



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2025 – 07:24 PM EDT

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

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

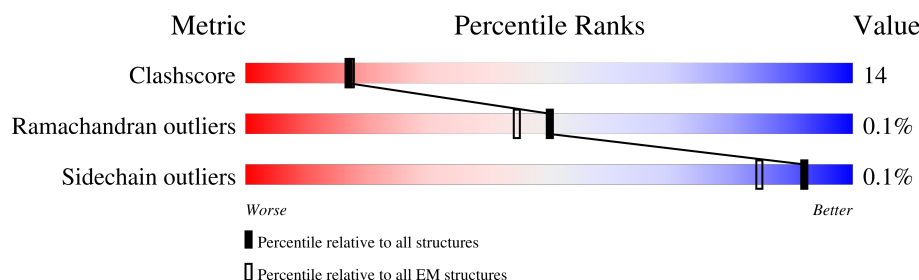
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	
3	E	492	
3	F	492	
4	G	96	
4	H	96	

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Mol	Chain	Length	Quality of chain
5	I	89	<div><div></div><div>25%</div><div>57%</div><div>43%</div></div>
5	J	89	<div><div></div><div>20%</div><div>56%</div><div>43%</div></div>
6	K	113	<div><div></div><div>85%</div><div>64%</div><div>36%</div></div>
6	L	113	<div><div></div><div>75%</div><div>72%</div><div>28%</div></div>

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		

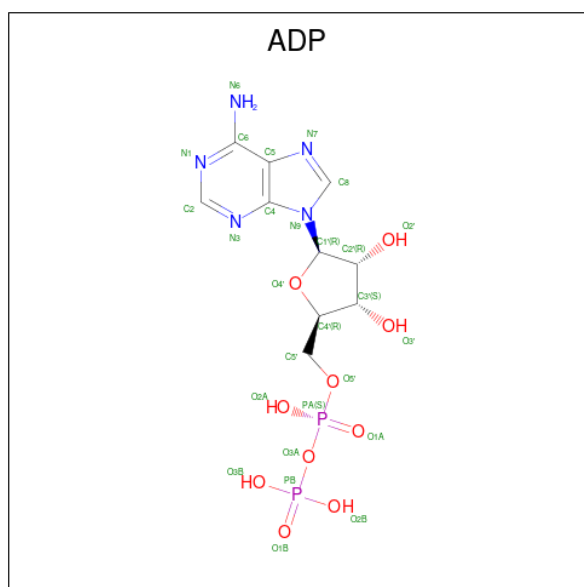
- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

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).



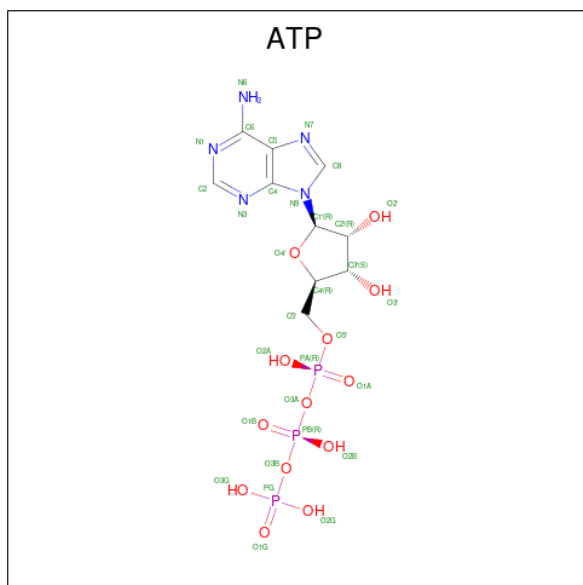
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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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

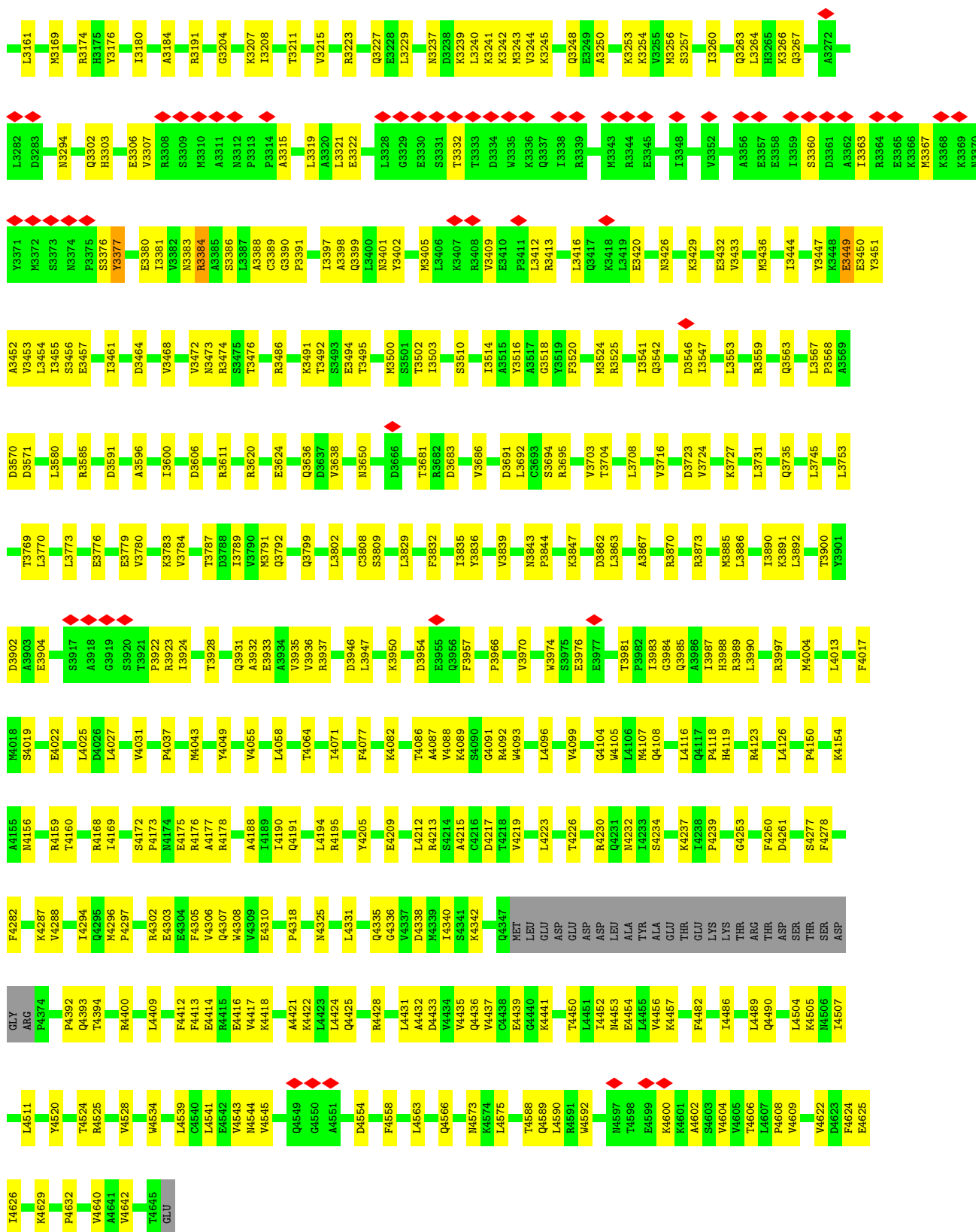


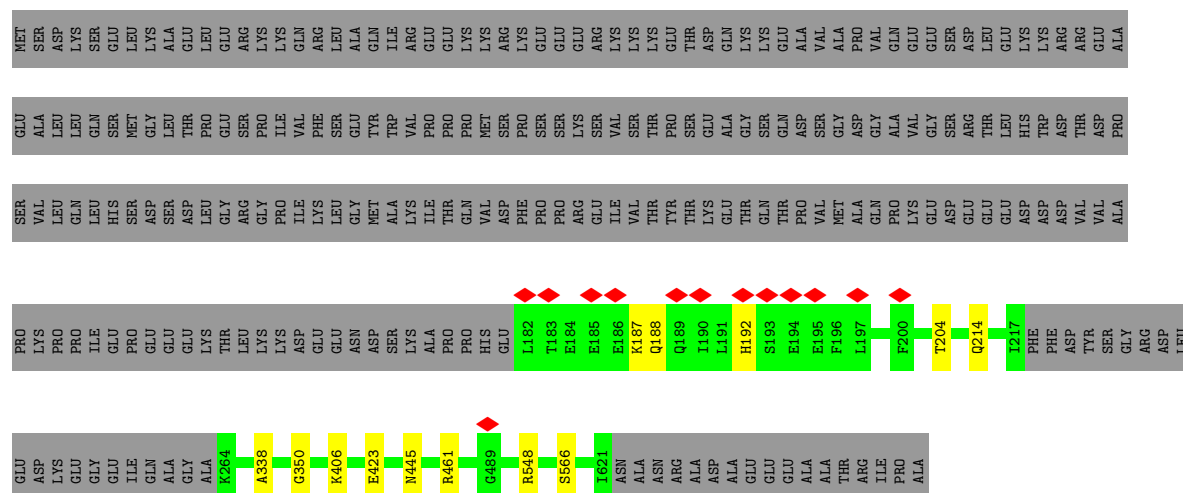
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E1215	Q1440	K1568	K1729	P1848	I1997	C2142	D2308	Q2416	P2570	P2722	D2917	Q3043	R3175
G1219	K1441	P1562	D1734	Q1850	L2001	V2146	N2314	I2422	T2571	L2723	D2917	M3043	R3176
F1221	B1442	Q1566	T1737	V1853	V2006	L2149	L2319	M2423	D2573	R2726	I2922	L3044	L3177
N1222	A1444	R1567	Q1746	Q1856	N2012	E2152	D2321	S2429	V2575	P2732	T2944	D3045	I3180
M1225	D1448	A1577	A1747	M1861	T2017	D2153	D2324	E2444	R2576	V2733	R2948	E3048	R3191
R1226	M1457	K1580	Q1748	A1862	L1750	L2154	L2324	H2445	L2581	S2743	L2934	E3049	S3192
K1228	A1458	L1751	V1751	Q1876	S2026	P2155	L2156	L2449	V2582	L2747	G2937	L3050	S3192
D1229	L1459	V1582	L1752	D1877	L2039	L2157	E2331	L2452	T2583	R2753	T2944	L3051	L3194
	E1461	S1583	Q1755	K1878	T2042	L2161	E2334	R2453	T2583	R2753	T2944	Q3057	R3195
I1232	K1464	L1584	I1756	L1890	Q2047	E2174	N2338	L2458	L2591	L2769	R2948	R3060	R3196
Q1233	Q1465	L1587	E1760	P1907	N2053	T2176	F2343	M2461	L2592	M2773	M2953	M3068	R3197
E1262	V1469	V1591	E1763	G1911	T2061	R2179	Q2346	L2462	L2603	F2776	L2956	P3070	K3207
N1270	L1477	L1619	T1764	S1915	A2062	E2180	D2347	H2463	L2605	M2779	T2961	T3081	T3211
L1306	V1478	R1623	A1765	S1915	E2063	E2181	L2348	Q2464	L2605	F2784	Y2967	L3085	T3212
D1308	L1486	R1628	M1769	E1934	V2064	E2205	V2356	A2465	D2614	Y2794	G2969	T3089	G3213
R1357	I1487	V1632	G1770	D1937	L2065	K2206	C2359	F2479	E2616	M2799	D2973	E3100	G3214
P1374	R1488	G1633	G1771	F1945	N2067	L2210	G2360	M2481	L2620	M2799	E2974	E3116	G3215
A1375	D1491	D1634	G1772	V1946	K2068	T2214	N2361	Q2482	L2623	L2813	D2975	Q3104	E3217
V1378	D1492	D1634	G1773	G1947	V2070	T2214	D2372	L2486	S2623	L2813	L2976	R3219	R3219
Q1379	L1493	L1638	A1775	Q1950	P2071	M2221	L2382	E2487	P2628	L2816	R2977	T3110	E3228
Y1380	V1497	V1647	A1776	V1951	F2072	M2222	L2382	Q2491	E2629	E2819	K2989	M3113	L3229
A1381	I1501	L1650	P1777	D1958	K2073	G2224	D2388	R2492	L2630	G2820	D2995	D3114	E3230
R1388	V1504	M1657	S1780	E1959	L2075	K2230	E2389	Y2493	T2634	L2824	N2998	L3115	V3231
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V1400	F1516	R1679	E1799	L1962	K2094	R2235	ASP	M2510	L2660	V2838	G3003	V3129	K3241
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D1519	D1519	E1680	P1802	E1965	V2096	L2244	ARG	E2517	E2665	R2843	L3005	D3131	K3243
E1402	E1518	E1680	L1803	M1967	L2097	E2248	ARG	Y2517	L2666	E2848	M3008	K3132	K3244
E1406	D1523	K1707	R1806	Q1973	V2098	K2257	LYS	I2521	I2667	T2852	L3011	L3133	K3245
A1407	E1524	V1711	K1807	Q1977	K2104	K2261	LYS	P2527	L2668	L2855	L3012	P3134	Q3248
L1408	K1526	L1717	H1810	I1978	R2107	L2279	GLU	N2531	L2671	R2863	E3016	Q3135	E3249
M1417	W1537	E1719	L1815	H1985	E2120	R2285	GLU	E2538	T2676	A2866	V3017	R3140	A3250
K1418	I1538	S1720	F1836	S1986	E2133	R2285	GLU	W2545	T2676	R2866	L3020	E3141	E3251
H1421	D1539	V1721	E1837	N1987	Q2134	S2290	GLU	W2548	F2682	K2879	L3026	V3148	K3252
V1425	V1540	E1722	M1838	N1988	E2135	L2295	ALA	Q2554	Q2698	Q2892	Y3026	F3149	K3253
V1426	R1543	V1724	L1839	Y1990	L2136	Q2296	S2410		Q2698	Q2892	R3030	V3150	K3254
E1428	Y1546	F1727	S1840	T1991	L2137	K2297	P2411		Q2707	R2896	T3031	T3153	V3255
D1436			R1843	K1992	T1993		M2412			L2897	E3035	L3154	S3257
													Q3258
													E3259
													T3260
													Q3263
													L3264





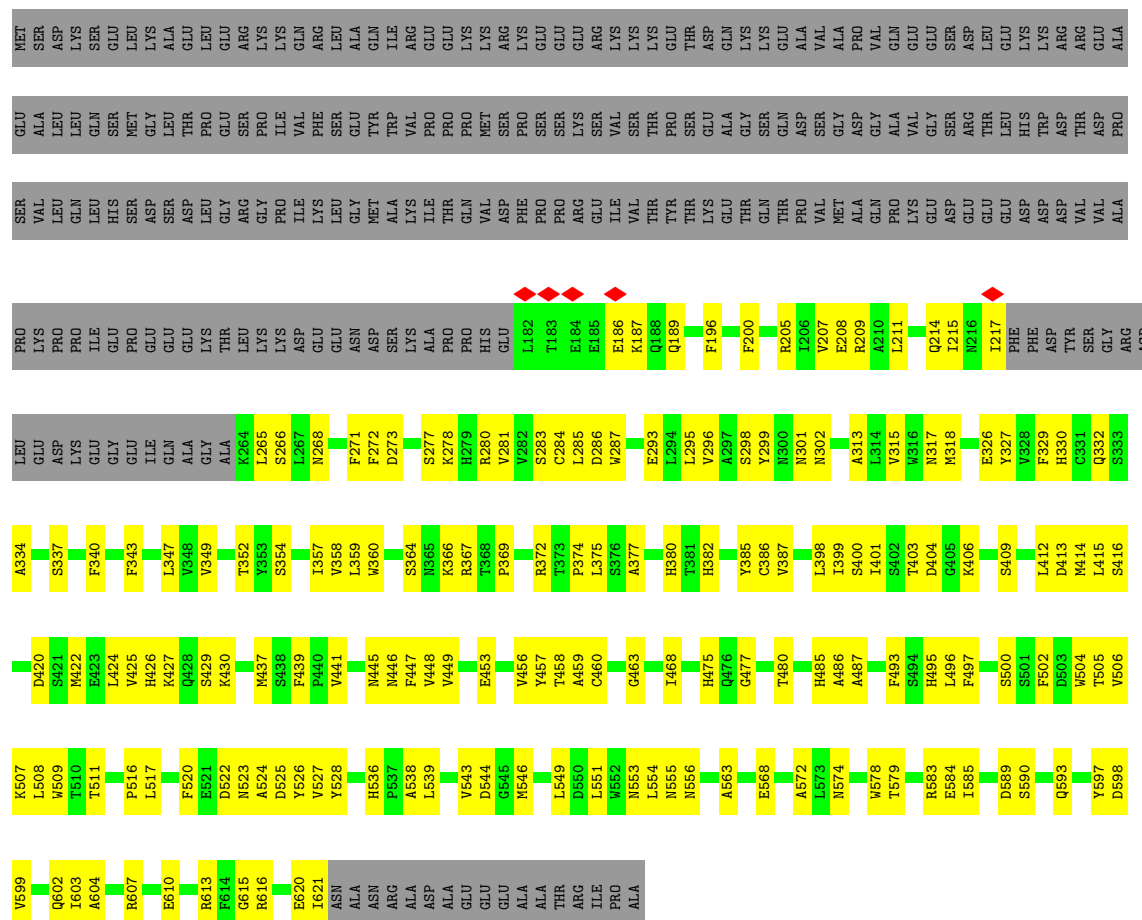
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D3045	Y2735	Y2734	V2569	H2463	F2375	D2262	S2140	P1988	R1806	S1678	Q1541	S1427	Q1203
S3046	D2917	Y2735	Q2464	H2463	L2382	T2267	C2142	Y1989	R1806	E1680	R1542	E1428	F1204
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R3060	L2933	F2751	F2480	F2480	ALA	R2285	L2157	Q2005	I1835	K1707	S1572	D1436	M1213
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D3114	T2968	L2816	T2634	T2634	ALA	P2309	V2185	N2067	Q1876	T1737	Q1612	E1464	S1230
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P3136	L2976	L2837	R2511	R2511	A2419	K2323	L2210	R2107	E1914	Q1746	F1629	L1486	K1347
P3137	R2977	L2837	R2511	R2511	A2420	L2324	T2214	I2108	E1914	A1747	V1632	D1491	P1350
R3140	K2989	V2838	L2514	L2514	T2421	E2331	Q2215	I2111	C1932	Q1755	D1636	D1492	P1350
T3143	N2998	E2840	G2515	G2515	T2422	S2334	M2222	K2112	D1933	I1756	L1637	L1493	P1350
V3144	D3001	E2841	G2515	G2515	T2422	S2334	M2222	K2112	E1934	E1760	E1639	V1497	R1357
V3148	S3002	R2843	E2544	E2544	L2437	M2342	G2224	K2113	F1945	T1764	I1640	I1501	Q1361
F3149	F3004	R2844	H2545	H2545	E2438	M2342	G2224	K2113	F1945	T1764	I1640	I1501	Q1361
V3150	V3017	E2848	W2545	W2545	Q2442	Q2346	S2231	E2115	Q1950	M1769	M1657	V1504	D1364
T3153	L3020	D2851	W2548	W2548	Q2442	Q2346	S2231	E2115	Q1950	M1769	M1657	V1504	D1364
L3154	D3024	T2852	W2548	W2548	L2443	L2348	R2235	G2126	D1958	G1771	F1658	K1508	S1382
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												V1516	V1516
												E1517	E1517





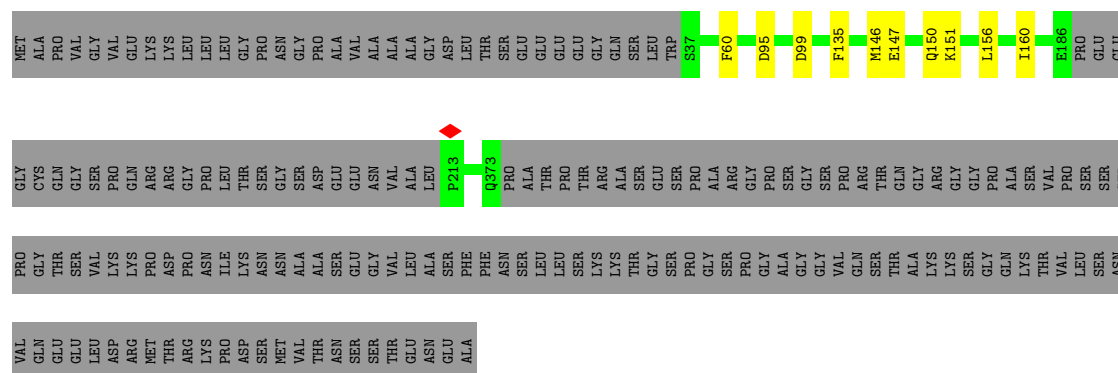
• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

Chain D: 35% 27% 38%



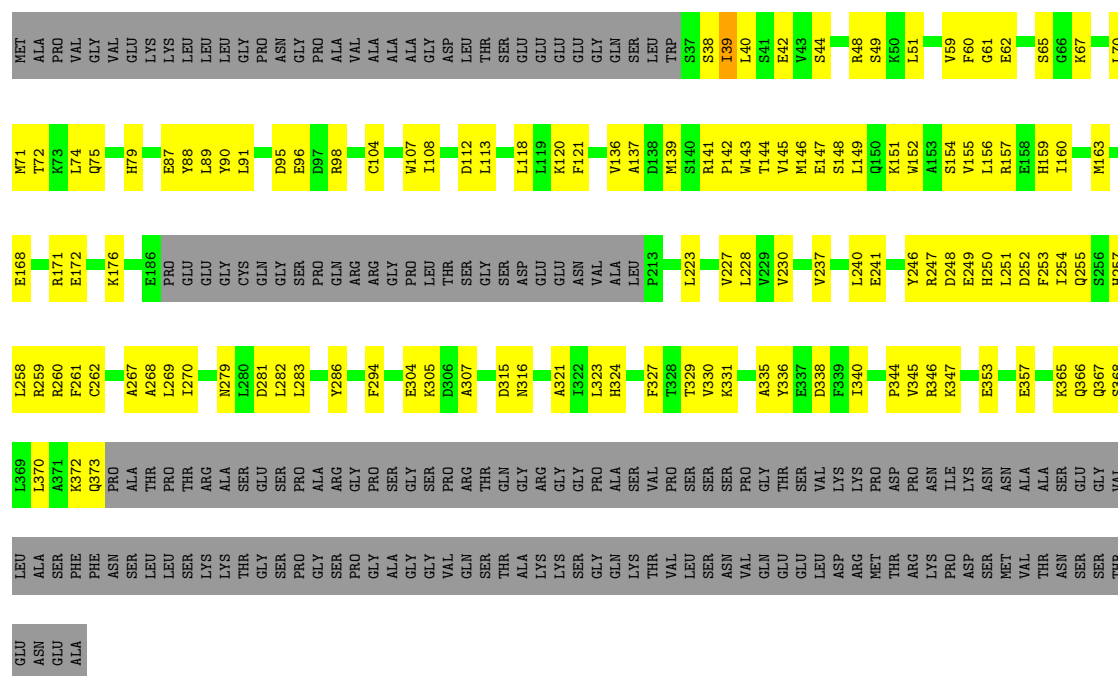
• Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

Chain E: 61% 37%



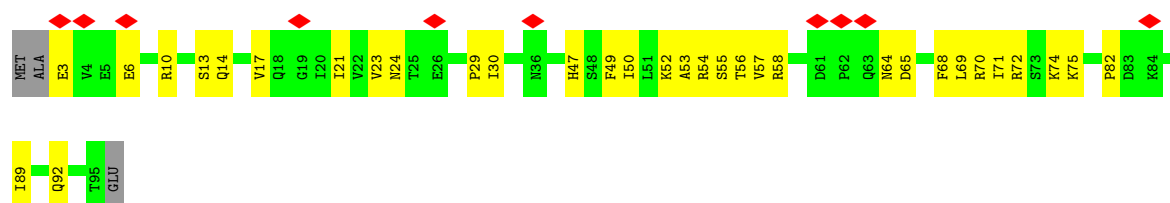
• Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

Chain F: 38% 25% 37%



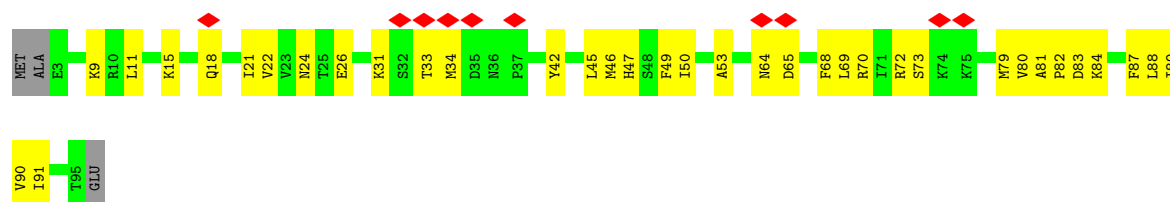
• Molecule 4: Dynein light chain roadblock-type 1

Chain G: 10% 63% 34%

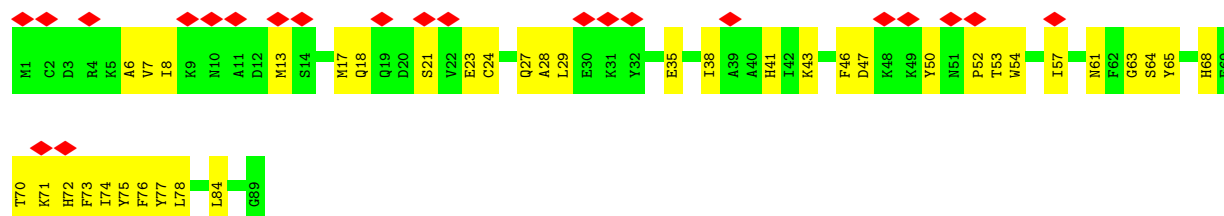


• Molecule 4: Dynein light chain roadblock-type 1

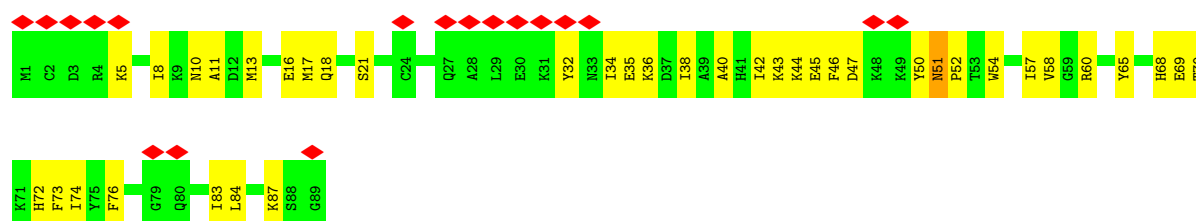
Chain H: 10% 59% 38%



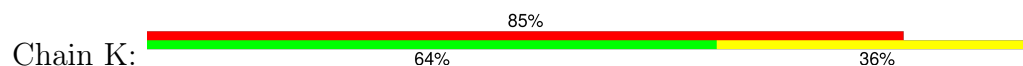
• Molecule 5: Dynein light chain 1, cytoplasmic



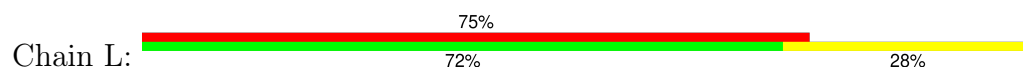
• Molecule 5: Dynein light chain 1, cytoplasmic

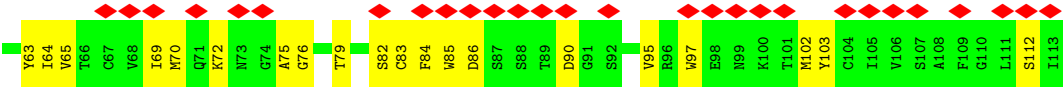


• Molecule 6: Dynein light chain Tctex-type 1



• 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: ADP, ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	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

Continued on next page...

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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%)	19	56
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%)	12	46
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%)	50	83

5 of 12 Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

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%)	92	94
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%)	92	94

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	28,33,33	0.71	0	34,52,52	0.59	1 (2%)
7	ADP	B	4703	-	24,29,29	0.86	0	29,45,45	1.23	2 (6%)
7	ADP	A	4704	-	24,29,29	0.86	0	29,45,45	1.17	2 (6%)
7	ADP	B	4701	9	24,29,29	0.88	0	29,45,45	1.18	2 (6%)
7	ADP	A	4703	-	24,29,29	0.88	0	29,45,45	1.22	2 (6%)
7	ADP	A	4701	9	24,29,29	0.89	0	29,45,45	1.20	2 (6%)
8	ATP	A	4702	9	28,33,33	0.71	0	34,52,52	0.60	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	B	4704	-	24,29,29	0.87	0	29,45,45	1.18	2 (6%)

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	-	6/18/38/38	0/3/3/3
7	ADP	B	4703	-	-	0/12/32/32	0/3/3/3
7	ADP	A	4704	-	-	2/12/32/32	0/3/3/3
7	ADP	B	4701	9	-	3/12/32/32	0/3/3/3
7	ADP	A	4703	-	-	2/12/32/32	0/3/3/3
7	ADP	A	4701	9	-	3/12/32/32	0/3/3/3
8	ATP	A	4702	9	-	6/18/38/38	0/3/3/3
7	ADP	B	4704	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4703	ADP	N3-C2-N1	-3.74	123.60	128.67
7	A	4703	ADP	N3-C2-N1	-3.72	123.63	128.67
7	A	4701	ADP	N3-C2-N1	-3.64	123.73	128.67
7	B	4701	ADP	N3-C2-N1	-3.64	123.74	128.67
7	B	4704	ADP	N3-C2-N1	-3.58	123.81	128.67

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

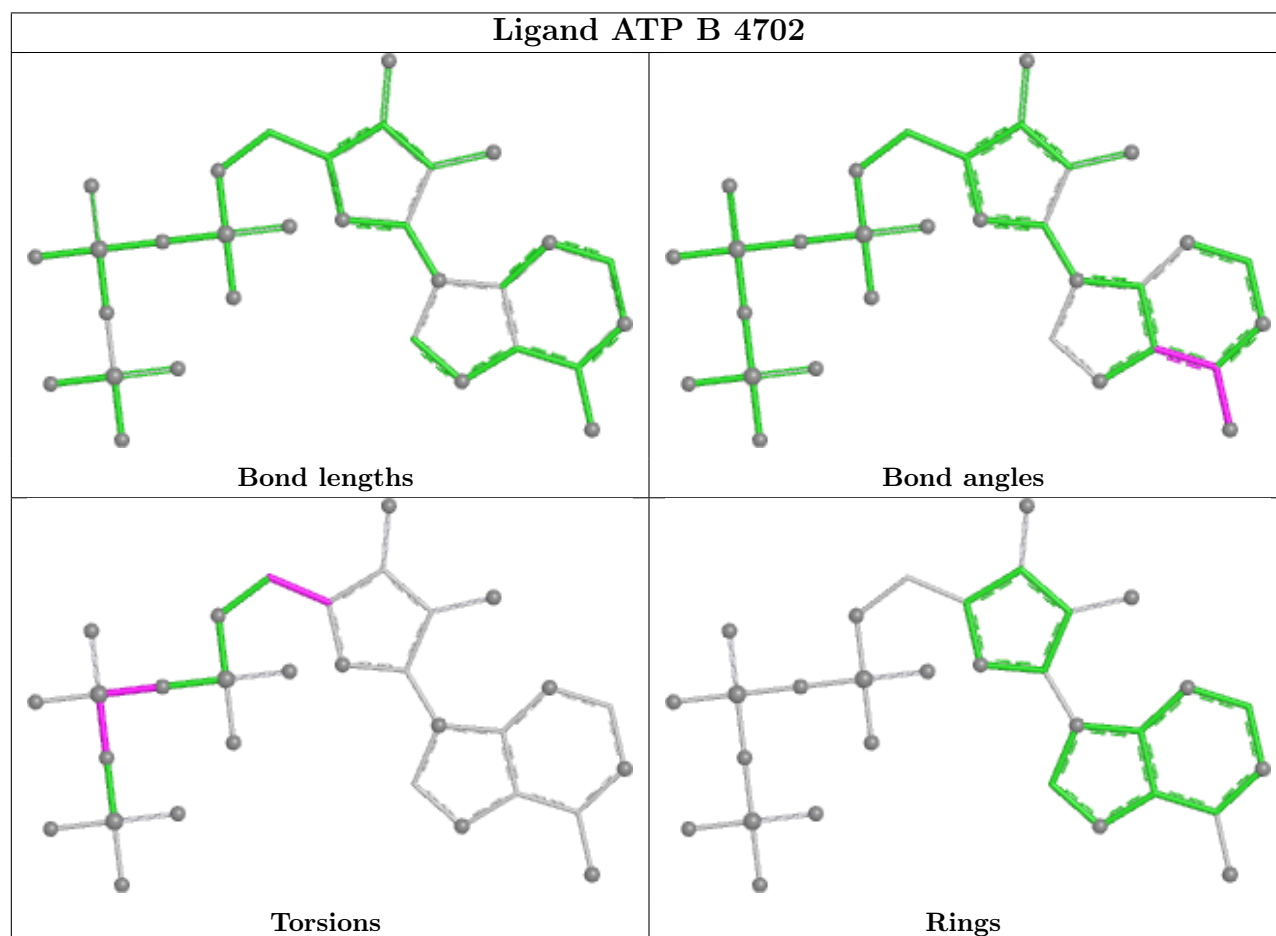
Mol	Chain	Res	Type	Atoms
7	A	4701	ADP	C5'-O5'-PA-O1A
7	A	4701	ADP	C5'-O5'-PA-O2A
7	A	4701	ADP	C5'-O5'-PA-O3A
7	A	4704	ADP	C5'-O5'-PA-O1A
7	B	4701	ADP	C5'-O5'-PA-O1A

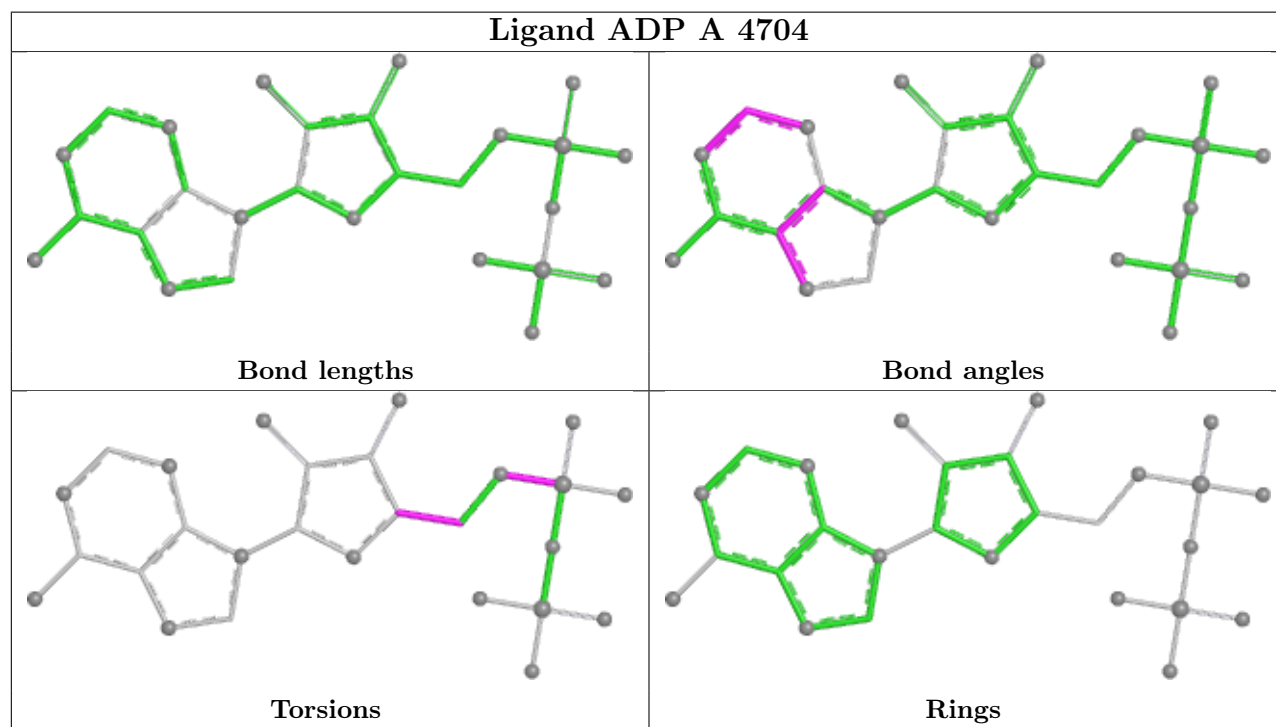
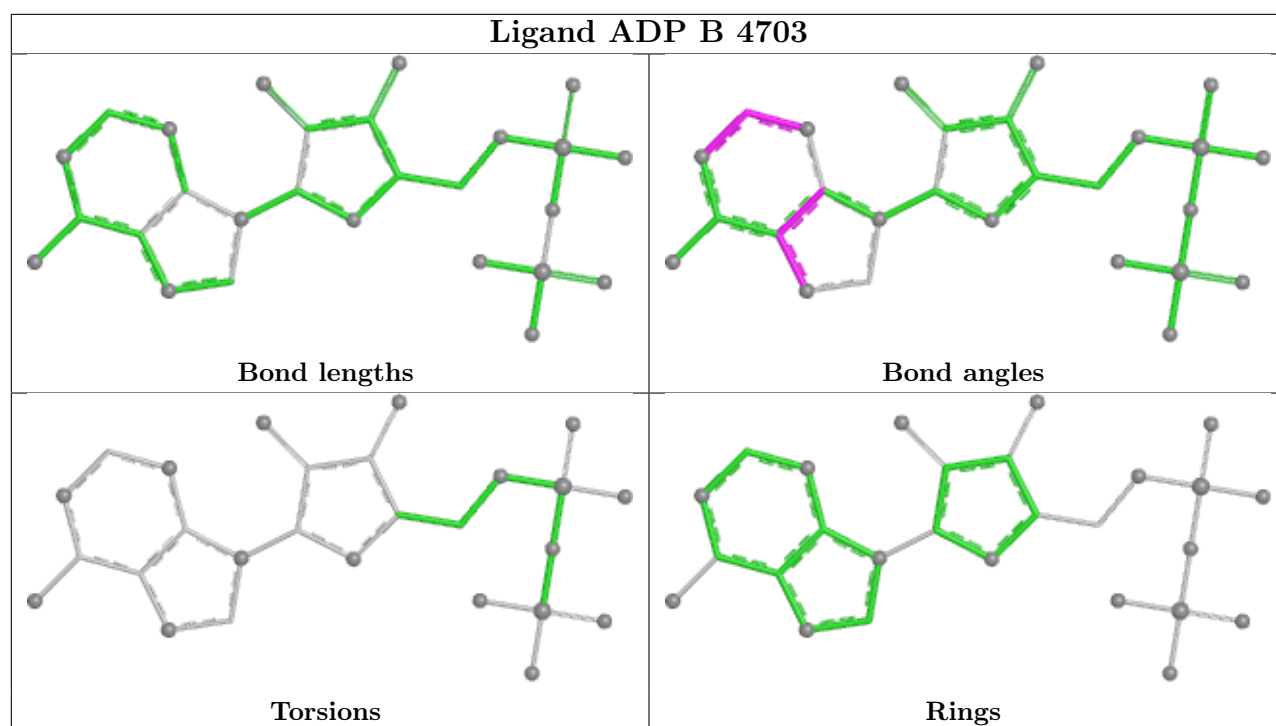
There are no ring outliers.

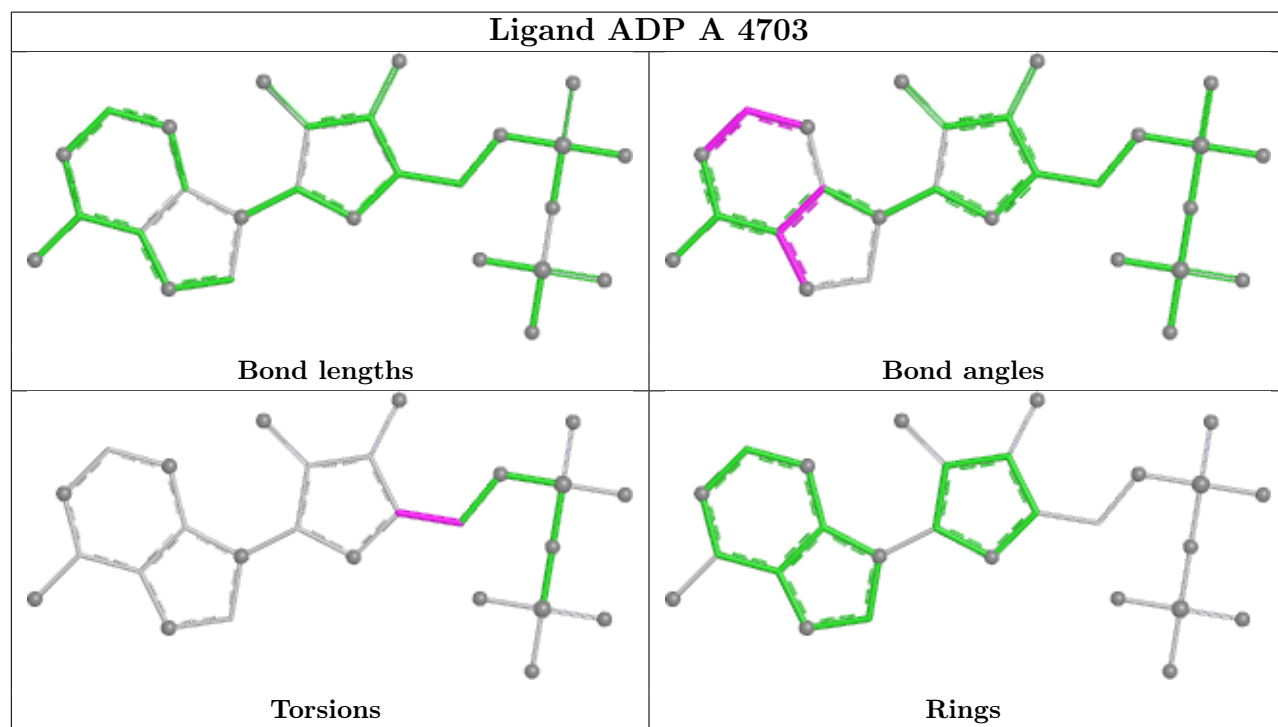
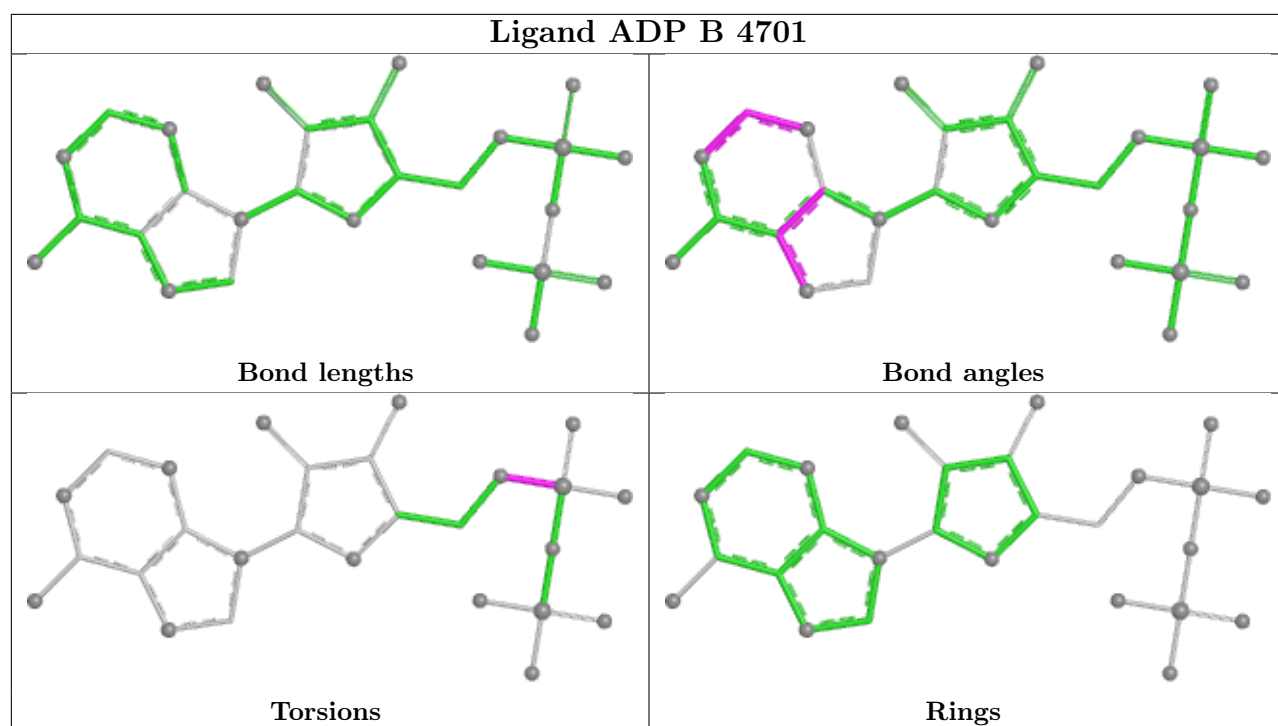
4 monomers are involved in 4 short contacts:

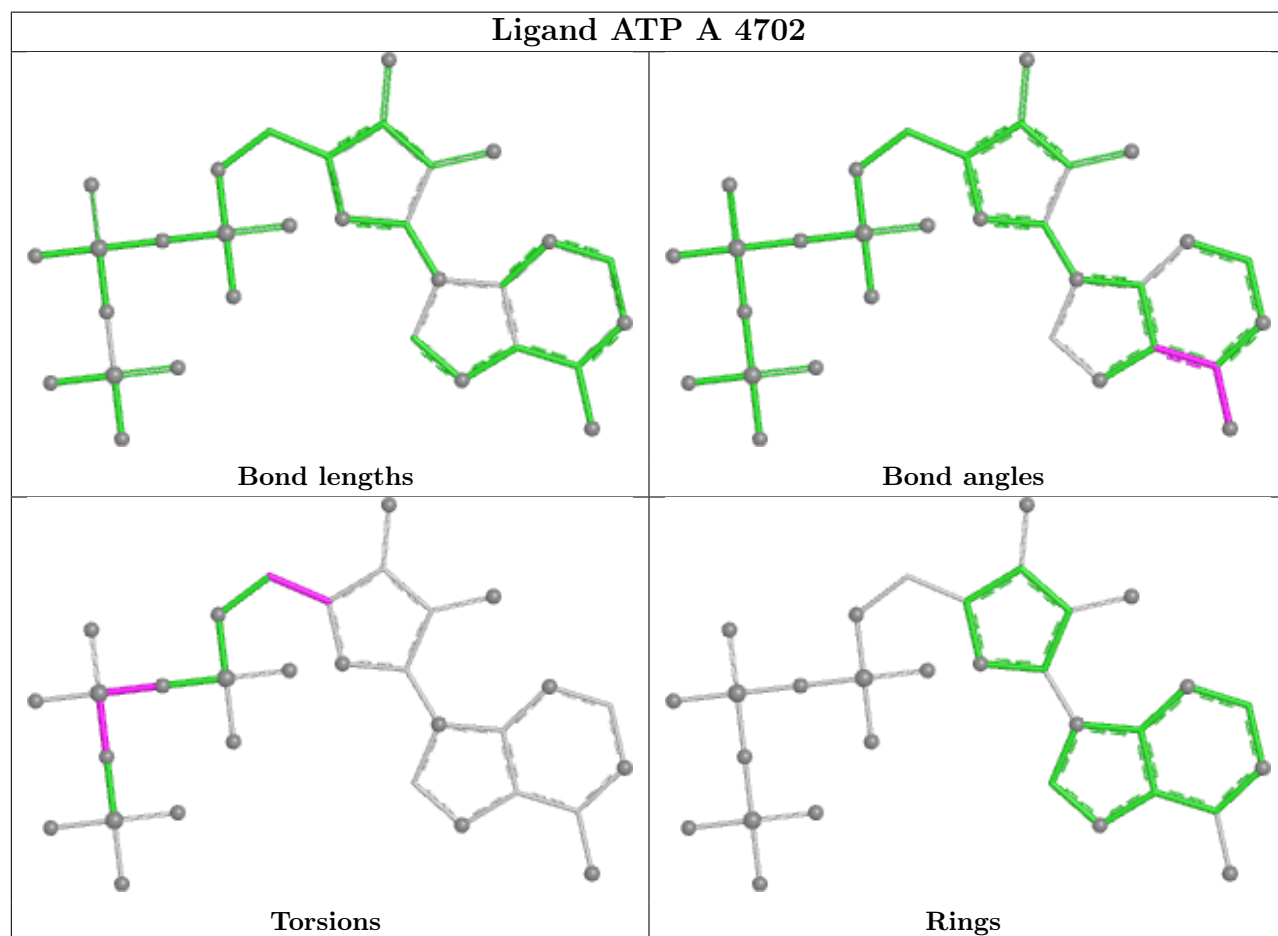
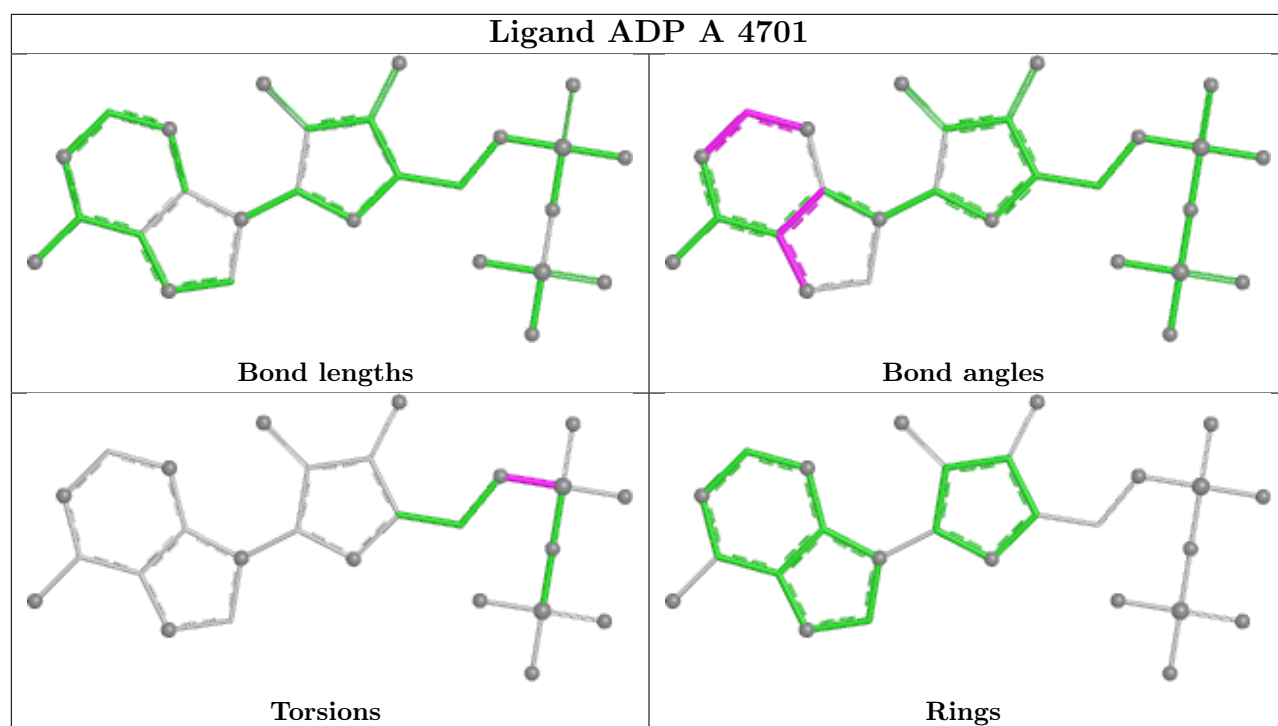
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	4701	ADP	1	0
7	A	4703	ADP	1	0
7	A	4701	ADP	1	0
7	B	4704	ADP	1	0

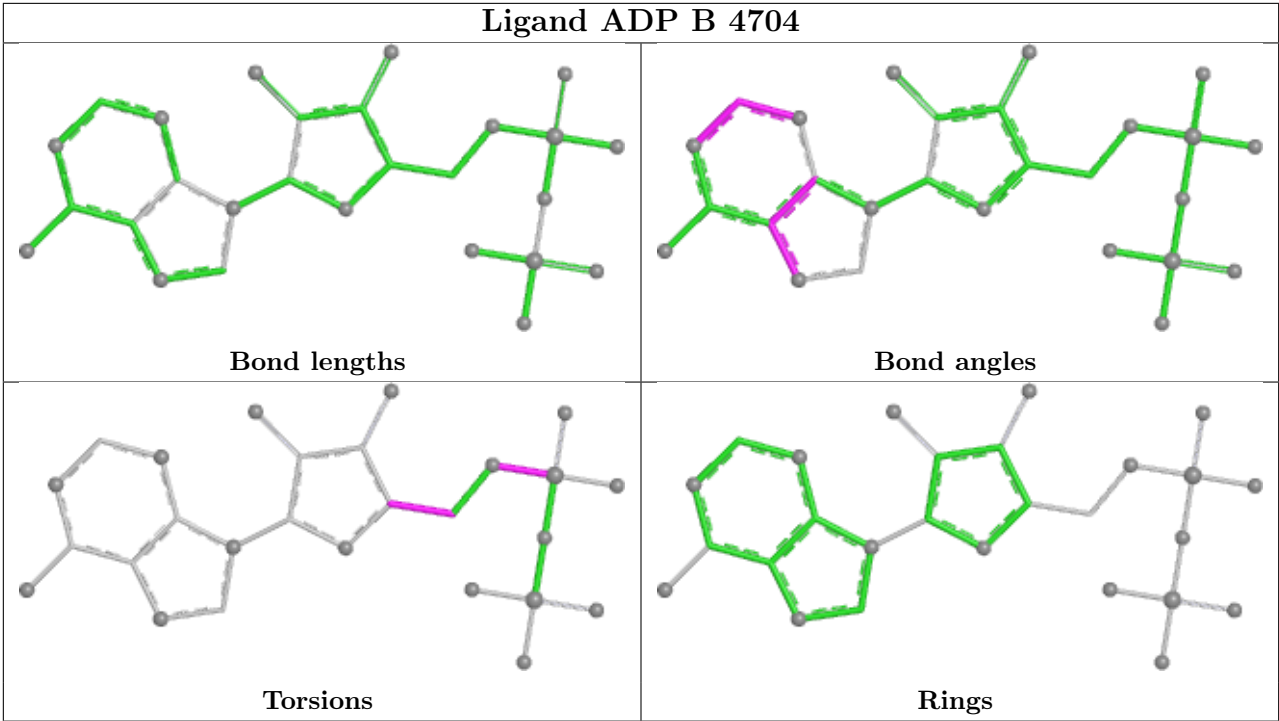
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

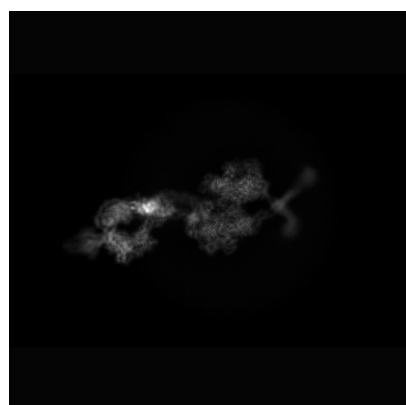
6 Map visualisation [i](#)

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.

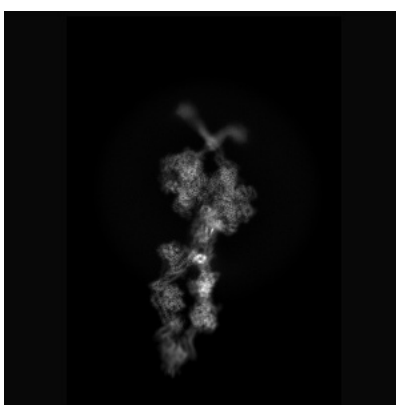
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

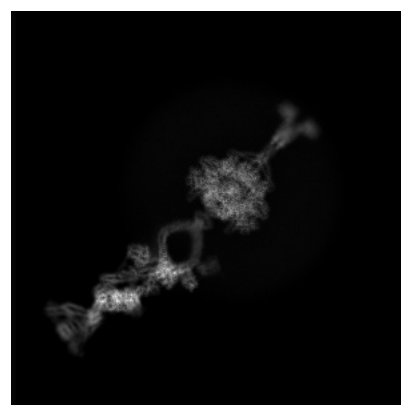
6.1.1 Primary map



X



Y

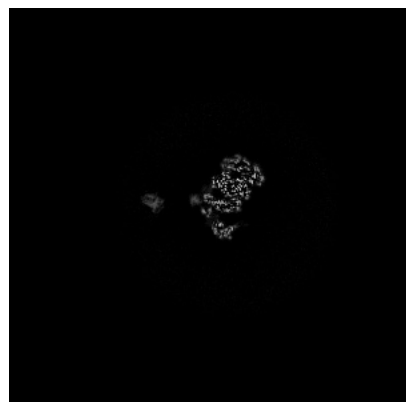


Z

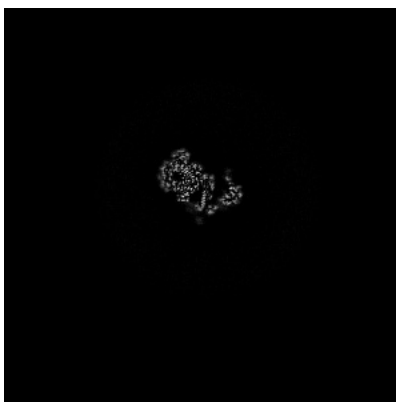
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210



Y Index: 210

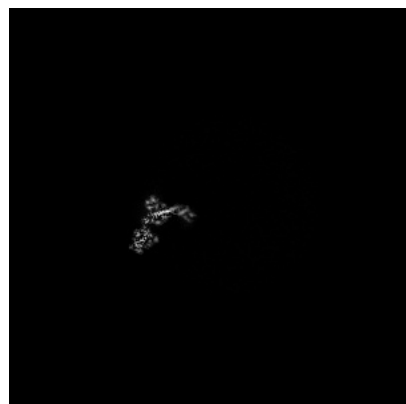


Z Index: 210

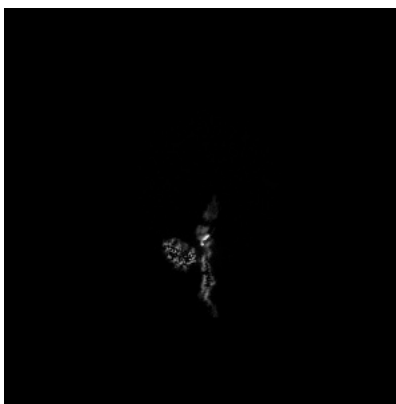
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

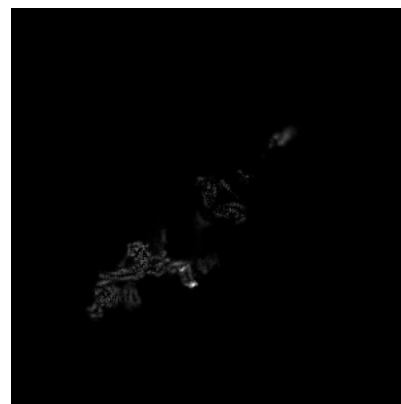
6.3.1 Primary map



X Index: 162



Y Index: 144

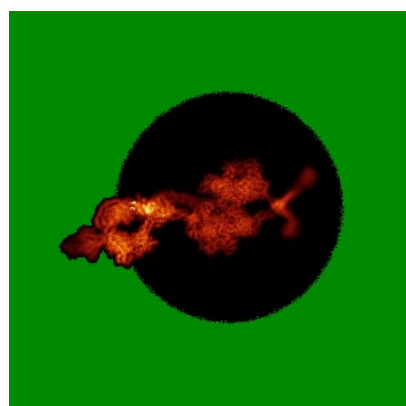


Z Index: 212

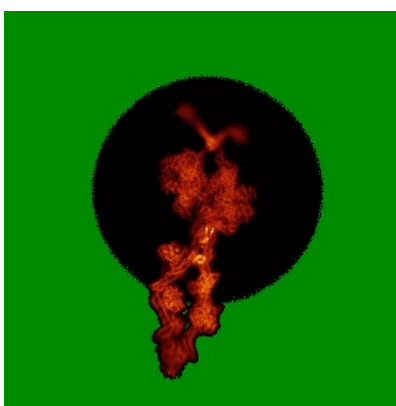
The images above show the largest variance slices of the map in three orthogonal directions.

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.

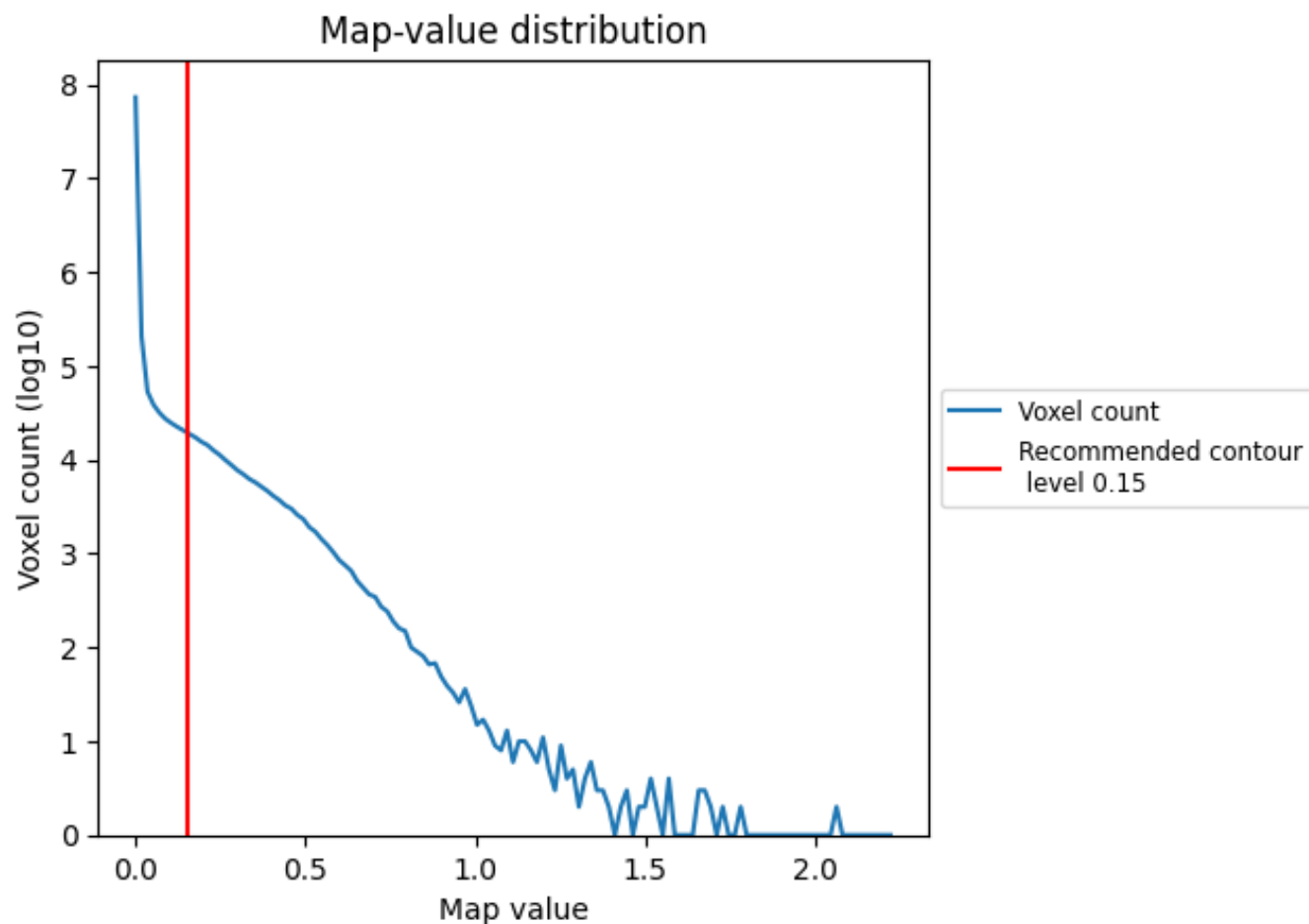
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

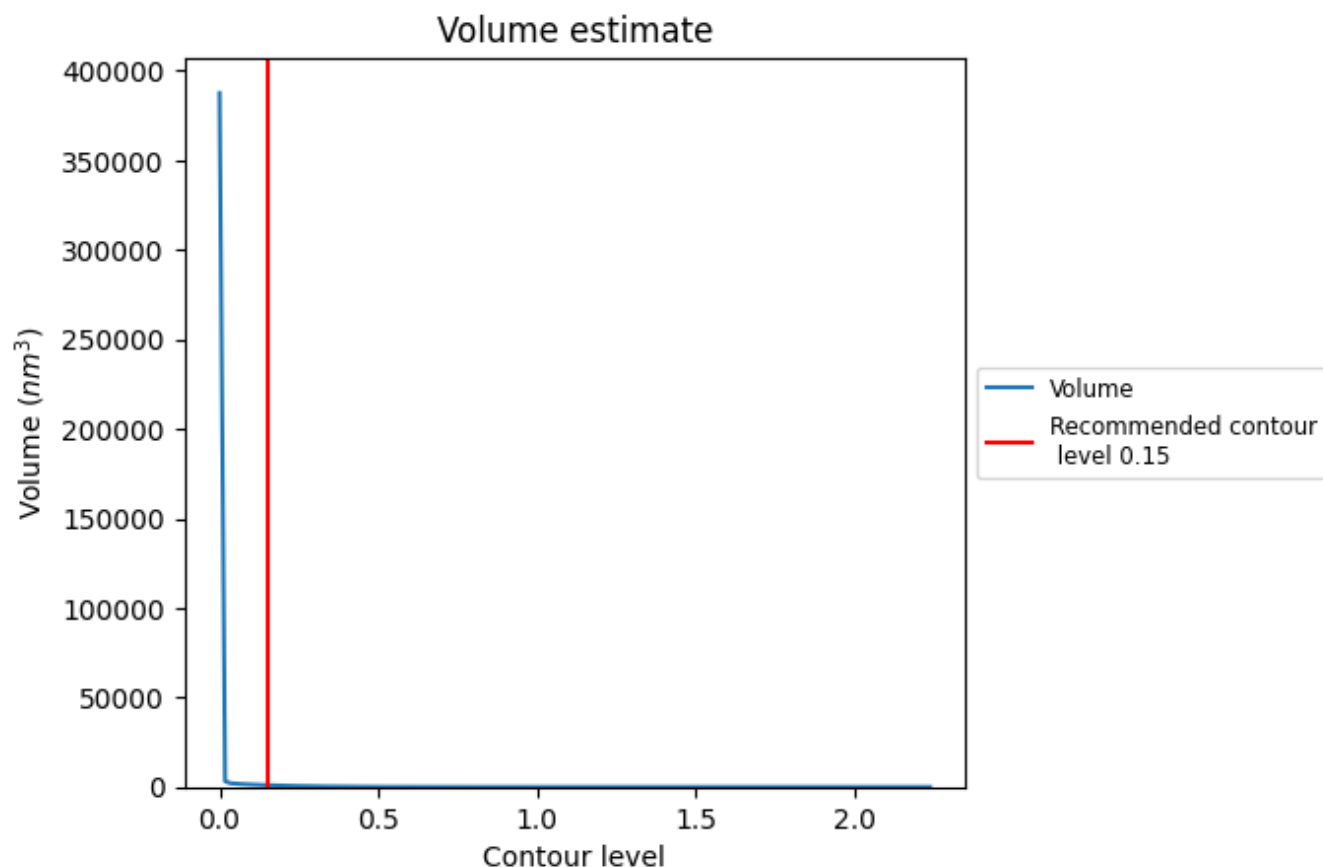
This section contains the results of statistical analysis of the map.

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.

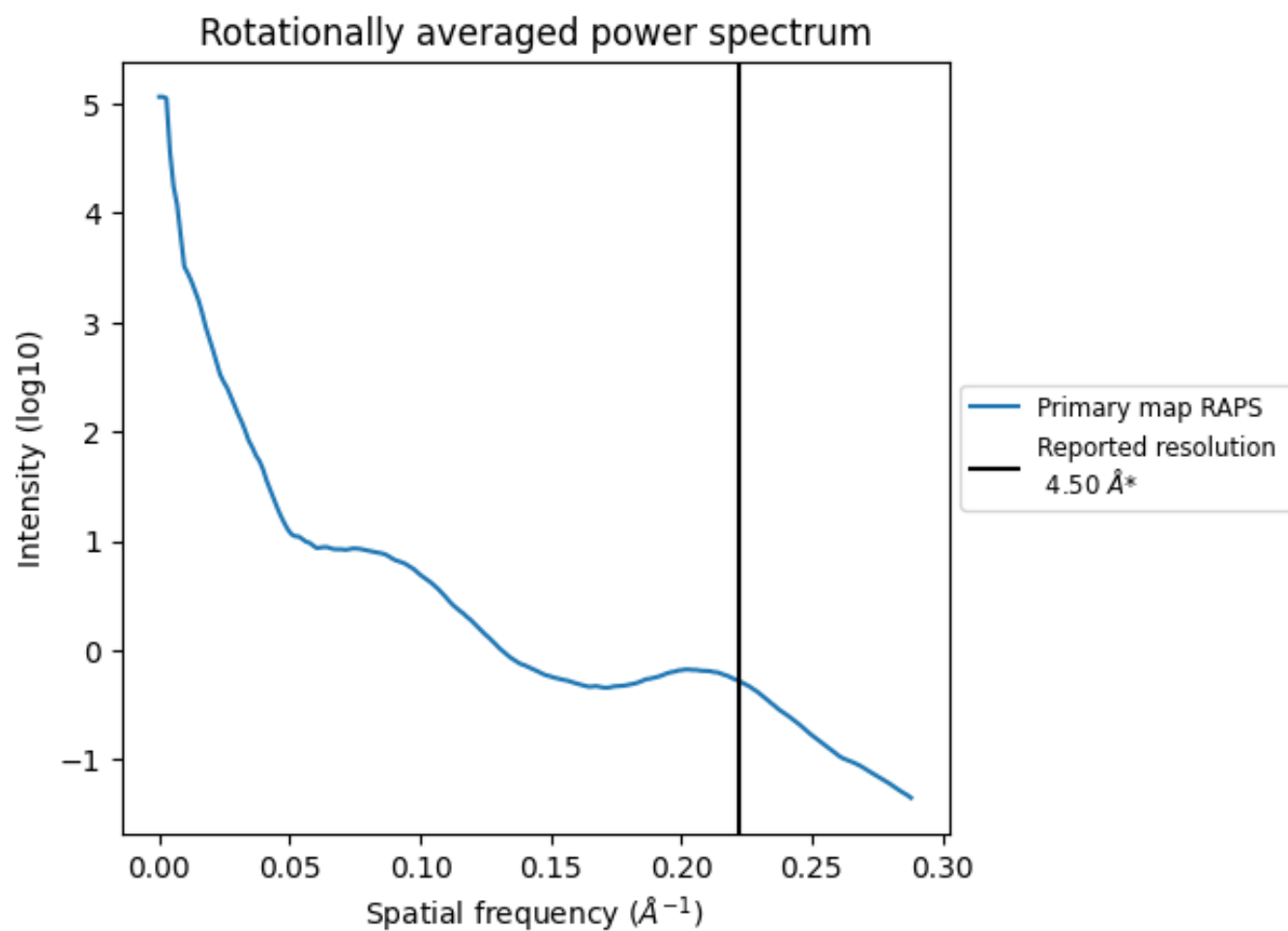
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 984 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 Å⁻¹

8 Fourier-Shell correlation

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

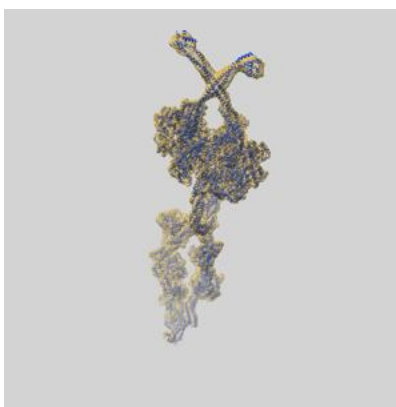
9 Map-model fit [i](#)

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](#).

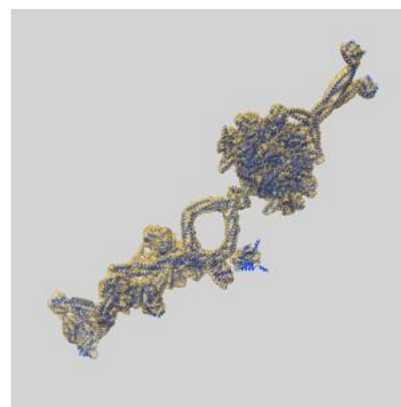
9.1 Map-model overlay [i](#)



X



Y



Z

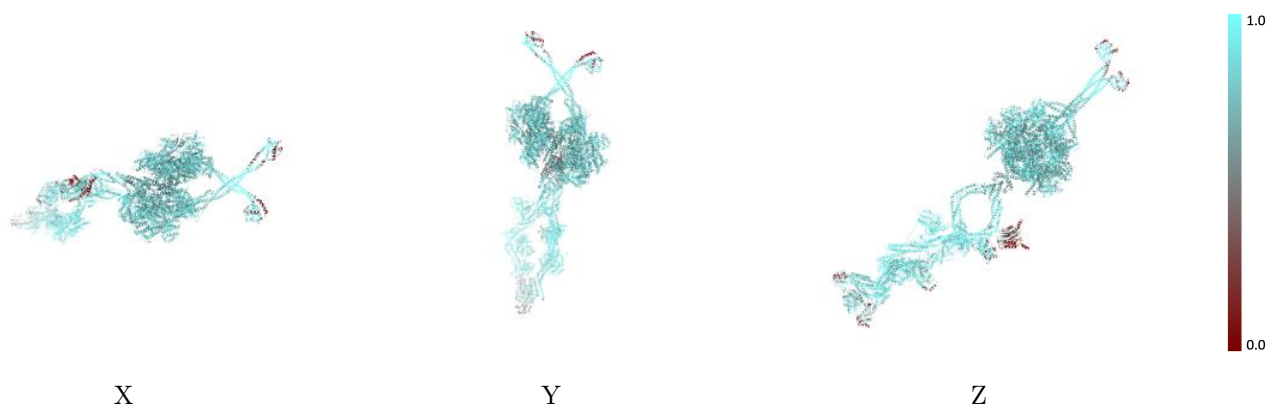
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



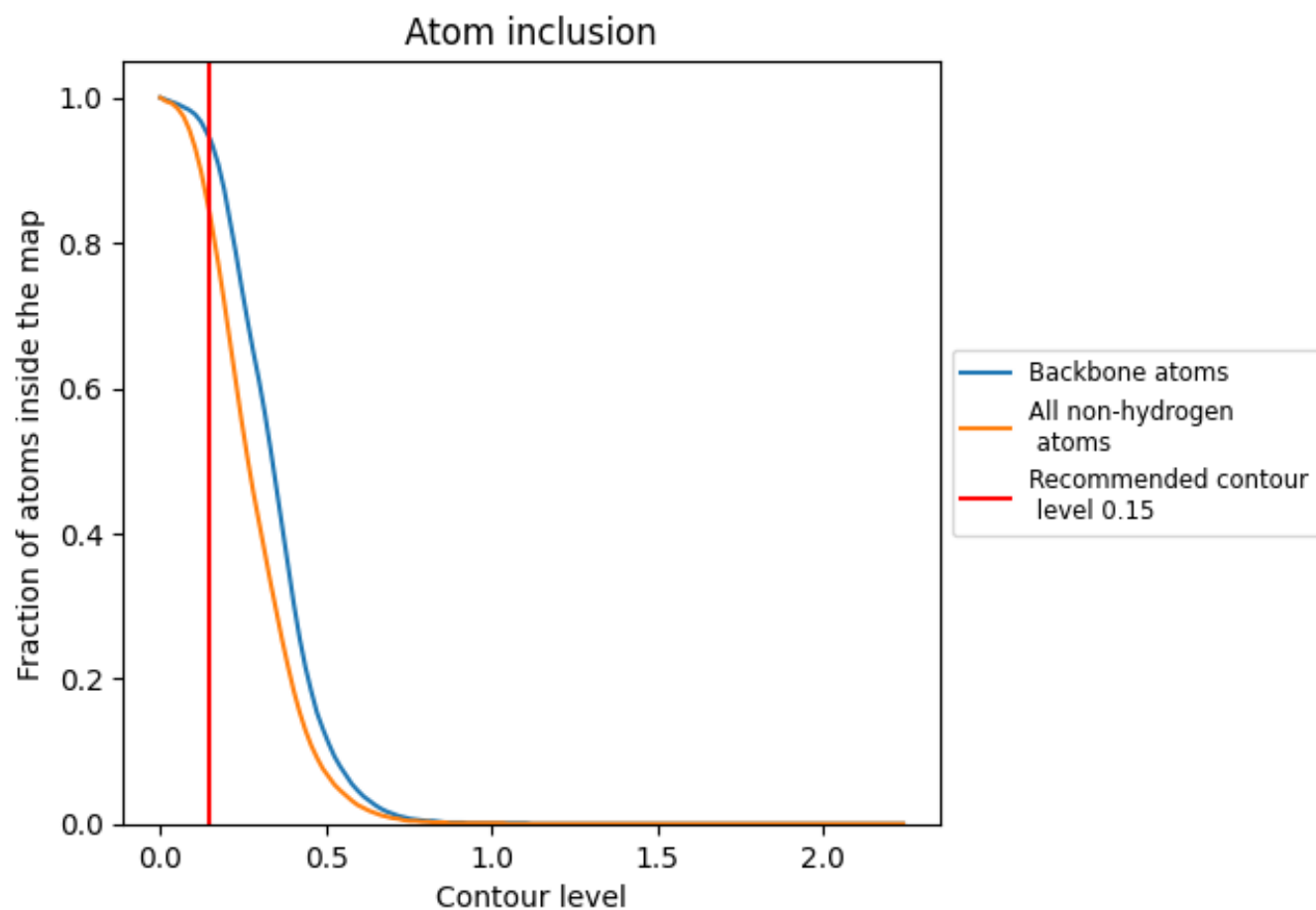
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 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

