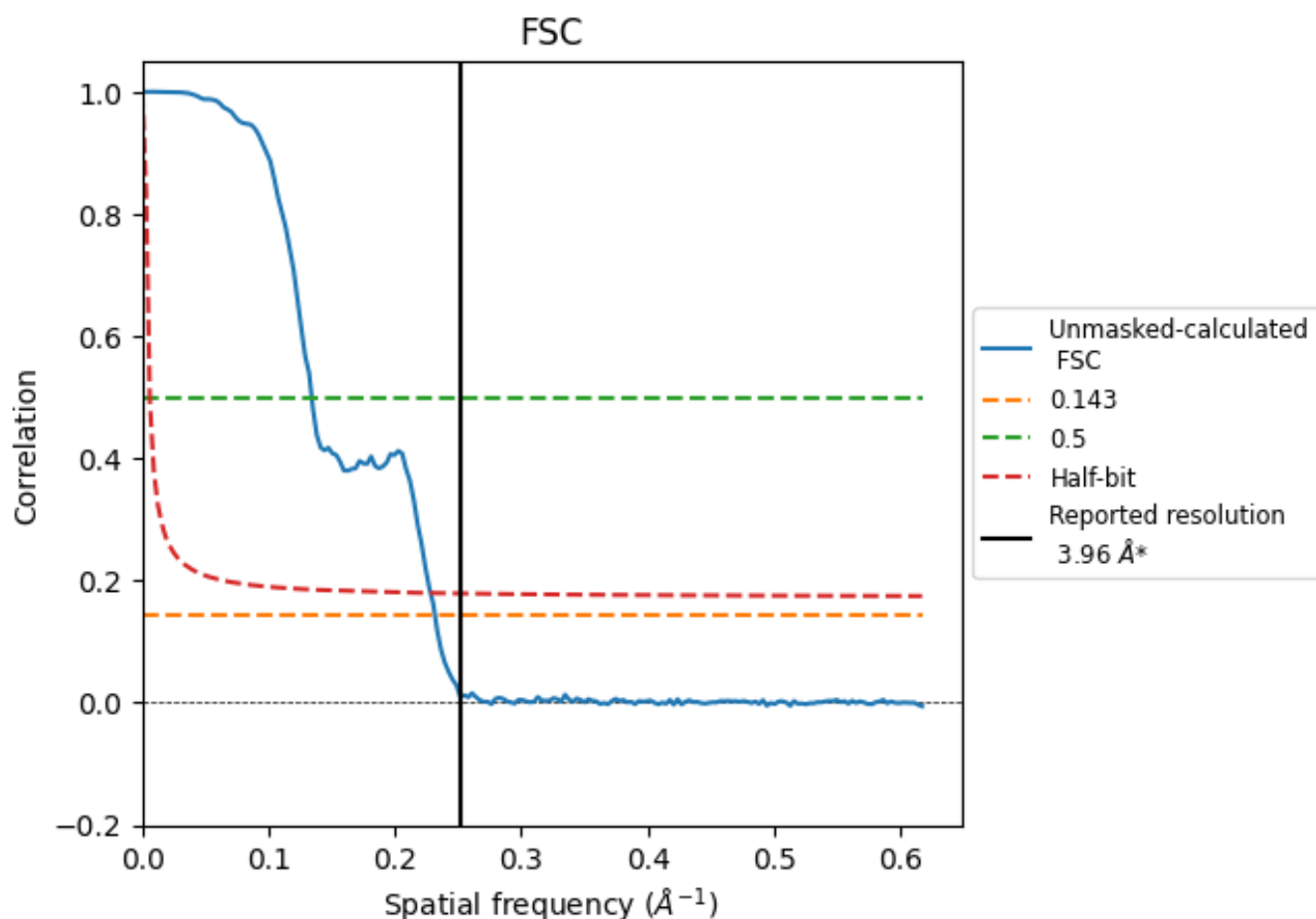


*Reported resolution corresponds to spatial frequency of 0.253 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.253 \AA^{-1}

8.2 Resolution estimates [i](#)

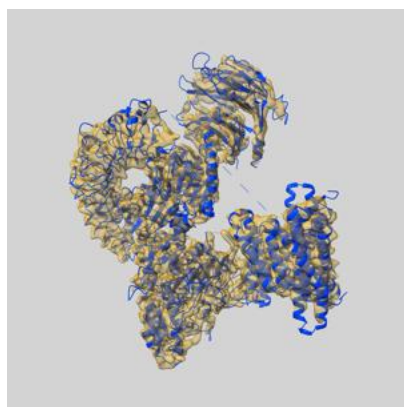
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.32	7.45	4.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

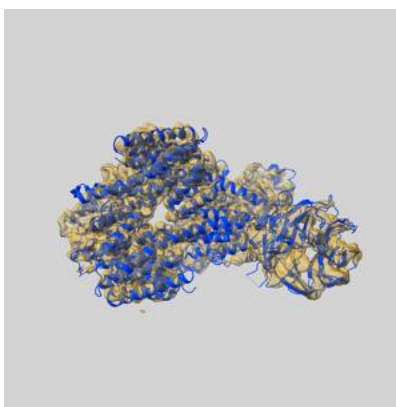
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45609 and PDB model 9CI3. Per-residue inclusion information can be found in section 3 on page 6.

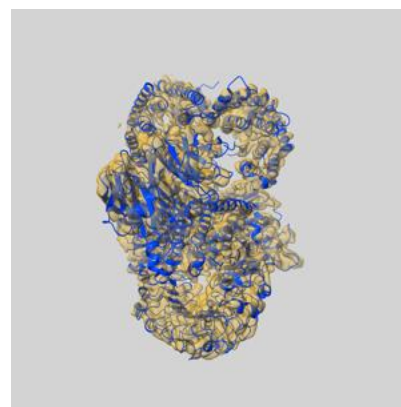
9.1 Map-model overlay [i](#)



X



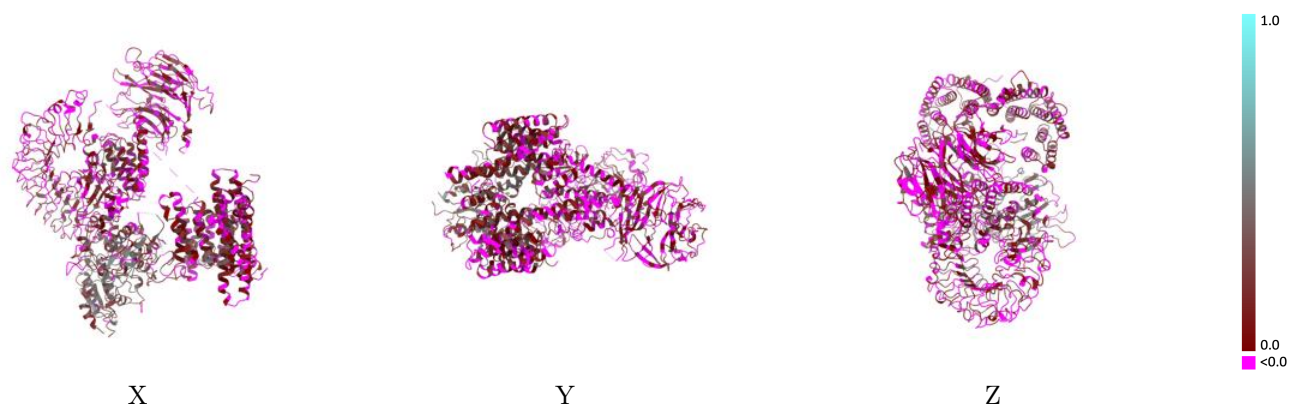
Y



Z

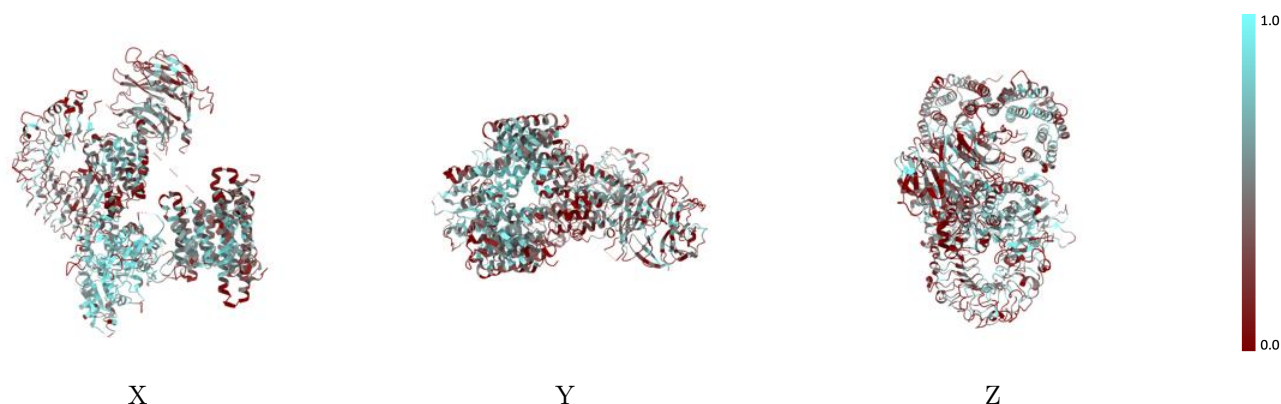
The images above show the 3D surface view of the map at the recommended contour level 0.122 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



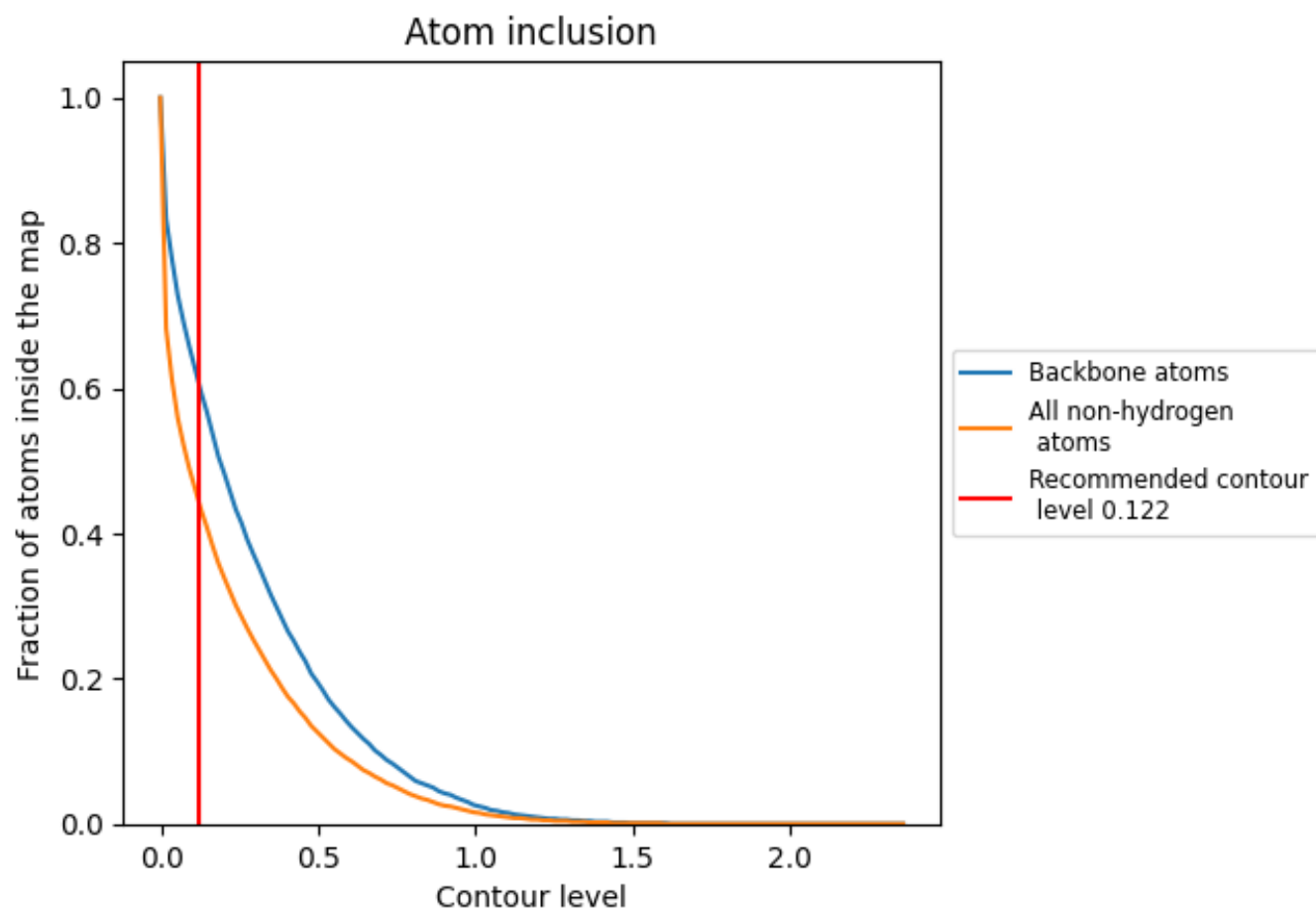
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.122).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 44% 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 (0.122) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4410	<div></div> 0.1120
A	<div></div> 0.4380	<div></div> 0.1170
B	<div></div> 0.3980	<div></div> 0.0800
C	<div></div> 0.5030	<div></div> 0.1170

