



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 11:34 PM UTC

PDB ID : 9F45 / pdb_00009f45
EMDB ID : EMD-50184
Title : cryo-EM structure of human LST2 bound to human mTOR complex 1
Authors : Craigie, L.M.; Maier, T.
Deposited on : 2024-04-26
Resolution : 3.74 Å(reported)
Based on initial model : 7PEB

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:

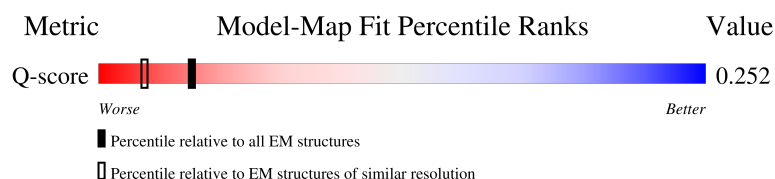
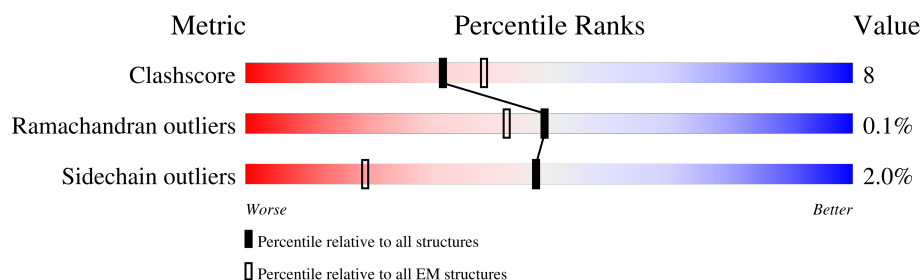
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.74 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.



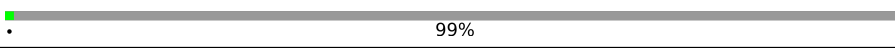
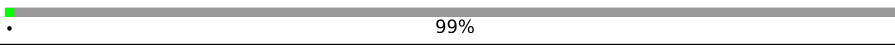
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10346 (3.24 - 4.24)

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	A	2549	 6% 67% 18% 14%
1	B	2549	 6% 68% 17% 14%
2	C	326	 1% 71% 26% 4%
2	D	326	 1% 70% 27% 4%

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Mol	Chain	Length	Quality of chain
3	E	1363	 59%18%23%
3	F	1363	 58%18%23%
4	G	887	 99%
4	H	887	 99%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 56848 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2192	Total	C	N	O	S	0	0
			17467	11158	3060	3137	112		
1	B	2192	Total	C	N	O	S	0	0
			17467	11158	3060	3137	112		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	317	Total	C	N	O	S	0	0
			2456	1526	436	476	18		
2	D	317	Total	C	N	O	S	0	0
			2456	1526	436	476	18		

- Molecule 3 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1052	Total	C	N	O	S	0	0
			8385	5361	1450	1518	56		
3	F	1052	Total	C	N	O	S	0	0
			8385	5361	1450	1518	56		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-27	HIS	-	expression tag	UNP Q8N122
E	-26	HIS	-	expression tag	UNP Q8N122
E	-25	HIS	-	expression tag	UNP Q8N122
E	-24	HIS	-	expression tag	UNP Q8N122
E	-23	HIS	-	expression tag	UNP Q8N122
E	-22	HIS	-	expression tag	UNP Q8N122
E	-21	HIS	-	expression tag	UNP Q8N122
E	-20	HIS	-	expression tag	UNP Q8N122
E	-19	HIS	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	HIS	-	expression tag	UNP Q8N122
E	-17	GLU	-	expression tag	UNP Q8N122
E	-16	GLN	-	expression tag	UNP Q8N122
E	-15	LYS	-	expression tag	UNP Q8N122
E	-14	LEU	-	expression tag	UNP Q8N122
E	-13	ILE	-	expression tag	UNP Q8N122
E	-12	SER	-	expression tag	UNP Q8N122
E	-11	GLU	-	expression tag	UNP Q8N122
E	-10	GLU	-	expression tag	UNP Q8N122
E	-9	ASP	-	expression tag	UNP Q8N122
E	-8	LEU	-	expression tag	UNP Q8N122
E	-7	ASP	-	expression tag	UNP Q8N122
E	-6	TYR	-	expression tag	UNP Q8N122
E	-5	LYS	-	expression tag	UNP Q8N122
E	-4	ASP	-	expression tag	UNP Q8N122
E	-3	ASP	-	expression tag	UNP Q8N122
E	-2	ASP	-	expression tag	UNP Q8N122
E	-1	ASP	-	expression tag	UNP Q8N122
E	0	LYS	-	expression tag	UNP Q8N122
F	-27	HIS	-	expression tag	UNP Q8N122
F	-26	HIS	-	expression tag	UNP Q8N122
F	-25	HIS	-	expression tag	UNP Q8N122
F	-24	HIS	-	expression tag	UNP Q8N122
F	-23	HIS	-	expression tag	UNP Q8N122
F	-22	HIS	-	expression tag	UNP Q8N122
F	-21	HIS	-	expression tag	UNP Q8N122
F	-20	HIS	-	expression tag	UNP Q8N122
F	-19	HIS	-	expression tag	UNP Q8N122
F	-18	HIS	-	expression tag	UNP Q8N122
F	-17	GLU	-	expression tag	UNP Q8N122
F	-16	GLN	-	expression tag	UNP Q8N122
F	-15	LYS	-	expression tag	UNP Q8N122
F	-14	LEU	-	expression tag	UNP Q8N122
F	-13	ILE	-	expression tag	UNP Q8N122
F	-12	SER	-	expression tag	UNP Q8N122
F	-11	GLU	-	expression tag	UNP Q8N122
F	-10	GLU	-	expression tag	UNP Q8N122
F	-9	ASP	-	expression tag	UNP Q8N122
F	-8	LEU	-	expression tag	UNP Q8N122
F	-7	ASP	-	expression tag	UNP Q8N122
F	-6	TYR	-	expression tag	UNP Q8N122
F	-5	LYS	-	expression tag	UNP Q8N122

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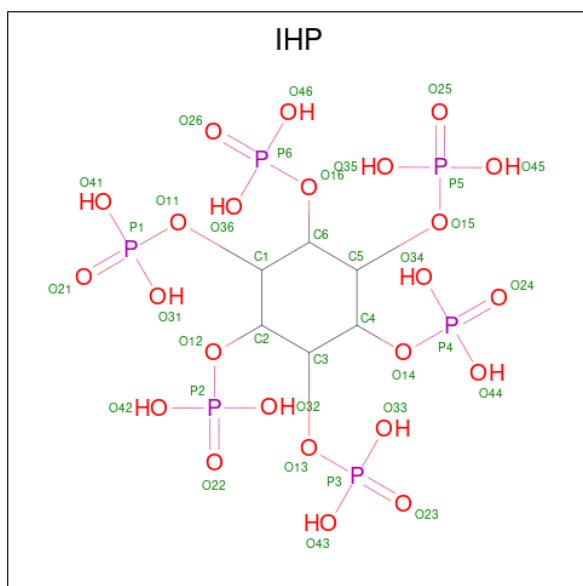
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ASP	-	expression tag	UNP Q8N122
F	-3	ASP	-	expression tag	UNP Q8N122
F	-2	ASP	-	expression tag	UNP Q8N122
F	-1	ASP	-	expression tag	UNP Q8N122
F	0	LYS	-	expression tag	UNP Q8N122

- Molecule 4 is a protein called Lateral signaling target protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	9	Total	C	N	O	S	0	0
			80	52	12	15	1		
4	H	9	Total	C	N	O	S	0	0
			80	52	12	15	1		

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).

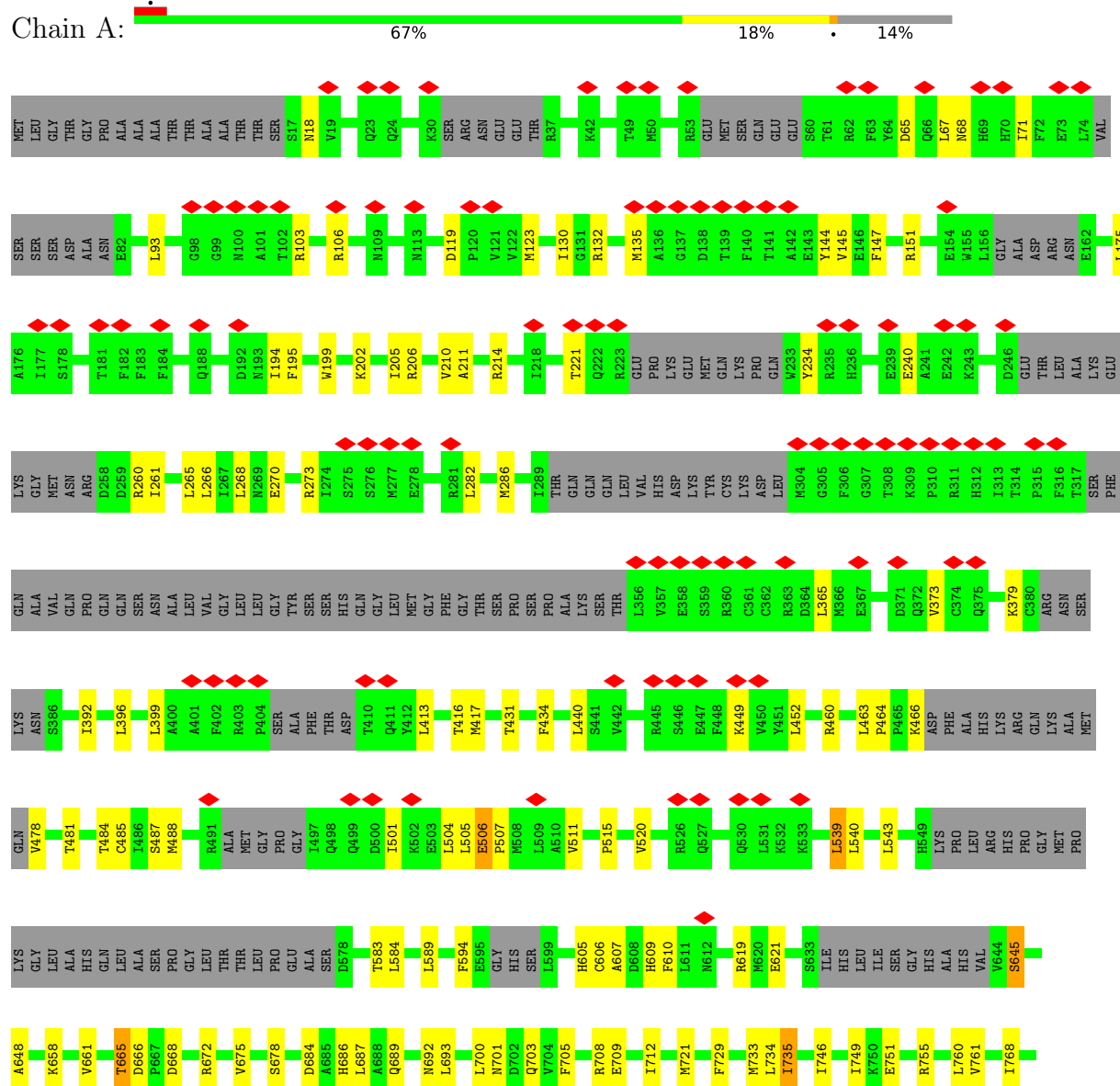


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			36	6	24	6	
5	B	1	Total	C	O	P	0
			36	6	24	6	

3 Residue-property plots

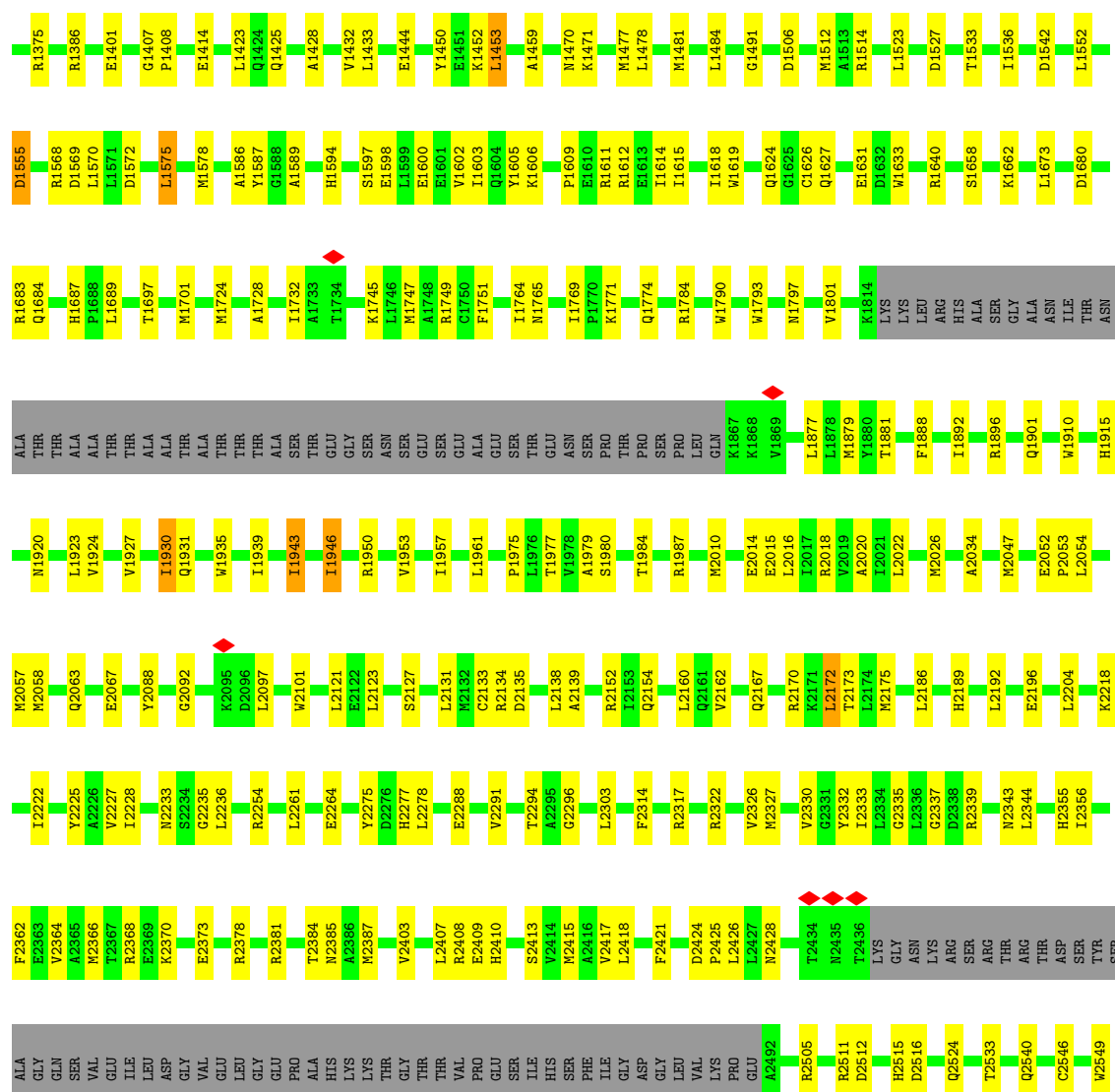
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

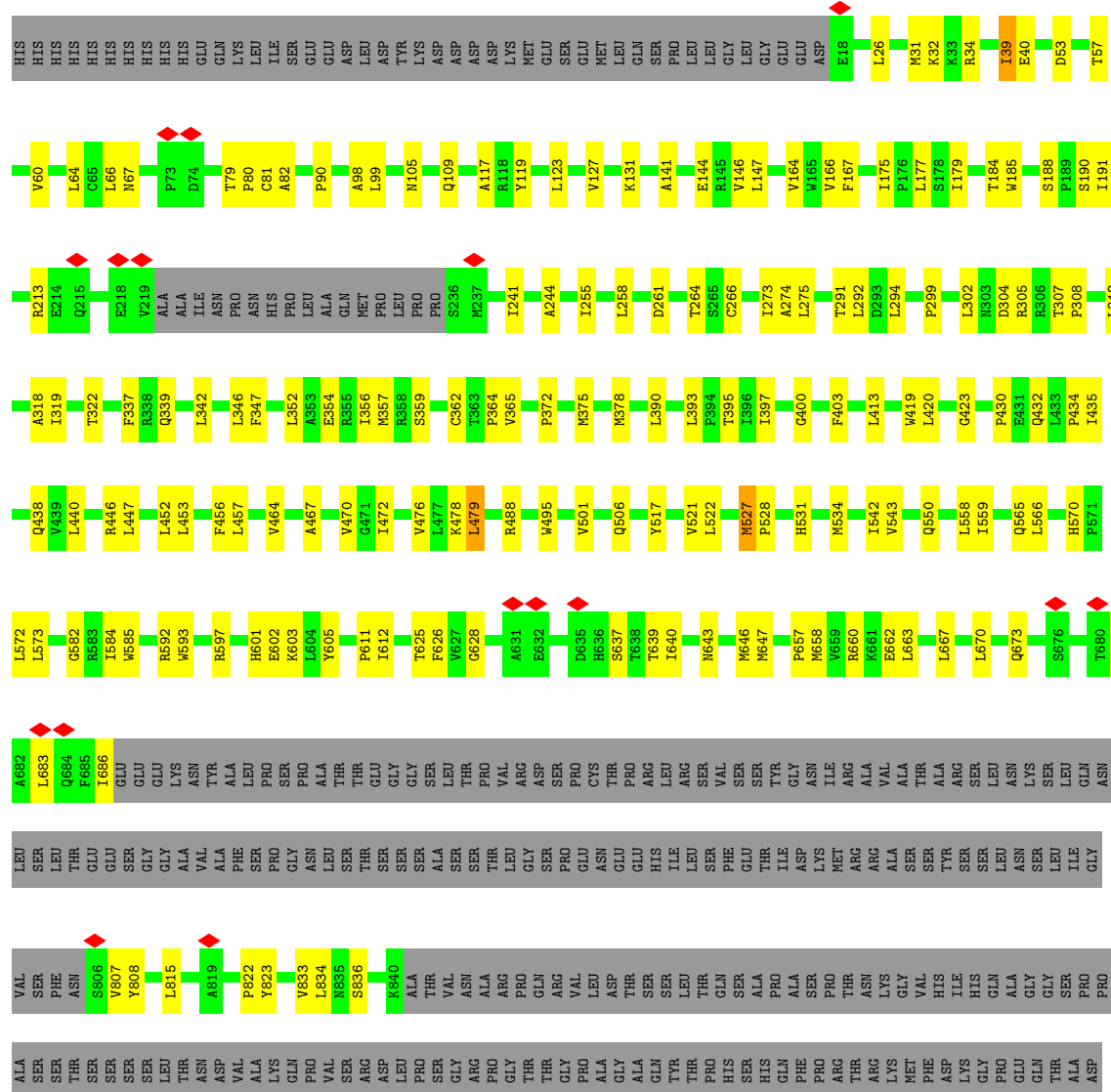
- Molecule 1: Serine/threonine-protein kinase mTOR

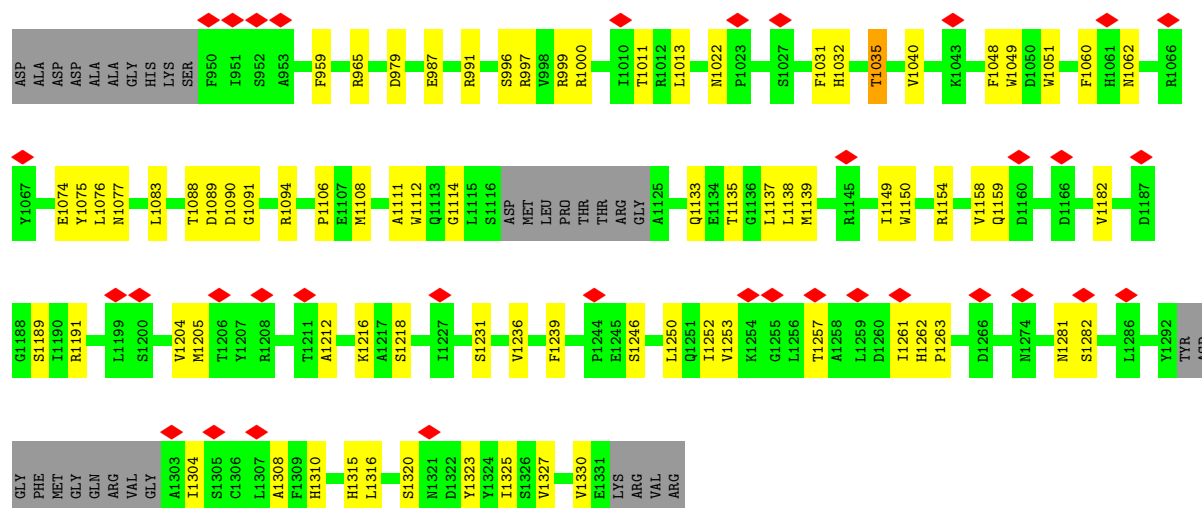


VAL	GLU	L2236	G2235	E2067	N1920	GLY	D1680	L1552	G1407	LEU	L1446	Y1030	ALA	I775
GLU	L2237	L2238	L2239	Y2088	L1923	ALA	R1683	D1569	P1408	ALA	DI147	M1031	VAL	L776
LEU	L2240	L2241	L2242	Y2089	V1924	ASN	Q1684	D1572	I1412	GLY	F1148	E1033	SER	I780
GLY	L2243	L2244	L2245	G2092	E1925	THR	H1687	L1575	L1413	PRO	T1149	I1034	LEU	L781
GLU	L2246	L2247	L2248	L2097	I1930	ASN	P1688	L1578	E1414	VAL	DI150	V1035	GLU	K762
ALA	L2249	L2250	L2251	L2101	I1943	THR	L1689	M1578	Q1425	THR	R1154	M1038	LYS	L783
HIS	L2252	L2253	L2254	W2101	I1946	THR	T1697	A1586	A1428	GLY	I1155	W1042	SER	P786
LYS	L2255	L2256	L2257	ALA	I1949	ALA	M1701	Y1587	V1432	MET	H1157	V1043	PRO	ASP
THR	L2258	L2259	L2260	THR	R1950	THR	M1724	V1591	L1433	LYS	P1158	M1044	ASP	ASP
GLY	L2261	L2262	L2263	ALA	V1953	ALA	A1728	M1595	E1444	LEU	DI164	N1045	SER	PRO
ASP	L2264	L2265	L2266	THR	L1961	ALA	A1732	M1596	Y1450	HIS	P1167	Q1049	ASP	M791
GLY	L2267	L2268	L2269	THR	I1973	THR	I1746	S1597	E1451	VAL	E1168	I1056	SER	V794
LEU	L2270	L2271	L2272	THR	I1974	THR	K1745	E1598	K1452	THR	L1169	I1055	THR	V798
GLY	L2273	L2274	L2275	THR	P1975	ALA	L1746	L1599	L1453	THR	R1170	A1062	SER	L799
ASP	L2276	L2277	L2278	ALA	A1979	SER	M1747	E1601	L1483	THR	S1178	L1063	THR	A800
GLY	L2279	L2280	L2281	THR	A1984	GLY	A1748	V1602	M1481	THR	I1190	G1064	THR	I802
LEU	L2282	L2283	L2284	GLY	T1984	GLY	R1749	I1603	N1470	THR	F1191	F1067	THR	G803
GLY	L2285	L2286	L2287	SER	T1985	SER	G1750	G1504	K1471	THR	V1195	I1075	THR	E804
ASP	L2288	L2289	L2290	ASN	T1986	SER	F1751	Y1605	E1472	THR	H1202	I1070	THR	Q807
GLY	L2291	L2292	L2293	ASN	R1987	ASN	K1753	K1606	D1473	THR	R1203	L1071	THR	L820
LEU	L2294	L2295	L2296	GLY	Q2007	SER	L1764	P1609	M1481	THR	R1208	Q1073	THR	D830
GLY	L2297	L2298	L2299	GLY	M2010	GLY	N1765	R1611	L1484	THR	H1202	I1075	THR	Q846
ASP	L2300	L2301	L2302	ALA	E2014	GLY	I1769	R1612	E1489	THR	R1203	L1079	THR	S850
GLY	L2303	L2304	L2305	GLU	E2015	SER	P1771	E1613	W1490	THR	I1204	D1085	THR	S850
LEU	L2306	L2307	L2308	THR	L2016	THR	K1771	I1615	N1505	THR	R1208	Q1090	THR	E856
GLY	L2309	L2310	L2311	ASN	L2017	ASN	Q1774	G1617	D1506	THR	L1222	R1090	THR	P857
ASP	L2312	L2313	L2314	SER	R2018	SER	R1784	I1618	W1509	THR	ALA	S1093	THR	M877
GLY	L2315	L2316	L2317	PRO	L2022	THR	S1785	W1619	Q1509	THR	ASP	I1094	THR	Q878
LEU	L2318	L2319	L2320	THR	M2026	PRO	W1786	R1622	M1512	THR	GLU	L1097	THR	G879
GLY	L2321	L2322	L2323	PRO	A2034	PRO	Y1787	L1623	A1513	THR	GLU	L1097	THR	T880
ASP	L2324	L2325	L2326	LEU	L2034	LEU	K1788	G1624	R1514	THR	ASP	I1100	THR	R881
GLY	L2327	L2328	L2329	GLN	G2040	GLN	A1789	C1626	A1519	THR	PRO	F1103	THR	R882
ASP	L2330	L2331	L2332	GLY	E2041	GLY	W1790	Q1627	D1527	THR	LEU	F1103	THR	I885
LEU	L2333	L2334	L2335	GLY	L2047	GLY	W1793	E1631	D1527	THR	TVR	N1106	THR	L890
GLY	L2336	L2337	L2338	GLY	M2047	GLY	N1797	R1640	E1530	THR	GLN	C1004	THR	L890
ASP	L2339	L2340	L2341	THR	E2052	THR	V1801	V1643	T1533	THR	HIS	L1111	THR	I303
GLY	L2342	L2343	L2344	THR	P2053	THR	K1814	V1644	T1533	THR	ARG	R1009	THR	GLY
LEU	L2345	L2346	L2347	THR	L2054	THR	LVS	LVS	I1536	THR	MET	V1020	THR	ILE
ASP	L2348	L2349	L2350	THR	M2057	THR	LVS	S1658	D1542	THR	ARG	V1119	THR	ASP
GLY	L2351	L2352	L2353	THR	M2058	THR	LEU	K1662	F1545	THR	GLY	F1122	THR	GLN
ASP	L2354	L2355	L2356	THR	E2059	THR	ARG	K1662	F1545	THR	GLY	F1122	THR	SER
GLY	L2357	L2358	L2359	THR	Q2063	THR	HIS	L1673	L1550	THR	GLY	L1129	THR	ARG
ASP	L2360	L2361	L2362	THR	L2063	THR	ALA	L1673	L1550	THR	GLY	L1129	THR	ASP
GLY	L2363	L2364	L2365	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	ALA
ASP	L2366	L2367	L2368	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2369	L2370	L2371	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2372	L2373	L2374	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2375	L2376	L2377	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2378	L2379	L2380	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2381	L2382	L2383	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2384	L2385	L2386	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2387	L2388	L2389	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2390	L2391	L2392	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2393	L2394	L2395	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2396	L2397	L2398	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2399	L2400	L2401	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2402	L2403	L2404	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2405	L2406	L2407	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2408	L2409	L2410	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2411	L2412	L2413	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2414	L2415	L2416	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2417	L2418	L2419	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2420	L2421	L2422	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2423	L2424	L2425	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2426	L2427	L2428	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2429	L2430	L2431	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2432	L2433	L2434	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2435	L2436	L2437	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2438	L2439	L2440	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2441	L2442	L2443	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2444	L2445	L2446	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2447	L2448	L2449	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2450	L2451	L2452	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2453	L2454	L2455	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2456	L2457	L2458	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2459	L2460	L2461	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2462	L2463	L2464	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2465	L2466	L2467	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2468	L2469	L2470	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2471	L2472	L2473	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2474	L2475	L2476	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2477	L2478	L2479	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2480	L2481	L2482	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2483	L2484	L2485	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2486	L2487	L2488	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2489	L2490	L2491	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2492	L2493	L2494	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2495	L2496	L2497	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2498	L2499	L2500	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2501	L2502	L2503	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2504	L2505	L2506	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2507	L2508	L2509	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2510	L2511	L2512	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2513	L2514	L2515	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2516	L2517	L2518	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2519	L2520	L2521	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2522	L2523	L2524	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2525	L2526	L2527	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2528	L2529	L2530	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2531	L2532	L2533	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
ASP	L2534	L2535	L2536	THR	L2063	THR	SER	L1673	L1550	THR	ALA	D1140	THR	SER
GLY	L2537	L2538	L2											



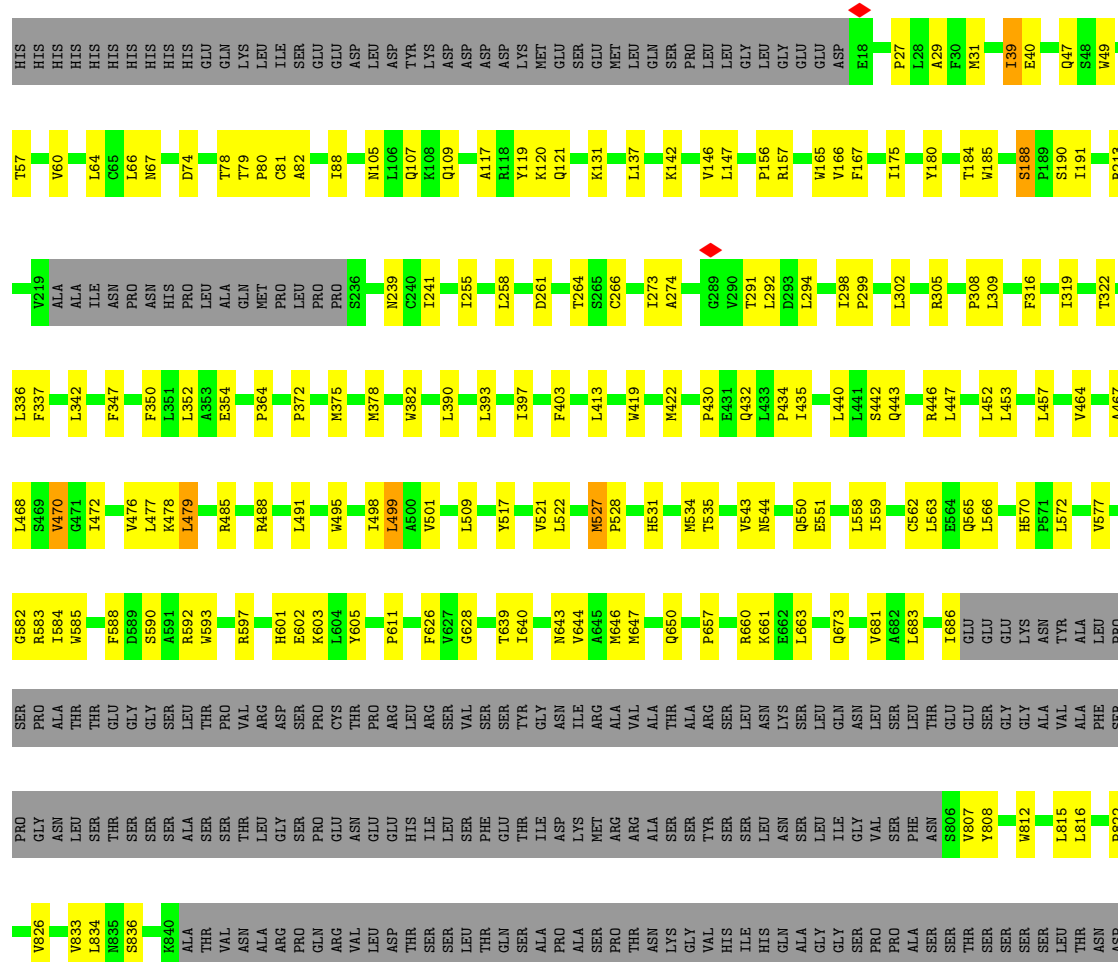


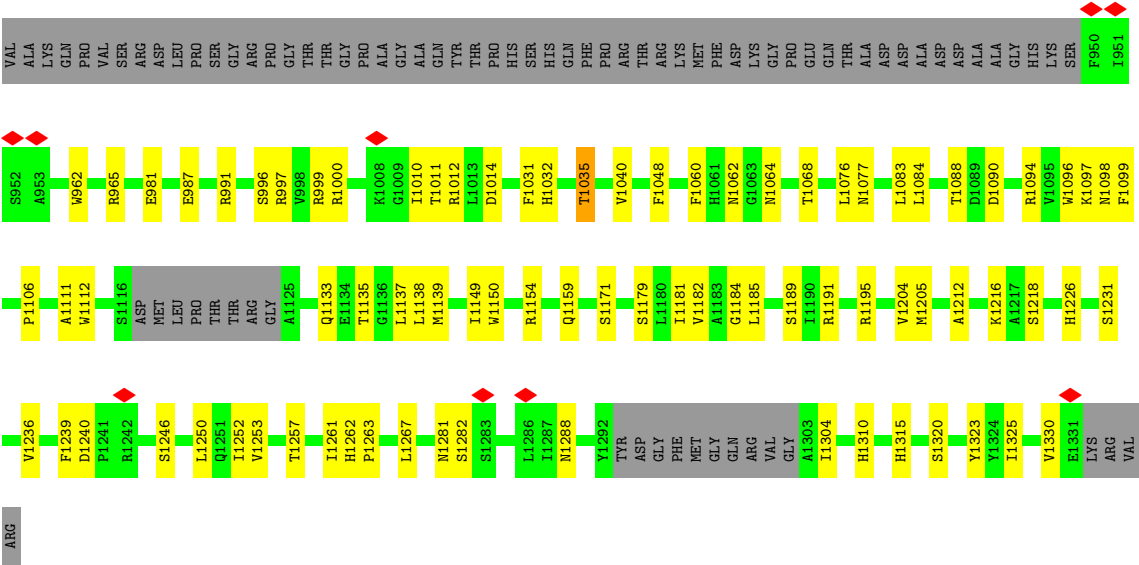




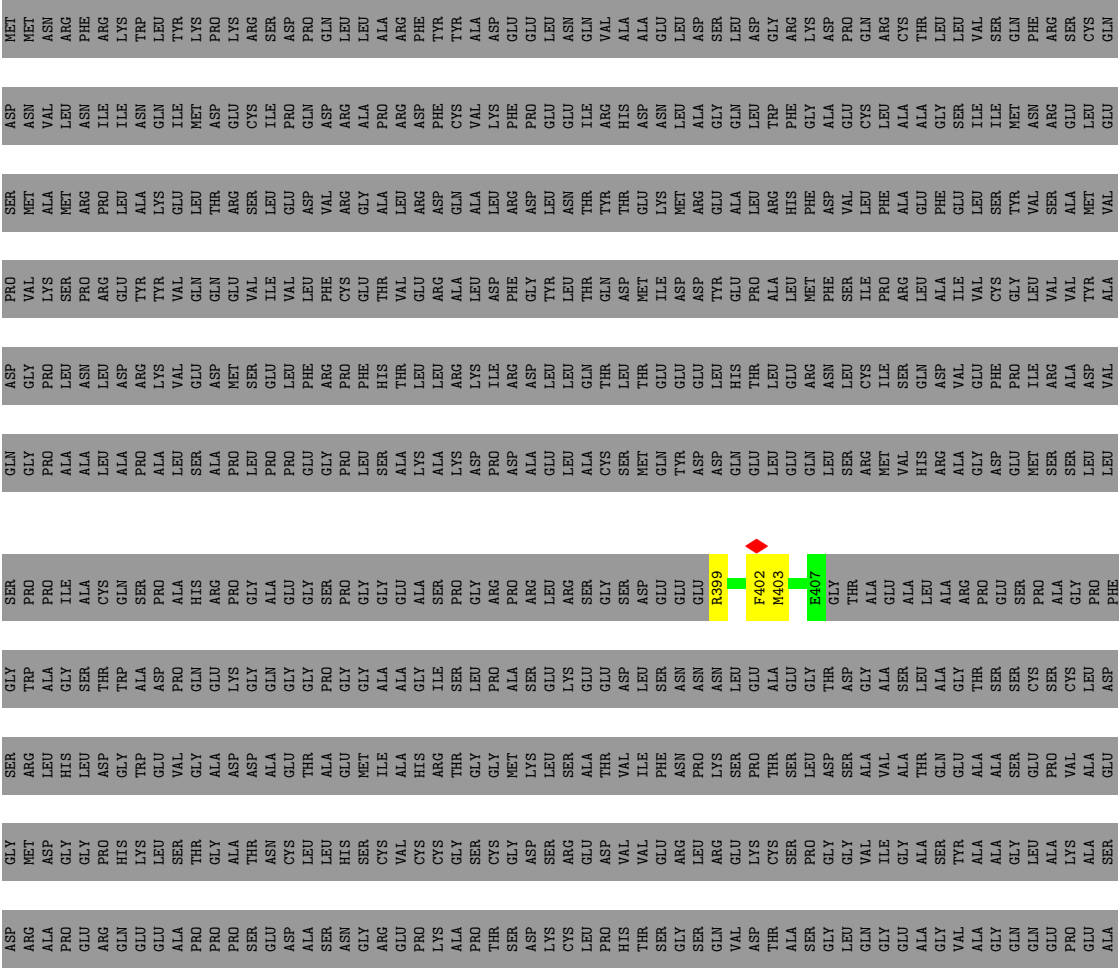
• Molecule 3: Regulatory-associated protein of mTOR

Chain F: 58% 18% 23%





• Molecule 4: Lateral signaling target protein 2 homolog



- Molecule 4: Lateral signaling target protein 2 homolog

Chain H: 99%

[illegible]

LYS
ILE
PHE
CYS
SER
ARG
CYS
SER
SER
HIS
SER
ALA
PRO
LEU
PRO
ARG
TYR
GLY
GLN
VAL
LYS
PRO
VAL
VAL
VAL
CYS
THR
HIS
CYS
TYR
MET
PHE
HIS
VAL
THR
PRO
PHE
TYR
SER
ASP
LYS
ALA
GLY
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	272762	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	61.816	Depositor
Minimum map value	-20.377	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	1.017	Depositor
Recommended contour level	8	Depositor
Map size (Å)	670.72, 670.72, 670.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.12	0/17814	0.28	0/24116
1	B	0.12	0/17814	0.28	0/24116
2	C	0.11	0/2514	0.31	0/3426
2	D	0.12	0/2514	0.32	0/3426
3	E	0.10	0/8585	0.27	0/11680
3	F	0.11	0/8585	0.27	0/11680
4	G	0.12	0/81	0.35	0/107
4	H	0.13	0/81	0.35	0/107
All	All	0.12	0/57988	0.28	0/78658

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	17467	0	17553	291	0
1	B	17467	0	17553	281	0
2	C	2456	0	2341	52	0
2	D	2456	0	2341	54	0
3	E	8385	0	8375	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	8385	0	8375	156	0
4	G	80	0	71	3	0
4	H	80	0	71	3	0
5	A	36	0	6	1	0
5	B	36	0	6	1	0
All	All	56848	0	56692	962	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 8.

All (962) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1943:ILE:HA	1:B:1946:ILE:HD13	1.59	0.83
1:A:1943:ILE:HA	1:A:1946:ILE:HD13	1.63	0.81
3:E:39:ILE:HD11	3:E:959:PHE:HA	1.63	0.80
1:A:1793:TRP:O	1:A:1797:ASN:ND2	2.19	0.75
1:B:751:GLU:HB2	1:B:794:VAL:HG22	1.68	0.74
3:F:660:ARG:NH2	3:F:1111:ALA:O	2.21	0.74
1:B:1042:TRP:HE1	1:B:1049:GLN:HG2	1.53	0.73
1:A:1943:ILE:HD12	1:A:1975:PRO:HB2	1.68	0.72
2:D:274:TRP:HE1	2:D:316:VAL:HA	1.54	0.72
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.72	0.72
1:A:689:GLN:HE22	3:F:419:TRP:HA	1.55	0.71
1:B:2222:ILE:HD11	1:B:2330:VAL:HG21	1.73	0.71
2:C:166:ILE:HD11	2:C:169:PRO:HA	1.72	0.71
2:C:194:CYS:HB3	2:C:216:ILE:HB	1.71	0.71
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.24	0.70
3:E:1252:ILE:HG22	3:E:1253:VAL:HG23	1.73	0.70
1:B:2277:HIS:O	2:D:87:ASN:ND2	2.21	0.69
2:D:19:GLY:HA2	2:D:316:VAL:HG22	1.73	0.69
2:C:63:GLN:HG2	2:C:85:ASN:HA	1.75	0.69
2:D:63:GLN:HG2	2:D:85:ASN:HA	1.73	0.69
3:E:413:LEU:HD12	3:E:452:LEU:HD12	1.75	0.69
3:F:628:GLY:O	3:F:673:GLN:NE2	2.26	0.69
1:A:2408:ARG:NH2	1:A:2524:GLN:OE1	2.26	0.69
3:E:660:ARG:NH2	3:E:1111:ALA:O	2.25	0.69
1:A:2222:ILE:HD11	1:A:2330:VAL:HG21	1.76	0.68
1:B:2170:ARG:HB2	1:B:2186:LEU:HB2	1.75	0.68
1:A:487:SER:HB3	1:A:520:VAL:HG13	1.75	0.68
1:B:689:GLN:HE22	3:E:419:TRP:HA	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:19:GLY:HA2	2:C:316:VAL:HG22	1.75	0.68
1:B:782:LYS:HD2	1:B:798:VAL:HG21	1.75	0.68
1:A:751:GLU:HB2	1:A:794:VAL:HG22	1.76	0.67
1:A:782:LYS:HD2	1:A:798:VAL:HG21	1.75	0.67
3:F:1212:ALA:HB3	3:F:1231:SER:HB2	1.75	0.67
1:A:1987:ARG:HH22	1:A:2426:LEU:HD11	1.58	0.67
1:B:68:ASN:HD21	1:B:93:LEU:HD12	1.60	0.67
2:D:101:TYR:HE2	2:D:136:LEU:HD13	1.60	0.67
1:B:686:HIS:O	1:B:692:ASN:ND2	2.28	0.66
2:C:275:GLY:HA3	2:C:288:ALA:H	1.60	0.66
3:E:184:THR:OG1	3:E:213:ARG:NH2	2.28	0.66
3:F:1252:ILE:HG22	3:F:1253:VAL:HG23	1.76	0.66
2:C:17:THR:HB	2:C:27:TRP:HE1	1.60	0.66
2:C:246:ILE:HD12	2:C:256:THR:HB	1.76	0.66
1:A:878:GLN:NE2	1:A:1572:ASP:OD2	2.28	0.66
1:B:1307:ALA:HB1	1:B:1314:ALA:HB2	1.78	0.66
1:A:1178:SER:OG	1:A:1208:ARG:NH2	2.28	0.65
1:B:487:SER:HB3	1:B:520:VAL:HG13	1.77	0.65
1:B:2218:LYS:O	1:B:2322:ARG:NH1	2.29	0.65
3:F:639:THR:O	3:F:643:ASN:ND2	2.27	0.65
2:D:198:ASN:HB2	2:D:211:ILE:HB	1.77	0.65
1:B:2204:LEU:HD22	1:B:2417:VAL:HG21	1.79	0.65
1:B:2332:TYR:OH	1:B:2512:ASP:OD2	2.15	0.65
1:B:1987:ARG:HH22	1:B:2426:LEU:HD11	1.61	0.65
3:F:1310:HIS:HB2	3:F:1315:HIS:HB2	1.79	0.65
3:E:1218:SER:HB3	3:E:1261:ILE:HD12	1.78	0.65
3:F:592:ARG:NH1	3:F:626:PHE:O	2.29	0.65
3:E:440:LEU:HD12	3:E:472:ILE:HD11	1.78	0.65
1:A:2332:TYR:OH	1:A:2512:ASP:OD2	2.15	0.65
3:E:1236:VAL:HB	3:E:1250:LEU:HB2	1.77	0.64
1:B:583:THR:HG23	1:B:621:GLU:HG3	1.78	0.64
1:B:2288:GLU:OE1	2:D:221:ARG:NH2	2.29	0.64
3:F:531:HIS:HA	3:F:534:MET:HE3	1.79	0.64
1:B:65:ASP:OD2	1:B:106:ARG:NH1	2.30	0.64
3:F:184:THR:OG1	3:F:213:ARG:NH2	2.26	0.64
1:A:1274:ARG:HH21	1:A:1283:TRP:HD1	1.46	0.64
1:B:2162:VAL:HG22	1:B:2170:ARG:HG3	1.80	0.64
1:A:1268:ALA:O	1:A:1283:TRP:NE1	2.29	0.64
2:D:166:ILE:HD11	2:D:169:PRO:HA	1.78	0.64
3:E:488:ARG:HD2	3:E:521:VAL:HG22	1.78	0.63
1:A:68:ASN:HD21	1:A:93:LEU:HD12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2018:ARG:NH1	1:A:2067:GLU:OE2	2.31	0.63
1:B:2254:ARG:NH2	1:B:2264:GLU:OE2	2.30	0.63
1:B:2408:ARG:NH2	1:B:2524:GLN:OE1	2.32	0.63
2:C:91:VAL:HG12	2:C:102:THR:HG22	1.80	0.63
2:D:46:ASN:N	2:D:60:ALA:O	2.25	0.63
1:A:583:THR:HG23	1:A:621:GLU:HG3	1.80	0.63
1:B:1425:GLN:HG3	1:B:2314:PHE:HZ	1.63	0.63
1:B:1697:THR:O	1:B:1701:MET:HG3	1.98	0.63
3:E:40:GLU:O	3:E:965:ARG:NH2	2.32	0.63
3:F:1236:VAL:HB	3:F:1250:LEU:HB2	1.79	0.63
3:E:592:ARG:NH1	3:E:626:PHE:O	2.32	0.62
1:B:506:GLU:HG3	1:B:507:PRO:HD3	1.82	0.62
1:A:1307:ALA:HB1	1:A:1314:ALA:HB2	1.81	0.62
1:A:661:VAL:O	1:A:665:THR:OG1	2.15	0.62
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.33	0.62
1:B:2018:ARG:NH1	1:B:2067:GLU:OE2	2.33	0.61
1:A:2170:ARG:HB2	1:A:2186:LEU:HB2	1.81	0.61
3:F:464:VAL:HB	3:F:501:VAL:HG21	1.82	0.61
1:A:2254:ARG:NH2	1:A:2264:GLU:OE2	2.31	0.61
3:E:531:HIS:HA	3:E:534:MET:HE3	1.82	0.61
2:C:198:ASN:HB2	2:C:211:ILE:HB	1.82	0.61
1:A:686:HIS:O	1:A:692:ASN:ND2	2.32	0.61
2:C:147:ASP:OD2	2:C:149:SER:OG	2.16	0.61
3:F:1083:LEU:HD23	3:F:1097:LYS:HD3	1.82	0.61
1:B:1915:HIS:HB3	1:B:1950:ARG:HD3	1.83	0.61
1:A:65:ASP:OD2	1:A:106:ARG:NH1	2.32	0.61
3:E:432:GLN:HG3	3:E:435:ILE:HD12	1.81	0.61
1:B:2016:LEU:HD12	1:B:2186:LEU:HD21	1.83	0.61
2:C:152:ILE:N	2:C:165:LEU:O	2.33	0.61
1:A:1444:GLU:N	1:A:1444:GLU:OE1	2.34	0.61
1:A:2052:GLU:HG3	1:A:2053:PRO:HD3	1.82	0.61
3:F:131:LYS:HZ3	3:F:185:TRP:CD1	2.19	0.61
1:A:1190:ILE:HG23	1:B:661:VAL:HG23	1.83	0.60
3:E:639:THR:O	3:E:643:ASN:ND2	2.28	0.60
3:F:646:MET:HE3	3:F:807:VAL:HG13	1.82	0.60
1:A:214:ARG:HE	1:A:273:ARG:HH22	1.49	0.60
1:A:1346:THR:HA	1:A:1386:ARG:HH21	1.66	0.60
1:A:776:LEU:HD11	1:A:820:LEU:HD21	1.82	0.60
1:B:1024:LYS:HA	1:B:1062:ALA:HB1	1.82	0.60
1:A:1552:LEU:O	1:A:1606:LYS:NZ	2.34	0.60
1:B:893:ALA:H	1:B:1594:HIS:HD2	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:305:ARG:NH2	4:H:402:PHE:O	2.34	0.60
3:F:1040:VAL:HG21	3:F:1325:ILE:HD13	1.84	0.60
3:F:266:CYS:HA	3:F:273:ILE:HG21	1.83	0.60
3:E:266:CYS:HA	3:E:273:ILE:HG21	1.84	0.59
1:A:2288:GLU:OE1	2:C:221:ARG:NH2	2.35	0.59
3:F:611:PRO:HB3	3:F:1154:ARG:HE	1.68	0.59
1:A:2016:LEU:HD12	1:A:2186:LEU:HD21	1.85	0.59
1:B:1943:ILE:HD12	1:B:1975:PRO:HB2	1.85	0.59
2:D:285:ILE:HG23	2:D:297:TRP:HB2	1.85	0.59
1:B:1552:LEU:O	1:B:1606:LYS:NZ	2.35	0.59
3:F:27:PRO:O	3:F:1133:GLN:NE2	2.36	0.59
1:A:2133:CYS:O	1:A:2134:ARG:NE	2.36	0.59
3:E:305:ARG:NH2	4:G:402:PHE:O	2.36	0.59
3:E:646:MET:HE3	3:E:807:VAL:HG13	1.83	0.59
3:E:1062:ASN:O	3:E:1094:ARG:NH1	2.36	0.59
3:F:1032:HIS:CG	3:F:1035:THR:HG22	2.38	0.59
1:A:701:ASN:O	1:B:1153:SER:OG	2.20	0.59
1:B:661:VAL:O	1:B:665:THR:OG1	2.19	0.59
2:D:147:ASP:OD2	2:D:149:SER:OG	2.20	0.59
1:B:396:LEU:HB3	1:B:416:THR:HG23	1.85	0.58
1:A:210:VAL:HG21	1:A:266:LEU:HD13	1.86	0.58
3:F:432:GLN:HG3	3:F:435:ILE:HD12	1.85	0.58
3:F:1149:ILE:HD12	3:F:1159:GLN:HB2	1.84	0.58
1:A:2277:HIS:O	2:C:87:ASN:ND2	2.27	0.58
3:F:1084:LEU:HB3	3:F:1096:TRP:HB2	1.85	0.58
1:A:1425:GLN:HG3	1:A:2314:PHE:HZ	1.68	0.58
1:B:145:VAL:HG13	1:B:175:LEU:HD13	1.85	0.58
1:B:1764:ILE:HG23	1:B:1769:ILE:HD11	1.86	0.58
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.85	0.58
1:A:1167:PRO:HA	1:A:1170:ARG:HG3	1.85	0.58
1:B:776:LEU:HD11	1:B:820:LEU:HD21	1.84	0.58
2:C:57:ILE:HB	2:C:70:LEU:HD21	1.86	0.58
1:A:145:VAL:HG13	1:A:175:LEU:HD13	1.86	0.58
3:F:390:LEU:HA	3:F:393:LEU:HD13	1.84	0.58
1:B:1167:PRO:HA	1:B:1170:ARG:HG3	1.86	0.57
3:F:413:LEU:HD12	3:F:452:LEU:HD12	1.85	0.57
1:B:1119:VAL:HA	1:B:1122:PHE:CE2	2.39	0.57
3:E:26:LEU:HD22	3:E:1133:GLN:HG3	1.85	0.57
1:A:211:ALA:HA	1:A:214:ARG:HD3	1.86	0.57
1:A:2162:VAL:HG22	1:A:2170:ARG:HG3	1.86	0.57
1:B:606:CYS:HA	1:B:609:HIS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:990:LEU:HD21	1:B:1023:VAL:HG21	1.86	0.57
3:E:657:PRO:HB3	3:E:660:ARG:HH21	1.69	0.57
1:A:1470:ASN:ND2	1:A:1471:LYS:O	2.37	0.57
1:B:1470:ASN:ND2	1:B:1471:LYS:O	2.38	0.57
1:B:1444:GLU:OE1	1:B:1444:GLU:N	2.36	0.57
2:D:91:VAL:HG12	2:D:102:THR:HG22	1.84	0.57
3:E:32:LYS:HZ1	3:E:34:ARG:HH12	1.53	0.57
1:B:1481:MET:HE1	1:B:1512:MET:HG2	1.85	0.57
1:B:2133:CYS:O	1:B:2134:ARG:NE	2.36	0.57
3:F:1236:VAL:N	3:F:1250:LEU:O	2.38	0.57
1:A:65:ASP:OD1	1:A:103:ARG:NH1	2.37	0.57
1:B:2052:GLU:HG3	1:B:2053:PRO:HD3	1.87	0.57
3:F:1262:HIS:HD2	3:F:1263:PRO:HD2	1.70	0.57
3:F:446:ARG:HD2	3:F:479:LEU:HD11	1.87	0.57
3:F:1062:ASN:O	3:F:1094:ARG:NH1	2.38	0.57
3:E:611:PRO:HB3	3:E:1154:ARG:HE	1.68	0.56
1:A:619:ARG:NH2	1:A:668:ASP:OD2	2.35	0.56
1:B:2384:THR:HA	1:B:2387:MET:HE3	1.86	0.56
2:D:296:LEU:O	2:D:305:LYS:N	2.38	0.56
3:E:1236:VAL:N	3:E:1250:LEU:O	2.35	0.56
1:A:1626:CYS:SG	1:A:1627:GLN:N	2.77	0.56
1:B:2189:HIS:HA	1:B:2233:ASN:HB3	1.86	0.56
3:E:657:PRO:HA	3:E:660:ARG:HE	1.70	0.56
3:F:1181:ILE:HD11	3:F:1195:ARG:HH11	1.70	0.56
1:A:396:LEU:HB3	1:A:416:THR:HG23	1.87	0.56
1:A:1284:LEU:HD12	1:A:1353:VAL:HG22	1.87	0.56
3:E:1032:HIS:CG	3:E:1035:THR:HG22	2.40	0.56
1:A:1024:LYS:HA	1:A:1062:ALA:HB1	1.87	0.56
1:B:210:VAL:HG21	1:B:266:LEU:HD13	1.87	0.56
1:B:1064:GLY:O	1:B:1106:ASN:ND2	2.25	0.56
3:E:815:LEU:HB3	3:E:834:LEU:HD21	1.87	0.56
1:A:703:GLN:OE1	1:B:1161:ARG:NH2	2.37	0.56
1:A:2204:LEU:HD22	1:A:2417:VAL:HG21	1.87	0.56
2:C:173:ILE:HD11	2:C:187:ALA:HB1	1.86	0.56
1:A:701:ASN:O	1:B:1154:ARG:HG3	2.06	0.56
1:B:2034:ALA:HB1	1:B:2047:MET:HG2	1.88	0.56
1:A:990:LEU:HD21	1:A:1023:VAL:HG21	1.88	0.55
1:B:211:ALA:HA	1:B:214:ARG:HD3	1.86	0.55
1:B:2409:GLU:OE2	1:B:2410:HIS:NE2	2.40	0.55
1:B:964:LEU:HG	1:B:968:HIS:CE1	2.40	0.55
1:B:1004:CYS:O	1:B:1009:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1281:ASN:OD1	3:F:1282:SER:N	2.38	0.55
3:F:660:ARG:HH12	3:F:1112:TRP:HA	1.71	0.55
1:A:2368:ARG:NH1	1:A:2370:LYS:O	2.40	0.55
1:B:1425:GLN:HG3	1:B:2314:PHE:CZ	2.42	0.55
1:B:1728:ALA:O	1:B:1732:ILE:HG13	2.06	0.55
1:B:2135:ASP:OD2	1:B:2154:GLN:NE2	2.39	0.55
1:A:1274:ARG:HH21	1:A:1283:TRP:CD1	2.24	0.55
1:B:1045:ASN:HD22	1:B:1048:ILE:HG13	1.72	0.55
3:F:1226:HIS:ND1	3:F:1240:ASP:OD1	2.40	0.55
3:F:1088:THR:OG1	3:F:1090:ASP:OD1	2.24	0.55
1:A:607:ALA:HA	1:A:610:PHE:CE2	2.42	0.55
1:B:1268:ALA:O	1:B:1283:TRP:NE1	2.37	0.55
1:B:431:THR:HG23	1:B:481:THR:HG21	1.88	0.55
1:A:780:ILE:HD13	1:A:783:LEU:HD12	1.89	0.54
3:E:667:LEU:HD23	3:E:815:LEU:HG	1.89	0.54
3:E:1149:ILE:HD12	3:E:1159:GLN:HB2	1.88	0.54
1:A:2189:HIS:HA	1:A:2233:ASN:HB3	1.90	0.54
1:A:2296:GLY:O	1:A:2385:ASN:ND2	2.40	0.54
1:B:214:ARG:HE	1:B:273:ARG:HH22	1.56	0.54
1:B:607:ALA:HA	1:B:610:PHE:CE2	2.42	0.54
2:C:46:ASN:ND2	2:C:61:GLY:O	2.41	0.54
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.88	0.54
2:C:129:ALA:HB3	2:C:147:ASP:HB2	1.90	0.54
1:A:1004:CYS:O	1:A:1009:ARG:NH2	2.36	0.54
3:E:997:ARG:HE	3:E:1000:ARG:HD3	1.72	0.54
1:A:2326:VAL:HG22	1:A:2403:VAL:HG21	1.89	0.54
1:A:2511:ARG:NH2	1:A:2515:HIS:O	2.41	0.54
1:A:705:PHE:HA	1:A:708:ARG:HD3	1.89	0.54
1:A:1728:ALA:O	1:A:1732:ILE:HG13	2.07	0.54
1:B:65:ASP:OD1	1:B:103:ARG:NH1	2.41	0.54
1:B:877:ASN:HB3	1:B:880:THR:HG22	1.90	0.54
2:D:254:LEU:HD21	2:D:257:GLU:HB2	1.90	0.54
3:E:1216:LYS:HE3	3:E:1218:SER:HB2	1.91	0.54
1:B:700:LEU:HD22	1:B:733:MET:HE2	1.91	0.53
1:A:396:LEU:HD13	1:A:416:THR:HA	1.90	0.53
1:A:1119:VAL:HA	1:A:1122:PHE:CE2	2.43	0.53
3:F:1135:THR:HG23	3:F:1137:LEU:H	1.73	0.53
1:A:877:ASN:HB3	1:A:880:THR:HG22	1.90	0.53
1:A:1506:ASP:N	1:A:1506:ASP:OD1	2.40	0.53
1:B:396:LEU:HD13	1:B:416:THR:HA	1.90	0.53
3:E:191:ILE:HG22	3:E:241:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:O	1:A:214:ARG:HG3	2.09	0.53
1:A:506:GLU:HG3	1:A:507:PRO:HD3	1.91	0.53
1:A:1764:ILE:HG23	1:A:1769:ILE:HD11	1.90	0.53
1:A:661:VAL:HG23	1:B:1190:ILE:HG23	1.91	0.53
1:A:1129:LEU:HD22	1:A:1169:LEU:HD21	1.89	0.53
1:A:1514:ARG:NH1	1:A:1542:ASP:OD2	2.42	0.53
1:B:2196:GLU:HA	1:B:2227:VAL:HG21	1.90	0.53
3:E:299:PRO:HD3	3:E:397:ILE:HD11	1.91	0.53
3:E:667:LEU:HA	3:E:670:LEU:HD12	1.89	0.53
1:B:1178:SER:OG	1:B:1208:ARG:NH2	2.38	0.53
1:B:1631:GLU:OE1	1:B:1631:GLU:N	2.41	0.53
1:B:2139:ALA:HA	1:B:2152:ARG:HA	1.89	0.53
3:F:563:LEU:HG	3:F:603:LYS:HD2	1.90	0.53
1:B:2154:GLN:HB3	1:B:2175:MET:HG3	1.91	0.53
3:E:628:GLY:O	3:E:673:GLN:NE2	2.41	0.53
3:F:81:CYS:SG	3:F:82:ALA:N	2.82	0.53
1:A:2264:GLU:HG3	1:A:2294:THR:HG21	1.89	0.53
1:B:1433:LEU:HD22	1:B:1453:LEU:HD13	1.89	0.53
1:B:1506:ASP:OD1	1:B:1506:ASP:N	2.41	0.53
1:B:1600:GLU:O	1:B:1603:ILE:HG12	2.09	0.53
1:A:964:LEU:HG	1:A:968:HIS:CE1	2.44	0.52
1:A:2415:MET:HE1	1:A:2505:ARG:HA	1.91	0.52
1:B:850:SER:HA	1:B:1611:ARG:HH22	1.73	0.52
2:D:224:LEU:HG	2:D:274:TRP:HE3	1.74	0.52
3:E:1022:ASN:HD21	3:E:1049:TRP:NE1	2.07	0.52
3:E:81:CYS:SG	3:E:82:ALA:N	2.82	0.52
1:A:1064:GLY:O	1:A:1106:ASN:ND2	2.28	0.52
1:B:210:VAL:O	1:B:214:ARG:HG3	2.09	0.52
1:B:1658:SER:OG	1:B:1662:LYS:NZ	2.43	0.52
3:F:299:PRO:HD3	3:F:397:ILE:HD11	1.91	0.52
1:A:449:LYS:HA	1:A:452:LEU:HG	1.92	0.52
3:E:464:VAL:HB	3:E:501:VAL:HG21	1.90	0.52
3:E:1304:ILE:HA	3:E:1320:SER:HA	1.91	0.52
3:F:1076:LEU:HB2	3:F:1083:LEU:HB2	1.92	0.52
1:B:130:ILE:HG23	1:B:144:TYR:HE2	1.74	0.52
2:D:57:ILE:HB	2:D:70:LEU:HD21	1.90	0.52
2:D:102:THR:OG1	2:D:112:TRP:NE1	2.34	0.52
3:F:372:PRO:HB2	3:F:375:MET:HE1	1.92	0.52
3:F:559:ILE:HD11	3:F:584:ILE:HG21	1.92	0.52
1:A:1111:LEU:HD21	1:A:1148:PHE:CE2	2.44	0.52
1:B:132:ARG:HA	1:B:135:MET:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ARG:HH21	1:B:478:VAL:HG11	1.75	0.52
1:B:2418:LEU:HD23	1:B:2421:PHE:HE2	1.75	0.52
2:C:78:ILE:HG22	2:C:79:ILE:HG12	1.90	0.52
3:E:131:LYS:HZ3	3:E:185:TRP:CD1	2.28	0.52
3:E:372:PRO:HB2	3:E:375:MET:HE1	1.92	0.52
2:D:25:ARG:HG2	2:D:37:THR:HG22	1.91	0.52
1:B:1277:LYS:HA	1:B:1350:ILE:HD13	1.91	0.52
1:B:1745:LYS:HE3	1:B:1749:ARG:HE	1.75	0.52
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.92	0.52
2:D:173:ILE:HA	2:D:189:ASN:HA	1.91	0.52
3:E:390:LEU:HA	3:E:393:LEU:HD13	1.92	0.52
3:E:559:ILE:HD11	3:E:584:ILE:HG21	1.92	0.52
2:C:44:GLN:NE2	2:C:46:ASN:OD1	2.38	0.51
2:D:89:ALA:N	2:D:103:GLY:O	2.41	0.51
3:F:815:LEU:HB3	3:F:834:LEU:HD21	1.92	0.51
1:A:1277:LYS:HA	1:A:1350:ILE:HD13	1.91	0.51
1:A:1684:GLN:HB3	1:A:1687:HIS:HB3	1.92	0.51
1:A:1425:GLN:HG3	1:A:2314:PHE:CZ	2.45	0.51
2:D:244:CYS:HB3	2:D:258:LEU:HB2	1.92	0.51
2:D:244:CYS:HB2	2:D:273:MET:SD	2.50	0.51
1:B:1793:TRP:O	1:B:1797:ASN:ND2	2.38	0.51
1:B:2415:MET:HE1	1:B:2505:ARG:HA	1.92	0.51
3:E:105:ASN:O	3:E:109:GLN:HG2	2.10	0.51
3:E:605:TYR:CD1	3:E:647:MET:HG2	2.45	0.51
1:B:1658:SER:OG	5:B:2601:IHP:O32	2.29	0.51
1:A:130:ILE:HG23	1:A:144:TYR:HE2	1.76	0.51
2:C:123:ARG:NH1	2:C:157:LEU:O	2.36	0.51
3:F:447:LEU:H	3:F:447:LEU:HD23	1.74	0.51
2:D:78:ILE:HG22	2:D:79:ILE:HG12	1.91	0.51
2:D:192:GLY:HA2	2:D:223:ALA:HB2	1.93	0.51
1:A:882:ARG:NH2	1:A:1569:ASP:OD2	2.44	0.51
1:B:449:LYS:HA	1:B:452:LEU:HG	1.92	0.51
1:B:1527:ASP:OD1	1:B:1527:ASP:N	2.42	0.51
3:F:602:GLU:HA	3:F:605:TYR:CD2	2.46	0.51
1:A:2010:MET:O	1:A:2014:GLU:HG2	2.11	0.51
1:A:2384:THR:HA	1:A:2387:MET:HE3	1.93	0.51
1:A:606:CYS:HA	1:A:609:HIS:HB2	1.92	0.51
1:A:890:LEU:HD12	1:A:1597:SER:HB2	1.93	0.51
1:A:1658:SER:OG	5:A:2601:IHP:O32	2.27	0.50
1:A:1689:LEU:HD12	1:A:1701:MET:HE3	1.91	0.50
1:B:1984:THR:HG23	1:B:1987:ARG:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2511:ARG:NH2	1:B:2515:HIS:O	2.44	0.50
1:A:2088:TYR:O	1:A:2092:GLY:N	2.43	0.50
1:B:645:SER:HB2	1:B:648:ALA:HB3	1.94	0.50
2:D:17:THR:HB	2:D:27:TRP:HE1	1.76	0.50
3:E:1088:THR:OG1	3:E:1090:ASP:OD1	2.24	0.50
1:B:882:ARG:NH2	1:B:1569:ASP:OD2	2.45	0.50
2:D:152:ILE:N	2:D:165:LEU:O	2.38	0.50
3:E:566:LEU:HD23	3:E:603:LYS:HG2	1.93	0.50
3:E:1076:LEU:HB2	3:E:1083:LEU:HB2	1.93	0.50
3:F:1138:LEU:O	3:F:1150:TRP:N	2.44	0.50
1:A:1164:ASP:OD1	1:A:1202:HIS:NE2	2.28	0.50
1:B:1626:CYS:SG	1:B:1627:GLN:N	2.84	0.50
1:A:850:SER:HA	1:A:1611:ARG:HH22	1.76	0.50
1:A:2154:GLN:HB3	1:A:2175:MET:HG3	1.92	0.50
3:E:1135:THR:HG23	3:E:1137:LEU:H	1.76	0.50
3:F:292:LEU:HD12	3:F:292:LEU:H	1.77	0.50
3:E:304:ASP:O	3:E:307:THR:OG1	2.27	0.50
3:E:833:VAL:O	3:E:836:SER:OG	2.27	0.50
3:F:74:ASP:HB3	3:F:157:ARG:HH21	1.76	0.50
1:A:1042:TRP:HE1	1:A:1049:GLN:HG2	1.77	0.50
1:A:1745:LYS:HE3	1:A:1749:ARG:HE	1.77	0.50
1:A:1428:ALA:O	1:A:1432:VAL:HG23	2.12	0.50
1:B:221:THR:OG1	1:B:234:TYR:OH	2.25	0.50
1:B:689:GLN:NE2	3:E:419:TRP:HA	2.26	0.50
1:B:1332:ASP:OD1	1:B:1332:ASP:N	2.45	0.50
3:E:527:MET:HG3	3:E:528:PRO:HD2	1.94	0.50
2:C:106:ASP:OD1	2:C:106:ASP:N	2.38	0.49
1:A:689:GLN:OE1	3:F:422:MET:HB2	2.12	0.49
1:B:1170:ARG:HH11	1:B:1204:ILE:HD11	1.76	0.49
3:E:322:THR:HA	3:E:434:PRO:HG3	1.94	0.49
3:F:107:GLN:OE1	3:F:121:GLN:NE2	2.46	0.49
3:F:605:TYR:CD1	3:F:647:MET:HG2	2.47	0.49
1:B:2054:LEU:O	1:B:2058:MET:HG2	2.12	0.49
2:D:129:ALA:HB3	2:D:147:ASP:HB2	1.93	0.49
1:A:940:ASN:HB2	1:A:941:LEU:HD12	1.93	0.49
3:E:478:LYS:HE2	4:G:399:ARG:HH22	1.77	0.49
3:F:1216:LYS:HE3	3:F:1218:SER:HB2	1.95	0.49
1:B:266:LEU:O	1:B:270:GLU:HG2	2.13	0.49
1:A:1450:TYR:HB2	1:A:1459:ALA:HB2	1.95	0.49
3:E:1077:ASN:OD1	3:E:1133:GLN:NE2	2.45	0.49
1:B:1329:LEU:HB2	1:B:1334:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:ASP:OD1	2:D:151:ALA:N	2.45	0.49
3:E:60:VAL:HG13	3:E:147:LEU:HD22	1.93	0.49
3:E:356:ILE:O	3:E:359:SER:OG	2.31	0.49
3:E:1060:PHE:CZ	3:E:1106:PRO:HB3	2.48	0.49
3:F:1239:PHE:CE1	3:F:1246:SER:HB3	2.48	0.49
1:A:956:MET:HE1	1:A:996:THR:OG1	2.13	0.49
1:B:1414:GLU:OE2	1:B:1452:LYS:NZ	2.30	0.49
3:E:64:LEU:HD23	3:E:66:LEU:HD11	1.94	0.49
1:A:132:ARG:HA	1:A:135:MET:HG2	1.95	0.48
1:A:396:LEU:HA	1:A:399:LEU:HD12	1.95	0.48
3:F:1304:ILE:HA	3:F:1320:SER:HA	1.95	0.48
1:A:761:VAL:HA	1:A:768:ILE:HD12	1.95	0.48
1:A:1072:PRO:HA	1:A:1075:ILE:HD12	1.95	0.48
1:A:1481:MET:HE1	1:A:1512:MET:HG2	1.94	0.48
1:B:1896:ARG:NH1	1:B:1931:GLN:OE1	2.46	0.48
1:B:2192:LEU:HD12	1:B:2235:GLY:HA3	1.94	0.48
2:C:287:THR:HB	2:C:297:TRP:HE1	1.77	0.48
3:F:60:VAL:HG13	3:F:147:LEU:HD22	1.95	0.48
3:F:166:VAL:HG23	3:F:175:ILE:HG13	1.95	0.48
3:F:1077:ASN:OD1	3:F:1133:GLN:NE2	2.46	0.48
1:A:539:LEU:HD22	1:A:594:PHE:HE1	1.78	0.48
1:B:2123:LEU:HB3	1:B:2131:LEU:HB2	1.95	0.48
3:E:602:GLU:HA	3:E:605:TYR:CD2	2.48	0.48
3:F:105:ASN:O	3:F:109:GLN:HG2	2.13	0.48
3:F:191:ILE:HG22	3:F:241:ILE:HB	1.93	0.48
3:F:354:GLU:HA	3:F:364:PRO:HG2	1.94	0.48
3:F:566:LEU:HD23	3:F:603:LYS:HG2	1.95	0.48
1:A:1470:ASN:ND2	1:A:1473:ASP:OD2	2.41	0.48
1:A:1598:GLU:O	1:A:1602:VAL:HG23	2.12	0.48
1:B:1514:ARG:NH1	1:B:1542:ASP:OD2	2.45	0.48
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.94	0.48
1:A:1195:VAL:O	1:A:1199:LEU:HG	2.14	0.48
1:A:2231:SER:HG	1:A:2234:SER:H	1.61	0.48
1:B:2512:ASP:N	1:B:2512:ASP:OD1	2.47	0.48
2:D:28:GLN:O	2:D:32:GLY:N	2.47	0.48
3:F:478:LYS:HE2	4:H:399:ARG:HH22	1.79	0.48
1:A:687:LEU:HD12	1:A:692:ASN:HB3	1.94	0.48
1:A:2135:ASP:OD2	1:A:2154:GLN:NE2	2.44	0.48
1:B:1598:GLU:O	1:B:1602:VAL:HG23	2.14	0.48
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	1.96	0.48
1:B:1977:THR:O	1:B:1980:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:254:LEU:HD21	2:C:257:GLU:HB2	1.96	0.48
3:E:318:ALA:HA	3:E:438:GLN:HG3	1.96	0.48
3:E:1040:VAL:HG21	3:E:1325:ILE:HD13	1.94	0.48
1:A:484:THR:O	1:A:487:SER:OG	2.27	0.48
1:A:1910:TRP:NE1	1:A:1953:VAL:HG13	2.29	0.48
1:B:760:LEU:HG	1:B:768:ILE:HD11	1.96	0.48
1:B:2225:TYR:CE2	1:B:2356:ILE:HG22	2.48	0.48
3:E:1212:ALA:HB3	3:E:1231:SER:HB2	1.95	0.48
3:F:522:LEU:O	3:F:565:GLN:NE2	2.46	0.48
1:A:1747:MET:HE2	1:A:1751:PHE:CE2	2.49	0.48
1:B:466:LYS:HZ1	1:B:478:VAL:N	2.12	0.48
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.96	0.48
3:F:308:PRO:HG3	3:F:403:PHE:CD1	2.49	0.48
1:A:515:PRO:HD3	1:A:584:LEU:HD11	1.96	0.48
1:A:705:PHE:HZ	1:A:755:ARG:HB3	1.79	0.48
1:A:2366:MET:HG2	1:A:2373:GLU:O	2.14	0.48
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.46	0.48
1:B:940:ASN:HB2	1:B:941:LEU:HD12	1.96	0.48
1:B:1346:THR:HA	1:B:1386:ARG:HH21	1.78	0.48
1:B:2254:ARG:NH1	1:B:2261:LEU:O	2.46	0.48
2:C:147:ASP:OD1	2:C:151:ALA:N	2.47	0.48
1:A:1349:ASP:OD1	1:A:1354:THR:OG1	2.24	0.48
1:A:1984:THR:HG23	1:A:1987:ARG:HB3	1.96	0.48
3:E:1189:SER:OG	3:E:1191:ARG:NH1	2.47	0.48
3:F:67:ASN:HB2	3:F:167:PHE:HZ	1.78	0.48
3:F:543:VAL:HB	3:F:550:GLN:HG2	1.95	0.48
1:A:214:ARG:HG2	1:A:270:GLU:CD	2.39	0.47
1:B:2088:TYR:O	1:B:2092:GLY:N	2.45	0.47
3:E:1281:ASN:OD1	3:E:1282:SER:N	2.43	0.47
1:A:266:LEU:O	1:A:270:GLU:HG2	2.14	0.47
1:A:1527:ASP:N	1:A:1527:ASP:OD1	2.45	0.47
1:A:1601:GLU:OE2	1:A:1622:ARG:NH2	2.42	0.47
3:F:681:VAL:HG21	3:F:808:TYR:HB2	1.96	0.47
1:B:1199:LEU:HD22	1:B:1204:ILE:HB	1.95	0.47
1:B:1450:TYR:HB2	1:B:1459:ALA:HB2	1.95	0.47
2:D:279:SER:HA	2:D:320:PHE:CE2	2.49	0.47
3:F:488:ARG:HD2	3:F:521:VAL:HG22	1.96	0.47
1:B:890:LEU:HD12	1:B:1597:SER:HB2	1.96	0.47
1:B:968:HIS:NE2	1:B:1004:CYS:SG	2.87	0.47
1:B:1119:VAL:HG13	1:B:1158:PRO:HG2	1.96	0.47
1:B:1274:ARG:NH2	1:B:1286:ARG:HH22	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2063:GLN:N	1:B:2067:GLU:OE1	2.45	0.47
3:F:40:GLU:HG3	3:F:965:ARG:HH22	1.78	0.47
1:A:1484:LEU:HD12	1:A:1489:GLU:HB2	1.97	0.47
1:A:1587:TYR:OH	1:A:1626:CYS:SG	2.72	0.47
1:A:1600:GLU:O	1:A:1603:ILE:HG12	2.15	0.47
1:B:214:ARG:HG2	1:B:270:GLU:CD	2.40	0.47
1:B:952:MET:O	1:B:956:MET:HG2	2.14	0.47
3:F:601:HIS:CD2	3:F:640:ILE:HD11	2.50	0.47
1:A:1765:ASN:O	1:A:1769:ILE:HG12	2.15	0.47
1:A:2409:GLU:OE2	1:A:2410:HIS:NE2	2.47	0.47
1:B:1598:GLU:OE2	1:B:1640:ARG:NE	2.43	0.47
2:C:223:ALA:HA	2:C:239:SER:HA	1.97	0.47
2:D:89:ALA:H	2:D:104:GLY:HA2	1.80	0.47
1:A:431:THR:HG23	1:A:481:THR:HG21	1.95	0.47
1:A:1605:TYR:CZ	1:A:1612:ARG:HD2	2.49	0.47
1:A:2054:LEU:O	1:A:2058:MET:HG2	2.14	0.47
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.96	0.47
1:B:2022:LEU:HD11	1:B:2121:LEU:HD21	1.97	0.47
1:B:2296:GLY:O	1:B:2385:ASN:ND2	2.47	0.47
2:C:224:LEU:HG	2:C:274:TRP:HB3	1.97	0.47
3:E:67:ASN:HB2	3:E:167:PHE:HZ	1.79	0.47
3:E:255:ILE:HG23	3:E:258:LEU:HB2	1.97	0.47
3:E:354:GLU:HA	3:E:364:PRO:HG2	1.96	0.47
3:E:1138:LEU:O	3:E:1150:TRP:N	2.47	0.47
3:F:188:SER:HB2	3:F:239:ASN:HD22	1.80	0.47
3:F:527:MET:HG3	3:F:528:PRO:HD2	1.96	0.47
1:A:373:VAL:HA	1:A:392:ILE:HD13	1.97	0.47
1:A:800:ALA:O	1:A:804:GLU:HG2	2.14	0.47
1:A:1680:ASP:HB2	1:A:1683:ARG:HG2	1.96	0.47
2:C:46:ASN:N	2:C:60:ALA:O	2.24	0.47
2:D:67:MET:HE2	2:D:79:ILE:HB	1.96	0.47
1:B:1569:ASP:HA	1:B:1572:ASP:OD2	2.15	0.47
1:A:1119:VAL:HG13	1:A:1158:PRO:HG2	1.97	0.47
1:B:2326:VAL:HG22	1:B:2403:VAL:HG21	1.96	0.47
1:B:2333:ILE:HD12	1:B:2407:LEU:HD13	1.96	0.47
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.97	0.47
3:E:683:LEU:HD23	3:E:686:ILE:HD12	1.97	0.47
3:F:64:LEU:HD23	3:F:66:LEU:HD11	1.97	0.47
3:F:440:LEU:HD12	3:F:472:ILE:HD11	1.96	0.47
1:A:700:LEU:HD22	1:A:733:MET:HE2	1.97	0.46
1:A:1915:HIS:HB3	1:A:1950:ARG:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:SER:HB2	1:B:678:SER:HB2	1.97	0.46
1:B:1765:ASN:O	1:B:1769:ILE:HG12	2.14	0.46
2:C:316:VAL:HG23	2:C:317:CYS:SG	2.55	0.46
3:E:164:VAL:O	3:E:177:LEU:N	2.47	0.46
3:E:1051:TRP:HB3	3:E:1327:VAL:HG21	1.96	0.46
1:A:1697:THR:O	1:A:1701:MET:HG3	2.15	0.46
1:A:1910:TRP:CD1	1:A:1923:LEU:HD13	2.50	0.46
1:A:2225:TYR:CE2	1:A:2356:ILE:HG22	2.50	0.46
1:B:437:LEU:HD21	1:B:455:VAL:HG22	1.98	0.46
3:E:64:LEU:HB3	3:E:66:LEU:HG	1.97	0.46
3:E:1074:GLU:OE1	3:E:1075:TYR:N	2.48	0.46
3:F:588:PHE:CE2	3:F:590:SER:HB3	2.50	0.46
3:F:1064:ASN:ND2	3:F:1068:THR:OG1	2.45	0.46
1:A:1154:ARG:HG3	1:B:701:ASN:O	2.15	0.46
1:A:2121:LEU:HD13	1:A:2162:VAL:HG21	1.97	0.46
1:B:1771:LYS:O	1:B:1774:GLN:HG2	2.16	0.46
1:B:1920:ASN:O	1:B:1924:VAL:HG13	2.15	0.46
3:F:255:ILE:HG23	3:F:258:LEU:HB2	1.97	0.46
1:A:645:SER:HB2	1:A:648:ALA:HB3	1.97	0.46
1:A:1414:GLU:OE2	1:A:1452:LYS:NZ	2.31	0.46
1:A:1784:ARG:HD3	1:A:1790:TRP:HZ2	1.80	0.46
1:B:282:LEU:O	1:B:286:MET:HG2	2.15	0.46
1:B:2425:PRO:HA	1:B:2428:ASN:OD1	2.15	0.46
2:C:18:ALA:HB2	2:C:24:VAL:HA	1.97	0.46
3:E:291:THR:HG23	3:E:294:LEU:H	1.80	0.46
3:E:446:ARG:HD2	3:E:479:LEU:HD11	1.96	0.46
3:F:47:GLN:HB3	3:F:49:TRP:CD1	2.50	0.46
3:F:558:LEU:HD23	3:F:584:ILE:HD11	1.96	0.46
3:F:987:GLU:HG2	3:F:991:ARG:NE	2.31	0.46
1:A:1045:ASN:HD22	1:A:1048:ILE:HG13	1.80	0.46
1:B:1100:ILE:HA	1:B:1103:PHE:CD2	2.50	0.46
1:B:1587:TYR:OH	1:B:1626:CYS:SG	2.74	0.46
2:C:285:ILE:HG23	2:C:297:TRP:HB2	1.98	0.46
2:D:92:GLY:N	2:D:101:TYR:O	2.27	0.46
2:D:156:ASP:OD2	2:D:159:THR:N	2.40	0.46
3:E:823:TYR:HA	3:E:1108:MET:HE1	1.97	0.46
3:F:996:SER:HA	3:F:999:ARG:HE	1.80	0.46
1:B:1935:TRP:O	1:B:1939:ILE:HG13	2.16	0.46
3:E:99:LEU:HG	3:E:123:LEU:HD13	1.97	0.46
1:A:952:MET:O	1:A:956:MET:HG2	2.15	0.46
1:B:619:ARG:NH2	1:B:668:ASP:OD2	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:PHE:CD2	1:B:986:CYS:HB2	2.51	0.46
2:C:16:ALA:HB3	2:C:319:ALA:HB3	1.96	0.46
1:A:268:LEU:HD13	1:A:365:LEU:HA	1.97	0.46
1:A:2034:ALA:HB1	1:A:2047:MET:HG2	1.98	0.46
1:A:2196:GLU:HA	1:A:2227:VAL:HG21	1.97	0.46
1:A:416:THR:HG21	1:A:440:LEU:HD21	1.98	0.46
1:B:373:VAL:HA	1:B:392:ILE:HD13	1.97	0.46
1:B:693:LEU:HG	1:B:697:PHE:CZ	2.51	0.46
1:B:956:MET:HE1	1:B:996:THR:OG1	2.15	0.46
3:E:67:ASN:HB2	3:E:167:PHE:CZ	2.51	0.46
3:E:166:VAL:HG23	3:E:175:ILE:HG13	1.98	0.46
3:E:244:ALA:HB3	3:E:365:VAL:HB	1.96	0.46
3:E:582:GLY:HA2	3:E:585:TRP:NE1	2.31	0.46
1:B:67:LEU:O	1:B:71:ILE:HG13	2.16	0.46
1:B:1024:LYS:HE2	1:B:1024:LYS:HB3	1.82	0.46
1:B:2010:MET:O	1:B:2014:GLU:HG2	2.16	0.46
2:C:197:TRP:HB3	2:C:210:LEU:HB3	1.97	0.46
1:A:2063:GLN:N	1:A:2067:GLU:OE1	2.49	0.45
1:B:1605:TYR:CZ	1:B:1612:ARG:HD2	2.51	0.45
1:B:2368:ARG:NH1	1:B:2370:LYS:O	2.49	0.45
1:A:675:VAL:O	1:A:678:SER:OG	2.29	0.45
1:A:807:GLN:NE2	1:A:846:GLN:OE1	2.47	0.45
1:A:2418:LEU:HD23	1:A:2421:PHE:HE2	1.81	0.45
1:B:1877:LEU:O	1:B:1881:THR:OG1	2.23	0.45
1:B:1946:ILE:HD11	1:B:1961:LEU:HD11	1.98	0.45
3:E:660:ARG:HH12	3:E:1112:TRP:HA	1.80	0.45
3:E:1239:PHE:CE1	3:E:1246:SER:HB3	2.52	0.45
3:F:822:PRO:HB2	3:F:1111:ALA:HB1	1.97	0.45
1:A:199:TRP:HA	1:A:206:ARG:HH21	1.80	0.45
1:A:689:GLN:NE2	3:F:419:TRP:HA	2.28	0.45
1:A:1035:VAL:HG21	1:A:1070:TYR:HB3	1.98	0.45
1:B:1342:GLU:OE2	1:B:1375:ARG:N	2.48	0.45
1:B:1401:GLU:CD	1:B:2317:ARG:HH12	2.24	0.45
3:F:1218:SER:HB3	3:F:1261:ILE:HD12	1.97	0.45
1:B:947:TYR:HB2	1:B:948:PRO:HD3	1.97	0.45
2:C:244:CYS:HB3	2:C:258:LEU:HB2	1.98	0.45
3:F:261:ASP:OD2	3:F:264:THR:HB	2.15	0.45
3:F:833:VAL:O	3:F:836:SER:OG	2.27	0.45
1:B:539:LEU:HD22	1:B:594:PHE:HE1	1.82	0.45
1:B:1020:VAL:HG22	1:B:1027:ILE:HG12	1.98	0.45
2:D:43:SER:HB3	2:D:64:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:VAL:HG23	1:A:1045:ASN:H	1.82	0.45
1:B:416:THR:HG21	1:B:440:LEU:HD21	1.97	0.45
1:B:1611:ARG:HG3	1:B:1615:ILE:HG12	1.97	0.45
1:B:1684:GLN:HB3	1:B:1687:HIS:HB3	1.99	0.45
1:B:1747:MET:HE2	1:B:1751:PHE:CE2	2.51	0.45
3:F:57:THR:HG21	3:F:342:LEU:HD23	1.98	0.45
3:F:997:ARG:HE	3:F:1000:ARG:HD3	1.80	0.45
1:A:1079:LEU:HD13	1:A:1117:PRO:HG3	1.99	0.45
1:B:1043:VAL:HG23	1:B:1045:ASN:H	1.82	0.45
1:B:1555:ASP:N	1:B:1555:ASP:OD1	2.49	0.45
3:E:822:PRO:HB2	3:E:1111:ALA:HB1	1.98	0.45
3:F:1060:PHE:HZ	3:F:1099:PHE:HA	1.82	0.45
1:A:413:LEU:HD11	1:A:417:MET:HE3	1.98	0.45
1:B:155:TRP:CE3	1:B:168:ALA:HB2	2.52	0.45
1:B:539:LEU:HD23	1:B:543:LEU:HD13	1.99	0.45
3:E:453:LEU:O	3:E:457:LEU:HG	2.16	0.45
3:F:322:THR:HA	3:F:434:PRO:HG3	1.98	0.45
3:F:499:LEU:HD21	3:F:509:LEU:HD11	1.98	0.45
3:F:544:ASN:HA	3:F:583:ARG:HD2	1.98	0.45
1:B:705:PHE:HZ	1:B:755:ARG:HB3	1.82	0.45
1:B:849:ALA:HB2	1:B:890:LEU:HD21	1.99	0.45
1:B:945:GLU:OE1	1:B:945:GLU:N	2.44	0.45
3:E:447:LEU:HD23	3:E:447:LEU:H	1.80	0.45
1:A:705:PHE:O	1:A:709:GLU:HG3	2.16	0.45
1:A:2132:MET:HE3	1:A:2132:MET:HB3	1.88	0.45
1:A:2310:SER:HA	1:A:2313:TRP:HB3	1.98	0.45
1:B:800:ALA:O	1:B:804:GLU:HG2	2.17	0.45
1:B:878:GLN:NE2	1:B:1572:ASP:OD2	2.50	0.45
1:B:1689:LEU:HD12	1:B:1701:MET:HE3	1.99	0.45
1:A:689:GLN:HE21	1:A:689:GLN:HA	1.83	0.44
1:A:1578:MET:HB3	1:A:1586:ALA:HA	1.98	0.44
2:D:43:SER:OG	2:D:44:GLN:N	2.49	0.44
3:E:53:ASP:OD1	3:E:339:GLN:NE2	2.50	0.44
3:E:395:THR:O	3:E:400:GLY:N	2.38	0.44
3:E:467:ALA:O	3:E:470:VAL:HG12	2.17	0.44
3:F:1012:ARG:HB3	3:F:1288:ASN:HD21	1.82	0.44
1:A:195:PHE:CD2	1:A:240:GLU:HG3	2.52	0.44
1:A:540:LEU:HD21	1:A:594:PHE:HB3	1.99	0.44
1:A:684:ASP:OD1	1:A:721:MET:HG3	2.17	0.44
3:F:67:ASN:HB2	3:F:167:PHE:CZ	2.52	0.44
1:B:1927:VAL:HA	1:B:1930:ILE:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ASP:OD1	2:D:71:ASN:ND2	2.49	0.44
3:E:274:ALA:HB2	3:E:352:LEU:HD21	2.00	0.44
3:E:488:ARG:HG2	3:E:517:TYR:OH	2.17	0.44
3:E:1091:GLY:O	3:E:1114:GLY:N	2.35	0.44
3:F:453:LEU:O	3:F:457:LEU:HG	2.17	0.44
3:F:1031:PHE:HD2	3:F:1310:HIS:HA	1.83	0.44
1:A:1591:VAL:O	1:A:1595:MET:HG3	2.16	0.44
1:A:1946:ILE:HD11	1:A:1961:LEU:HD11	1.99	0.44
1:B:1428:ALA:O	1:B:1432:VAL:HG23	2.17	0.44
3:F:479:LEU:HB3	3:F:491:LEU:HD11	1.99	0.44
1:A:221:THR:OG1	1:A:234:TYR:OH	2.25	0.44
1:A:485:CYS:HA	1:A:488:MET:HE2	1.99	0.44
1:A:1032:ASP:OD1	1:A:1032:ASP:N	2.50	0.44
1:A:1199:LEU:HD22	1:A:1204:ILE:HB	1.99	0.44
1:B:645:SER:HG	3:E:979:ASP:CG	2.22	0.44
2:D:16:ALA:HB3	2:D:319:ALA:HB3	2.00	0.44
3:F:582:GLY:HA2	3:F:585:TRP:NE1	2.32	0.44
1:A:947:TYR:HB2	1:A:948:PRO:HD3	1.98	0.44
1:A:979:PHE:CD2	1:A:986:CYS:HB2	2.52	0.44
2:D:287:THR:HB	2:D:297:TRP:HE1	1.81	0.44
3:E:79:THR:HB	3:E:80:PRO:HD3	1.99	0.44
3:E:146:VAL:H	3:E:190:SER:HA	1.82	0.44
3:F:499:LEU:HD13	3:F:499:LEU:HA	1.86	0.44
1:A:1484:LEU:HD13	1:A:1484:LEU:HA	1.89	0.44
2:C:65:ILE:HD11	2:C:88:ILE:HG12	1.99	0.44
2:D:65:ILE:HB	2:D:81:TYR:HB2	2.00	0.44
3:E:337:PHE:CZ	3:E:347:PHE:HB3	2.53	0.44
3:F:570:HIS:CE1	3:F:572:LEU:HB3	2.53	0.44
1:A:282:LEU:O	1:A:286:MET:HG2	2.18	0.44
1:A:968:HIS:NE2	1:A:1004:CYS:SG	2.91	0.44
1:A:1643:VAL:HG23	1:A:1644:VAL:HG23	2.00	0.44
1:B:1030:TYR:O	1:B:1034:ILE:HG13	2.18	0.44
1:B:1164:ASP:OD1	1:B:1202:HIS:NE2	2.28	0.44
1:B:1325:CYS:O	1:B:1329:LEU:HG	2.17	0.44
2:C:139:ASN:ND2	2:C:141:ALA:HB3	2.33	0.44
3:E:261:ASP:OD2	3:E:264:THR:HB	2.18	0.44
3:E:1310:HIS:HB2	3:E:1315:HIS:HB2	1.99	0.44
3:F:146:VAL:H	3:F:190:SER:HA	1.83	0.44
3:F:479:LEU:HD22	4:H:403:MET:HE1	2.00	0.44
1:A:543:LEU:HD23	1:A:589:LEU:HD13	2.00	0.44
1:B:807:GLN:NE2	1:B:846:GLN:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1111:LEU:HD21	1:B:1148:PHE:CE2	2.53	0.44
1:B:1910:TRP:NE1	1:B:1953:VAL:HG13	2.32	0.44
1:B:2339:ARG:HH21	1:B:2343:ASN:HB3	1.83	0.44
2:D:248:ARG:HD2	2:D:251:ASN:HB3	2.00	0.44
3:E:681:VAL:HG21	3:E:808:TYR:HB2	1.99	0.44
3:F:347:PHE:HA	3:F:350:PHE:HB3	2.00	0.44
3:F:1060:PHE:CZ	3:F:1106:PRO:HB3	2.52	0.44
1:A:802:ILE:HD13	1:A:820:LEU:HD11	2.00	0.43
1:B:261:ILE:O	1:B:265:LEU:HG	2.18	0.43
1:B:589:LEU:HG	1:B:629:LEU:HD11	2.00	0.43
1:B:1045:ASN:ND2	1:B:1048:ILE:HG13	2.33	0.43
1:B:1491:GLY:HA2	1:B:1523:LEU:HD11	1.99	0.43
1:B:1724:MET:HE2	1:B:1724:MET:HA	2.00	0.43
1:B:1801:VAL:HG13	1:B:1877:LEU:HD22	2.00	0.43
2:C:28:GLN:O	2:C:32:GLY:N	2.48	0.43
2:D:65:ILE:HD11	2:D:88:ILE:HG21	2.00	0.43
3:F:467:ALA:O	3:F:470:VAL:HG12	2.18	0.43
1:A:658:LYS:O	1:A:661:VAL:HG12	2.17	0.43
1:A:666:ASP:O	1:A:672:ARG:NE	2.45	0.43
1:A:1024:LYS:HG3	1:A:1025:SER:H	1.83	0.43
1:A:1343:LEU:O	1:A:1347:SER:OG	2.31	0.43
1:A:1490:TRP:CE3	1:A:1519:ALA:HA	2.54	0.43
1:A:1605:TYR:CE2	1:A:1612:ARG:HD2	2.54	0.43
1:A:1946:ILE:HA	1:A:1946:ILE:HD12	1.78	0.43
1:B:700:LEU:HD13	1:B:729:PHE:HE2	1.83	0.43
1:B:1533:THR:HA	1:B:1536:ILE:HG13	1.99	0.43
1:B:1979:ALA:HB1	1:B:1987:ARG:HD2	2.00	0.43
3:E:1089:ASP:N	3:E:1089:ASP:OD1	2.51	0.43
3:E:1158:VAL:HG12	3:E:1159:GLN:HG3	1.99	0.43
3:F:1048:PHE:HE2	3:F:1060:PHE:CE2	2.36	0.43
3:E:57:THR:HG21	3:E:342:LEU:HD23	2.00	0.43
3:E:528:PRO:HG2	3:E:531:HIS:ND1	2.33	0.43
3:F:419:TRP:CZ2	3:F:430:PRO:HD3	2.53	0.43
3:F:661:LYS:HB2	3:F:826:VAL:HG22	2.01	0.43
1:A:1623:LEU:HB2	1:A:1640:ARG:HH22	1.84	0.43
1:A:1786:TRP:CE2	1:A:1788:LYS:HB2	2.53	0.43
1:A:2122:GLU:HG2	1:A:2124:GLN:HG2	2.00	0.43
1:B:854:VAL:O	1:B:856:GLU:N	2.48	0.43
1:B:1034:ILE:HG22	1:B:1038:MET:SD	2.58	0.43
1:B:1174:MET:HE3	1:B:1204:ILE:HG21	2.01	0.43
1:B:1195:VAL:O	1:B:1199:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1910:TRP:CD1	1:B:1923:LEU:HD13	2.53	0.43
1:B:2327:MET:HE2	1:B:2355:HIS:CG	2.54	0.43
3:E:40:GLU:HG3	3:E:965:ARG:HH22	1.82	0.43
3:E:131:LYS:HD3	3:E:185:TRP:CD1	2.53	0.43
3:E:292:LEU:HD12	3:E:292:LEU:H	1.82	0.43
3:F:337:PHE:CZ	3:F:347:PHE:HB3	2.54	0.43
1:A:67:LEU:O	1:A:71:ILE:HG13	2.18	0.43
1:A:434:PHE:HB3	1:A:485:CYS:SG	2.59	0.43
1:A:945:GLU:OE1	1:A:945:GLU:N	2.49	0.43
1:A:1332:ASP:OD1	1:A:1332:ASP:N	2.44	0.43
1:A:1598:GLU:OE2	1:A:1640:ARG:NE	2.49	0.43
1:A:1771:LYS:O	1:A:1774:GLN:HG2	2.18	0.43
1:A:1910:TRP:HA	1:A:1923:LEU:HD11	2.01	0.43
1:B:2015:GLU:OE1	1:B:2127:SER:OG	2.33	0.43
2:D:25:ARG:NH1	2:D:310:GLY:O	2.51	0.43
2:D:197:TRP:HB3	2:D:210:LEU:HB3	2.00	0.43
3:E:127:VAL:HG23	3:E:175:ILE:HD12	2.01	0.43
3:E:479:LEU:HD22	4:G:403:MET:HE1	1.99	0.43
3:E:601:HIS:CD2	3:E:640:ILE:HD11	2.54	0.43
3:F:74:ASP:HB3	3:F:157:ARG:NH2	2.34	0.43
1:A:645:SER:OG	3:F:981:GLU:HB2	2.18	0.43
1:A:2123:LEU:HB3	1:A:2131:LEU:HB2	2.01	0.43
1:A:2321:THR:HG21	1:A:2395:ASN:HB2	2.00	0.43
1:B:396:LEU:HA	1:B:399:LEU:HD12	1.99	0.43
1:B:675:VAL:O	1:B:678:SER:OG	2.33	0.43
1:B:1627:GLN:O	1:B:1633:TRP:NE1	2.43	0.43
1:B:1680:ASP:HB2	1:B:1683:ARG:HG2	2.01	0.43
1:A:1067:PHE:HB3	1:A:1106:ASN:ND2	2.33	0.43
1:A:1747:MET:HE2	1:A:1751:PHE:HE2	1.82	0.43
1:B:705:PHE:O	1:B:709:GLU:HG3	2.19	0.43
1:B:1614:ILE:O	1:B:1618:ILE:HG13	2.19	0.43
3:E:1204:VAL:HG12	3:E:1205:MET:HG2	2.00	0.43
3:E:1262:HIS:HD2	3:E:1263:PRO:HD2	1.84	0.43
3:F:683:LEU:HD23	3:F:686:ILE:HD12	2.00	0.43
3:F:1189:SER:OG	3:F:1191:ARG:NH1	2.51	0.43
1:A:700:LEU:HD13	1:A:729:PHE:HE2	1.83	0.43
1:A:1724:MET:HA	1:A:1724:MET:HE2	2.00	0.43
1:B:1032:ASP:N	1:B:1032:ASP:OD1	2.52	0.43
1:B:2339:ARG:NH2	1:B:2343:ASN:HB3	2.34	0.43
3:E:440:LEU:HD23	3:E:440:LEU:HA	1.87	0.43
3:E:558:LEU:HD23	3:E:584:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:47:GLN:HB3	3:F:49:TRP:HD1	1.84	0.43
3:F:79:THR:HB	3:F:80:PRO:HD3	2.01	0.43
3:F:88:ILE:HD11	3:F:105:ASN:HD22	1.82	0.43
3:F:156:PRO:HG2	3:F:165:TRP:CG	2.54	0.43
3:F:1048:PHE:CE2	3:F:1099:PHE:HB2	2.54	0.43
1:A:1530:GLU:HA	1:A:1550:LEU:HD11	2.01	0.43
1:A:1619:TRP:HB3	1:A:1640:ARG:CZ	2.49	0.43
1:A:2022:LEU:HD11	1:A:2121:LEU:HD21	2.00	0.43
1:B:824:ILE:O	1:B:828:LEU:HB2	2.18	0.43
3:F:39:ILE:HD12	3:F:962:TRP:CG	2.54	0.43
1:A:712:ILE:HD11	1:A:760:LEU:HD13	2.01	0.43
1:A:1056:ILE:HD11	1:A:1074:LEU:HD13	2.00	0.43
1:A:1609:PRO:HA	1:A:1612:ARG:NE	2.33	0.43
1:A:2057:MET:HE3	1:A:2057:MET:HB3	1.85	0.43
1:A:2097:LEU:HG	1:A:2101:TRP:CD1	2.54	0.43
1:B:2020:ALA:O	1:B:2170:ARG:NH1	2.52	0.43
2:C:143:LEU:HD23	2:C:155:TRP:HE3	1.84	0.43
2:D:238:CYS:HB3	2:D:273:MET:O	2.19	0.43
3:F:274:ALA:HB2	3:F:352:LEU:HD21	2.01	0.43
3:F:1010:ILE:HG21	3:F:1267:LEU:HD11	2.01	0.43
1:A:2407:LEU:HD23	1:A:2407:LEU:HA	1.85	0.42
1:B:780:ILE:HD13	1:B:783:LEU:HD12	2.01	0.42
1:B:1575:LEU:HG	1:B:1589:ALA:HB1	2.01	0.42
1:B:1888:PHE:O	1:B:1892:ILE:HG13	2.19	0.42
3:F:308:PRO:HG3	3:F:403:PHE:CG	2.53	0.42
1:A:1100:ILE:HA	1:A:1103:PHE:CD2	2.54	0.42
1:A:2131:LEU:O	1:A:2134:ARG:NH2	2.52	0.42
1:B:1274:ARG:HH21	1:B:1283:TRP:HD1	1.66	0.42
1:B:1568:ARG:HH22	1:B:1600:GLU:CD	2.27	0.42
3:F:1179:SER:HB3	3:F:1195:ARG:HG2	2.01	0.42
1:A:1979:ALA:HB1	1:A:1987:ARG:HD2	2.01	0.42
1:B:658:LYS:O	1:B:661:VAL:HG12	2.19	0.42
1:B:1177:LEU:O	1:B:1181:VAL:HG23	2.18	0.42
1:B:2097:LEU:HG	1:B:2101:TRP:CD1	2.54	0.42
2:D:39:GLN:HB3	2:D:41:GLN:HE22	1.85	0.42
2:D:147:ASP:O	2:D:173:ILE:HG22	2.19	0.42
3:E:996:SER:HA	3:E:999:ARG:HE	1.85	0.42
3:E:1031:PHE:HD2	3:E:1310:HIS:HA	1.85	0.42
1:A:1122:PHE:CZ	1:A:1158:PRO:HB2	2.55	0.42
1:A:1156:ILE:HD13	1:A:1191:PHE:CG	2.55	0.42
1:A:1505:ASN:O	1:A:1509:GLN:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2281:MET:HA	1:A:2281:MET:HE2	2.01	0.42
1:B:69:HIS:NE2	1:B:73:GLU:OE2	2.53	0.42
1:B:768:ILE:HG23	1:B:775:ILE:HD12	2.01	0.42
1:B:1478:LEU:HA	1:B:1481:MET:HE2	2.01	0.42
1:B:1605:TYR:CE2	1:B:1612:ARG:HD2	2.55	0.42
2:C:192:GLY:HA2	2:C:223:ALA:HB2	2.01	0.42
3:E:117:ALA:HB3	3:E:119:TYR:CE1	2.55	0.42
3:F:442:SER:O	3:F:446:ARG:HB2	2.19	0.42
3:F:468:LEU:HD21	3:F:498:ILE:HD12	2.02	0.42
3:F:657:PRO:HA	3:F:660:ARG:HE	1.83	0.42
1:A:1631:GLU:OE1	1:A:1631:GLU:N	2.41	0.42
1:B:579:VAL:HG13	1:B:618:ILE:HD11	2.00	0.42
1:B:2275:TYR:HA	1:B:2278:LEU:HG	2.02	0.42
1:B:2344:LEU:HD21	1:B:2378:ARG:HD3	2.00	0.42
2:D:47:ALA:HB3	2:D:60:ALA:HB3	2.01	0.42
3:F:582:GLY:HA2	3:F:585:TRP:CE2	2.55	0.42
1:A:261:ILE:O	1:A:265:LEU:HG	2.19	0.42
1:A:1020:VAL:HG22	1:A:1027:ILE:HG12	2.02	0.42
1:A:2317:ARG:NH2	1:A:2388:GLU:HG3	2.34	0.42
1:B:501:ILE:HD11	1:B:524:LEU:HD11	2.01	0.42
1:B:2022:LEU:O	1:B:2026:MET:HG3	2.20	0.42
2:D:136:LEU:HD21	2:D:140:GLN:OE1	2.19	0.42
3:E:31:MET:HE2	3:E:31:MET:HB3	1.96	0.42
3:E:90:PRO:HA	3:E:98:ALA:HB1	2.02	0.42
3:F:291:THR:HG23	3:F:294:LEU:H	1.84	0.42
3:F:476:VAL:HG13	3:F:495:TRP:CZ2	2.55	0.42
1:A:147:PHE:CE2	1:A:151:ARG:HD2	2.54	0.42
1:A:463:LEU:N	1:A:464:PRO:HD2	2.34	0.42
1:A:1801:VAL:HG13	1:A:1877:LEU:HD22	2.01	0.42
1:B:312:HIS:CD2	1:B:313:ILE:HG12	2.54	0.42
1:B:684:ASP:OD1	1:B:721:MET:HG3	2.20	0.42
1:B:2167:GLN:HB3	1:B:2189:HIS:HE1	1.84	0.42
3:F:640:ILE:O	3:F:644:VAL:HG23	2.20	0.42
1:A:1265:LEU:N	1:A:1290:GLU:OE2	2.53	0.42
1:A:2432:MET:HE1	1:A:2493:LEU:HA	2.01	0.42
3:E:308:PRO:HG3	3:E:403:PHE:CG	2.55	0.42
3:F:485:ARG:HA	3:F:488:ARG:HG3	2.02	0.42
1:A:746:ILE:HD12	1:A:749:ILE:HD12	2.01	0.42
1:A:1027:ILE:HD12	1:A:1027:ILE:HA	1.94	0.42
1:A:2244:ASP:OD1	1:A:2244:ASP:N	2.53	0.42
3:F:316:PHE:HB2	3:F:382:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:488:ARG:HG2	3:F:517:TYR:OH	2.20	0.42
3:F:1097:LYS:HD2	3:F:1098:ASN:H	1.84	0.42
1:A:460:ARG:HH21	1:A:504:LEU:HD21	1.84	0.42
1:A:735:ILE:HD13	1:A:735:ILE:HA	1.95	0.42
1:B:761:VAL:HA	1:B:768:ILE:HD12	2.01	0.42
1:B:1060:VAL:HG11	1:B:1103:PHE:CE1	2.55	0.42
3:E:141:ALA:HB1	3:E:144:GLU:HB2	2.01	0.42
3:E:357:MET:HB3	3:E:362:CYS:HB2	2.01	0.42
3:E:522:LEU:O	3:E:565:GLN:NE2	2.52	0.42
3:E:987:GLU:HG2	3:E:991:ARG:NE	2.34	0.42
1:A:2015:GLU:OE1	1:A:2127:SER:OG	2.31	0.41
1:B:1784:ARG:O	1:B:1790:TRP:NE1	2.51	0.41
1:B:1879:MET:HE3	1:B:1879:MET:HB3	1.86	0.41
2:C:274:TRP:CZ2	2:C:316:VAL:HG12	2.55	0.41
2:D:272:TRP:N	2:D:290:SER:HB3	2.35	0.41
3:E:1048:PHE:HE2	3:E:1060:PHE:CE2	2.37	0.41
1:A:501:ILE:O	1:A:505:LEU:HG	2.19	0.41
1:B:268:LEU:HD13	1:B:365:LEU:HA	2.02	0.41
1:B:515:PRO:HD3	1:B:584:LEU:HD11	2.02	0.41
1:B:1005:ASP:HA	1:B:1009:ARG:HH21	1.85	0.41
1:B:1953:VAL:O	1:B:1957:ILE:HG13	2.19	0.41
1:B:2167:GLN:HB3	1:B:2189:HIS:CE1	2.54	0.41
2:C:226:CYS:SG	2:C:237:THR:HG23	2.60	0.41
3:E:593:TRP:O	3:E:597:ARG:HG3	2.21	0.41
3:E:1308:ALA:O	3:E:1316:LEU:HD12	2.20	0.41
3:F:131:LYS:HD3	3:F:185:TRP:CE2	2.55	0.41
1:A:221:THR:HG1	1:A:234:TYR:HH	1.59	0.41
1:A:1611:ARG:HG3	1:A:1615:ILE:HG12	2.01	0.41
1:A:2300:ALA:HB2	1:A:2386:ALA:HA	2.02	0.41
1:B:463:LEU:N	1:B:464:PRO:HD2	2.35	0.41
1:B:485:CYS:HA	1:B:488:MET:HE2	2.02	0.41
2:C:173:ILE:HA	2:C:189:ASN:HA	2.02	0.41
3:E:476:VAL:HG13	3:E:495:TRP:CZ2	2.54	0.41
1:A:507:PRO:O	1:A:511:VAL:HG23	2.21	0.41
1:A:1085:ASP:OD2	1:A:1093:SER:OG	2.27	0.41
1:A:1658:SER:OG	1:A:1662:LYS:NZ	2.53	0.41
1:B:199:TRP:HE3	1:B:260:ARG:HG2	1.84	0.41
1:B:1155:ILE:C	1:B:1158:PRO:HD2	2.45	0.41
1:B:1319:ASN:OD1	1:B:1319:ASN:N	2.53	0.41
1:B:1386:ARG:HD3	1:B:1386:ARG:HA	1.75	0.41
1:B:1609:PRO:HA	1:B:1612:ARG:NE	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:319:ILE:HG23	3:E:378:MET:HG3	2.03	0.41
3:E:419:TRP:O	3:E:423:GLY:N	2.53	0.41
3:E:570:HIS:CE1	3:E:572:LEU:HB3	2.56	0.41
3:F:120:LYS:HD2	3:F:137:LEU:HD21	2.01	0.41
1:B:504:LEU:O	1:B:507:PRO:HD2	2.20	0.41
1:B:2228:ILE:HB	1:B:2236:LEU:HB3	2.02	0.41
2:C:69:ASP:OD1	2:C:71:ASN:ND2	2.53	0.41
2:C:300:GLU:HG2	2:C:301:THR:HG23	2.03	0.41
3:E:543:VAL:HB	3:E:550:GLN:HG2	2.02	0.41
1:A:202:LYS:HG3	1:A:205:ILE:HD12	2.02	0.41
1:A:1045:ASN:ND2	1:A:1048:ILE:HG13	2.35	0.41
1:A:1745:LYS:HE3	1:A:1749:ARG:NE	2.35	0.41
1:A:1899:ASN:O	1:A:1903:THR:OG1	2.32	0.41
3:E:420:LEU:HD21	3:E:456:PHE:HD1	1.86	0.41
3:E:452:LEU:HD23	3:E:452:LEU:HA	1.91	0.41
3:F:477:LEU:HA	3:F:495:TRP:HZ2	1.85	0.41
1:A:1071:LEU:N	1:A:1072:PRO:HD2	2.35	0.41
3:E:506:GLN:NE2	3:E:542:ILE:O	2.50	0.41
3:E:570:HIS:HB3	3:E:573:LEU:HB3	2.03	0.41
1:A:1090:ARG:O	1:A:1094:ILE:HG13	2.19	0.41
1:A:2415:MET:HE2	1:A:2415:MET:HB2	1.98	0.41
1:B:2264:GLU:HG3	1:B:2294:THR:HG21	2.02	0.41
3:F:64:LEU:HB3	3:F:66:LEU:HG	2.02	0.41
3:F:647:MET:O	3:F:650:GLN:HG3	2.21	0.41
1:A:119:ASP:O	1:A:123:MET:HG3	2.21	0.41
1:A:504:LEU:O	1:A:507:PRO:HD2	2.21	0.41
1:A:1322:PHE:CD1	1:A:1360:LEU:HD11	2.56	0.41
1:A:1323:VAL:HG21	1:A:1363:PHE:HE2	1.86	0.41
1:A:1433:LEU:HD22	1:A:1453:LEU:HD13	2.02	0.41
1:A:2022:LEU:O	1:A:2026:MET:HG3	2.20	0.41
1:A:2332:TYR:CZ	1:A:2528:LEU:HD21	2.55	0.41
1:A:2516:ASP:OD1	1:A:2516:ASP:N	2.54	0.41
1:B:155:TRP:HE3	1:B:168:ALA:HB2	1.86	0.41
1:B:830:ASP:N	1:B:830:ASP:OD1	2.54	0.41
1:B:2335:GLY:O	1:B:2362:PHE:N	2.53	0.41
1:B:2366:MET:HG2	1:B:2373:GLU:O	2.21	0.41
1:B:2516:ASP:OD1	1:B:2516:ASP:N	2.53	0.41
2:C:15:LEU:HA	2:C:319:ALA:O	2.21	0.41
2:C:32:GLY:HA3	2:C:306:ARG:NH2	2.36	0.41
2:C:65:ILE:HD11	2:C:88:ILE:HG21	2.02	0.41
2:C:238:CYS:HB3	2:C:273:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:ILE:O	2:C:270:ARG:NH1	2.54	0.41
3:E:582:GLY:HA2	3:E:585:TRP:CE2	2.56	0.41
3:F:78:THR:O	3:F:81:CYS:HB3	2.21	0.41
3:F:298:ILE:HD13	3:F:309:LEU:HD13	2.02	0.41
3:F:443:GLN:OE1	3:F:446:ARG:NH2	2.49	0.41
3:F:562:CYS:HB3	3:F:577:VAL:HG13	2.03	0.41
3:F:593:TRP:O	3:F:597:ARG:HG3	2.21	0.41
1:A:199:TRP:HE3	1:A:260:ARG:HG2	1.85	0.41
1:A:1920:ASN:O	1:A:1924:VAL:HG13	2.20	0.41
1:A:2353:ILE:HD13	1:A:2353:ILE:HA	1.98	0.41
1:A:2425:PRO:HA	1:A:2428:ASN:OD1	2.21	0.41
1:B:1423:LEU:HD12	1:B:1423:LEU:HA	1.87	0.41
2:D:139:ASN:ND2	2:D:141:ALA:HB3	2.35	0.41
3:E:308:PRO:HG3	3:E:403:PHE:CD1	2.56	0.41
3:F:31:MET:HE2	3:F:31:MET:HB3	1.99	0.41
3:F:142:LYS:HE3	3:F:142:LYS:HB2	1.95	0.41
1:A:466:LYS:HZ1	1:A:478:VAL:N	2.20	0.40
1:A:1030:TYR:O	1:A:1034:ILE:HG13	2.21	0.40
1:A:1613:GLU:HG3	1:A:1616:ARG:NH2	2.36	0.40
1:A:2344:LEU:HD21	1:A:2378:ARG:HD3	2.03	0.40
1:B:631:THR:HB	1:B:632:PRO:HD3	2.03	0.40
1:B:714:THR:HG23	1:B:717:ARG:NH2	2.36	0.40
1:B:856:GLU:N	1:B:857:PRO:HD2	2.36	0.40
1:B:2546:CYS:HB3	1:B:2549:TRP:HB2	2.04	0.40
2:C:171:VAL:HG21	2:C:189:ASN:HD22	1.85	0.40
2:D:68:TYR:HE1	2:D:77:PRO:HG3	1.86	0.40
3:E:346:LEU:HD23	3:E:346:LEU:HA	1.90	0.40
3:F:29:ALA:N	3:F:1077:ASN:HD21	2.19	0.40
1:A:734:LEU:HD21	1:A:775:ILE:HD11	2.03	0.40
1:A:1034:ILE:HG22	1:A:1038:MET:SD	2.61	0.40
1:A:1533:THR:HA	1:A:1536:ILE:HG13	2.04	0.40
1:A:2228:ILE:HB	1:A:2236:LEU:HB3	2.02	0.40
1:A:2340:HIS:CE1	1:A:2342:SER:HB3	2.56	0.40
1:B:214:ARG:HG2	1:B:270:GLU:OE1	2.21	0.40
1:B:501:ILE:O	1:B:505:LEU:HG	2.21	0.40
1:B:1129:LEU:N	1:B:1130:PRO:HD2	2.37	0.40
1:B:2291:VAL:HG13	1:B:2381:ARG:HE	1.87	0.40
1:B:2339:ARG:O	1:B:2378:ARG:HD2	2.21	0.40
3:E:164:VAL:HG23	3:E:179:ILE:HD11	2.02	0.40
3:F:1185:LEU:HD11	3:F:1191:ARG:HD3	2.03	0.40
3:F:1204:VAL:HG12	3:F:1205:MET:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:LEU:HD13	1:A:1146:LEU:HA	1.91	0.40
1:A:1403:GLU:HG2	1:A:1412:ILE:HD11	2.02	0.40
1:A:1614:ILE:O	1:A:1618:ILE:HG13	2.21	0.40
1:A:1753:LYS:HD3	1:A:1753:LYS:HA	1.86	0.40
1:B:783:LEU:HD23	1:B:795:ILE:HD11	2.02	0.40
2:C:101:TYR:HE2	2:C:136:LEU:HD13	1.86	0.40
2:C:277:ALA:HB3	2:C:286:VAL:HB	2.04	0.40
3:E:611:PRO:HG2	3:E:612:ILE:HD12	2.03	0.40
3:E:637:SER:HA	3:E:640:ILE:HG22	2.02	0.40
3:F:117:ALA:HB3	3:F:119:TYR:CE1	2.56	0.40
3:F:258:LEU:HD23	3:F:258:LEU:HA	1.94	0.40
1:A:856:GLU:N	1:A:857:PRO:HD2	2.36	0.40
1:A:1407:GLY:HA2	1:A:1408:PRO:HD3	1.95	0.40
1:A:1599:LEU:O	1:A:1603:ILE:HG23	2.21	0.40
1:B:588:THR:O	1:B:591:SER:OG	2.34	0.40
1:B:615:HIS:HB2	1:B:618:ILE:HB	2.03	0.40
1:B:1407:GLY:HA2	1:B:1408:PRO:HD3	1.97	0.40
1:B:1578:MET:HB3	1:B:1586:ALA:HA	2.03	0.40
2:D:15:LEU:HD22	2:D:27:TRP:HB2	2.03	0.40
3:E:275:LEU:HD21	3:E:312:LEU:HD13	2.03	0.40
3:F:457:LEU:HD22	3:F:464:VAL:HG22	2.04	0.40
3:F:812:TRP:CZ3	3:F:816:LEU:HD11	2.55	0.40
1:A:1155:ILE:C	1:A:1158:PRO:HD2	2.47	0.40
1:A:1545:PHE:CZ	1:A:1595:MET:HE2	2.56	0.40
1:A:2218:LYS:O	1:A:2322:ARG:NH1	2.55	0.40
1:B:959:PHE:O	1:B:964:LEU:HD22	2.21	0.40
1:B:1477:MET:HE1	1:B:1512:MET:SD	2.61	0.40
1:B:1619:TRP:HB3	1:B:1640:ARG:CZ	2.51	0.40
3:E:419:TRP:CZ2	3:E:430:PRO:HD3	2.56	0.40
3:F:180:TYR:O	3:F:184:THR:OG1	2.36	0.40
3:F:319:ILE:HG23	3:F:378:MET:HG3	2.04	0.40
3:F:1171:SER:O	3:F:1184:GLY:N	2.51	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	A	2150/2549 (84%)	2101 (98%)	47 (2%)	2 (0%)	48	78
1	B	2150/2549 (84%)	2101 (98%)	47 (2%)	2 (0%)	48	78
2	C	315/326 (97%)	304 (96%)	11 (4%)	0	100	100
2	D	315/326 (97%)	303 (96%)	12 (4%)	0	100	100
3	E	1040/1363 (76%)	1004 (96%)	36 (4%)	0	100	100
3	F	1040/1363 (76%)	1009 (97%)	31 (3%)	0	100	100
4	G	7/887 (1%)	6 (86%)	1 (14%)	0	100	100
4	H	7/887 (1%)	7 (100%)	0	0	100	100
All	All	7024/10250 (68%)	6835 (97%)	185 (3%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	LYS
1	B	379	LYS
1	A	18	ASN
1	B	18	ASN

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	1876/2220 (84%)	1833 (98%)	43 (2%)	44	62
1	B	1876/2220 (84%)	1840 (98%)	36 (2%)	50	65
2	C	269/276 (98%)	265 (98%)	4 (2%)	57	68
2	D	269/276 (98%)	264 (98%)	5 (2%)	50	65
3	E	928/1191 (78%)	911 (98%)	17 (2%)	51	66
3	F	928/1191 (78%)	909 (98%)	19 (2%)	48	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	9/730 (1%)	9 (100%)	0	100	100
4	H	9/730 (1%)	9 (100%)	0	100	100
All	All	6164/8834 (70%)	6040 (98%)	124 (2%)	48	64

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ILE
1	A	506	GLU
1	A	539	LEU
1	A	605	HIS
1	A	645	SER
1	A	665	THR
1	A	693	LEU
1	A	735	ILE
1	A	794	VAL
1	A	820	LEU
1	A	830	ASP
1	A	885	ILE
1	A	966	HIS
1	A	968	HIS
1	A	969	THR
1	A	1056	ILE
1	A	1097	LEU
1	A	1140	ASP
1	A	1150	ASP
1	A	1197	LYS
1	A	1262	THR
1	A	1284	LEU
1	A	1453	LEU
1	A	1484	LEU
1	A	1575	LEU
1	A	1624	GLN
1	A	1673	LEU
1	A	1899	ASN
1	A	1925	GLU
1	A	1943	ILE
1	A	1946	ILE
1	A	1973	ILE
1	A	1985	THR
1	A	2007	GLN

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Mol	Chain	Res	Type
1	A	2057	MET
1	A	2138	LEU
1	A	2172	LEU
1	A	2173	THR
1	A	2303	LEU
1	A	2353	ILE
1	A	2371	PHE
1	A	2533	THR
1	A	2540	GLN
1	B	194	ILE
1	B	506	GLU
1	B	539	LEU
1	B	605	HIS
1	B	645	SER
1	B	665	THR
1	B	689	GLN
1	B	820	LEU
1	B	830	ASP
1	B	938	MET
1	B	966	HIS
1	B	968	HIS
1	B	1097	LEU
1	B	1140	ASP
1	B	1150	ASP
1	B	1197	LYS
1	B	1262	THR
1	B	1284	LEU
1	B	1453	LEU
1	B	1484	LEU
1	B	1555	ASP
1	B	1570	LEU
1	B	1575	LEU
1	B	1624	GLN
1	B	1673	LEU
1	B	1930	ILE
1	B	1943	ILE
1	B	1946	ILE
1	B	2057	MET
1	B	2138	LEU
1	B	2172	LEU
1	B	2173	THR
1	B	2303	LEU

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Mol	Chain	Res	Type
1	B	2364	VAL
1	B	2533	THR
1	B	2540	GLN
2	C	128	ASN
2	C	132	ASN
2	C	274	TRP
2	C	292	ASN
2	D	49	GLU
2	D	93	PHE
2	D	128	ASN
2	D	274	TRP
2	D	292	ASN
3	E	39	ILE
3	E	188	SER
3	E	302	LEU
3	E	479	LEU
3	E	527	MET
3	E	625	THR
3	E	658	MET
3	E	662	GLU
3	E	663	LEU
3	E	1011	THR
3	E	1013	LEU
3	E	1035	THR
3	E	1139	MET
3	E	1182	VAL
3	E	1257	THR
3	E	1323	TYR
3	E	1330	VAL
3	F	39	ILE
3	F	188	SER
3	F	302	LEU
3	F	336	LEU
3	F	470	VAL
3	F	479	LEU
3	F	499	LEU
3	F	527	MET
3	F	535	THR
3	F	551	GLU
3	F	663	LEU
3	F	1011	THR
3	F	1014	ASP

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Mol	Chain	Res	Type
3	F	1035	THR
3	F	1139	MET
3	F	1182	VAL
3	F	1257	THR
3	F	1323	TYR
3	F	1330	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	418	ASN
1	A	689	GLN
1	A	701	ASN
1	A	1058	GLN
1	A	1359	ASN
1	A	1405	GLN
1	A	1424	GLN
1	A	1627	GLN
1	A	1684	GLN
1	A	1737	GLN
1	A	1791	HIS
1	A	1920	ASN
1	A	2007	GLN
1	A	2008	GLN
1	A	2099	GLN
1	A	2401	HIS
1	B	68	ASN
1	B	418	ASN
1	B	689	GLN
1	B	838	GLN
1	B	1045	ASN
1	B	1058	GLN
1	B	1207	GLN
1	B	1359	ASN
1	B	1509	GLN
1	B	1541	HIS
1	B	1624	GLN
1	B	1627	GLN
1	B	1737	GLN
1	B	1760	ASN
1	B	1915	HIS

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Mol	Chain	Res	Type
1	B	2007	GLN
1	B	2008	GLN
1	B	2114	GLN
1	B	2515	HIS
2	C	39	GLN
2	C	71	ASN
2	D	40	HIS
2	D	71	ASN
3	E	107	GLN
3	E	121	GLN
3	E	151	ASN
3	E	392	GLN
3	E	481	GLN
3	E	586	GLN
3	E	673	GLN
3	E	1022	ASN
3	E	1062	ASN
3	F	121	GLN
3	F	242	GLN
3	F	506	GLN
3	F	586	GLN
3	F	601	HIS
3	F	673	GLN
3	F	1248	ASN
3	F	1262	HIS
3	F	1310	HIS
3	F	1315	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IHP	B	2601	-	36,36,36	0.76	1 (2%)	60,60,60	0.56	1 (1%)
5	IHP	A	2601	-	36,36,36	0.77	1 (2%)	60,60,60	0.56	1 (1%)

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
5	IHP	B	2601	-	-	1/30/54/54	0/1/1/1
5	IHP	A	2601	-	-	1/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2601	IHP	P3-O13	3.06	1.64	1.59
5	B	2601	IHP	P3-O13	2.94	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2601	IHP	P2-O12-C2	2.73	130.73	123.43
5	B	2601	IHP	P2-O12-C2	2.72	130.69	123.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

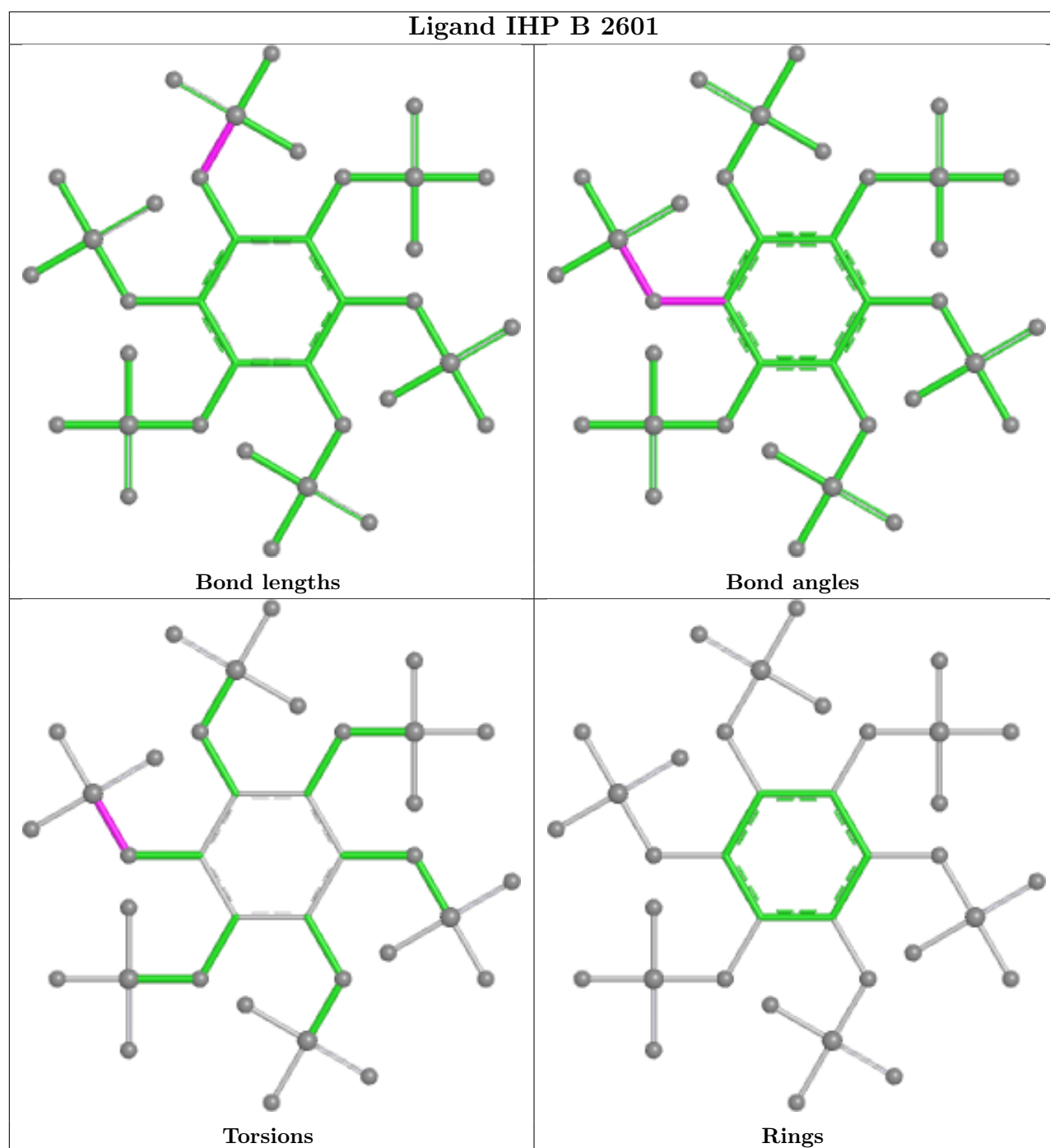
Mol	Chain	Res	Type	Atoms
5	A	2601	IHP	C2-O12-P2-O22
5	B	2601	IHP	C2-O12-P2-O22

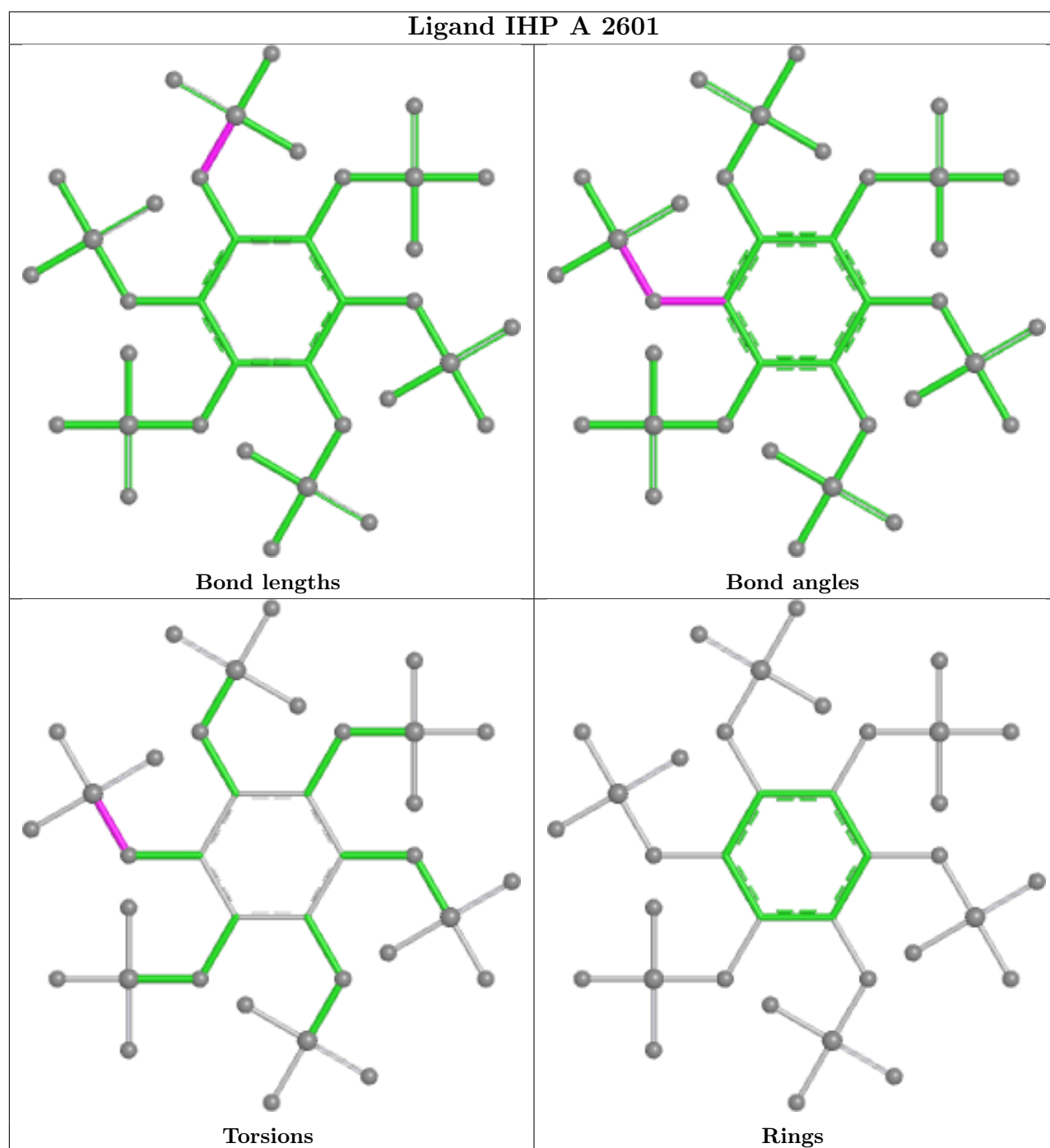
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2601	IHP	1	0
5	A	2601	IHP	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.

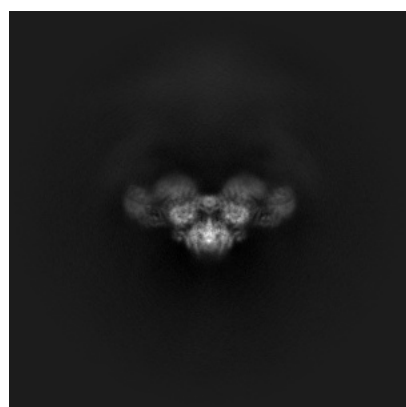
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50184. These allow visual inspection of the internal detail of the map and identification of artifacts.

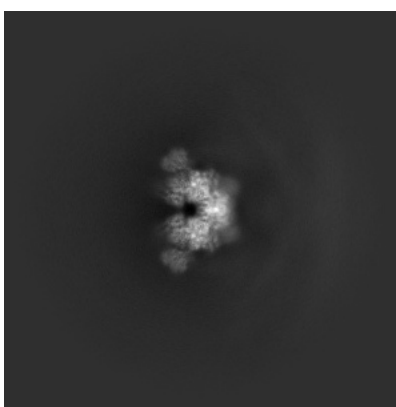
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

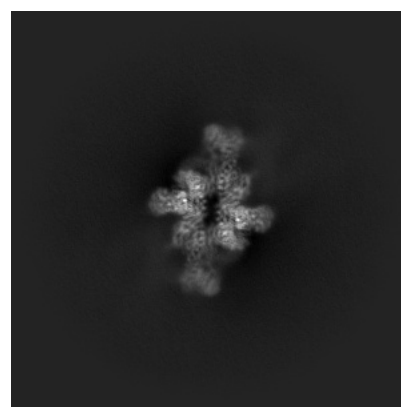
6.1.1 Primary map



X



Y

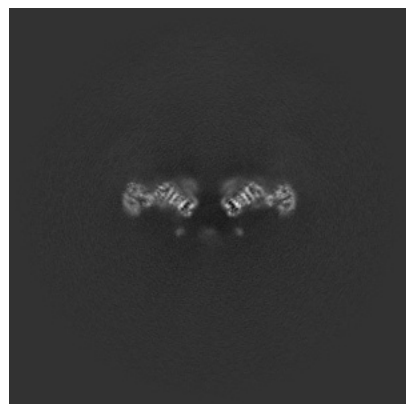


Z

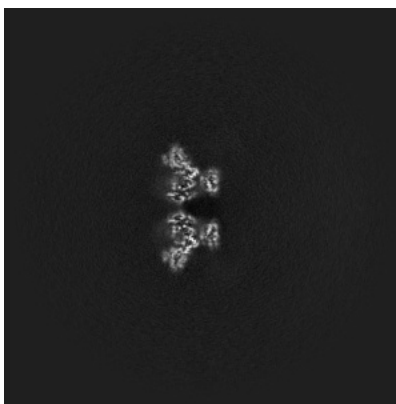
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

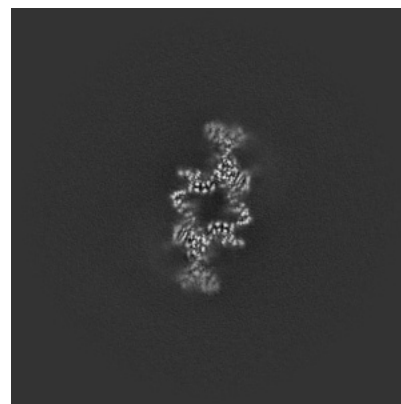
6.2.1 Primary map



X Index: 256



Y Index: 256

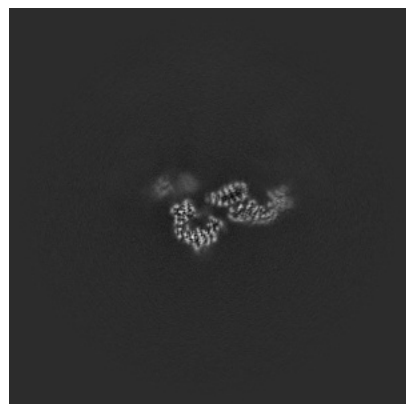


Z Index: 256

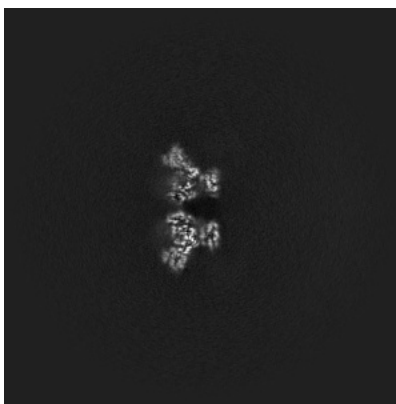
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

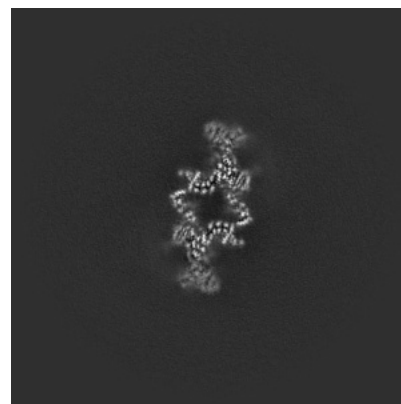
6.3.1 Primary map



X Index: 273



Y Index: 257



Z Index: 257

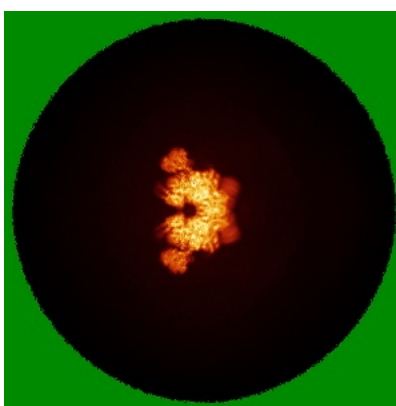
The images above show the largest variance slices of the map in three orthogonal directions.

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

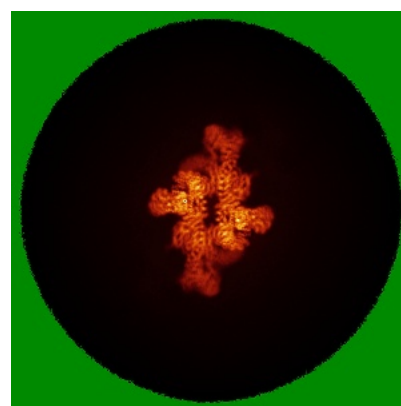
6.4.1 Primary map



X



Y

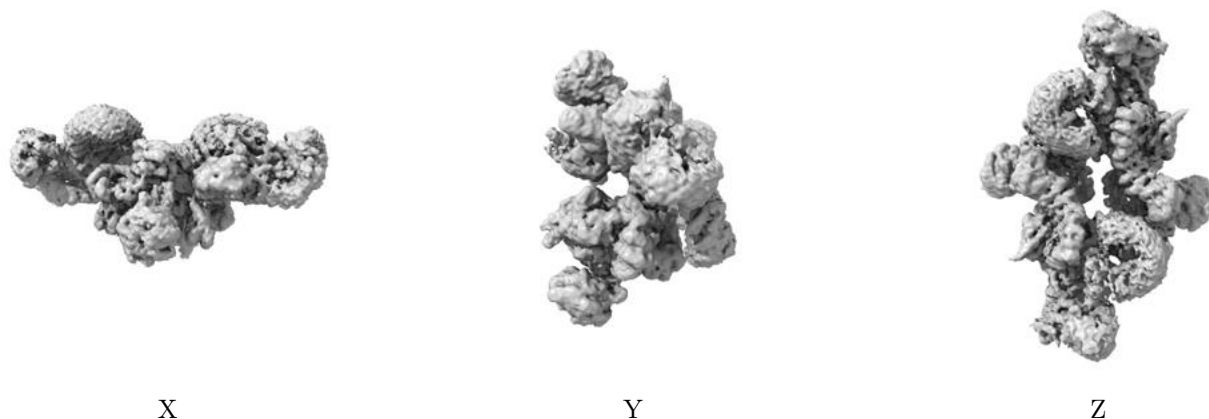


Z

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 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

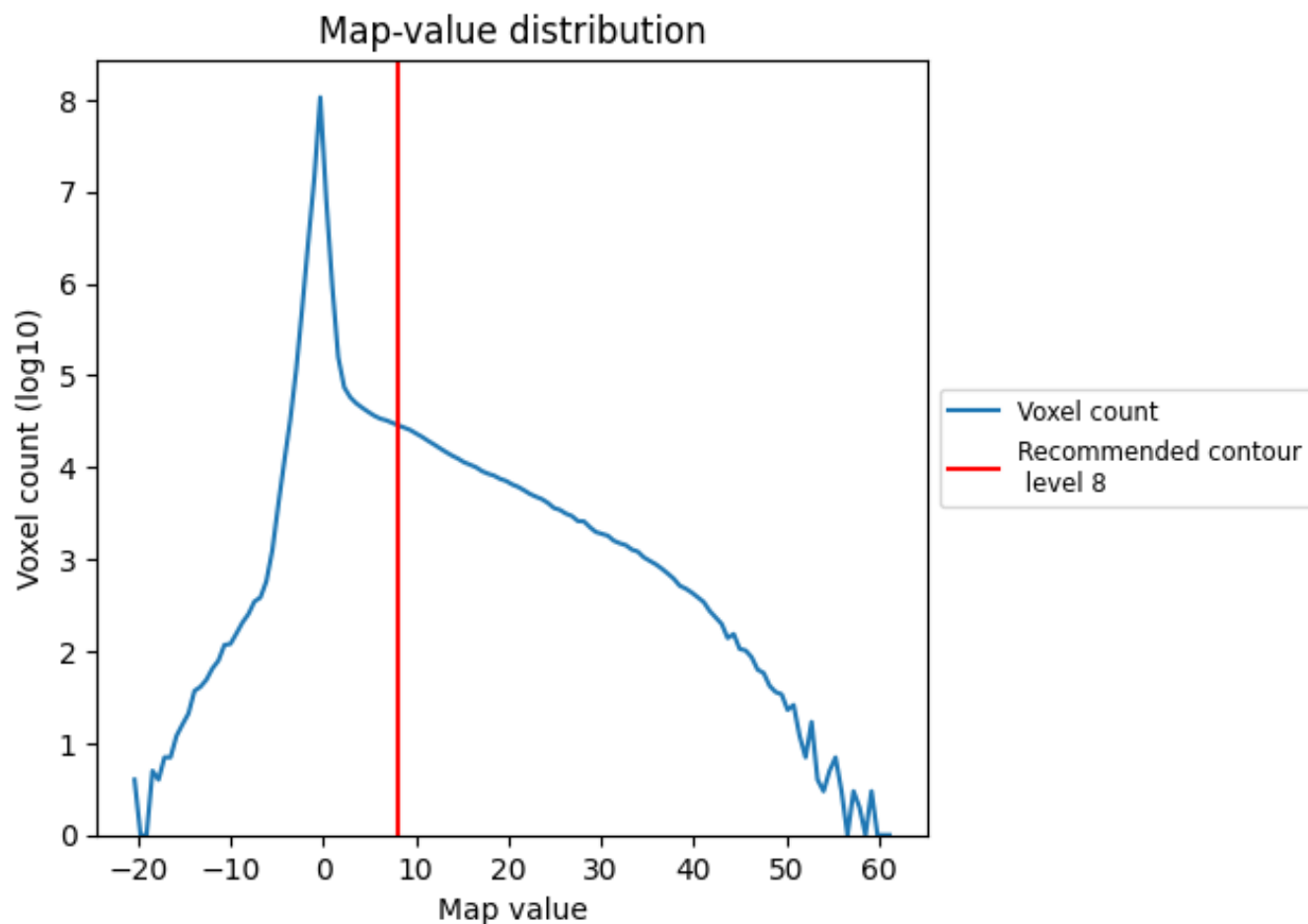
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

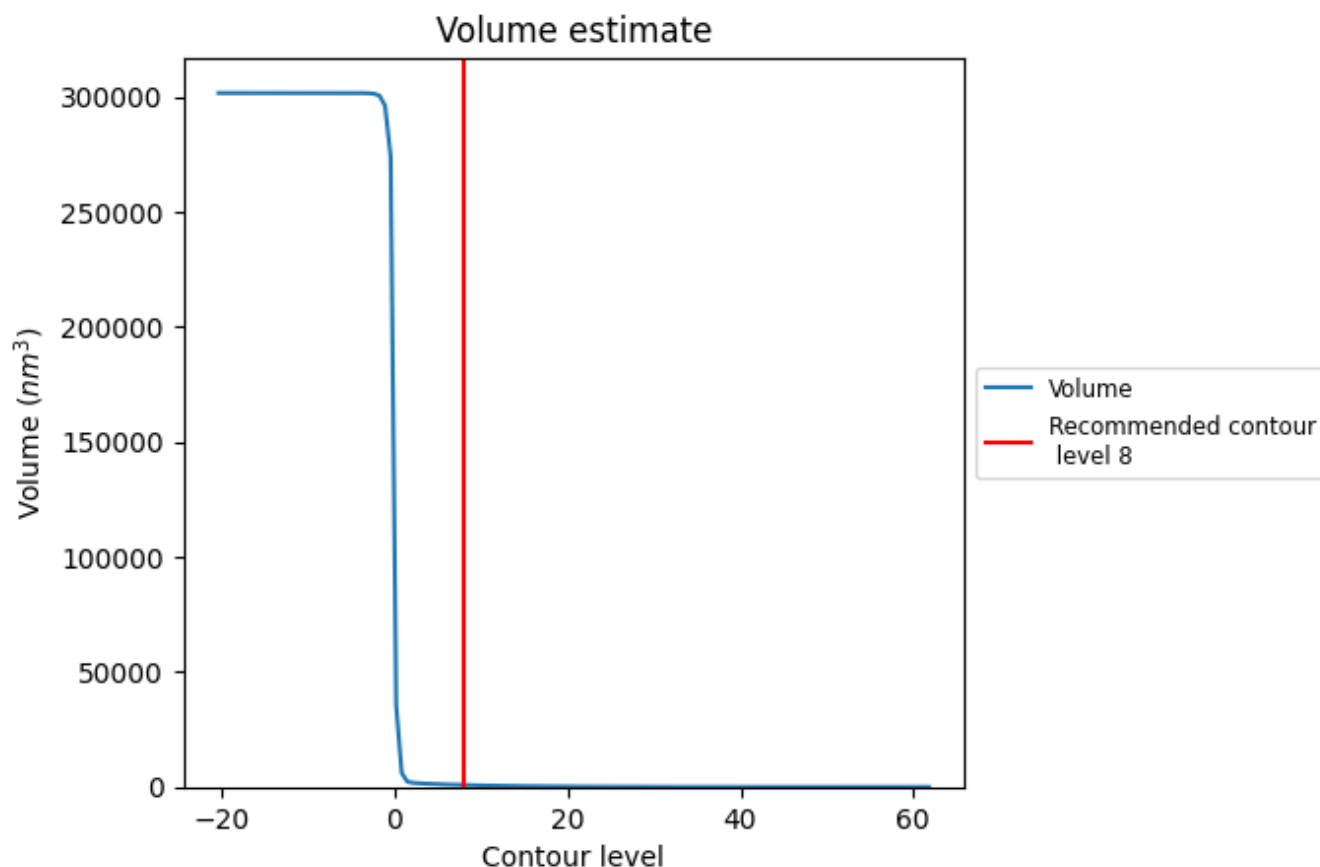
This section contains the results of statistical analysis of the map.

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.

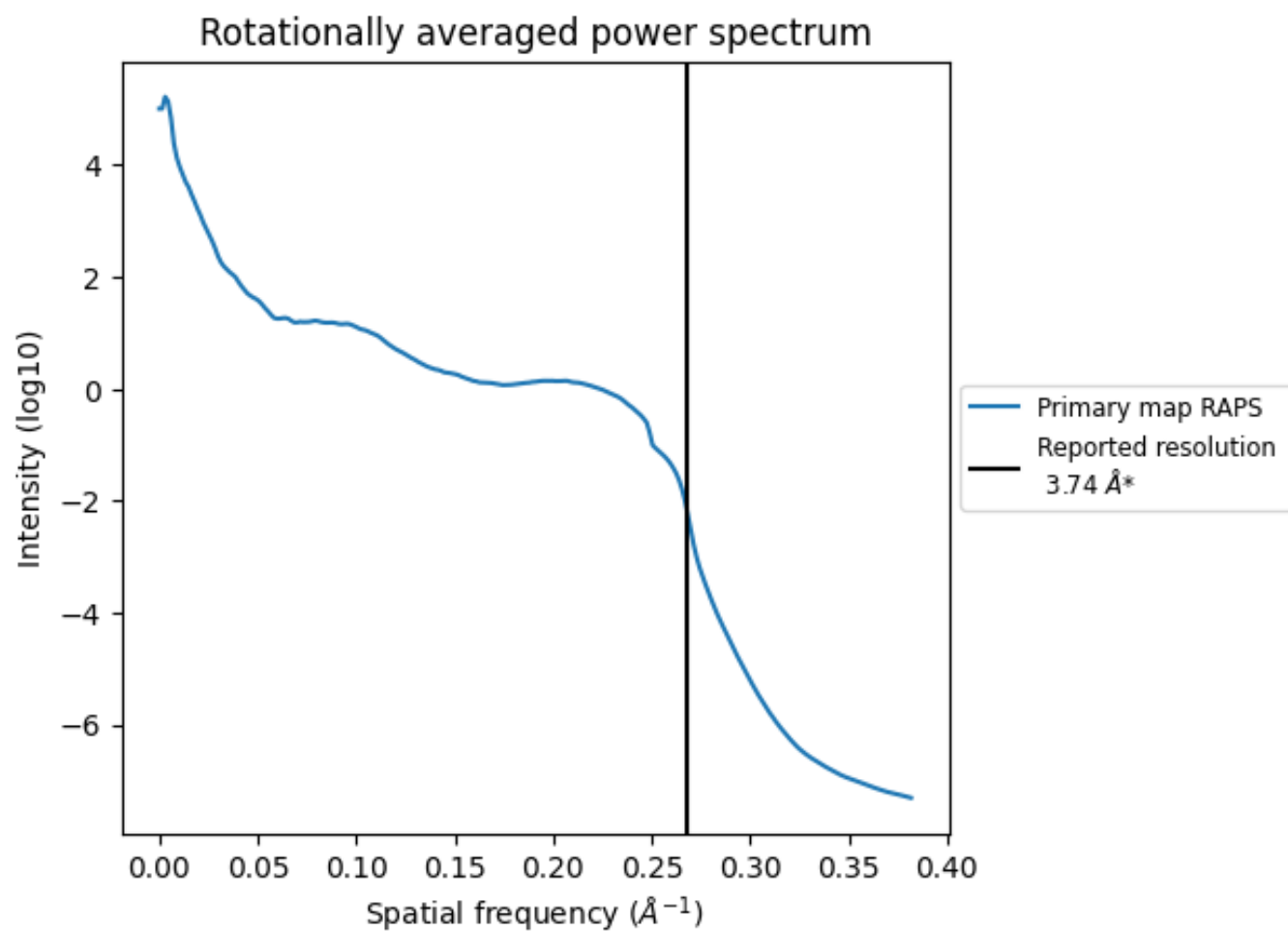
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 847 nm^3 ; this corresponds to an approximate mass of 765 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 ⓘ

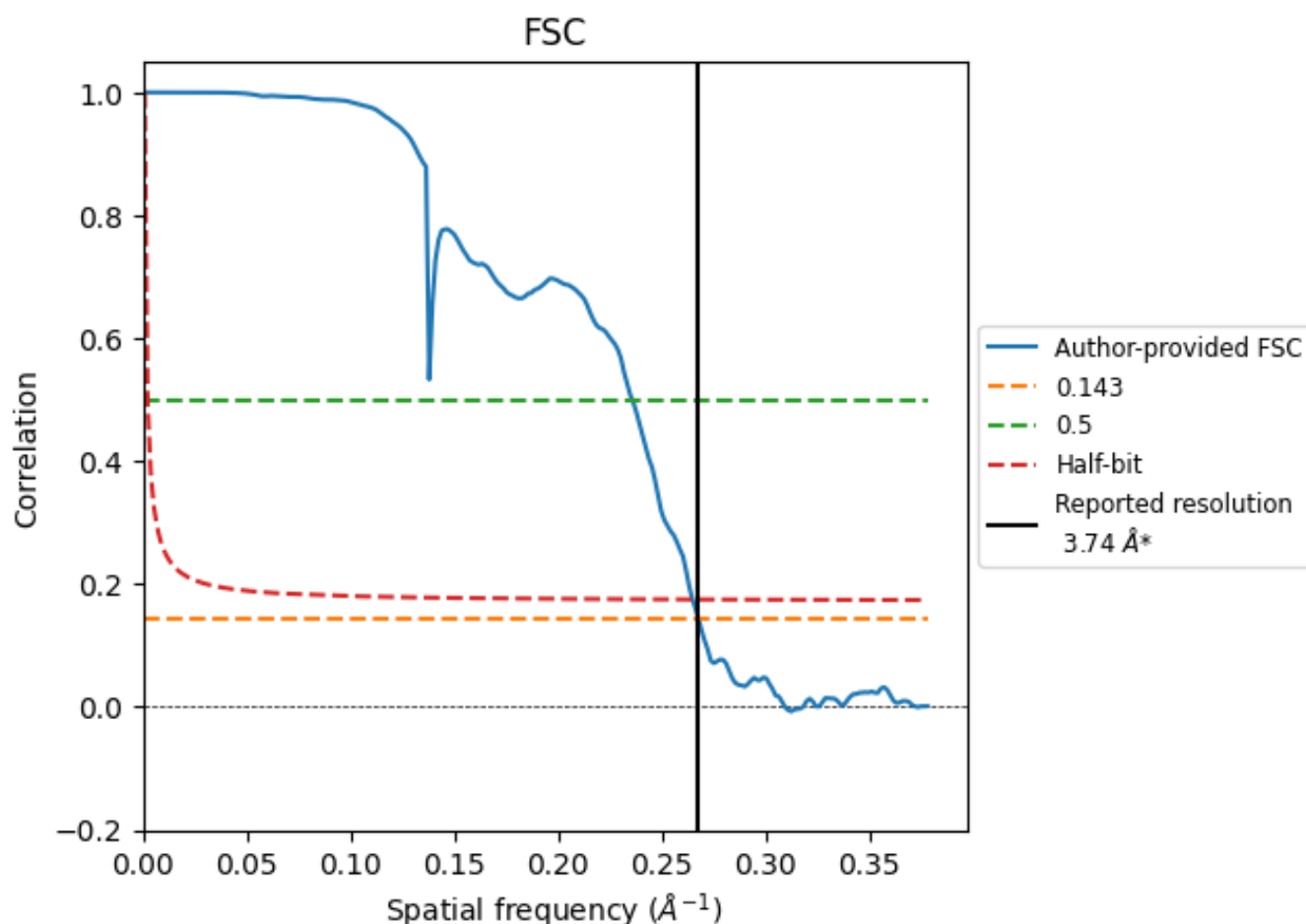


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

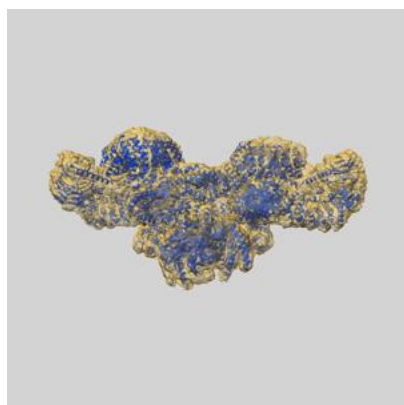
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.74	-	-
Author-provided FSC curve	3.73	4.24	3.78
Unmasked-calculated*	-	-	-

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

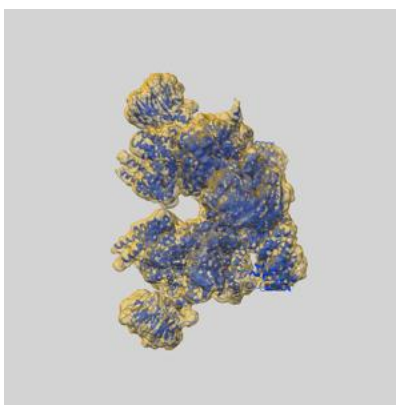
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50184 and PDB model 9F45. Per-residue inclusion information can be found in section [3](#) on page [7](#).

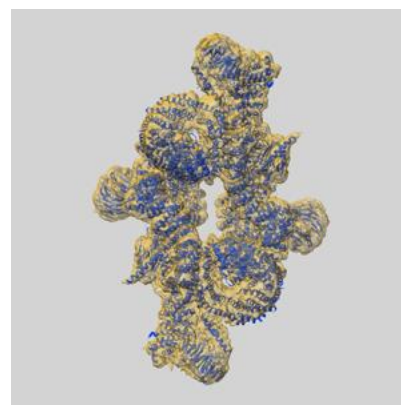
9.1 Map-model overlay [i](#)



X



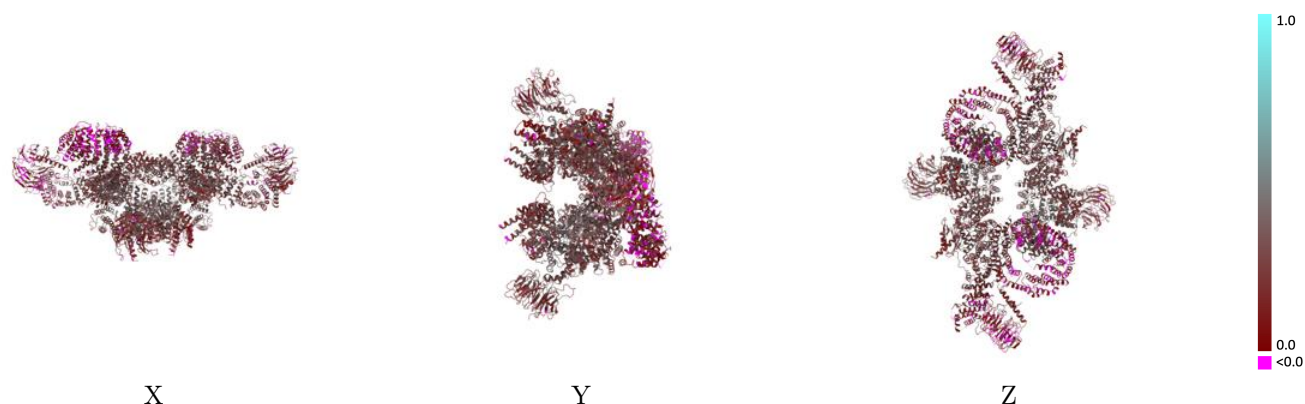
Y



Z

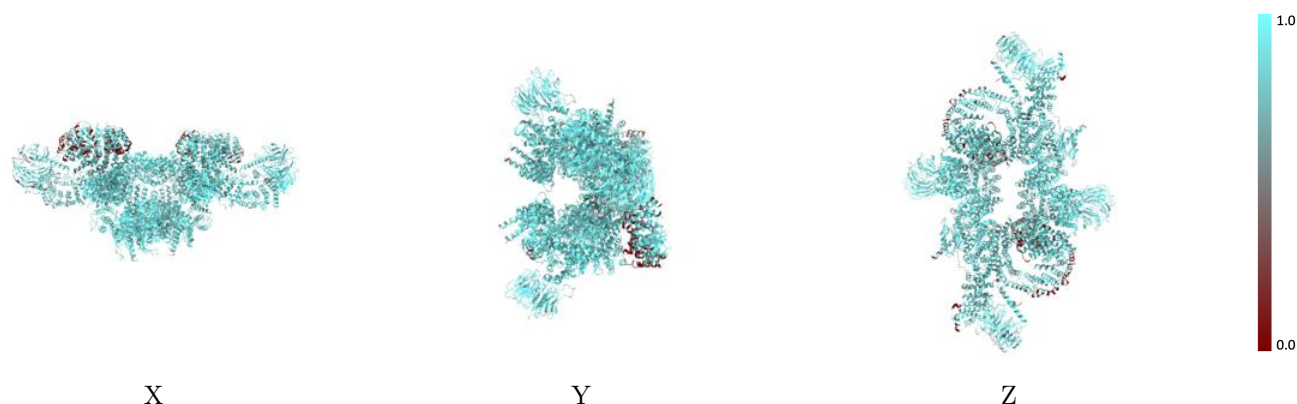
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



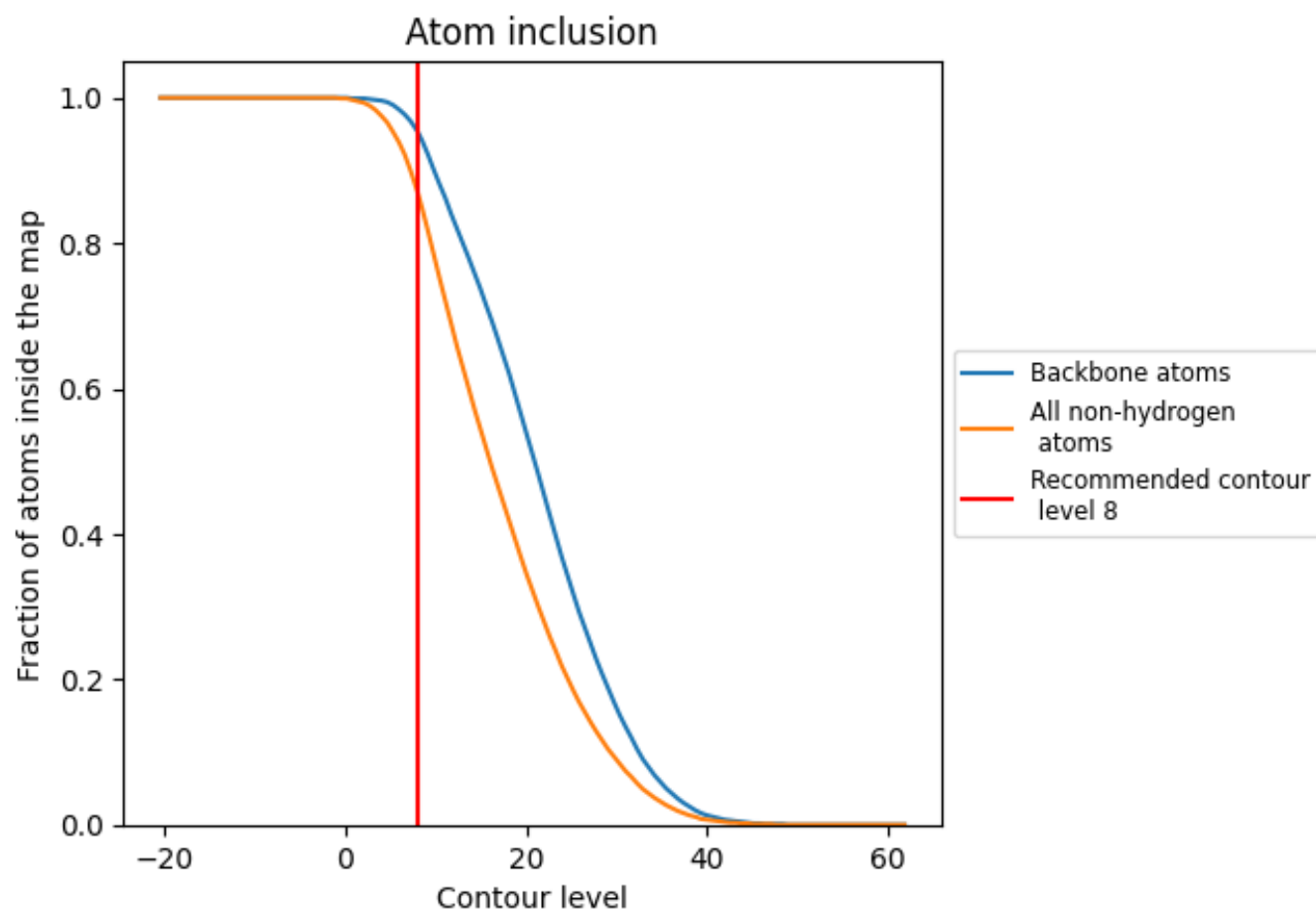
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 87% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.2520
A	0.8750	0.2690
B	0.8590	0.2580
C	0.9350	0.2550
D	0.9110	0.2170
E	0.8450	0.2090
F	0.8880	0.2570
G	0.6540	0.1090
H	0.6410	0.1990

1.0

0.0

<0.0