



## wwPDB EM Validation Summary Report ⓘ

Aug 4, 2025 – 05:45 PM EDT

PDB ID : 9E13 / pdb\_00009e13  
EMDB ID : EMD-47382  
Title : Full-length human dynein-1 in phi-like conformation bound to a Lis1 dimer under Lis1 condition  
Authors : Yang, J.; Zhang, K.  
Deposited on : 2024-10-21  
Resolution : 4.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

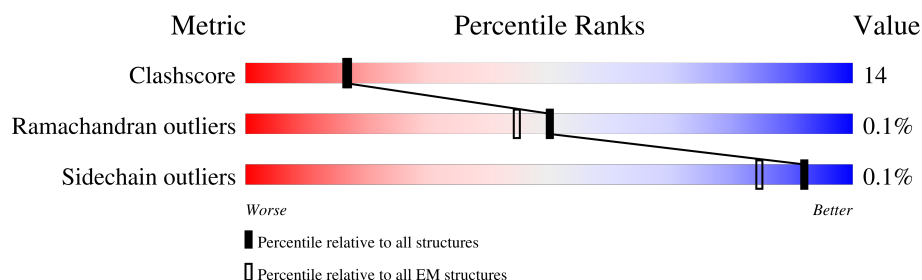
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	<div> <div>6%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	B	4646	<div> <div>.</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
2	C	638	<div> <div>57%</div> <div>38%</div> </div>
2	D	638	<div> <div>33%</div> <div>29%</div> <div>38%</div> </div>
3	E	492	<div> <div>62%</div> <div>37%</div> </div>
3	F	492	<div> <div>36%</div> <div>27%</div> <div>37%</div> </div>
4	G	96	<div> <div>14%</div> <div>47%</div> <div>50%</div> <div>.</div> </div>
4	H	96	<div> <div>5%</div> <div>59%</div> <div>38%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	89	<div><div></div><div>17%</div><div>49%</div><div>51%</div></div>
5	J	89	<div><div></div><div>16%</div><div>54%</div><div>46%</div></div>
6	K	113	<div><div></div><div>56%</div><div>73%</div><div>27%</div></div>
6	L	113	<div><div></div><div>36%</div><div>73%</div><div>27%</div></div>
7	O	410	<div><div></div><div>58%</div><div>20%</div><div>21%</div></div>
7	P	410	<div><div></div><div>51%</div><div>27%</div><div>22%</div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 94479 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4542	Total	C	N	O	S	0	0
			36692	23323	6381	6822	166		
1	B	4521	Total	C	N	O	S	0	0
			36527	23221	6349	6791	166		

- Molecule 2 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		
2	D	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		

- Molecule 3 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		
3	F	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		

- Molecule 4 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	93	Total	C	N	O	S	0	0
			742	468	128	143	3		
4	H	93	Total	C	N	O	S	0	0
			742	468	128	143	3		

- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
5	J	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

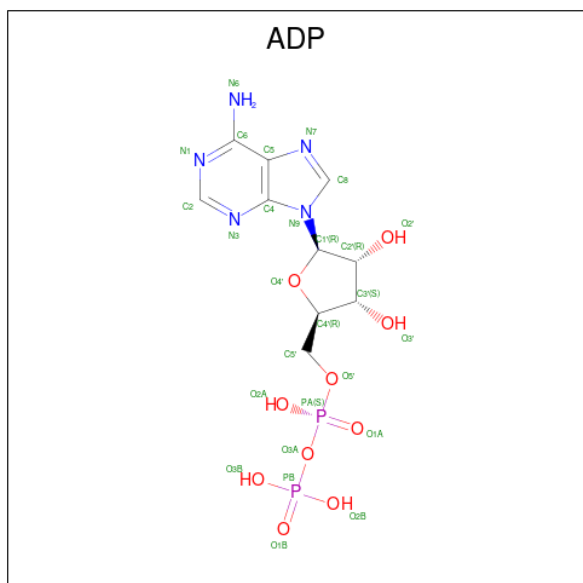
- Molecule 6 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
6	L	113	Total	C	N	O	S	0	0
			872	548	142	175	7		

- Molecule 7 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
7	P	319	Total	C	N	O	S	0	0
			2531	1593	446	472	20		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



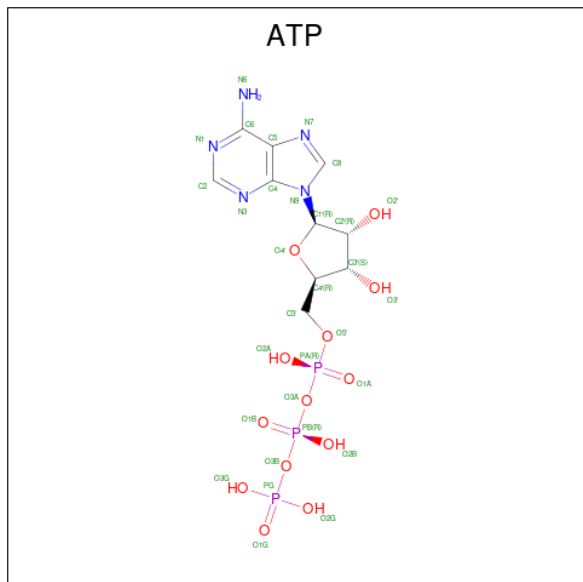
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total	Mg	0
			2	2	

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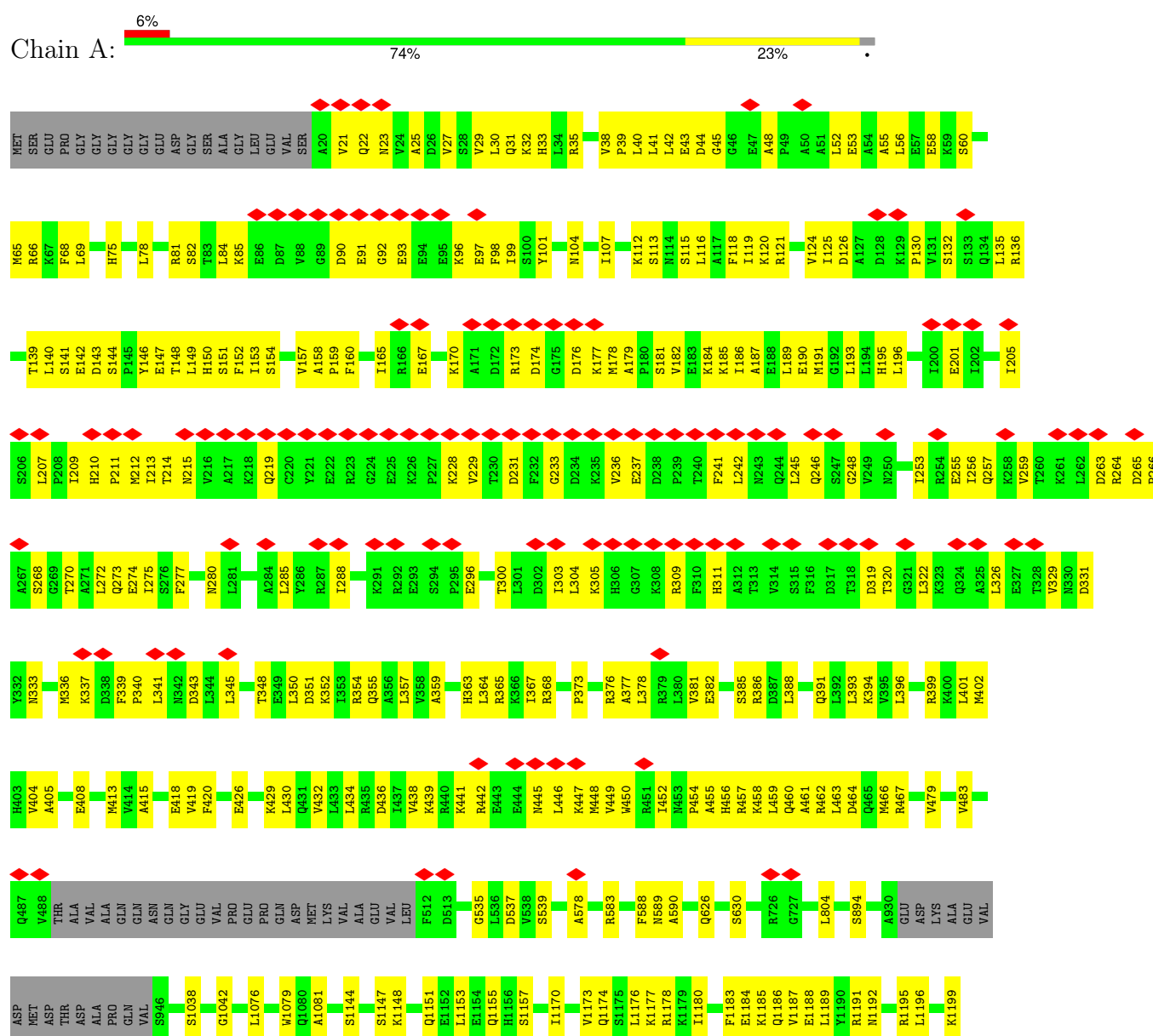
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	B	2	2	2	0

### 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: Cytoplasmic dynein 1 heavy chain 1





R2804	R2807	R2811	R2812	R2836	L2837	D2840	E2841	E2842	S2874	L2877	S2878	K2879	V2884	K2894	A2895	R2896	L2905	L2911	L2925	L2933	L2934	K2943	L2956	T2961	K2962	V2963	H2964	Y2967	D2973	K2989	M2994	V2998	V2999	L3000	D3001	S3002	L3005									
Y2641	R2642	T2644	P2645	N2646	G2647	V2648	L2661	L2666	N2667	P2669	F2692	V2701	K2702	L2703	F2708	C2712	D2717	R2726	R2729	H2730	V2731	P2732	V2733	V2734	Y2735	T2747	R2753	L2757	L2758	R2763	F2776	N2779	R2783	F2784	P2790	H2791	Y2792	L2793	Y2794							
E2513	L2514	R2519	L2526	T2534	L2535	E2538	V2548	K2551	E2556	V2557	E2558	T2559	H2560	K2561	V2562	A2563	D2566	V2567	V2568	V2569	D2573	T2574	V2575	R2576	H2577	E2578	L2581	V2584	P2590	L2591	V2592	L2593	L2605	F2606	S2607	A2608	L2609	R2610	L2620	N2621	F2622	K2626	K2633			
ALA	ALA	S2410	L2413	Q2416	A2419	A2420	M2423	L2437	E2444	H2445	L2446	L2449	T2450	R2451	L2452	R2453	C2454	S2457	L2458	A2465	C2466	R2467	N2468	Q2471	Y2472	D2478	F2479	P2480	M2481	Q2482	L2483	L2486	Y2493	L2494	V2495	T2498	L2499	W2500	S2503	K2509	M2510	T2511	A2512			
W2275	T2276	D2277	R2285	S2290	L2295	D2304	D2308	L2319	D2320	H2329	G2330	E2331	F2343	Q2346	S2357	R2358	C2359	G2360	M2361	T2371	N2377	L2382	T2385	P2386	L2387	D2388	E2389	GLY	GLU	ASP	GLU	ALA	L2494	GLN	ARG	ARG	ARG	LYS	GLY	LYS	GLU	ASP	GLU	GLY	GLU	
E2133	Q2134	T2138	T2144	M2145	L2149	L2157	L2161	F2165	R2172	E2181	C2186	Y2190	L2191	W2203	Y2204	K2206	Y2211	T2214	Q2215	L2220	M2221	G2224	G2227	S2228	S2231	N2232	A2233	W2234	R2235	V2236	L2244	K2257	D2269	P2270	N2271	T2272	R2273	E2274								
T2017	R2037	S2038	L2039	A2040	N2041	T2042	K2043	Q2044	C2047	Q2051	M2052	L2054	R2060	E2063	V2064	A2066	L2069	P2071	F2072	G2073	K2074	L2075	Q2079	L2080	H2085	R2091	A2092	L2093	K2094	S2095	V2096	L2097	Q2109	R2113	R2118	G2119	E2120	A2121	A2128	E2129	N2130	L2131	P2132			
Q1856	Q1860	K1865	L1879	V1880	Q1881	C1888	M1892	A1895	L1896	L1897	A1898	R1899	Q1902	K1912	A1918	R1943	C1949	D1958	E1959	F1960	N1961	R1962	L1963	S1795	Q1800	P1801	K1807	L1811	E1814	H1817	S1835	F1836	E1837	W1838	L1839	R1843	E2000	L2001	P2010							
V1721	V1724	K1729	Y1738	W1741	Y1745	L1749	V1750	Q1755	I1756	E1760	M1769	G1770	G1772	G1773	D1774	P1777	L1778	T1788	L1792	S1795	Q1800	P1801	K1807	L1811	E1814	H1817	S1835	F1836	E1837	W1838	L1839	R1843	E2000	L2001	P2010											
Q1595	G1596	Y1597	R1598	R1599	E1602	R1603	D1606	L1607	L1608	G1609	K1610	I1611	Q1612	Y1618	L1619	E1620	R1621	E1622	R1623	P1627	V1632	G1633	D1634	E1635	D1636	L1637	L1638	I1641	V1647	L1650	M1657	I1665	E1683	H1695	I1698	N1699	E1700	W1701	V1705	E1708	V1711	L1717				
P1511	Y1512	E1517	E1518	L1521	S1522	W1523	K1526	L1527	N1528	I1530	M1531	A1532	L1533	W1537	R1543	Y1546	L1547	S1554	K1558	H1559	L1560	V1563	E1564	T1565	Q1566	R1567	F1568	Q1569	S1570	I1571	S1572	T1573	L1576	M1579	K1580	V1582	S1583	K1584	L1587	V1588	M1589	D1590	V1591	I1594		
T1430	D1436	L1439	Q1440	N1441	N1442	E1443	A1444	K1447	D1448	V1452	E1456	M1457	A1458	L1459	E1460	F1462	K1463	K1464	Q1465	I1466	L1467	E1468	V1469	W1470	N1471	T1472	Y1473	D1476	L1477	V1478	N1482	T1487	R1488	D1491	D1492	L1493	F1494	N1495	K1496	V1497	K1498	E1499	H1500	I1501	M1507	S1510
R1200	R1201	F1202	Q1203	L1209	E1215	W1218	G1219	N1222	M1225	R1226	R1227	K1228	D1229	I1232	Q1233	Q1234	L1306	D1344	P1350	S1353	K1358	P1374	L1377	R1378	K1391	M1398	L1399	E1402	L1403	K1404	S1405	E1406	A1407	L1408	L1416	R1419	L1420	H1421	V1426	S1427						

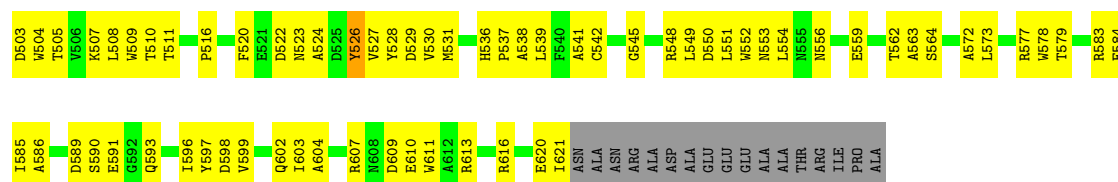




E2767	L2605	V2433	M2342	F1629	E1517	R1411	R1201	M139	L1060	Q967
P2768	A2608	T2494	F2343	D1634	E1524	H1412	F1204	T1140	W1061	Y968
V2774	L2609	K2435	E2344	T2042	D1525	W1413		E1141	Q1064	
E2775		E2438	K2346	L1638	L1527	M1417	W1208	F1142	N1067	L971
F2776	P2613	D2347	D2347	V1647	R1528	L1420	L1209	H1143	I1068	N972
M2779	D2614	E2444	L2348		R1529	H1421	Y1210	S1144	P973	
M2815	M2615	H2445		I1665	L1529	V1422	I1211	Q1145	Y1069	
E2782	E2616	L2446	C2359	L1666	L1533	W1423	D1212	Q1147	M1070	E977
E2783	V2617	L2449	M2221	M1667	L1543	W1424	I1213	S1148	R1071	A978
F2784	L2620	L2452	M2222	E1668	R1543	Y1425	I1214	S1149	L1072	C979
		R2453	M2223		Y1546	V1426	G1216	R1150	Y980	
Y2794	S2623	S2457	G2224	V1672	L1547	S1427	E1217	Q1151	D1075	
M2799	P2628	E2629	N2067	V1673	L1547		W1218	E1152	K1078	N986
W2802	L2630	Q2464	K2068	E1683	L1547		G1219	L1153	F987	A988
L2631	A2465	A2465	V2070	W1684	S1554		A1220	Q1154	W1079	
L2632			P2071	M1685	T1557	D1436	F1221	Q1155	L1082	N991
K2633					K1558	K1441	D1223	D1159	L1083	Y992
Q2654			H2085		L1561	M1442	I1224	T1160	V1084	N993
			R2091		E1564	E1443	M1225	A1161	Q1085	L994
A2829	K2657	L2486	K2094	K1707	T1585	V1446	K1227	S1162	R1087	L996
E2839	W2658	E2487	R2242	E1708	Q1569	K1447	K1228	D1165	A1089	S1001
L2855	Y2488	Y2489	L2244	M1709				T1168	R1090	GLN
L2855	L2490	Q2491	A2100	R1710	T1573	L1450	Q1245	F1093	TYR	ARG
D2862	L2668	R2492	G2101	V1711	K1580	A1453	D1256	F1169	GLN	GLN
R2863	P2669	Y2493	W1202	V1721	K1581	Q1454	T1259	T1170	VAL	VAL
E2864	F2682	R2498	C1949	V1724	K1584	M1457	K1263	T1171	GLY	GLY
K2865	L2683	L2498	Q1950	V1724	V1588	E1460	V1267	Q1177	VAL	VAL
R2869	Q2685	M2510	E1959	F1727	V1597	K1464		K1178	GLY	GLY
K2879	L2686	L2514	R1962	G1728	Q1598	R1467	N1270	I1179	VAL	VAL
R2896	E2688	L2518	L1963	K1729	E1599			I1180	GLY	GLY
Y2901	Q2707	E2538	E1965	L1752	S1600	W1470	I1282	I1181	VAL	VAL
L2905	V2709		M1967	Q1755	R1603			Q1182	TYR	TYR
F2912	P2714	W2548	L1968	M1769		L1475	T1309	F1183	LEU	
N2913	K2721	D2573	H1985	G1770	D1606	D1476	G1310	K1184	T1013	T1013
E2914	R2726	R2576	D1991	G1771	L1607	L1477	L1311	K1185	E1014	E1014
K2943		H2577	K1992	G1773	L1608	V1478		Q1186	K1017	K1017
L2956	R2729	E2578	T1993	D1774	G1609	C1484	R1357	E1188	F1018	F1018
L2956	H2730	E2578	S1994		K1610	R1485		Y1190	Y1019	Y1019
L2961	V2731	T2583	N2003	P1777	L1611	R1488	Q1379	N1191	R1020	R1020
K2962	P2732	V2312	Q2005	L1778	E1612			N1192	L1023	L1023
Y2967	P2760	V2592	W2006	T1788	E1620	D1492	S1382	G1193	T1024	T1024
G2969	R2763	T2604	M2012	L1792	R1623	F1493		Q1194	R1025	R1025
			S2026	R1306	P1627	N1495	R1388	R1195	M1026	M1026
				E1814	R1628	K1498	S1405	L1196	P1030	P1030
						K1508	E1406	K1129	L1033	L1033
						Y1513	A1407	S1045	G1042	G1042
						K1514	L1408	F1131	S1045	S1045
							K1409	E1198	E1048	E1048
							D1410	K1199	C1059	C1059

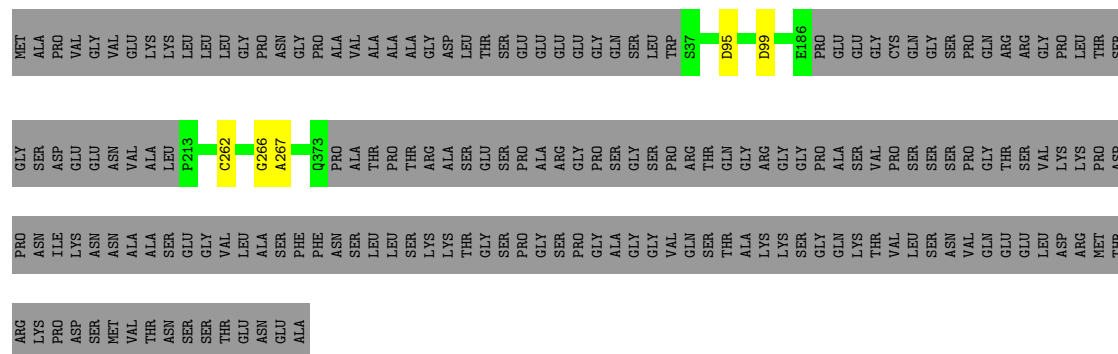






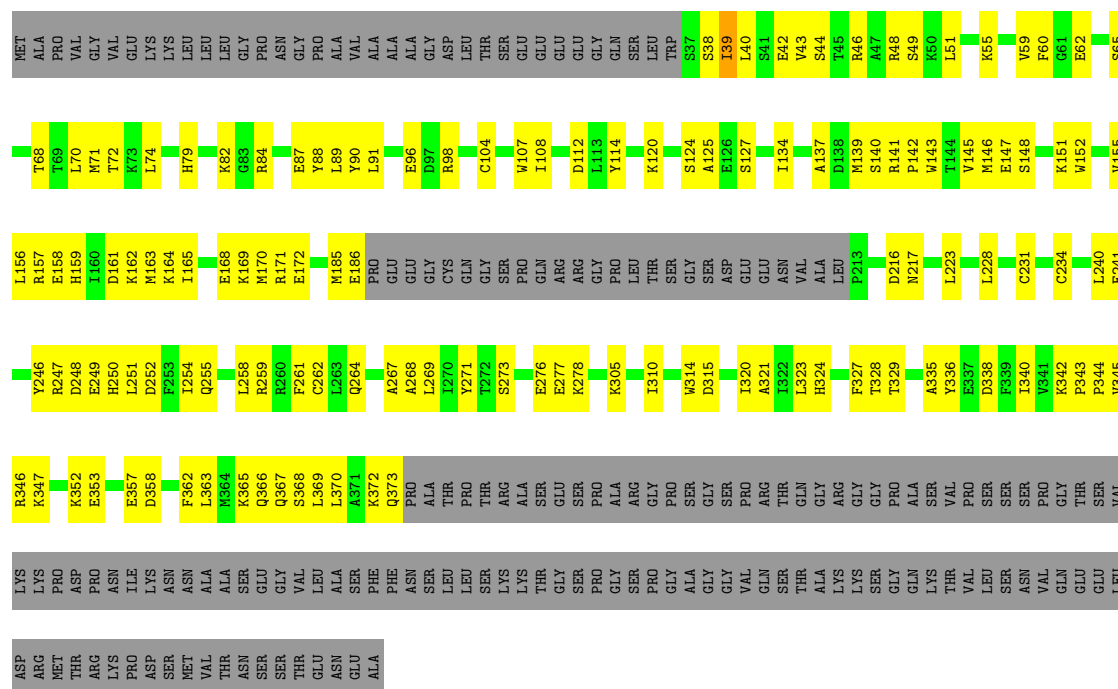
• Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

Chain E: 62% 37%



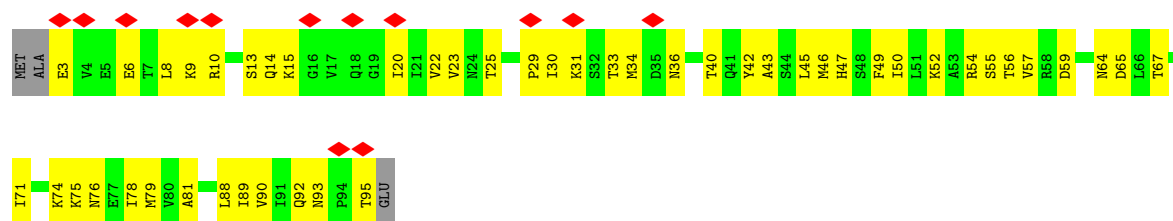
• Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

Chain F: 36% 27% 37%

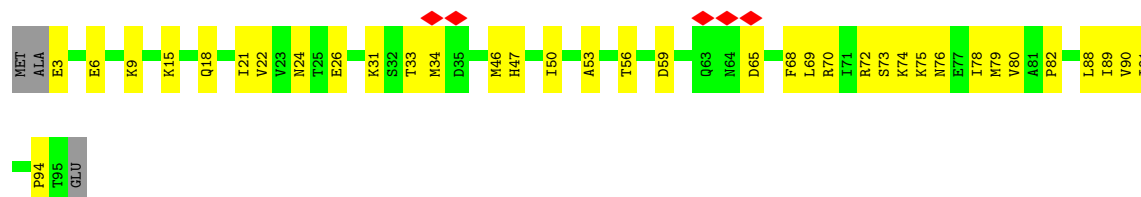


• Molecule 4: Dynein light chain roadblock-type 1

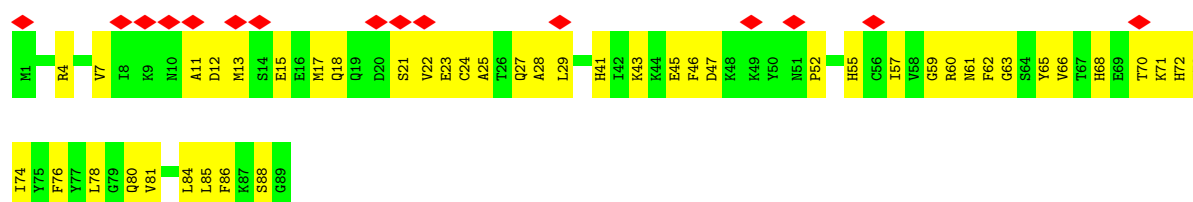
Chain G: 14% 47% 50%



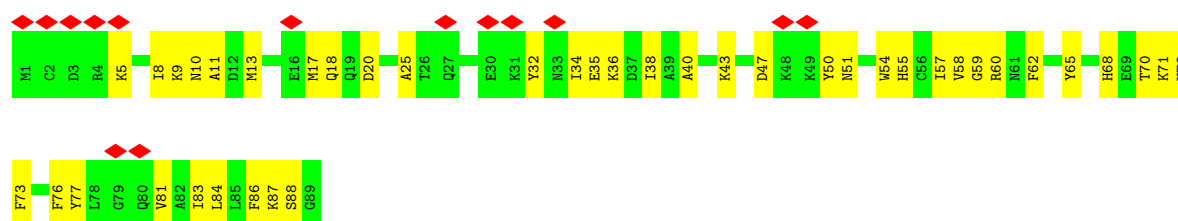
• Molecule 4: Dynein light chain roadblock-type 1



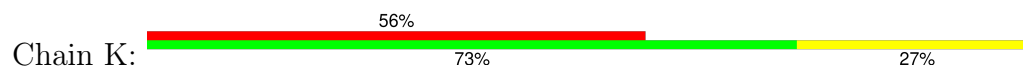
• Molecule 5: Dynein light chain 1, cytoplasmic



• Molecule 5: Dynein light chain 1, cytoplasmic

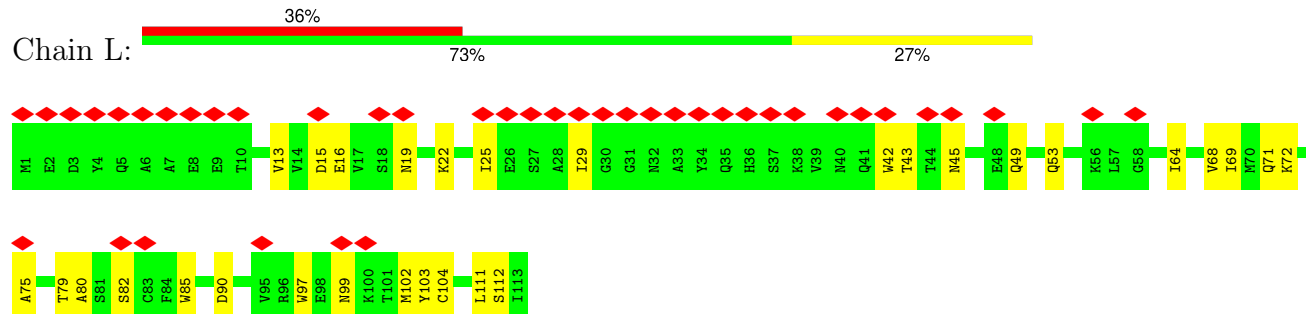


• Molecule 6: Dynein light chain Tctex-type 1

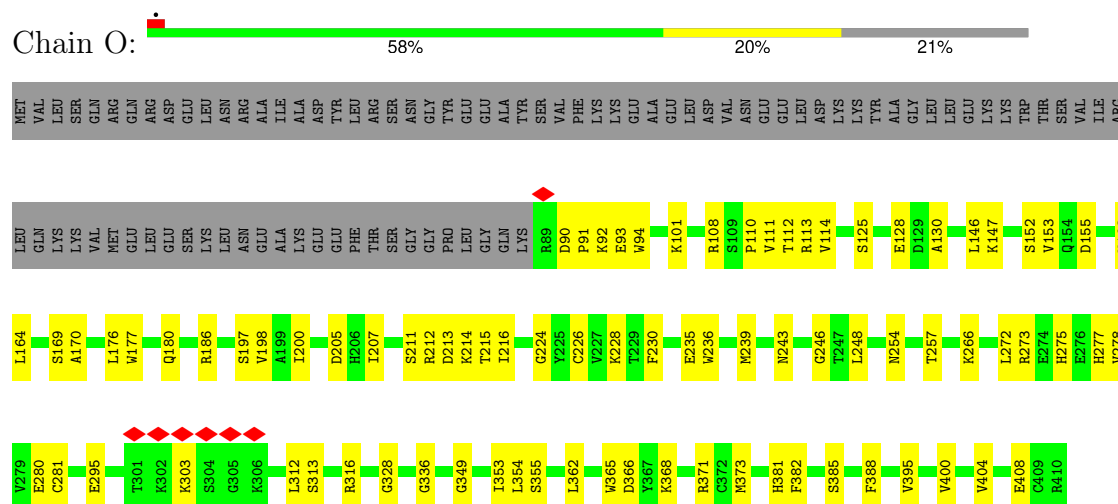




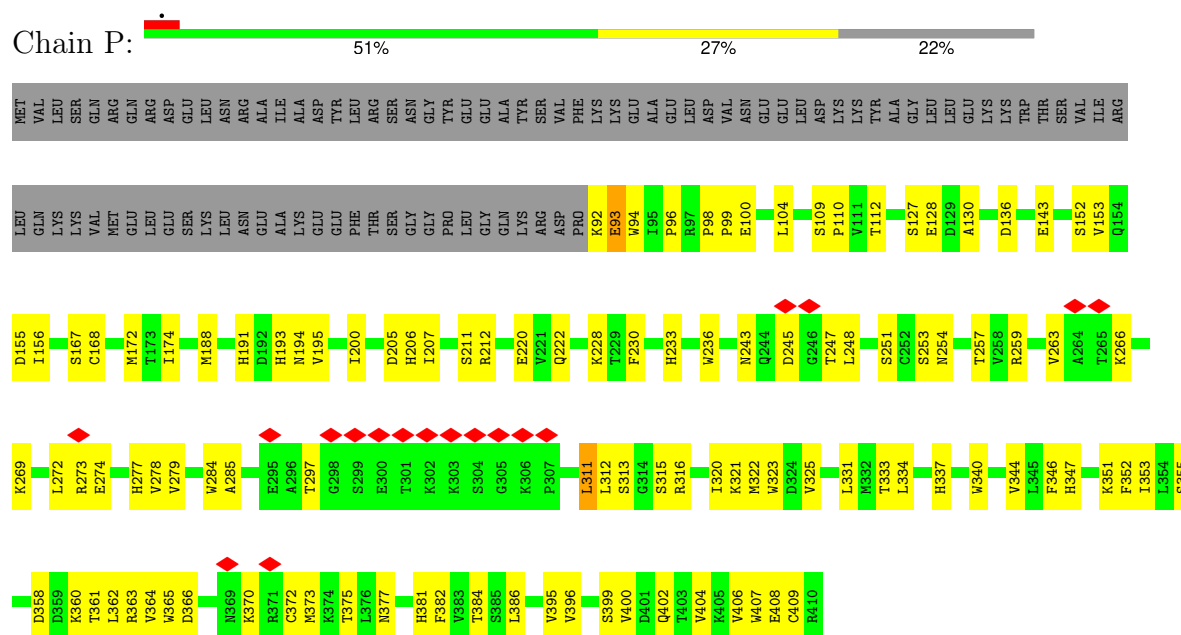
- Molecule 6: Dynein light chain Tctex-type 1



- Molecule 7: Platelet-activating factor acetylhydrolase IB subunit beta



- Molecule 7: Platelet-activating factor acetylhydrolase IB subunit beta



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.743	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	729.12, 729.12, 729.12	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.736, 1.736, 1.736	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: ATP, ADP, MG

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	0.21	2/37419 (0.0%)	0.43	15/50625 (0.0%)
1	B	0.20	1/37248 (0.0%)	0.41	3/50392 (0.0%)
2	C	0.23	0/3195	0.46	1/4351 (0.0%)
2	D	0.20	0/3195	0.46	0/4351
3	E	0.20	0/2573	0.42	0/3473
3	F	0.18	0/2573	0.38	0/3473
4	G	0.17	0/752	0.44	0/1017
4	H	0.16	0/752	0.40	0/1017
5	I	0.35	0/744	0.78	0/997
5	J	0.21	0/744	0.48	0/997
6	K	0.17	0/888	0.46	0/1203
6	L	0.12	0/888	0.33	0/1203
7	O	0.17	0/2624	0.42	0/3555
7	P	0.16	0/2597	0.42	1/3518 (0.0%)
All	All	0.20	3/96192 (0.0%)	0.42	20/130172 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
2	D	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3242	LYS	C-O	-9.86	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3242	LYS	C-O	-7.30	1.15	1.24
1	A	1801	PRO	CA-C	6.87	1.55	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3242	LYS	O-C-N	-11.27	110.47	122.07
1	A	3242	LYS	O-C-N	-8.21	111.42	122.43
1	A	3262	GLU	N-CA-C	-7.84	102.73	111.28
1	A	3438	ARG	N-CA-C	-6.66	102.90	111.02
1	A	3250	ALA	N-CA-C	-6.52	104.25	111.82

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1076	LEU	Peptide
1	A	3223	ARG	Sidechain
1	A	3242	LYS	Mainchain
1	A	3446	ARG	Sidechain
1	B	3219	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	36692	0	36962	814	0
1	B	36527	0	36805	994	0
2	C	3112	0	2964	20	0
2	D	3112	0	2964	163	0
3	E	2518	0	2525	3	0
3	F	2518	0	2525	114	0
4	G	742	0	768	48	0
4	H	742	0	768	33	0
5	I	728	0	714	56	0
5	J	728	0	714	46	0
6	K	872	0	846	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	872	0	846	25	0
7	O	2557	0	2487	66	0
7	P	2531	0	2463	89	0
8	A	81	0	36	2	0
8	B	81	0	36	6	0
9	A	31	0	12	2	0
9	B	31	0	12	2	0
10	A	2	0	0	0	0
10	B	2	0	0	0	0
All	All	94479	0	94447	2368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 2368 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:3426:ASN:HA	1:B:3429:LYS:CE	1.28	1.56
1:B:3426:ASN:CA	1:B:3429:LYS:HE3	1.09	1.34
1:B:3426:ASN:HA	1:B:3429:LYS:CD	1.78	1.13
1:B:3426:ASN:N	1:B:3429:LYS:HE3	1.67	1.07
1:B:3256:MET:HG2	1:B:3433:VAL:HG21	1.42	1.01

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	4530/4646 (98%)	4368 (96%)	157 (4%)	5 (0%)	48	83
1	B	4507/4646 (97%)	4365 (97%)	137 (3%)	5 (0%)	48	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	390/638 (61%)	363 (93%)	27 (7%)	0	100	100
2	D	390/638 (61%)	365 (94%)	25 (6%)	0	100	100
3	E	307/492 (62%)	296 (96%)	11 (4%)	0	100	100
3	F	307/492 (62%)	291 (95%)	14 (5%)	2 (1%)	19	56
4	G	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
4	H	91/96 (95%)	85 (93%)	6 (7%)	0	100	100
5	I	87/89 (98%)	73 (84%)	14 (16%)	0	100	100
5	J	87/89 (98%)	83 (95%)	3 (3%)	1 (1%)	12	46
6	K	111/113 (98%)	110 (99%)	1 (1%)	0	100	100
6	L	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
7	O	320/410 (78%)	306 (96%)	14 (4%)	0	100	100
7	P	317/410 (77%)	297 (94%)	19 (6%)	1 (0%)	37	72
All	All	11646/12968 (90%)	11197 (96%)	435 (4%)	14 (0%)	50	83

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	ASN
1	A	3270	VAL
1	A	3271	ILE
1	A	3384	ARG
1	A	3444	ILE

### 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	4044/4125 (98%)	4036 (100%)	8 (0%)	92	93
1	B	4028/4125 (98%)	4021 (100%)	7 (0%)	92	93
2	C	344/557 (62%)	344 (100%)	0	100	100
2	D	344/557 (62%)	344 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	279/422 (66%)	279 (100%)	0	100	100
3	F	279/422 (66%)	279 (100%)	0	100	100
4	G	87/89 (98%)	87 (100%)	0	100	100
4	H	87/89 (98%)	87 (100%)	0	100	100
5	I	78/78 (100%)	78 (100%)	0	100	100
5	J	78/78 (100%)	78 (100%)	0	100	100
6	K	97/97 (100%)	97 (100%)	0	100	100
6	L	97/97 (100%)	97 (100%)	0	100	100
7	O	287/364 (79%)	287 (100%)	0	100	100
7	P	284/364 (78%)	284 (100%)	0	100	100
All	All	10413/11464 (91%)	10398 (100%)	15 (0%)	92	94

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3454	LEU
1	B	3436	MET
1	B	3243	MET
1	B	3440	LEU
1	B	3428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1056	GLN
1	B	2464	GLN
7	O	381	HIS
3	F	115	HIS
1	B	1186	GLN

### 5.3.3 RNA ⓘ

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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ADP	A	4701	10	24,29,29	0.85	0	29,45,45	1.26	2 (6%)
8	ADP	B	4703	-	24,29,29	0.88	0	29,45,45	1.25	2 (6%)
8	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.24	2 (6%)
9	ATP	B	4702	10	28,33,33	0.78	0	34,52,52	0.60	1 (2%)
8	ADP	A	4704	-	24,29,29	0.87	0	29,45,45	1.17	2 (6%)
8	ADP	B	4704	-	24,29,29	0.84	0	29,45,45	1.20	2 (6%)
8	ADP	B	4701	10	24,29,29	0.86	0	29,45,45	1.24	2 (6%)
9	ATP	A	4702	10	28,33,33	0.72	0	34,52,52	0.59	1 (2%)

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
8	ADP	A	4701	10	-	0/12/32/32	0/3/3/3
8	ADP	B	4703	-	-	5/12/32/32	0/3/3/3
8	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
9	ATP	B	4702	10	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	A	4704	-	-	1/12/32/32	0/3/3/3
8	ADP	B	4704	-	-	3/12/32/32	0/3/3/3
8	ADP	B	4701	10	-	3/12/32/32	0/3/3/3
9	ATP	A	4702	10	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	4703	ADP	N3-C2-N1	-3.68	123.67	128.67
8	A	4701	ADP	N3-C2-N1	-3.66	123.70	128.67
8	A	4703	ADP	N3-C2-N1	-3.66	123.71	128.67
8	B	4704	ADP	N3-C2-N1	-3.63	123.75	128.67
8	A	4704	ADP	N3-C2-N1	-3.61	123.77	128.67

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	4703	ADP	C5'-O5'-PA-O1A
8	A	4703	ADP	C5'-O5'-PA-O3A
8	B	4701	ADP	C5'-O5'-PA-O1A
8	B	4701	ADP	C5'-O5'-PA-O2A
8	B	4701	ADP	C5'-O5'-PA-O3A

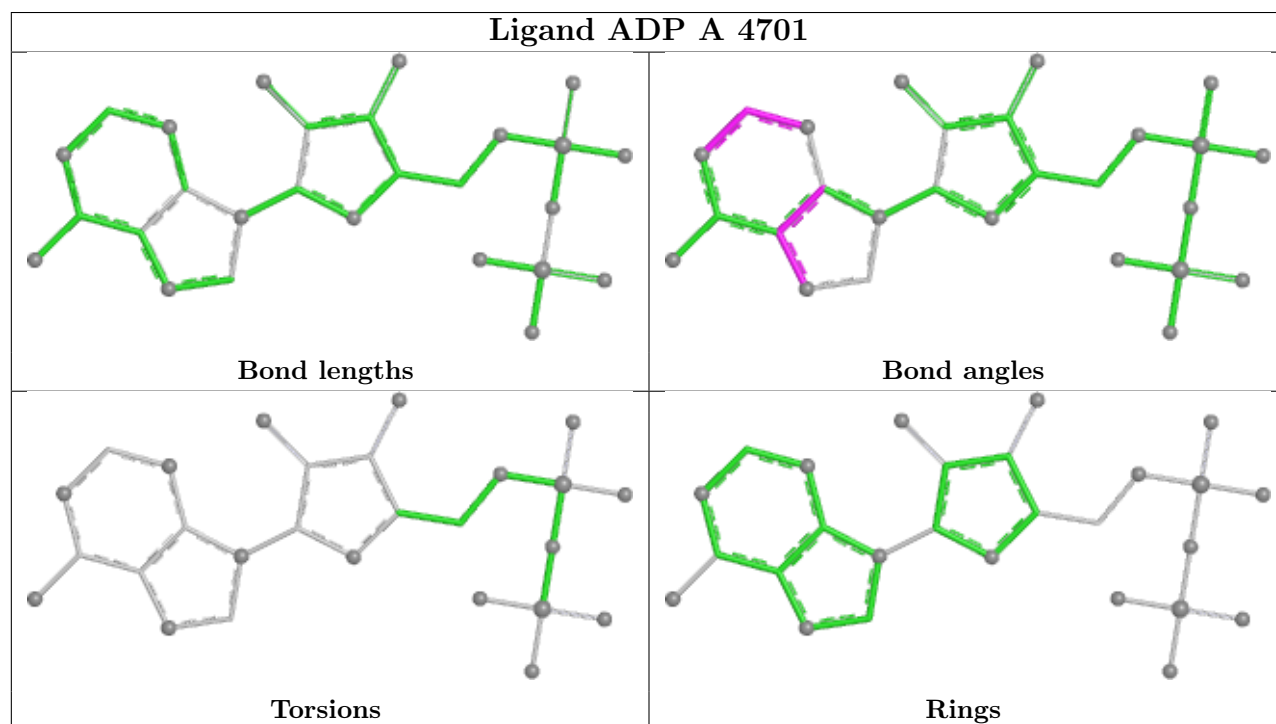
There are no ring outliers.

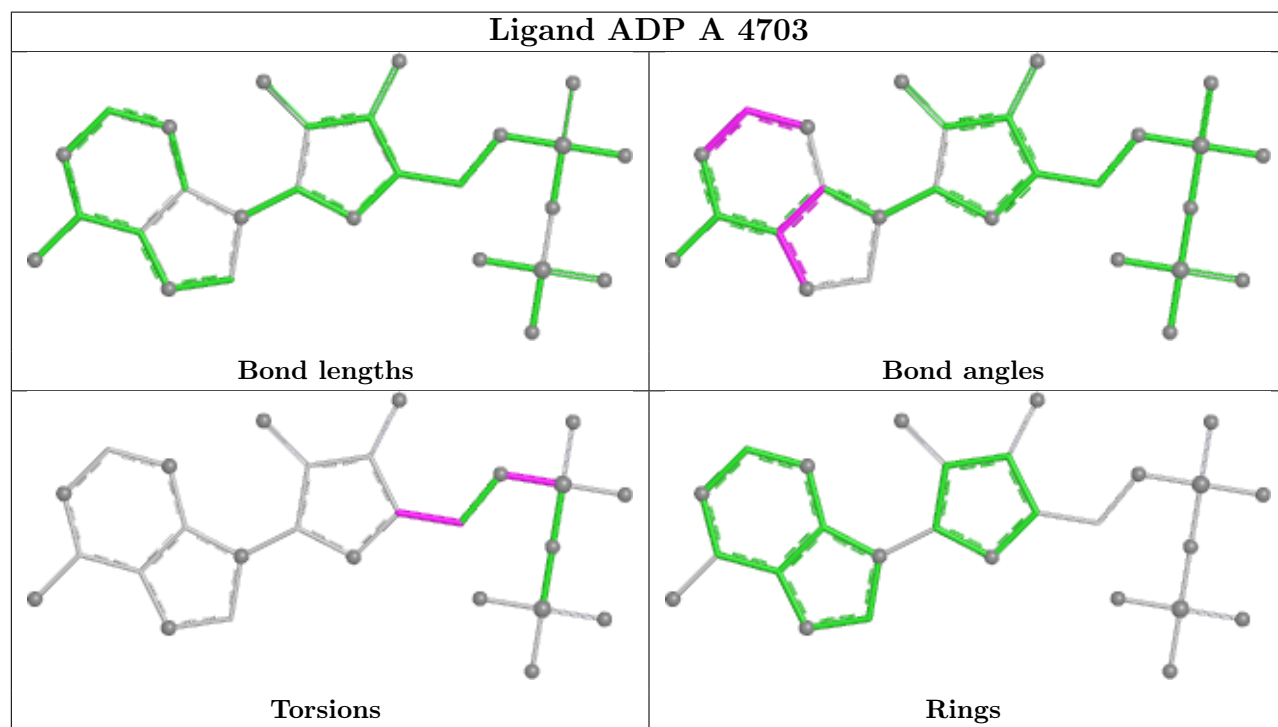
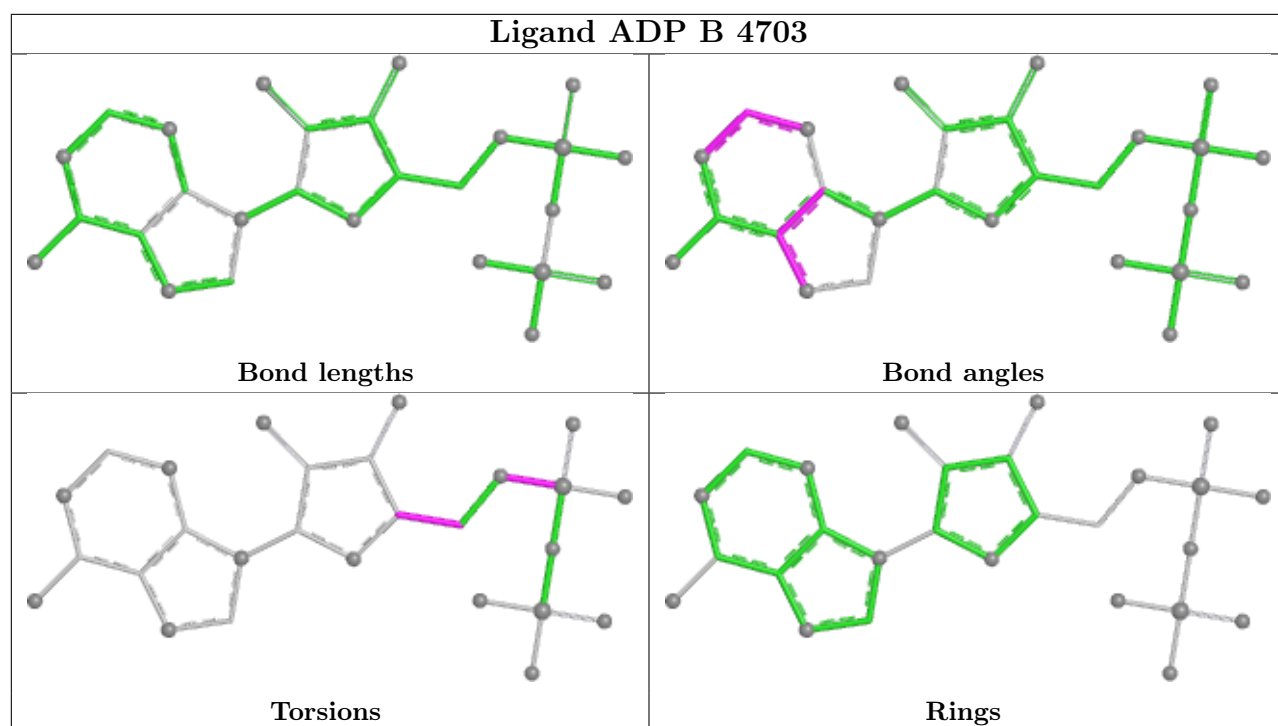
7 monomers are involved in 12 short contacts:

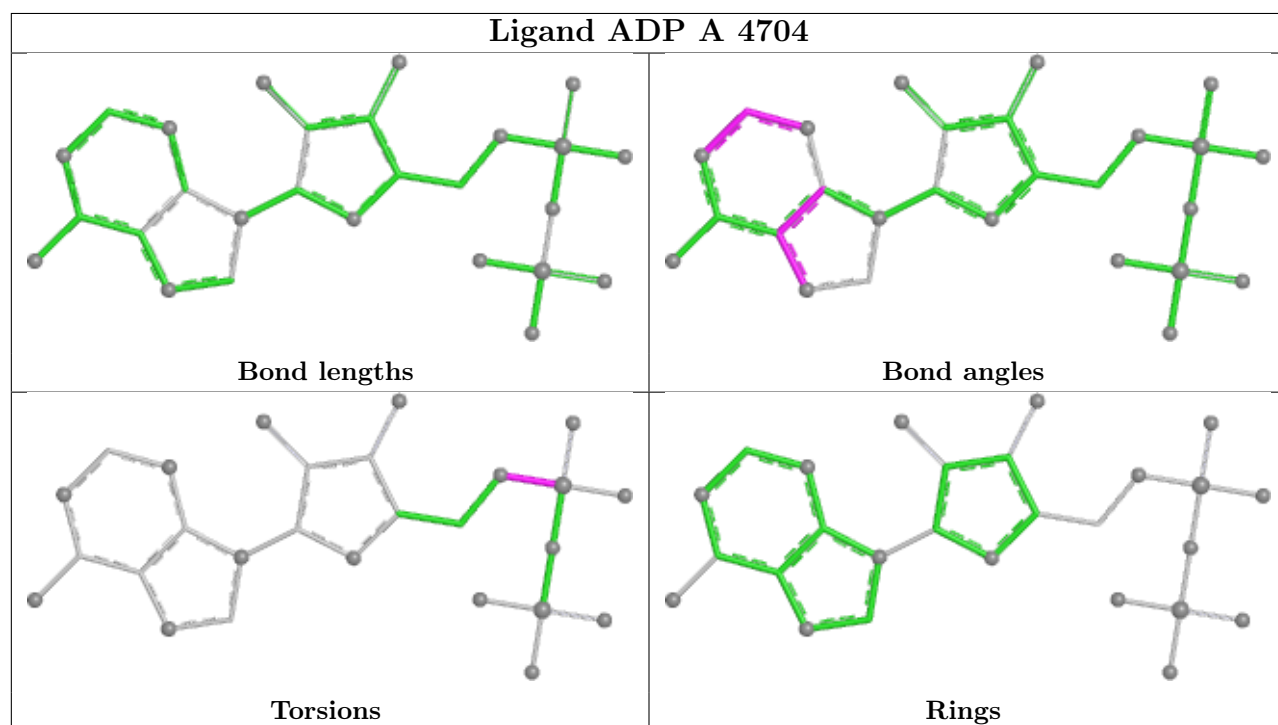
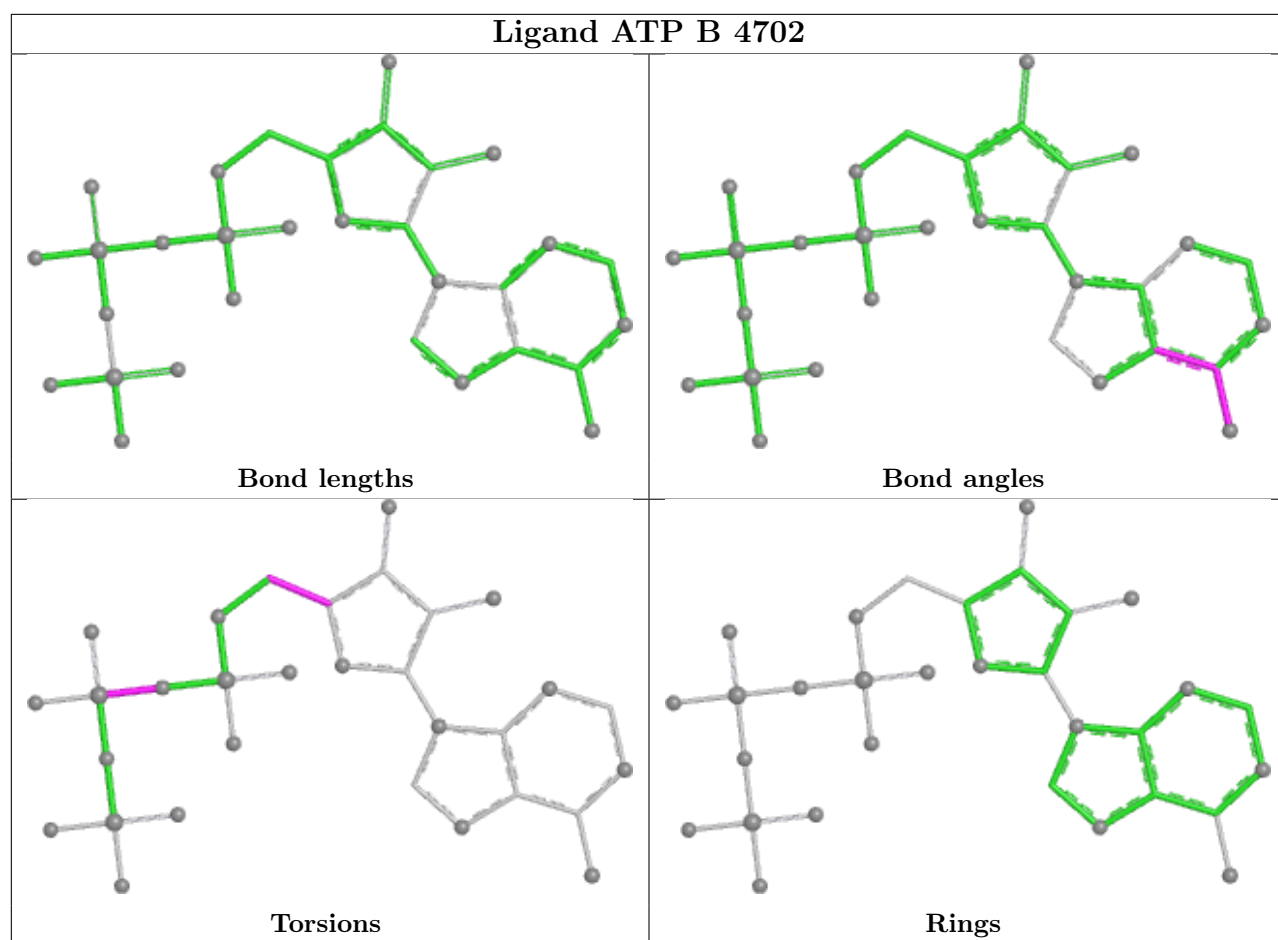
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	4701	ADP	1	0
8	B	4703	ADP	2	0
9	B	4702	ATP	2	0
8	A	4704	ADP	1	0
8	B	4704	ADP	1	0
8	B	4701	ADP	3	0
9	A	4702	ATP	2	0

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

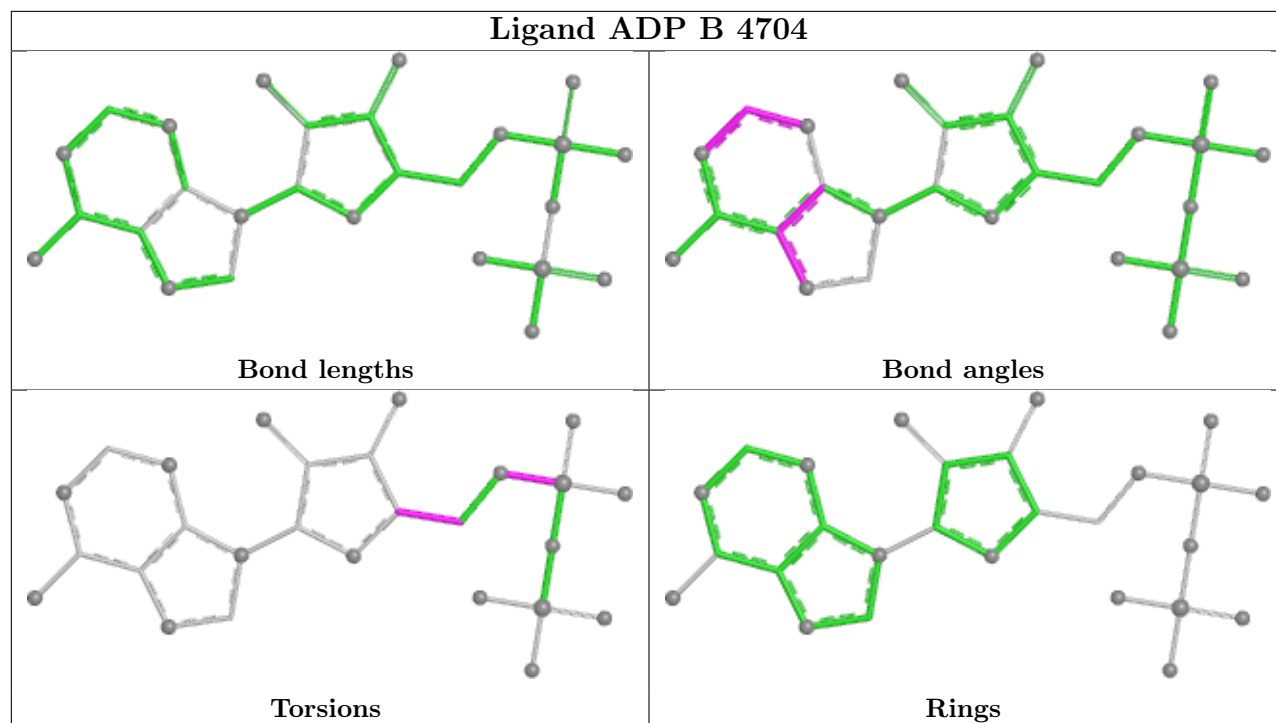
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



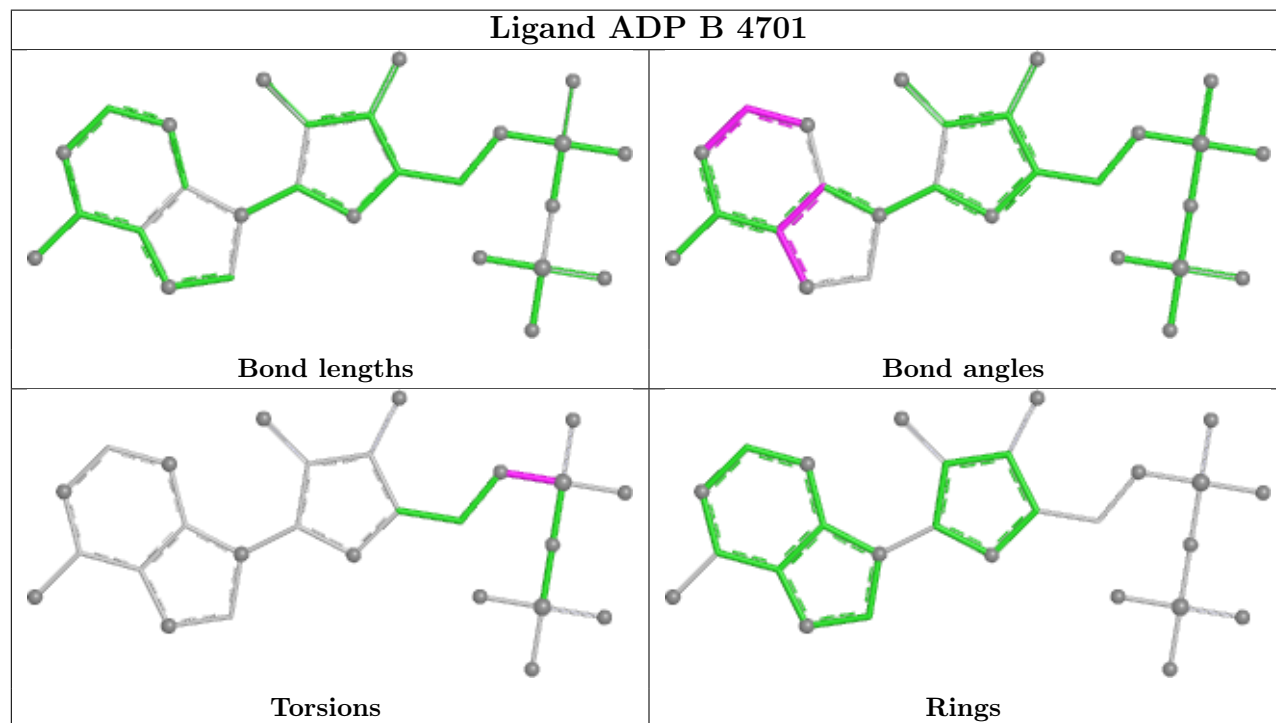


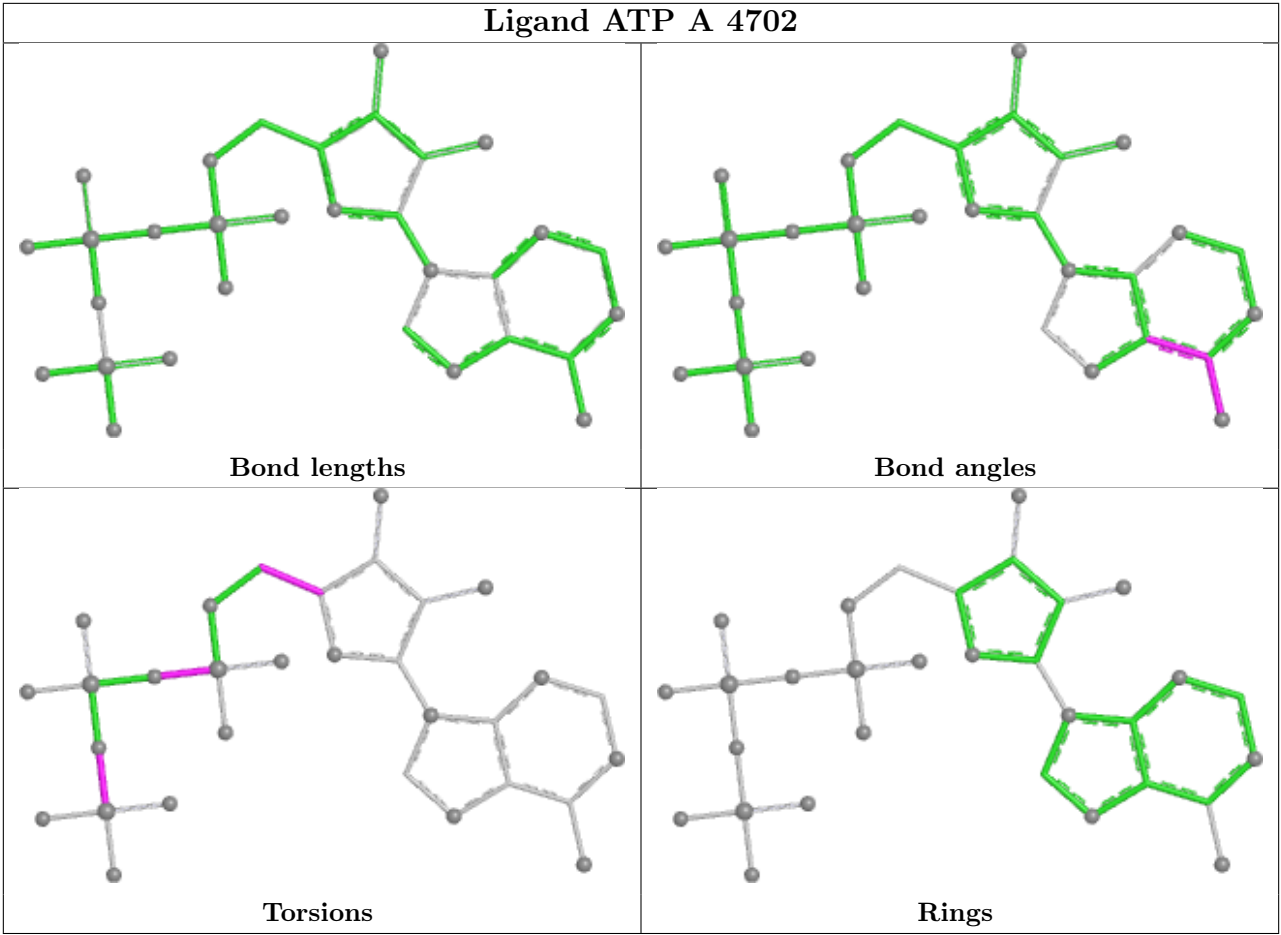


## Ligand ADP B 4704



## Ligand ADP B 4701





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1394:MET	C	1395:LYS	N	8.64
1	A	1394:MET	C	1395:LYS	N	5.37

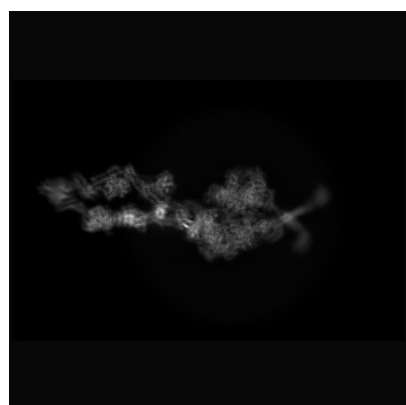
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47382. These allow visual inspection of the internal detail of the map and identification of artifacts.

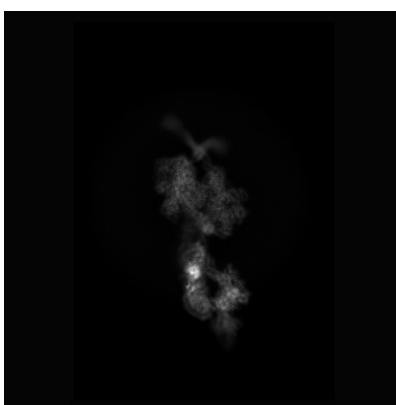
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

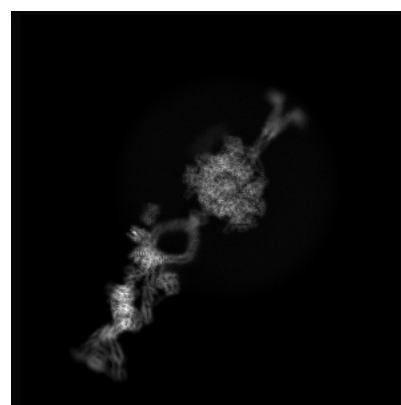
#### 6.1.1 Primary map



X



Y

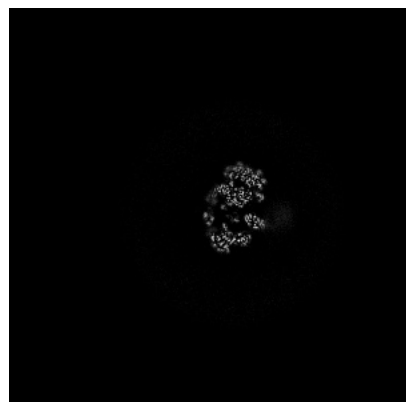


Z

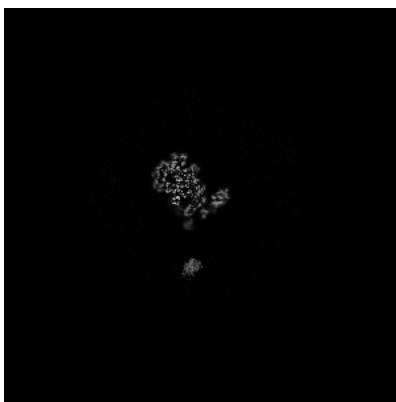
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 210



Y Index: 210

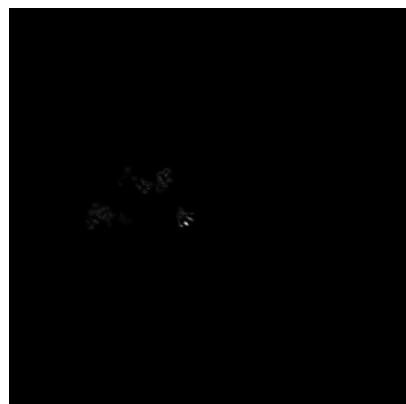


Z Index: 210

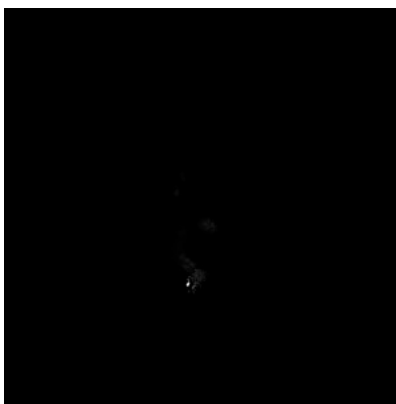
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 130



Y Index: 186

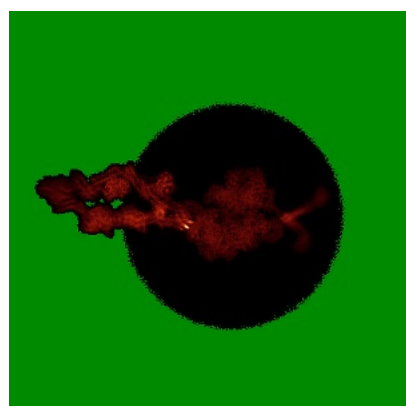


Z Index: 198

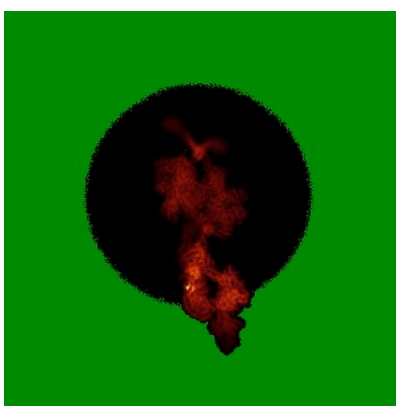
The images above show the largest variance slices of the map in three orthogonal directions.

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

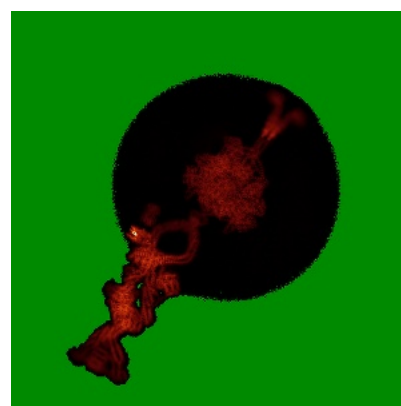
### 6.4.1 Primary map



X



Y



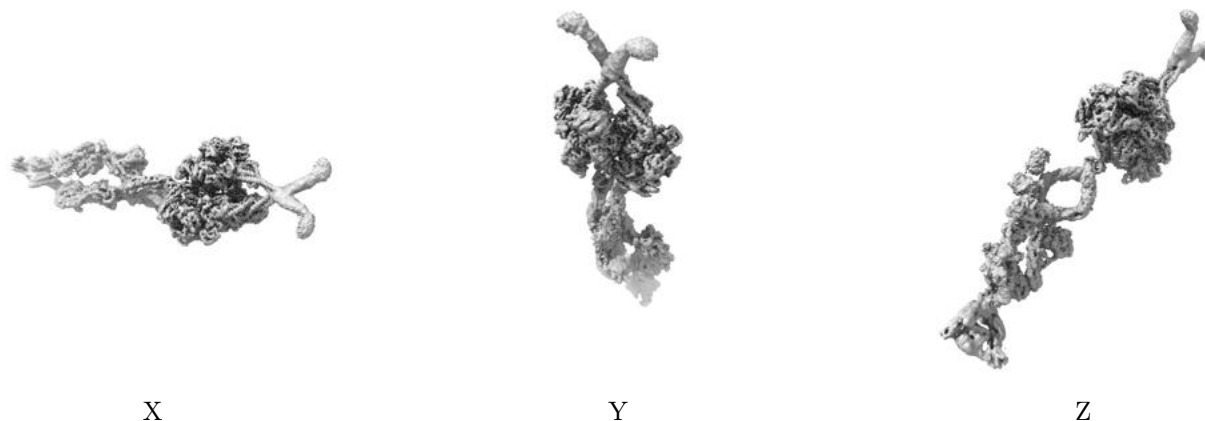
Z

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

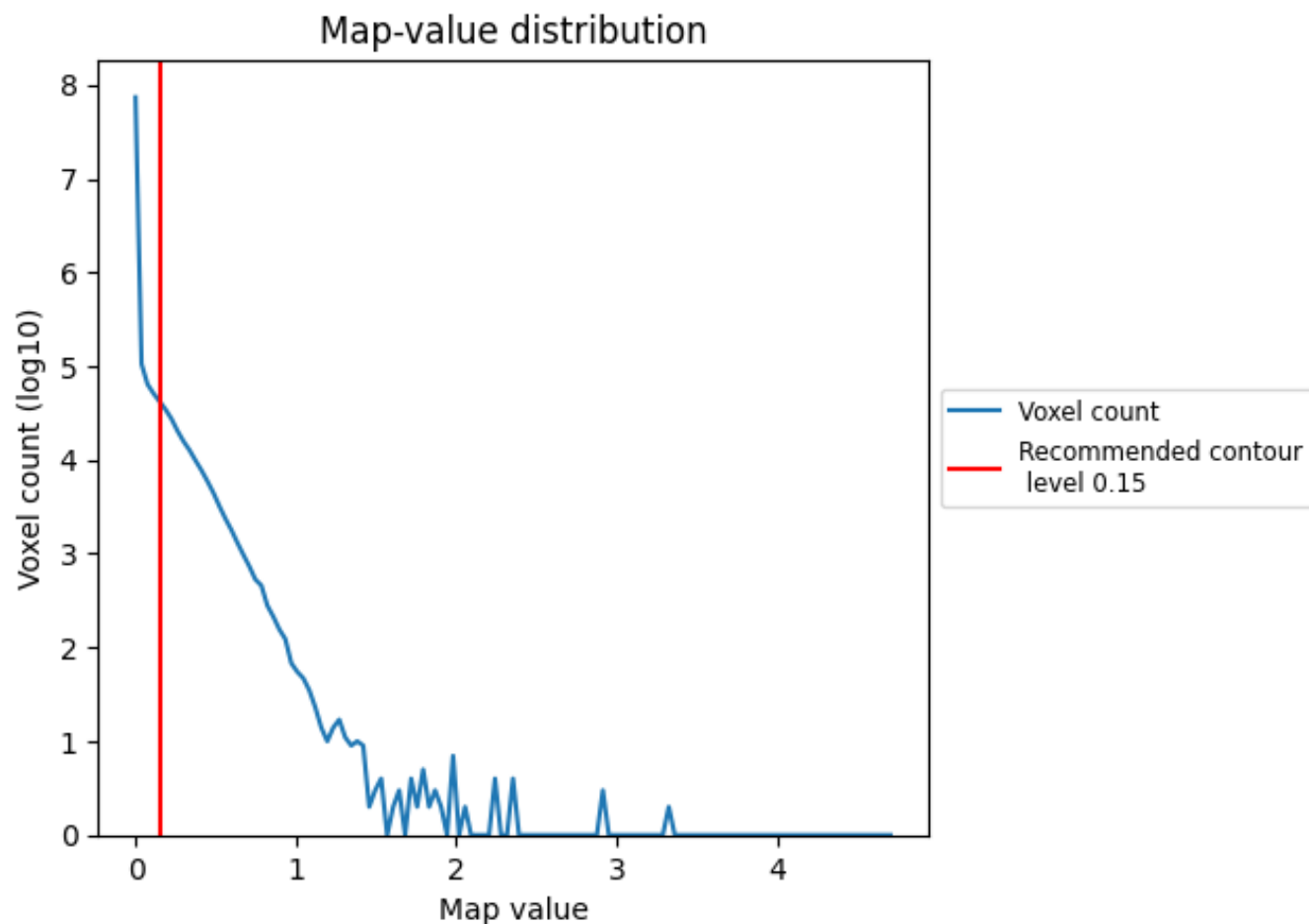
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

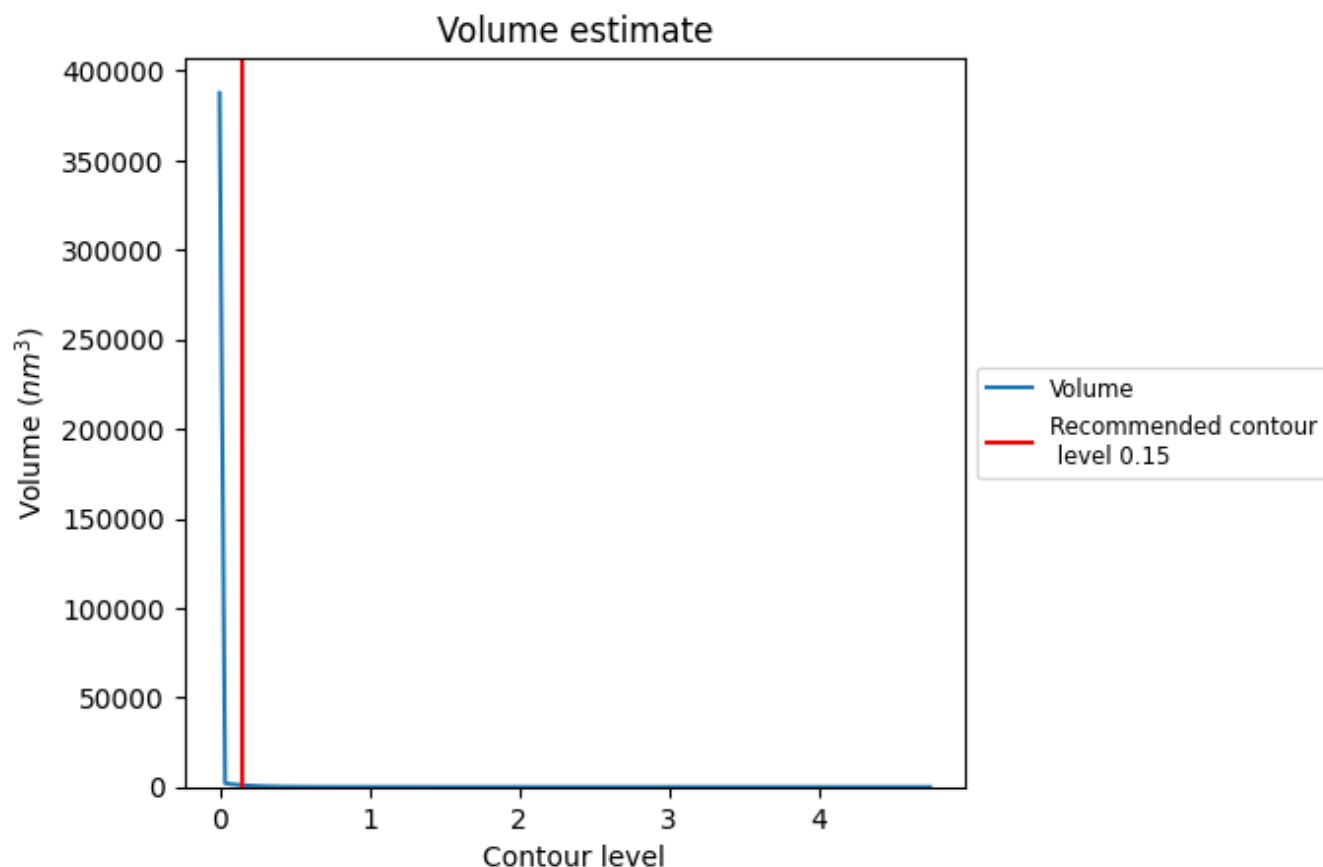
This section contains the results of statistical analysis of the map.

### 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.

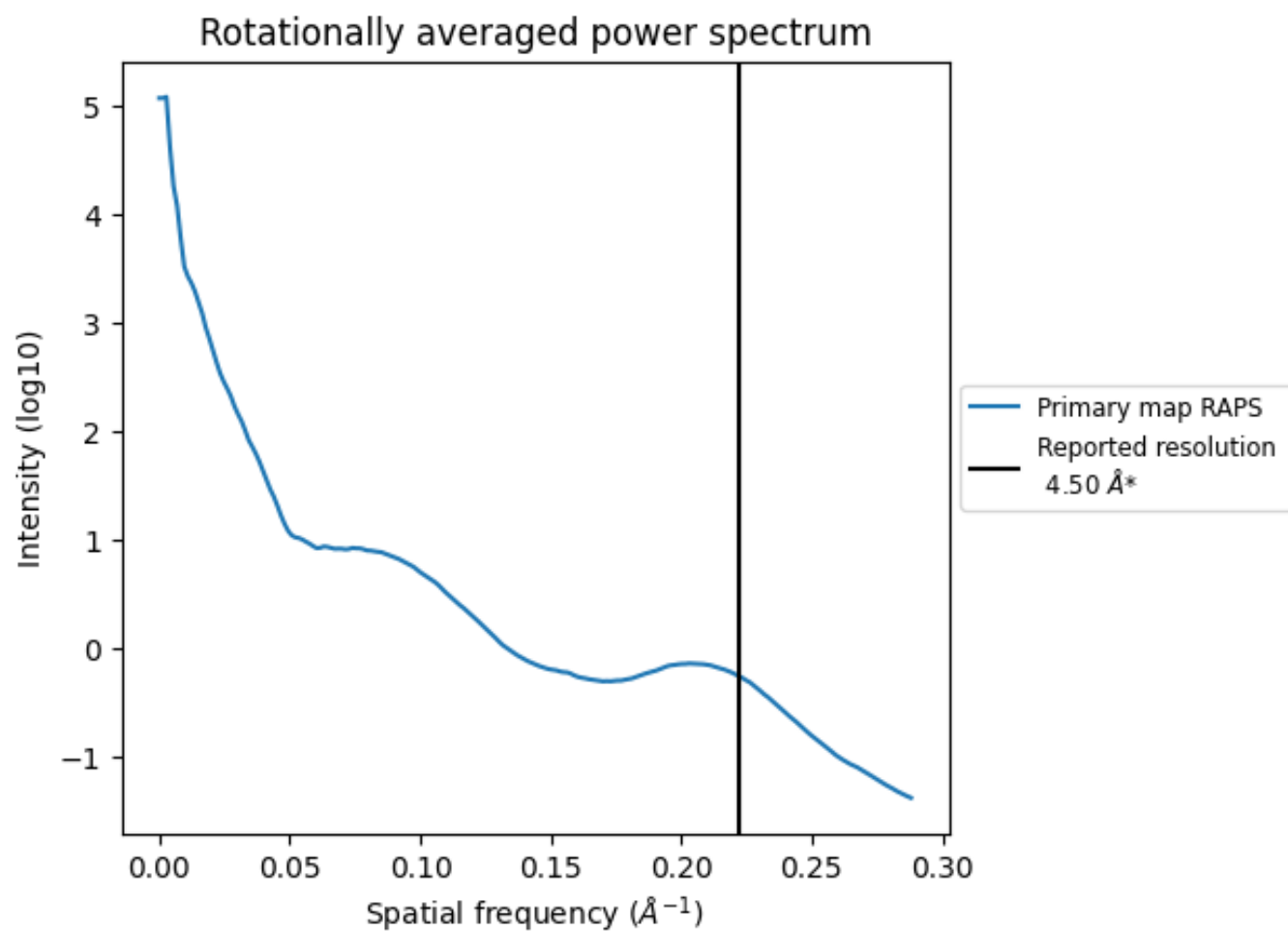
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1011  $\text{nm}^3$ ; this corresponds to an approximate mass of 913 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 0.222  $\text{\AA}^{-1}$

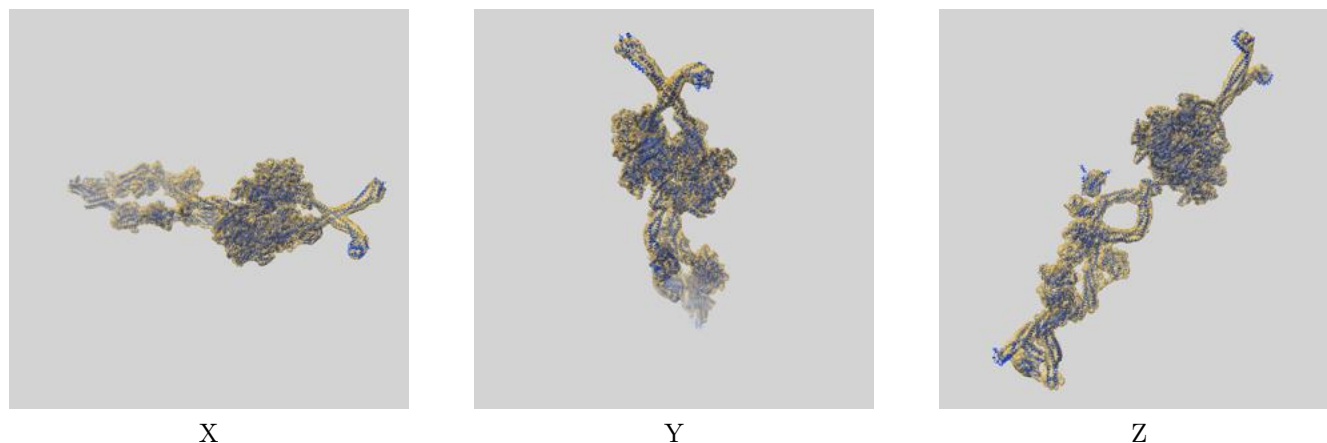
## 8 Fourier-Shell correlation

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

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

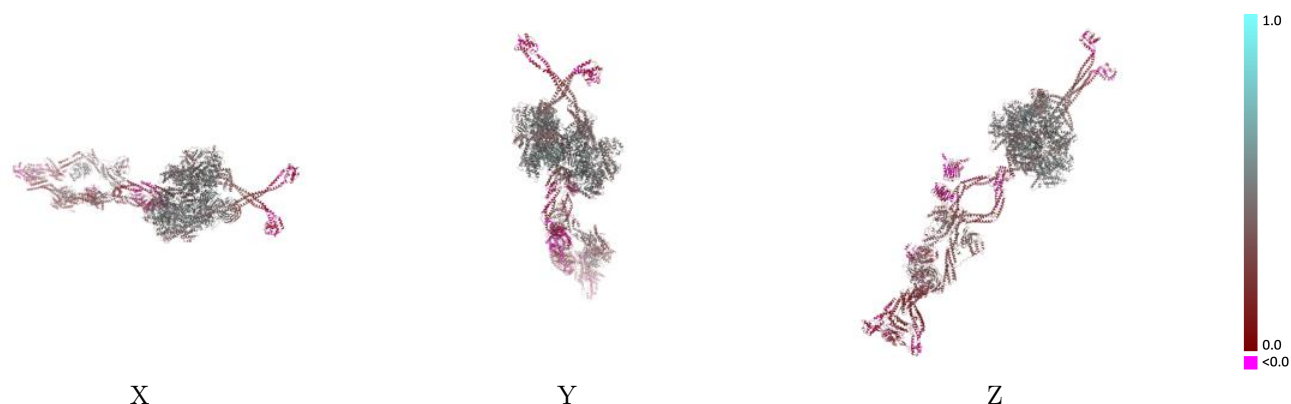
This section contains information regarding the fit between EMDB map EMD-47382 and PDB model 9E13. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.15 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](#)



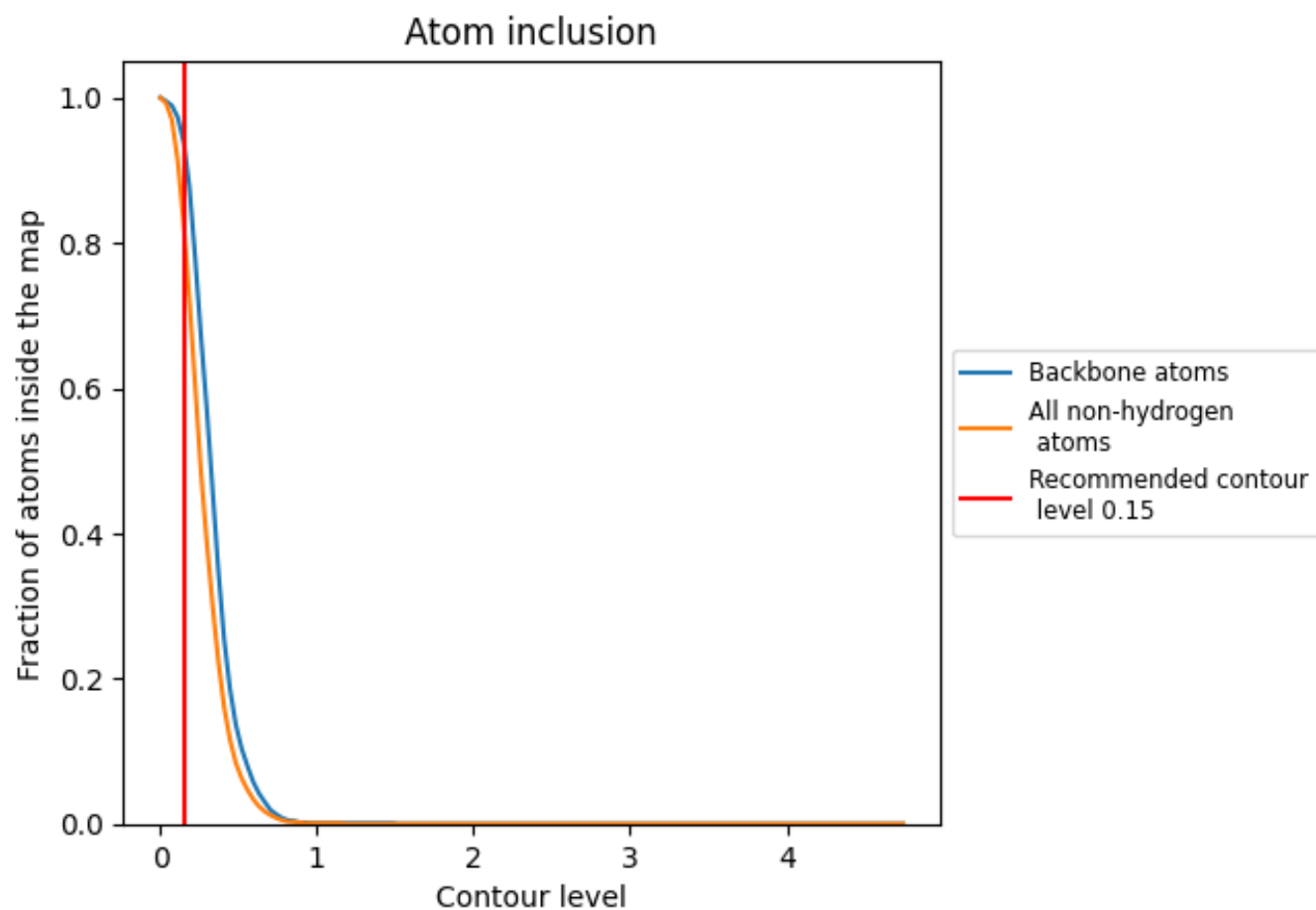
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)

































At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.3450
A	 0.8020	 0.3540
B	 0.8320	 0.3620
C	 0.9310	 0.3560
D	 0.9320	 0.2890
E	 0.9490	 0.3300
F	 0.9530	 0.3150
G	 0.7640	 0.1010
H	 0.8580	 0.1450
I	 0.7760	 0.1040
J	 0.8010	 0.0940
K	 0.3960	 0.0350
L	 0.5500	 0.0770
O	 0.8570	 0.4980
P	 0.7510	 0.3890

