



wwPDB EM Validation Summary Report ⓘ

Mar 4, 2026 – 08:30 PM UTC

PDB ID : 8BX8 / pdb_00008bx8
EMDB ID : EMD-16312
Title : In situ outer dynein arm from Chlamydomonas reinhardtii in the post-power stroke state
Authors : Zimmermann, N.E.L.; Noga, A.; Obbineni, J.M.; Ishikawa, T.
Deposited on : 2022-12-08
Resolution : 30.30 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:

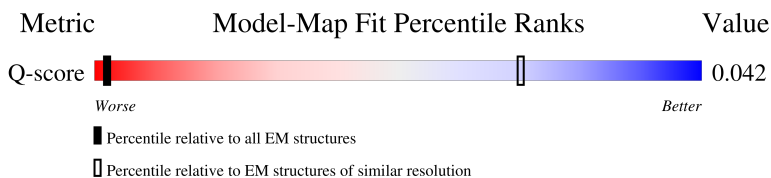
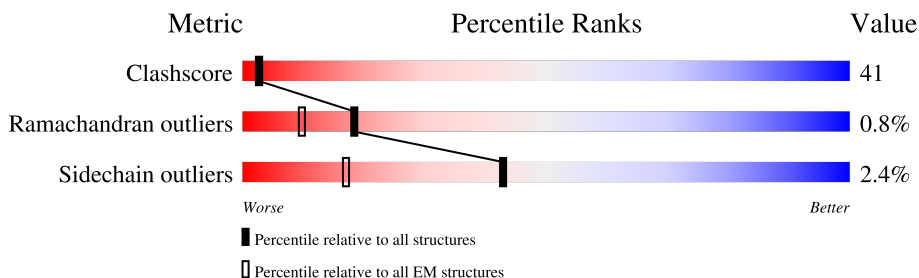
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 30.30 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.



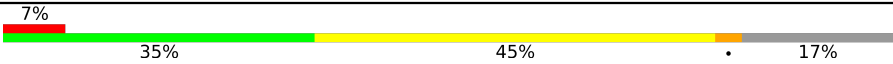
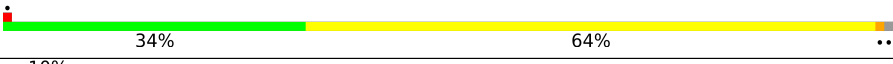
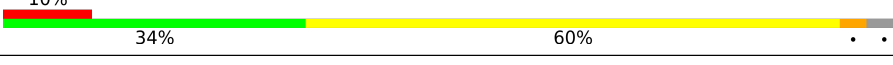
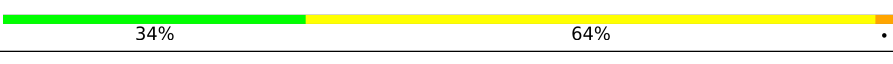
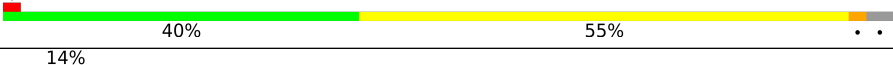
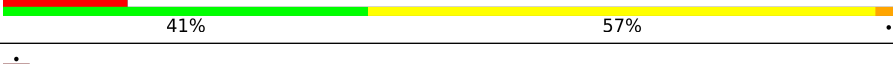
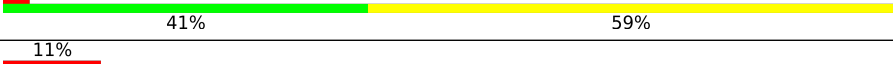
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10 (30.00 - 30.60)

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	4620	
2	B	4595	
3	C	4168	
4	D	657	

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Mol	Chain	Length	Quality of chain
5	E	670	
6	F	133	
7	G	159	
8	H	92	
9	I	110	
10	J	95	
11	K	93	
12	L	111	
13	M	87	
14	N	117	
15	O	132	
16	P	122	
17	Q	202	
18	R	160	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	ADP	A	4701	-	-	X	-
19	ADP	A	4703	-	-	X	-
19	ADP	B	5405	-	-	X	-
19	ADP	C	4305	-	-	X	-
19	ADP	C	4306	-	-	X	-
20	ATP	A	4702	-	-	X	-
20	ATP	B	5403	-	-	X	-
21	MG	A	4705	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 119530 atoms, of which 156 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 heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4453	Total	C	N	O	S	0	0
			33975	21575	5801	6441	158		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4488	LYS	GLY	conflict	UNP Q22A67

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4519	Total	C	N	O	S	0	0
			34713	22055	5945	6563	150		

- Molecule 3 is a protein called Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	3947	Total	C	N	O	S	0	0
			30427	19395	5159	5724	149		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	579	Total	C	N	O	S	0	0
			4680	2975	791	883	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	555	Total	C	N	O	S	0	0
			4440	2798	762	858	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	128	Total	C	N	O	S	0	0
			996	625	176	193	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1024	636	184	203	1		

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	91	Total	C	N	O	S	0	0
			750	483	124	139	4		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	106	Total	C	N	O	S	0	0
			827	526	134	161	6		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	95	Total	C	N	O	S	0	0
			807	527	135	140	5		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	90	Total	C	N	O	S	0	0
			754	489	124	137	4		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	111	Total	C	N	O	S	0	0
			855	555	145	152	3		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	87	Total	C	N	O	S	0	0
			735	477	123	130	5		

- Molecule 14 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	N	O	S	0	0
			852	542	142	165	3		

- Molecule 15 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	120	Total	C	N	O	S	0	0
			994	639	173	179	3		

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	109	Total	C	N	O	0	0
			541	323	109	109		

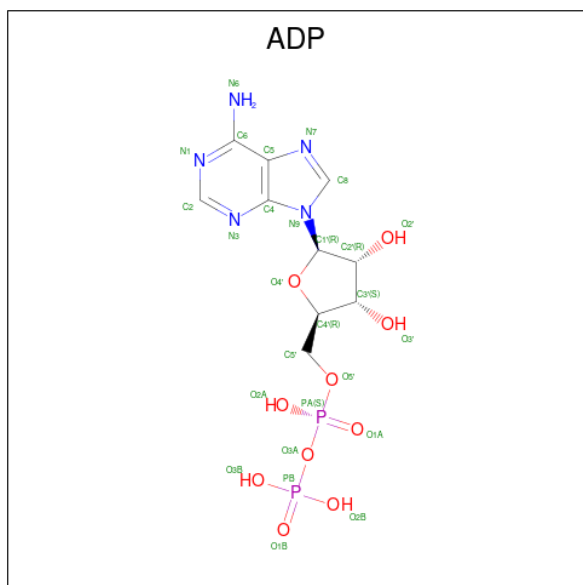
- Molecule 17 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	191	Total	C	N	O	0	0
			1001	607	202	192		

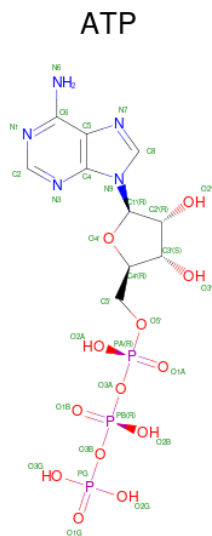
- Molecule 18 is a protein called Dynein light chain 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	150	Total	C	H	N	O	0	0
			895	439	156	150	150		

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

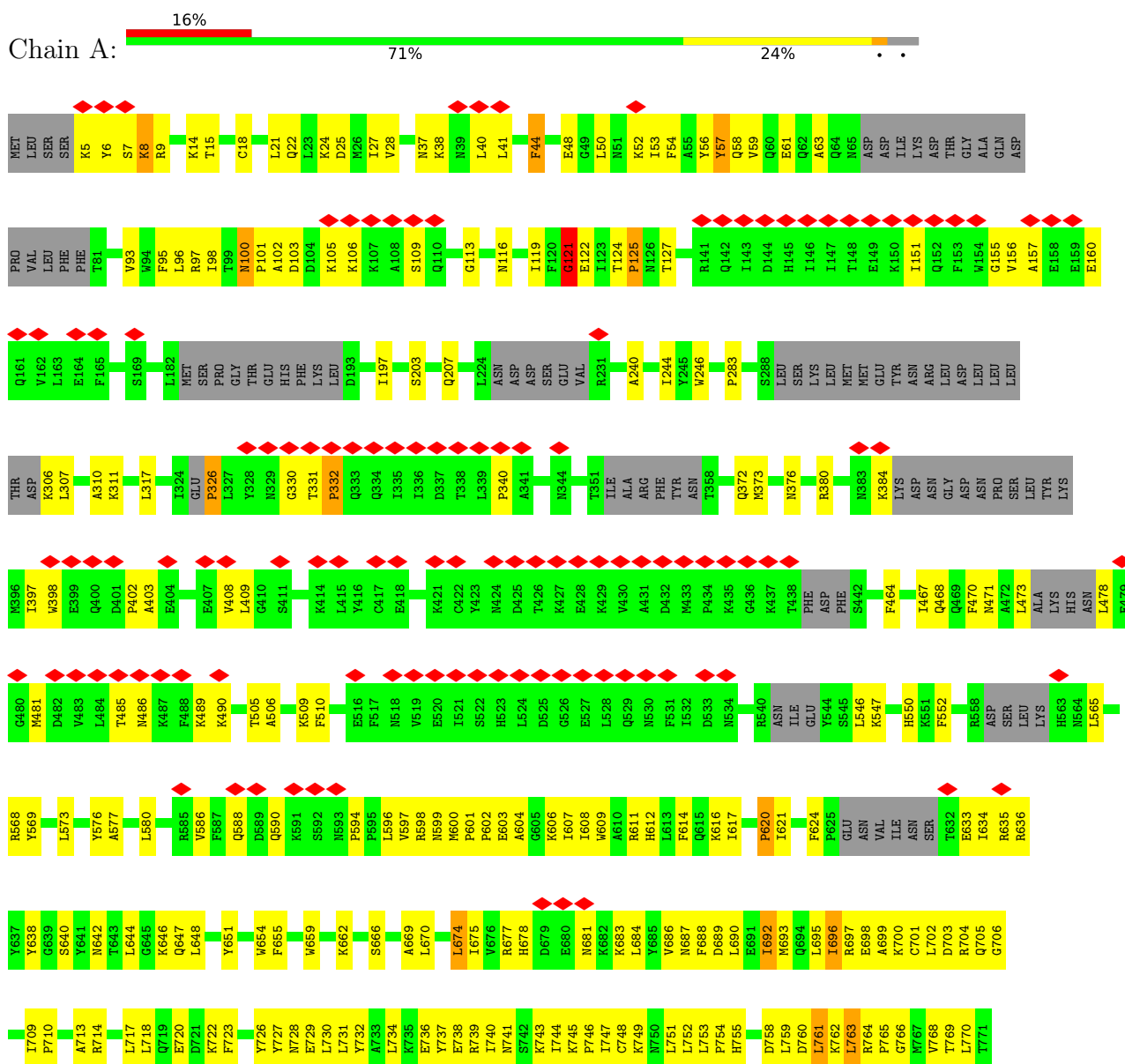
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	A	3	Total Mg 3 3	0
21	B	3	Total Mg 3 3	0
21	C	3	Total Mg 3 3	0

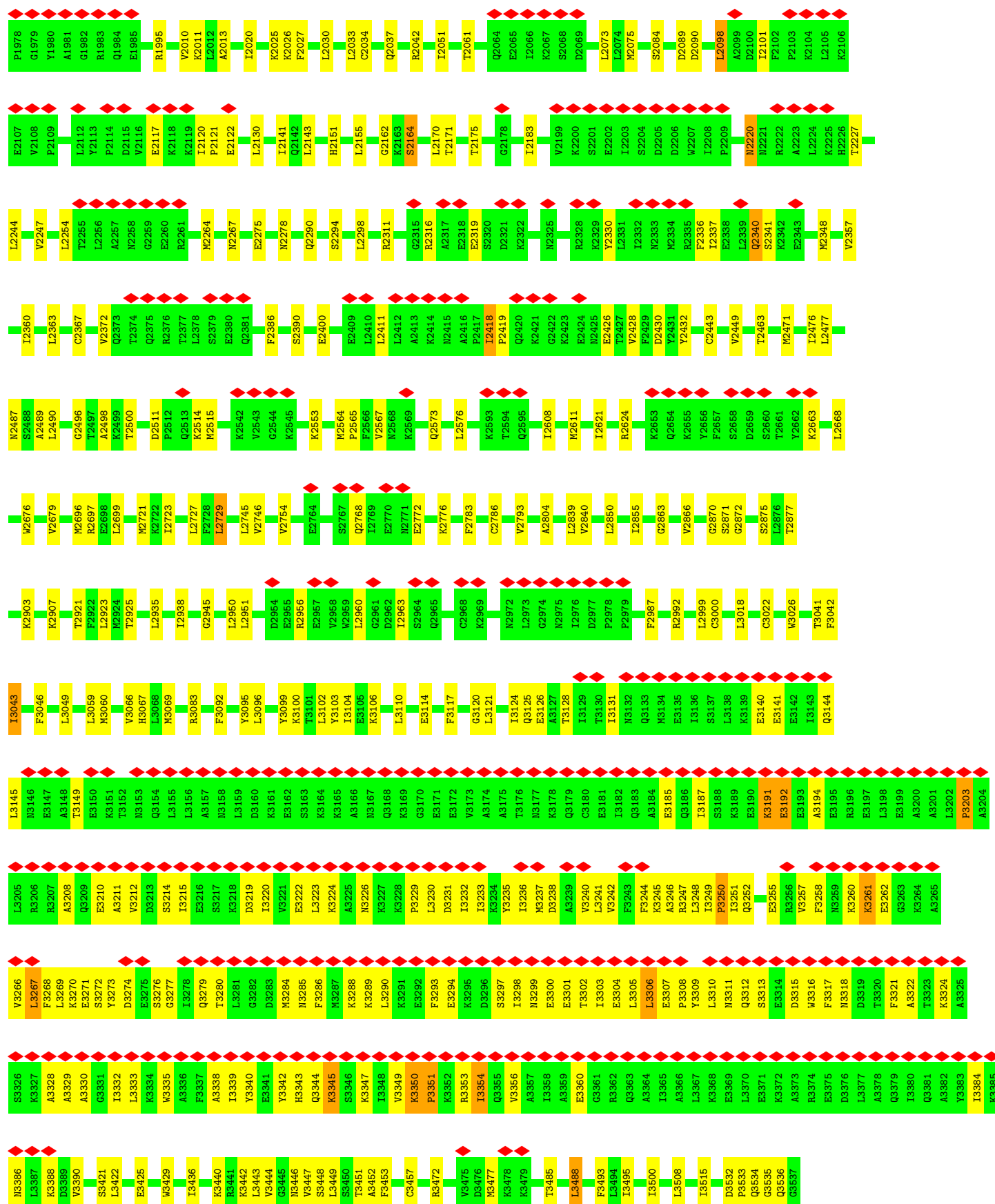
3 Residue-property plots

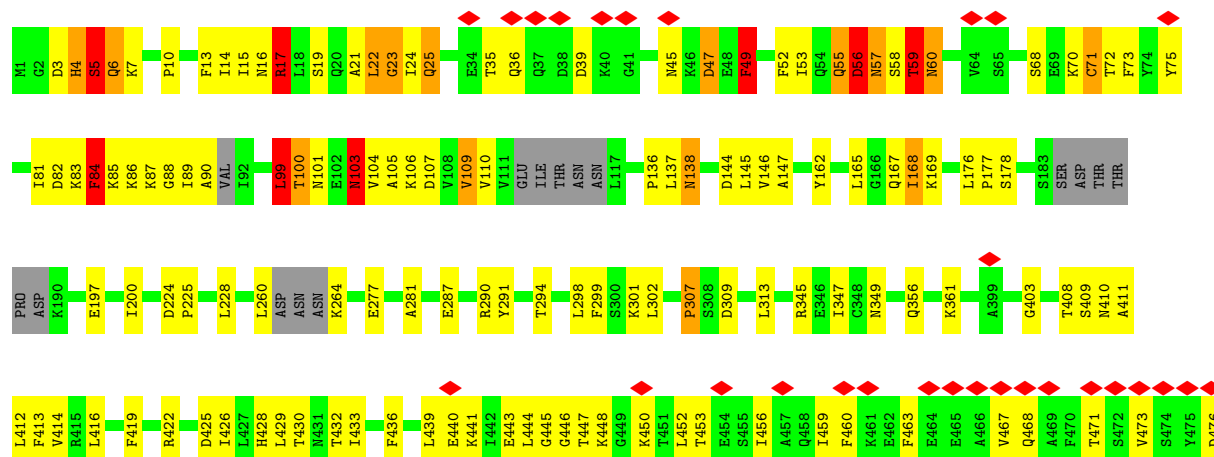
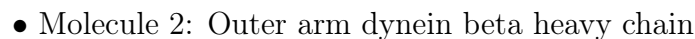
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

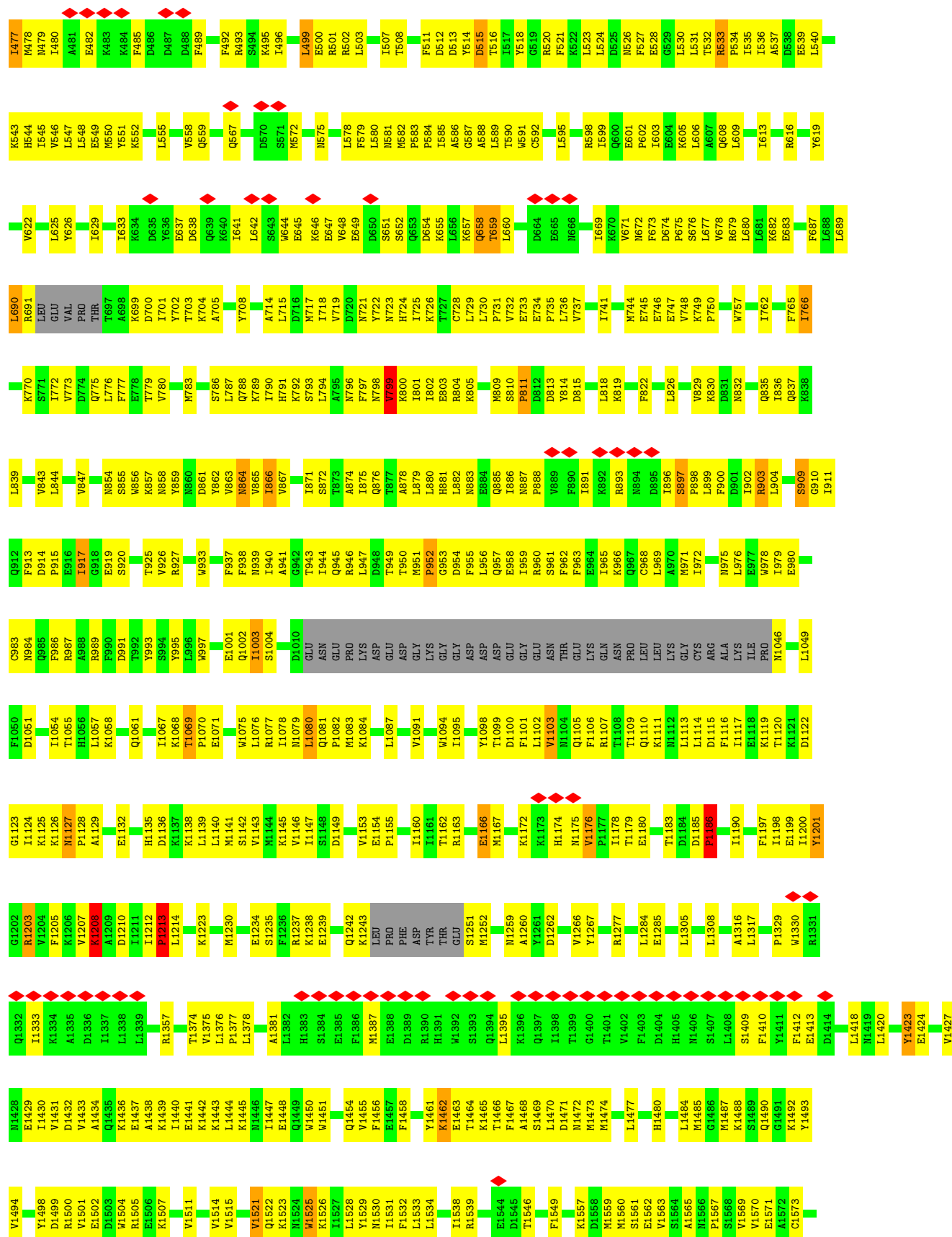
- Molecule 1: Dynein heavy chain, outer arm protein



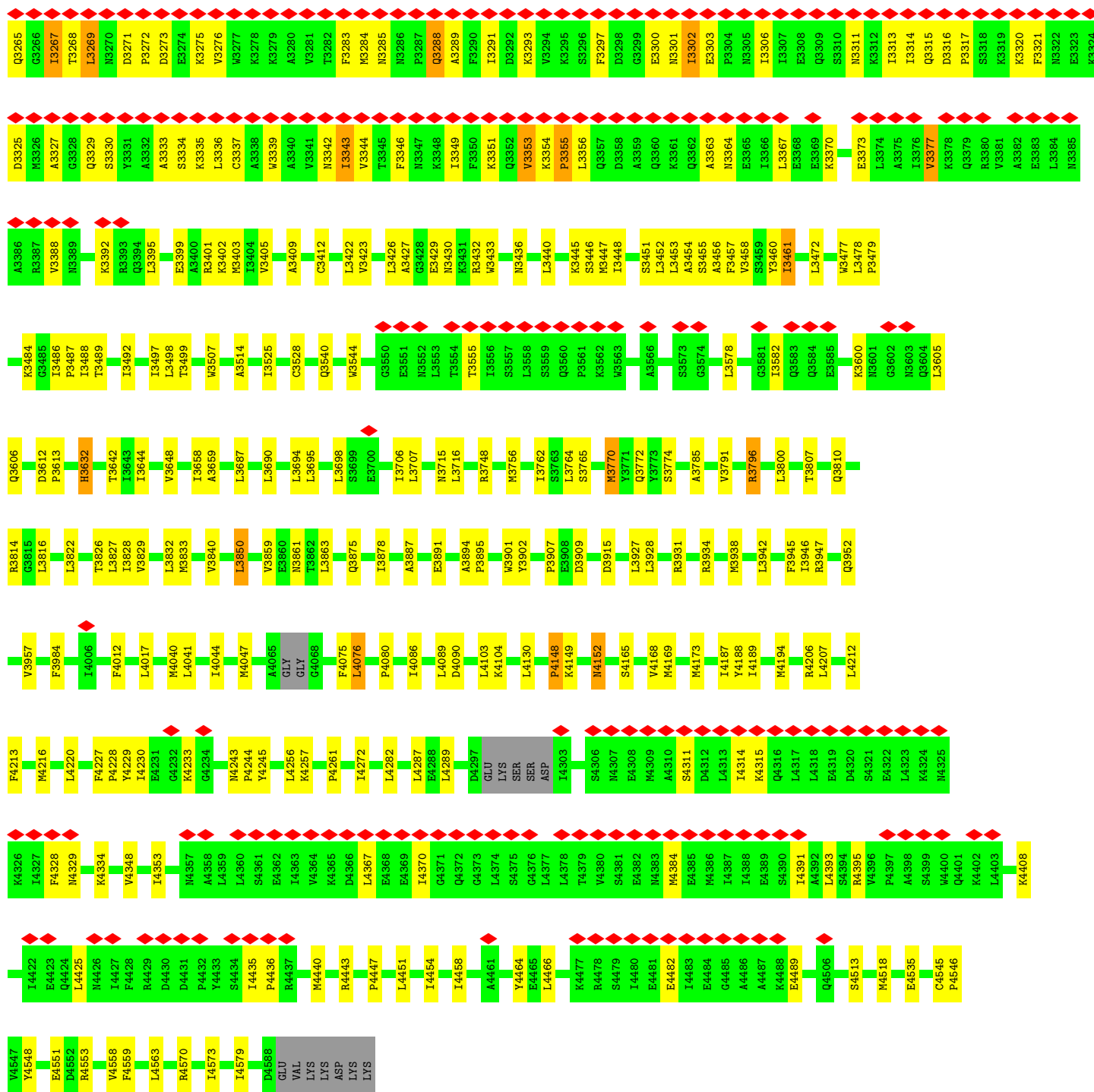
G1868	A1749	T1835	K1571	M1505	I1436	LYS	I1207	V1135	G1045	D973	K910	I841	W772
G1872	M1750	K1636	D1572	D1506	W1440	ASP	Y1208	M1136	N1047	Q974	Y911	K844	T773
A1874	D1751	V1637	F1573	T1507	N1441	L1323	K1210	E1137	Y1048	GLN	R912	T845	S774
G1875	I1752	T1638	L1574	D1509	D1442	D1329	E1211	L1138	Q1061	LYS	CYS	D846	I777
E1880	K1758	F1639	P1575	M1510	M1443	S1338	E1212	L1140	L1052	ASP	GLY	F847	Y780
L1889	L1764	S1641	D1576	W1511	F1444	Q1348	I1216	I1142	E1059	THR	LYS	L848	L761
L1892	L1769	K1645	L1577	W1512	F1445	Q1348	F1219	E1145	E1060	ASP	ILE	T849	
T1896	E1770	K1645	M1578	K1516	F1446	S1388	F1219	E1146	E1061	LYS	PRO	K851	H785
N1897	D1771	K1580	R1579	Q1515	F1447	Q1348	Y1223	Q1145	E1062	ALA	ASN	G787	G787
C1898	L1772	L1581	L1581	K1516	G1448	S1388	Y1223	Q1146	E1063	THR	THR	L788	K789
S1899	L1774	E1582	Q1585	W1518	W1449	LEU	Y1230	E1147	F985	Y986	LEU	K790	K790
D1900	L1774	Q1585	K1585	W1518	W1450	LYS	Y1230	E1148	F985	Y986	GLN	L791	L791
Q1901	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	ASN	E854	E854
H1902	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	THR	R857	R857
R1903	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	LEU	A858	A858
K1909	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	GLN	V859	V859
I1910	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	ASN	D860	D860
L1914	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	LYS	D861	D861
V1915	L1774	E1582	K1585	W1518	W1450	THR	Y1230	E1149	R989	Y986	PRO	L862	L862
Q1917	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	LEU	I866	I866
G1918	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	GLN	L868	L868
L1919	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	ASN	V869	V869
S1917	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	THR	P870	P870
G1918	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	GLN	L871	L871
L1919	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	ASN	N802	N802
N1925	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	PRO	E803	E803
E1925	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	THR	N804	N804
N1926	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	LEU	P873	P873
N1927	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	GLN	R874	R874
R1928	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	ASN	E807	E807
I1929	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	THR	N808	N808
D1930	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	GLN	K811	K811
L1931	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	ASN	V813	V813
E1932	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	PRO	S814	S814
V1933	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	THR	E815	E815
L1934	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	LEU	V816	V816
S1935	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	GLN	L818	L818
I1962	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	ASN	H820	H820
I1967	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	THR	P822	P822
V1970	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	LEU	Y890	Y890
F1973	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	GLN	F891	F891
I1974	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	ASN	W892	W892
T1975	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	THR	F894	F894
M1976	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	GLN	L898	L898
N1977	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	ASN	L899	L899
	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	PRO	N900	N900
	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	THR	S901	S901
	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	LEU	T902	T902
	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	GLN	S905	S905
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	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	GLN	A908	A908
	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	ASN	N971	N971
	L1774	E1582	K1585	W1518	W1450	PRO	Y1230	E1149	R989	Y986	PRO	W972	W972
	L1774	E1582	K1585	W1518	W1450	SER	Y1230	E1149	R989	Y986	THR	L836	L836
	L1774	E1582	K1585	W1518	W1450	LEU	Y1230	E1149	R989	Y986	LEU	Q837	Q837
	L1774	E1582	K1585	W1518	W1450	LYS	Y1230	E1149	R989	Y986	GLN	Y840	Y840

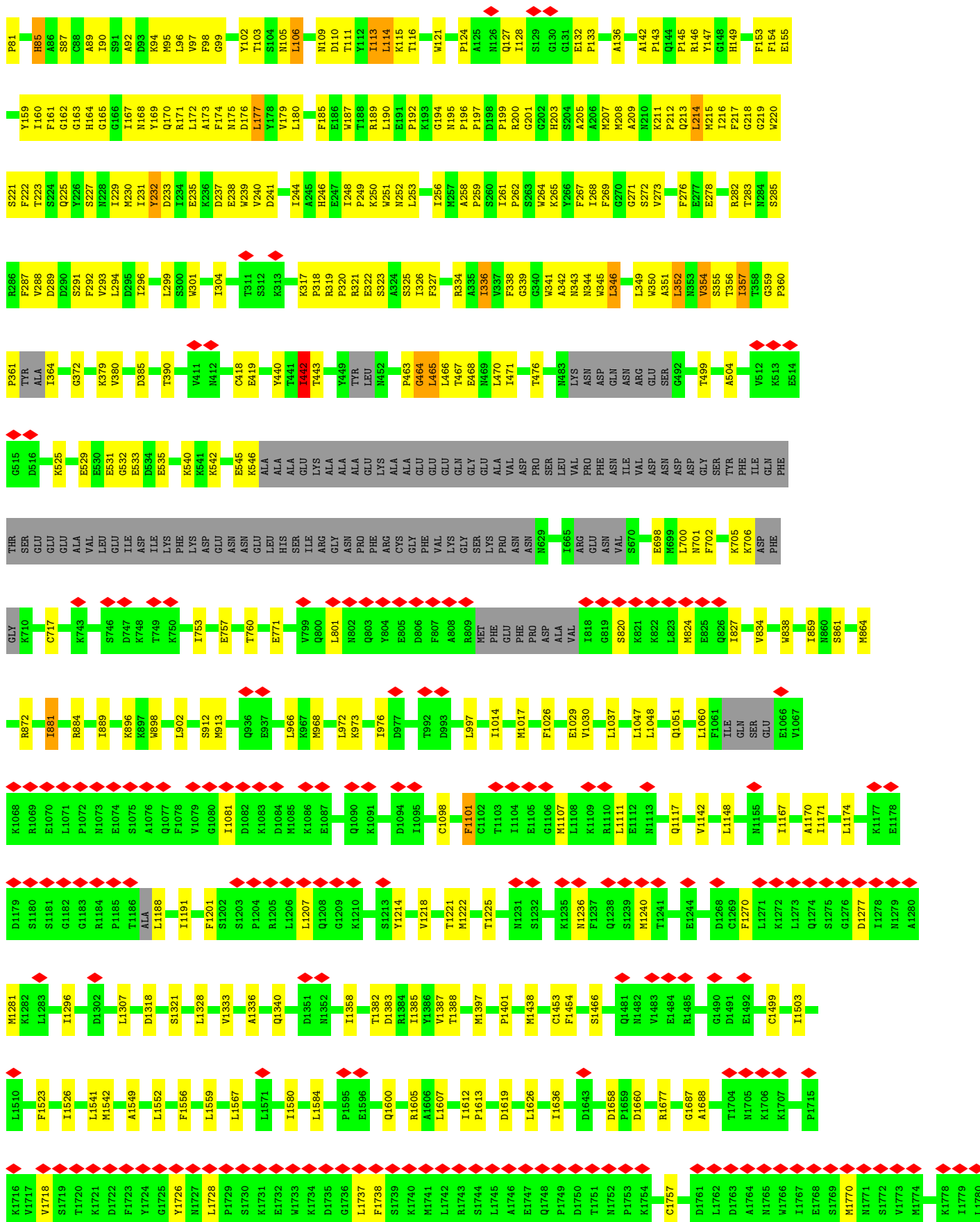




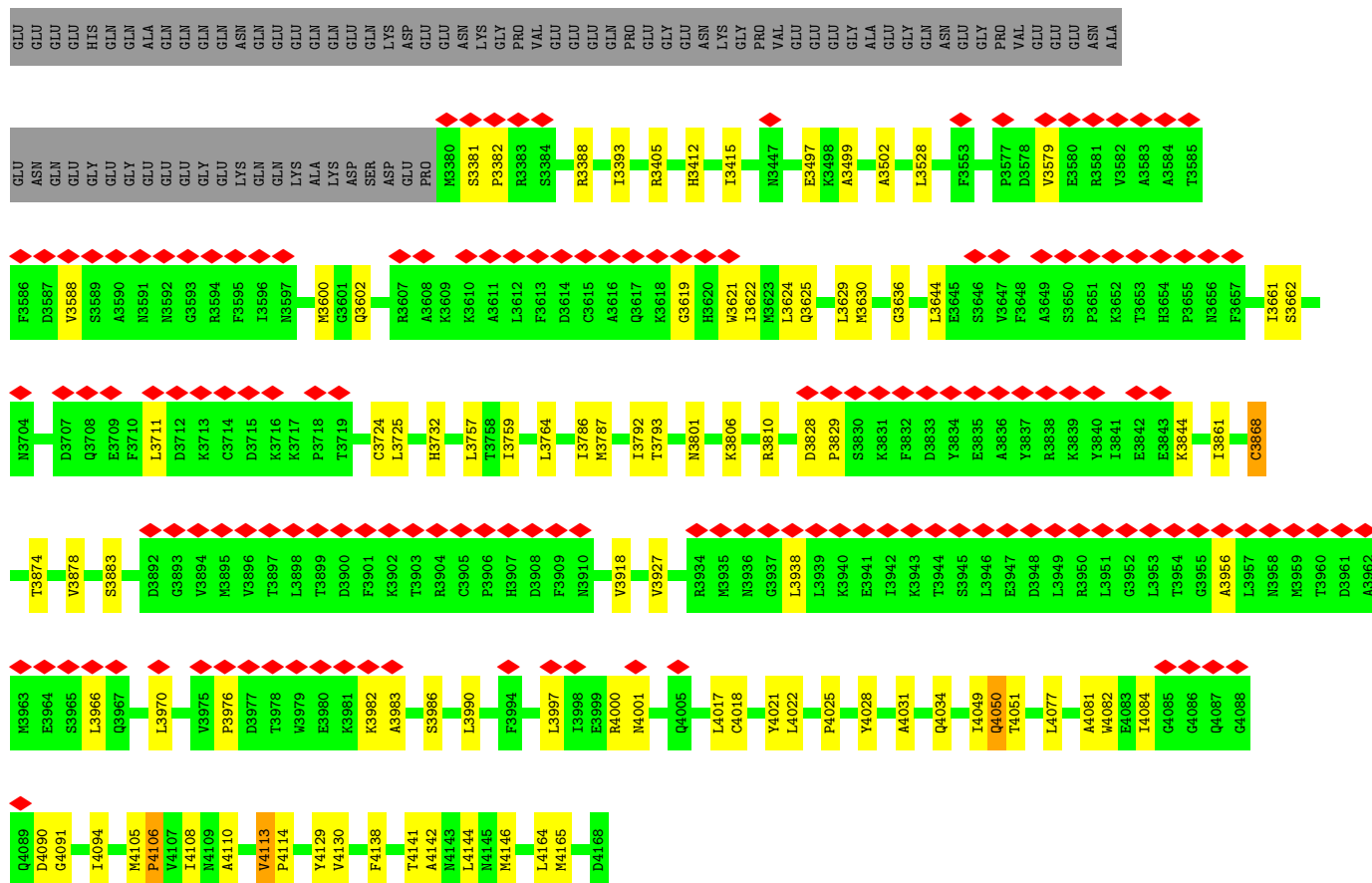


E3205	G3139	T3031	Q2930	T2755	P2610	N2487	N2345	N2235	K2070	Y1863	A1681	R1577
A3206	L3140	N3041	E2931	P2756	K2614	E2488	K2348	V2237	D2073	I1868	V1682	W1584
E3207	L3143	N3042	K2934	G2757	G2615	N2489	Q2349	V2240	A2078	L1687	H1684	S1585
K3208	A3144	T3043	K2935	Y2759	G2616	W2491	Q2349	K2243	L2083	C1591	L1687	C1591
K3209	Q3147	D3046	I2936	S2760	T2617	N2492	A2354	Q2085	L2083	L1595	K1705	L1595
S3210	V3059	V3059	A2937	G2761	S2619	T2493	K2358	Q2085	Q2085	L1599	A1708	L1599
K3211	F3063	F3063	K2938	G2762	I2621	W2494	E2358	K2247	D2085	K1912	A1708	L1599
E3212	L3153	L3153	P2939	L2767	Q2622	L2500	P2359	N2248	D2085	V1922	W1711	K1602
A3213	Q3154	Q3154	E2944	L2770	R2625	P2501	P2360	E2249	T2116	M1923	D1712	K1603
T3214	E3155	E3155	L2960	K2776	R2636	N2502	V2361	Y2252	D2117	W1925	D1712	K1604
E3215	E3156	E3156	P2961	D2781	E2637	D2503	D2362	K2253	D2118	F1924	G1714	S1605
A3216	L3157	L3157	L2962	L2800	Q2638	V2512	D2363	A2254	D2118	F1925	G1714	S1605
L3217	K3160	K3161	N2963	L2800	E2640	T2514	D2364	W2260	I2121	C1927	Q1728	P1607
A3218	S3077	S3077	L2966	L2812	E2641	H2516	D2367	D2264	T2126	S1928	L1731	P1608
E3219	Q3162	Q3162	L2966	P2813	E2641	H2516	K2367	D2264	G2127	S1928	L1731	P1609
A3220	E3163	E3163	L2966	P2813	E2641	H2516	K2367	D2264	D2128	F1610	L1731	P1610
L3221	N3081	N3081	L2966	P2813	E2641	H2516	K2367	D2264	L2129	F1611	L1731	P1611
P3222	M3082	M3082	L2971	P2814	E2641	H2516	K2367	D2264	L2129	F1612	L1731	P1612
A3223	V3085	V3085	L2974	A2815	P2644	R2519	S2368	D2268	K2132	M1936	T1734	L1617
L3224	E3169	E3170	F2975	E2816	L2649	M2523	K2395	P2269	L2133	G1942	T1735	L1618
K3225	T3171	T3171	P2976	P2817	L2649	I2526	K2396	E2270	L1749	G1942	D1748	L1621
A3226	L3172	L3172	P2976	L2818	N2655	R2531	L2409	W2271	D2134	Q1945	A1750	S1622
L3227	S3077	S3077	E2978	L2819	N2655	R2531	L2409	W2271	P2135	Q1946	G1751	N1623
E3228	Q3173	Q3173	E2978	F2820	V2663	L2534	D2410	E2273	P2136	C1947	G1752	A1627
A3229	L3174	L3174	D2979	Y2834	D2664	L2534	L2412	S2274	T2150	E1954	G1752	P1628
K3230	I3175	I3175	K2980	T2835	L2665	A2540	L2413	K2283	V2176	F1955	S1753	P1628
A3231	E3176	E3176	D2981	Q2836	R2666	G2543	T2414	V2284	R2177	N1956	E1754	C1637
L3232	K3177	K3177	S2982	C2837	L2667	T2545	Q2415	L2285	P2185	R1957	T1755	F1638
C3233	V3178	V3178	L2983	T2838	Q2668	A2546	H2416	L2286	P2185	R1957	T1755	F1638
A3234	Q3179	Q3179	V2984	P2840	M2676	A2546	L2417	L2287	S2188	V1966	K1758	L1641
K3235	L3180	L3180	S2985	L2846	K2685	R2556	P2418	V2288	G2189	N2005	L1771	T1645
S3236	E3181	E3181	Q2986	L2846	L2686	P2557	K2419	V2288	K2190	P2006	I1772	F1646
P3237	S3182	S3182	V2987	L2862	L2687	E2558	L2420	S2289	T2191	P2006	E1783	E1647
E3238	A3183	A3183	R2988	L2864	S2690	Q2559	K2421	N2290	C2192	Q2007	R1784	P1648
L3239	L3184	L3184	N2989	E2870	L2696	V2560	Q2422	D2291	N2203	Y2008	W1785	P1649
A3240	E3185	E3185	E2990	H2871	S2697	S2569	K2423	R2292	N2214	A2009	K1786	P1649
K3241	S3186	S3186	A2991	Y2872	T2698	L2674	E2425	I2293	G2219	R2011	I1787	A1650
L3242	E3187	E3187	K2992	S2873	L2699	L2674	E2426	F2294	N2219	G2010	I1788	N1651
C3243	Q3188	Q3188	G2993	L2879	D2700	Q2577	D2427	L2295	S2220	R2023	T1792	P1652
L3245	T3189	T3189	E2994	N2885	D2701	Q2577	E2428	R2300	D2221	R2023	I1793	A1653
G3246	I3191	I3191	V2996	G2893	K2702	K2586	K2429	L2301	S2221	N2038	D1794	E1654
S3247	A3192	A3192	D2997	G2893	A2707	K2587	Q2430	F2303	G2225	M2039	V1795	T1655
P3248	Q3193	Q3193	V2998	T2904	V2711	N2588	A2431	E2304	A2226	M2041	R1798	S1656
A3249	L3194	L3194	N2999	T2904	V2711	N2588	A2431	L2305	Y2227	G2044	I1806	T1657
E3250	E3195	E3195	N3000	L2911	S2731	G2590	L2432	L2308	T2228	G2044	S1819	V1658
G3251	S3196	S3196	L3001	I2911	A2732	N2591	F2436	R2309	T2229	R2049	S1819	G1659
V3252	E3197	E3197	T3002	N2927	R2742	Y2592	L2441	A2311	T2230	L2068	W1825	I1660
L3253	K3198	K3198	A3003	N2927	R2742	Y2592	L2441	E2326	K2231	L2068	W1825	G1661
V3254	T3199	T3199	L3004	N2927	T2754	I2601	G2445	E2326	E2232	L2068	W1825	M1662
T3255	N3200	N3200	T3005	N2927	T2754	I2601	G2445	E2326	W2233	L2068	W1825	K1675
A3256	S3201	S3201	S3006	N2927	T2754	I2601	G2445	E2326	E2233	L2068	W1825	K1675
K3257	V3201	V3201	Y3007	N2927	T2754	I2601	G2445	E2326	E2233	L2068	W1825	K1675
A3258	A3203	A3203	F3008	N2927	T2754	I2601	G2445	E2326	E2233	L2068	W1825	K1675
V3259	L3260	L3260	K3017	N2927	T2754	I2601	G2445	E2326	E2233	L2068	W1825	K1675
L3260	L3261	L3261	V3018	N2927	T2754	I2601	G2445	E2326	E2233	L2068	W1825	K1675
L3262	L3262	L3262	F3263	N2927	T2754	I2601	G2445	E2326	E2233	L2068	W1825	K1675
F3263	L3264	L3264	N3264	N2927	T2754	I2601	G2445	E2326	E2233	L2068	W1825	K1675

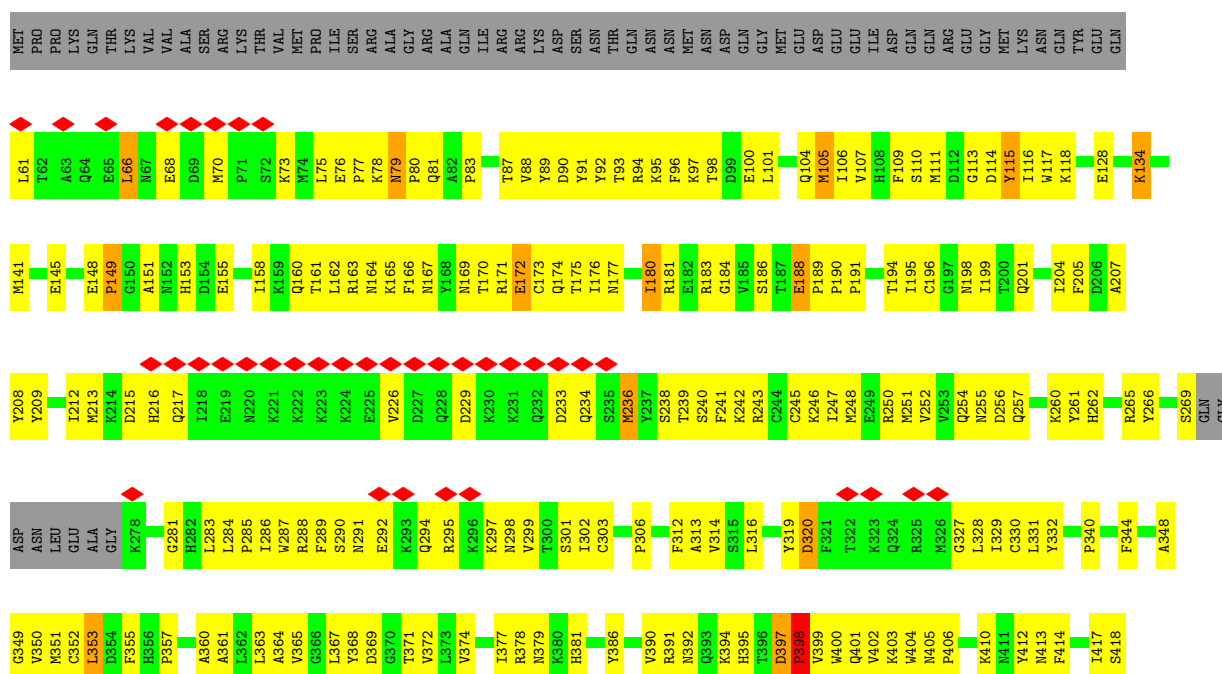


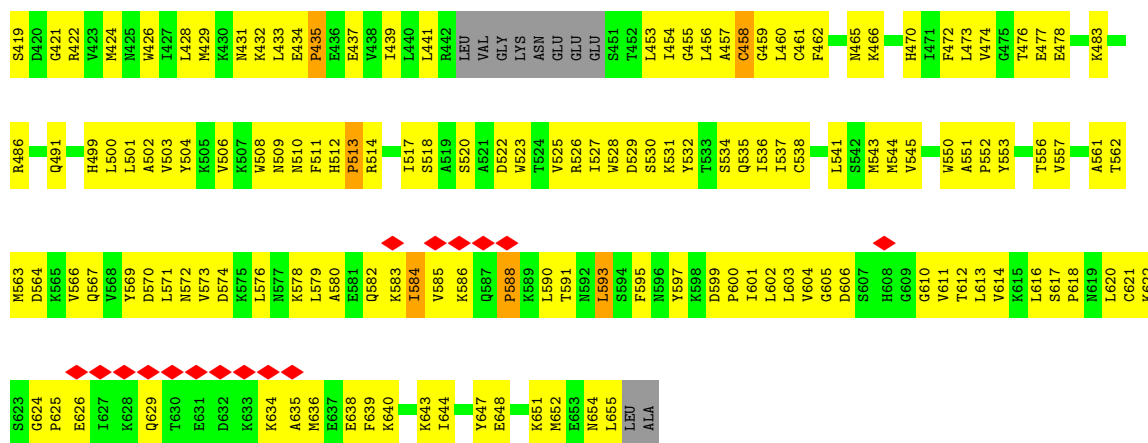


K3151	L2989	A3785	S2815	L2755	K2695	V2480	G2365	K2113	R1923	T1781
F3161	P2990	L2876	W2816	K2756	S2696	W2486	K2366	L2114	K1924	L1782
L3184	V2994	A2877	V2817	L2757	A2697	A2487	Q2367	A2115	A1783	A1783
D3185	V2994	E2878	V2818	M2758	L2698	L2488	S2368	I2119	W1784	W1784
I3190	I3001	R2879	N2819	K2759	N2699	T2512	D2226	T2122	W1785	W1785
I3010	I3010	N2880	N2820	S2760	S2700	D2513	P2227	Q2123	W1929	W1929
M3011	M3011	A2881	V2821	P2761	I2701	W2514	N2228	V2124	W1930	W1930
I3012	I3012	R2892	K2822	E2762	S2702	L2531	K2229	M2128	N1981	N1981
D3013	D3013	L2895	Y2823	E2763	K2703	E2532	F2230	T2131	I1982	I1982
P3014	P3014	L2899	Y2824	F2764	K2704	P2533	F2231	T2132	T1983	T1983
E3204	E3204	L2899	D2825	M2765	D2705	L2536	R2396	S2131	T1983	T1983
E3205	E3205	L2899	V2826	E2766	F2706	R2646	N2397	A2132	K1791	K1791
A3208	A3208	L2902	L2827	K2767	Q2707	R2647	D2398	G2133	P1792	P1792
I3212	I3212	L2903	Q2828	L2768	Q2708	E2648	L2399	S2133	H1793	H1793
I3217	I3217	L2908	D2829	L2769	A2709	K2649	Q2400	F2135	L2007	L2007
R3225	R3225	R2909	V2830	N2770	K2710	D2650	Q2401	P2136	S2012	S2012
A3227	A3227	K2912	E2831	F2771	S2711	K2651	L2402	V2137	G2013	G2013
V3244	V3244	L2914	P2832	K2772	F2712	F2577	Y2403	Y2141	C2014	C2014
S3267	S3267	L2915	K2833	D2773	A2713	L2581	F2404	F2145	G2015	G2015
E3268	E3268	L2916	R2834	V2774	S2714	T2582	K2405	T2247	K2016	K2016
N3269	N3269	Q2916	K2835	V2775	K2654	L2583	C2406	F2152	T2017	T2017
I3057	I3057	L2917	A2836	D2776	P2715	L2584	L2416	S2159	Q2018	Q2018
E3058	E3058	E2918	L2837	A2777	P2716	F2585	F2417	T2172	T2023	T2023
N3059	N3059	D2919	K2838	K2778	A2717	L2589	N2424	R2172	N2043	N2043
I3064	I3064	Q2920	E2839	Q2779	G2718	K2592	E2425	F2173	Y2044	Y2044
I3072	I3072	L2922	E2840	Q2780	V2719	R2593	R2426	K2174	Y2045	Y2045
A3073	A3073	L2923	T2841	PR0	E2721	L2596	I2431	S2175	L2055	L2055
R3074	R3074	L2924	E2842	ALA	V2722	E2597	N2432	T2176	L2059	L2059
H3095	H3095	D2927	Q2843	N2784	F2723	K2600	Y2444	E2179	E2060	E2060
P3096	P3096	L2928	E2844	V2785	A2724	L2607	T2445	K2184	K2061	K2061
N3097	N3097	V2929	E2845	V2786	A2725	E2615	L2446	Y2185	K2062	K2062
F3101	F3101	L2930	E2846	L2787	T2726	L2618	D2447	L2189	A2063	A2063
L3102	L3102	A2931	E2847	V2788	L2727	L2619	E2448	L2189	Y2067	Y2067
P3113	P3113	F2934	E2848	K2789	Y2728	L2619	K2449	L2189	I2079	I2079
E3114	E3114	V2935	E2849	N2790	L2729	L2619	E2450	H2192	L2082	L2082
I3115	I3115	S2936	L2851	Q2791	A2731	V2622	A2451	Q2193	Q2086	Q2086
L3121	L3121	S2937	L2852	Y2792	G2732	E2623	M2452	A2194	L2087	L2087
T3125	T3125	S2938	E2853	L2793	Y2733	V2624	L2453	V2195	D2088	D2088
L3131	L3131	F2941	V2854	N2794	F2734	K2625	N2454	T2196	A2089	A2089
VAL	VAL	N2942	E2855	K2795	N2735	E2626	Q2455	Q2197	Y2090	Y2090
PRO	PRO	L2943	E2856	P2796	E2736	K2627	R2457	N2198	D2091	D2091
TYR	TYR	K2944	E2857	P2797	A2737	Q2628	K2459	F2199	T2092	T2092
GLY	GLY	M2949	E2858	F2798	I2738	Q2629	K2461	R2200	Q2093	Q2093
ASP	ASP	S2966	E2859	T2799	S2678	A2631	G2462	T2202	I2096	I2096
GLU	GLU	L2974	K2860	P2800	S2679	E2632	E2463	L2204	D2110	D2110
THR	THR	W2984	L2861	E2801	D2741	K2633	K2464	H2207	V2111	V2111
ALA	ALA		L2862	E2802	K2742	K2633	E2465	R2213	S2112	S2112
ASN	ASN		E2863	A2804	K2744	K2634	K2466			
GLN	GLN		L2865	S2805	K2745		P2466			
HIS	HIS		K2867	K2806	P2746		D2467			
LYS	LYS		L2868	A2808	K2747		R2469			
GLU	GLU		K2869	A2809	D2748					
GLU	GLU		A2870	A2810	V2749					
GLU	GLU		E2871	A2811	S2750					
GLU	GLU		N2872	K2751	W2751					
GLU	GLU		D2873	L2813	K2752					
GLU	GLU		K2874	C2814	S2753					
					S2754					
					A2694					

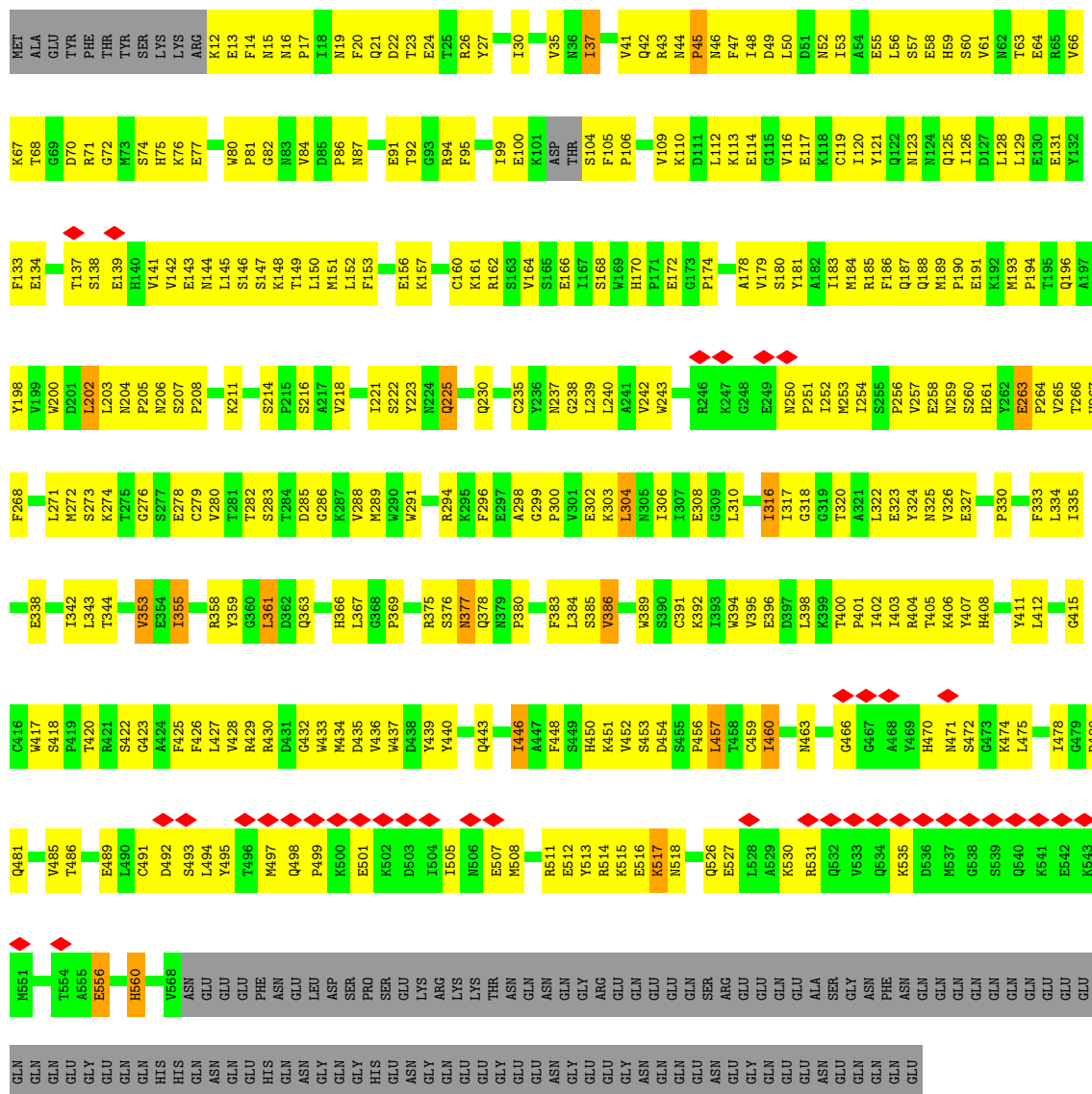


• Molecule 4: Dynein intermediate chain 2

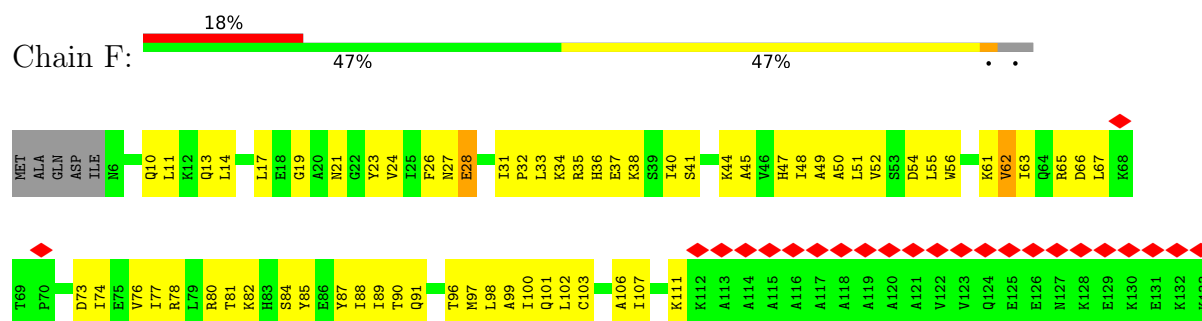




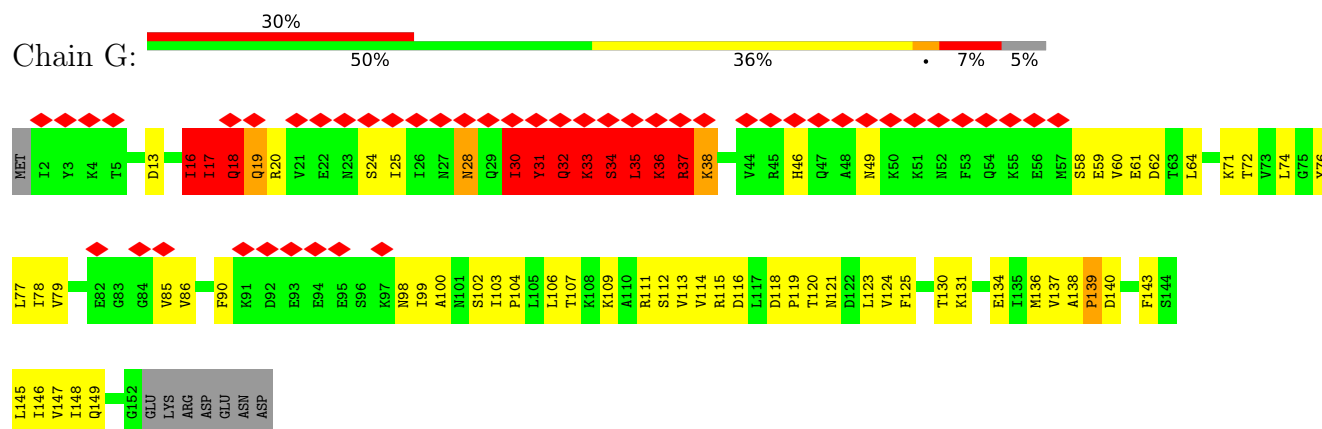
• Molecule 5: Flagellar outer dynein arm intermediate protein, putative



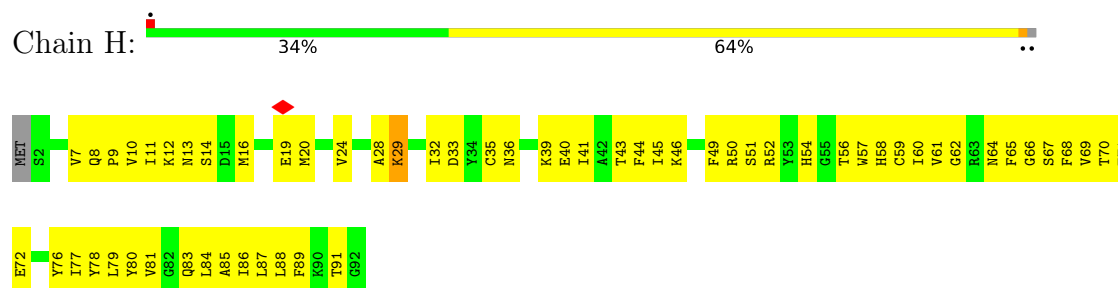
- Molecule 6: Dynein light chain roadblock-type 2 protein



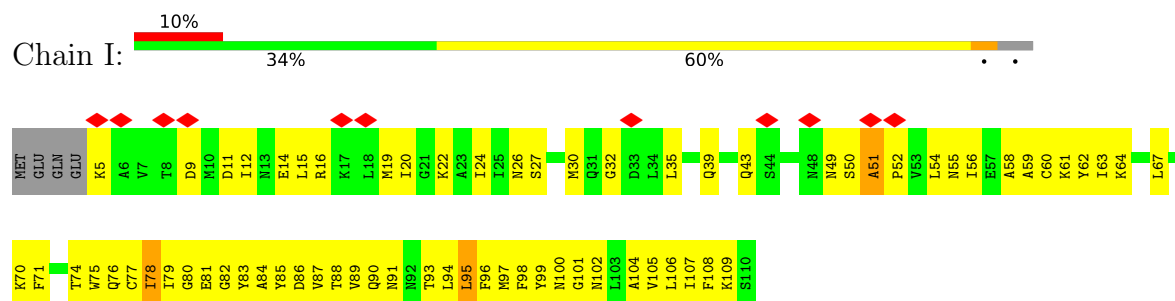
- Molecule 7: Dynein light chain roadblock-type 2 protein



- Molecule 8: Dynein light chain

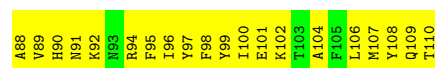


- Molecule 9: Dynein light chain

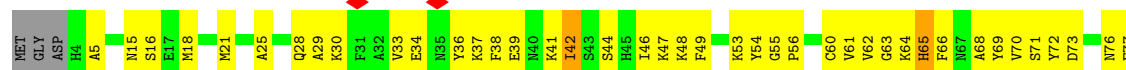


- Molecule 10: Dynein light chain

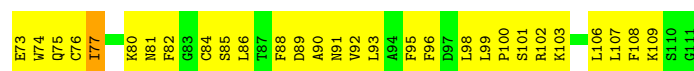




• Molecule 11: Dynein light chain



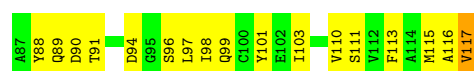
• Molecule 12: Dynein light chain



• Molecule 13: Dynein light chain

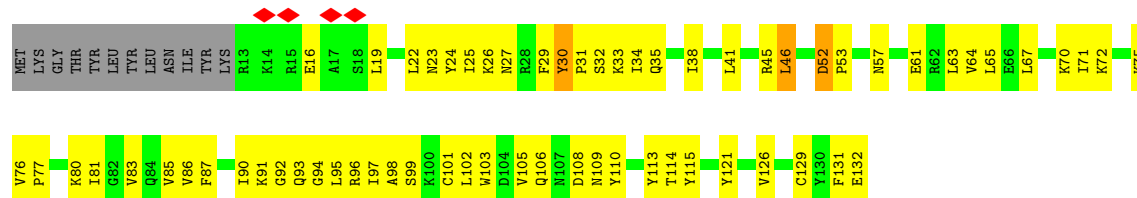


• Molecule 14: Dynein light chain tctex-type 1 protein



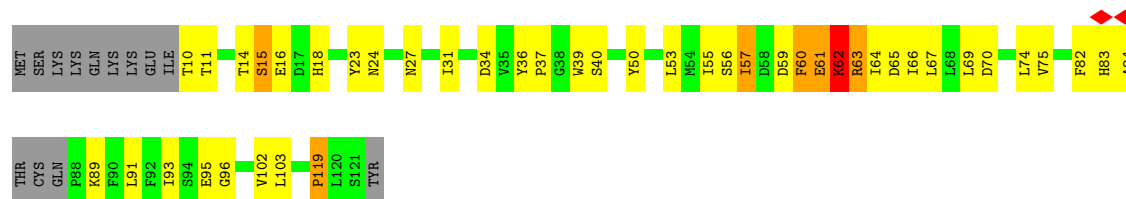
• Molecule 15: Dynein light chain 2A

Chain O: 



• Molecule 16: Thioredoxin

Chain P: 



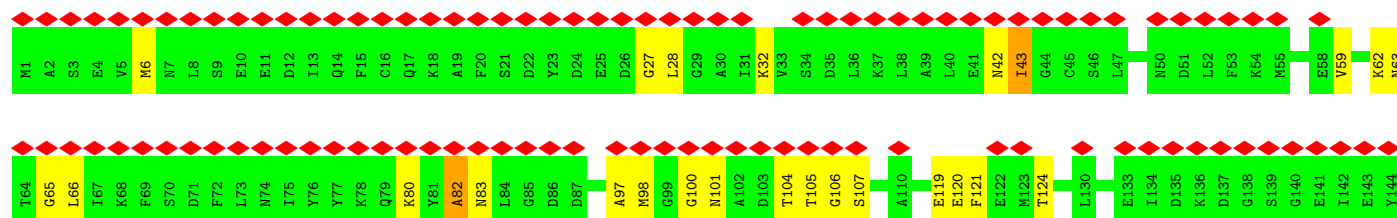
• Molecule 17: Dynein light chain 1

Chain Q: 



• Molecule 18: Dynein light chain 4A

Chain R: 



L149
L150
LEU
LYS
SER
GLY
PHE
ALA
ASN
GLU
GLY
ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	2131	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80.0	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.222	Depositor
Minimum map value	-0.797	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.196	Depositor
Recommended contour level	0.14	Depositor
Map size ($\text{\AA}$)	628.26, 628.26, 628.26	wwPDB
Map dimensions	74, 74, 74	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	8.49, 8.49, 8.49	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.04	16/34544 (0.0%)	1.54	59/46728 (0.1%)
2	B	1.12	18/35318 (0.1%)	1.61	88/47792 (0.2%)
3	C	1.30	278/31033 (0.9%)	1.70	278/42007 (0.7%)
4	D	0.98	1/4789 (0.0%)	1.27	10/6477 (0.2%)
5	E	0.94	0/4540	1.18	3/6136 (0.0%)
6	F	0.87	0/1008	1.06	0/1355
7	G	0.96	0/1030	1.67	14/1403 (1.0%)
8	H	0.98	0/767	1.13	0/1031
9	I	1.01	0/838	1.15	0/1131
10	J	0.93	0/832	1.14	1/1119 (0.1%)
11	K	0.95	0/776	1.08	0/1038
12	L	0.94	0/872	1.18	2/1176 (0.2%)
13	M	0.96	0/752	1.11	0/1006
14	N	1.01	0/864	1.20	0/1175
15	O	0.97	0/1012	1.18	0/1358
16	P	3.15	6/538 (1.1%)	2.40	20/746 (2.7%)
17	Q	0.50	2/1004 (0.2%)	1.24	9/1385 (0.6%)
18	R	1.42	1/738 (0.1%)	1.72	4/1025 (0.4%)
All	All	1.14	322/121255 (0.3%)	1.56	488/164088 (0.3%)

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
2	B	0	11
3	C	0	2
4	D	0	1
7	G	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	2
All	All	0	32

The worst 5 of 322 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	59	THR	C-N	-63.97	0.44	1.33
1	A	1067	PRO	N-CD	51.30	2.19	1.47
16	P	62	LYS	C-N	-49.84	0.64	1.33
16	P	15	SER	C-N	35.33	1.81	1.34
18	R	82	ALA	C-N	30.51	1.71	1.33

The worst 5 of 488 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1171	ILE	CA-C-N	-61.26	4.53	121.54
1	A	1171	ILE	C-N-CA	-61.26	4.53	121.54
2	B	59	THR	O-C-N	-50.09	59.73	122.34
2	B	49	PHE	O-C-N	-38.45	78.05	123.04
2	B	137	LEU	N-CA-C	31.92	152.81	113.23

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1171	ILE	Mainchain,Peptide
1	A	121	GLY	Mainchain
1	A	1649	ALA	Mainchain
2	B	25	GLN	Peptide
2	B	49	PHE	Mainchain

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	33975	0	32349	2921	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	34713	0	33234	2580	0
3	C	30427	0	29349	1432	0
4	D	4680	0	4509	1343	0
5	E	4440	0	4304	1029	0
6	F	996	0	1019	266	0
7	G	1024	0	883	191	0
8	H	750	0	734	231	0
9	I	827	0	826	300	0
10	J	807	0	772	269	0
11	K	754	0	715	133	0
12	L	855	0	854	212	0
13	M	735	0	735	237	0
14	N	852	0	796	196	0
15	O	994	0	1017	308	0
16	P	541	0	217	58	0
17	Q	1001	0	490	289	0
18	R	739	156	339	38	0
19	A	54	0	23	34	0
19	B	54	0	24	19	0
19	C	54	0	22	34	0
20	A	31	0	12	10	0
20	B	31	0	12	44	0
20	C	31	0	12	1	0
21	A	3	0	0	2	0
21	B	3	0	0	0	0
21	C	3	0	0	0	0
All	All	119374	156	113247	9584	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 41.

The worst 5 of 9584 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)
10:J:86:CYS:SG	11:K:61:VAL:HG22	1.24	1.74
2:B:1474:MET:SD	2:B:1515:VAL:HG11	1.32	1.66
1:A:935:VAL:HG22	1:A:944:LEU:CD2	1.23	1.65
1:A:3232:ILE:HG12	1:A:3316:TRP:CZ3	1.14	1.65
3:C:196:PRO:HA	3:C:239:TRP:CZ2	1.23	1.64

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	4391/4620 (95%)	4177 (95%)	189 (4%)	25 (1%)	21	59
2	B	4491/4595 (98%)	4255 (95%)	199 (4%)	37 (1%)	16	54
3	C	3923/4168 (94%)	3692 (94%)	208 (5%)	23 (1%)	21	59
4	D	569/657 (87%)	546 (96%)	16 (3%)	7 (1%)	10	44
5	E	551/670 (82%)	531 (96%)	18 (3%)	2 (0%)	30	67
6	F	126/133 (95%)	120 (95%)	6 (5%)	0	100	100
7	G	147/159 (92%)	134 (91%)	7 (5%)	6 (4%)	2	18
8	H	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
9	I	104/110 (94%)	100 (96%)	3 (3%)	1 (1%)	12	49
10	J	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
11	K	88/93 (95%)	85 (97%)	3 (3%)	0	100	100
12	L	109/111 (98%)	104 (95%)	4 (4%)	1 (1%)	14	51
13	M	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
14	N	112/117 (96%)	105 (94%)	7 (6%)	0	100	100
15	O	118/132 (89%)	112 (95%)	4 (3%)	2 (2%)	7	36
16	P	103/122 (84%)	90 (87%)	7 (7%)	6 (6%)	1	14
17	Q	189/202 (94%)	173 (92%)	13 (7%)	3 (2%)	7	38
18	R	148/160 (92%)	121 (82%)	19 (13%)	8 (5%)	1	15
All	All	15436/16323 (95%)	14606 (95%)	709 (5%)	121 (1%)	18	54

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	PRO
1	A	125	PRO
1	A	127	THR
1	A	151	ILE

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Mol	Chain	Res	Type
1	A	1171	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	3430/4197 (82%)	3331 (97%)	99 (3%)	37	58
2	B	3520/4145 (85%)	3432 (98%)	88 (2%)	42	63
3	C	3139/3691 (85%)	3081 (98%)	58 (2%)	51	68
4	D	511/600 (85%)	498 (98%)	13 (2%)	42	63
5	E	488/597 (82%)	469 (96%)	19 (4%)	28	49
6	F	105/109 (96%)	103 (98%)	2 (2%)	50	67
7	G	86/149 (58%)	86 (100%)	0	100	100
8	H	82/83 (99%)	81 (99%)	1 (1%)	63	75
9	I	91/95 (96%)	89 (98%)	2 (2%)	45	64
10	J	82/82 (100%)	81 (99%)	1 (1%)	63	75
11	K	80/82 (98%)	78 (98%)	2 (2%)	42	63
12	L	90/99 (91%)	87 (97%)	3 (3%)	33	55
13	M	78/78 (100%)	78 (100%)	0	100	100
14	N	84/104 (81%)	82 (98%)	2 (2%)	43	64
15	O	108/119 (91%)	107 (99%)	1 (1%)	70	79
17	Q	11/186 (6%)	11 (100%)	0	100	100
All	All	11985/14416 (83%)	11694 (98%)	291 (2%)	43	64

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3131	LEU
12	L	66	GLU
3	C	3868	CYS
5	E	139	GLU

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Mol	Chain	Res	Type
1	A	4562	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 280 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	493	GLN
5	E	44	ASN
9	I	39	GLN
2	B	1081	GLN
2	B	967	GLN

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](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	$\# Z > 2$
20	ATP	B	5403	21	32,33,33	0.54	0	48,52,52	0.62	0
19	ADP	A	4703	21	28,29,29	1.36	4 (14%)	43,45,45	1.83	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	ATP	C	4302	21	32,33,33	0.49	0	48,52,52	0.64	0
19	ADP	A	4701	21	28,29,29	1.41	5 (17%)	43,45,45	1.88	10 (23%)
19	ADP	B	5405	21	28,29,29	0.46	0	43,45,45	0.60	0
20	ATP	A	4702	21	32,33,33	1.31	4 (12%)	48,52,52	1.74	10 (20%)
19	ADP	B	5406	21	28,29,29	0.47	0	43,45,45	0.47	0
19	ADP	C	4305	21	28,29,29	0.52	0	43,45,45	0.82	1 (2%)
19	ADP	C	4306	21	28,29,29	0.47	0	43,45,45	0.60	0

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
20	ATP	B	5403	21	-	2/22/38/38	0/3/3/3
19	ADP	A	4703	21	-	6/16/32/32	0/3/3/3
20	ATP	C	4302	21	-	3/22/38/38	0/3/3/3
19	ADP	A	4701	21	-	8/16/32/32	0/3/3/3
19	ADP	B	5405	21	-	3/16/32/32	0/3/3/3
20	ATP	A	4702	21	-	3/22/38/38	0/3/3/3
19	ADP	B	5406	21	-	1/16/32/32	0/3/3/3
19	ADP	C	4305	21	-	7/16/32/32	0/3/3/3
19	ADP	C	4306	21	-	4/16/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	4703	ADP	C5-C4	4.48	1.47	1.39
19	A	4701	ADP	C5-C4	4.43	1.47	1.39
20	A	4702	ATP	C5-C4	4.17	1.46	1.39
19	A	4703	ADP	C5-C6	2.77	1.48	1.41
20	A	4702	ATP	C5-N7	-2.62	1.34	1.39

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	4701	ADP	C5-C4-N3	-6.21	118.17	126.72
20	A	4702	ATP	C5-C4-N3	-5.79	118.74	126.72
19	A	4703	ADP	C5-C4-N3	-5.77	118.78	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	4702	ATP	N3-C4-N9	4.59	134.97	127.17
19	A	4703	ADP	N3-C4-N9	4.58	134.96	127.17

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

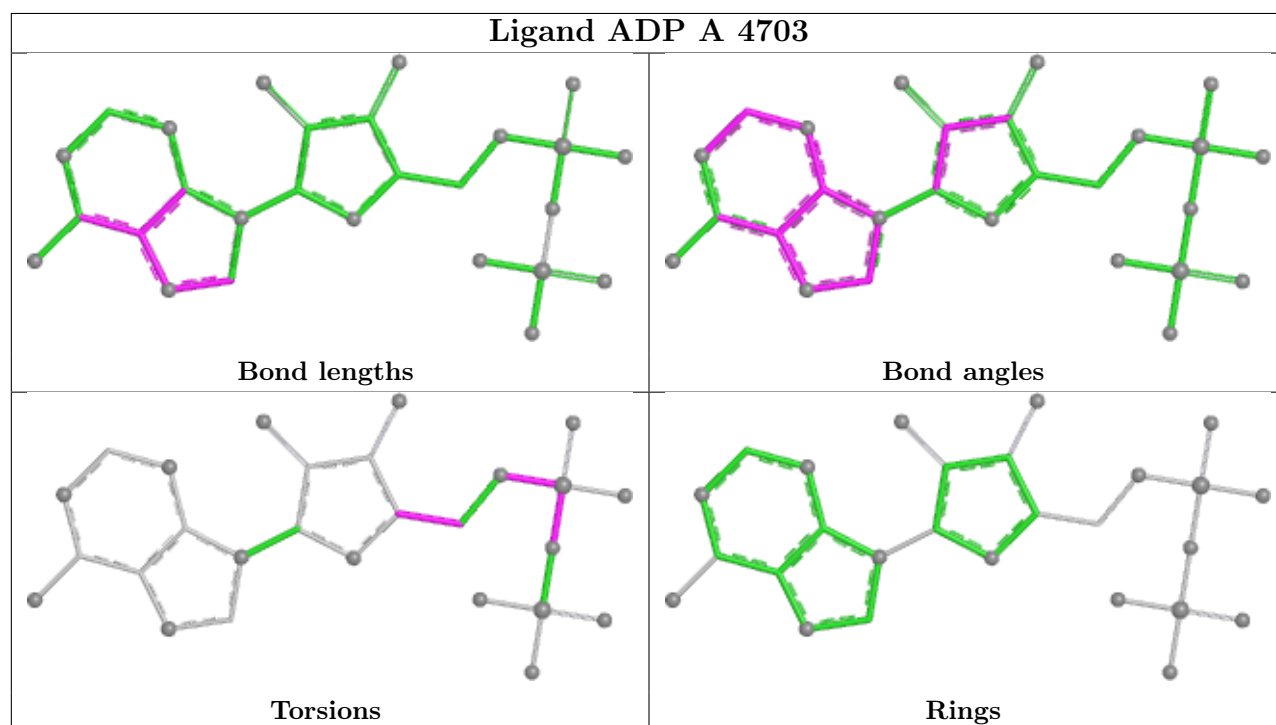
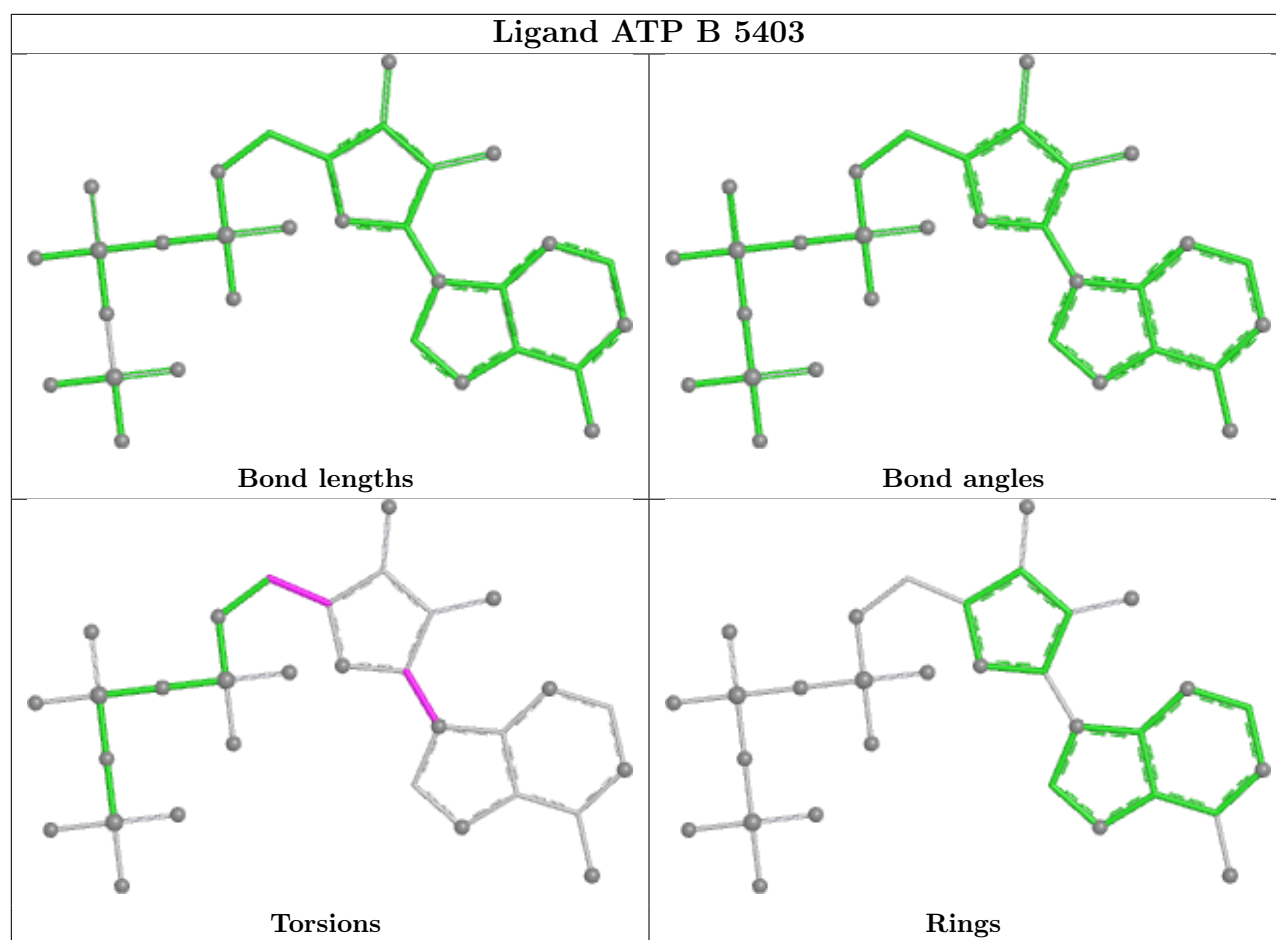
Mol	Chain	Res	Type	Atoms
19	A	4701	ADP	PB-O3A-PA-O5'
19	A	4701	ADP	C5'-O5'-PA-O1A
19	A	4701	ADP	C5'-O5'-PA-O2A
19	A	4701	ADP	C5'-O5'-PA-O3A
19	A	4703	ADP	PB-O3A-PA-O5'

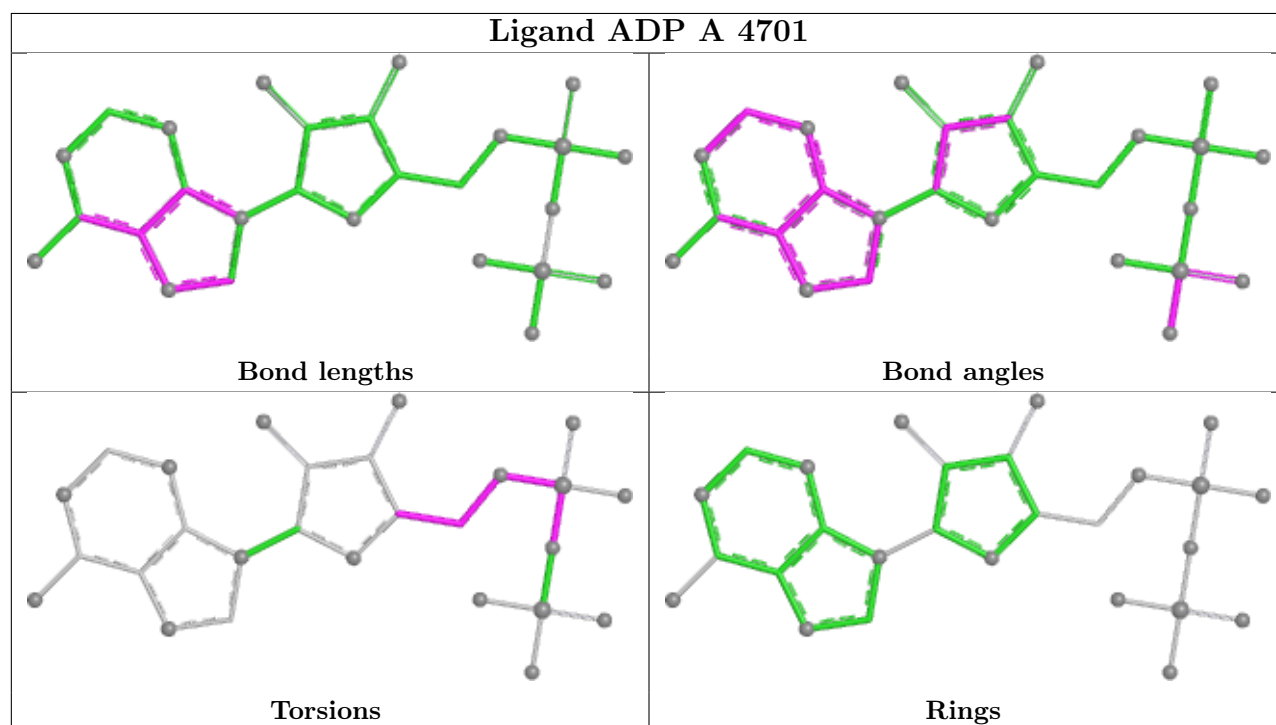
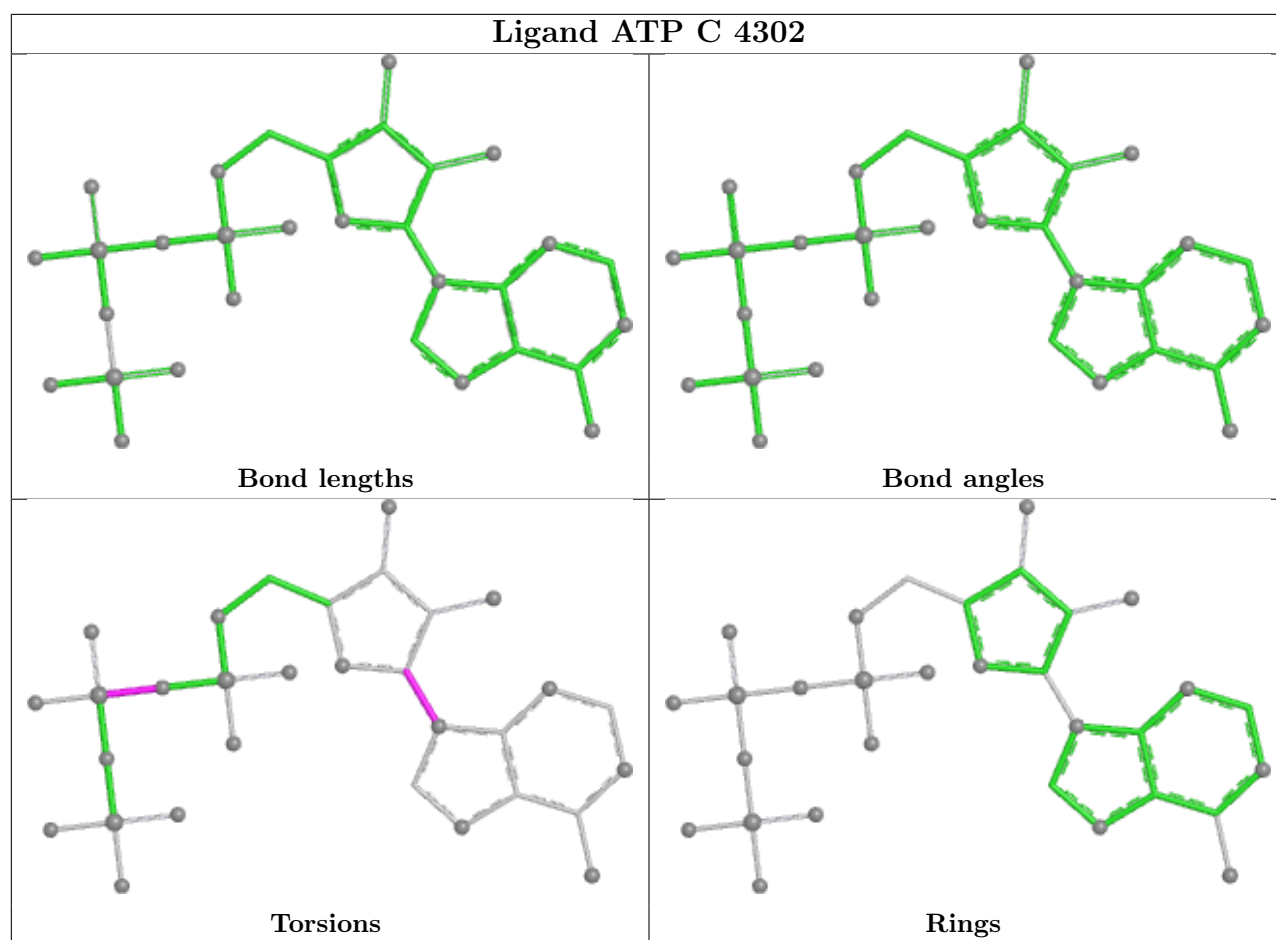
There are no ring outliers.

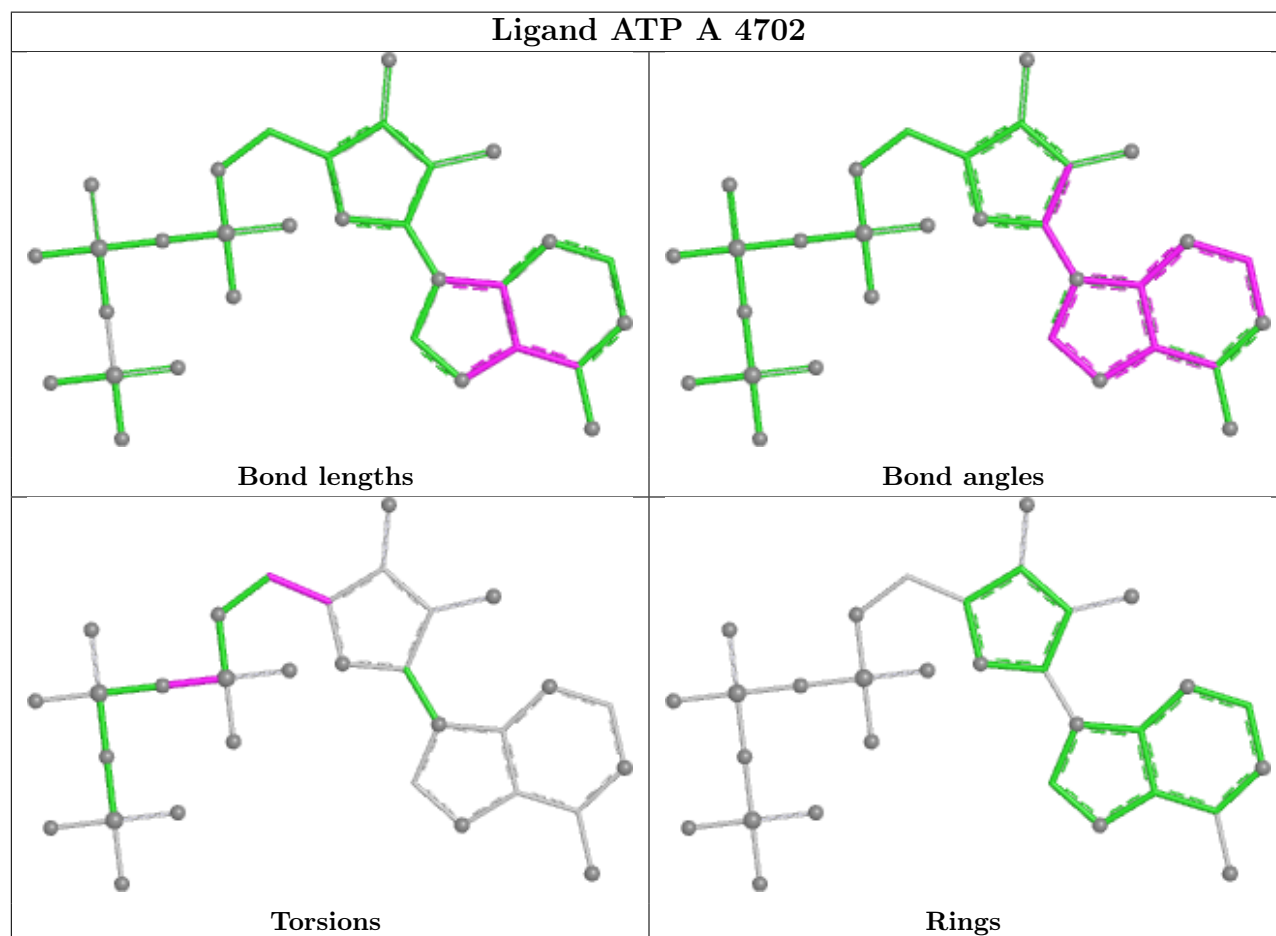
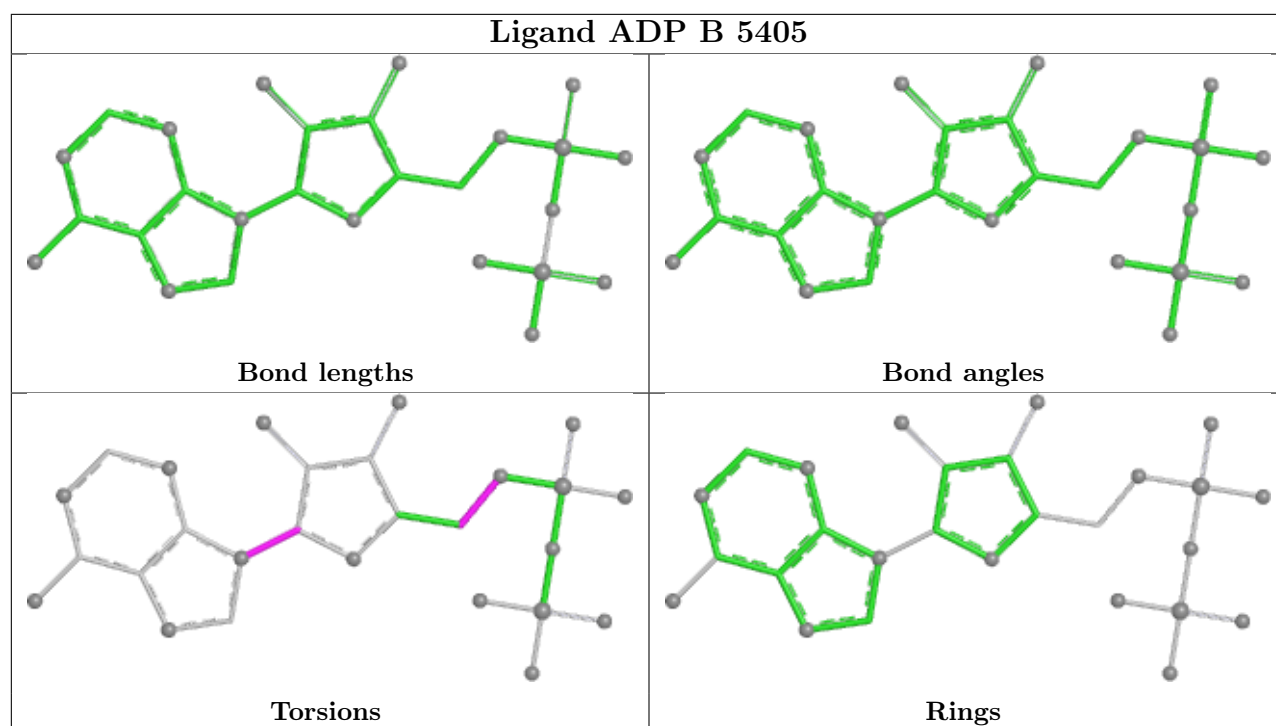
9 monomers are involved in 142 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	5403	ATP	44	0
19	A	4703	ADP	21	0
20	C	4302	ATP	1	0
19	A	4701	ADP	13	0
19	B	5405	ADP	16	0
20	A	4702	ATP	10	0
19	B	5406	ADP	3	0
19	C	4305	ADP	25	0
19	C	4306	ADP	9	0

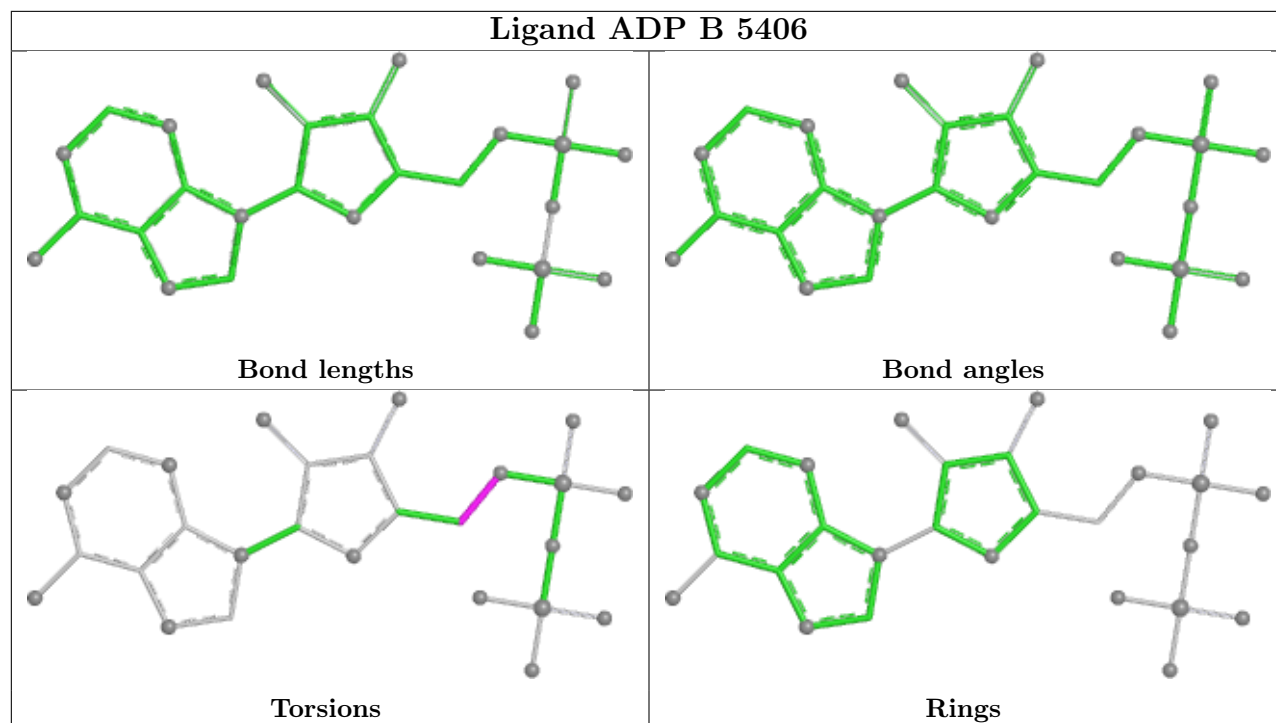
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



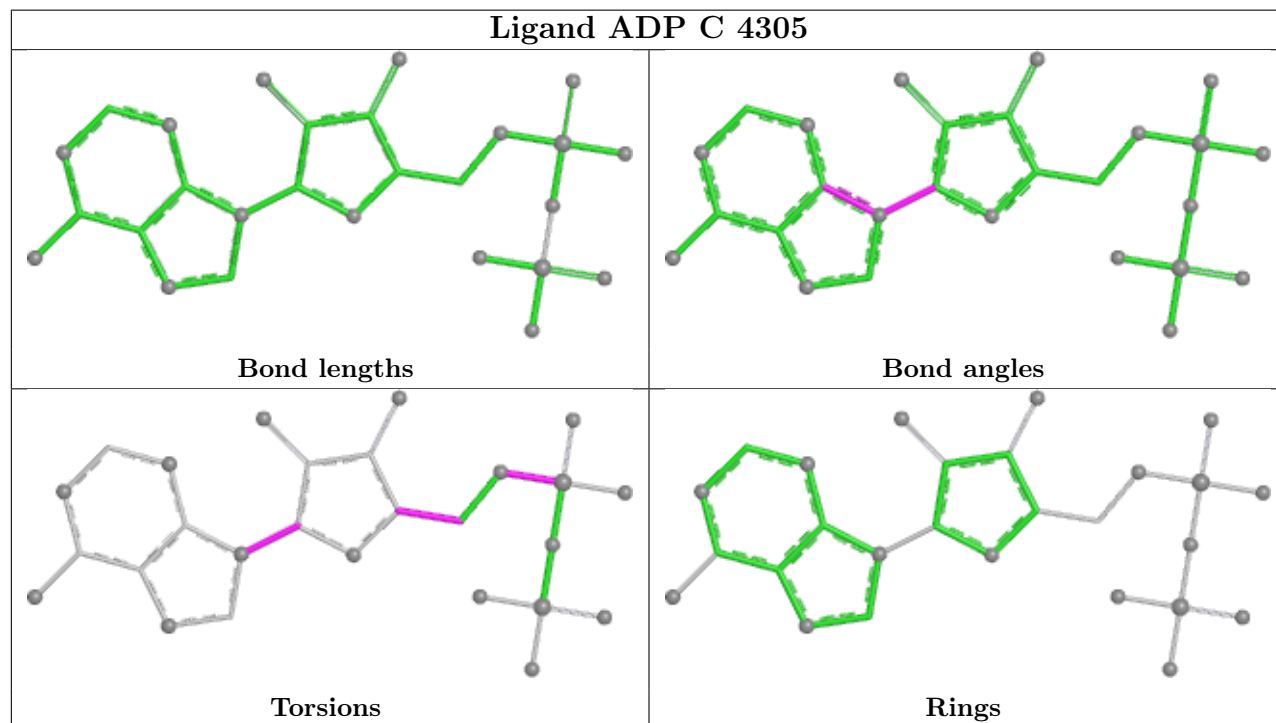


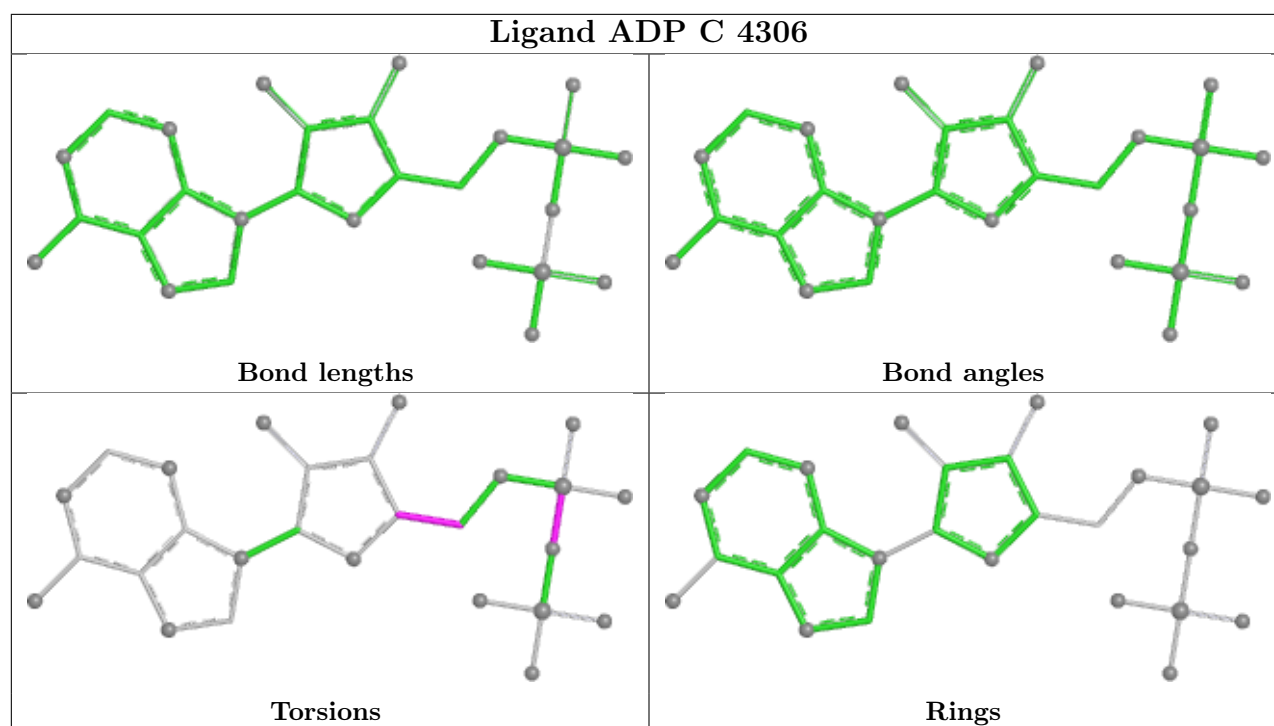


Ligand ADP B 5406



Ligand ADP C 4305





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
2	B	10
1	A	9
16	P	4
4	D	2
7	G	1
18	R	1

The worst 5 of 27 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3250:PRO	C	3251:ILE	N	5.80
1	A	3251:ILE	C	3252:GLN	N	4.89
1	A	24:LYS	C	25:ASP	N	3.36
1	B	79:PRO	C	80:PRO	N	3.22
1	D	216:HIS	C	217:GLN	N	2.93

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16312. These allow visual inspection of the internal detail of the map and identification of artifacts.

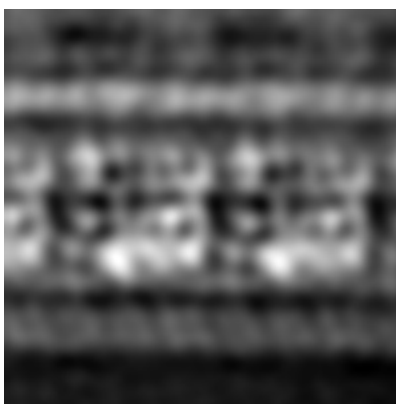
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

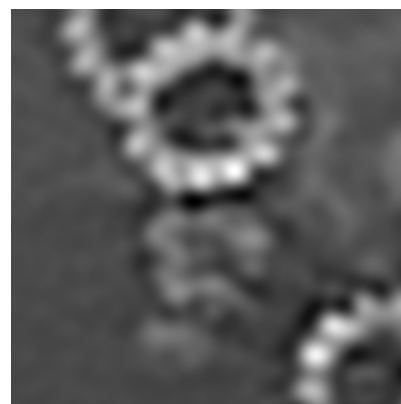
6.1.1 Primary map



X

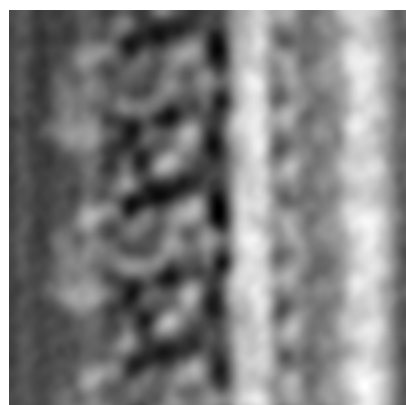


Y

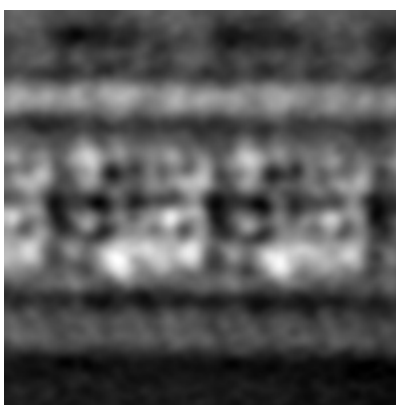


Z

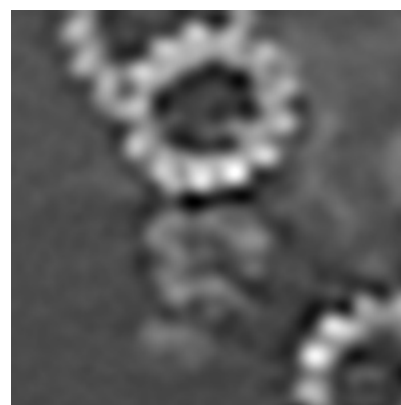
6.1.2 Raw map



X



Y



Z

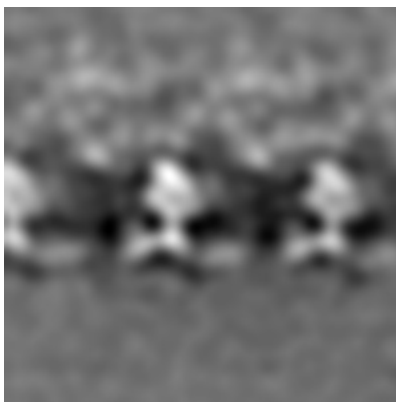
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 37

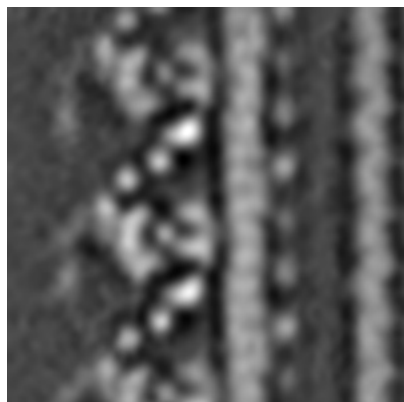


Y Index: 37

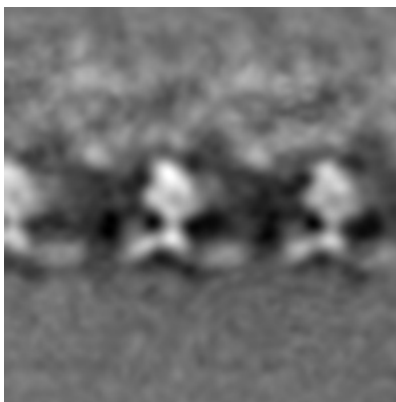


Z Index: 37

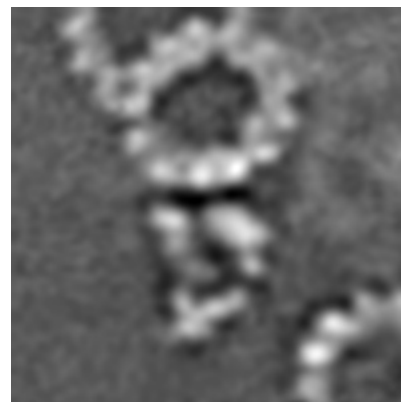
6.2.2 Raw map



X Index: 37



Y Index: 37



Z Index: 37

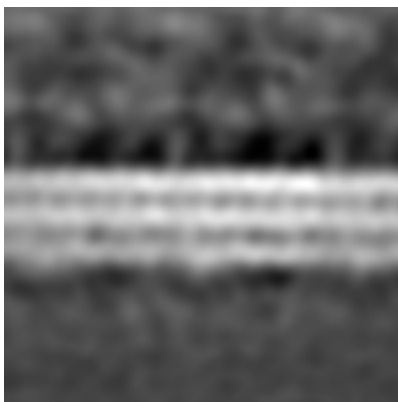
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 41



Y Index: 43

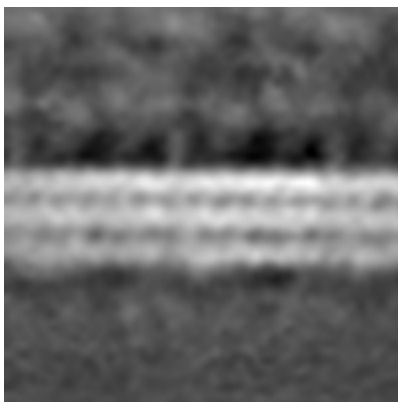


Z Index: 21

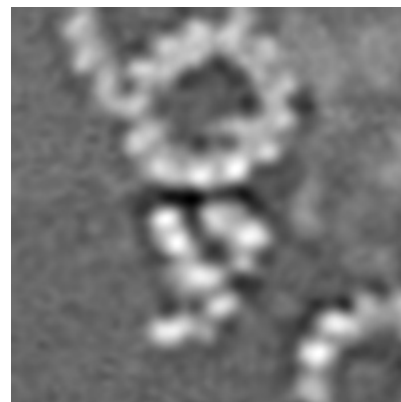
6.3.2 Raw map



X Index: 41



Y Index: 43

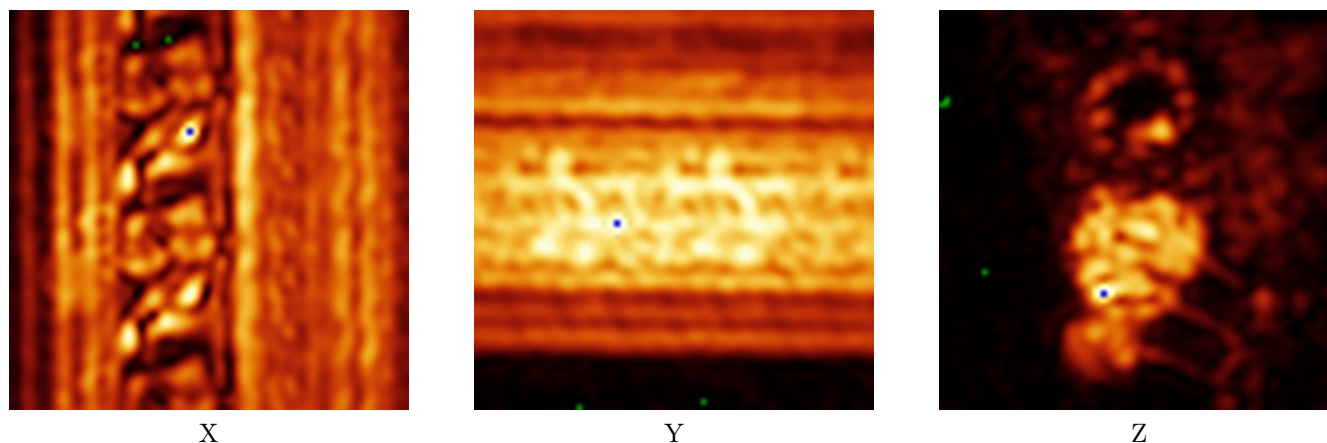


Z Index: 35

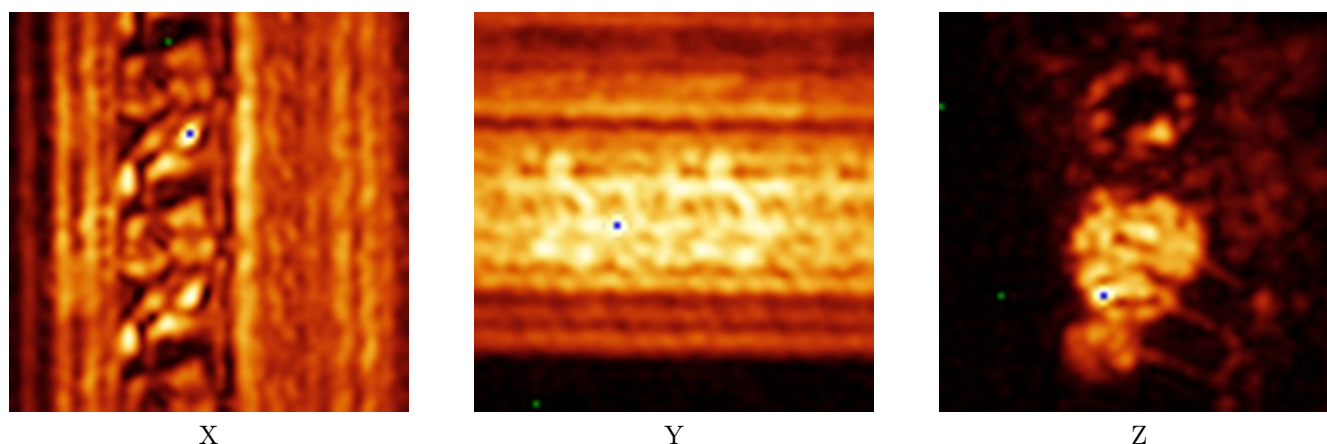
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

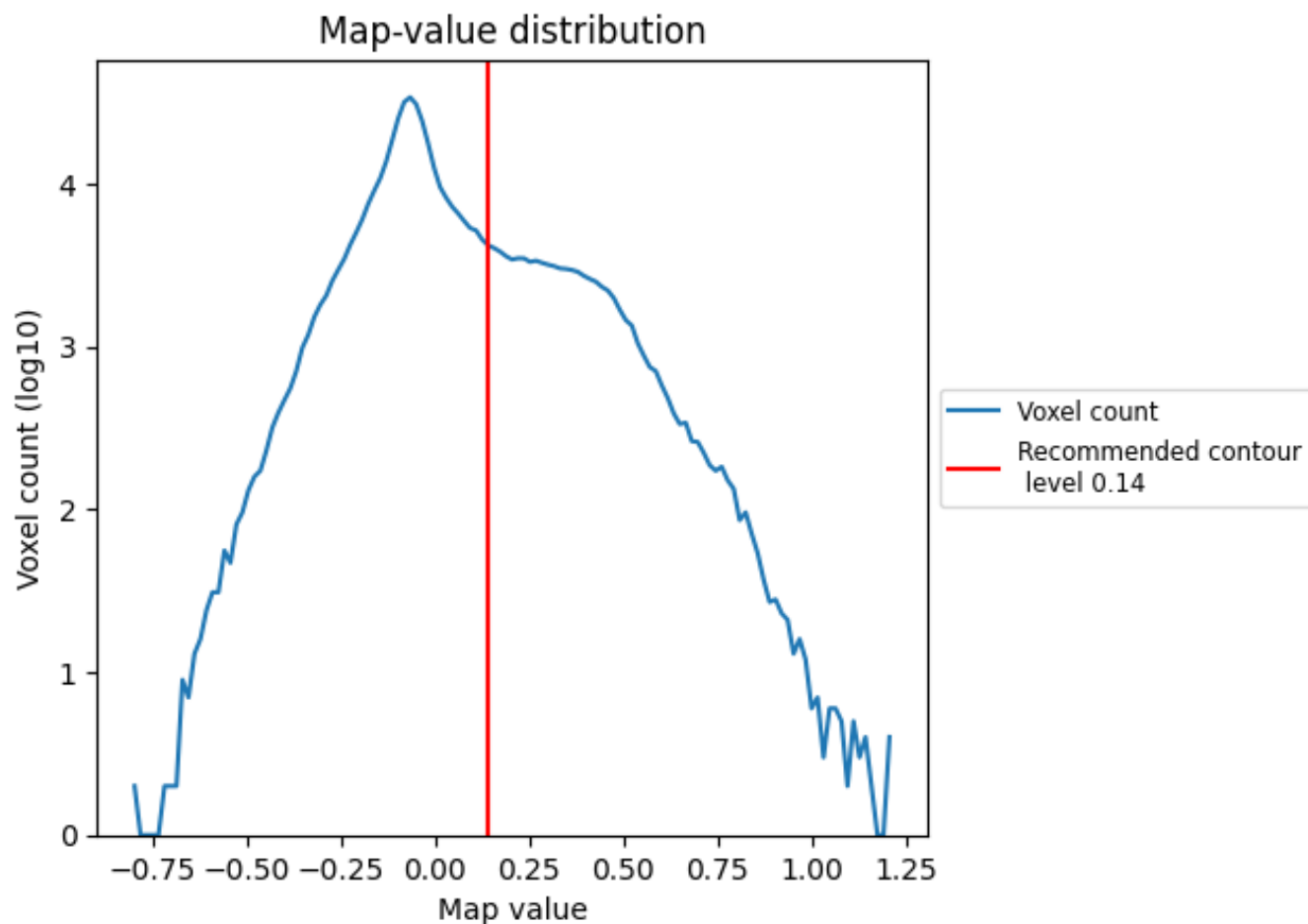
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

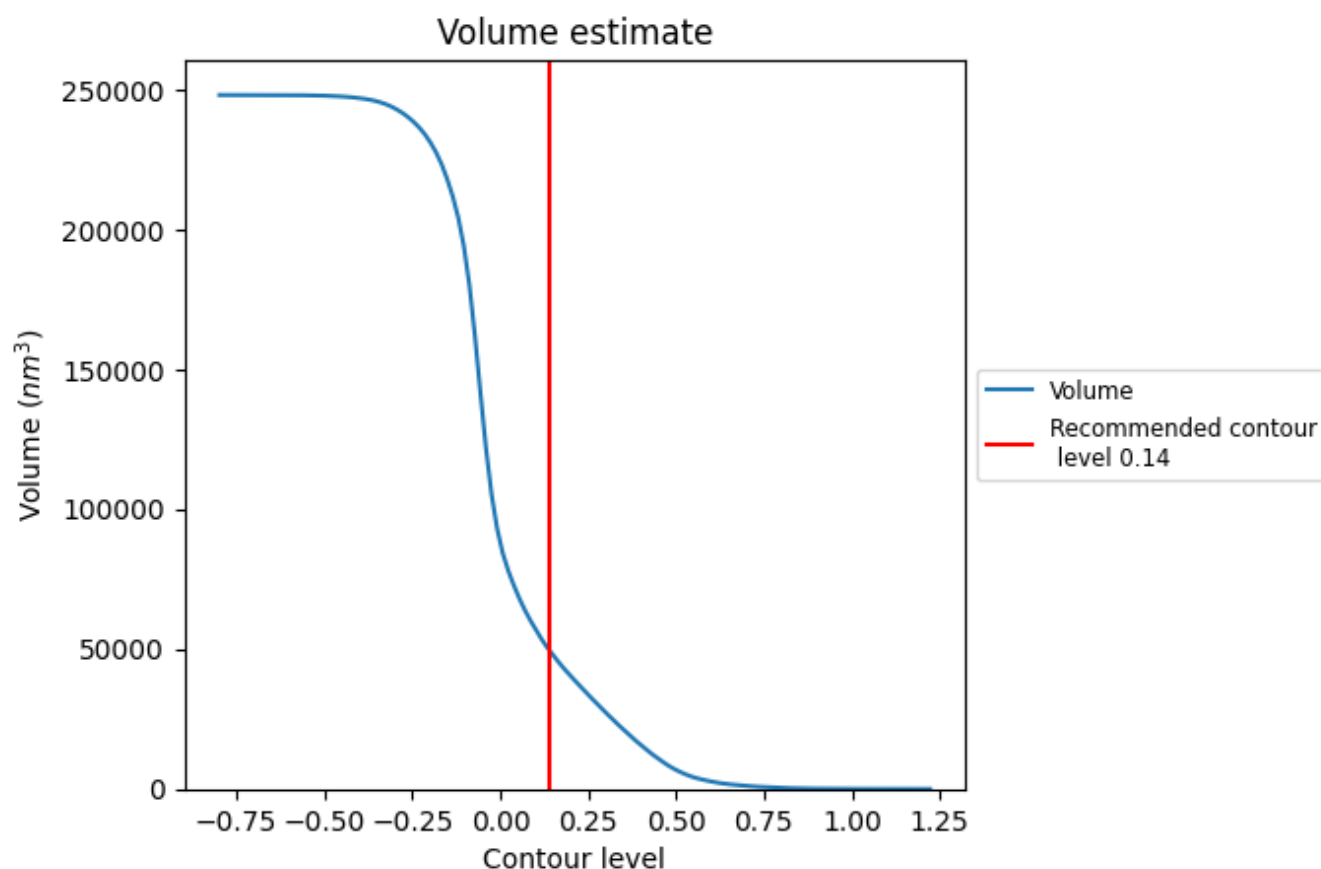
This section contains the results of statistical analysis of the map.

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.

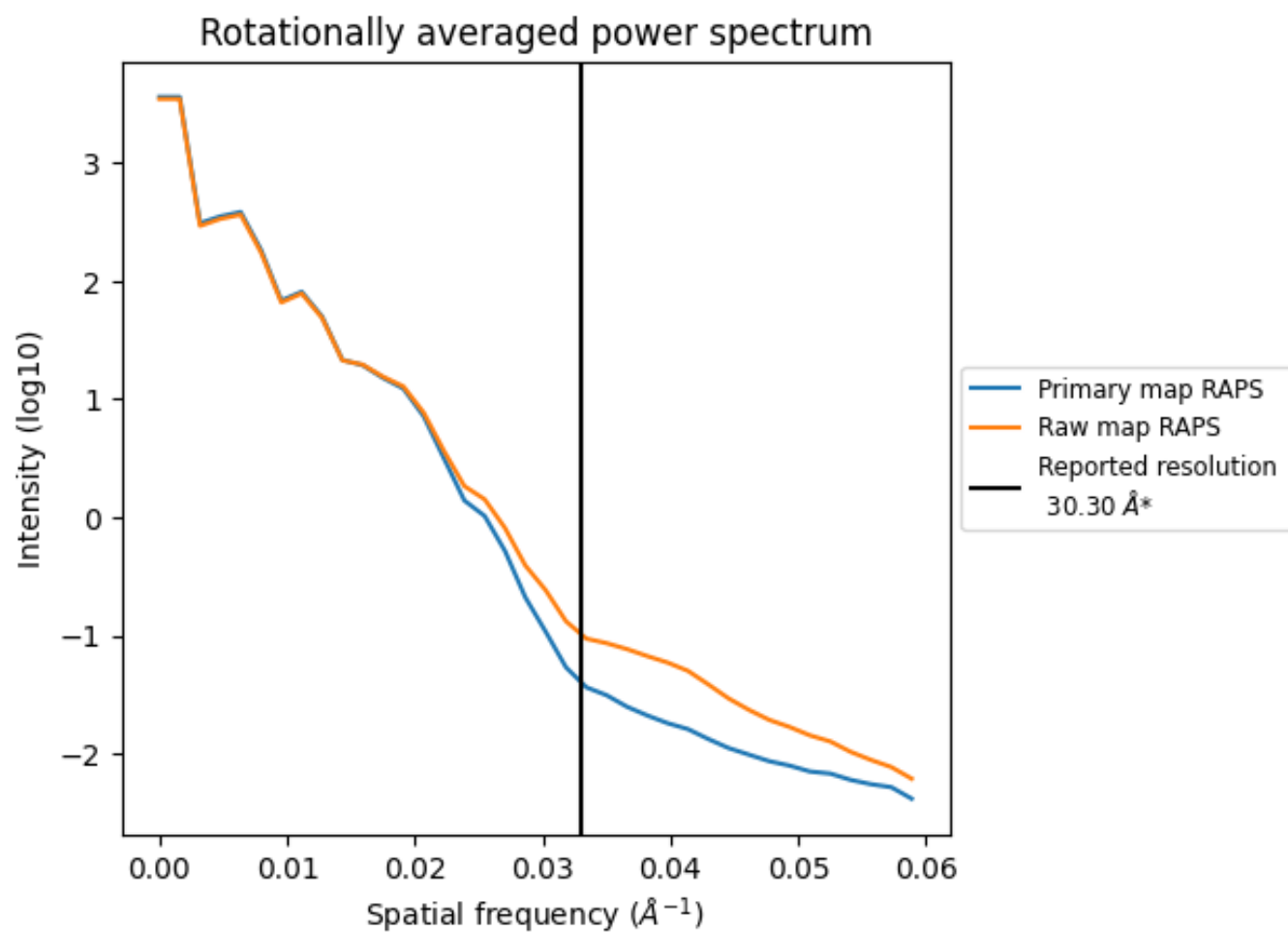
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49562 nm³; this corresponds to an approximate mass of 44771 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 ⓘ

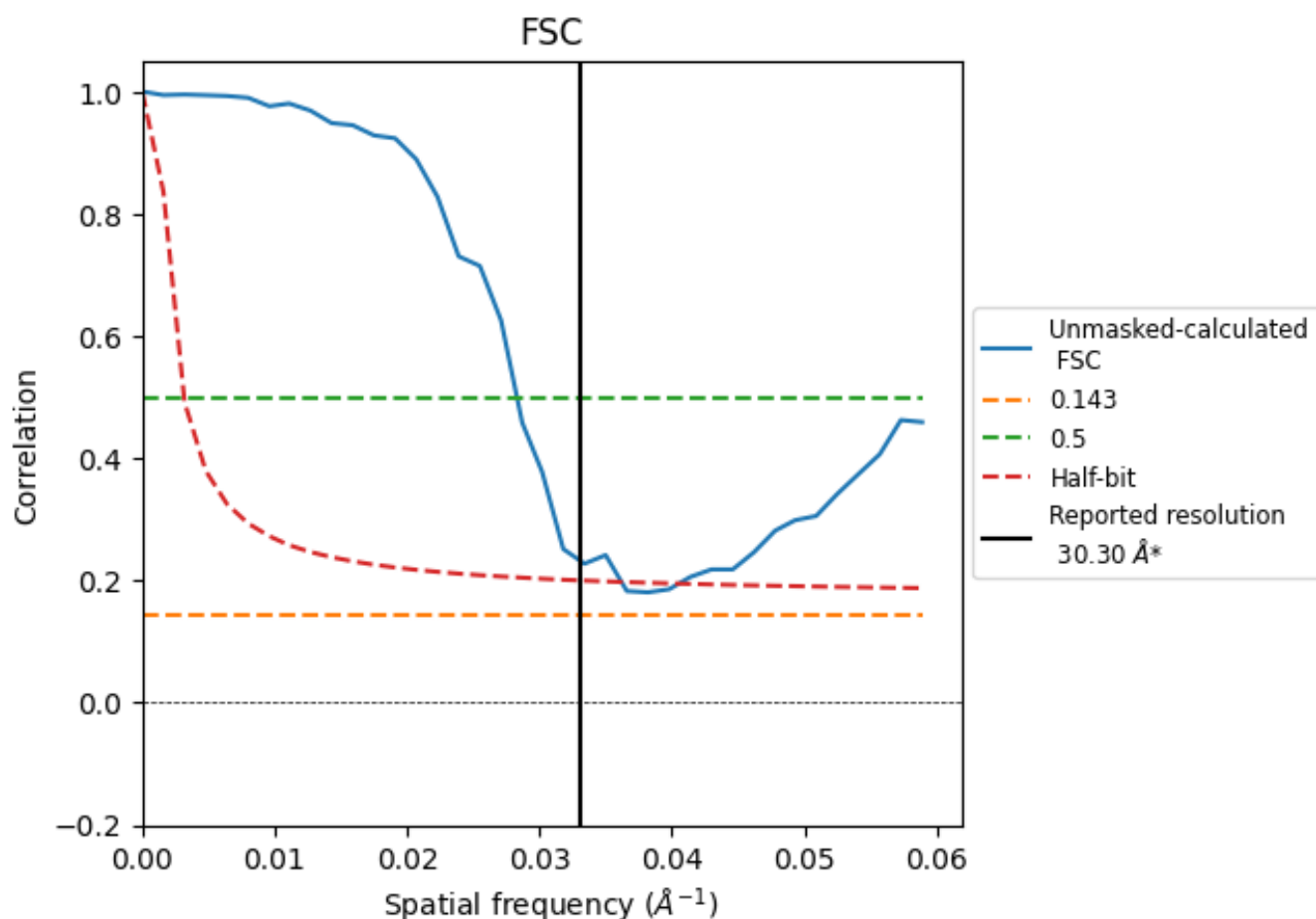


*Reported resolution corresponds to spatial frequency of $0.033 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.033 Å⁻¹

8.2 Resolution estimates [i](#)

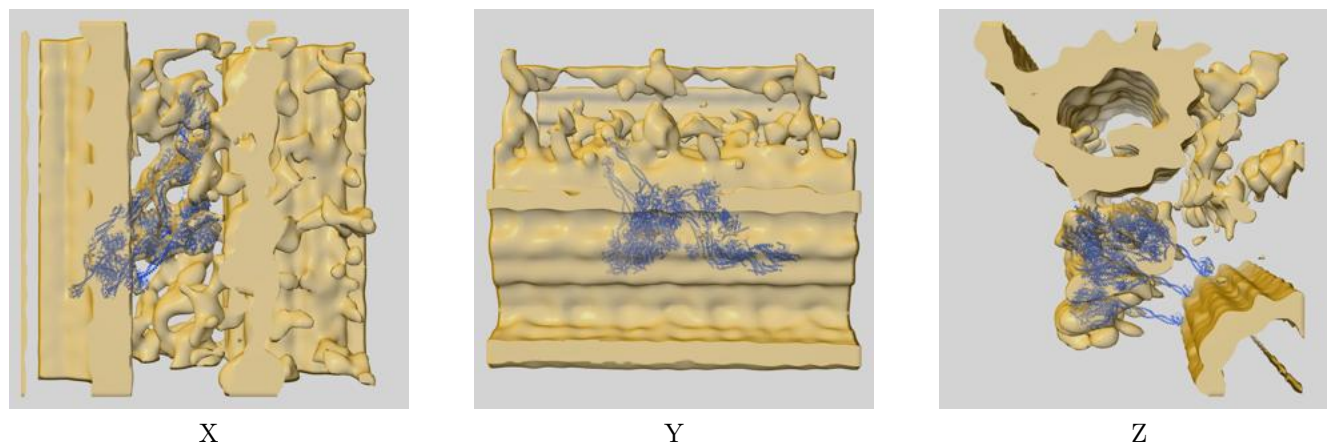
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	30.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	35.34	27.62

*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-16312 and PDB model 8BX8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



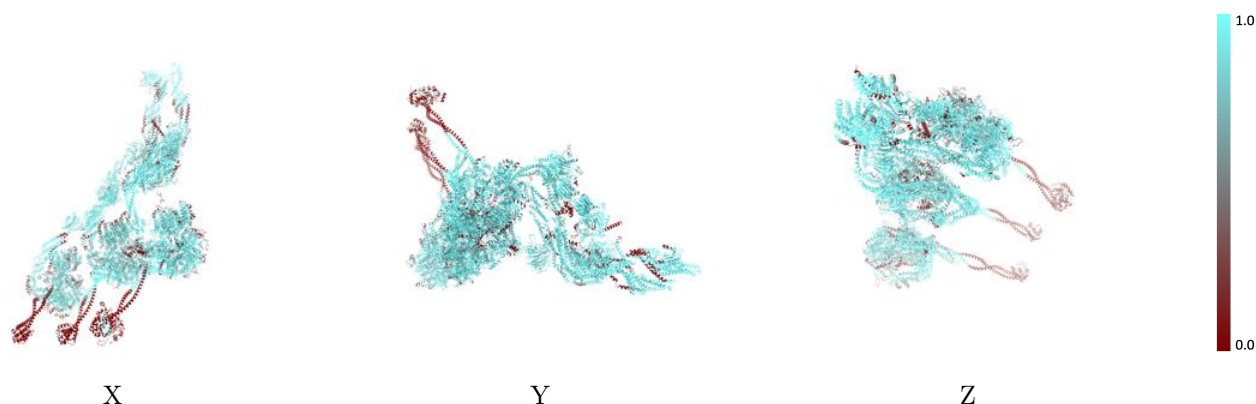
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



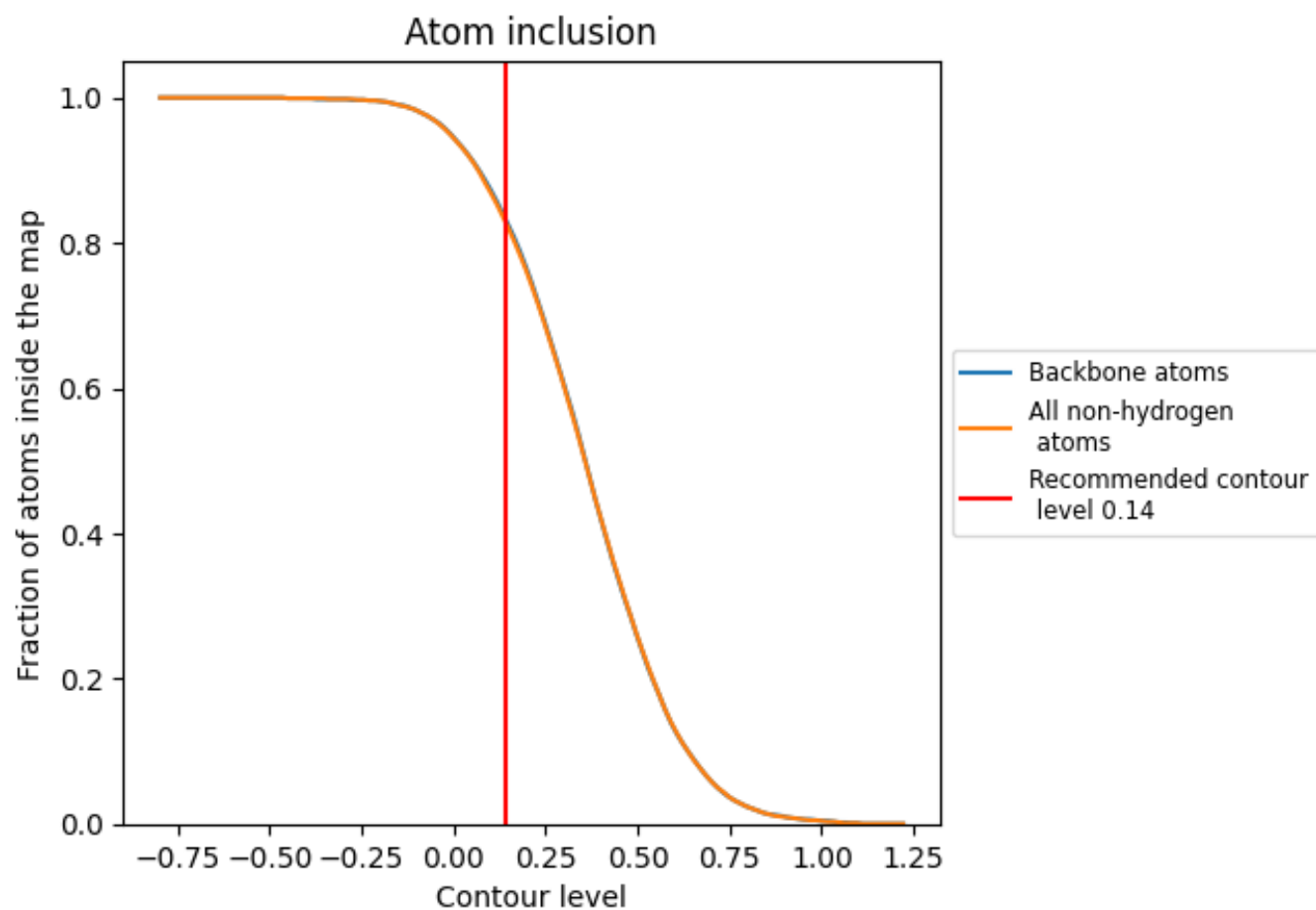
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8300	 0.0420
A	 0.8230	 0.0460
B	 0.8570	 0.0450
C	 0.7930	 0.0350
D	 0.9090	 0.0370
E	 0.9000	 0.0390
F	 0.8060	 0.0430
G	 0.7350	 0.0120
H	 0.9840	 0.0390
I	 0.8590	 0.0400
J	 0.9870	 0.0630
K	 0.9720	 0.0530
L	 0.8830	 0.0290
M	 0.9310	 0.0400
N	 0.8960	 0.0440
O	 0.9600	 0.0410
P	 0.9850	 0.0630
Q	 0.2450	 0.0610
R	 0.3110	 -0.0180

