



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 10:49 PM UTC

PDB ID : 7KEK / pdb_00007kek
EMDB ID : EMD-22840
Title : Structure of the free outer-arm dynein in pre-parallel state
Authors : Rao, Q.; Zhang, K.
Deposited on : 2020-10-11
Resolution : 8.00 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:

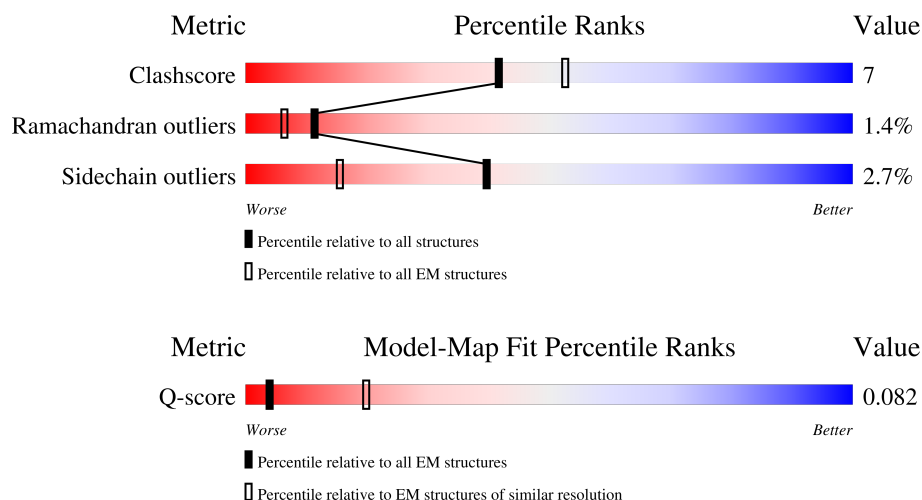
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 8.00 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.



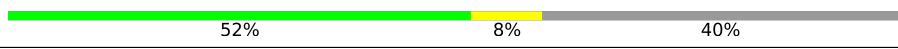
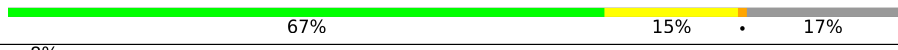
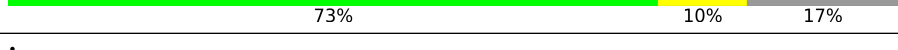
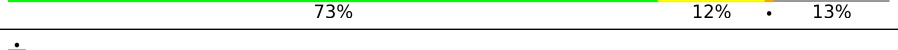
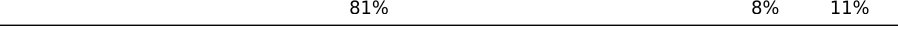
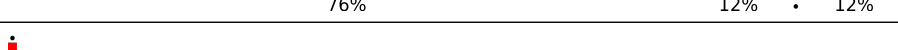
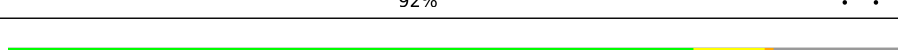
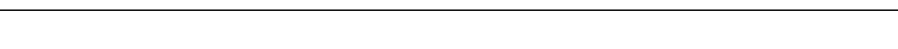
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

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	12% 85% 10% ..
2	C	4168	8% 83% 11% 5%
3	Q	202	95% 90% 5% 5%
4	B	4595	13% 84% 13% ..

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Mol	Chain	Length	Quality of chain
5	I	110	
6	H	92	
7	G	159	
8	F	133	
9	N	117	
10	O	132	
11	E	670	
12	D	667	
13	P	122	
14	L	111	
15	K	93	
16	J	111	
17	M	87	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 117936 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 alpha heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4443	Total	C	N	O	S	0	0
			33894	21519	5788	6429	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 Dynein gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	3943	Total	C	N	O	S	0	0
			30436	19390	5162	5735	149		

- Molecule 3 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Q	192	Total	C	N	O	2	0
			1002	607	202	193		

- Molecule 4 is a protein called Dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	4516	Total	C	N	O	S	0	0
			34604	21978	5928	6547	151		

- Molecule 5 is a protein called Dynein light chain LC8_1a (LC10).

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

- Molecule 6 is a protein called Dynein light chain LC8_1b (DLC82).

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

- Molecule 7 is a protein called Dynein light chain roadblock LC7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	96	Total	C	N	O	S	0	0
			749	471	129	148	1		

- Molecule 8 is a protein called Dynein light chain roadblock LC7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	110	Total	C	N	O	S	0	0
			863	544	152	165	2		

- Molecule 9 is a protein called Dynein light chain Tctex_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	114	Total	C	N	O	S	0	0
			855	543	143	166	3		

- Molecule 10 is a protein called Dynein light chain Tctex_a (LC2A).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	120	Total	C	N	O	S	0	0
			986	634	172	177	3		

- Molecule 11 is a protein called Dynein intermediate chain DIC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	555	Total	C	N	O	S	0	0
			4423	2786	759	856	22		

- Molecule 12 is a protein called Dynein intermediate chain DIC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	579	Total	C	N	O	S	0	0
			4664	2964	787	883	30		

- Molecule 13 is a protein called Thioredoxin LC3BL.

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

- Molecule 14 is a protein called Dynein light chain LC8_3b.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	98	Total	C	N	O	S	0
			783	511	132	137	3	0

- Molecule 15 is a protein called Dynein light chain LC8_2a (LC8E).

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

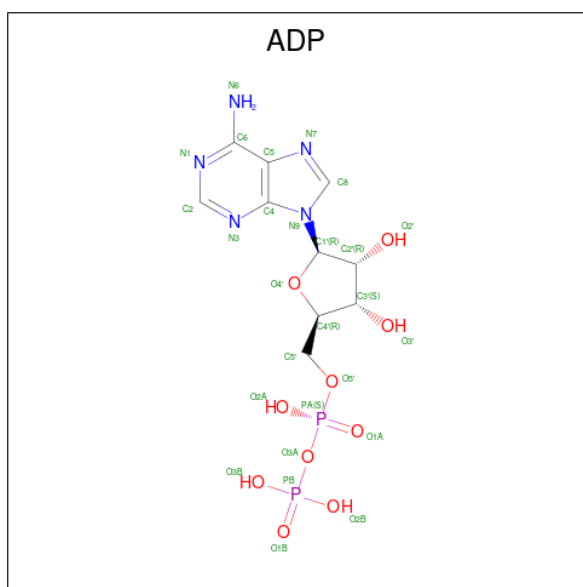
- Molecule 16 is a protein called Dynein light chain LC8_2b.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	J	95	Total	C	N	O	S	0
			806	527	135	140	4	0

- Molecule 17 is a protein called Dynein light chain LC8_3a.

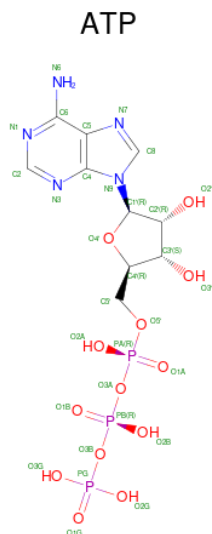
Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	87	Total	C	N	O	S	0
			735	477	123	130	5	0

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

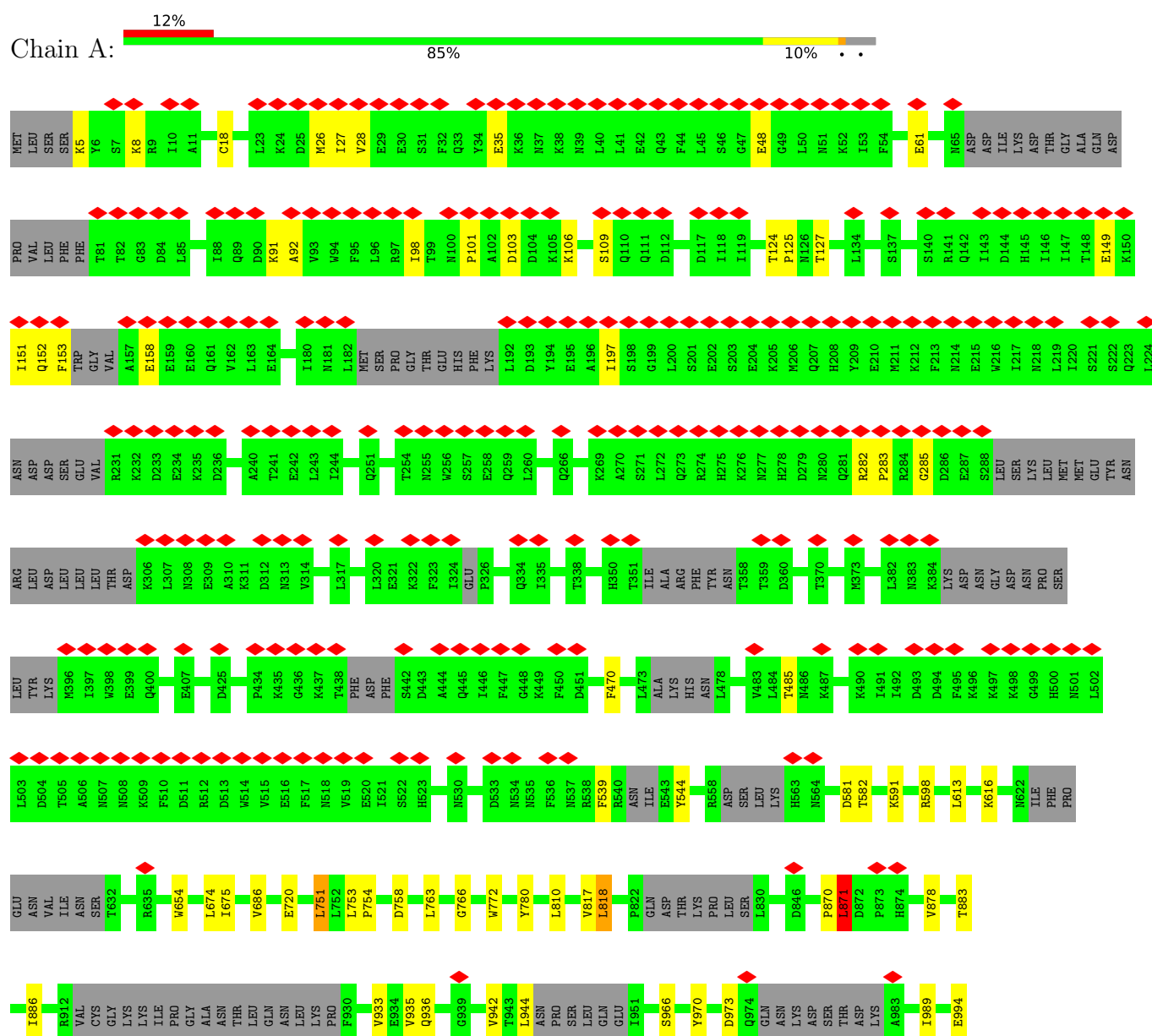
- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

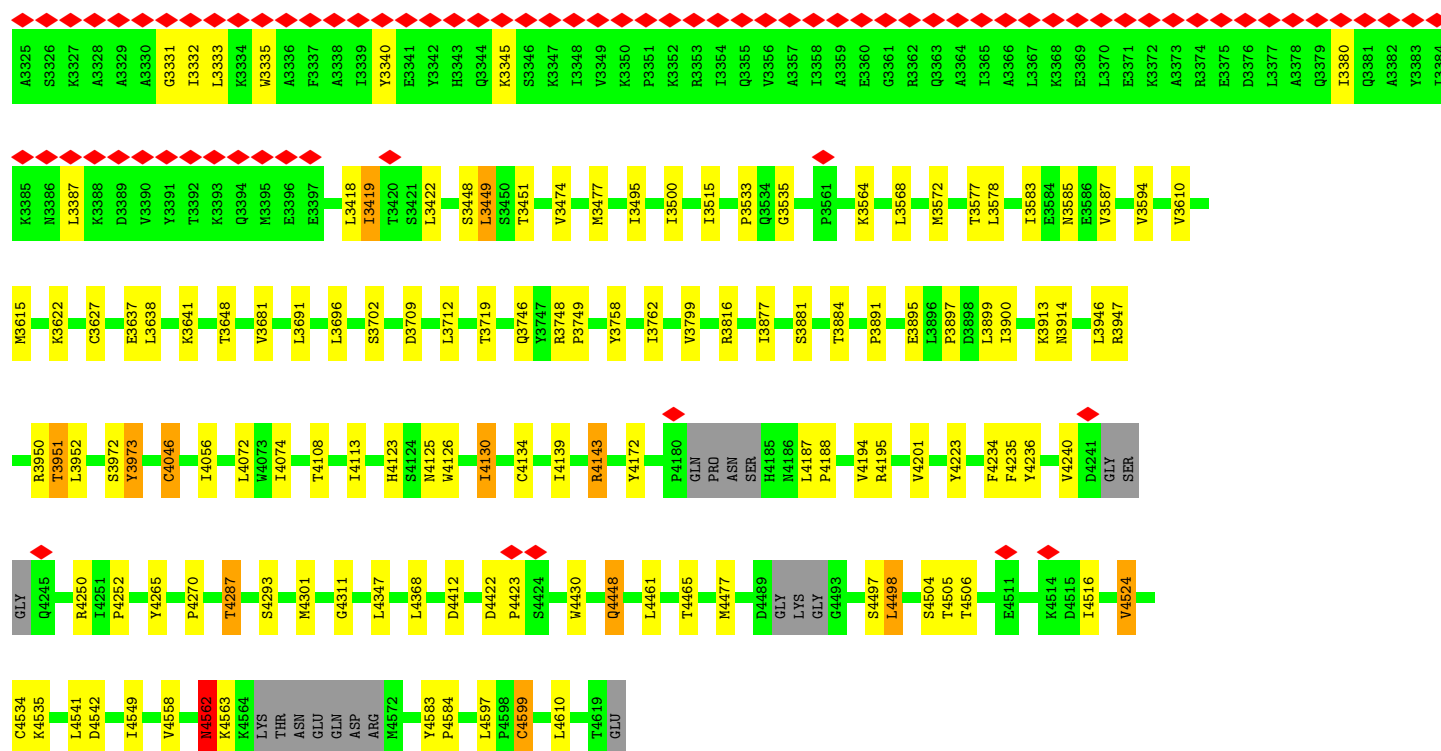
3 Residue-property plots [i](#)

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.

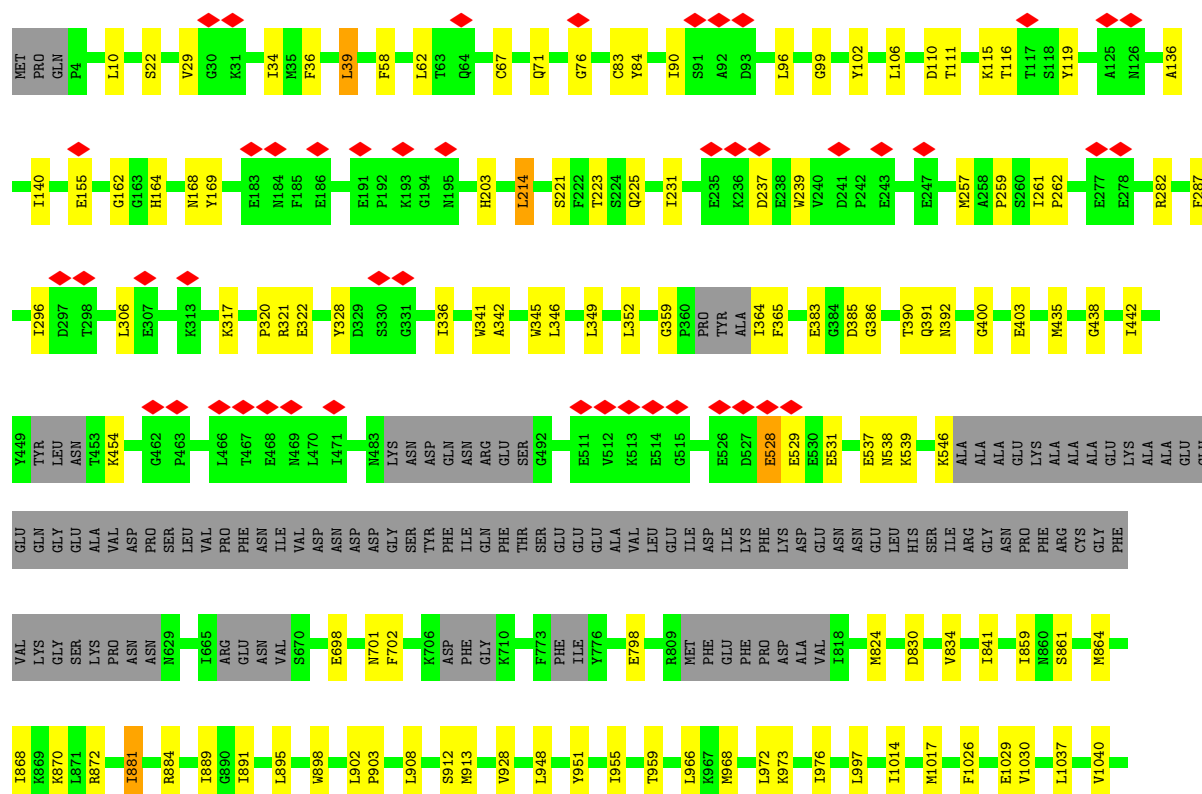
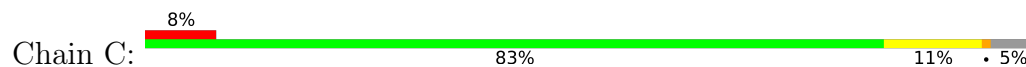
• Molecule 1: Dynein alpha heavy chain



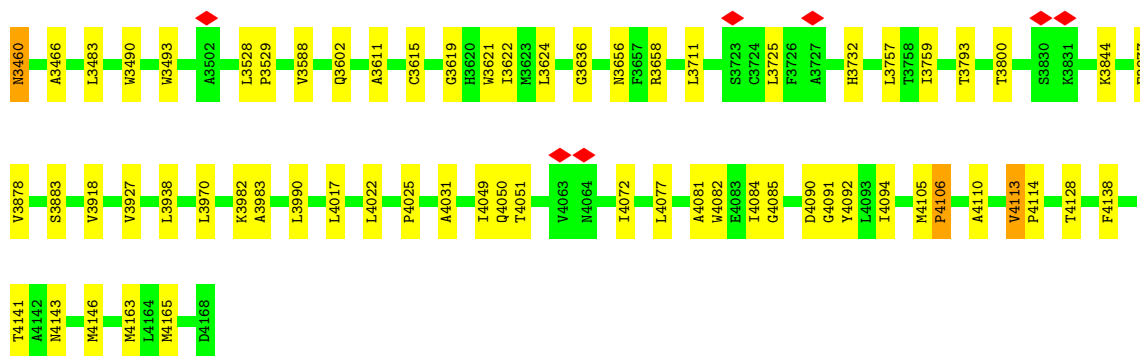
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V3266	R3206	N3146	L2866	E2400	K2011	I1787	F1631	H1486	Q1276	D1150	Y998
L3287	R3207	E3147	V2866	L2411	K2026	Q1788	D1632	V1487	K1279	M1151	T1009
F3268	A3208	A3148	T2877	L2418	F2027	V1789	I1634	Y1280	F1281	S1161	V1013
L3269	Q3209	R2624	T2923	Q2419	L2030	Q1791	V1637	F1490	E1282	L1162	L1013
Q3270	F3210	Y2656	L2923	P2420	L2033	K1792	F1639	T1500	L1283	D1163	F1016
A3211	K3151	Y2656	L2935	Q2421	R2042	D1793	F1639	V1504	T1286	D1164	L1017
S3272	T3152	D2659	L2935	G2422	R2042	I1794	S1641	V1504	E1289	M1165	F1020
Y3273	T2938	W2676	L2938	G2423	I2051	F1806	A1642	L1508	I1290	T1021	T1021
Q3274	T2963	T2686	T2963	E2424	L2097	D1819	K1643	E1522	S1319	K1022	F1023
E3275	L2963	R2697	L2972	N2425	L2098	I1825	D1644	V1523	LYS	C1027	C1027
S3276	F2968	F2698	L2973	E2426	L2098	Y1836	K1645	F1524	ASP	S1030	S1030
G3277	L2974	L2699	Q2974	T2427	I2101	E1837	K1646	T1526	ASP	I1031	I1031
T3278	Q2974	L2699	V2428	V2428	I2101	F1838	N1647	L1536	L1323	L1190	L1190
Q3279	N2975	K2704	Y2432	Y2432	V2116	I1847	P1648	L1536	L1323	Y1201	L1052
T3280	T2976	T2708	V2433	S2434	E2117	T1847	A1649	K1539	W1347	Q1205	I1065
L3281	D2977	K2711	T2437	T2437	I2124	T1857	Q1652	Q1540	I1368	V1066	V1066
G3282	F2987	I2723	C2443	C2443	I2131	M1862	I1653	F1541	LEU	Y1069	Y1069
D3283	V2981	L2727	Q2455	Q2455	I2141	G1868	Q1655	I1544	LYS	Y1208	Y1208
M3284	L2999	L2727	Q2455	Q2455	I2141	G1868	I1656	W1548	LYS	L1209	L1209
N3285	L3018	L2727	Q2455	Q2455	I2141	G1868	I1656	M1549	PRO	K1210	K1210
M3287	C3022	L2745	E2470	E2470	I2171	L1889	I1667	M1552	ILE	E1075	E1075
K3288	W3026	V2754	M2471	M2471	E2172	T1670	T1670	M1552	MET	L1076	L1076
Q3289	T3041	V2754	L2490	L2490	E2172	T1670	T1670	M1552	MET	I1081	I1081
L3290	H3062	E2772	D2511	D2511	V2173	F1892	V1674	K1589	F1219	C1082	C1082
K3291	Y3099	C2786	P2512	P2512	W1920	N1897	K1875	K1560	T1220	S1086	S1086
E3292	L3102	L2789	Q2513	Q2513	G1921	Y1915	C1676	I1562	V1223	T1087	T1087
F3293	G3120	V2793	M2515	M2515	C1922	G1918	W1683	C1563	R1227	Q1096	Q1096
Q3294	N3122	I2799	G2544	G2544	I2203	G1918	W1683	C1563	Y1230	L1108	L1108
K3295	I3124	I2800	A2548	A2548	S2204	L1919	L1687	C1565	Y1230	L1108	L1108
L3296	T3128	E2802	K2514	K2514	D2205	W1920	E1688	N1567	P1235	T1112	T1112
Q3297	T3131	E2803	V2567	V2567	W2216	G1921	E1688	N1567	MET	E1113	E1113
E3298	N3132	I2811	V2567	V2567	W2216	C1922	K1696	F1573	VAL	K1116	K1116
M3299	T3136	C2821	Q2573	Q2573	N2220	F1926	D1697	F1573	GLY	M1117	M1117
E3300	E3140	V2840	L2576	L2576	T2228	L1934	I1698	K1580	ILE	L1118	L1118
S3301	E3141	L2841	M2602	M2602	T2231	I1967	L1711	L1581	SER	V1126	V1126
T3302	E3142	D2844	K2603	K2603	L2254	V1970	I1722	R1596	ALA	T1129	T1129
L3303	T3143				N2278	F1973	M1745	R1601	GLU	L1132	L1132
E3304	Q3144				S2320	I1974	K1758	F1602	ALA	M1246	M1246
L3305					Q2340	G1979	E1759	Y1603	ALA	Y1135	Y1135
K3306					M2348	Y1980	H1760	V1605	VAL	M1136	M1136
L3307					M2602	A1981	H1760	V1605	PRO	I1142	I1142
E3308					K2603	V1997	L1764	T1609	CYS	R1143	R1143
Y3309							K1780	P1620		F1273	F1273
L3310							V1781	K1629		G1274	G1274
N3311							E1782				
Q3312											
S3313											
E3314											
D3315											
M3316											
F3317											
N3318											
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K3320											
F3321											
A3322											
T3323											
K3324											



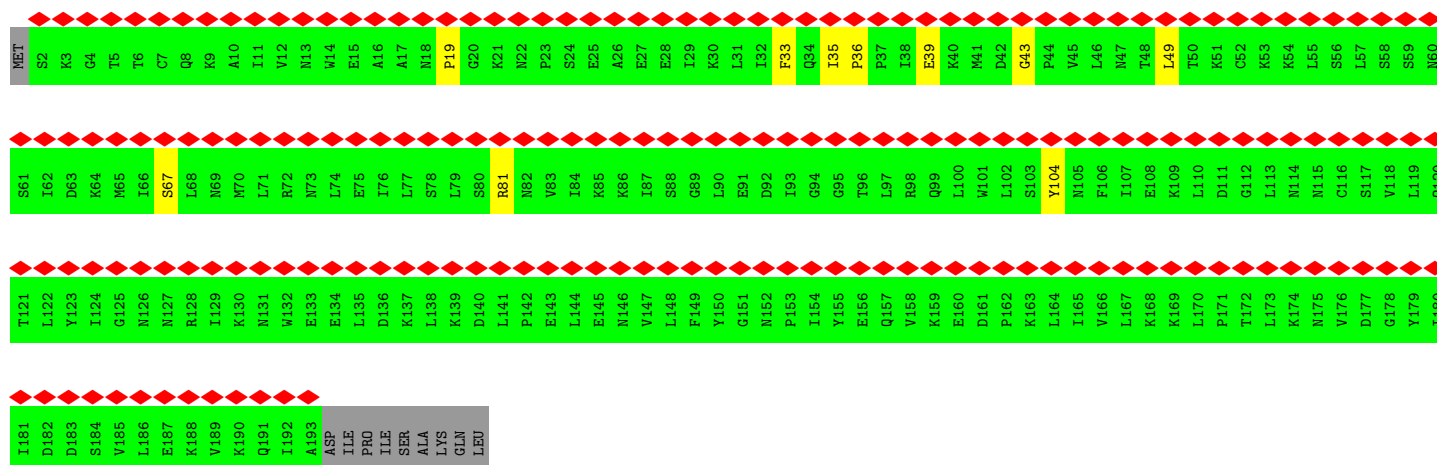
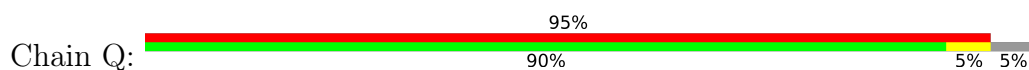
• Molecule 2: Dynein gamma heavy chain



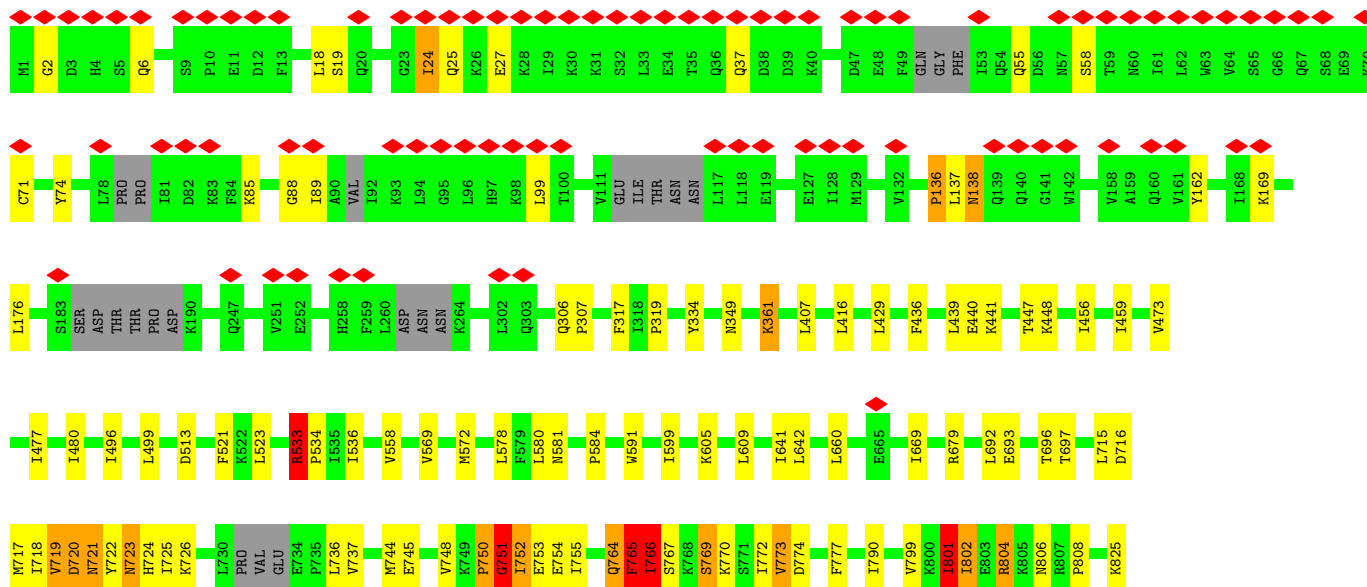
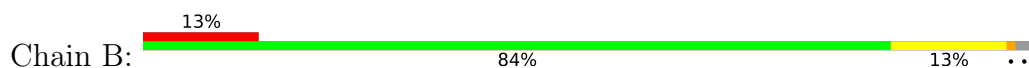




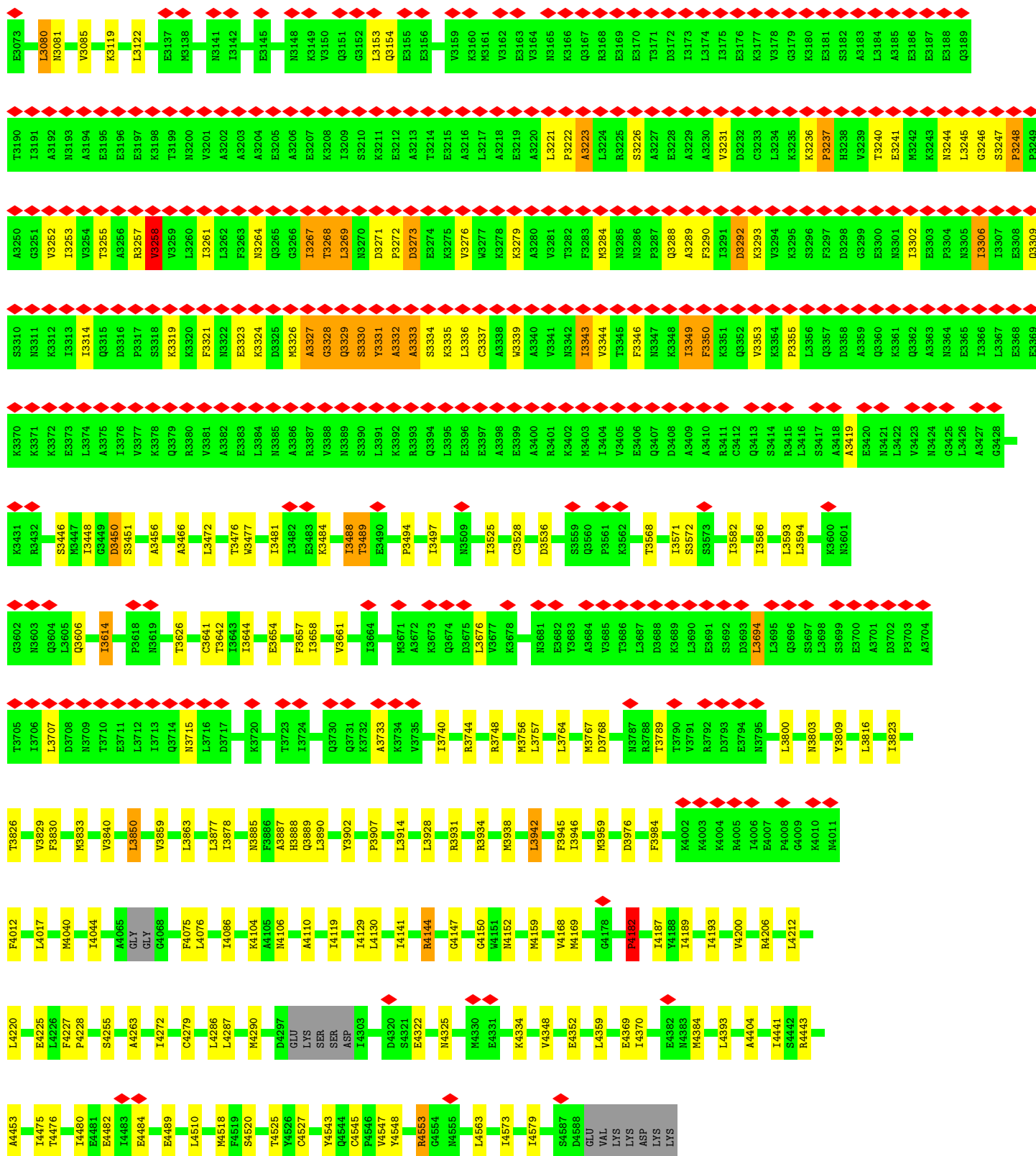
• Molecule 3: Dynein light chain 1

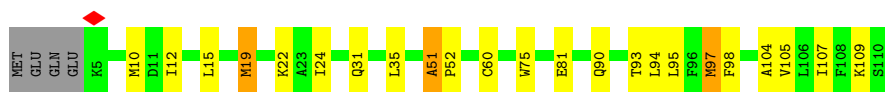


• Molecule 4: Dynein beta heavy chain

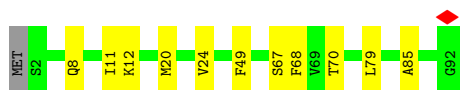
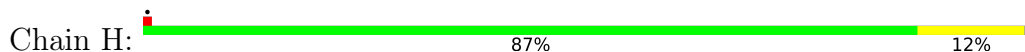




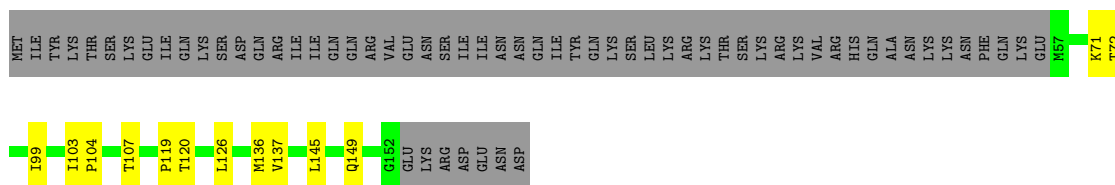




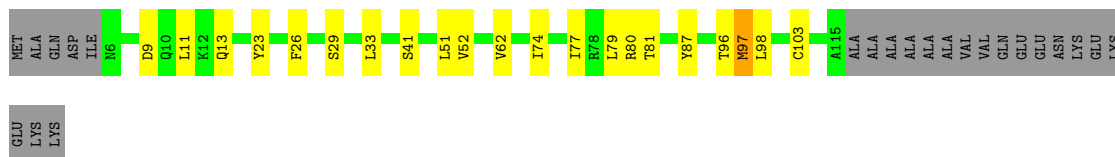
- Molecule 6: Dynein light chain LC8_1b (DLC82)



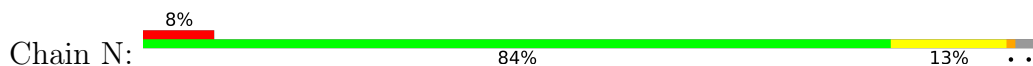
- Molecule 7: Dynein light chain roadblock LC7B



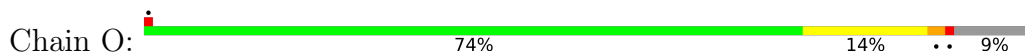
- Molecule 8: Dynein light chain roadblock LC7A



- Molecule 9: Dynein light chain Tctex_b

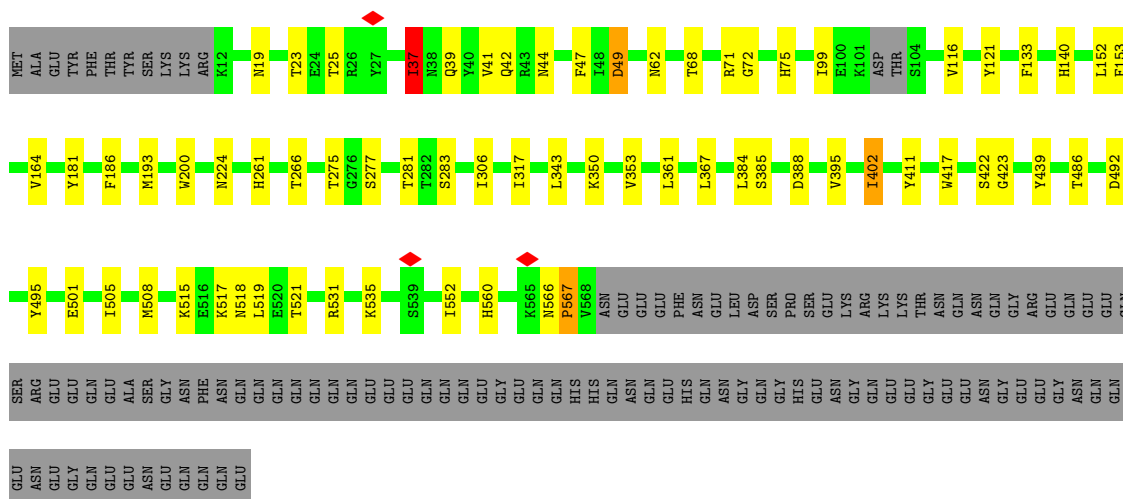


- Molecule 10: Dynein light chain Tctex_a (LC2A)



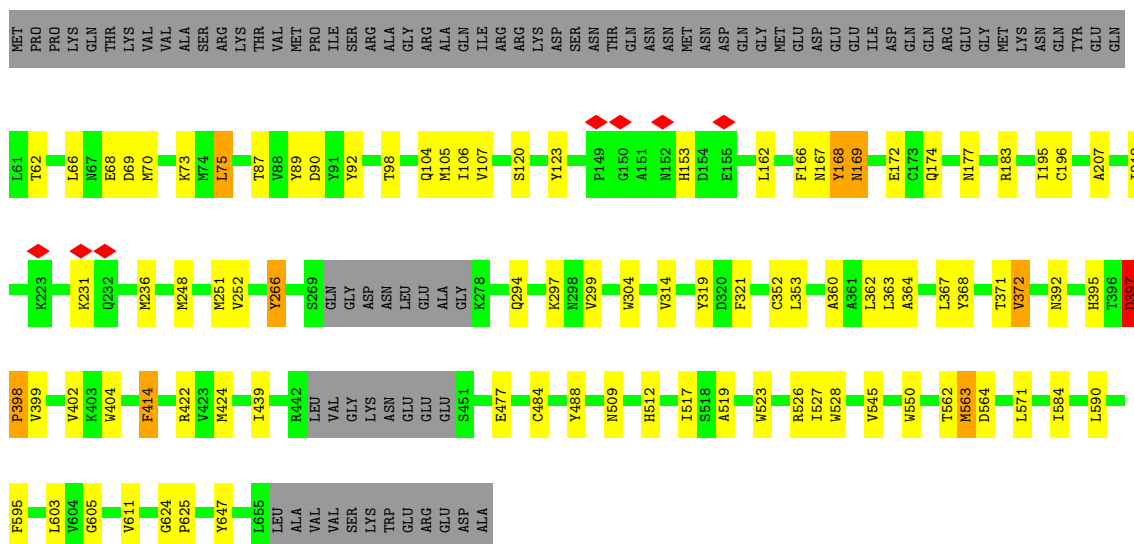
- Molecule 11: Dynein intermediate chain DIC3





• Molecule 12: Dynein intermediate chain DIC2

Chain D: 73% 12% 13%



• Molecule 13: Thioredoxin LC3BL

Chain P: 81% 8% 11%

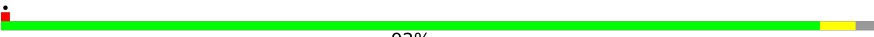


• Molecule 14: Dynein light chain LC8_3b

Chain L: 76% 12% 12%



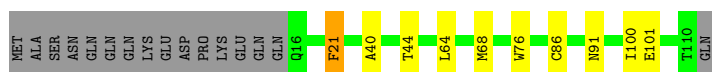
- Molecule 15: Dynein light chain LC8_2a (LC8E)

Chain K:  92%



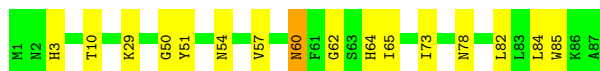
- Molecule 16: Dynein light chain LC8_2b

Chain J:  77% 8% 14%



- Molecule 17: Dynein light chain LC8_3a

Chain M:  82% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	9.863	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	1015.746, 1061.068, 970.42395	wwPDB
Map dimensions	381, 398, 364	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.666, 2.666, 2.666	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	1.05	0/34464	1.65	14/46623 (0.0%)
2	C	1.06	1/31037 (0.0%)	1.67	15/42000 (0.0%)
3	Q	1.32	0/1005	1.76	0/1388
4	B	1.06	1/35205 (0.0%)	1.70	30/47647 (0.1%)
5	I	1.06	0/838	1.57	2/1131 (0.2%)
6	H	1.03	0/767	1.51	0/1031
7	G	1.06	0/755	1.54	0/1018
8	F	1.05	0/875	1.51	0/1178
9	N	1.06	0/867	1.54	2/1179 (0.2%)
10	O	1.01	0/1004	1.47	0/1349
11	E	1.04	0/4522	1.45	2/6114 (0.0%)
12	D	1.02	0/4772	1.44	1/6458 (0.0%)
13	P	1.33	0/538	1.83	0/746
14	L	1.03	0/800	1.50	0/1076
15	K	1.00	0/776	1.45	0/1038
16	J	0.98	0/831	1.42	0/1118
17	M	1.00	0/752	1.42	0/1006
All	All	1.05	2/119808 (0.0%)	1.65	66/162100 (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	2
2	C	0	3
4	B	0	4
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1136	PHE	C-N	24.82	1.65	1.34
4	B	1606	PHE	C-N	16.80	1.73	1.33

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1136	PHE	O-C-N	53.07	171.08	121.19
2	C	1136	PHE	CA-C-N	-51.88	67.16	119.56
2	C	1136	PHE	C-N-CA	-51.88	67.16	119.56
4	B	1606	PHE	CA-C-N	37.30	166.47	119.84
4	B	1606	PHE	C-N-CA	37.30	166.47	119.84

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	GLU	Peptide
1	A	4250	ARG	Peptide
2	C	2717	ALA	Peptide
2	C	2746	PRO	Peptide
2	C	528	GLU	Peptide

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	33894	0	32284	339	0
2	C	30436	0	29388	343	0
3	Q	1002	0	498	6	0
4	B	34604	0	33084	736	0
5	I	827	0	829	17	0
6	H	750	0	735	7	0
7	G	749	0	772	11	0
8	F	863	0	881	10	0
9	N	855	0	800	13	0
10	O	986	0	1002	13	0
11	E	4423	0	4291	44	0
12	D	4664	0	4484	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	P	541	0	220	2	0
14	L	783	0	811	12	0
15	K	754	0	716	3	0
16	J	806	0	769	4	0
17	M	735	0	738	9	0
18	A	54	0	24	2	0
18	B	54	0	24	0	0
18	C	54	0	24	3	0
19	A	31	0	12	0	0
19	B	31	0	12	1	0
19	C	31	0	12	0	0
20	A	3	0	0	0	0
20	B	3	0	0	0	0
20	C	3	0	0	0	0
All	All	117936	0	112410	1554	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 7.

The worst 5 of 1554 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)
4:B:1223:LYS:HE2	4:B:1277:ARG:CB	1.23	1.63
4:B:1599:LEU:HB3	4:B:1617:LEU:CG	1.18	1.61
1:A:1219:PHE:HZ	1:A:1263:TYR:CD2	1.17	1.60
1:A:1219:PHE:CE1	1:A:1263:TYR:HA	1.26	1.60
1:A:1219:PHE:CZ	1:A:1263:TYR:CD2	1.89	1.60

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	4381/4620 (95%)	4081 (93%)	258 (6%)	42 (1%)	12	49
2	C	3914/4168 (94%)	3582 (92%)	283 (7%)	49 (1%)	9	42
3	Q	190/202 (94%)	163 (86%)	24 (13%)	3 (2%)	7	38
4	B	4488/4595 (98%)	4017 (90%)	383 (8%)	88 (2%)	6	31
5	I	104/110 (94%)	95 (91%)	8 (8%)	1 (1%)	12	49
6	H	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
7	G	92/159 (58%)	87 (95%)	5 (5%)	0	100	100
8	F	108/133 (81%)	96 (89%)	11 (10%)	1 (1%)	14	51
9	N	112/117 (96%)	92 (82%)	17 (15%)	3 (3%)	4	25
10	O	118/132 (89%)	103 (87%)	10 (8%)	5 (4%)	2	17
11	E	551/670 (82%)	496 (90%)	51 (9%)	4 (1%)	18	56
12	D	569/667 (85%)	510 (90%)	51 (9%)	8 (1%)	9	40
13	P	103/122 (84%)	86 (84%)	11 (11%)	6 (6%)	1	14
14	L	96/111 (86%)	91 (95%)	4 (4%)	1 (1%)	12	49
15	K	88/93 (95%)	79 (90%)	9 (10%)	0	100	100
16	J	93/111 (84%)	84 (90%)	8 (9%)	1 (1%)	11	46
17	M	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	4	27
All	All	15181/16189 (94%)	13817 (91%)	1150 (8%)	214 (1%)	11	40

5 of 214 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO
1	A	197	ILE
1	A	871	LEU
1	A	973	ASP
1	A	3251	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	3420/4197 (82%)	3332 (97%)	88 (3%)	40	62
2	C	3149/3691 (85%)	3090 (98%)	59 (2%)	50	67
3	Q	10/186 (5%)	10 (100%)	0	100	100
4	B	3497/4145 (84%)	3398 (97%)	99 (3%)	38	60
5	I	91/95 (96%)	87 (96%)	4 (4%)	25	47
6	H	82/83 (99%)	80 (98%)	2 (2%)	43	64
7	G	86/149 (58%)	86 (100%)	0	100	100
8	F	93/109 (85%)	85 (91%)	8 (9%)	10	29
9	N	85/104 (82%)	83 (98%)	2 (2%)	43	64
10	O	106/119 (89%)	98 (92%)	8 (8%)	12	33
11	E	484/597 (81%)	468 (97%)	16 (3%)	33	55
12	D	507/609 (83%)	486 (96%)	21 (4%)	27	49
14	L	87/99 (88%)	84 (97%)	3 (3%)	32	54
15	K	80/82 (98%)	79 (99%)	1 (1%)	61	74
16	J	81/97 (84%)	77 (95%)	4 (5%)	22	43
17	M	78/78 (100%)	74 (95%)	4 (5%)	21	42
All	All	11936/14440 (83%)	11617 (97%)	319 (3%)	40	61

5 of 319 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	4012	PHE
12	D	62	THR
4	B	4369	GLU
9	N	18	ASP
12	D	399	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 252 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	4068	ASN
11	E	196	GLN
4	B	1770	ASN
11	E	87	ASN
12	D	298	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
18	ADP	C	4203	20	28,29,29	0.50	0	43,45,45	0.83	1 (2%)
19	ATP	A	4702	20	32,33,33	0.51	0	48,52,52	0.59	0
19	ATP	C	4201	20	32,33,33	0.47	0	48,52,52	0.59	0
18	ADP	A	4703	-	28,29,29	0.50	0	43,45,45	0.58	0
19	ATP	B	4701	20	32,33,33	0.50	0	48,52,52	0.62	0
18	ADP	C	4206	20	28,29,29	0.46	0	43,45,45	0.60	0
18	ADP	B	4706	20	28,29,29	0.48	0	43,45,45	0.44	0
18	ADP	B	4705	20	28,29,29	0.54	0	43,45,45	0.51	0
18	ADP	A	4701	20	28,29,29	0.47	0	43,45,45	0.52	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
18	ADP	C	4203	20	-	7/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ATP	A	4702	20	-	5/22/38/38	0/3/3/3
19	ATP	C	4201	20	-	6/22/38/38	0/3/3/3
18	ADP	A	4703	-	-	1/16/32/32	0/3/3/3
19	ATP	B	4701	20	-	0/22/38/38	0/3/3/3
18	ADP	C	4206	20	-	4/16/32/32	0/3/3/3
18	ADP	B	4706	20	-	2/16/32/32	0/3/3/3
18	ADP	B	4705	20	-	5/16/32/32	0/3/3/3
18	ADP	A	4701	20	-	5/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	4203	ADP	C4-N9-C1'	2.03	131.39	126.63

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	4701	ADP	PA-O3A-PB-O3B
18	C	4203	ADP	C5'-O5'-PA-O1A
18	C	4203	ADP	C5'-O5'-PA-O2A
18	C	4203	ADP	C5'-O5'-PA-O3A
18	C	4206	ADP	O4'-C4'-C5'-O5'

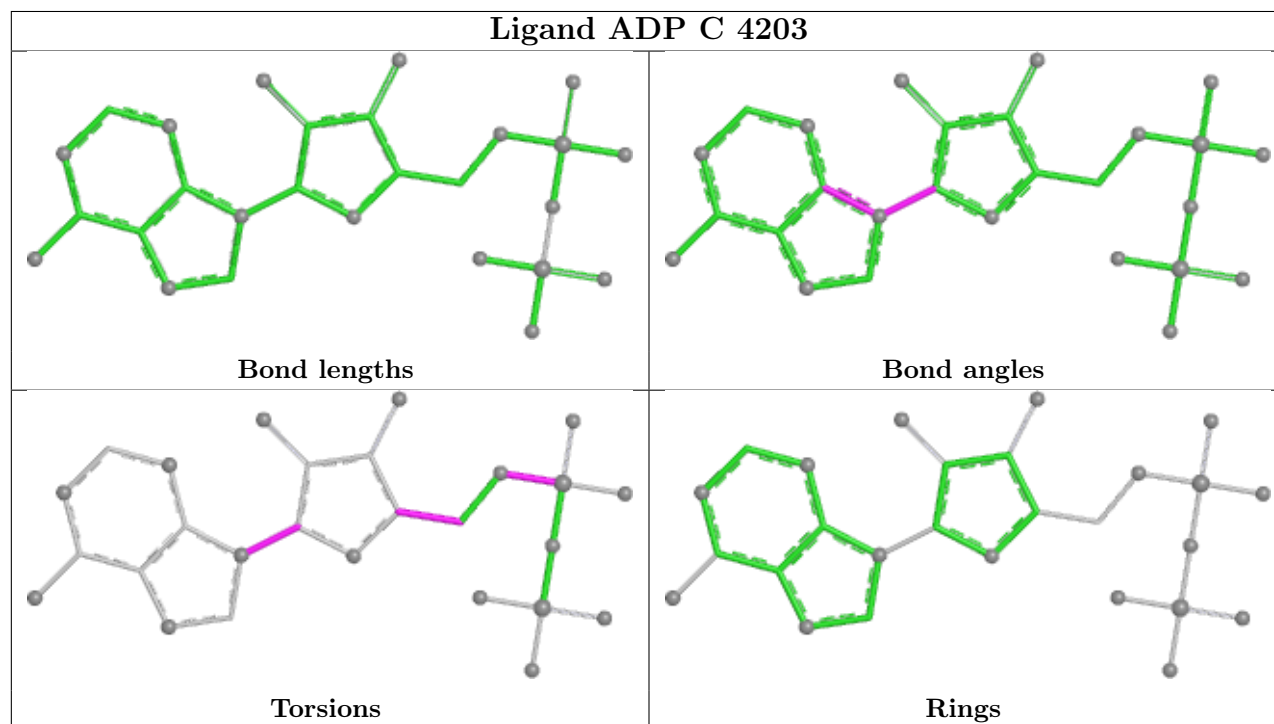
There are no ring outliers.

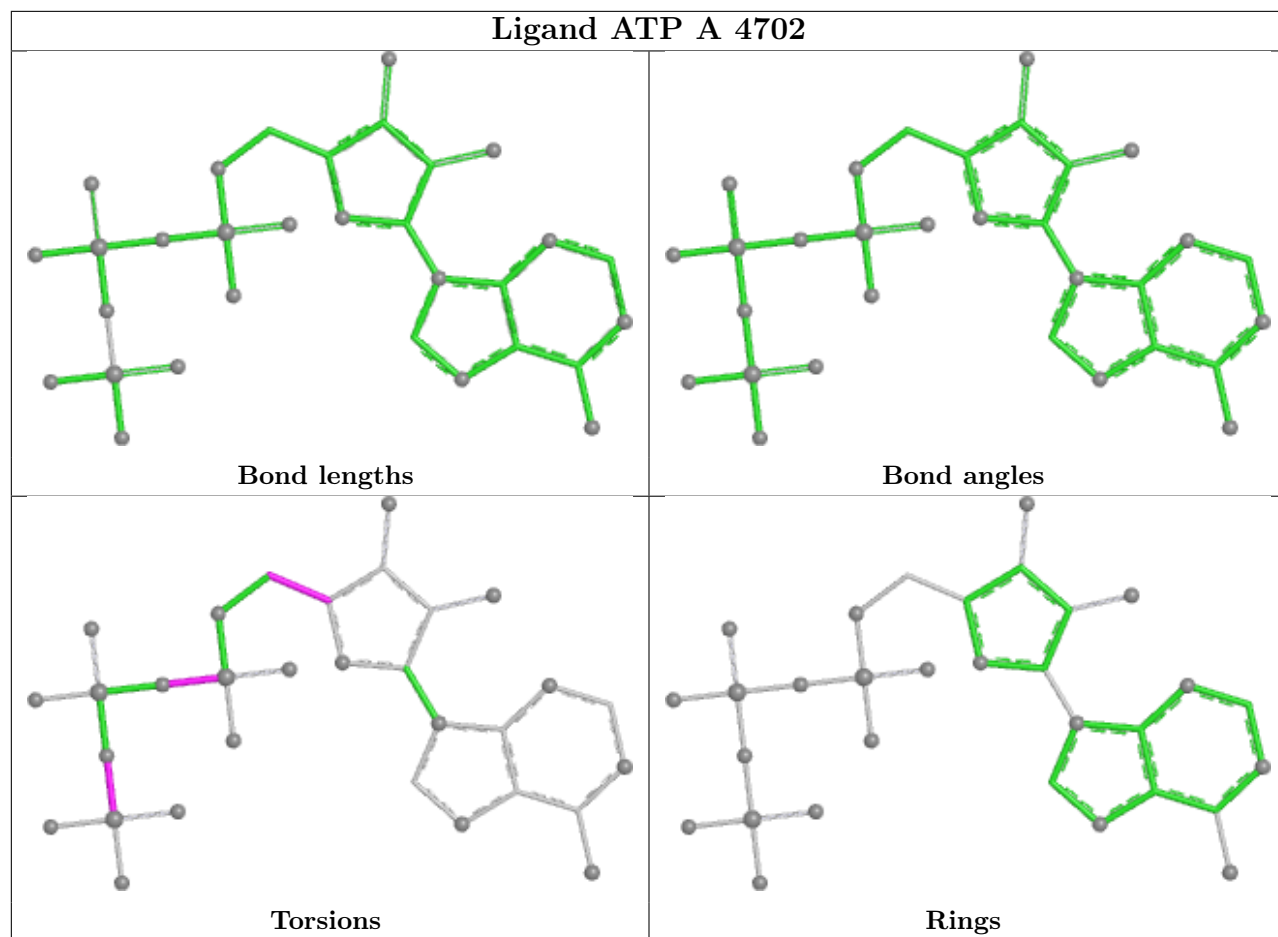
5 monomers are involved in 6 short contacts:

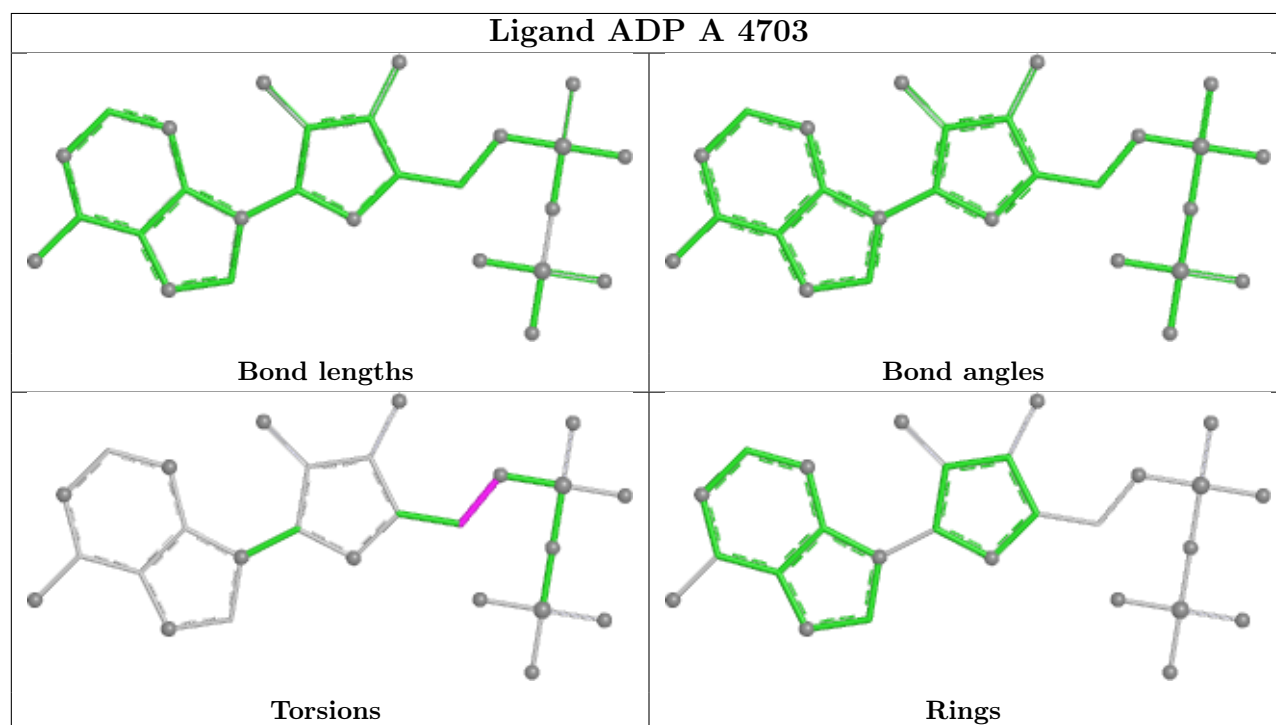
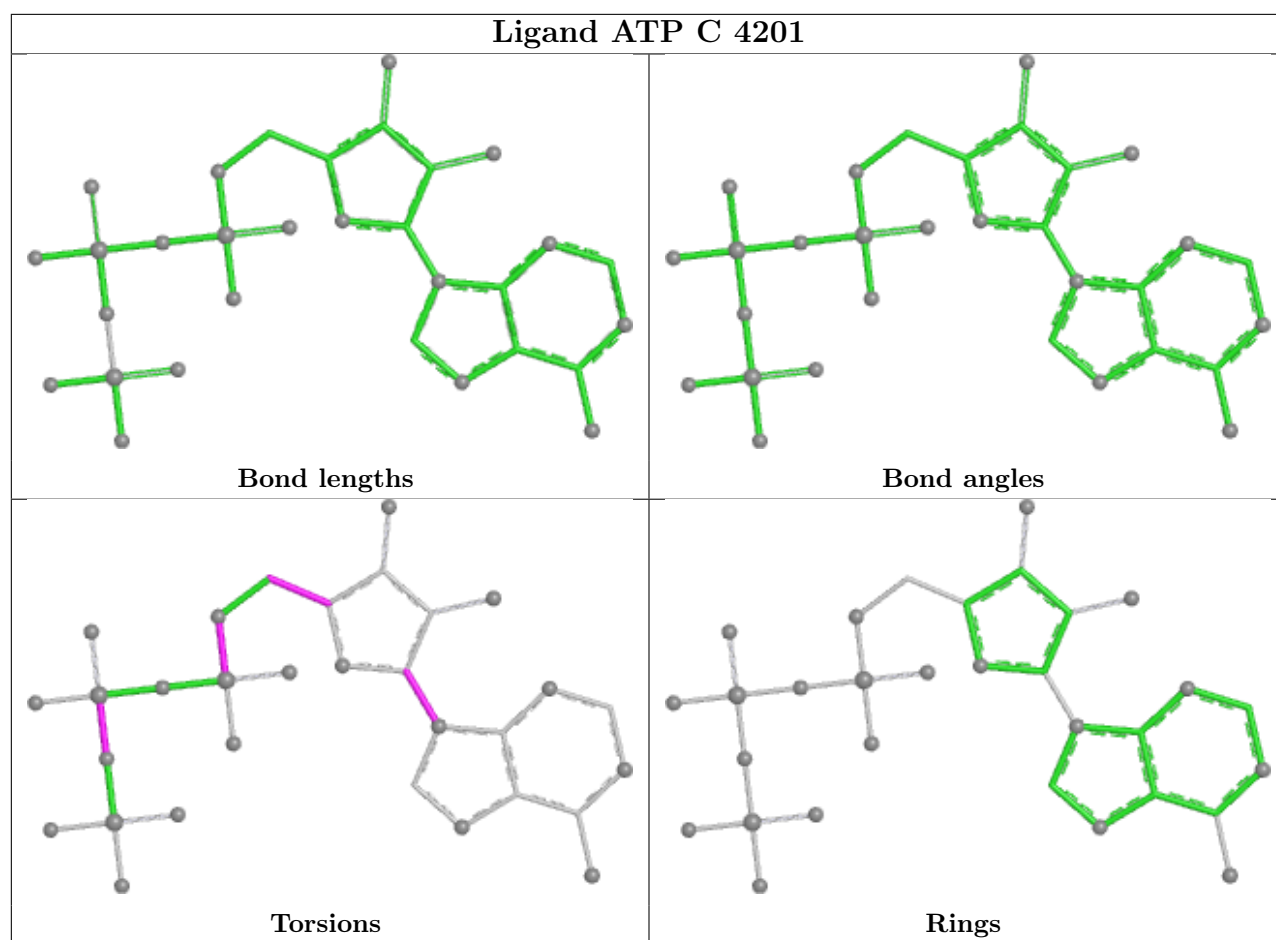
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	4203	ADP	1	0
18	A	4703	ADP	1	0
19	B	4701	ATP	1	0
18	C	4206	ADP	2	0
18	A	4701	ADP	1	0

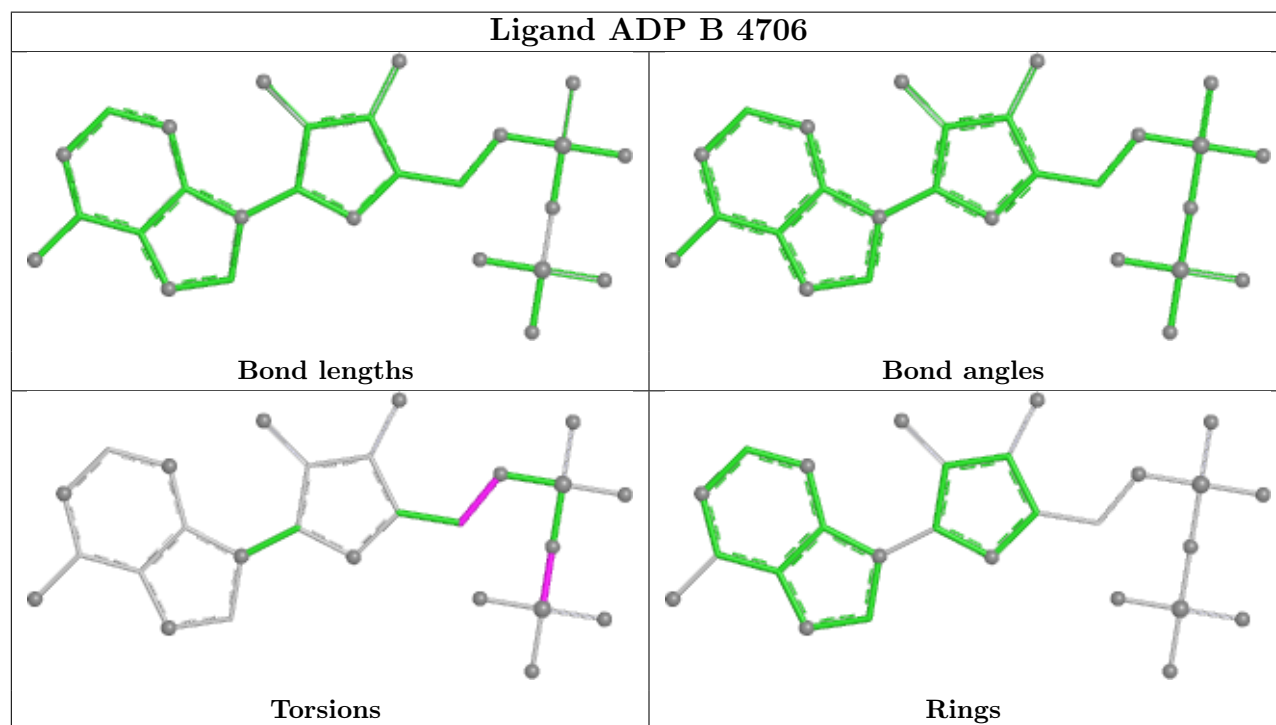
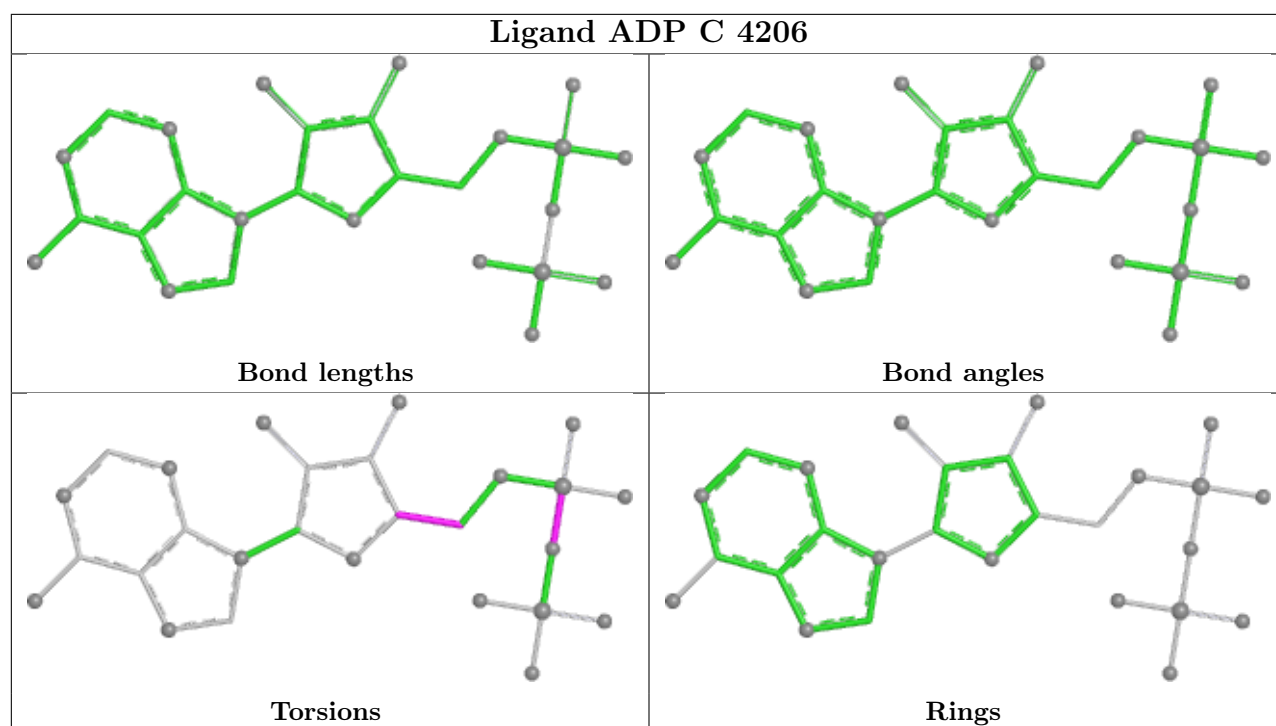
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

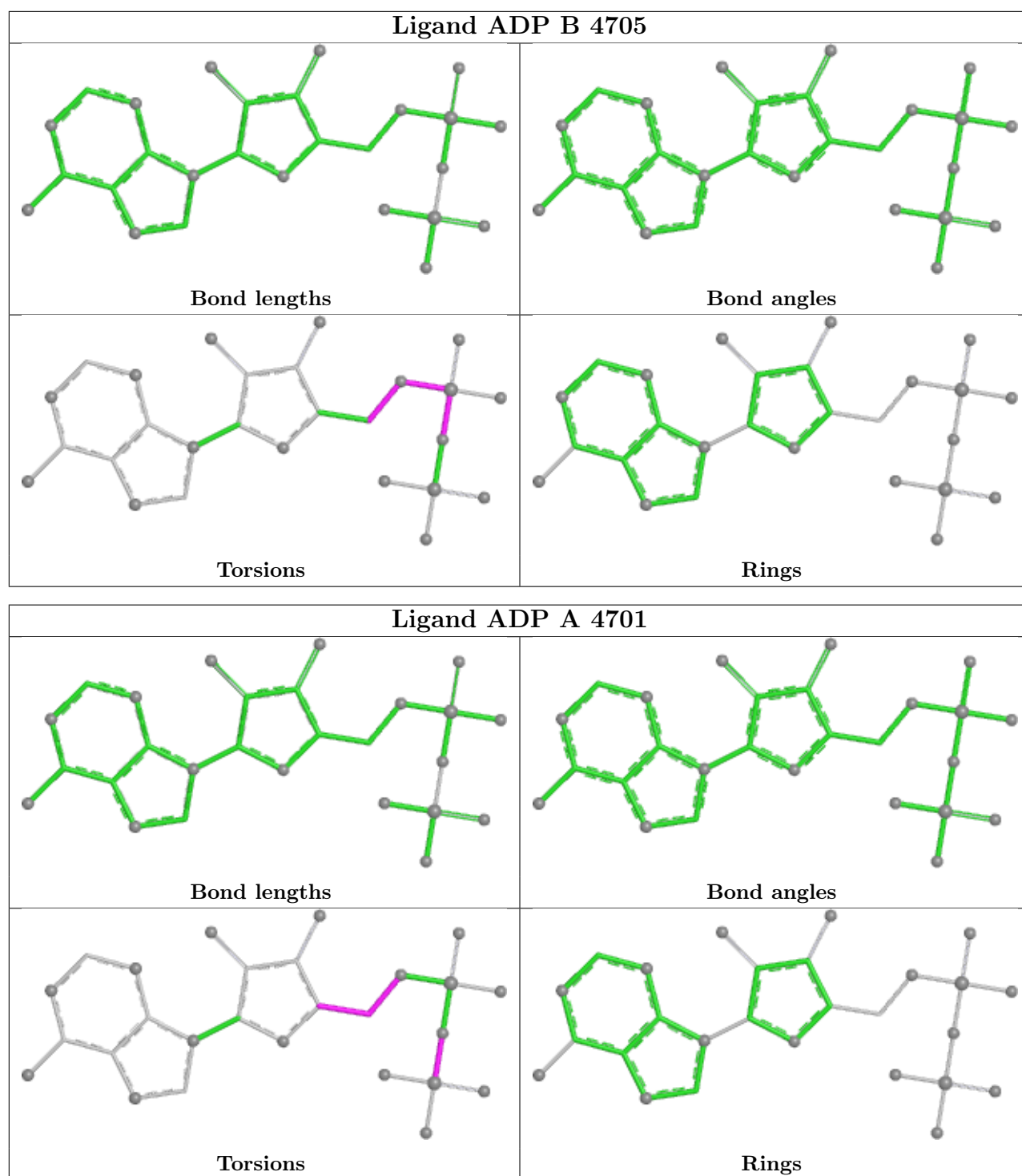
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers ⓘ

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	A	4
2	C	3
4	B	3
12	D	2
13	P	1
7	G	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	364:ILE	C	365:PHE	N	4.18
1	B	25:GLN	C	26:LYS	N	3.78
1	D	216:HIS	C	217:GLN	N	3.67
1	A	53:ILE	C	54:PHE	N	3.57
1	A	115:ASP	C	116:ASN	N	3.46

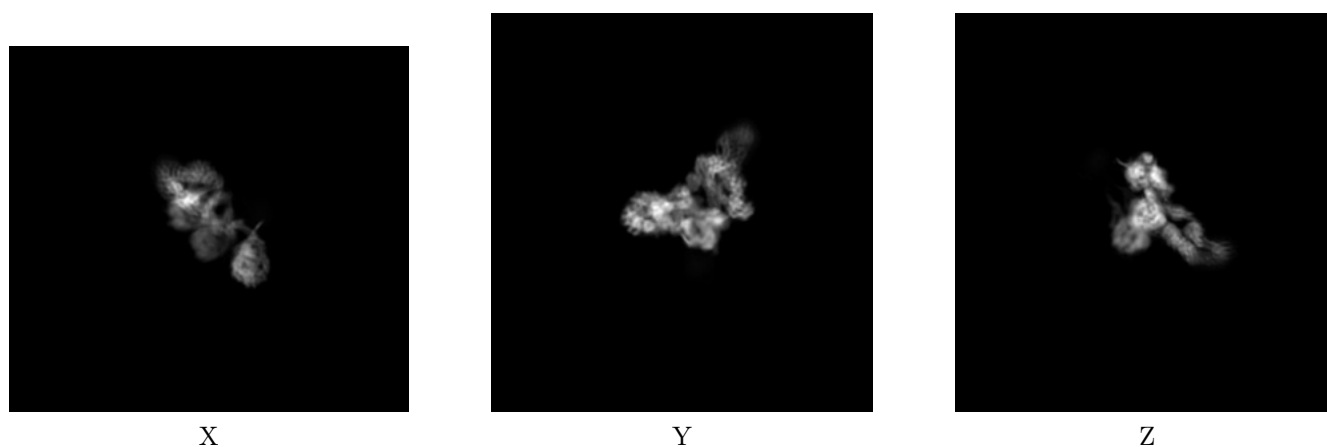
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22840. 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](#)

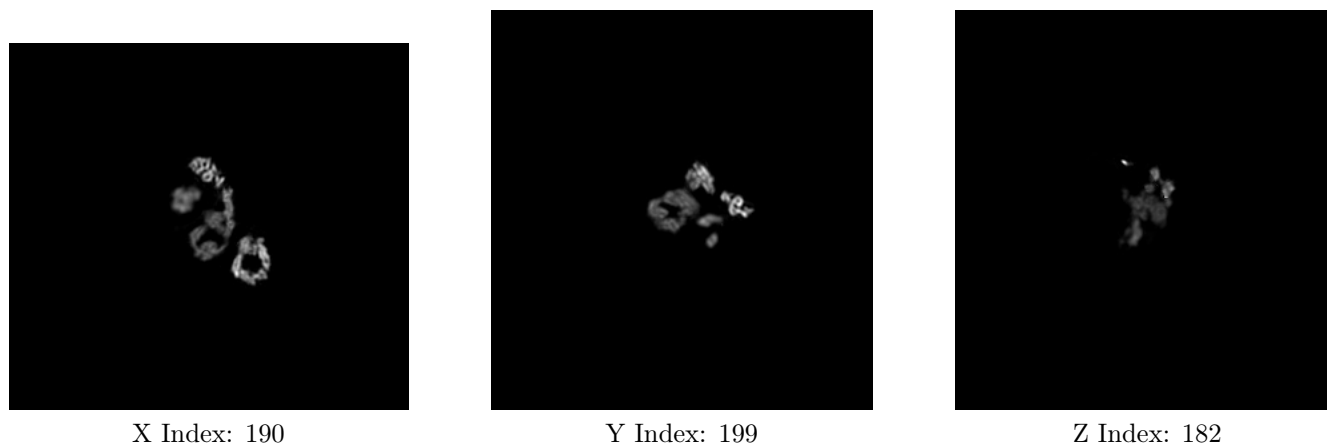
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



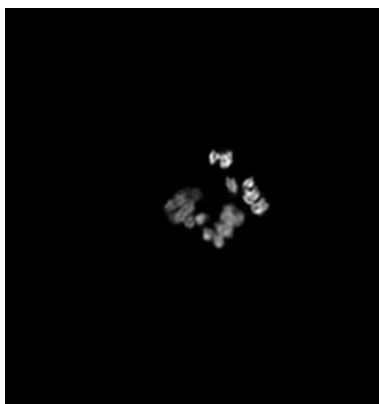
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 189



Y Index: 186

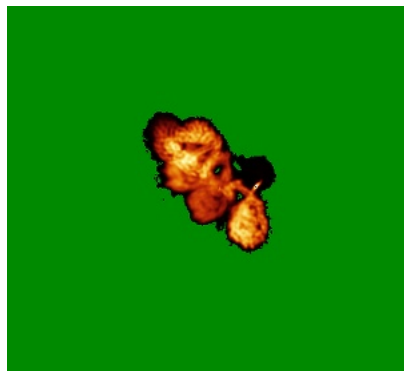


Z Index: 209

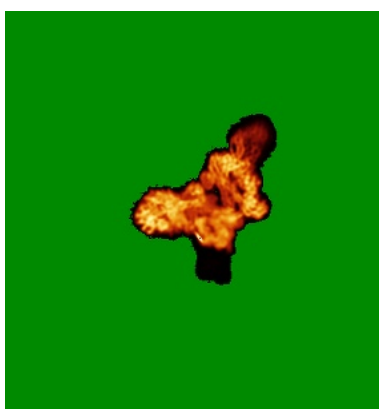
The images above show the largest variance slices of the map in three orthogonal directions.

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

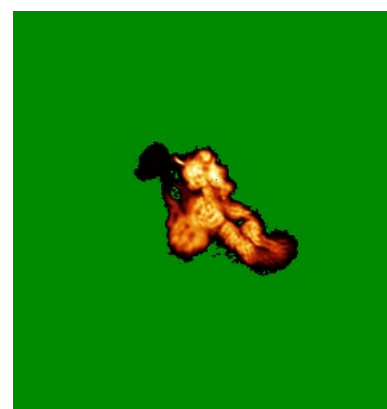
6.4.1 Primary map



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

This section was not generated.

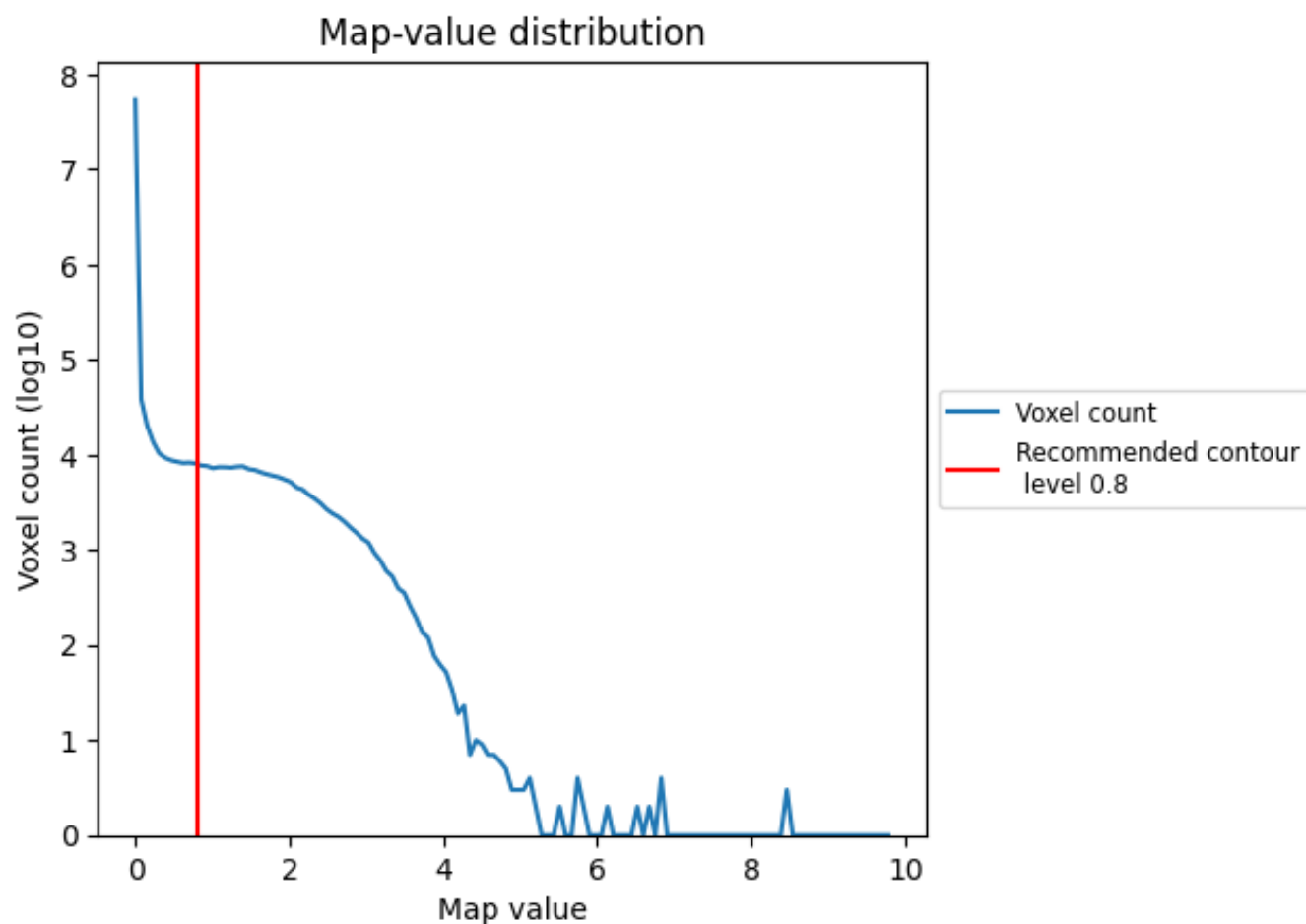
6.6 Mask visualisation

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

7 Map analysis ⓘ

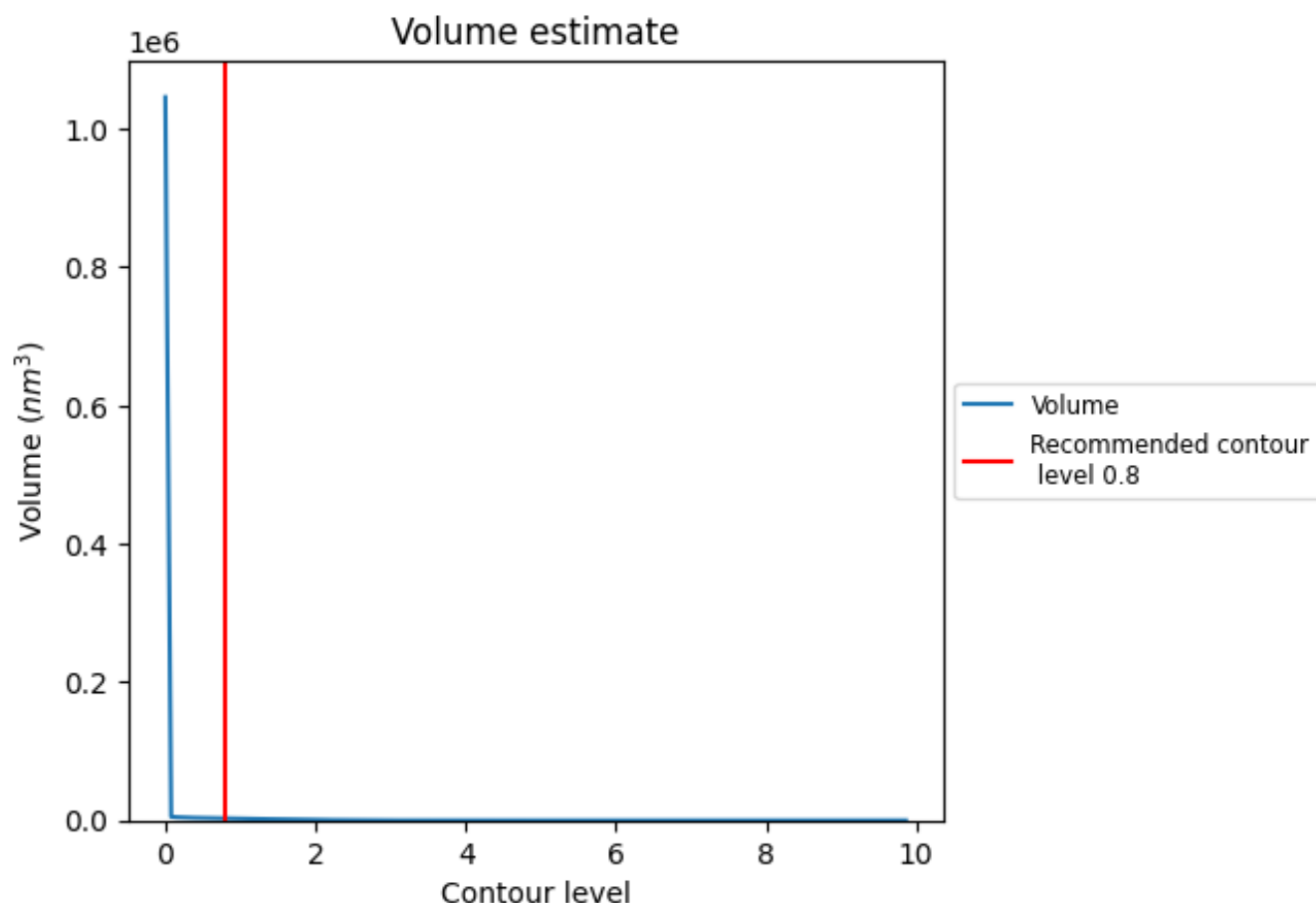
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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 2909 nm³; this corresponds to an approximate mass of 2628 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

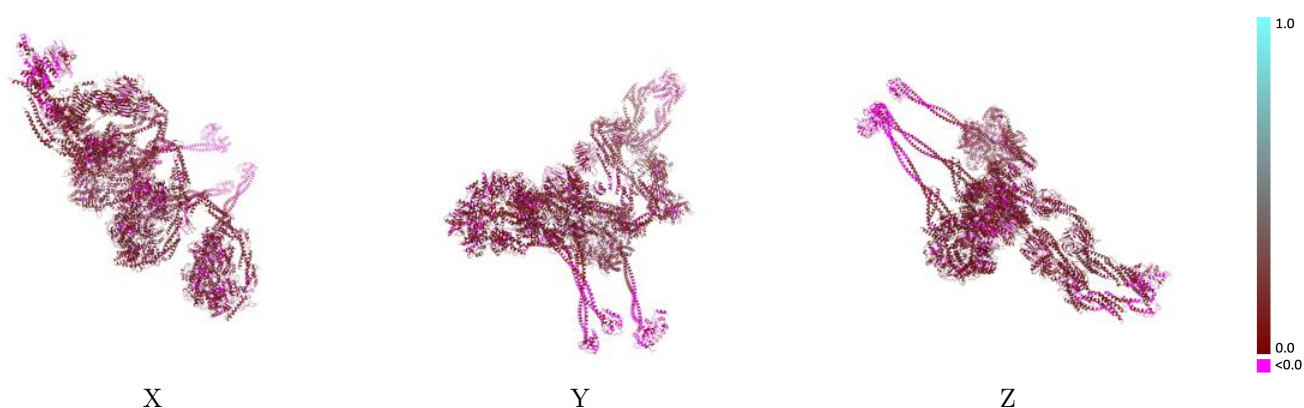
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22840 and PDB model 7KEK. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

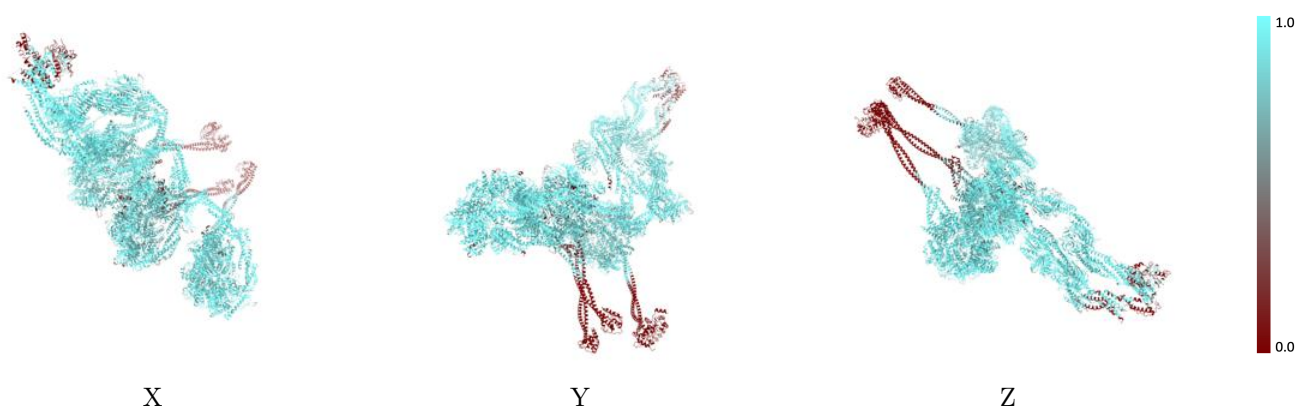
This section was not generated.

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



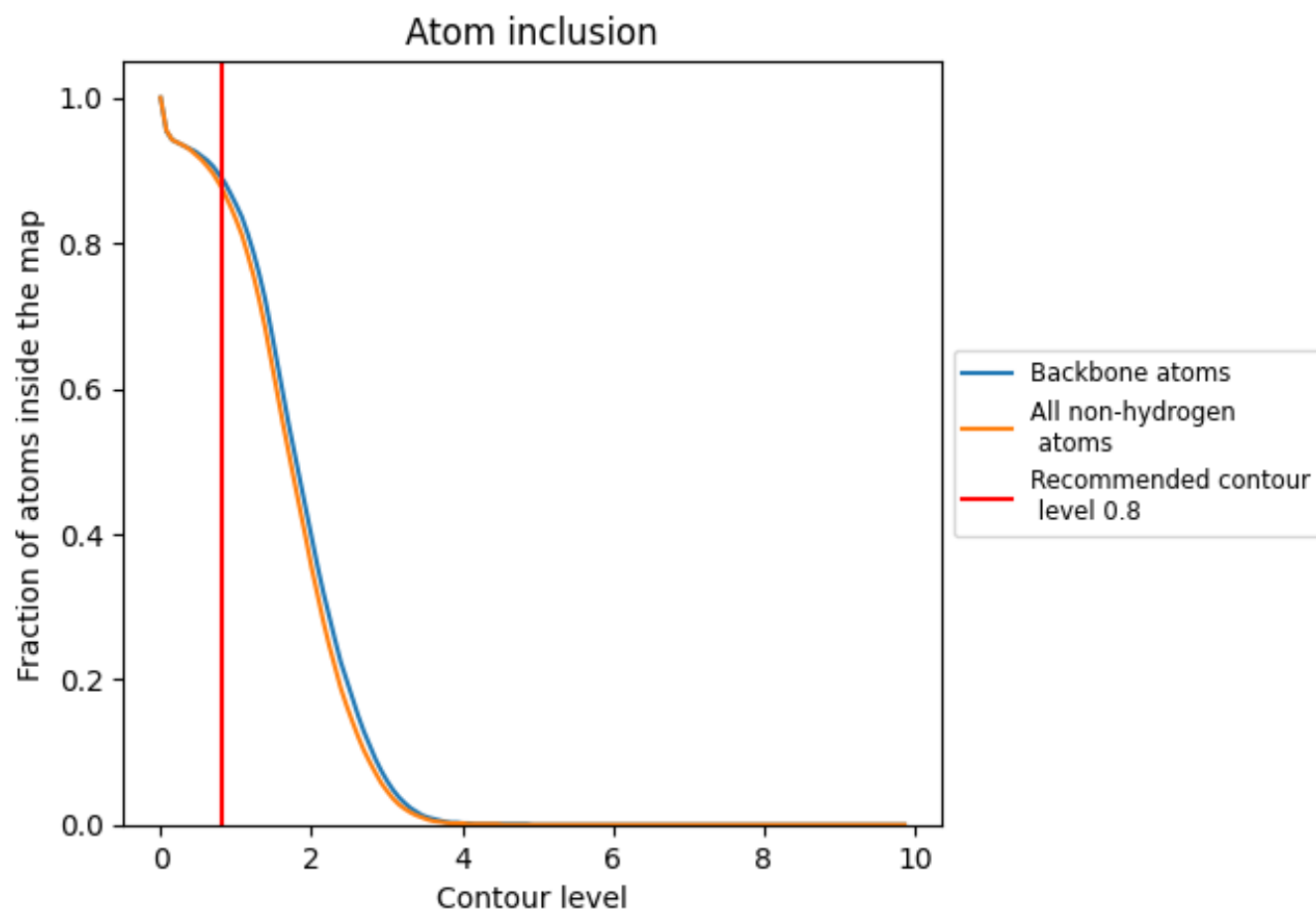
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.0820
A	 0.8690	 0.0750
B	 0.8440	 0.0940
C	 0.9000	 0.0720
D	 0.9770	 0.0930
E	 0.9660	 0.0980
F	 0.9940	 0.1150
G	 0.9730	 0.1140
H	 0.9880	 0.1000
I	 0.9670	 0.1140
J	 0.9860	 0.0810
K	 0.9850	 0.0970
L	 0.9870	 0.1020
M	 0.9720	 0.0830
N	 0.9110	 0.0660
O	 0.9670	 0.0780
P	 0.9760	 0.1150
Q	 0.0000	 -0.0530

