



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:10 PM UTC

PDB ID : 9E12 / pdb\_00009e12  
EMDB ID : EMD-47381  
Title : Full-length human dynein-1 in phi conformation 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.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

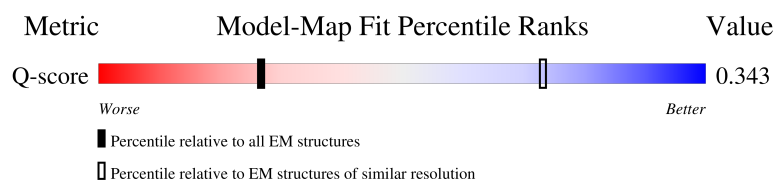
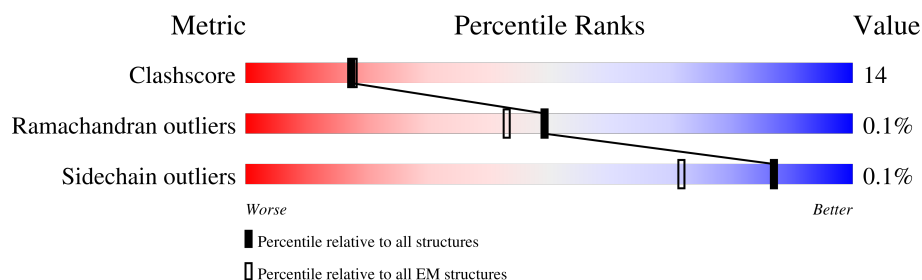
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




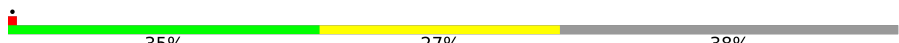
The reported resolution of this entry is 4.50 Å.

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.




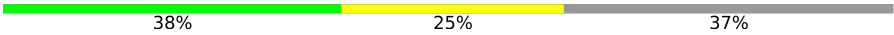






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 ( 4.00 - 5.00 )

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	
1	B	4646	
2	C	638	
2	D	638	

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Mol	Chain	Length	Quality of chain
3	E	492	
3	F	492	
4	G	96	
4	H	96	
5	I	89	
5	J	89	
6	K	113	
6	L	113	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 89391 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		

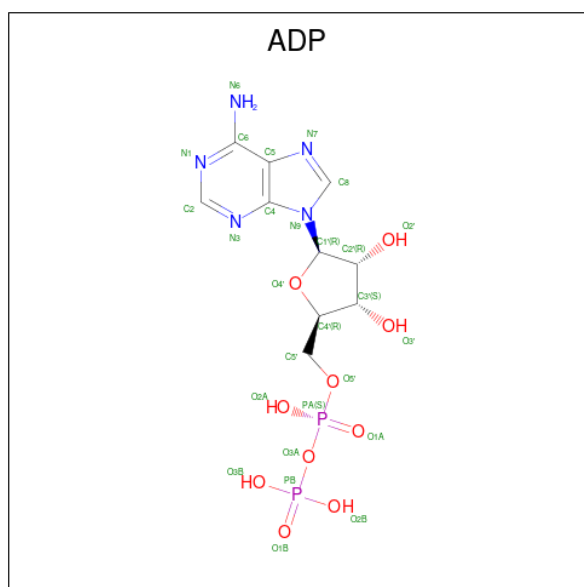
- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

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



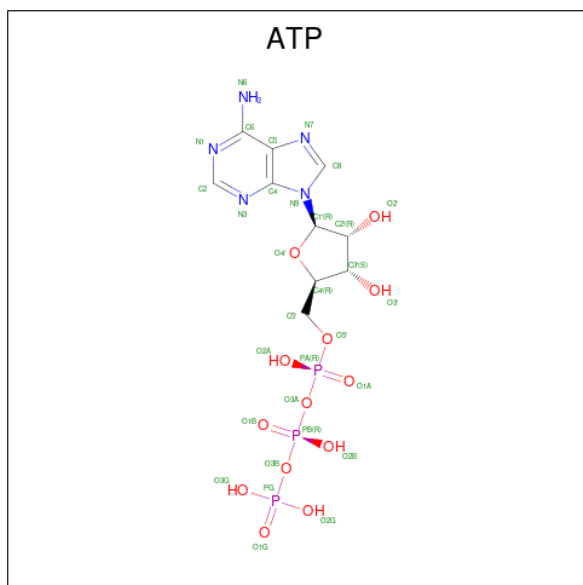
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

- Molecule 8 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
8	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

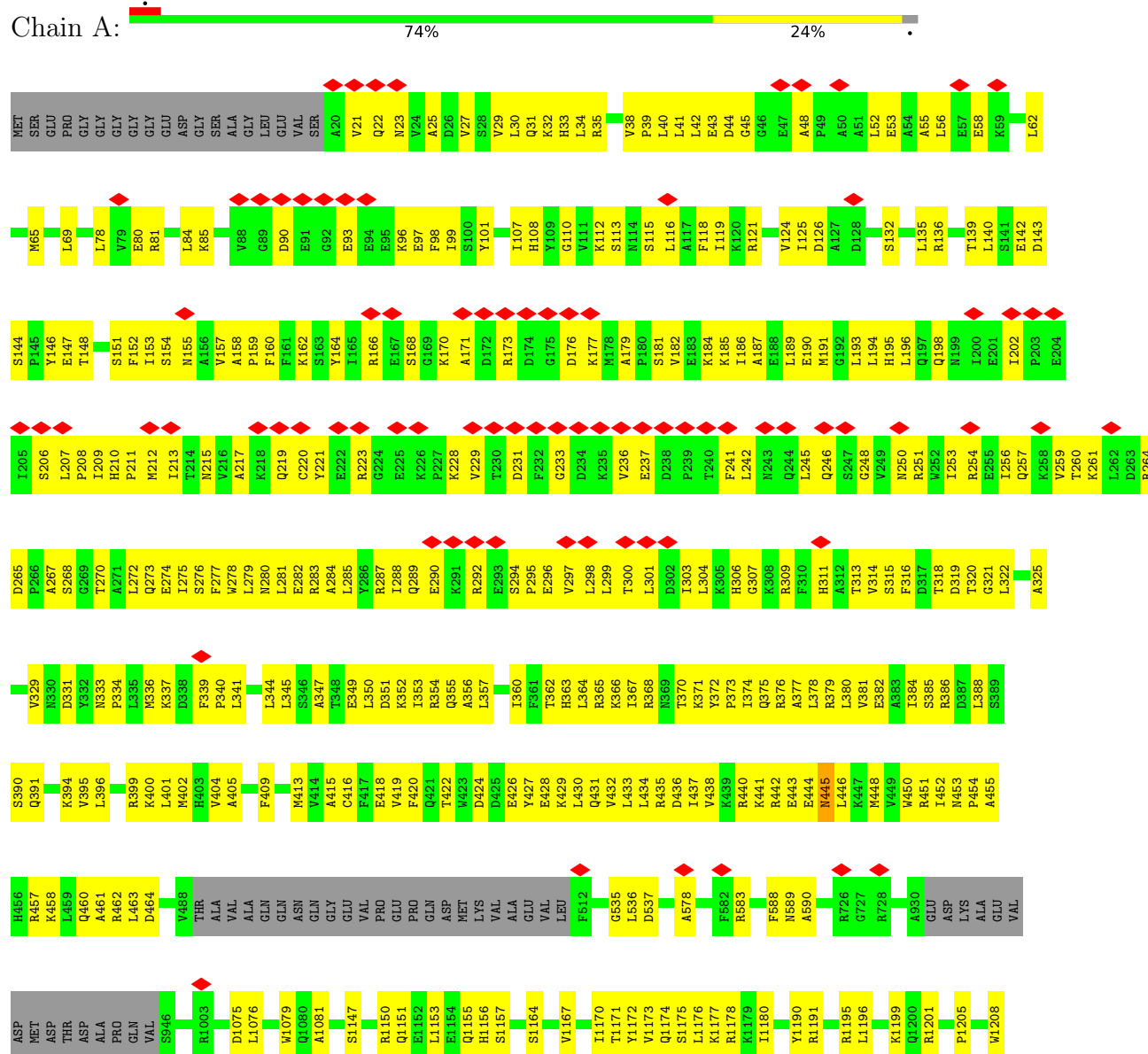
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	Mg	0
			2	2	
9	B	2	Total	Mg	0
			2	2	

### 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.

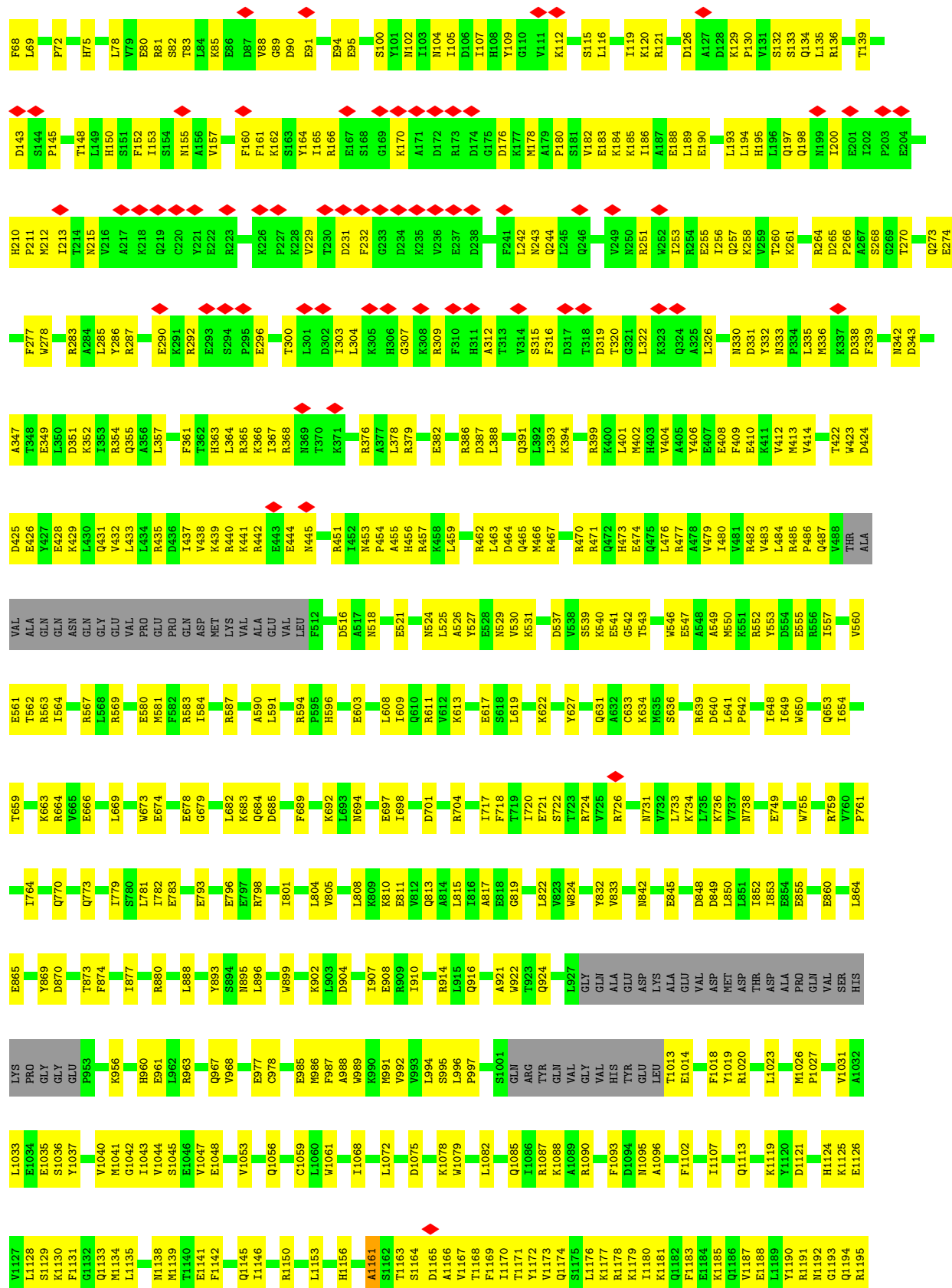
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1



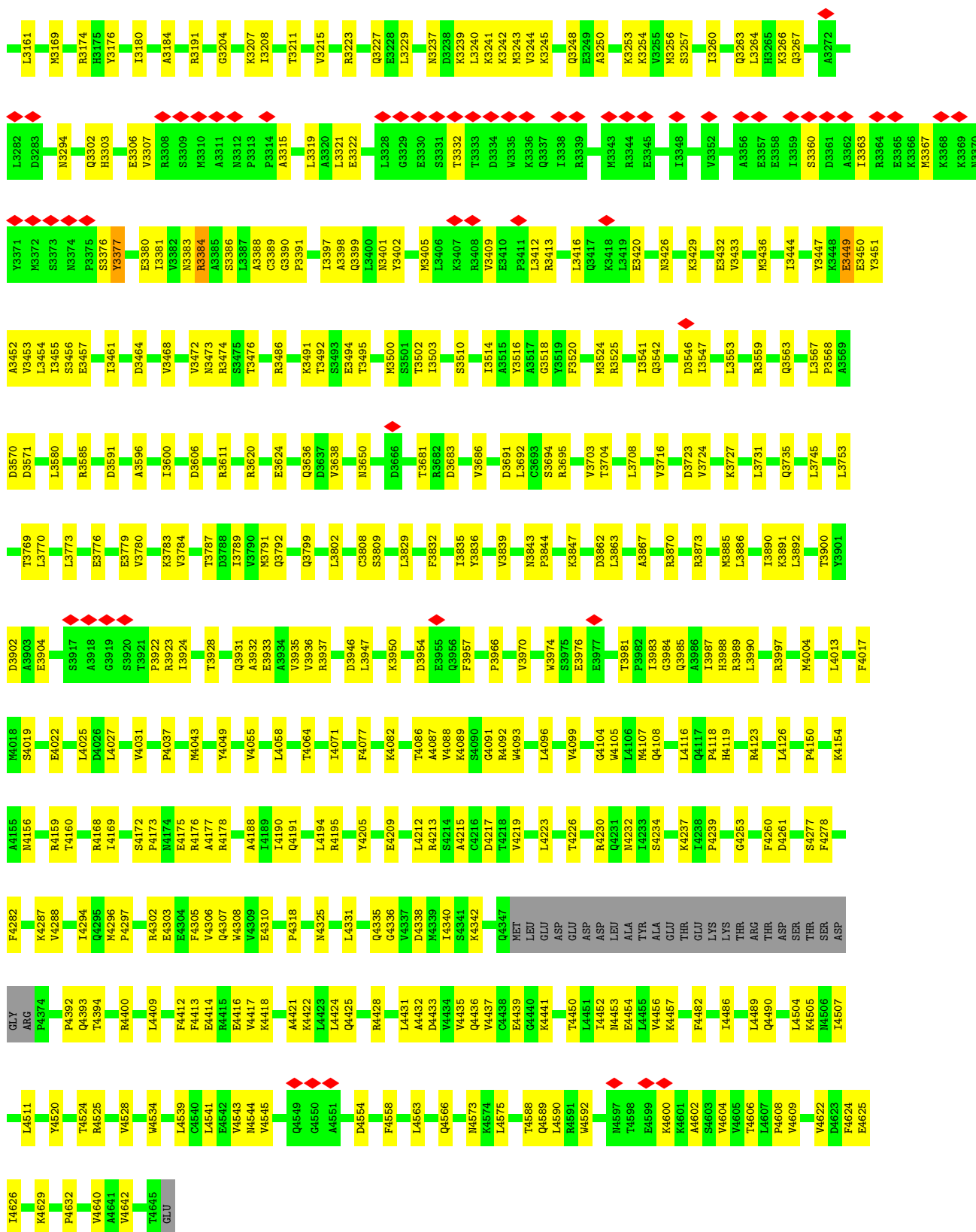






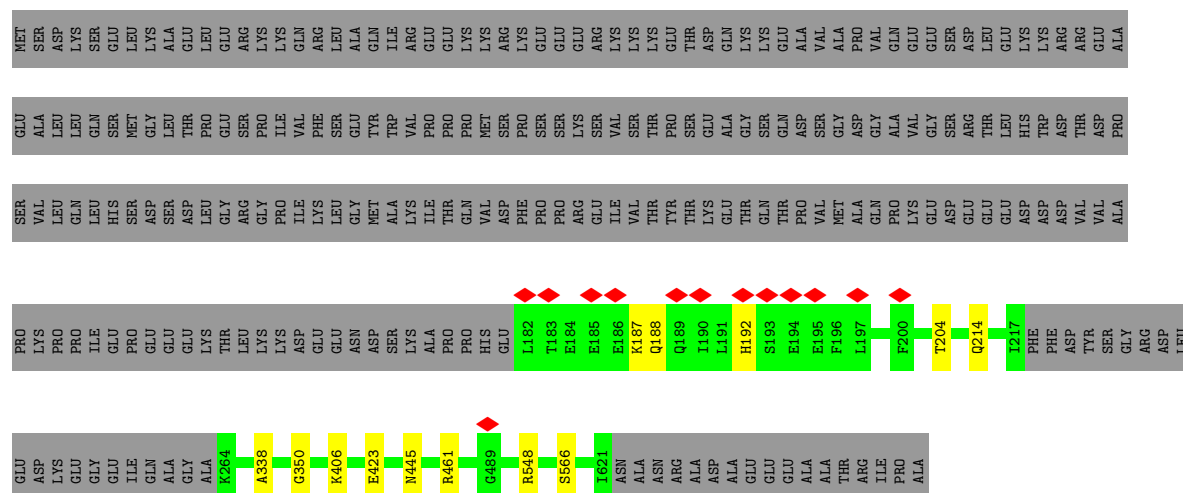


T3028	M2867	C9712	E2558	T2450	F2364	E2248	E2133	E1965	V1785	L1666	S1405	L1196
Q3032	D2885	L2723	H2560	R2451	L2369	K2257	Q2133	Q1973	M1798	V1672	E1406	L1197
C3033	Q2886	R2726	V2562	R2453	L2369	K2257	I2136	C1977	E1799	V1673	A1407	E1198
K3034	Q2886	R2726	V2562	R2453	L2369	K2257	I2136	C1977	Q1800	V1673	L1408	K1199
M3043	Y2892	P2732	V2568	S2457	M2373	S2260	I2137	I1978	R1804	I1676	V1426	Q1201
L3044	R2896	V2733	V2569	L2462	I2374	D2262	Q2139	N1987	R1805	S1677	F1203	F1202
D3045	D2917	Y2735	V2572	H2463	F2375	H2263	S2140	P1988	R1806	S1678	S1427	Q1203
S3046	H2918	Y2738	A2465	Q2464	L2382	T2267	C2142	Y1999	R1806	E1680	E1428	F1204
E3049	H2918	Y2738	A2465	Q2464	L2382	T2267	E2143	D1991	H1810	K1687	L1429	P1205
K3052	R2921	S2743	R2576	A2465	L2387	P2270	T2144	D1991	E1814	K1687	G1432	V1208
Q3057	I2922	L2744	H2577	N2468	E2389	R2273	V2146	T1993	L1815	S1691	Q1433	L1209
V3058	I2922	L2744	H2577	N2468	E2389	R2273	V2146	T1993	L1815	S1691	I1211	V1210
I3059	I2925	I2747	T2583	Q2471	GLY	L2279	L2149	K1994	L1825	L1704	I1434	D1212
R3060	I2925	I2747	T2583	Q2471	ASP	L2279	E2152	E2000	I1830	K1707	W1435	N1213
P3070	I2925	I2747	T2583	Q2471	ALA	L2284	L2157	Q2005	I1830	K1707	D1436	I1214
T3081	Q2930	Y2748	P2590	D2478	GLN	R2285	L2161	Q2005	S1835	V1711	L1439	E1215
R3088	L2933	F2751	L2592	F2480	ARG	I2288	F2165	Q2005	F1836	K1715	Q1440	G1216
F3094	L2937	M2755	P2596	M2481	ARG	D2289	L2176	T2017	W1837	K1715	K1441	E1217
T3099	G2937	L2756	P2596	M2481	ARG	S2290	A2177	L2061	W1838	K1715	G1452	W1218
E3100	K2943	L2758	M2603	E2484	GLY	S2290	L2178	T2061	L1839	V1721	V1452	G1219
Q3104	T2944	F2784	M2607	Q2485	LYS	L2296	E2174	T2061	L1839	V1721	A1453	K1228
T3110	R2948	Y2794	S2607	L2486	LYS	Q2296	M2175	Q2047	R1843	V1724	Q1454	D1229
M3113	Y2952	Y2794	F2622	Q2489	ASP	R2298	L2176	L2054	Q1850	F1727	G1455	S1230
D3114	M2953	V2803	T2627	Q2491	GLY	Q2299	A2177	L2054	Q1850	F1727	E1456	Q1233
Y3130	L2956	R2804	T2627	Q2491	GLY	Q2299	L2178	T2061	Q1856	K1729	M1457	V1267
D3131	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	K1464
K3132	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	Q1465
Q3135	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	I1466
P3137	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	E1467
R3140	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	V1469
T3143	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	T1472
V3144	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	T1473
V3148	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	L1486
F3149	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	D1491
V3150	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	D1492
T3153	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	L1493
L3154	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	V1497
N3158	L2961	F2807	P2628	Q2493	ALA	D2308	E2180	A2066	M1861	D1734	E1460	I1501
												V1504
												K1508
												Y1512
												Y1513
												K1514
												V1515
												E1517

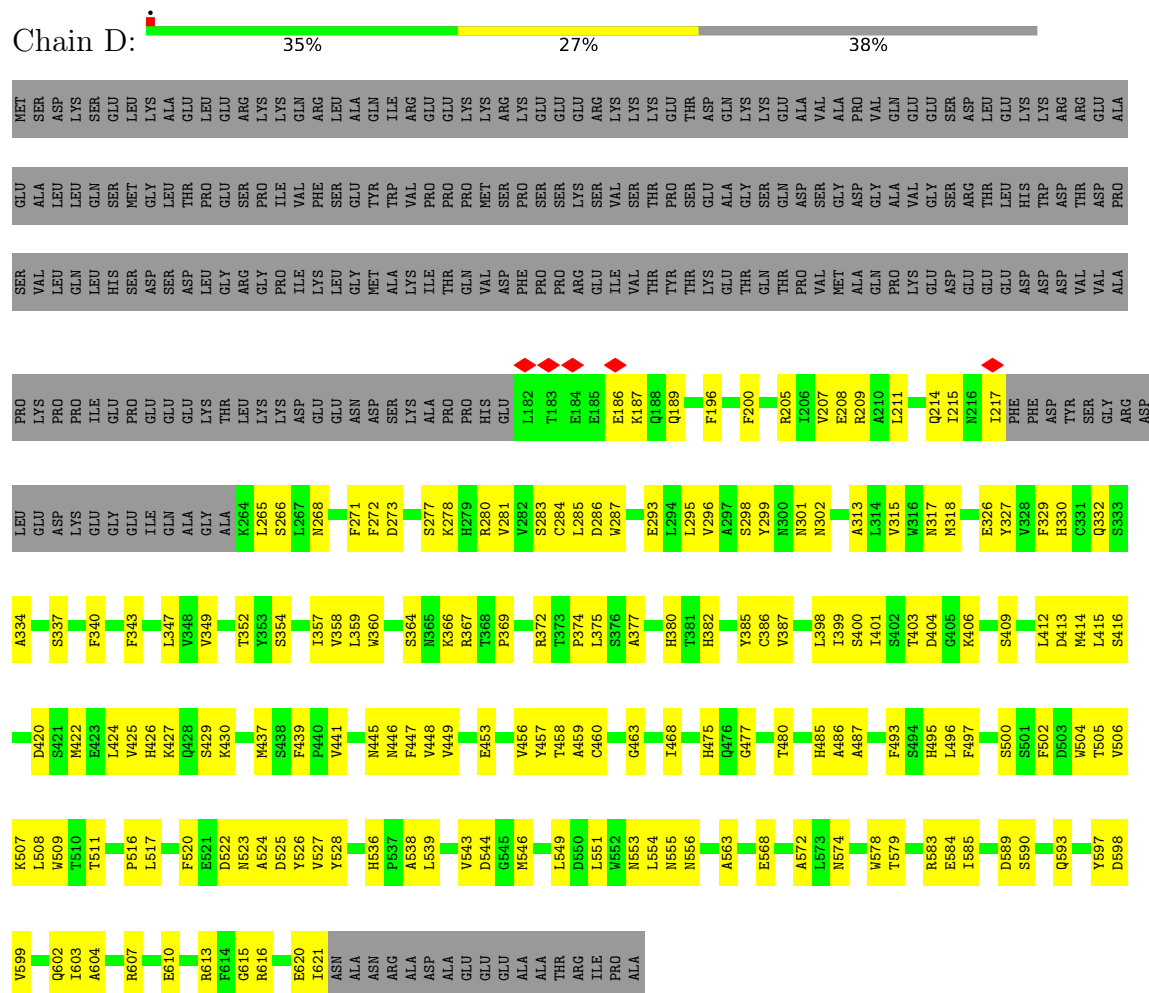


- Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

Chain C:  60% 38%

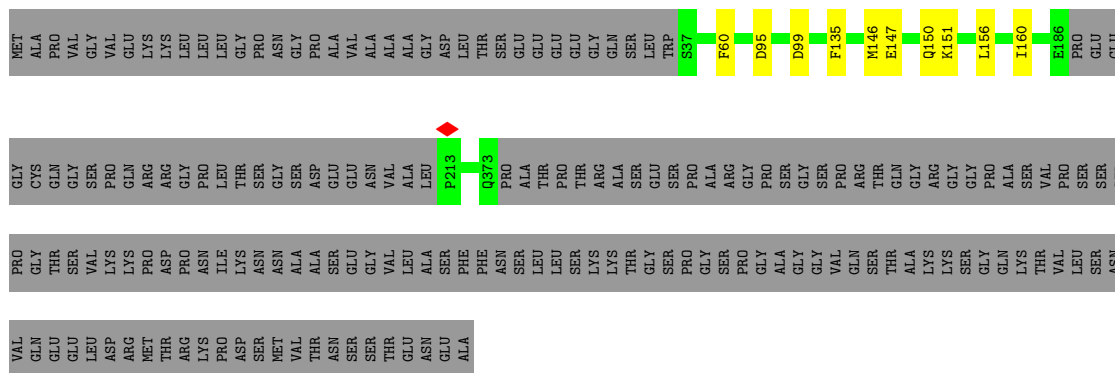


• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

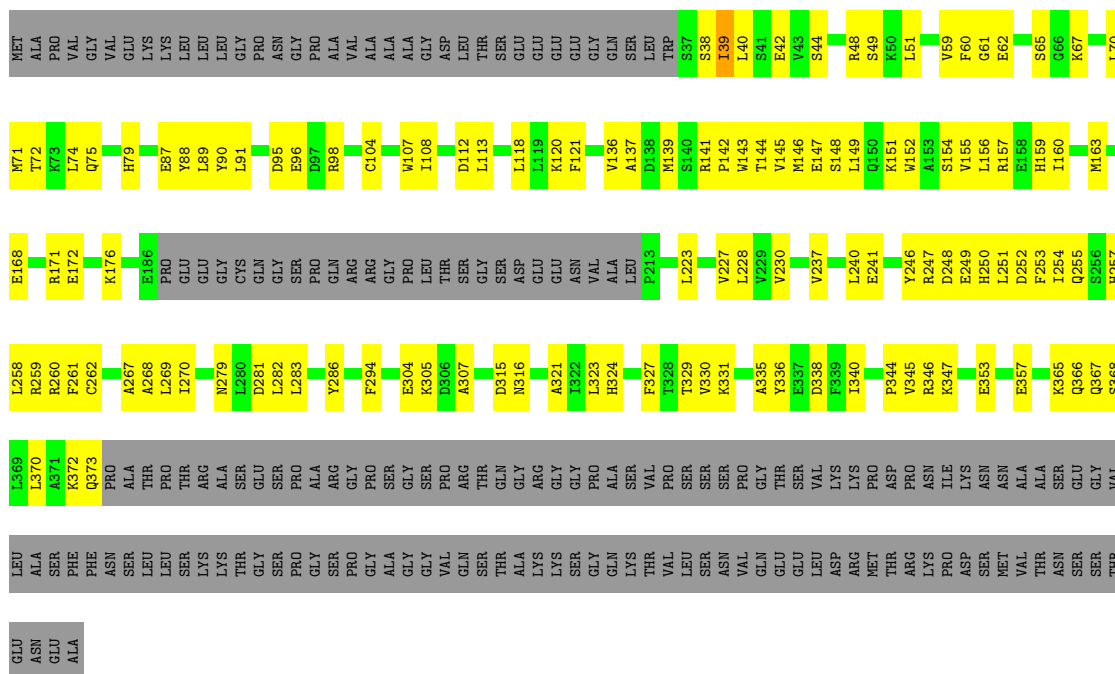
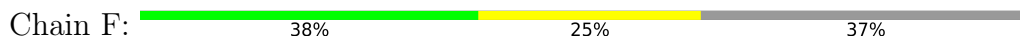


• Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

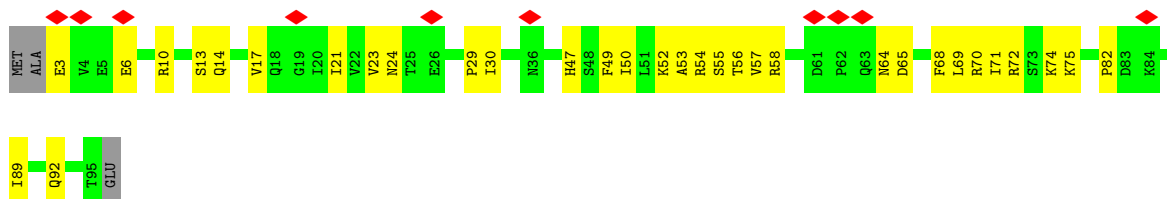




- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

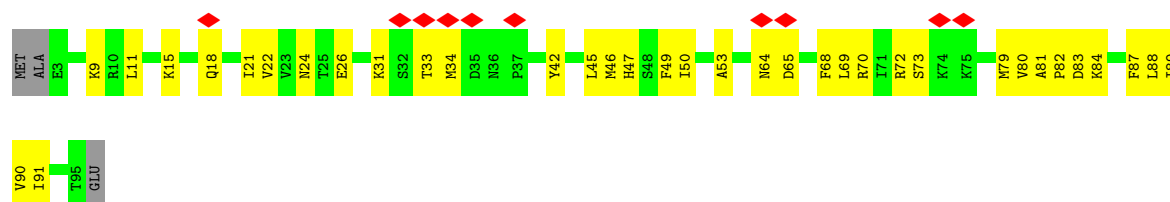


- Molecule 4: Dynein light chain roadblock-type 1

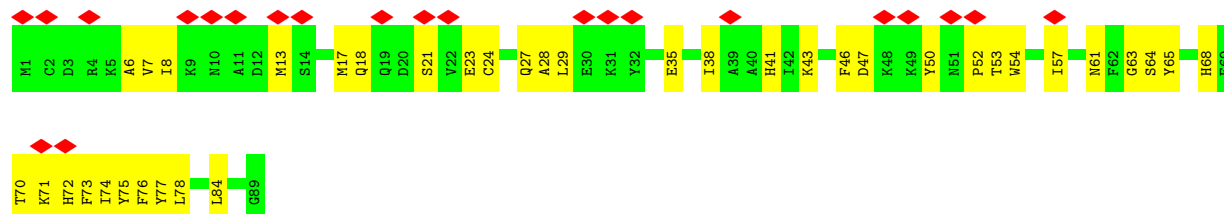


- Molecule 4: Dynein light chain roadblock-type 1

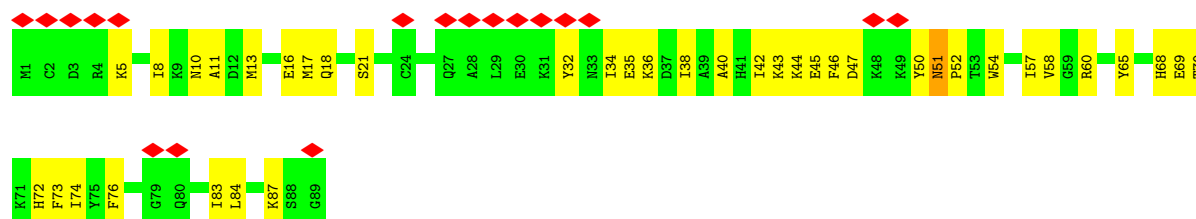




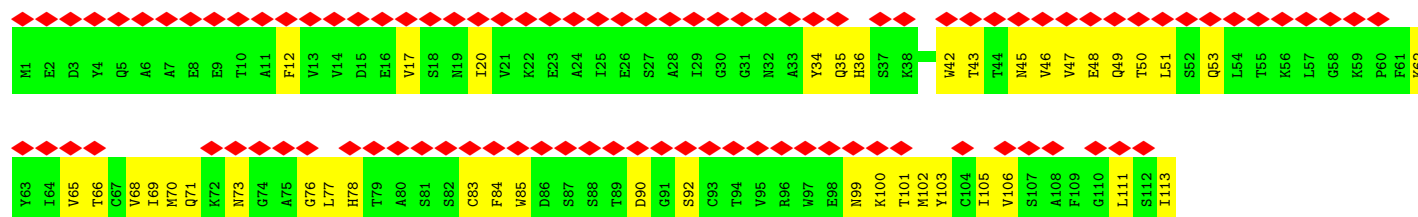
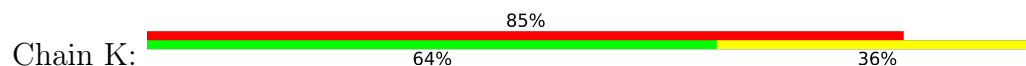
• Molecule 5: Dynein light chain 1, cytoplasmic



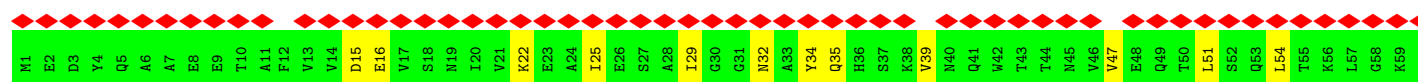
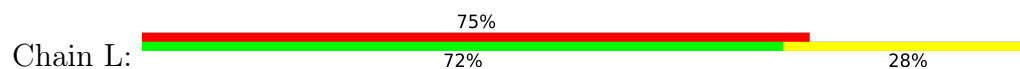
• Molecule 5: Dynein light chain 1, cytoplasmic

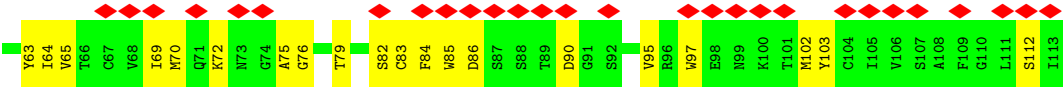


• Molecule 6: Dynein light chain Tctex-type 1



• Molecule 6: Dynein light chain Tctex-type 1







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103097	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	2.240	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

### 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	0.19	0/37419	0.42	1/50625 (0.0%)
1	B	0.15	0/37249	0.37	2/50395 (0.0%)
2	C	0.18	0/3195	0.40	0/4351
2	D	0.15	0/3195	0.41	0/4351
3	E	0.16	0/2573	0.38	0/3473
3	F	0.16	0/2573	0.38	0/3473
4	G	0.14	0/752	0.37	0/1017
4	H	0.15	0/752	0.42	0/1017
5	I	0.21	0/744	0.48	0/997
5	J	0.17	0/744	0.47	0/997
6	K	0.15	0/888	0.40	0/1203
6	L	0.15	0/888	0.38	0/1203
All	All	0.17	0/90972	0.40	3/123102 (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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3449	GLU	CA-C-N	-7.56	108.82	120.31
1	B	3449	GLU	C-N-CA	-7.56	108.82	120.31
1	A	1402	GLU	N-CA-C	-6.67	106.35	114.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3438	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	848	0
1	B	36527	0	36809	988	0
2	C	3112	0	2964	10	0
2	D	3112	0	2964	129	0
3	E	2518	0	2525	5	0
3	F	2518	0	2525	99	0
4	G	742	0	768	29	0
4	H	742	0	768	32	0
5	I	728	0	714	41	0
5	J	728	0	714	51	0
6	K	872	0	846	37	0
6	L	872	0	846	32	0
7	A	81	0	36	2	0
7	B	81	0	36	2	0
8	A	31	0	12	0	0
8	B	31	0	12	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
All	All	89391	0	89501	2182	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 2182 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:A:3257:SER:HA	1:A:3260:ILE:HD12	1.20	1.10
1:A:185:LYS:HE3	1:B:189:LEU:HD13	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3441:GLU:HA	1:A:3444:ILE:HD12	1.54	0.89
1:B:333:ASN:HA	1:B:336:MET:HE3	1.56	0.88
1:A:457:ARG:O	1:A:461:ALA:N	2.08	0.87

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	4530/4646 (98%)	4360 (96%)	165 (4%)	5 (0%)	48	83
1	B	4509/4646 (97%)	4383 (97%)	122 (3%)	4 (0%)	48	83
2	C	390/638 (61%)	364 (93%)	26 (7%)	0	100	100
2	D	390/638 (61%)	367 (94%)	23 (6%)	0	100	100
3	E	307/492 (62%)	292 (95%)	15 (5%)	0	100	100
3	F	307/492 (62%)	291 (95%)	14 (5%)	2 (1%)	18	55
4	G	91/96 (95%)	87 (96%)	4 (4%)	0	100	100
4	H	91/96 (95%)	85 (93%)	6 (7%)	0	100	100
5	I	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
5	J	87/89 (98%)	82 (94%)	4 (5%)	1 (1%)	11	45
6	K	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
6	L	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
All	All	11011/12148 (91%)	10610 (96%)	389 (4%)	12 (0%)	49	83

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	ASN
1	A	3384	ARG

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Mol	Chain	Res	Type
1	B	540	LYS
1	B	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%)	4038 (100%)	6 (0%)	88	88
1	B	4028/4125 (98%)	4028 (100%)	0	100	100
2	C	344/557 (62%)	344 (100%)	0	100	100
2	D	344/557 (62%)	344 (100%)	0	100	100
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
All	All	9842/10736 (92%)	9836 (100%)	6 (0%)	87	88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3447	TYR
1	A	3454	LEU
1	A	3461	ILE
1	A	3437	ILE
1	A	3434	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2476	HIS
1	B	3563	GLN
1	B	2560	HIS
1	B	3104	GLN
1	B	4156	ASN

### 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 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	ATP	B	4702	9	32,33,33	0.38	0	48,52,52	0.29	0
8	ATP	A	4702	9	32,33,33	0.38	0	48,52,52	0.29	0
7	ADP	B	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
7	ADP	B	4701	9	28,29,29	1.40	5 (17%)	43,45,45	1.81	9 (20%)
7	ADP	A	4704	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	8 (18%)
7	ADP	A	4701	9	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
7	ADP	B	4703	-	28,29,29	1.39	4 (14%)	43,45,45	1.88	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)

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	ATP	B	4702	9	-	6/22/38/38	0/3/3/3
8	ATP	A	4702	9	-	6/22/38/38	0/3/3/3
7	ADP	B	4704	-	-	3/16/32/32	0/3/3/3
7	ADP	B	4701	9	-	3/16/32/32	0/3/3/3
7	ADP	A	4704	-	-	2/16/32/32	0/3/3/3
7	ADP	A	4701	9	-	3/16/32/32	0/3/3/3
7	ADP	B	4703	-	-	0/16/32/32	0/3/3/3
7	ADP	A	4703	-	-	2/16/32/32	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4703	ADP	C5-C4	4.67	1.47	1.39
7	B	4703	ADP	C5-C4	4.66	1.47	1.39
7	A	4704	ADP	C5-C4	4.63	1.47	1.39
7	B	4704	ADP	C5-C4	4.62	1.47	1.39
7	B	4701	ADP	C5-C4	4.56	1.47	1.39

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	4703	ADP	C5-C4-N3	-6.15	118.25	126.72
7	B	4703	ADP	C5-C4-N3	-6.02	118.42	126.72
7	B	4704	ADP	C5-C4-N3	-5.87	118.63	126.72
7	A	4704	ADP	C5-C4-N3	-5.79	118.75	126.72
7	B	4701	ADP	C5-C4-N3	-5.78	118.77	126.72

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4701	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
7	A	4701	ADP	C5'-O5'-PA-O2A
7	A	4701	ADP	C5'-O5'-PA-O3A
7	A	4704	ADP	C5'-O5'-PA-O1A
7	B	4701	ADP	C5'-O5'-PA-O1A

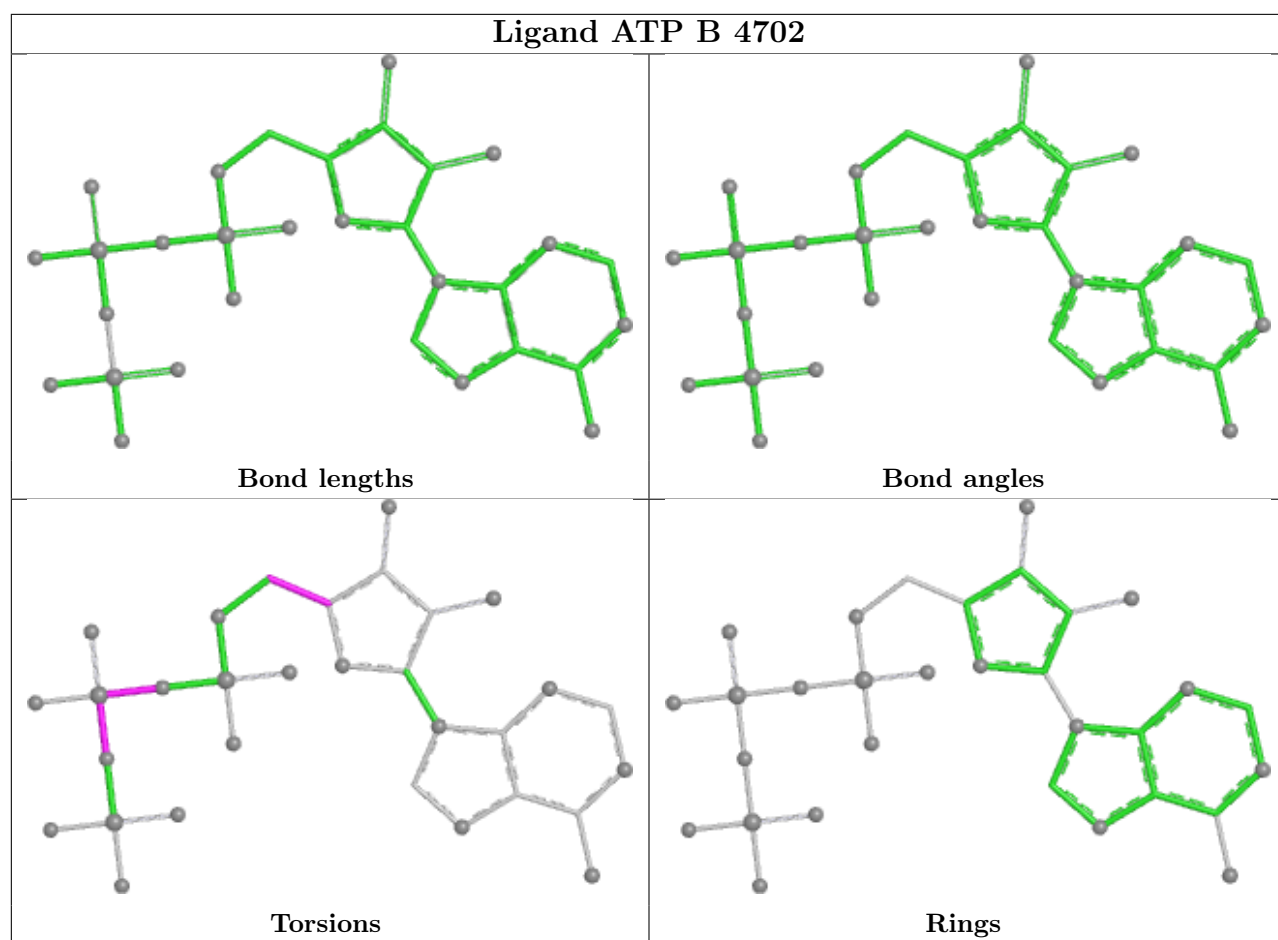
There are no ring outliers.

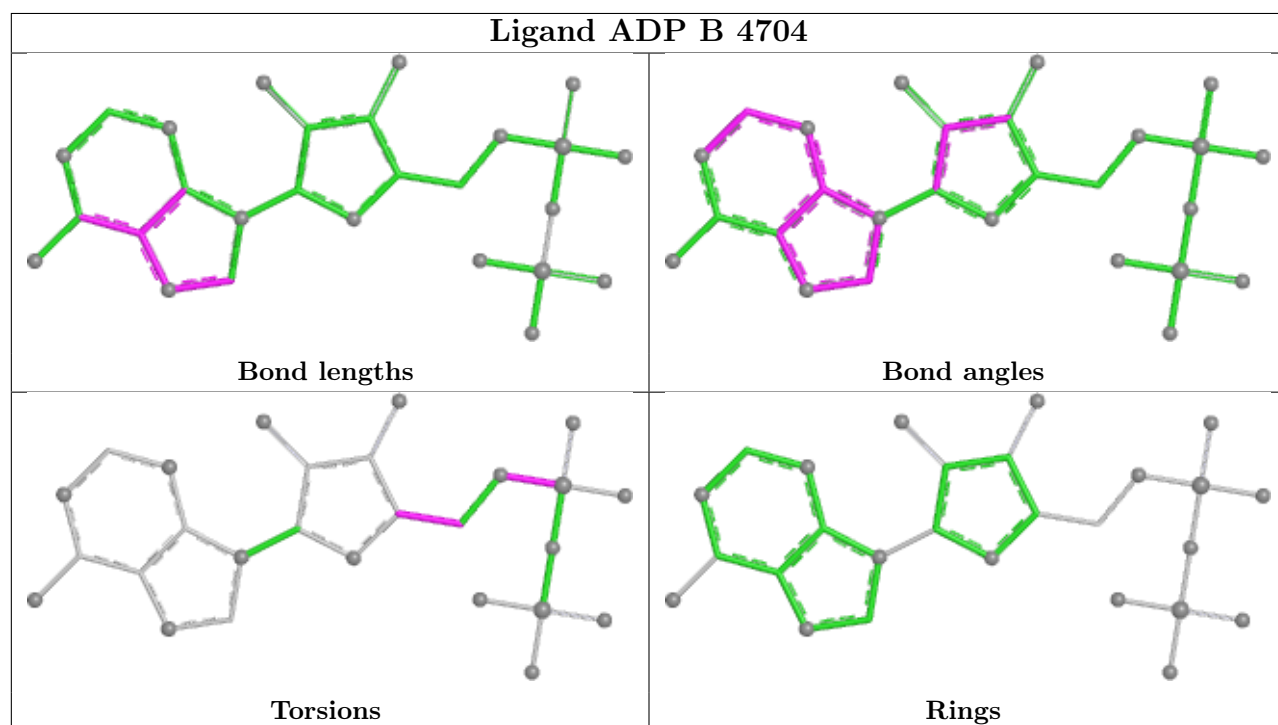
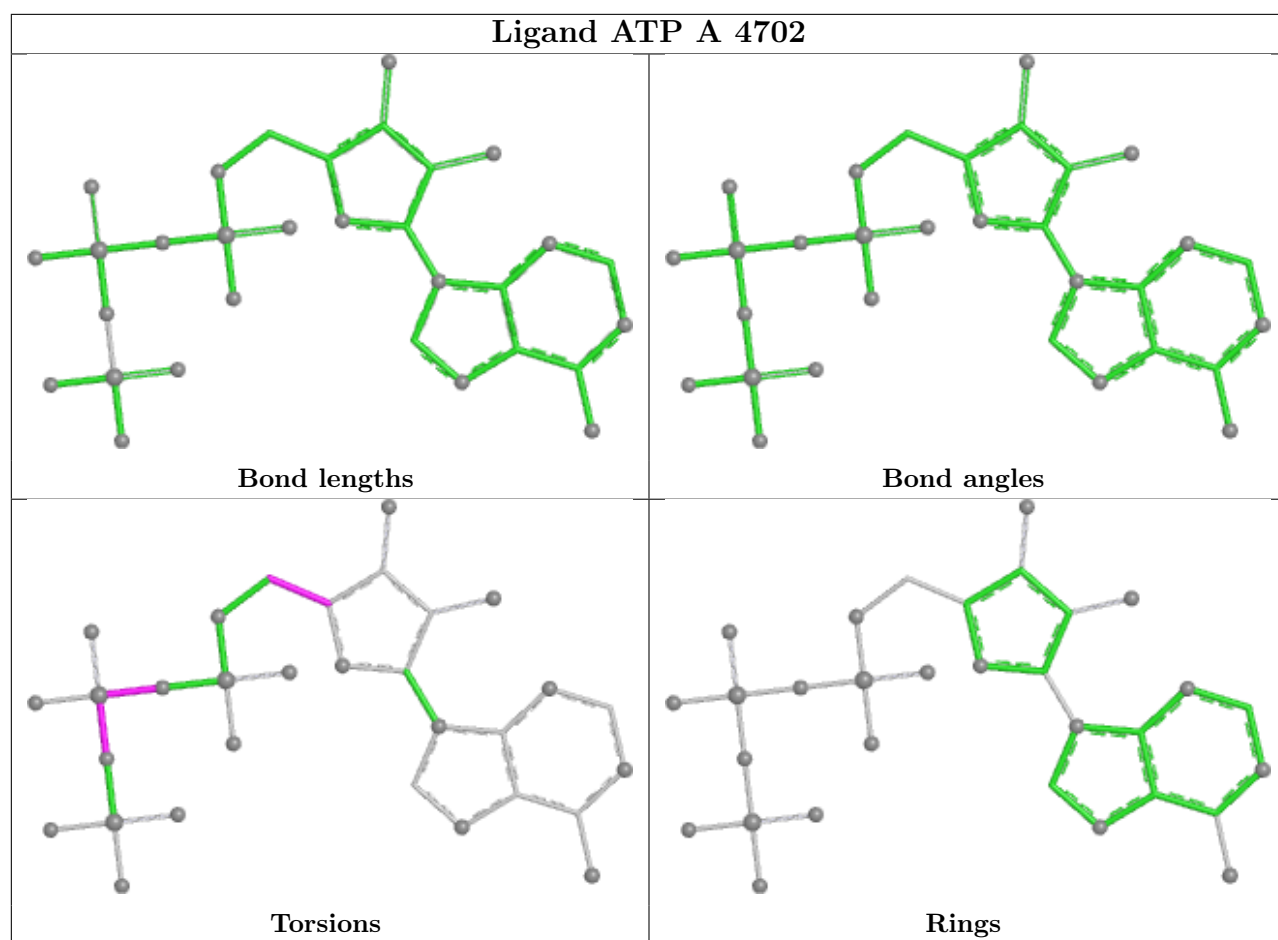
4 monomers are involved in 4 short contacts:

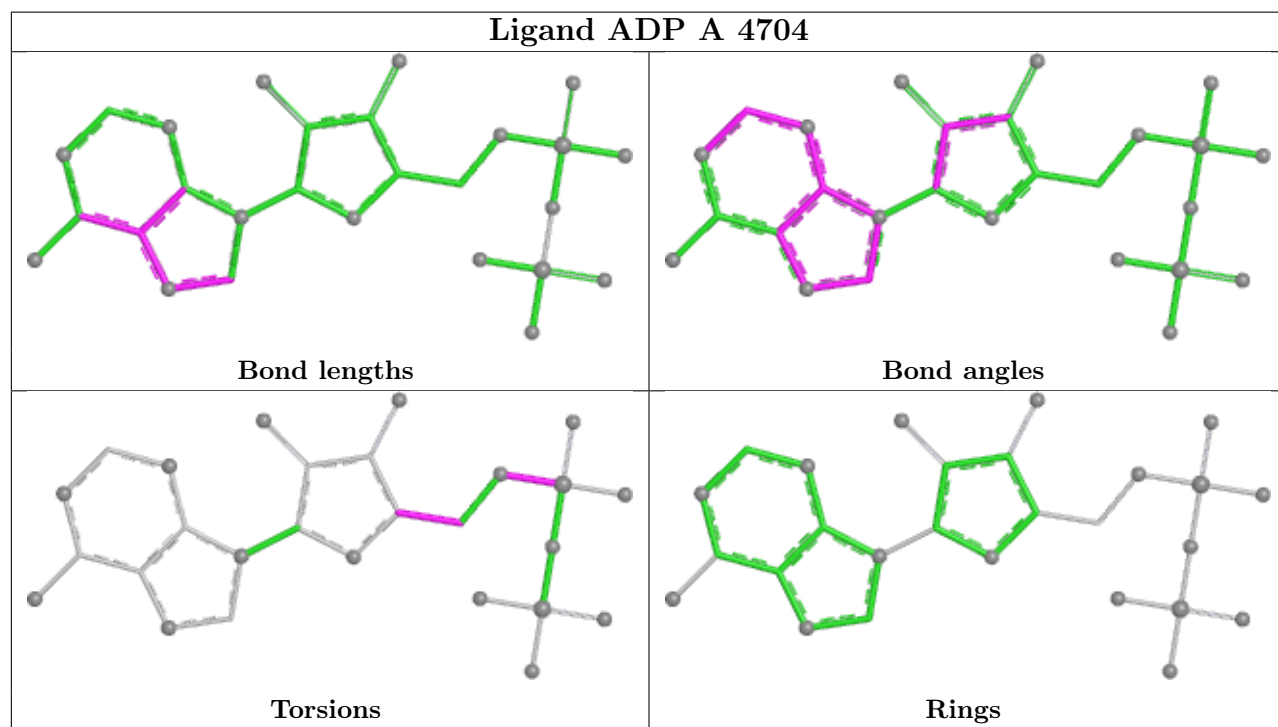
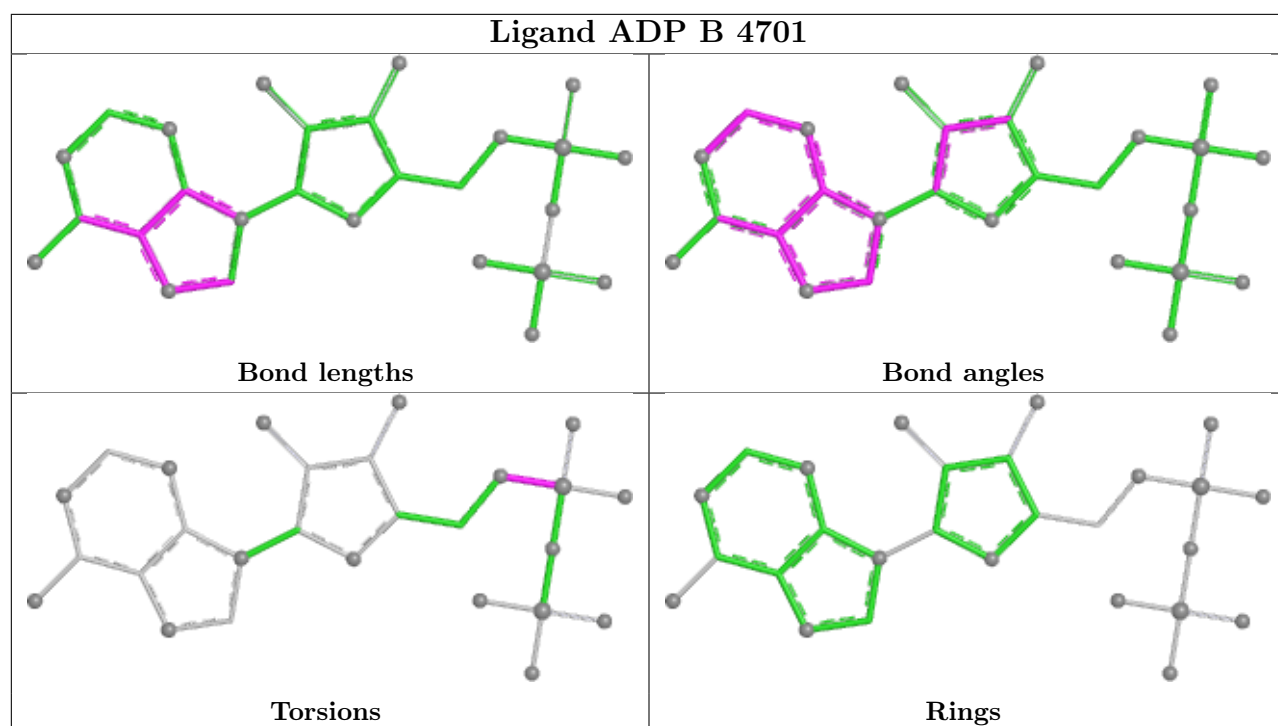
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	4704	ADP	1	0
7	B	4701	ADP	1	0
7	A	4701	ADP	1	0
7	A	4703	ADP	1	0

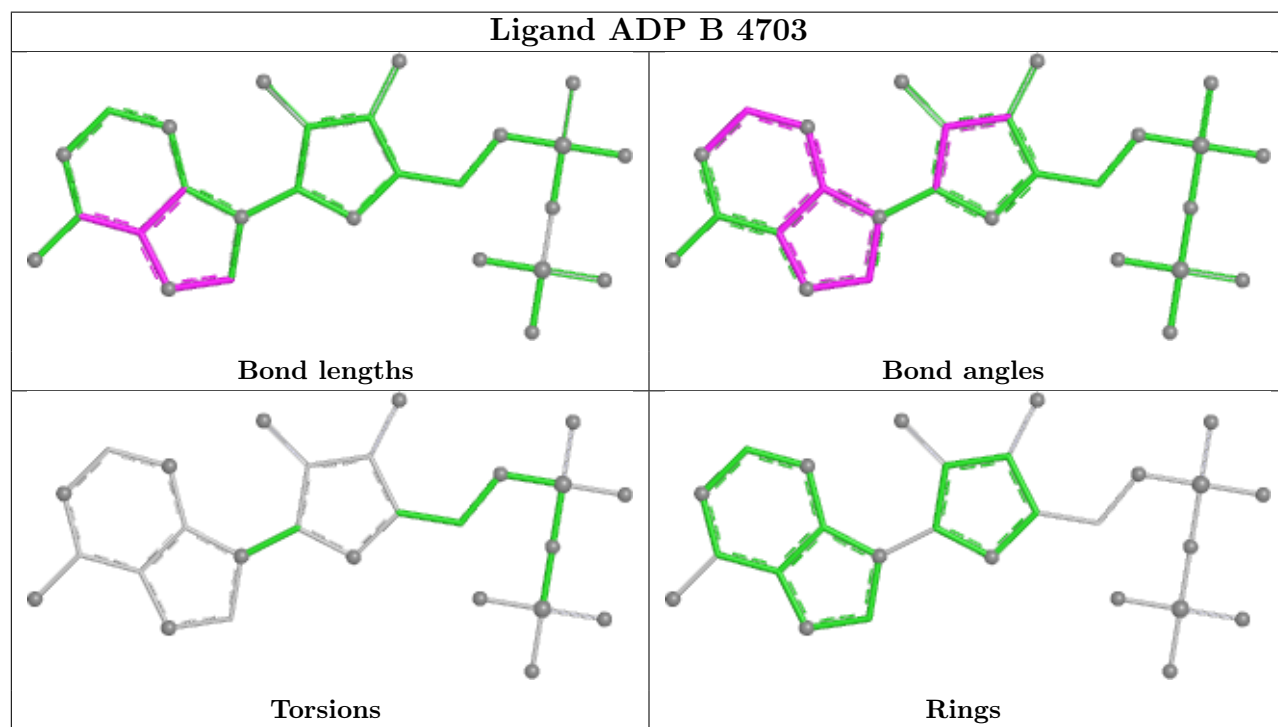
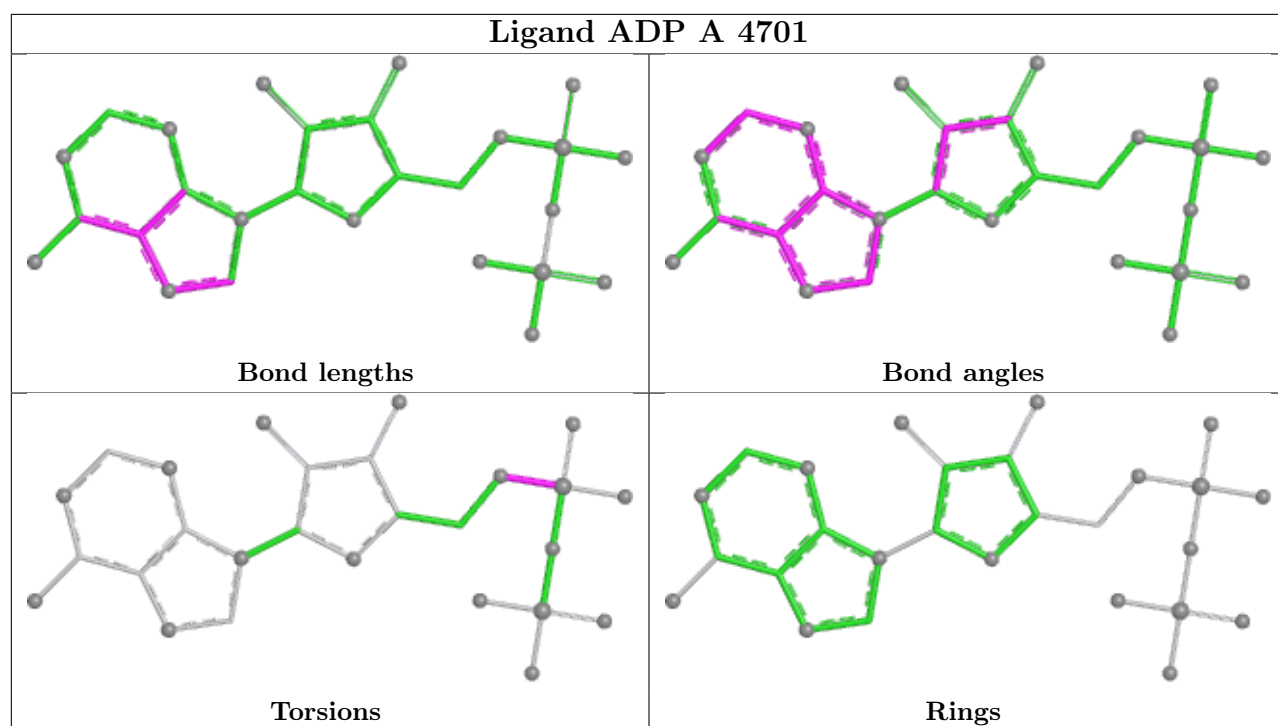
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

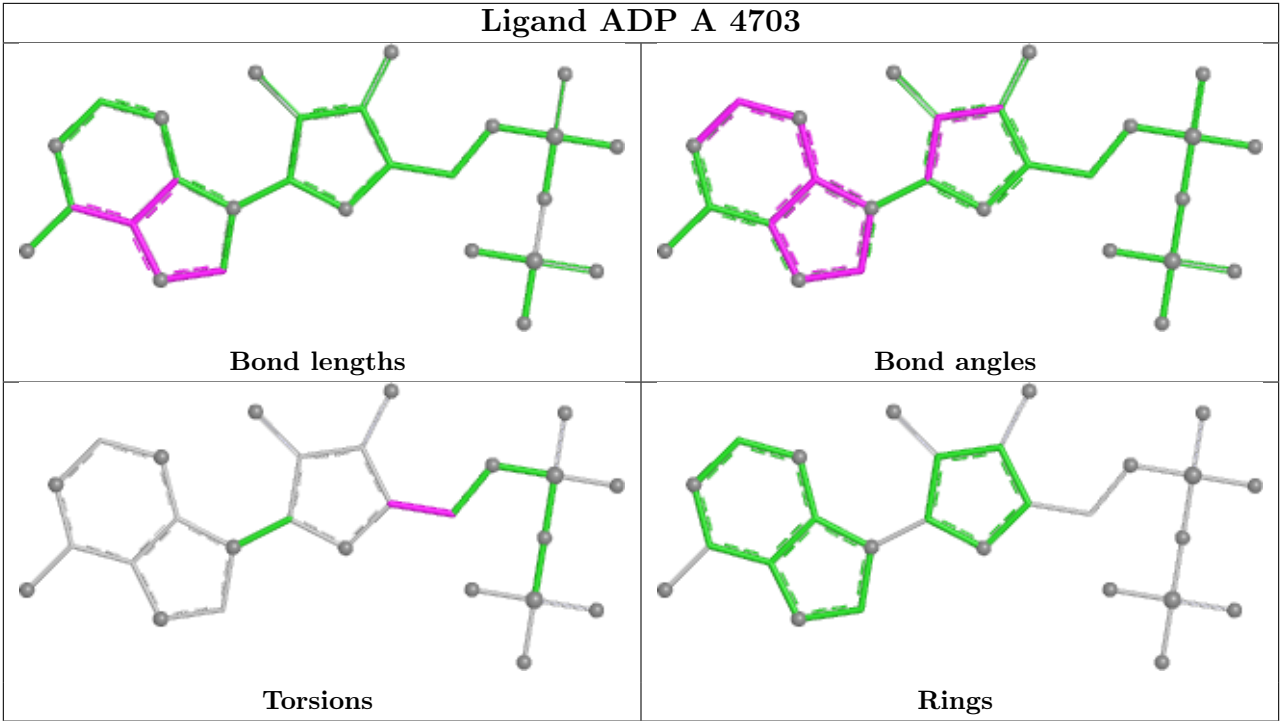












5.7 Other polymers ⓘ

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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1456:GLU	C	1457:MET	N	2.96

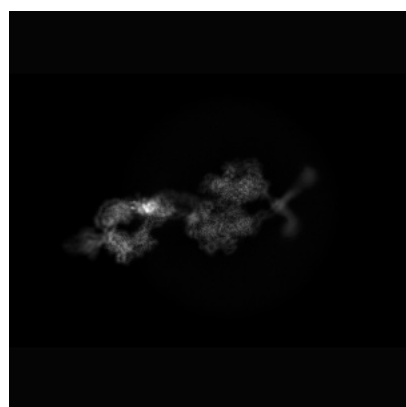
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47381. These allow visual inspection of the internal detail of the map and identification of artifacts.

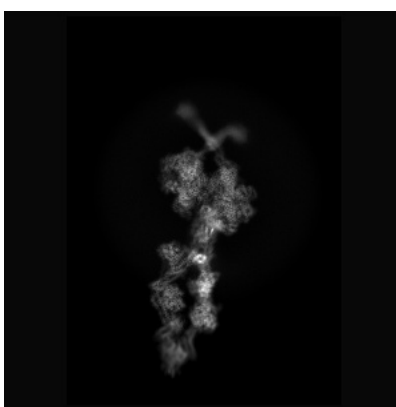
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

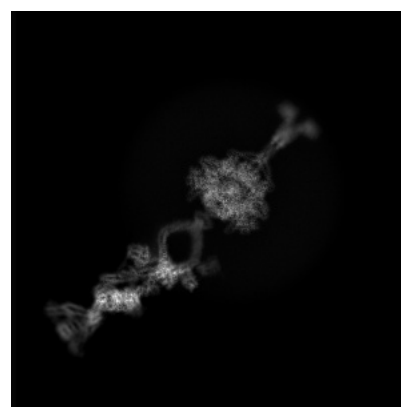
#### 6.1.1 Primary map



X



Y

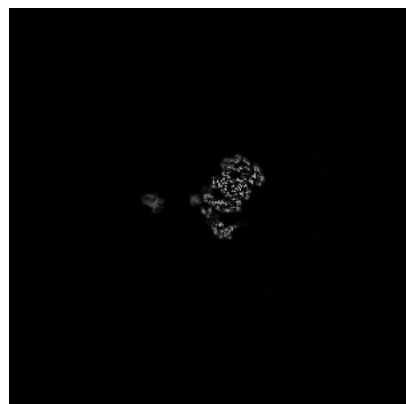


Z

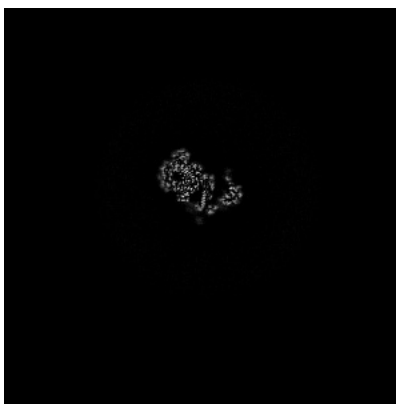
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 210



Y Index: 210

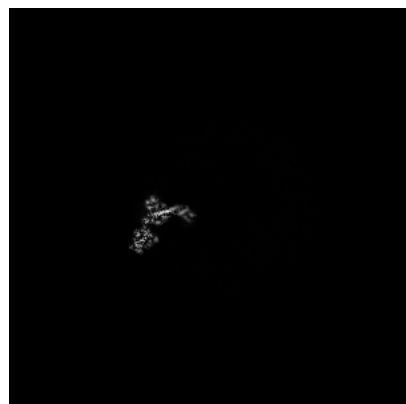


Z Index: 210

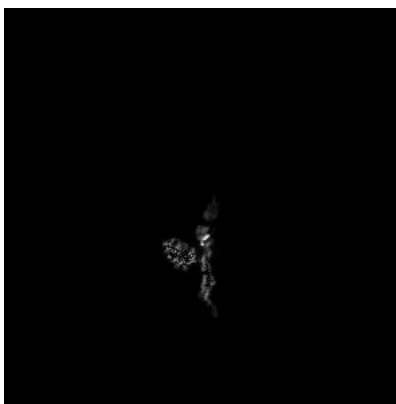
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 162



Y Index: 144

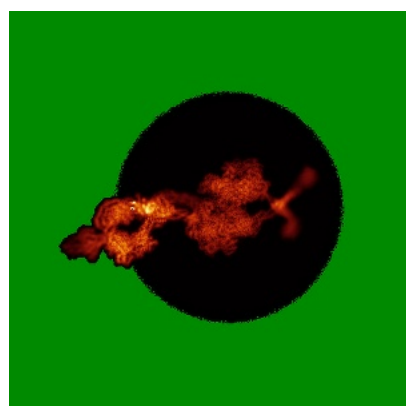


Z Index: 212

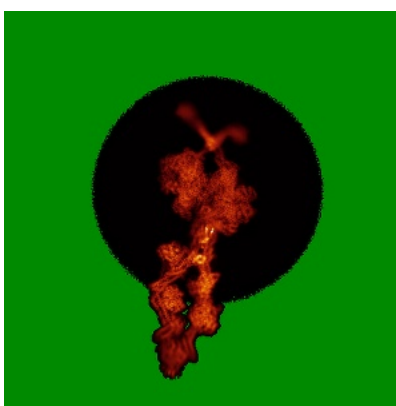
The images above show the largest variance slices of the map in three orthogonal directions.

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

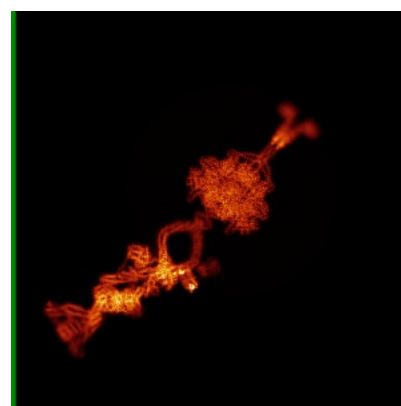
### 6.4.1 Primary map



X



Y

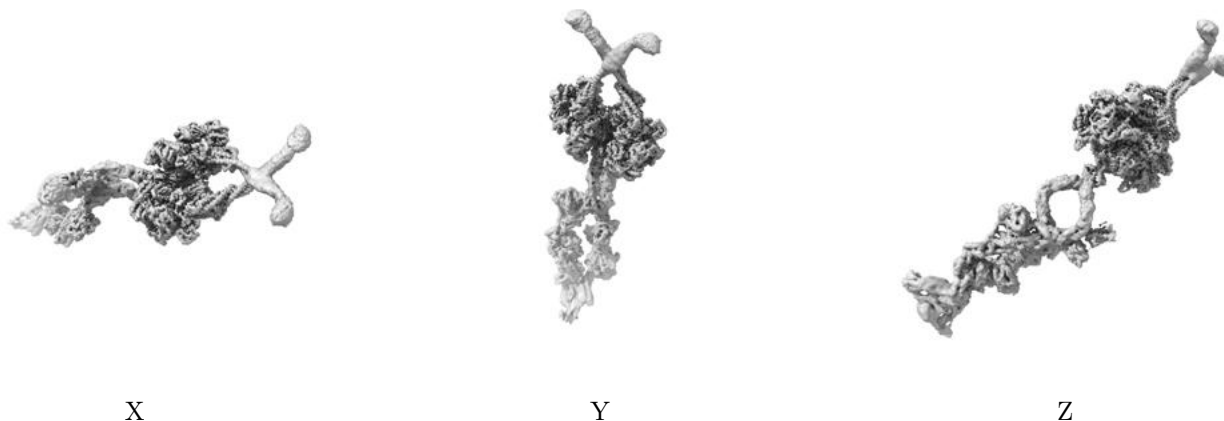


Z

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](#)

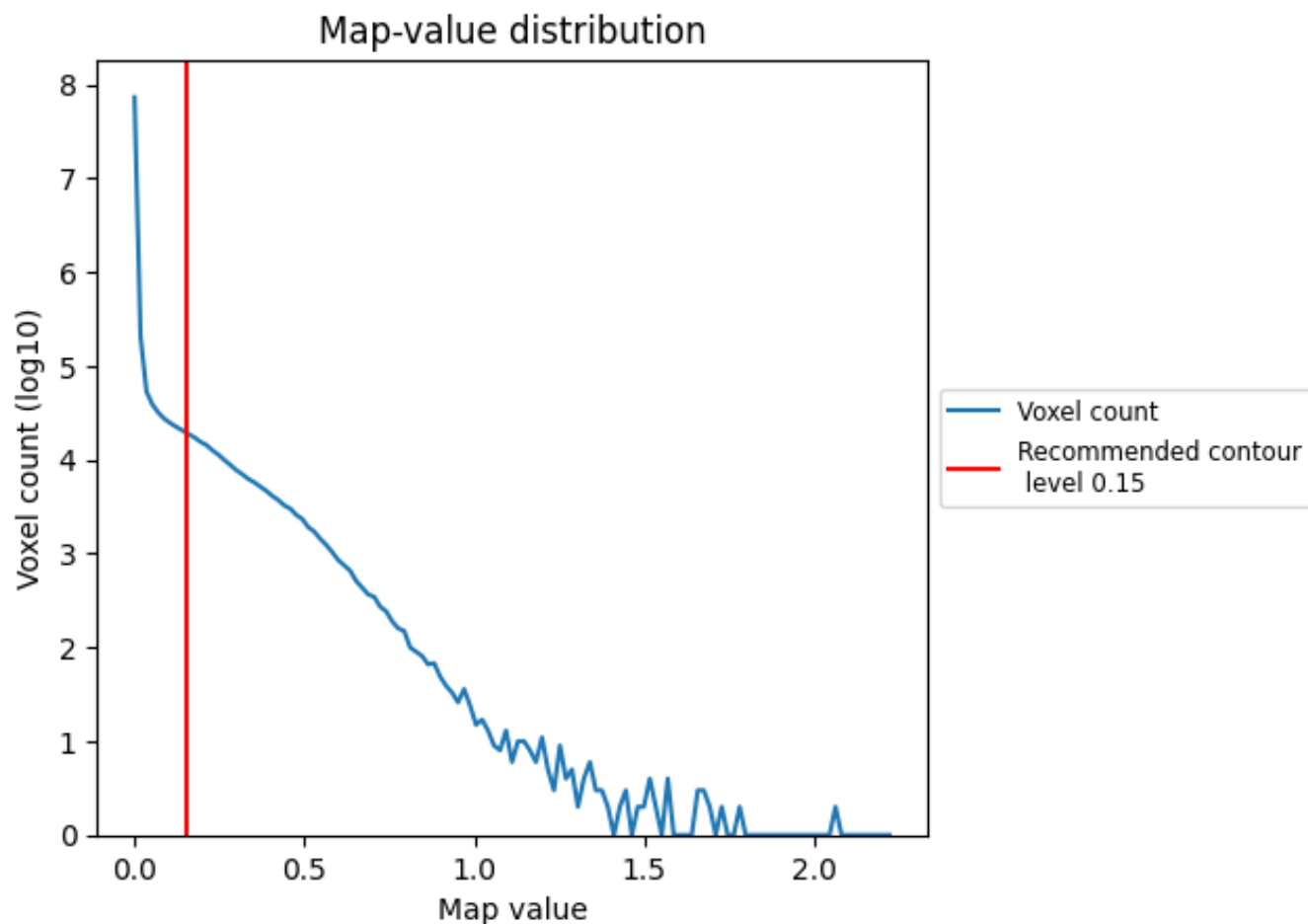
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

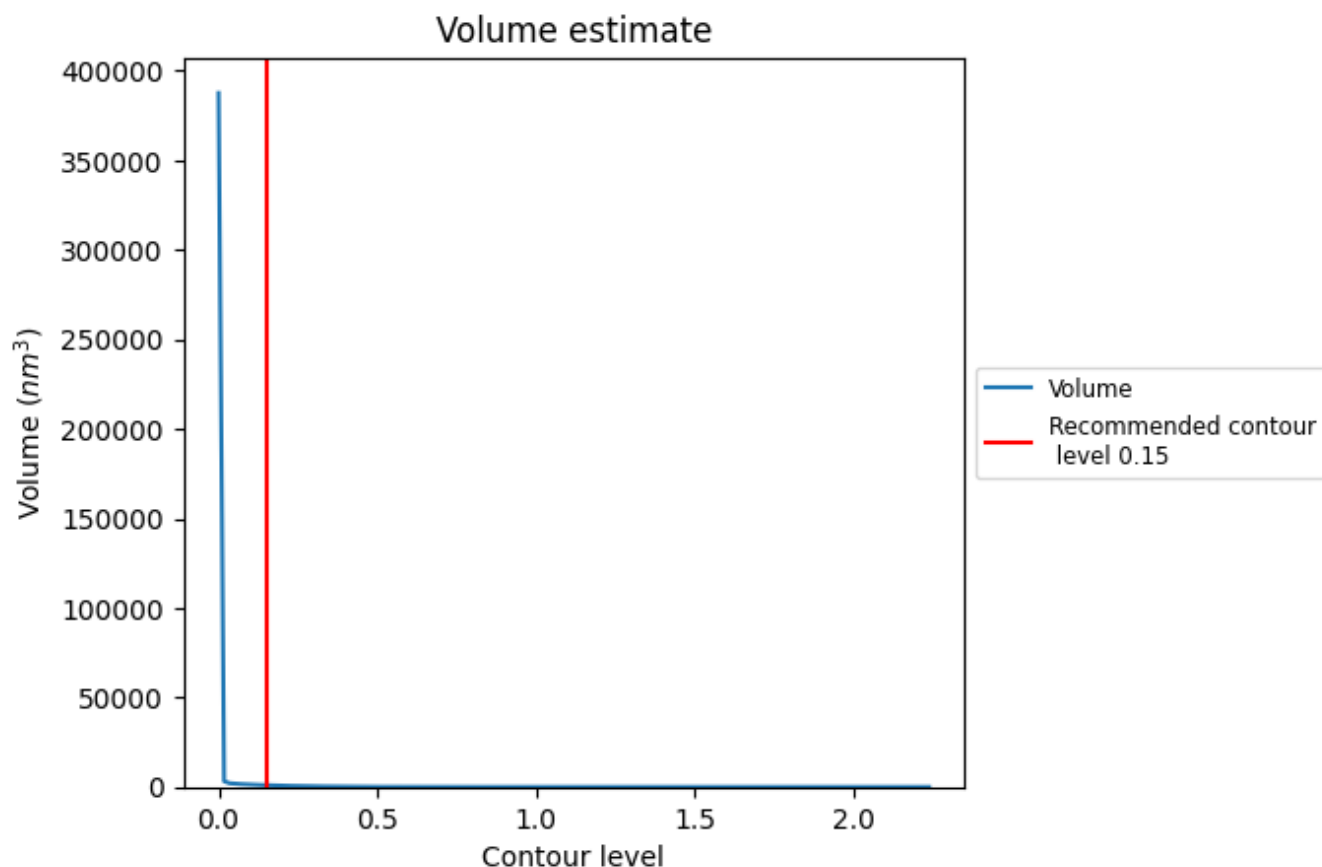
This section contains the results of statistical analysis of the map.

### 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.

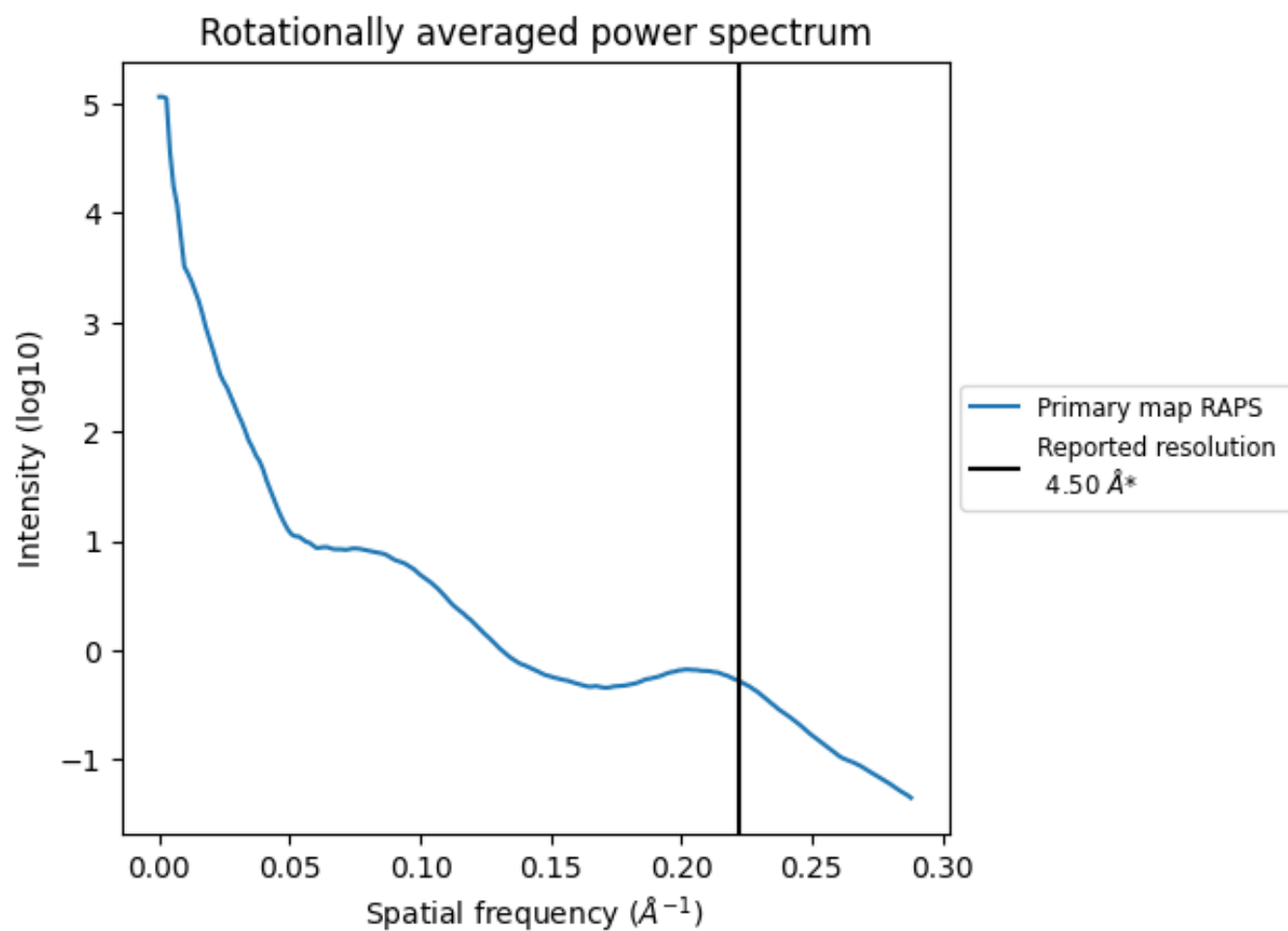
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 984  $\text{nm}^3$ ; this corresponds to an approximate mass of 888 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.

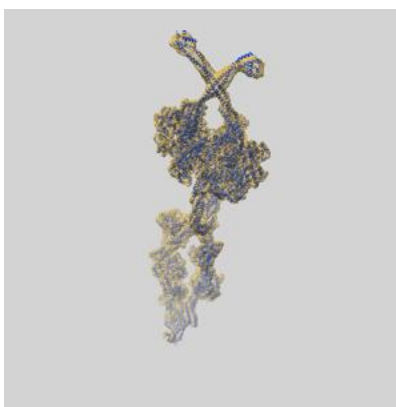
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47381 and PDB model 9E12. Per-residue inclusion information can be found in section [3](#) on page [7](#).

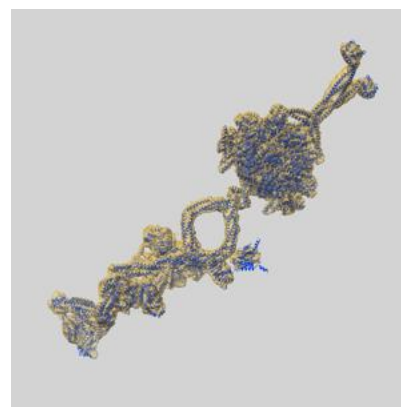
### 9.1 Map-model overlay [i](#)



X



Y



Z

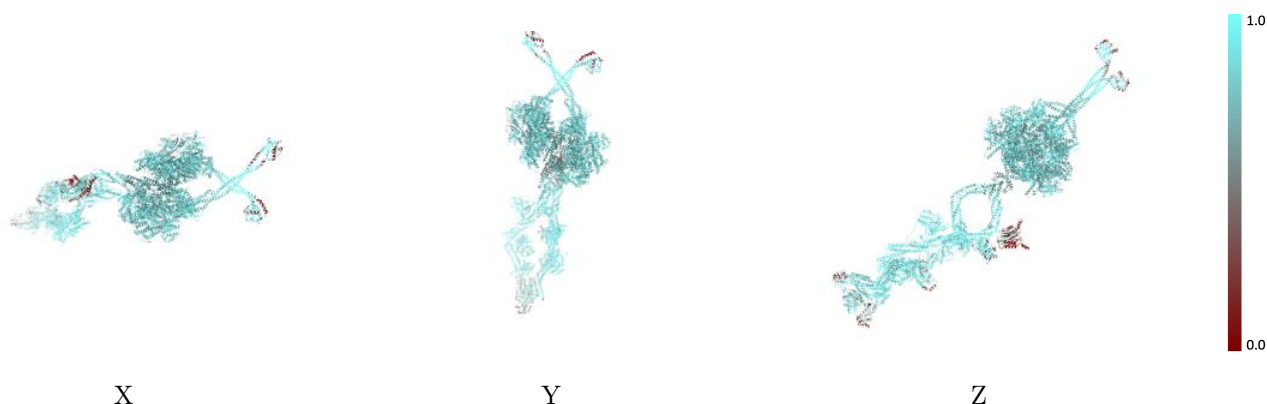
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



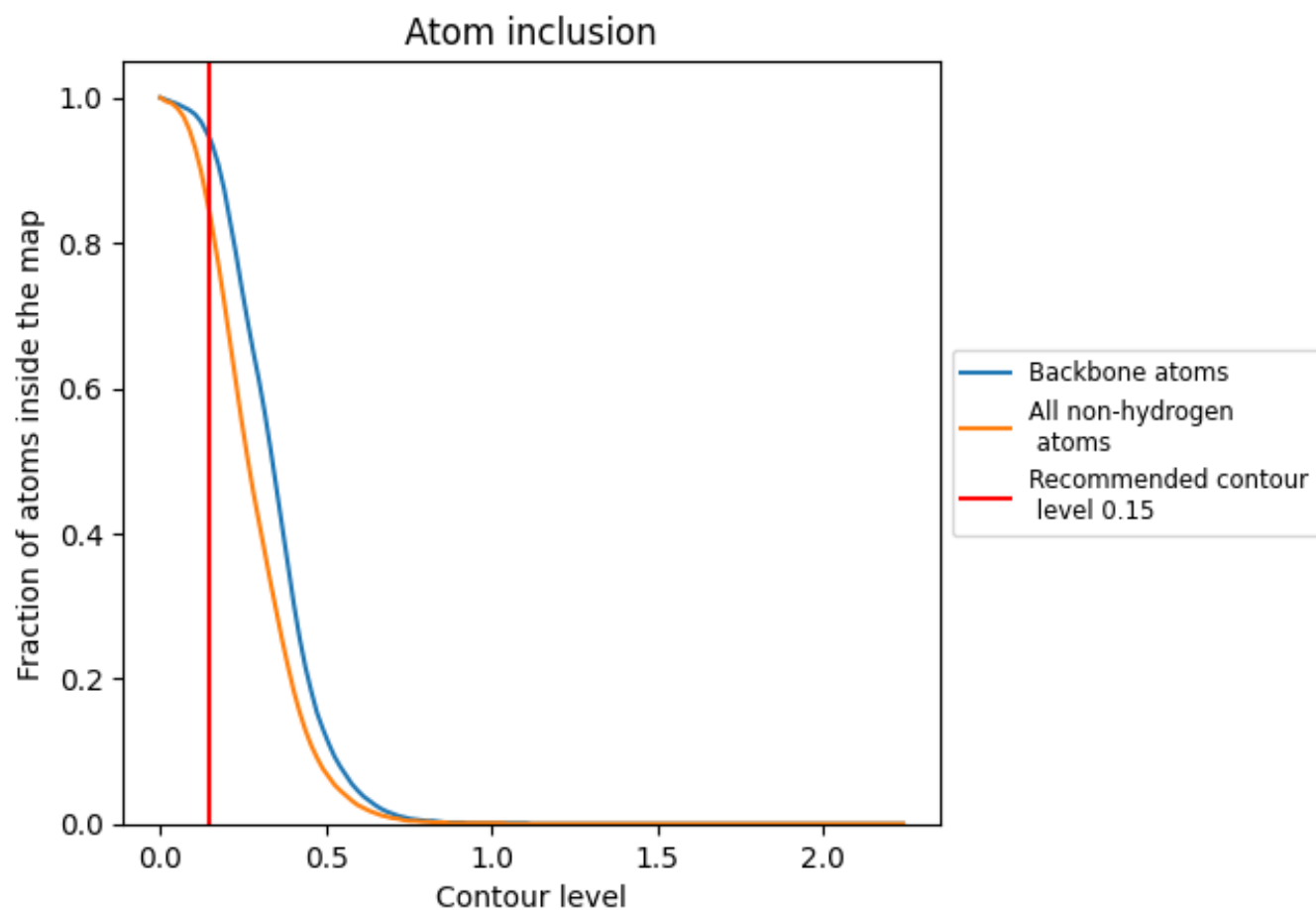
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



























## 9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 84% 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	 0.8380	 0.3430
A	 0.8390	 0.3700
B	 0.8430	 0.3640
C	 0.9250	 0.3340
D	 0.9340	 0.2750
E	 0.9430	 0.3160
F	 0.9380	 0.2850
G	 0.7930	 0.1060
H	 0.7960	 0.1400
I	 0.6740	 0.0410
J	 0.7800	 0.0680
K	 0.1630	 0.0320
L	 0.2470	 0.0410

