



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 02:43 PM UTC

PDB ID : 6ZYW / pdb_00006zyw
EMDB ID : EMD-11576
Title : Outer Dynein Arm-Shulin complex - overall structure (Tetrahymena thermophila)
Authors : Mali, G.R.; Abid Ali, F.; Lau, C.K.; Carter, A.P.
Deposited on : 2020-08-03
Resolution : 8.78 Å(reported)

This is a wwPDB EM Validation Summary 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:

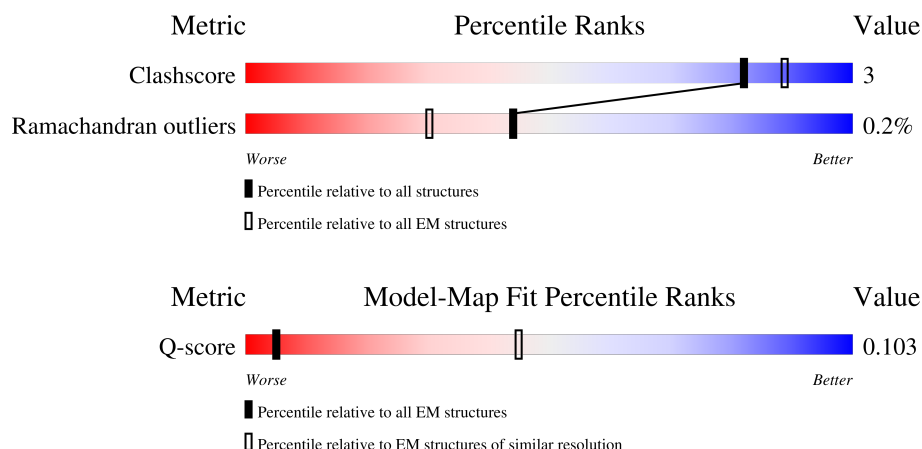
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 8.78 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.



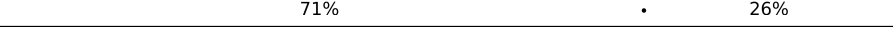
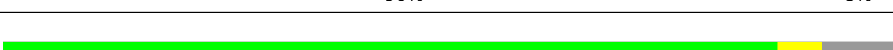
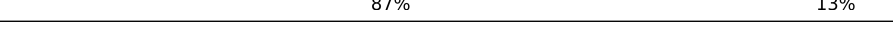
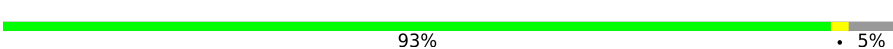
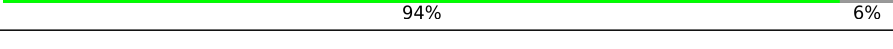
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	250 (8.30 - 9.25)

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	4168	
2	B	4595	
3	C	4620	
4	D	667	
4	d	667	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	670	
5	e	670	
6	F	133	
7	G	103	
8	H	92	
9	I	110	
10	J	93	
11	K	111	
12	L	111	
13	M	87	
14	N	132	
15	O	117	
16	P	110	
17	Y	1200	

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 73897 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 Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	3795	Total	C	N	O	0	0
			18787	11198	3795	3794		

- Molecule 2 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	4370	Total	C	N	O	0	417
			20008	12102	3953	3953		

- Molecule 3 is a protein called Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	4433	Total	C	N	O	0	563
			19737	11997	3870	3870		

- Molecule 4 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	321	Total	C	N	O	0	0
			1588	946	321	321		
4	d	128	Total	C	N	O	0	0
			637	381	128	128		

- Molecule 5 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	341	Total	C	N	O	0	0
			1678	996	341	341		
5	e	102	Total	C	N	O	0	0
			501	297	102	102		

- Molecule 6 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	98	Total	C	N	O	0	0
			486	290	98	98		

- Molecule 7 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	95	Total	C	N	O	0	0
			470	280	95	95		

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	85	Total	C	N	O	0	0
			420	250	85	85		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	89	Total	C	N	O	0	0
			439	261	89	89		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	95	Total	C	N	O	0	0
			470	280	95	95		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	97	Total	C	N	O	0	0
			479	285	97	97		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	86	Total	C	N	O	0	0
			426	254	86	86		

- Molecule 14 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	109	Total	C	N	O	0	0
			537	319	109	109		

- Molecule 15 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	111	Total	C	N	O	0	0
			550	328	111	111		

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	103	Total	C	N	O	0	0
			513	307	103	103		

- Molecule 17 is a protein called Shulin.

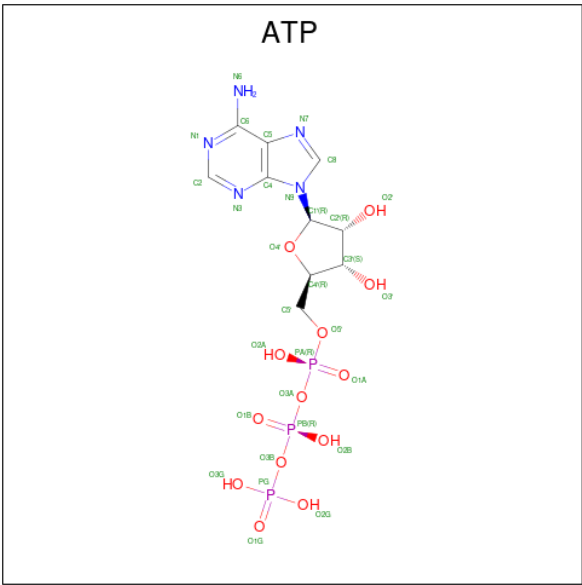
Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	1133	Total	C	N	O	0	0
			5611	3345	1133	1133		

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



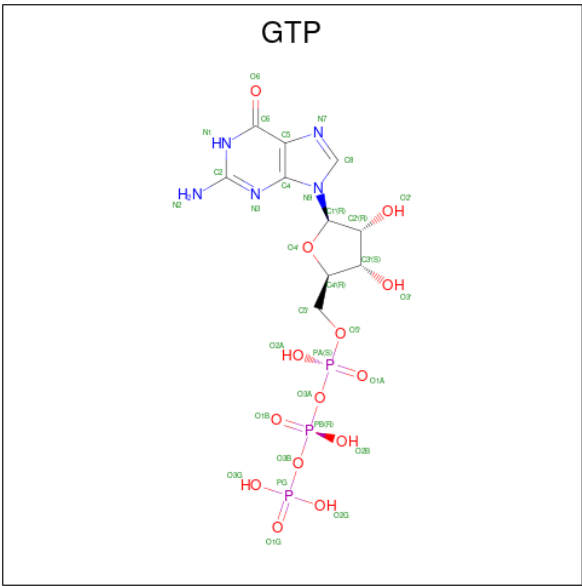
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
19	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

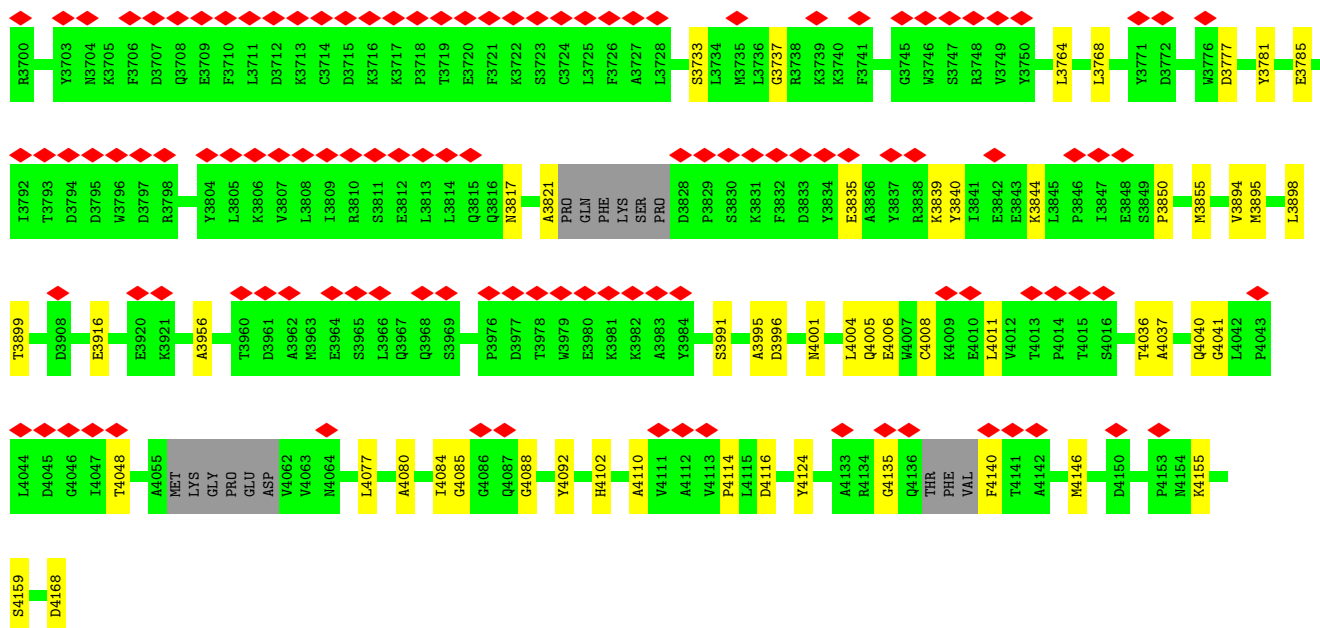
- Molecule 20 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



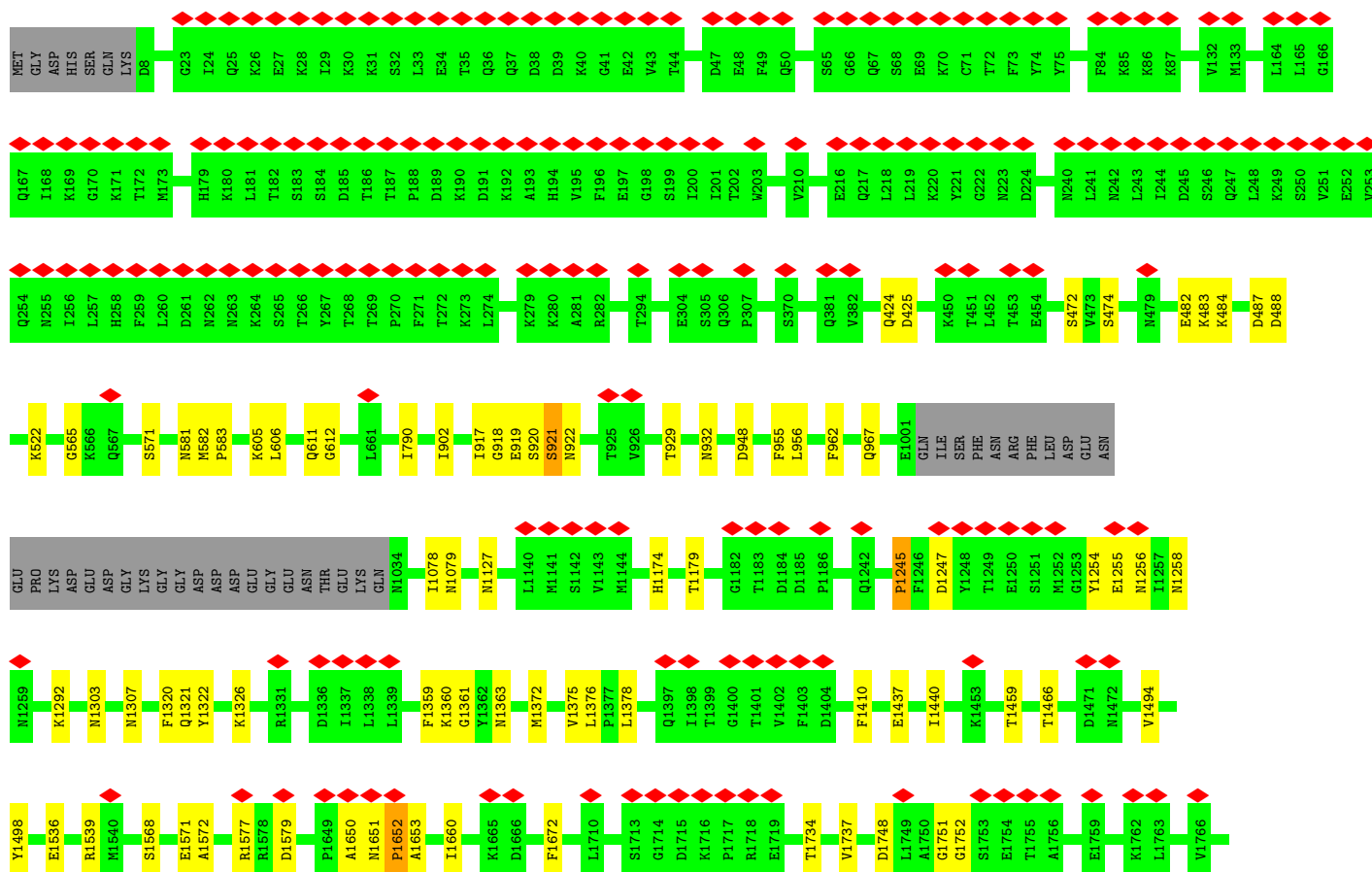
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	Y	1	32	10	5	14	3	0

K2671	N2672	V2673	E2674	A2675	Q2676	K2677	S2678	T2679	T2680	Q2681	Q2682	D2683	L2684	D2685	A2686	A2687	Q2688	P2689	L2690	V2691	E2692	Q2693	A2694	K2695	S2696	A2697	L2698	N2699	S2700	I2701	S2702	K2703	K2704	D2705	F2706	Q2707	Q2708	A2709	K2710	S2711	F2712	A2713	S2714	P2715	T2716	A2717	Q2718	V2719	P2720	E2721	V2722	F2723	A2724	A2725	T2726	I2727	L2728	L2729	L2730
K2611	E2612	T2613	A2614	Q2615	Q2616	V2617	A2618	I2619	L2620	E2621	V2622	E2623	V2624	K2625	E2626	Q2627	Q2628	V2629	E2630	A2631	E2632	A2633	K2634	K2635	K2636	E2637	A2638	D2639	A2640	F2641	A2642	E2643	V2644	V2645	Q2646	R2647	E2648	K2649	K2650	K2651	V2652	E2653	K2654	E2655	N2656	S2657	K2658	A2659	T2660	I2661	E2662	A2663	D2664	K2665	G2666	L2668	I2669	K2670	
E2463	Q2464	K2465	P2466	D2467	T2468	R2469	A2487	G2494	D2495	W2496	D2497	R2498	D2499	A2500	K2501	Q2502	F2503	V2511	I2512	D2513	W2514	F2515	Q2516	P2517	W2518	V2519	Y2520	E2521	A2522	L2523	F2524	N2525	V2526	A2527	K2528	S2529	F2530	L2531	E2532	P2533	V2534	D2535	LEU	GLY	ASP	ASP	LYS	VAL	ARG	E2543	A2544	V2545	V2546	K2547	F2548	M2549			
P2550	F2551	S2552	F2553	T2554	L2555	V2556	ASN	ASP	LEU	GLY	LVS	LEU	GLU	GLN	GLU	ARG	R2569	Y2572	T2573	T2574	P2575	K2576	S2577	F2578	L2579	E2580	L2581	T2582	S2583	L2584	F2585	T2586	N2587	M2588	D2589	A2590	Q2591	K2592	R2593	E2594	S2595	L2596	E2597	R2598	N2599	K2600	E2601	R2602	Y2603	E2604	T2605	G2606	L2607	V2608	K2609	L2610			
H2242	E2243	C2244	E2245	R2246	T2247	Y2248	Q2249	D2250	R2251	L2252	V2253	S2254	T2255	D2256	N2257	L2258	K2259	T2260	Y2261	K2262	E2263	N2264	T2265	F2266	D2267	L2268	V2269	K2270	K2271	S2272	F2273	S2274	K2275	F2276	N2277	F2278	S2279	R2280	Y2281	F2282	G2283	N2284	N2285	P2286	E2287	N2293	F2294	G2297	D2305	Q2306	M2307	P2308	N2309	N2310	E2311	M2312			
E2313	K2314	N2324	D2325	W2326	N2327	F2335	E2336	D2337	A2338	M2339	K2340	H2341	V2342	C2343	R2344	V2359	G2360	V2361	G2362	G2363	S2364	S2374	F2375	G2378	C2406	G2407	P2408	L2409	E2410	F2417	E2425	L2434	G2438	D2447	E2450	A2451	M2452	T2453	N2454	Q2455	V2456	R2457	A2458	K2459	V2460	K2461	G2462												
G2022	I2023	L2024	K2025	E2026	T2027	VAL	GLN	ALA	LYS	PRO	E2033	Y2044	D2047	Y2077	P2085	Q2086	L2087	D2088	A2089	Y2090	D2091	T2092	L2102	G2106	Y2109	D2110	V2111	S2112	K2113	L2114	Q2123	S2134	F2135	F2136	P2139	D2154	N2155	E2156	S2157	L2158	S2159	L2160	T2161	Y2162	T2163	T2164	F2165	L2166											
T1928	W1929	W1930	K1931	GLY	ALA	TRP	LYS	THR	ALA	V1938	K1939	F1940	P1941	K1942	G1944	T1945	I1946	D1948	F1947	Y1949	V1951	D1952	Q1953	S1954	GLY	ASP	S1957	S1958	K1959	F1960	V1961	E1962	W1963	S1964	K1965	R1966	L1967	E1968	N1969	K1970	E1971	F1972	P1974	Q1975	V1976	E1977	T1978	I1982	T1983	V1984	M1985	K1997	S1998						
Y1818	I1819	S1820	V1823	G1824	H1825	Q1826	S1829	S1833	K1836	Q1837	E1838	F1839	S1840	Q1841	D1842	E1844	K1847	N1848	L1849	D1850	T1851	L1852	F1853	G1854	K1855	I1877	T1889	L1890	L1891	K1892	GLY	ASP	VAL	LYS	ASN	LEU	E1899	A1915	E1916	K1917	D1918	S1919	I1920	D1921	Y1922	R1923	K1924	D1925	F1926	S1927									
D1750	T1751	M1752	P1753	K1754	W1755	I1756	C1757	L1758	D1759	G1760	L1762	D1763	A1764	M1765	W1766	I1767	D1768	S1769	M1770	M1771	S1772	V1773	M1774	D1775	D1776	M1777	K1778	I1779	L1780	T1781	L1782	A1783	M1784	W1785	E1786	R1787	I1788	P1789	L1790	K1791	P1792	H1793	M1794	R1795	A1796	L1797	F1798	D1802	L1803	R1804	F1805	A1806	A1814	G1815	I1816	L1817			
C1679	V1680	F1681	V1682	M1683	G1684	G1689	T1693	A1700	Q1701	D1702	K1703	T1704	N1705	K1706	K1707	T1708	T1709	W1710	I1711	D1714	P1715	K1716	V1717	L1718	S1719	T1720	K1721	D1722	F1723	Y1724	G1725	Y1726	N1727	L1728	P1729	M1730	K1731	E1732	W1733	K1734	D1735	G1736	L1737	F1738	S1739	K1740	M1741	L1742	R1743	S1744	L1745	A1746	E1747	Q1748	P1749				
K1555	F1556	V1557	T1558	L1559	M1560	M1561	L1562	C1563	R1564	D1565	L1566	L1567	S1568	K1569	Q1570	L1571	H1572	D1573	D1574	W1575	G1576	L1577	A1578	L1579	I1580	R1592	S1593	E1594	P1595	E1596	I1597	L1598	E1599	Q1600	A1601	L1602	L1603	M1604	R1605	A1606	A1616	L1620	P1632	Q1633	T1634	M1635	I1636	S1671	L1674	A1675	T1676	R1677	H1678						

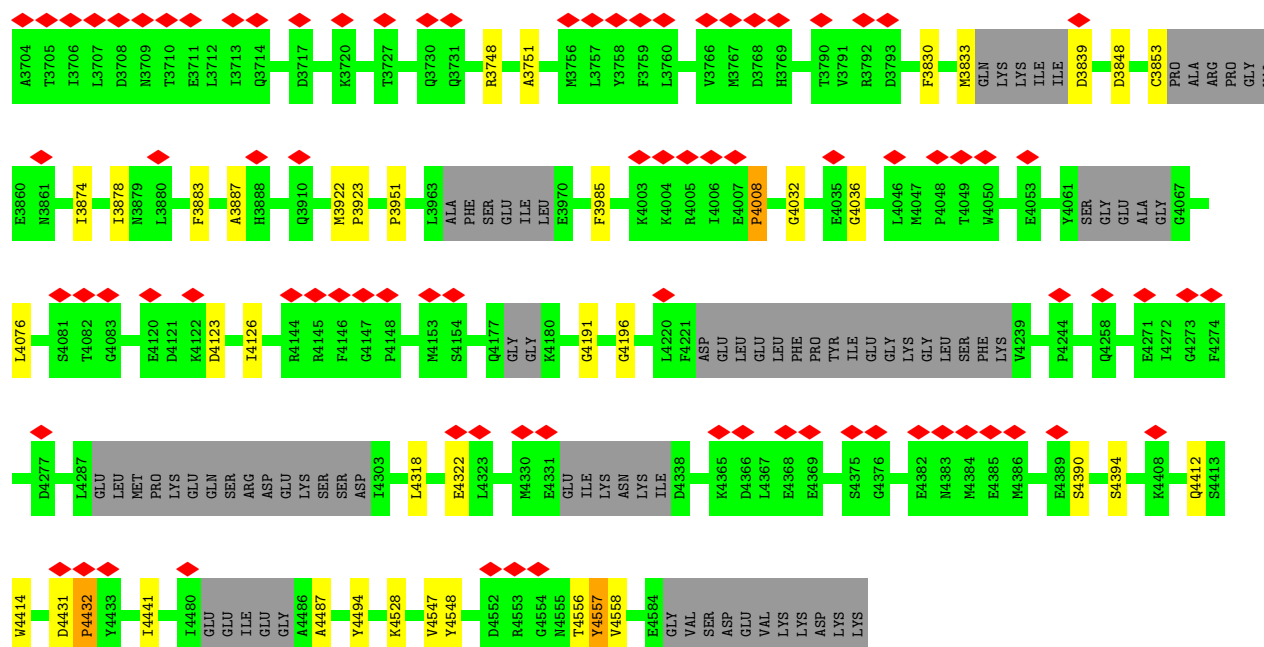




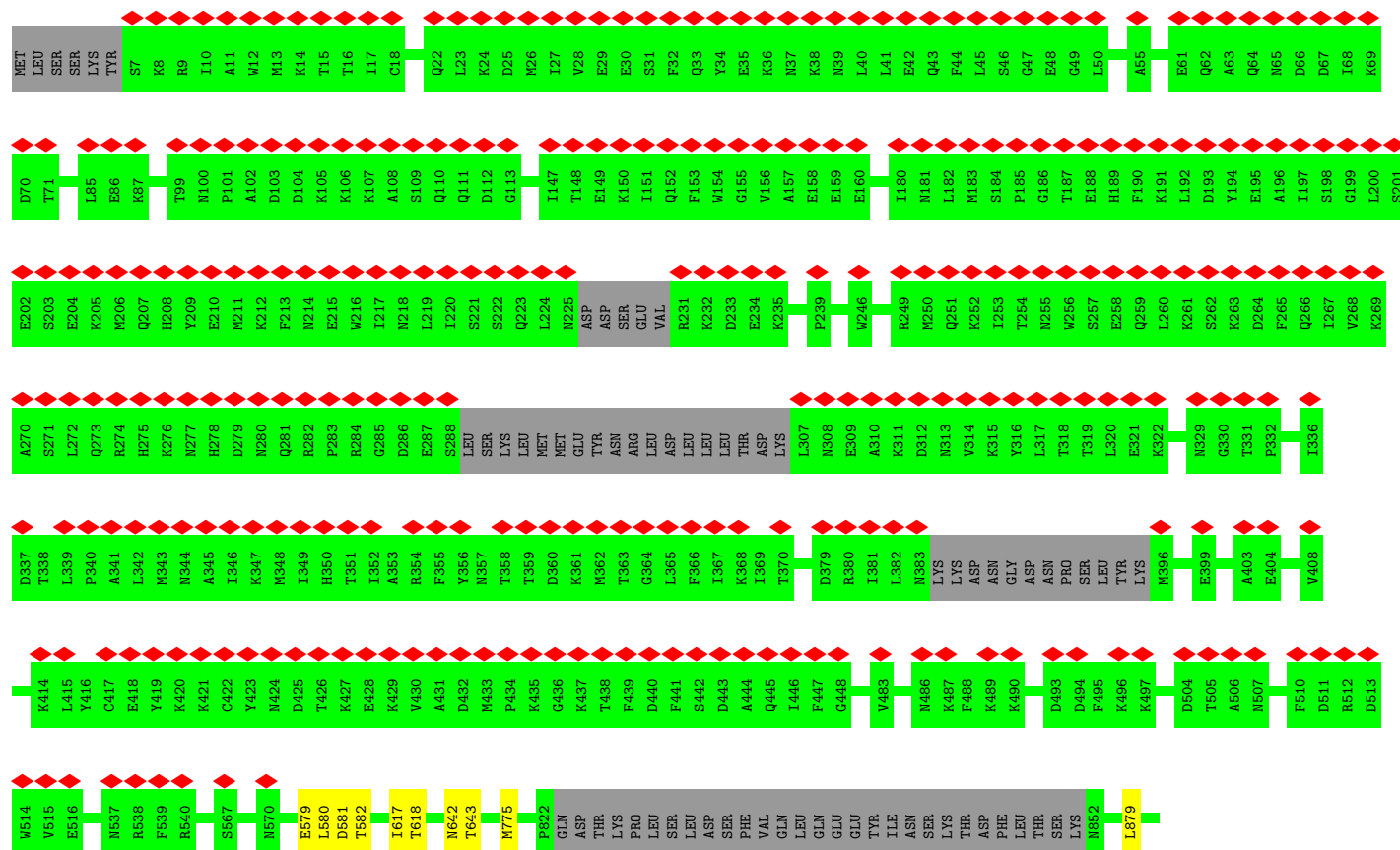
• Molecule 2: Outer arm dynein beta heavy chain

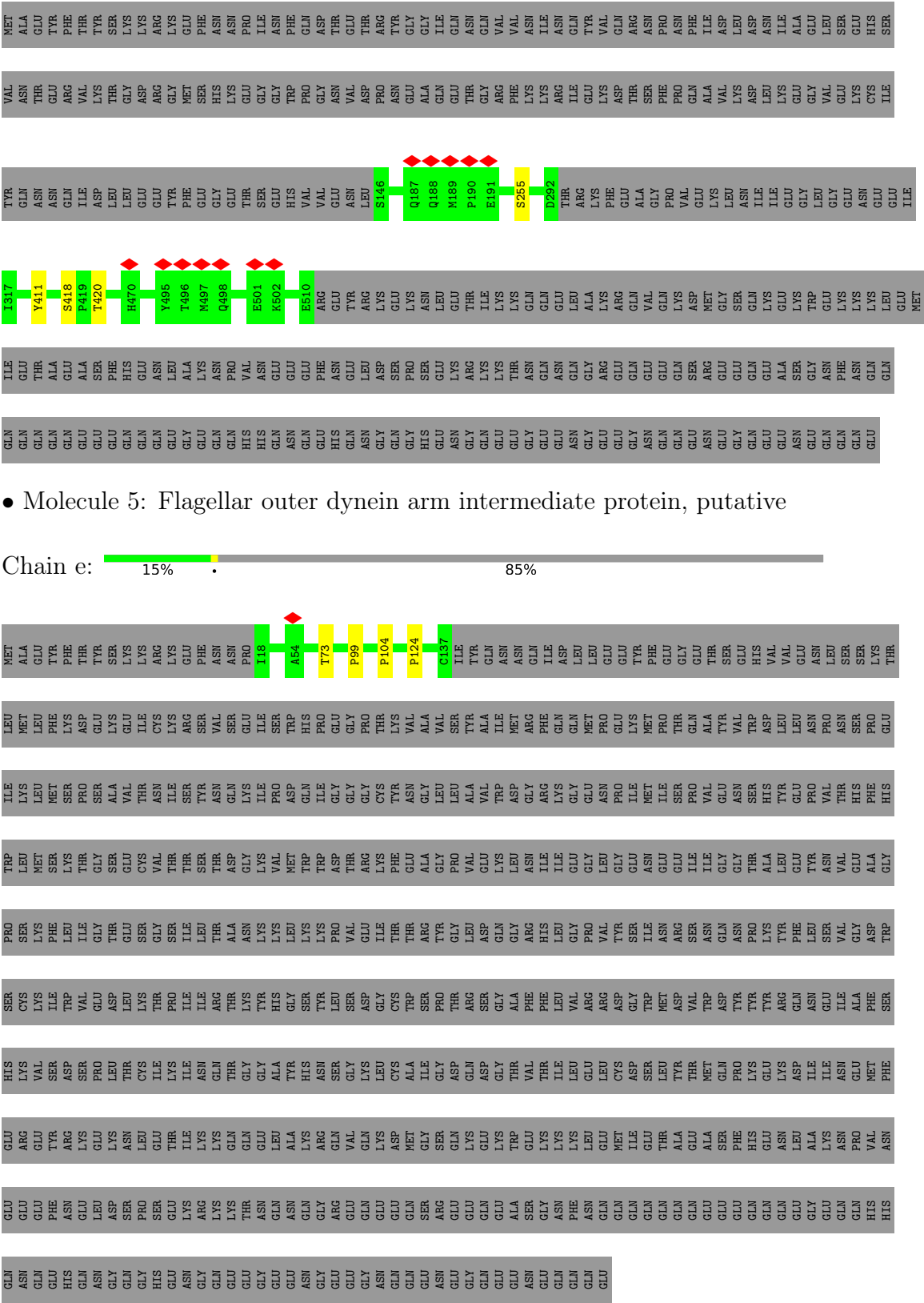






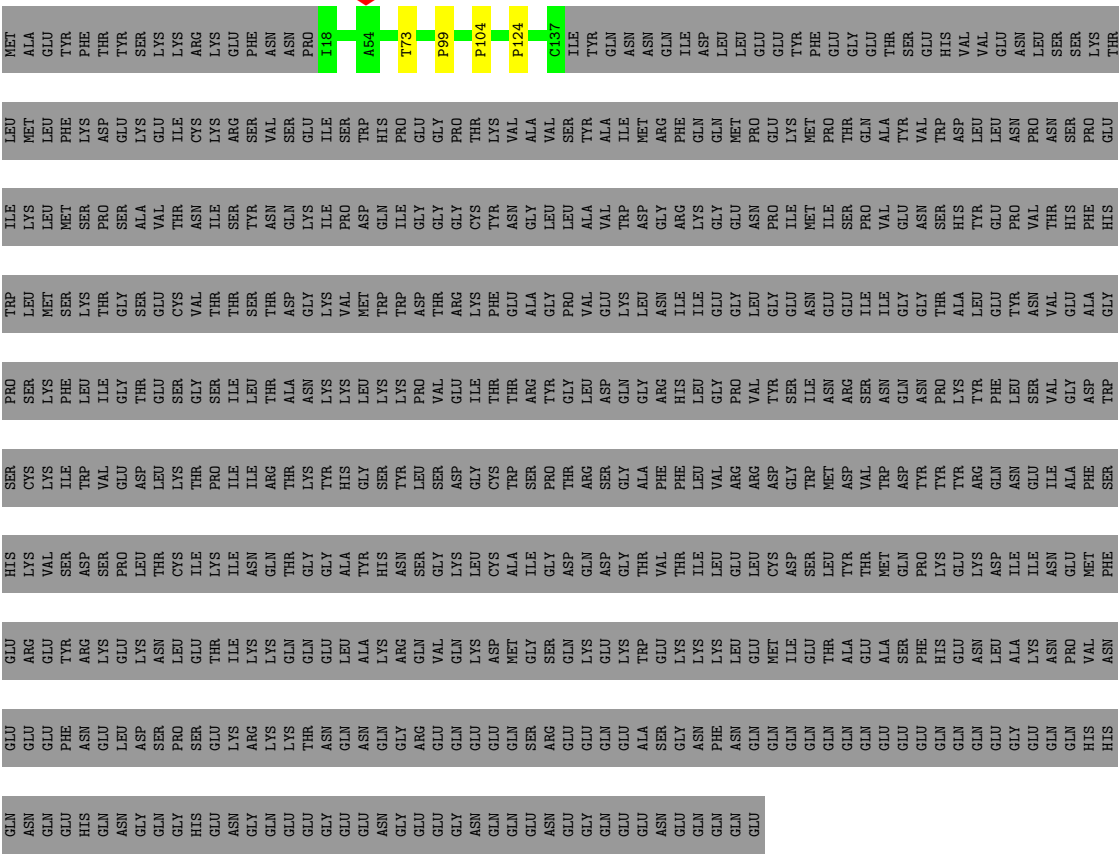
• Molecule 3: Dynein heavy chain, outer arm protein





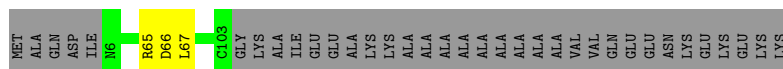
• Molecule 5: Flagellar outer dynein arm intermediate protein, putative

Chain e: 15% . 85%



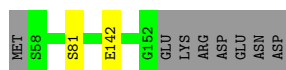
• Molecule 6: Dynein light chain roadblock-type 2 protein

Chain F: 71% . 26%



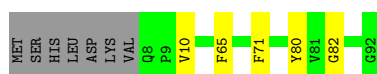
- Molecule 7: Dynein light chain roadblock-type 2 protein

Chain G: 90% 8%



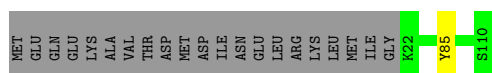
- Molecule 8: Dynein light chain

Chain H: 87% 5% 8%



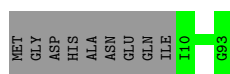
- Molecule 9: Dynein light chain

Chain I: 80% 19%



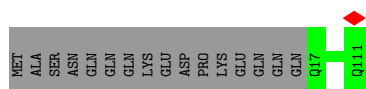
- Molecule 10: Dynein light chain

Chain J: 90% 10%



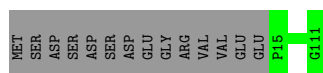
- Molecule 11: Dynein light chain

Chain K: 86% 14%



- Molecule 12: Dynein light chain

Chain L: 87% 13%

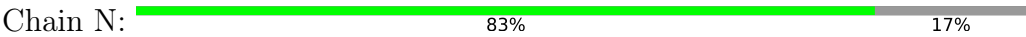


- Molecule 13: Dynein light chain

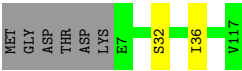
Chain M: 99%



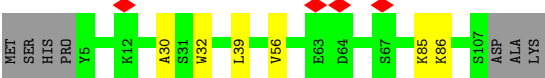
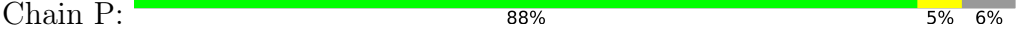
- Molecule 14: Dynein light chain 2A



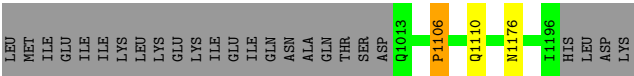
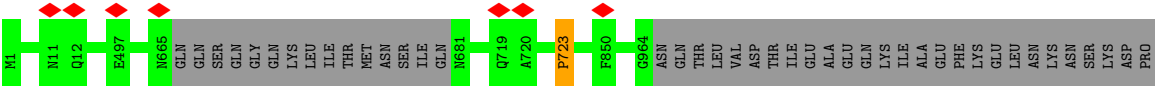
- Molecule 15: Dynein light chain tctex-type 1 protein



- Molecule 16: Thioredoxin



- Molecule 17: Shulin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0008	Depositor
Map size (Å)	499.5, 499.5, 499.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, GTP

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	0.42	0/18743	0.90	23/26057 (0.1%)
2	B	0.50	2/19561 (0.0%)	0.85	39/27233 (0.1%)
3	C	0.35	3/19162 (0.0%)	0.66	17/26702 (0.1%)
4	D	0.43	0/1584	1.03	2/2201 (0.1%)
4	d	0.35	0/634	0.72	0/881
5	E	0.43	0/1676	0.97	2/2327 (0.1%)
5	e	0.57	0/498	0.95	3/687 (0.4%)
6	F	0.59	0/485	1.11	4/675 (0.6%)
7	G	0.47	0/469	0.92	0/652
8	H	0.51	0/419	1.02	2/582 (0.3%)
9	I	0.51	0/438	1.09	0/608
10	J	0.32	0/415	0.63	0/577
11	K	0.28	0/469	0.59	0/652
12	L	0.29	0/478	0.68	0/664
13	M	0.28	0/425	0.58	0/591
14	N	0.28	0/536	0.63	0/744
15	O	0.20	0/549	0.43	0/764
16	P	1.20	0/512	1.47	2/714 (0.3%)
17	Y	0.30	1/5608 (0.0%)	0.56	3/7814 (0.0%)
All	All	0.43	6/72661 (0.0%)	0.81	97/101125 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	1176	ASN	C-N	10.26	1.47	1.33
3	C	879	LEU	C-O	8.28	1.27	1.23
2	B	1174	HIS	CA-C	6.50	1.56	1.52
2	B	487	ASP	C-N	-6.48	1.25	1.33
3	C	1091	GLU	C-N	-5.49	1.26	1.33

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3951	PRO	N-CA-CB	10.21	109.65	102.81
2	B	4432	PRO	N-CA-CB	10.05	113.80	103.25
1	A	502	ASN	CA-C-N	8.89	128.54	118.85
1	A	502	ASN	C-N-CA	8.89	128.54	118.85
1	A	83	CYS	N-CA-C	8.47	123.24	109.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18787	0	8282	134	0
2	B	20008	0	8566	93	0
3	C	19737	0	8300	29	0
4	D	1588	0	693	3	0
4	d	637	0	261	2	0
5	E	1678	0	724	1	0
5	e	501	0	215	1	0
6	F	486	0	218	0	0
7	G	470	0	203	1	0
8	H	420	0	185	2	0
9	I	439	0	202	1	0
10	J	416	0	184	0	0
11	K	470	0	215	0	0
12	L	479	0	209	0	0
13	M	426	0	189	0	0
14	N	537	0	231	0	0
15	O	550	0	247	1	0
16	P	513	0	213	2	0
17	Y	5611	0	2410	0	0
18	C	81	0	36	0	0
19	C	31	0	12	0	0
20	Y	32	0	12	0	0
All	All	73897	0	31807	268	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 3.

The worst 5 of 268 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:B:917:ILE:O	2:B:921:SER:CB	2.17	0.92
3:C:617:ILE:C	3:C:618:THR:CA	2.46	0.89
2:B:4318:LEU:O	2:B:4322:GLU:N	2.12	0.83
3:C:642:ASN:CA	3:C:643:THR:N	2.43	0.81
2:B:2229:LYS:O	2:B:2230:THR:N	2.13	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3707/4168 (89%)	3206 (86%)	493 (13%)	8 (0%)	43	78
2	B	3893/4595 (85%)	3484 (90%)	398 (10%)	11 (0%)	36	72
3	C	3846/4620 (83%)	3509 (91%)	330 (9%)	7 (0%)	43	78
4	D	313/667 (47%)	268 (86%)	45 (14%)	0	100	100
4	d	122/667 (18%)	112 (92%)	10 (8%)	0	100	100
5	E	337/670 (50%)	287 (85%)	50 (15%)	0	100	100
5	e	96/670 (14%)	86 (90%)	10 (10%)	0	100	100
6	F	96/133 (72%)	79 (82%)	17 (18%)	0	100	100
7	G	93/103 (90%)	81 (87%)	12 (13%)	0	100	100
8	H	83/92 (90%)	76 (92%)	7 (8%)	0	100	100
9	I	87/110 (79%)	79 (91%)	8 (9%)	0	100	100
10	J	82/93 (88%)	77 (94%)	5 (6%)	0	100	100
11	K	93/111 (84%)	83 (89%)	10 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	95/111 (86%)	90 (95%)	5 (5%)	0	100	100
13	M	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
14	N	107/132 (81%)	100 (94%)	7 (6%)	0	100	100
15	O	109/117 (93%)	99 (91%)	10 (9%)	0	100	100
16	P	101/110 (92%)	97 (96%)	4 (4%)	0	100	100
17	Y	1127/1200 (94%)	1071 (95%)	54 (5%)	2 (0%)	43	78
All	All	14471/18456 (78%)	12961 (90%)	1482 (10%)	28 (0%)	44	78

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1823	VAL
2	B	1651	ASN
2	B	1652	PRO
2	B	2557	PRO
2	B	3703	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
18	ADP	C	4703	-	28,29,29	1.32	4 (14%)	43,45,45	1.98	10 (23%)
20	GTP	Y	1301	-	33,34,34	0.89	2 (6%)	50,54,54	1.61	8 (16%)
19	ATP	C	4702	-	32,33,33	1.23	5 (15%)	48,52,52	1.80	9 (18%)
18	ADP	C	4701	-	28,29,29	1.37	5 (17%)	43,45,45	1.85	10 (23%)
18	ADP	C	4704	-	28,29,29	1.34	4 (14%)	43,45,45	1.87	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ADP	C	4703	-	-	3/16/32/32	0/3/3/3
20	GTP	Y	1301	-	-	6/22/38/38	0/3/3/3
19	ATP	C	4702	-	-	4/22/38/38	0/3/3/3
18	ADP	C	4701	-	-	1/16/32/32	0/3/3/3
18	ADP	C	4704	-	-	3/16/32/32	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	4704	ADP	C5-C4	4.37	1.46	1.39
18	C	4701	ADP	C5-C4	4.27	1.46	1.39
18	C	4703	ADP	C5-C4	4.19	1.46	1.39
19	C	4702	ATP	C5-C4	4.05	1.46	1.39
18	C	4703	ADP	C5-N7	-2.58	1.34	1.39

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	4703	ADP	C5-C4-N3	-6.20	118.17	126.72
18	C	4704	ADP	C5-C4-N3	-5.94	118.53	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	4702	ATP	C5-C4-N3	-5.93	118.55	126.72
18	C	4701	ADP	C5-C4-N3	-5.49	119.16	126.72
18	C	4703	ADP	N3-C4-N9	5.26	136.11	127.17

There are no chirality outliers.

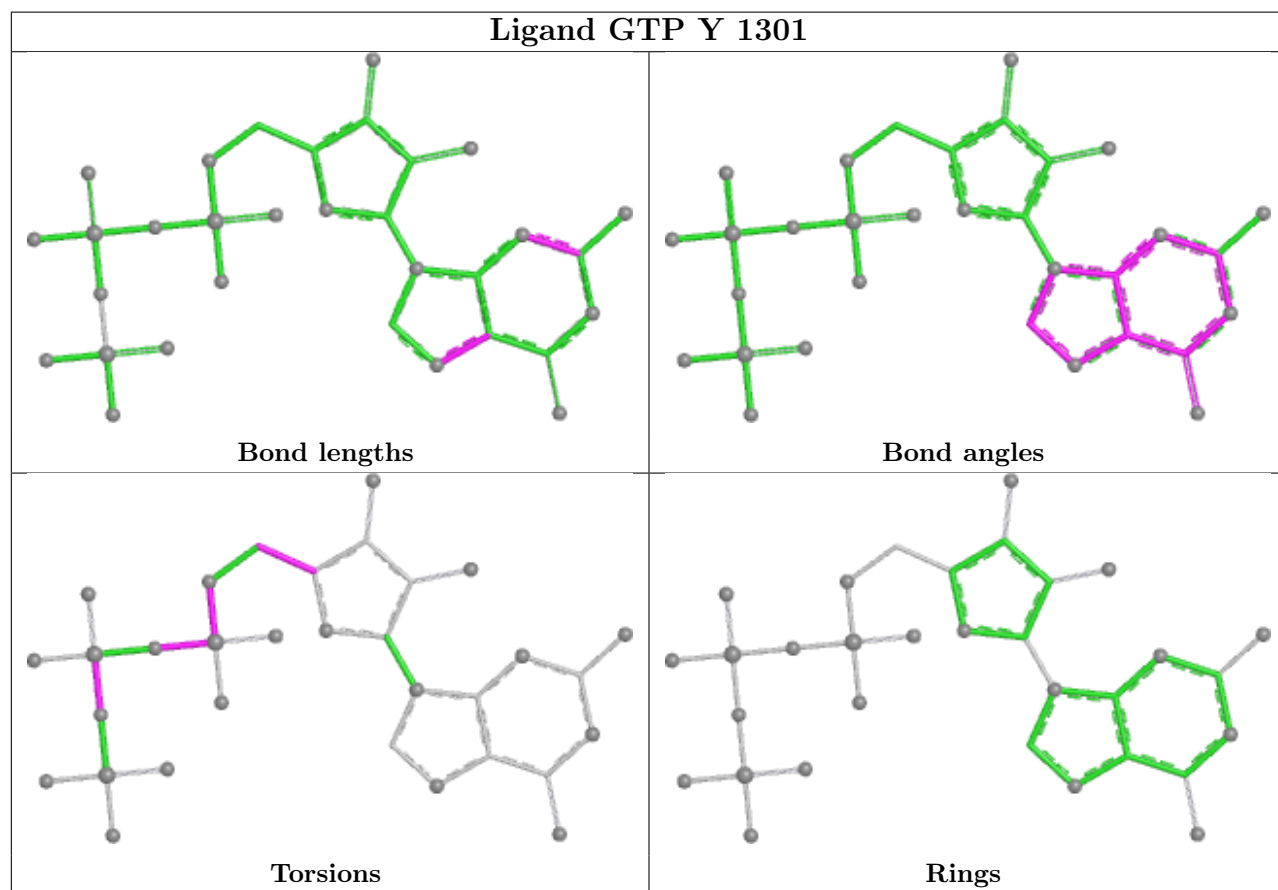
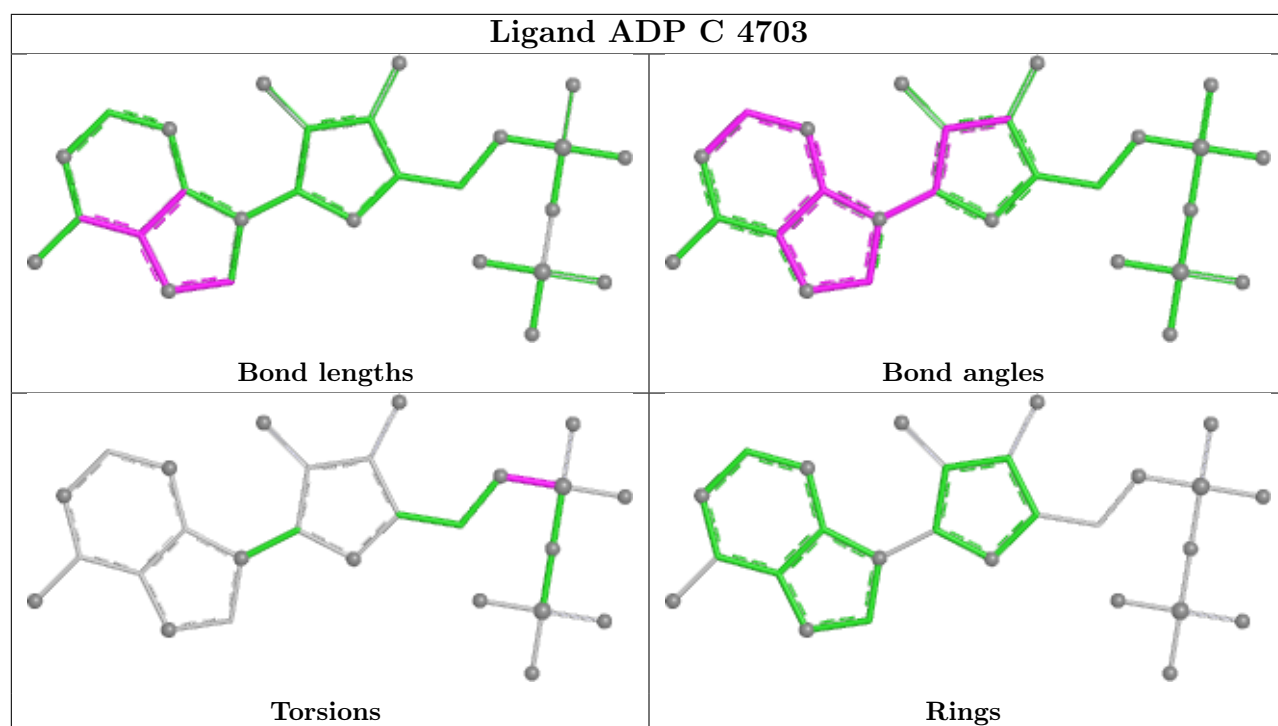
5 of 17 torsion outliers are listed below:

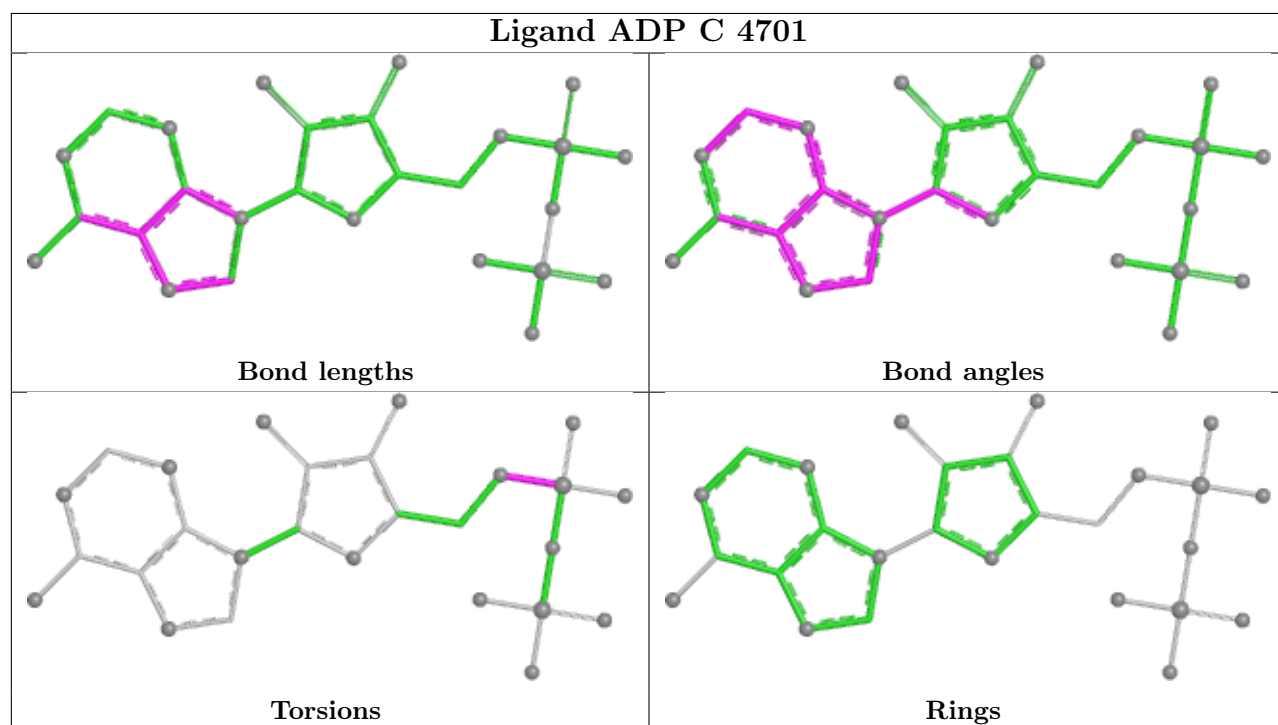
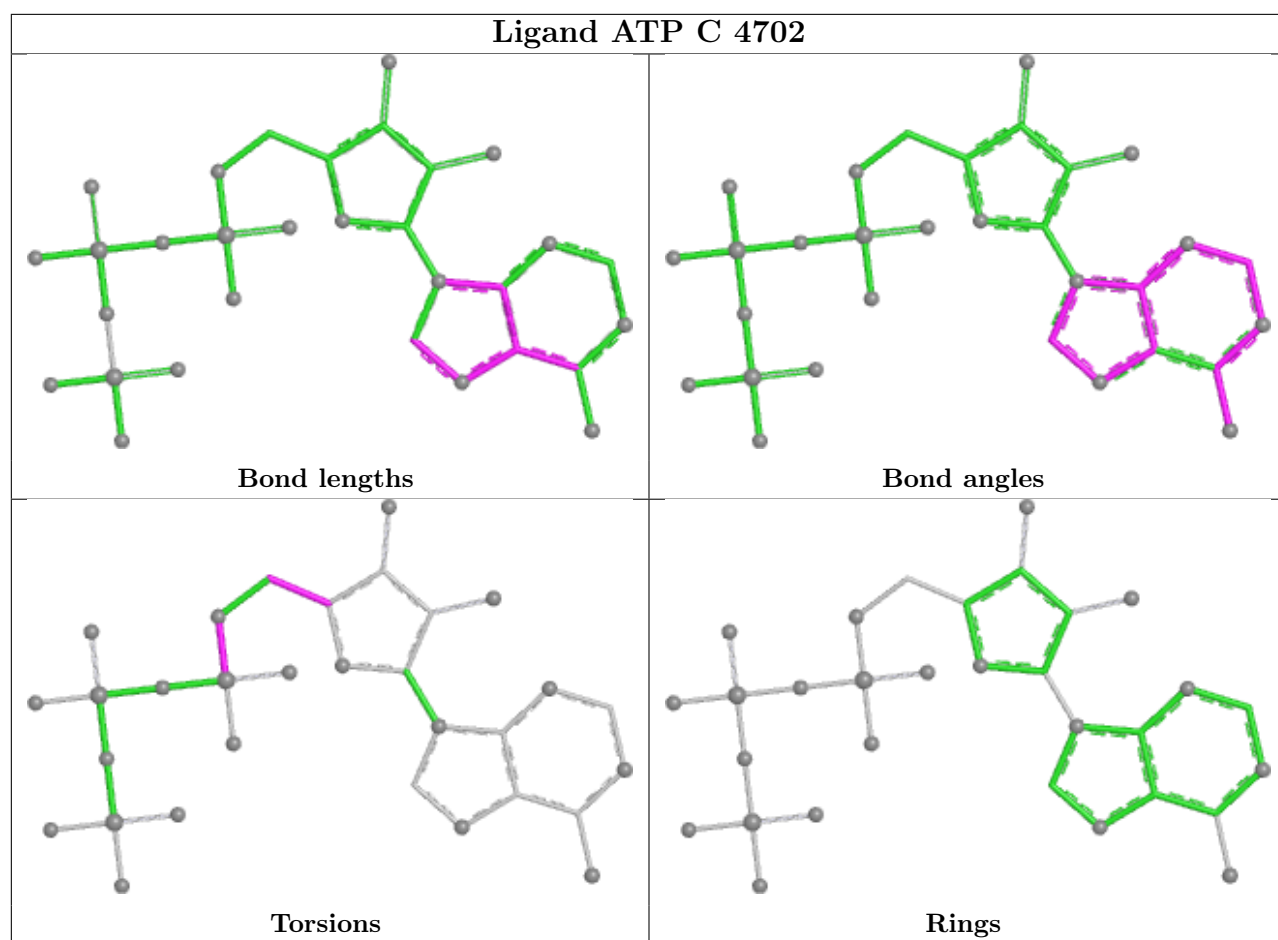
Mol	Chain	Res	Type	Atoms
18	C	4703	ADP	C5'-O5'-PA-O1A
18	C	4703	ADP	C5'-O5'-PA-O2A
18	C	4703	ADP	C5'-O5'-PA-O3A
18	C	4704	ADP	C5'-O5'-PA-O2A
18	C	4704	ADP	C5'-O5'-PA-O3A

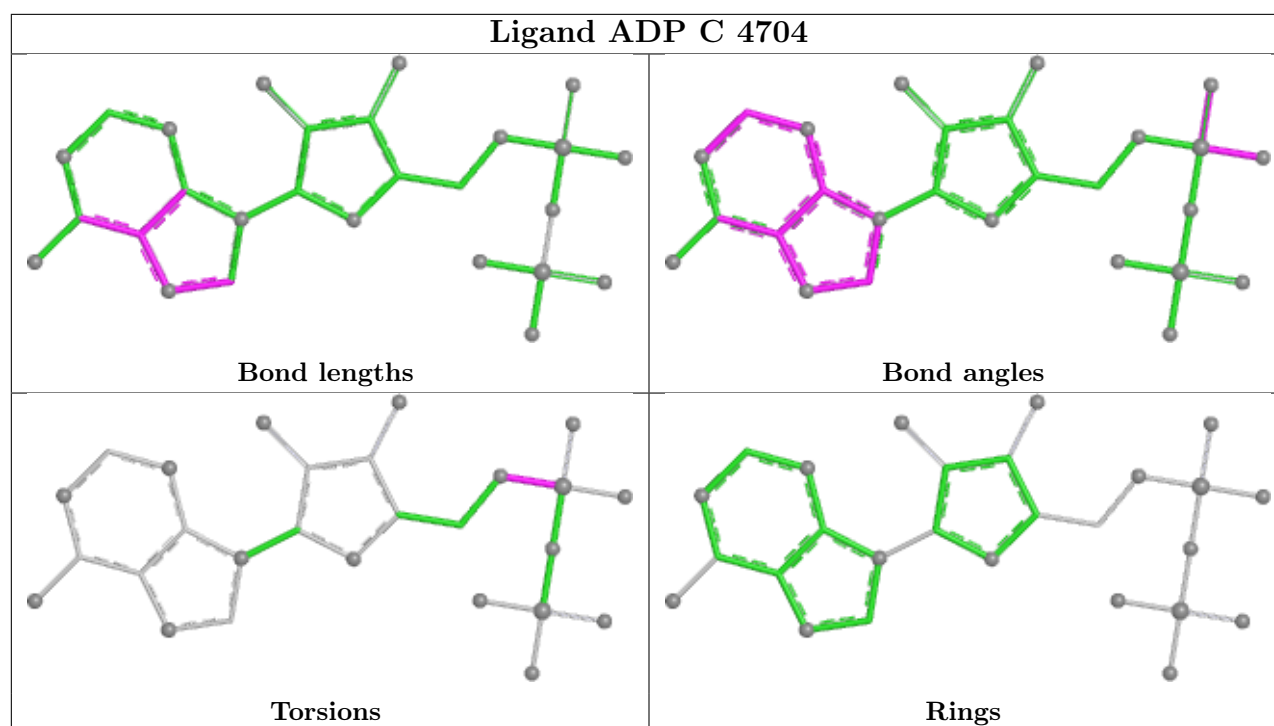
There are no ring outliers.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	23
2	B	12
5	e	2
4	d	1

The worst 5 of 38 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	201:GLN	C	235:TRP	N	31.73
1	A	389:ASP	C	390:THR	N	29.62
1	A	486:ASP	C	487:GLN	N	21.39
1	A	1299:VAL	C	1300:GLN	N	17.01
1	A	2300:SER	C	2301:ASP	N	13.90

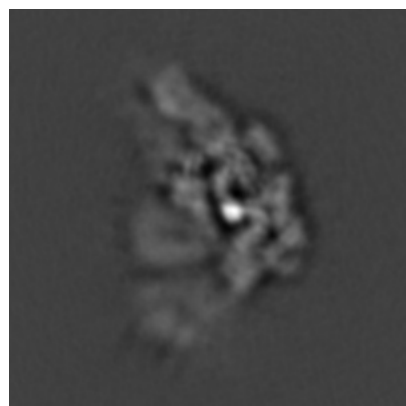
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11576. These allow visual inspection of the internal detail of the map and identification of artifacts.

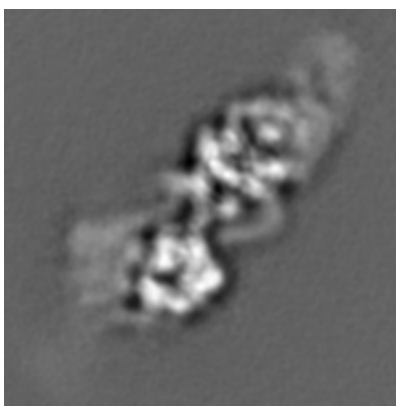
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

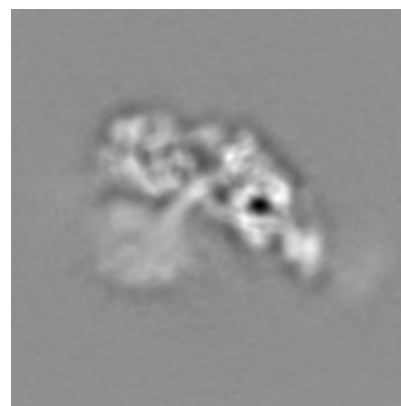
6.1.1 Primary map



X

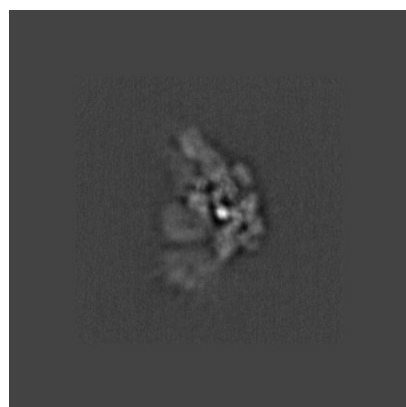


Y

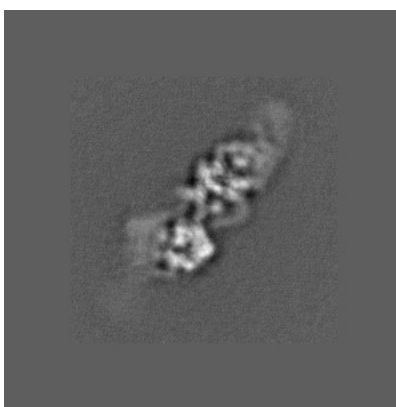


Z

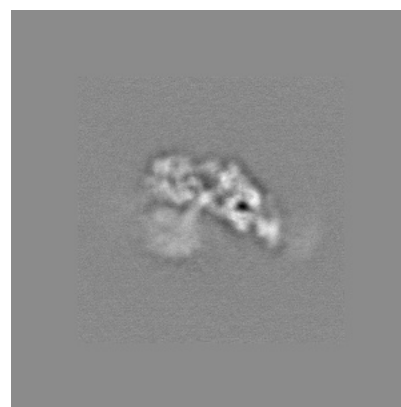
6.1.2 Raw map



X



Y

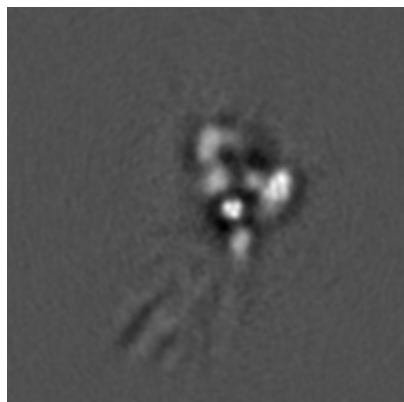


Z

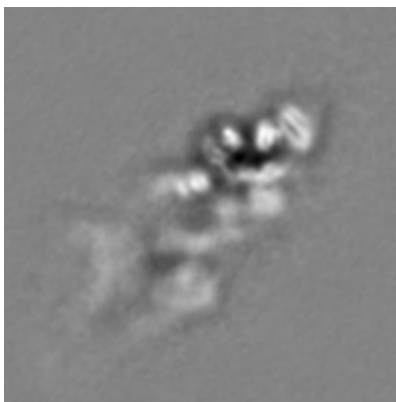
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

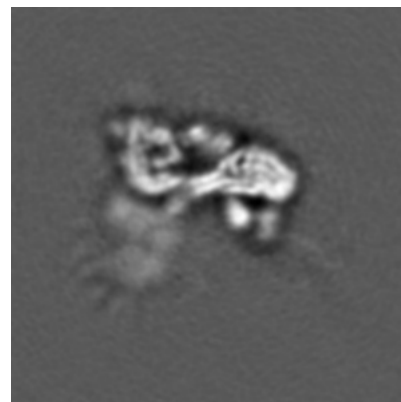
6.2.1 Primary map



X Index: 225

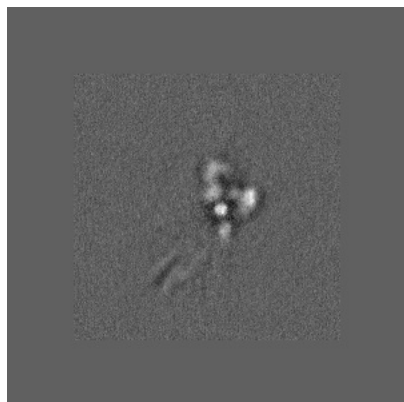


Y Index: 225

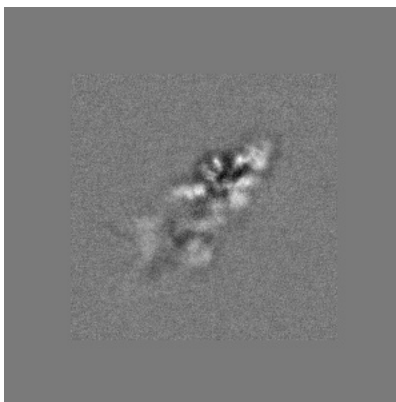


Z Index: 225

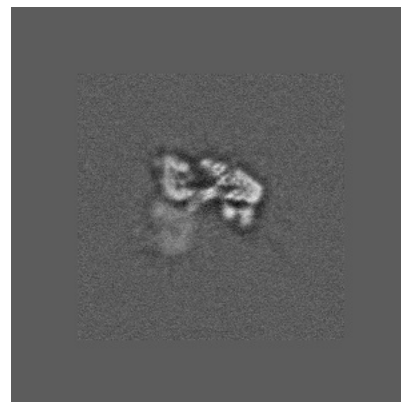
6.2.2 Raw map



X Index: 384



Y Index: 384

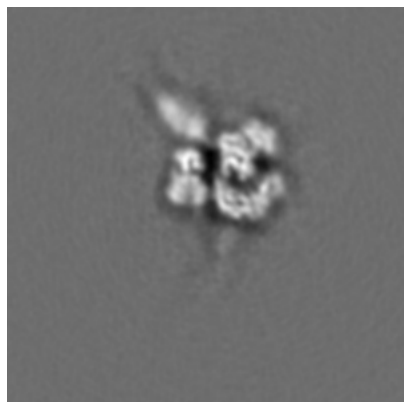


Z Index: 384

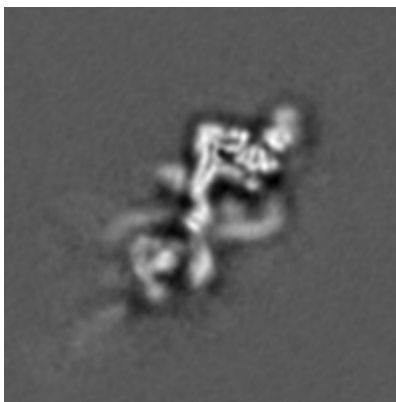
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

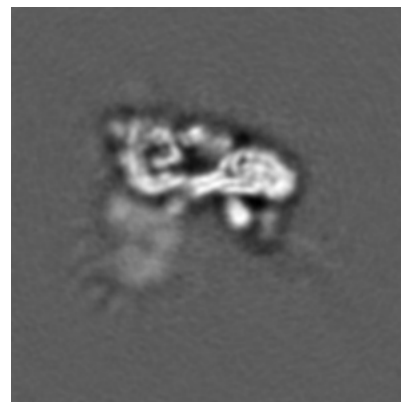
6.3.1 Primary map



X Index: 274

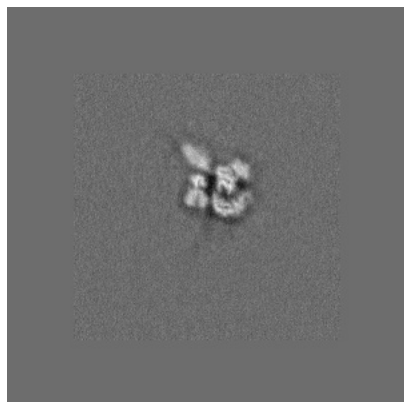


Y Index: 246

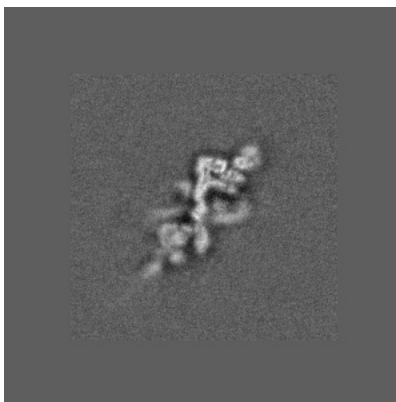


Z Index: 223

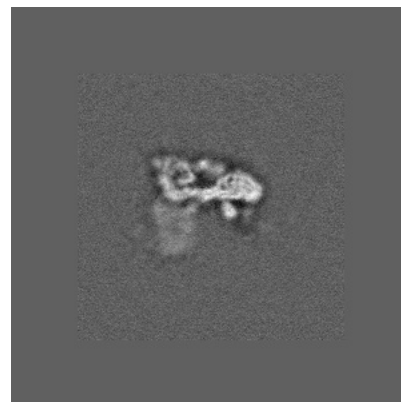
6.3.2 Raw map



X Index: 438



Y Index: 405

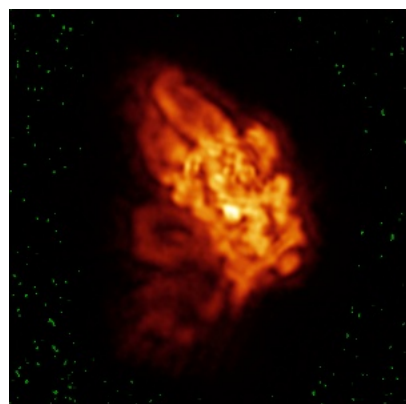


Z Index: 378

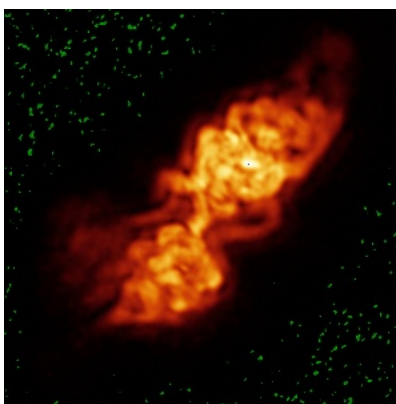
The images above show the largest variance slices of the map in three orthogonal directions.

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

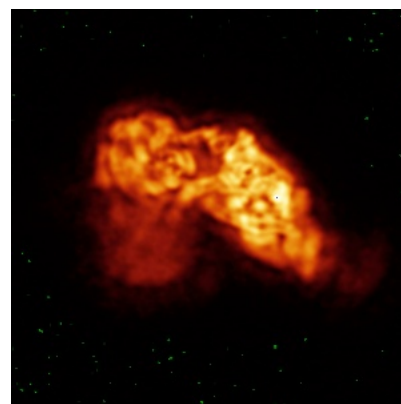
6.4.1 Primary map



X

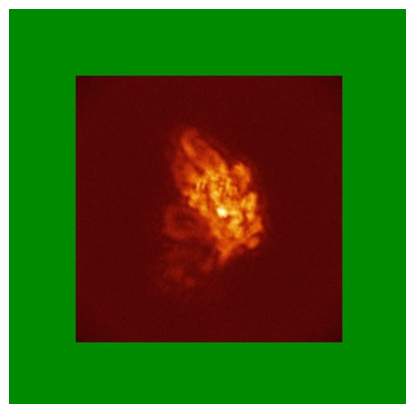


Y

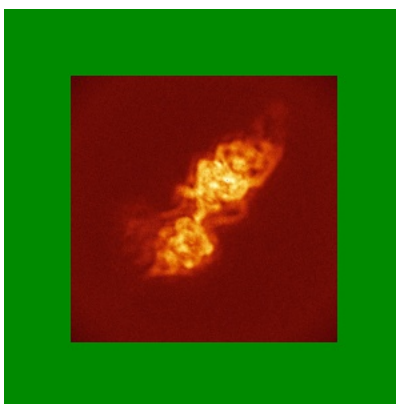


Z

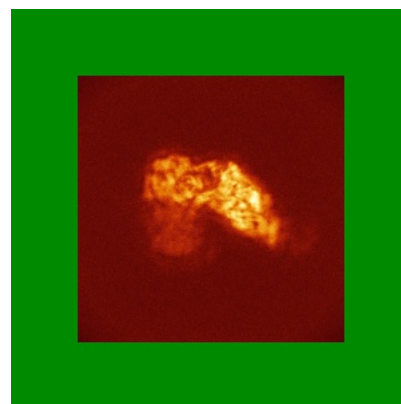
6.4.2 Raw map



X



Y

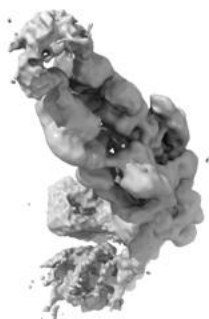


Z

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



X



Y



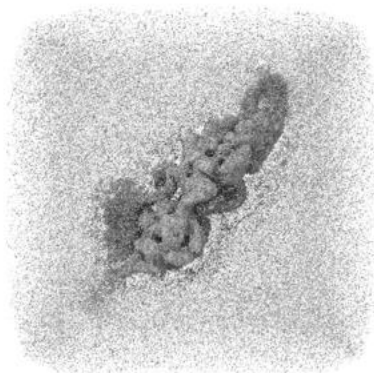
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

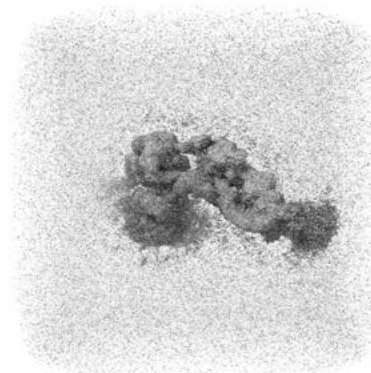
6.5.2 Raw map



X



Y



Z

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.

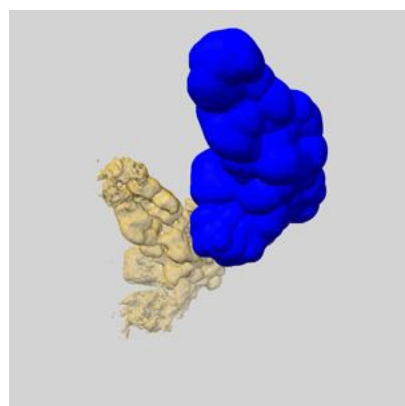
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

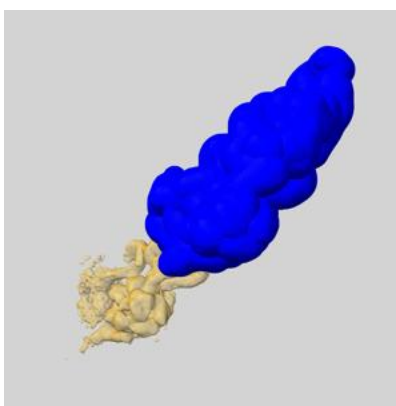
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

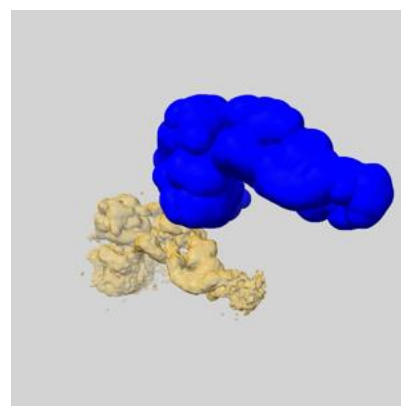
6.6.1 emd_11576_msk_1.map [i](#)



X



Y

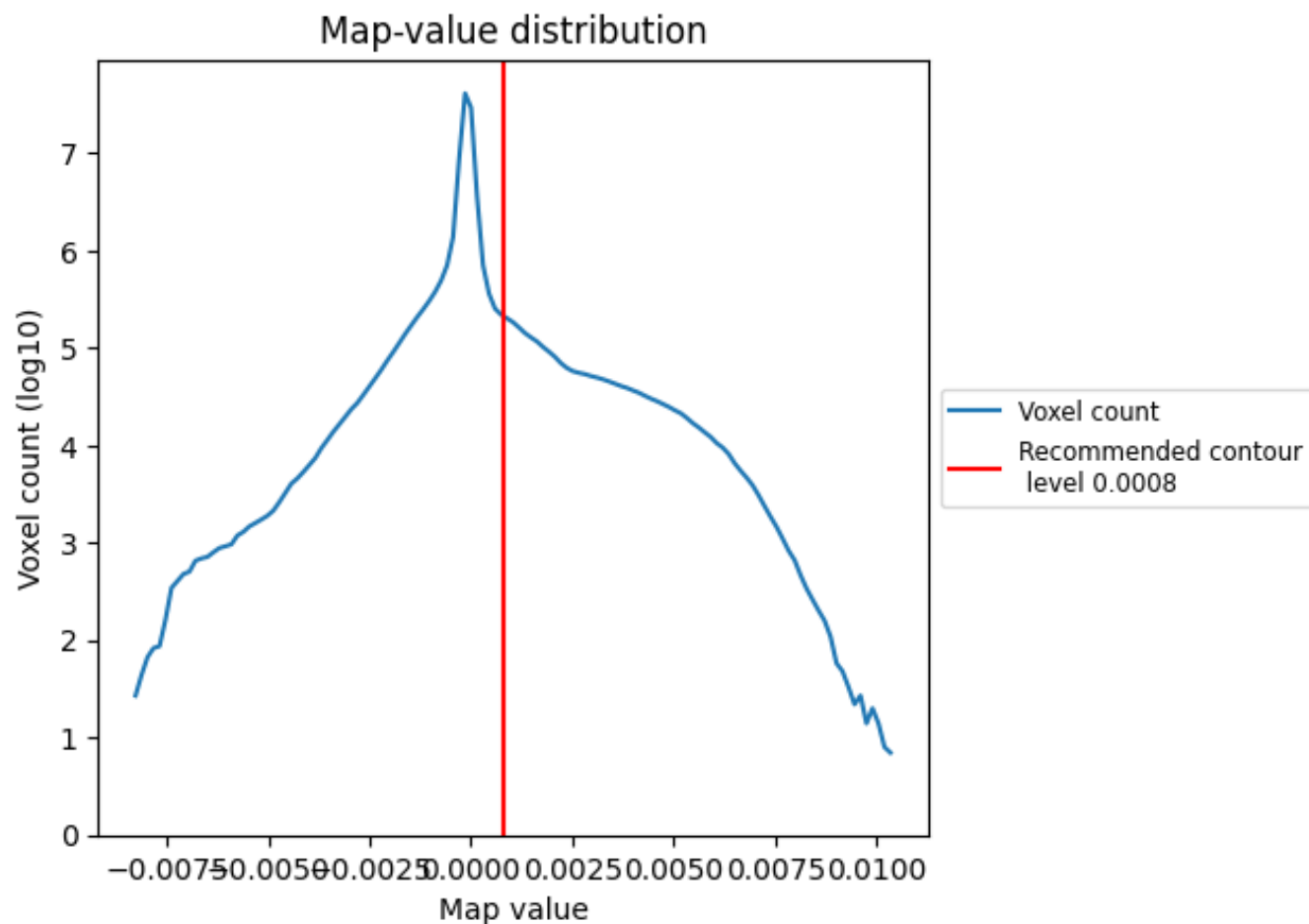


Z

7 Map analysis [i](#)

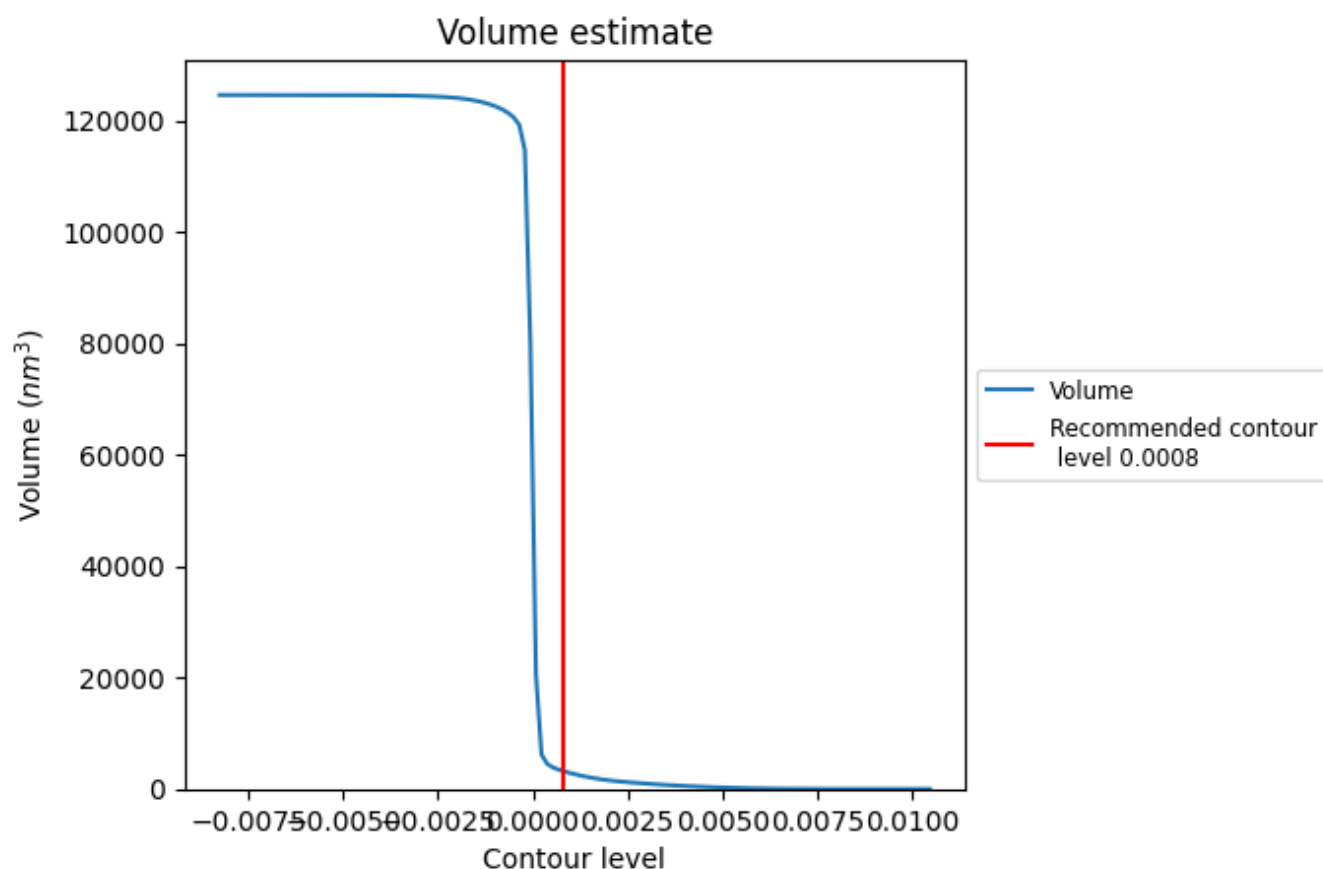
This section contains the results of statistical analysis of the map.

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.

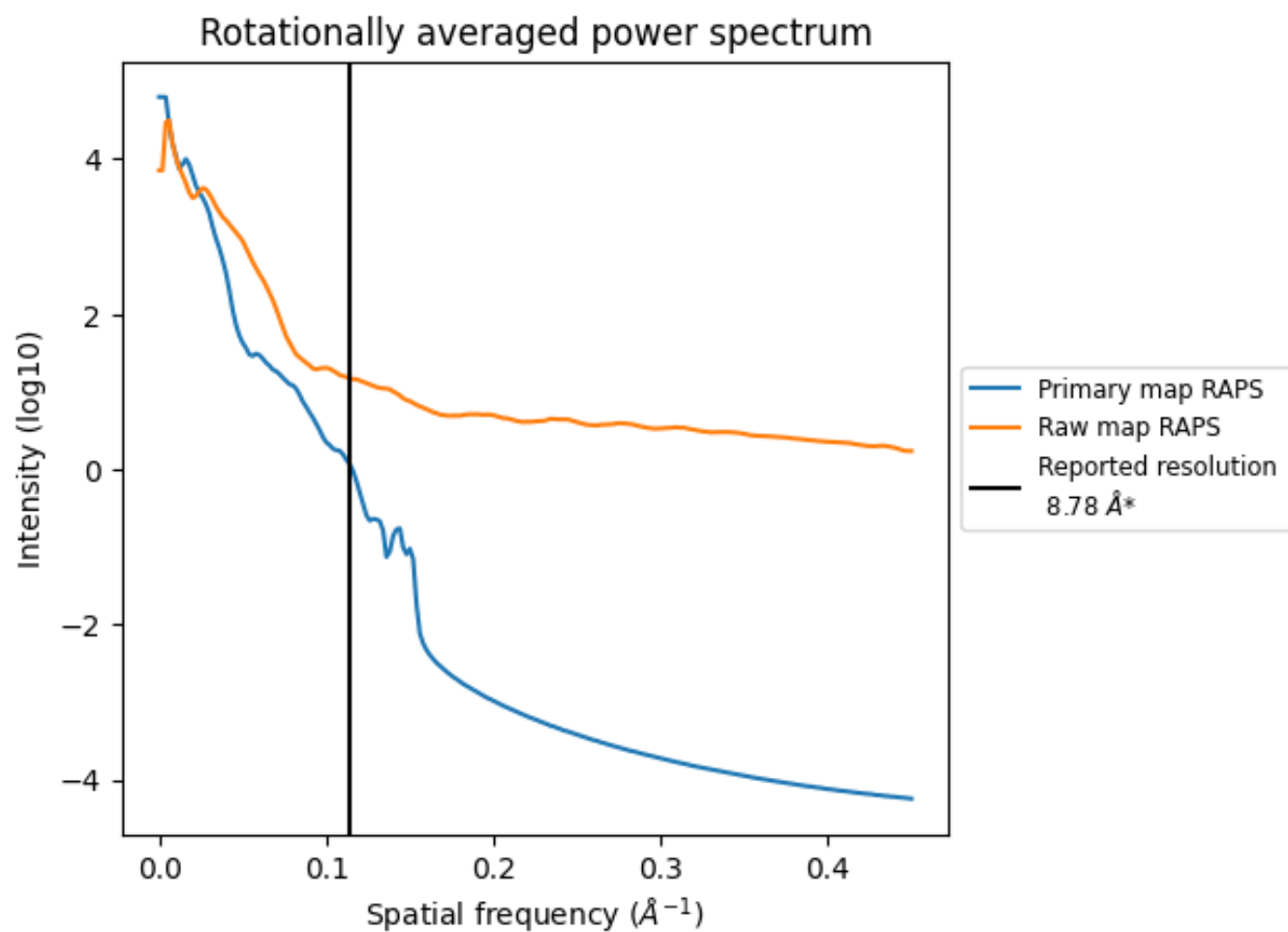
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3222 nm^3 ; this corresponds to an approximate mass of 2910 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 ⓘ

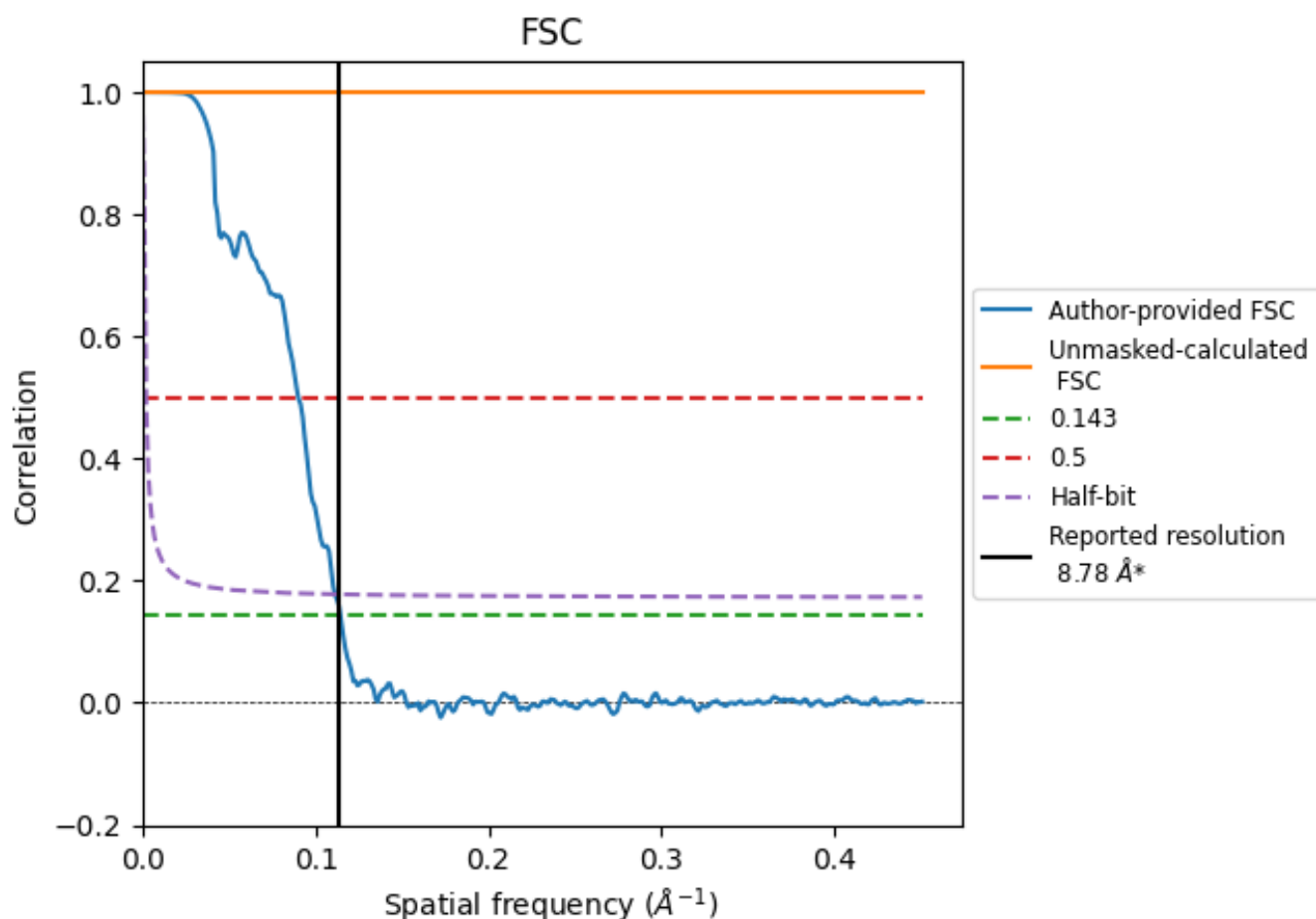


*Reported resolution corresponds to spatial frequency of 0.114 Å⁻¹

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 0.114 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

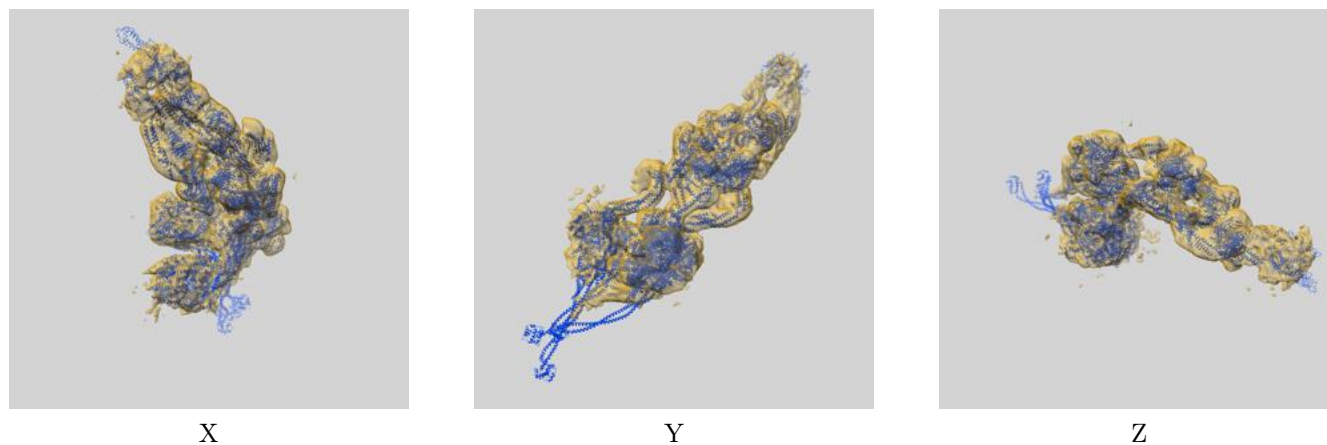
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.78	-	-
Author-provided FSC curve	8.73	11.09	8.98
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

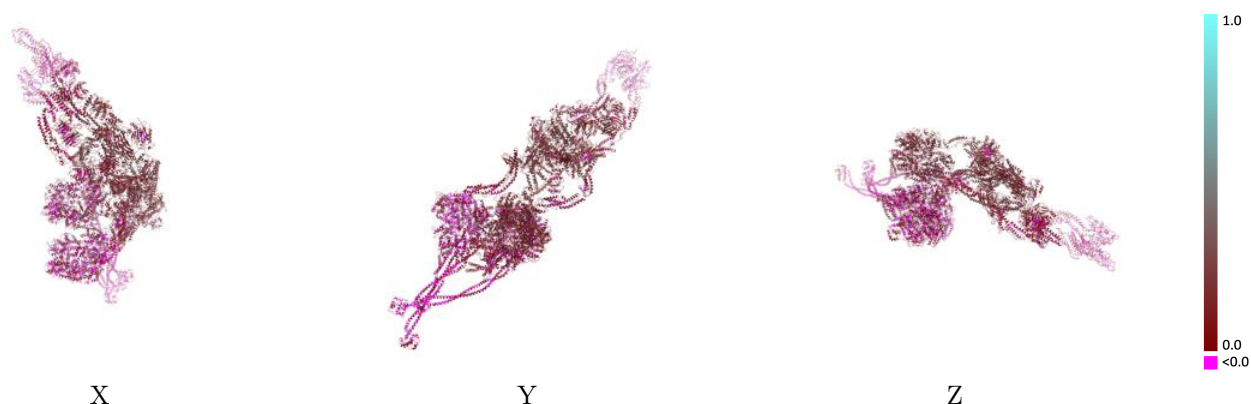
This section contains information regarding the fit between EMDB map EMD-11576 and PDB model 6ZYW. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



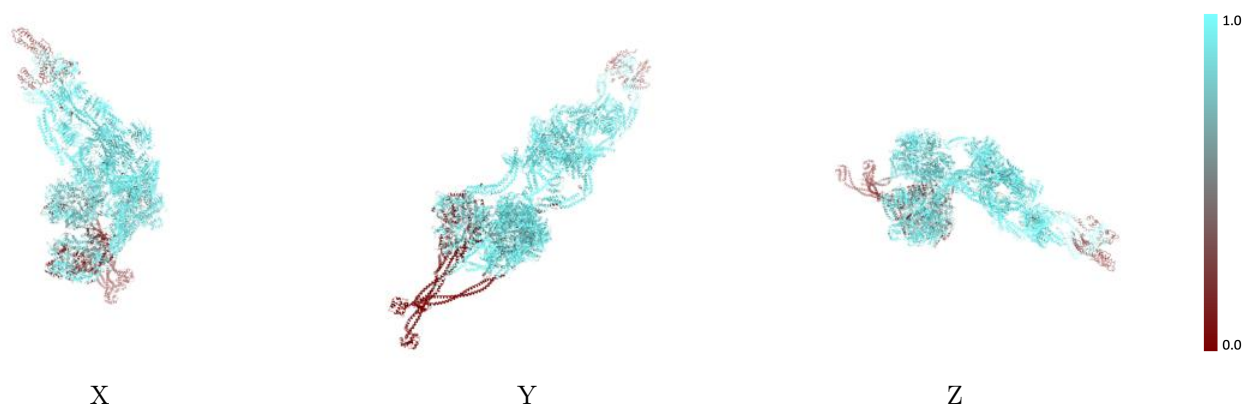
The images above show the 3D surface view of the map at the recommended contour level 0.0008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



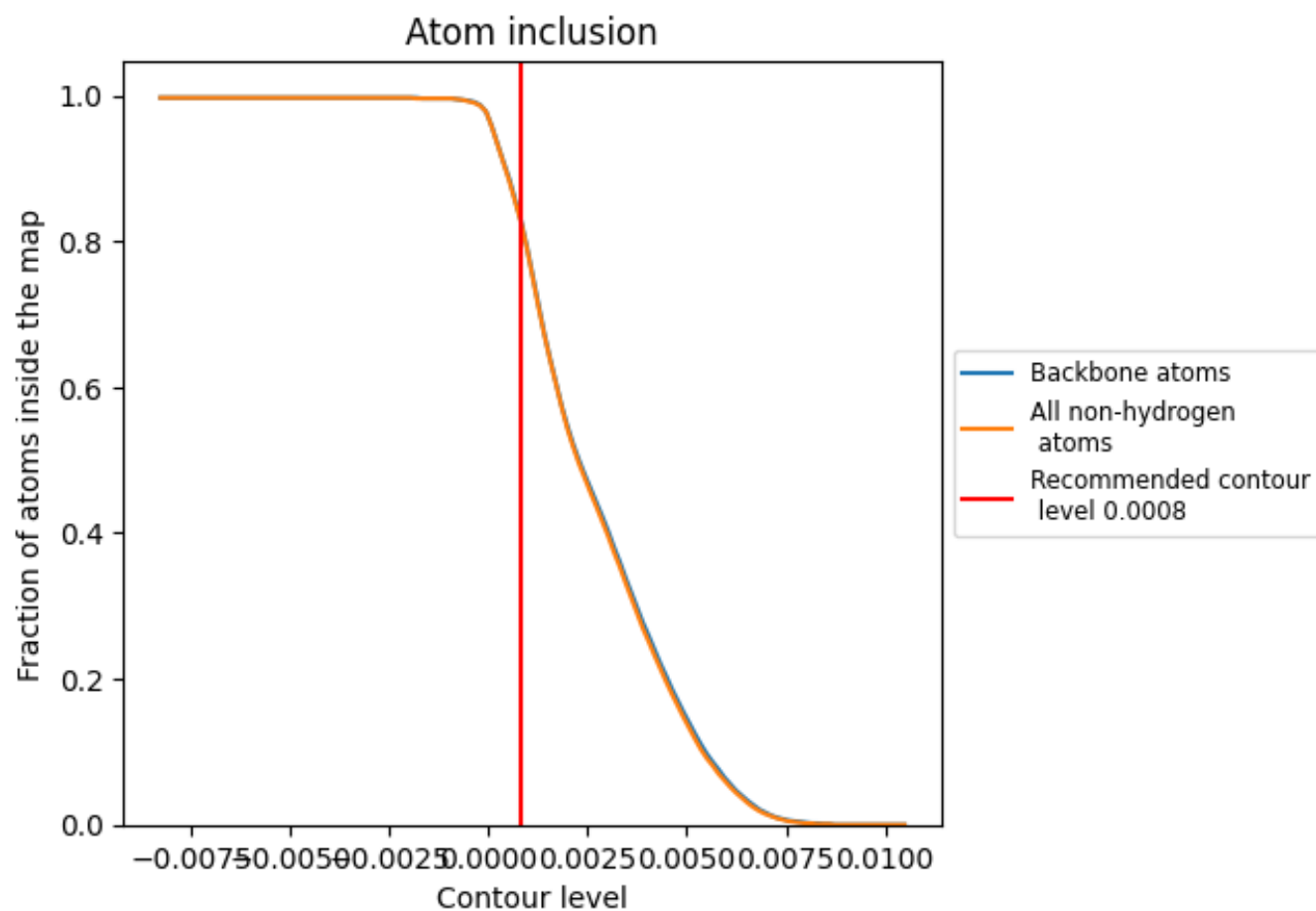
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.0008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8310	 0.1030
A	 0.6150	 0.0490
B	 0.8390	 0.0730
C	 0.9060	 0.1350
D	 0.9990	 0.1040
E	 0.9640	 0.0940
F	 0.9980	 0.1610
G	 0.9960	 0.1840
H	 1.0000	 0.1760
I	 0.9930	 0.2000
J	 0.9950	 0.2100
K	 0.9920	 0.2000
L	 0.9940	 0.2030
M	 0.9980	 0.2150
N	 1.0000	 0.1660
O	 0.9980	 0.1580
P	 0.9550	 0.0670
Y	 0.9910	 0.2020
d	 0.9500	 0.1750
e	 0.9860	 0.1510

