



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 11:21 AM UTC

PDB ID : 9E14 / pdb_00009e14
EMDB ID : EMD-47383
Title : Full-length human dynein-1 in phi-like conformation bound to a Lis1 dimer under Nde1-Lis1 condition
Authors : Yang, J.; Zhang, K.
Deposited on : 2024-10-21
Resolution : 5.00 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

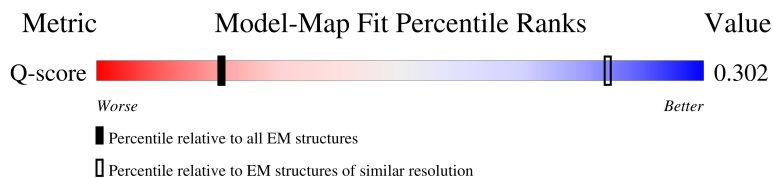
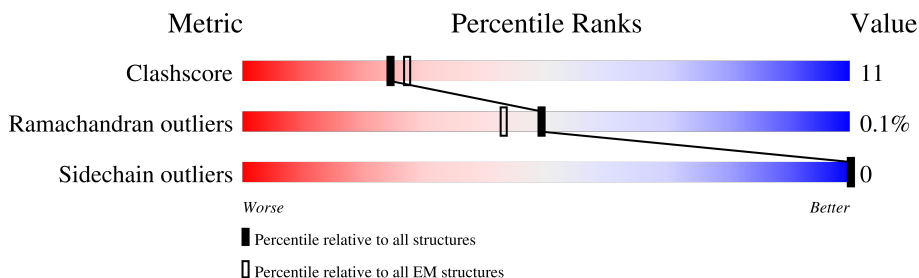
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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.




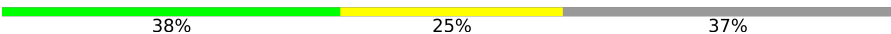








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1057 (4.50 - 5.50)

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	4646	<div> <div>10%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	B	4646	<div> <div>6%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
2	C	638	<div> <div>56%</div> <div>6%</div> <div>38%</div> </div>
2	D	638	<div> <div>36%</div> <div>26%</div> <div>38%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	492	 61% 37%
3	F	492	 38% 25% 37%
4	G	96	 14% 54% 43%
4	H	96	 70% 27%
5	I	89	 15% 49% 51%
5	J	89	 34% 57% 43%
6	K	113	 60% 75% 25%
6	L	113	 65% 73% 27%
7	O	410	 58% 21% 21%
7	P	410	 53% 25% 22%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 94479 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

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

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

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

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

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

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

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

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

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

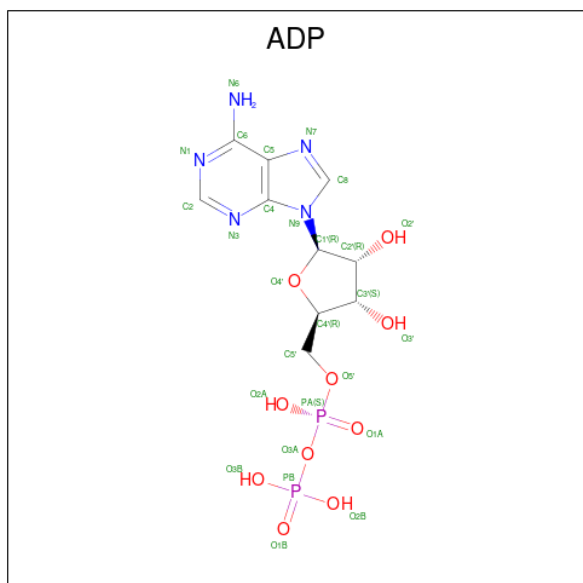
- Molecule 6 is a protein called Dynein light chain Tctex-type 1.

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

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

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

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



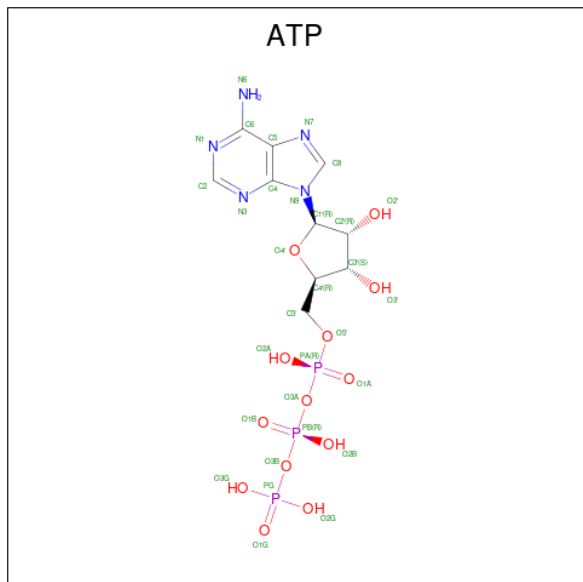
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

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



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

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

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

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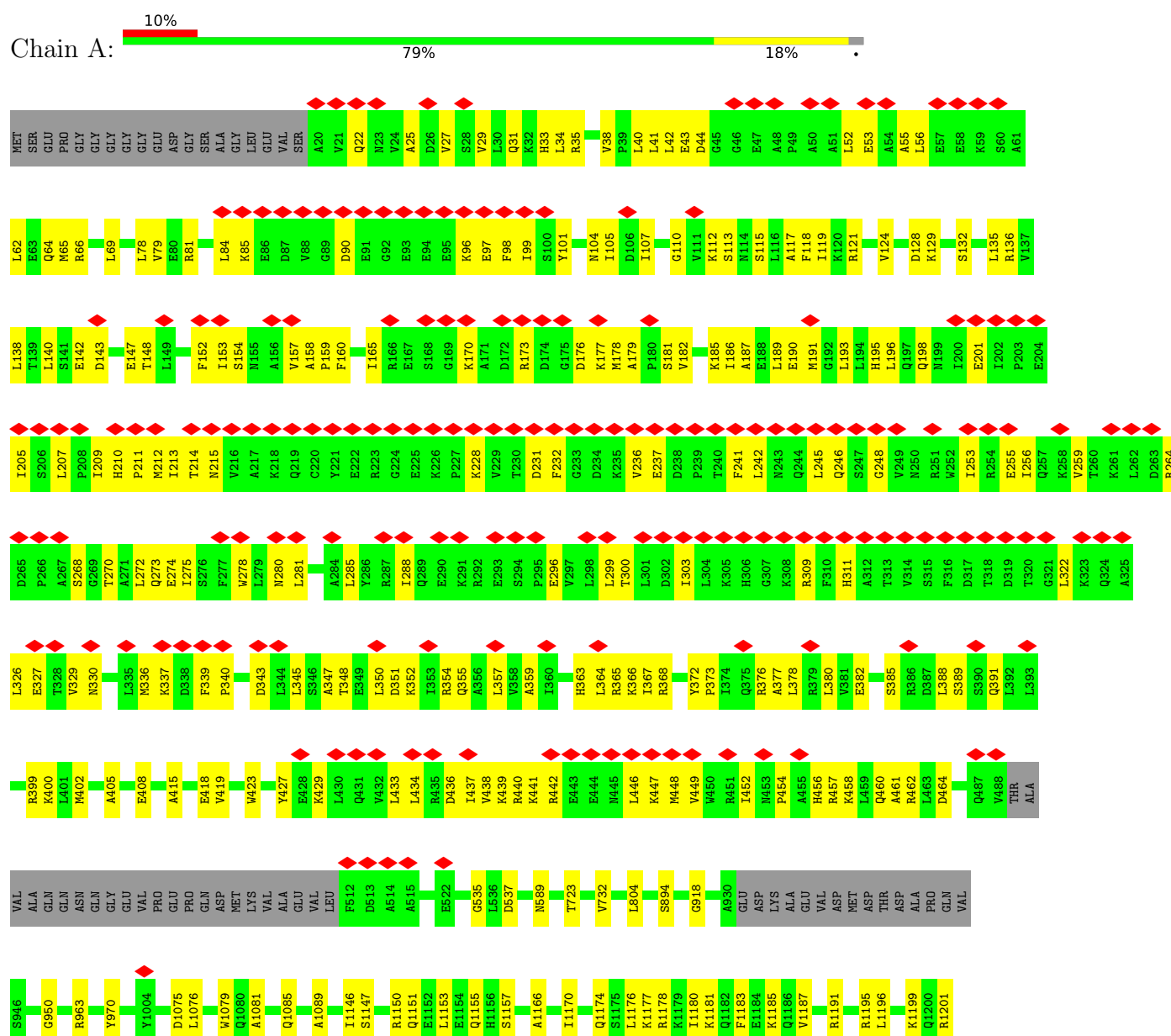
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	B	2	2	2	0

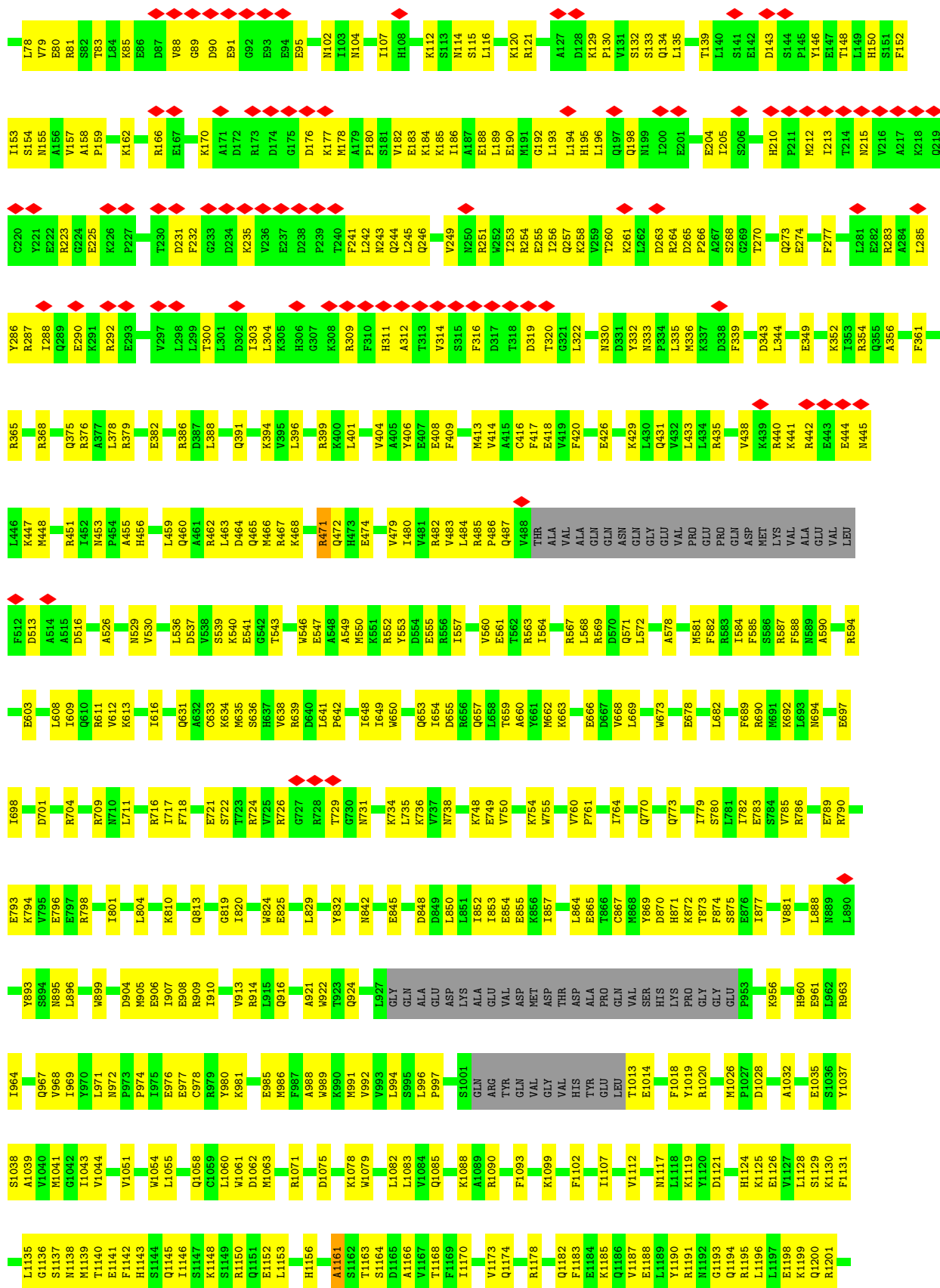
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

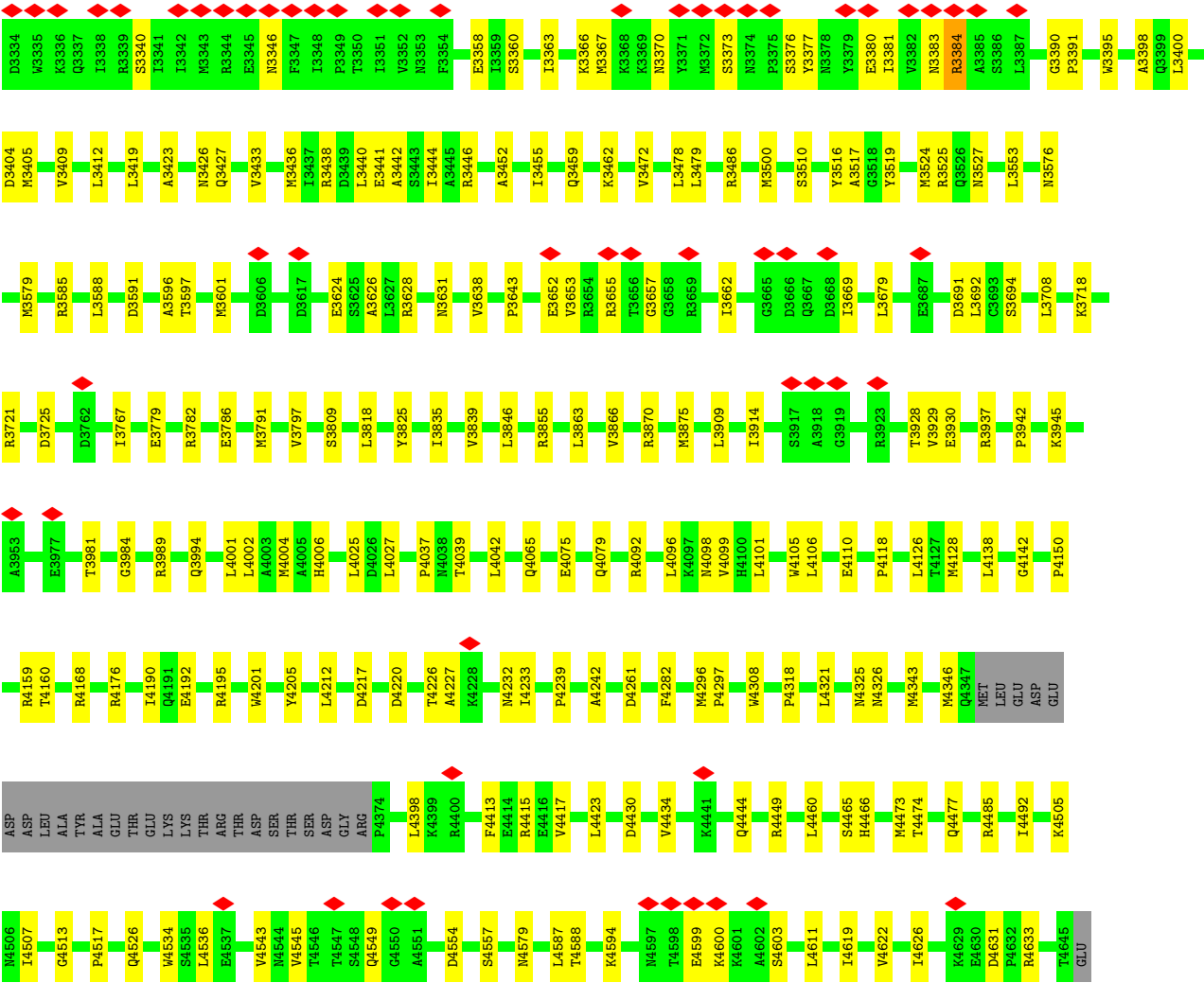
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1



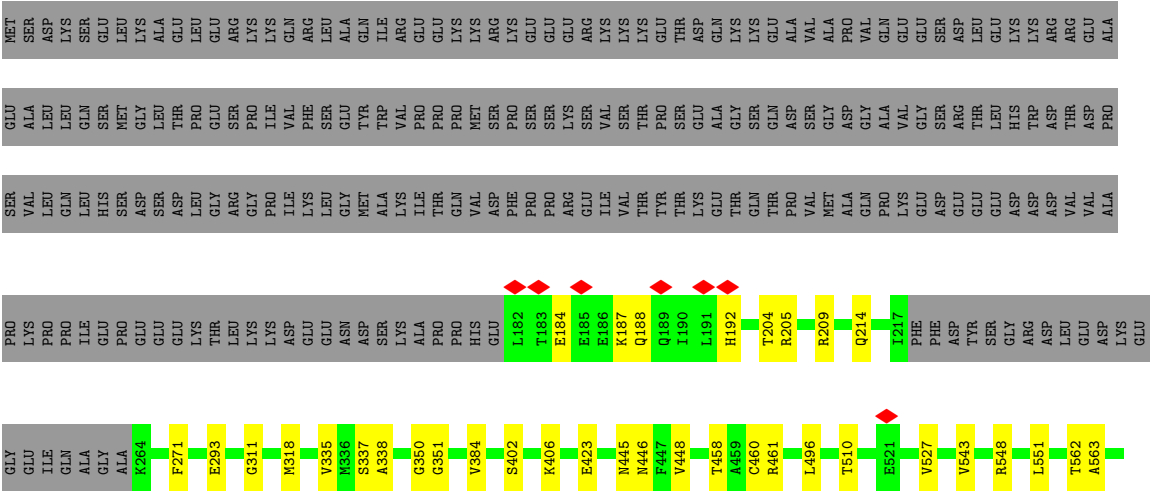
D2975	R2763	G2598	L2449	N2314	E2188	L2039	M1867	I1676	A1577	R1485	K1409	F1302
R2981	F2784	K2601	L2452	D2320	E2189	L2047	Y1868	R1679	K1581	L1486	D1410	Q1203
L2989	I2793	L2605	R2453	D2321	Y2190	Q2051	E1871	I1692	K1584	I1487	R1411	L1209
A2991	Y2794	F2606	C2454	L2324	L2191	L2065	L1879	T1693	S1585	L1415	Q1415	E1215
E2996	S2795	S2607	S2457	E2331	D2195	L2069	C1888	H1695	M1589	M1417	G1219	G1219
S2997	E2814	R2610	S2460	R2332	G2200	I2069	Y1889	I1698	D1590	K1418	N1222	N1222
N2998	R2836	D2614	L2462	M2342	W2203	V2070	M1892	V1699	V1591	K1419	M1225	M1225
V2999	R2836	H2615	H2463	F2343	V2204	P2071	E1700	E1700	K1498	L1420	H1421	K1228
L3000	E2841	E2616	R2467	Q2346	K2206	L2080	K1912	W1701	M1507	H1421	D1229	D1229
F3004	E2841	G2619	D2475	S2357	M2221	D2087	E1914	K1707	Y1512	W1424	W1424	W1424
L3005	R2844	S2623	D2475	S2357	M2222	D2087	R1925	V1721	Y1513	V1425	I1232	I1232
E3006	N2860	T2626	M2481	W2362	W2223	R2091	F1926	V1724	K1514	V1426	Q1233	Q1233
R3007	R2877	Q2485	Q2485	W2363	G2224	K2094	Y1946	Y1729	V1515	S1427	S1427	S1427
K3008	S2878	R2640	R2492	F2364	S2228	R2105	Q1950	K1729	E1517	E1428	E1428	E1428
A3013	K2879	R2643	R2492	S2365	V2236	R2105	V1951	Y1745	S1600	D1429	T1430	T1430
N3014	V2884	P2645	W2500	L2382	E2242	R2113	G1952	Y1750	L1601	L1439	L1439	L1439
E3025	A2895	N2646	L2514	L2382	R2243	E2117	A1953	V1763	E1602	Q1440	Q1440	Q1440
G3036	K2898	Q2654	R2519	D2387	L2244	E2117	W1954	L1766	R1603	K1441	K1441	K1441
K3039	E2902	K2657	L2526	D2388	E2248	E2120	D1958	L1766	D1606	N1442	N1442	N1442
E3040	E2903	V2660	L2534	D2388	K2257	A2121	E1959	L1766	L1607	E1524	E1524	E1524
G3041	E2904	L2661	E2538	D2389	K2257	V2122	G1952	M1769	L1608	D1525	D1525	D1525
K3043	L2905	L2661	E2538	D2389	K2257	D2123	A1953	Q1973	Q1609	K1526	K1526	K1526
L3044	D2906	P2669	E2538	D2389	K2257	N2130	W1954	Q1973	I1611	R1529	R1529	R1529
D3045	E2912	R2684	W2545	D2388	K2257	Q2134	D1958	Q1973	I1612	I1530	I1530	I1530
S3046	E2913	Q2685	W2545	D2388	K2257	Q2134	E1959	Q1973	K1613	L1533	L1533	L1533
H3047	E2914	Q2686	W2548	D2388	K2257	Q2134	E1959	Q1973	K1613	W1537	W1537	W1537
E3048	H2918	L2703	W2548	D2388	K2257	Q2134	E1959	Q1973	K1613	I1538	I1538	I1538
E3049	I2922	L2703	W2548	D2388	K2257	Q2134	E1959	Q1973	K1613	D1539	D1539	D1539
K3052	L2934	Q2707	Q2554	D2388	K2257	Q2134	E1959	Q1973	K1613	A1453	A1453	A1453
Q3057	L2935	F2708	I2555	D2388	K2257	Q2134	E1959	Q1973	K1613	Q1454	Q1454	Q1454
R3060	K2943	V2709	E2556	D2388	K2257	Q2134	E1959	Q1973	K1613	G1455	G1455	G1455
N3061	V2714	P2714	D2573	D2388	K2257	Q2134	E1959	Q1973	K1613	A1458	A1458	A1458
V3064	R2726	R2726	R2576	D2388	K2257	Q2134	E1959	Q1973	K1613	E1460	E1460	E1460
T3067	L2956	R2729	R2576	D2388	K2257	Q2134	E1959	Q1973	K1613	F1462	F1462	F1462
N3068	I2961	H2730	L2580	D2388	K2257	Q2134	E1959	Q1973	K1613	L1463	L1463	L1463
R3078	K2962	V2731	W2584	D2388	K2257	Q2134	E1959	Q1973	K1613	M1393	M1393	M1393
K3088	H2964	P2732	P2590	D2388	K2257	Q2134	E1959	Q1973	K1613	K1395	K1395	K1395
R3088	R2965	Y2738	L2591	D2388	K2257	Q2134	E1959	Q1973	K1613	I1466	I1466	I1466
K3113	K2966	Y2738	V2592	D2388	K2257	Q2134	E1959	Q1973	K1613	R1467	R1467	R1467
D3114	Y2967	R2753	V2592	D2388	K2257	Q2134	E1959	Q1973	K1613	N1471	N1471	N1471
V3129	D2973	R2757	P2596	D2388	K2257	Q2134	E1959	Q1973	K1613	E1402	E1402	E1402
Y3130	E2974	R2757	P2596	D2388	K2257	Q2134	E1959	Q1973	K1613	L1475	L1475	L1475
										D1476	D1476	D1476
										L1477	L1477	L1477
										V1478	V1478	V1478
										Q1481	Q1481	Q1481
										N1482	N1482	N1482
										E1406	E1406	E1406
										S1405	S1405	S1405
										A1407	A1407	A1407
										L1408	L1408	L1408

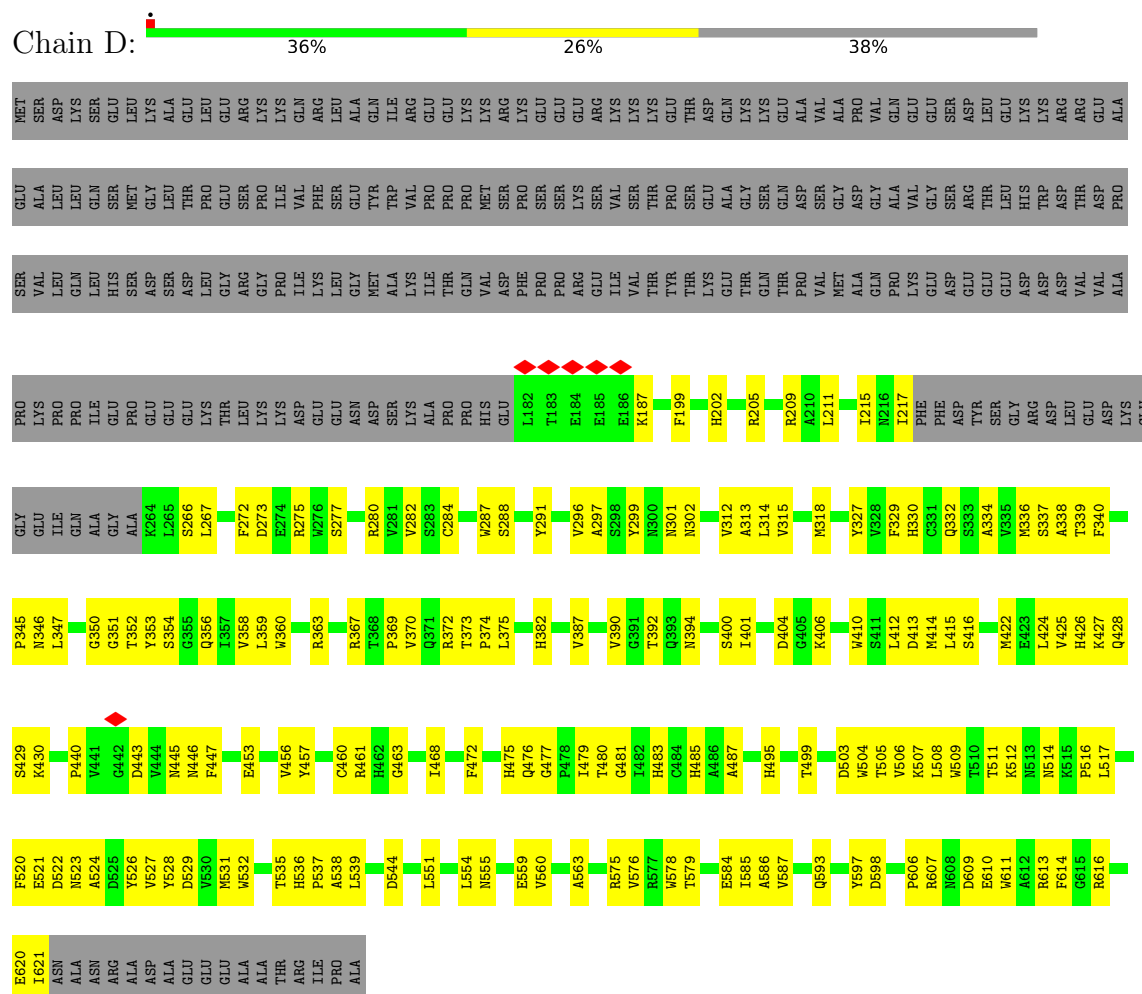




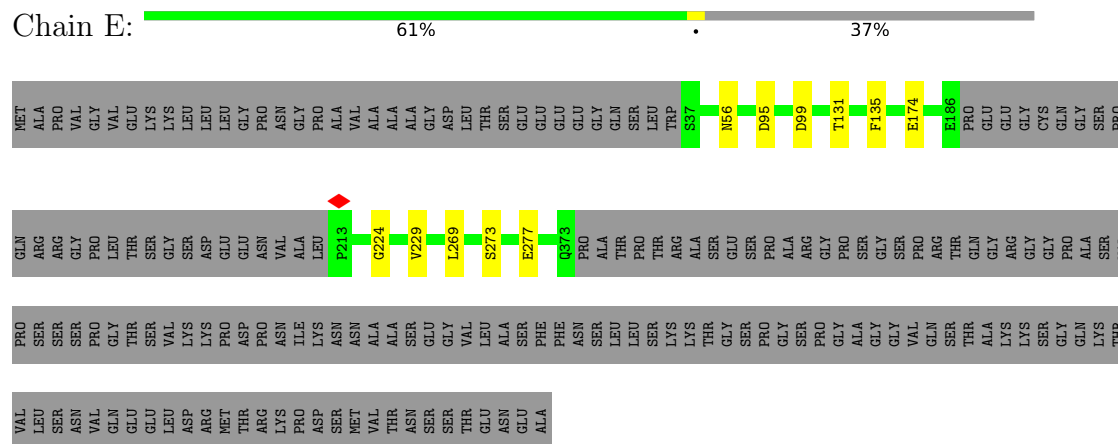


● Molecule 2: Cytoplasmic dynein 1 intermediate chain 2



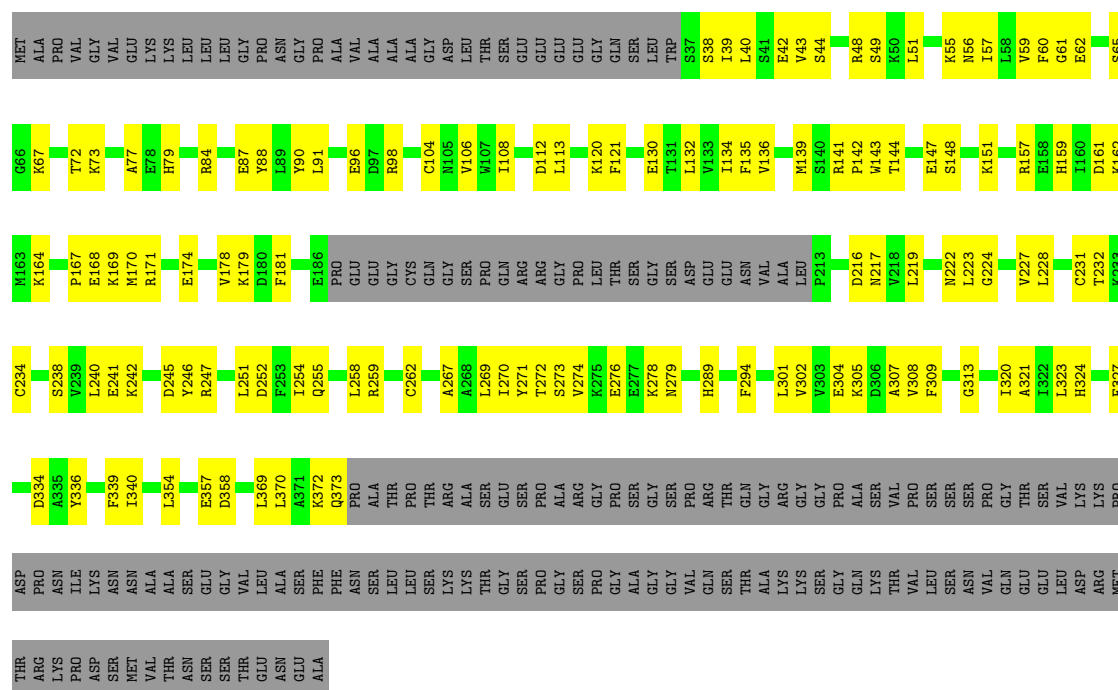


- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2



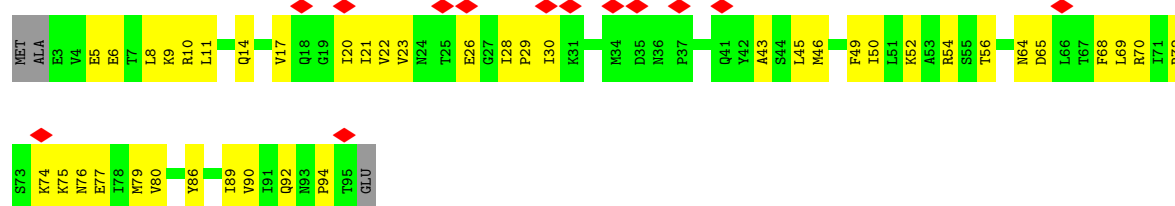
- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

Chain F:  38% 25% 37%



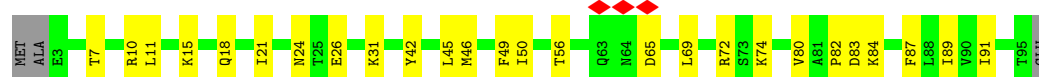
• Molecule 4: Dynein light chain roadblock-type 1

Chain G:  14% 54% 43%



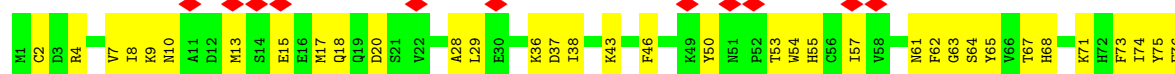
• Molecule 4: Dynein light chain roadblock-type 1

Chain H:  70% 27%



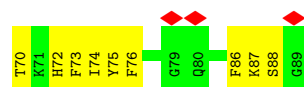
• Molecule 5: Dynein light chain 1, cytoplasmic

Chain I:  15% 49% 51%

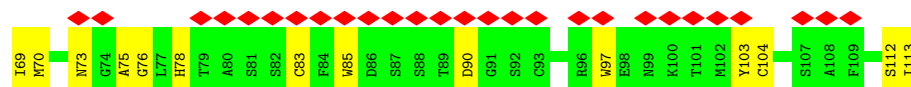
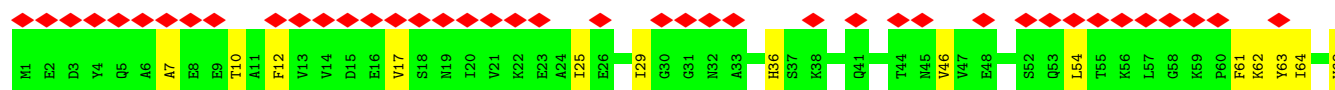
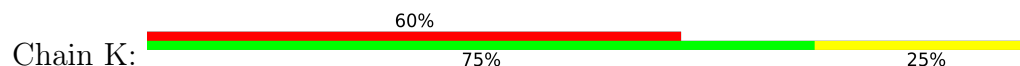




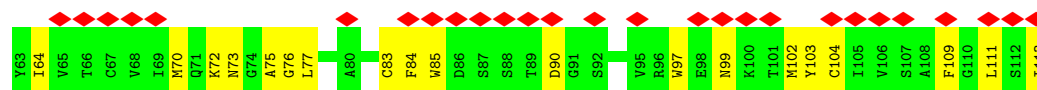
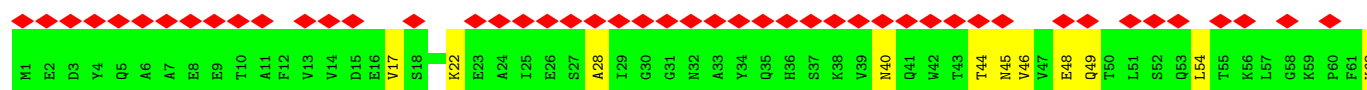
• Molecule 5: Dynein light chain 1, cytoplasmic



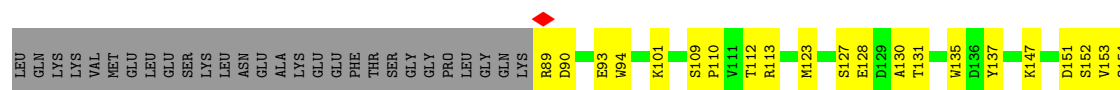
• Molecule 6: Dynein light chain Tctex-type 1



• Molecule 6: Dynein light chain Tctex-type 1

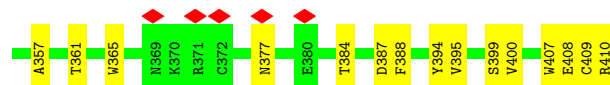
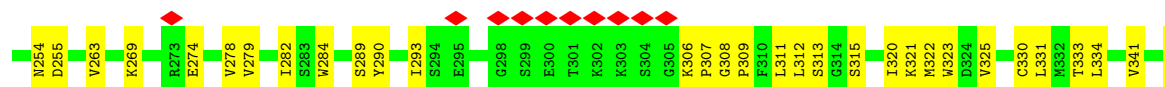
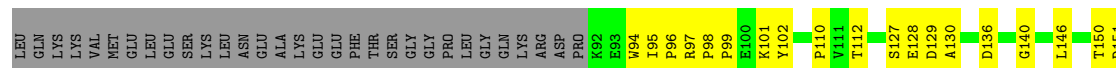
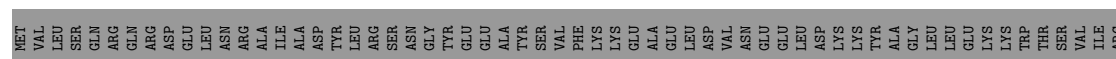


• Molecule 7: Platelet-activating factor acetylhydrolase IB subunit beta





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61684	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	1.773	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	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: ATP, MG, ADP

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	0.10	0/37419	0.28	0/50625
1	B	0.11	0/37248	0.29	0/50392
2	C	0.11	0/3195	0.32	0/4351
2	D	0.10	0/3195	0.30	0/4351
3	E	0.13	0/2573	0.34	0/3473
3	F	0.11	0/2573	0.32	0/3473
4	G	0.15	0/752	0.41	0/1017
4	H	0.12	0/752	0.31	0/1017
5	I	0.18	0/744	0.43	0/997
5	J	0.13	0/744	0.35	0/997
6	K	0.10	0/888	0.28	0/1203
6	L	0.10	0/888	0.30	0/1203
7	O	0.12	0/2624	0.29	0/3555
7	P	0.13	0/2597	0.33	0/3518
All	All	0.11	0/96192	0.29	0/130172

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	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	471	ARG	Sidechain
2	D	526	TYR	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	36692	0	36961	580	0
1	B	36527	0	36808	753	0
2	C	3112	0	2964	25	0
2	D	3112	0	2964	116	0
3	E	2518	0	2525	6	0
3	F	2518	0	2525	101	0
4	G	742	0	768	40	0
4	H	742	0	768	22	0
5	I	728	0	714	54	0
5	J	728	0	714	45	0
6	K	872	0	846	27	0
6	L	872	0	846	24	0
7	O	2557	0	2487	61	0
7	P	2531	0	2463	73	0
8	A	81	0	36	5	0
8	B	81	0	36	3	0
9	A	31	0	12	1	0
9	B	31	0	12	1	0
10	A	2	0	0	0	0
10	B	2	0	0	0	0
All	All	94479	0	94449	1824	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 11.

The worst 5 of 1824 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1937:ASP:HA	1:B:1967:MET:HE1	1.44	0.98
1:B:471:ARG:NH1	1:B:472:GLN:HG3	1.81	0.95

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ARG:HH12	1:B:472:GLN:HG3	1.29	0.92
1:B:4296:MET:HE3	1:B:4297:PRO:HD2	1.53	0.90
7:P:306:LYS:HD3	7:P:308:GLY:H	1.37	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%)	4400 (97%)	128 (3%)	2 (0%)	100	100
1	B	4507/4646 (97%)	4375 (97%)	129 (3%)	3 (0%)	48	83
2	C	390/638 (61%)	369 (95%)	21 (5%)	0	100	100
2	D	390/638 (61%)	369 (95%)	21 (5%)	0	100	100
3	E	307/492 (62%)	298 (97%)	9 (3%)	0	100	100
3	F	307/492 (62%)	294 (96%)	12 (4%)	1 (0%)	36	72
4	G	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
4	H	91/96 (95%)	83 (91%)	8 (9%)	0	100	100
5	I	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
5	J	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
6	K	111/113 (98%)	110 (99%)	1 (1%)	0	100	100
6	L	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
7	O	320/410 (78%)	306 (96%)	14 (4%)	0	100	100
7	P	317/410 (77%)	303 (96%)	14 (4%)	0	100	100
All	All	11646/12968 (90%)	11263 (97%)	377 (3%)	6 (0%)	49	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3384	ARG
1	B	540	LYS
1	B	3384	ARG
1	A	589	ASN
1	B	1161	ALA

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%)	4044 (100%)	0	100	100
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
7	O	287/364 (79%)	287 (100%)	0	100	100
7	P	284/364 (78%)	284 (100%)	0	100	100
All	All	10413/11464 (91%)	10413 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	731	ASN

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Mol	Chain	Res	Type
6	K	41	GLN
1	B	2067	ASN
5	I	51	ASN
1	B	4477	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	ADP	A	4701	10	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)
8	ADP	B	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
9	ATP	B	4702	10	32,33,33	0.31	0	48,52,52	0.28	0
8	ADP	B	4701	10	28,29,29	1.39	4 (14%)	43,45,45	1.86	8 (18%)
8	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
8	ADP	B	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.88	8 (18%)
9	ATP	A	4702	10	32,33,33	0.30	0	48,52,52	0.28	0
8	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	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	ADP	A	4701	10	-	1/16/32/32	0/3/3/3
8	ADP	B	4704	-	-	1/16/32/32	0/3/3/3
9	ATP	B	4702	10	-	3/22/38/38	0/3/3/3
8	ADP	B	4701	10	-	2/16/32/32	0/3/3/3
8	ADP	A	4704	-	-	1/16/32/32	0/3/3/3
8	ADP	B	4703	-	-	5/16/32/32	0/3/3/3
9	ATP	A	4702	10	-	5/22/38/38	0/3/3/3
8	ADP	A	4703	-	-	5/16/32/32	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	4703	ADP	C5-C4	4.73	1.47	1.39
8	B	4703	ADP	C5-C4	4.68	1.47	1.39
8	B	4701	ADP	C5-C4	4.66	1.47	1.39
8	B	4704	ADP	C5-C4	4.65	1.47	1.39
8	A	4704	ADP	C5-C4	4.63	1.47	1.39

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	4703	ADP	C5-C4-N3	-6.16	118.24	126.72
8	A	4703	ADP	C5-C4-N3	-6.01	118.44	126.72
8	B	4701	ADP	C5-C4-N3	-5.90	118.59	126.72
8	B	4704	ADP	C5-C4-N3	-5.81	118.72	126.72
8	A	4701	ADP	C5-C4-N3	-5.80	118.72	126.72

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

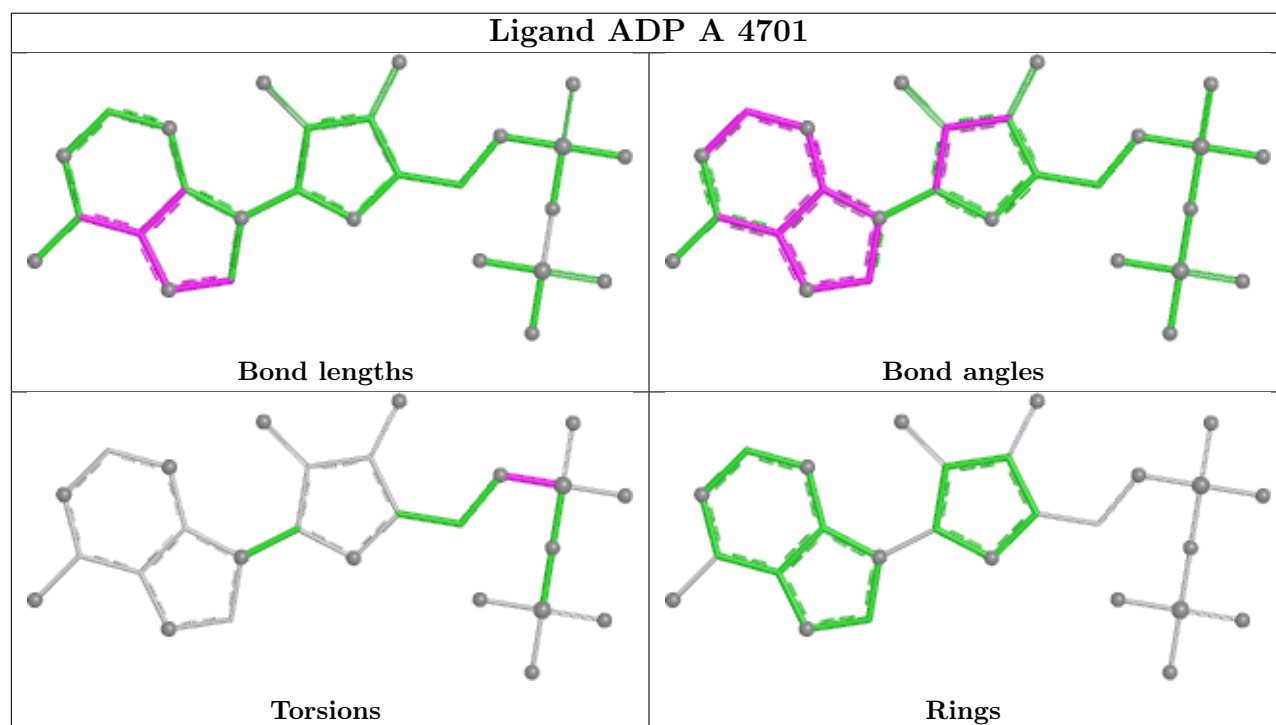
Mol	Chain	Res	Type	Atoms
8	A	4701	ADP	C5'-O5'-PA-O2A
8	A	4703	ADP	C5'-O5'-PA-O1A
8	A	4703	ADP	C5'-O5'-PA-O3A
8	B	4701	ADP	C5'-O5'-PA-O2A
8	B	4701	ADP	C5'-O5'-PA-O3A

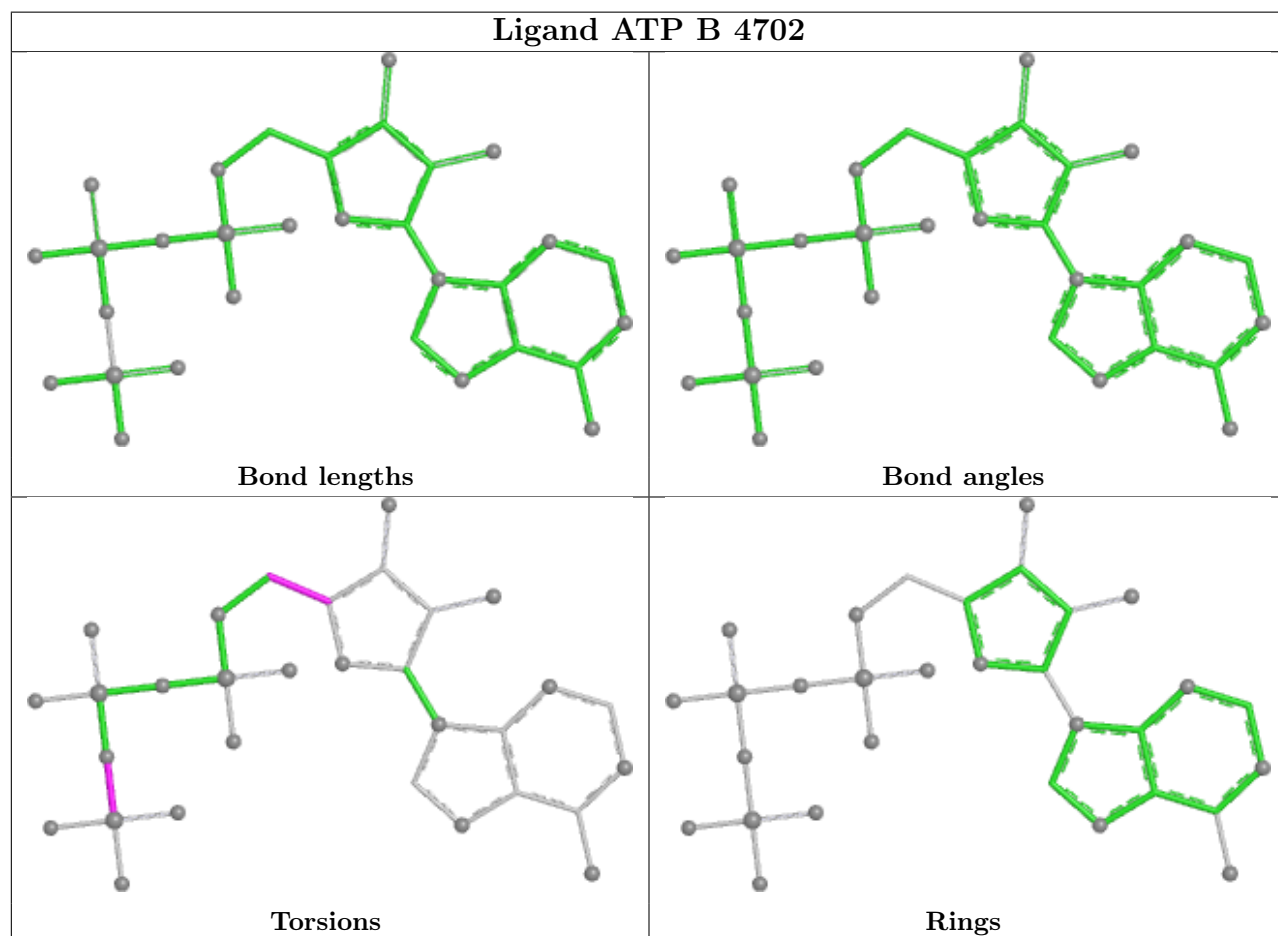
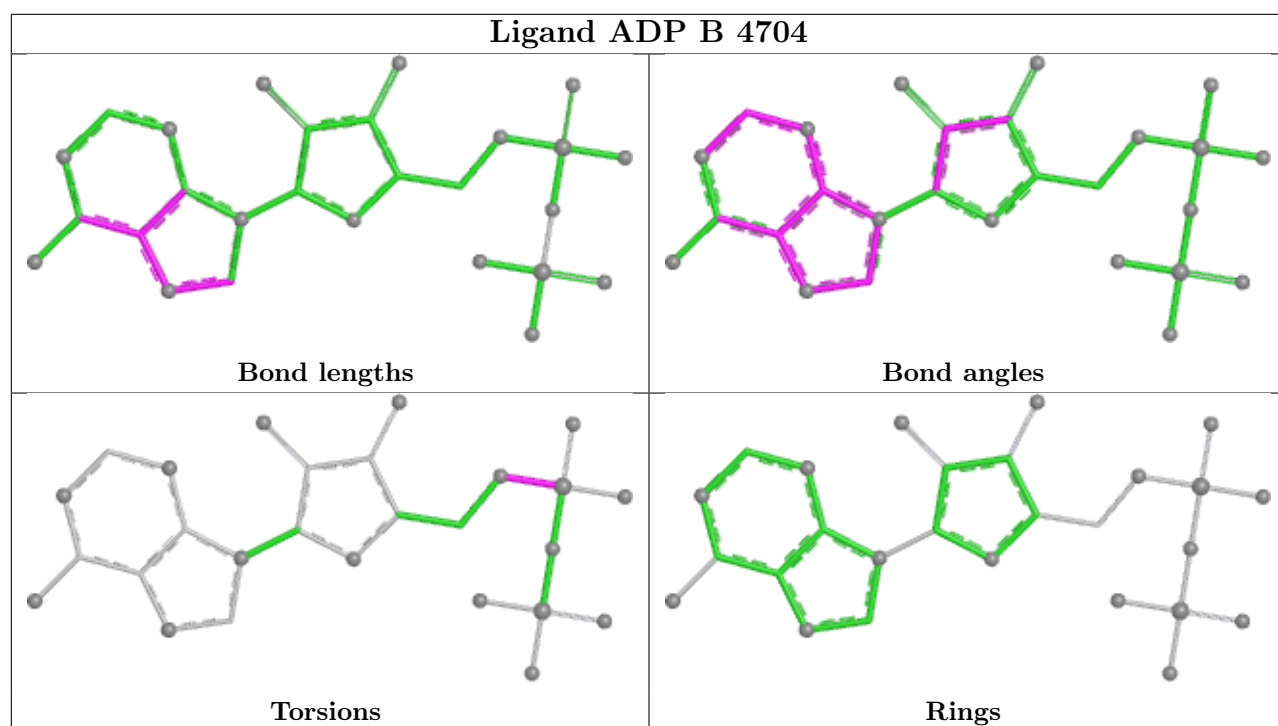
There are no ring outliers.

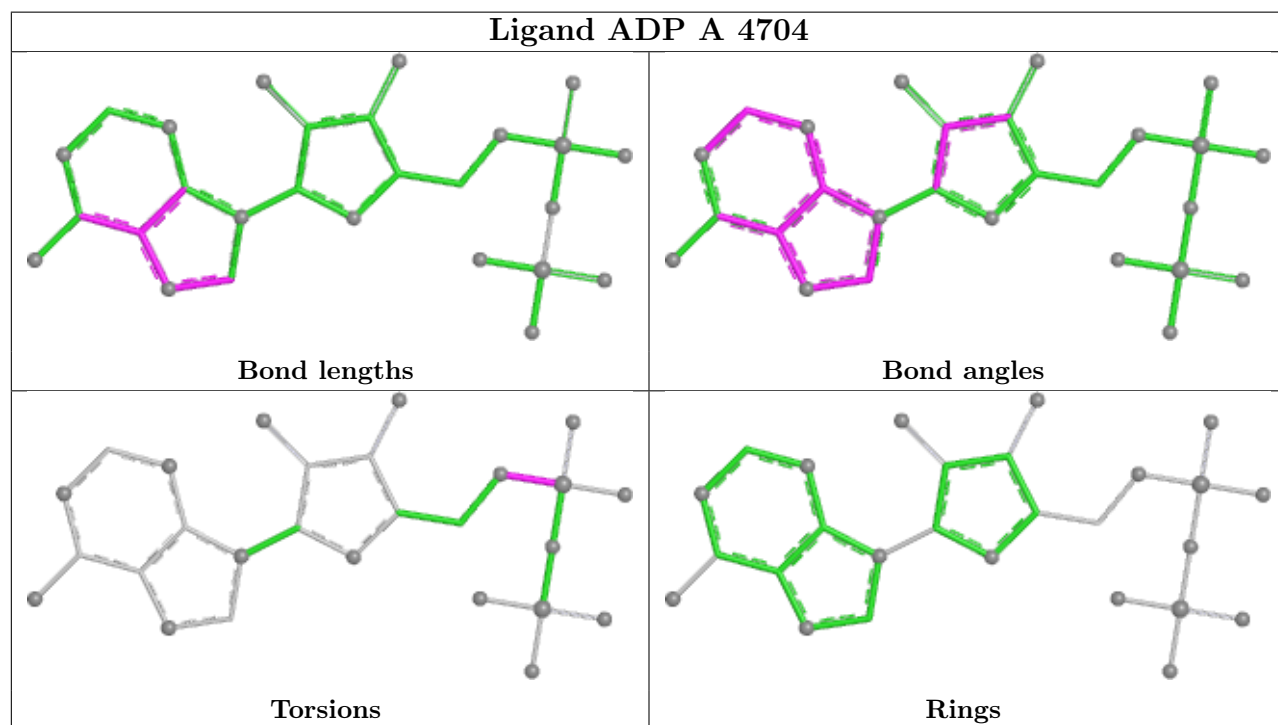
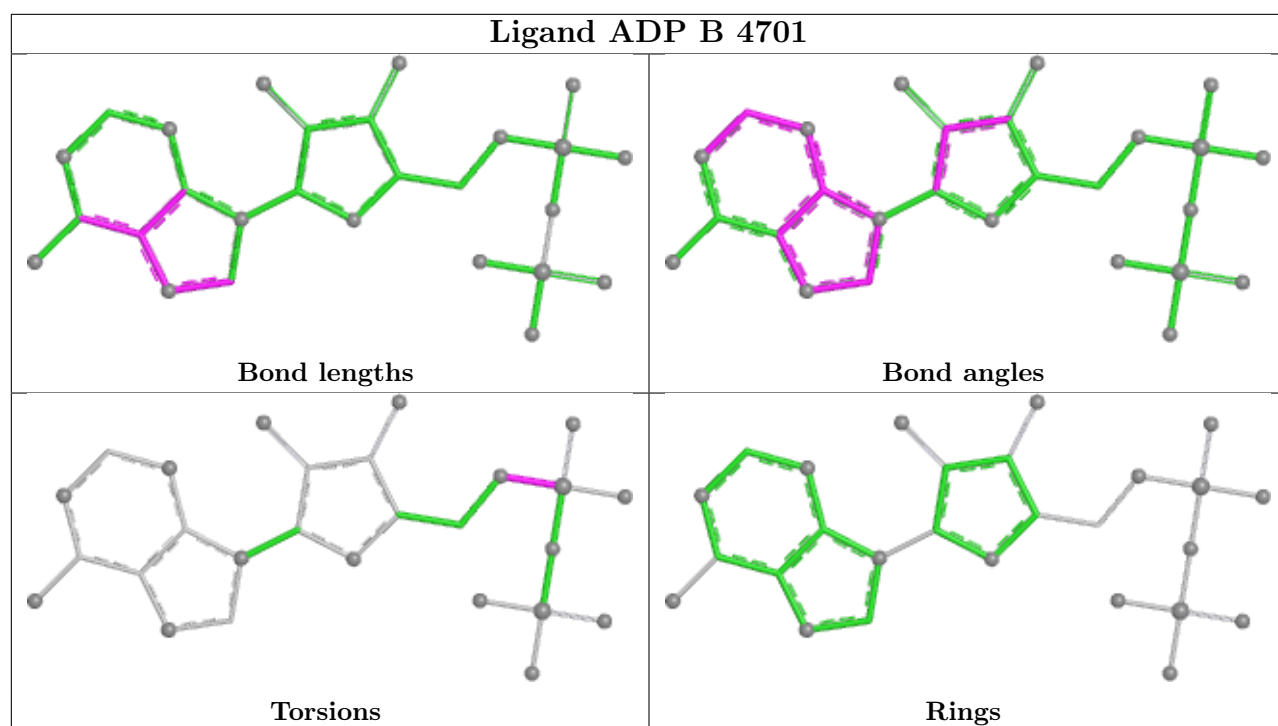
7 monomers are involved in 10 short contacts:

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

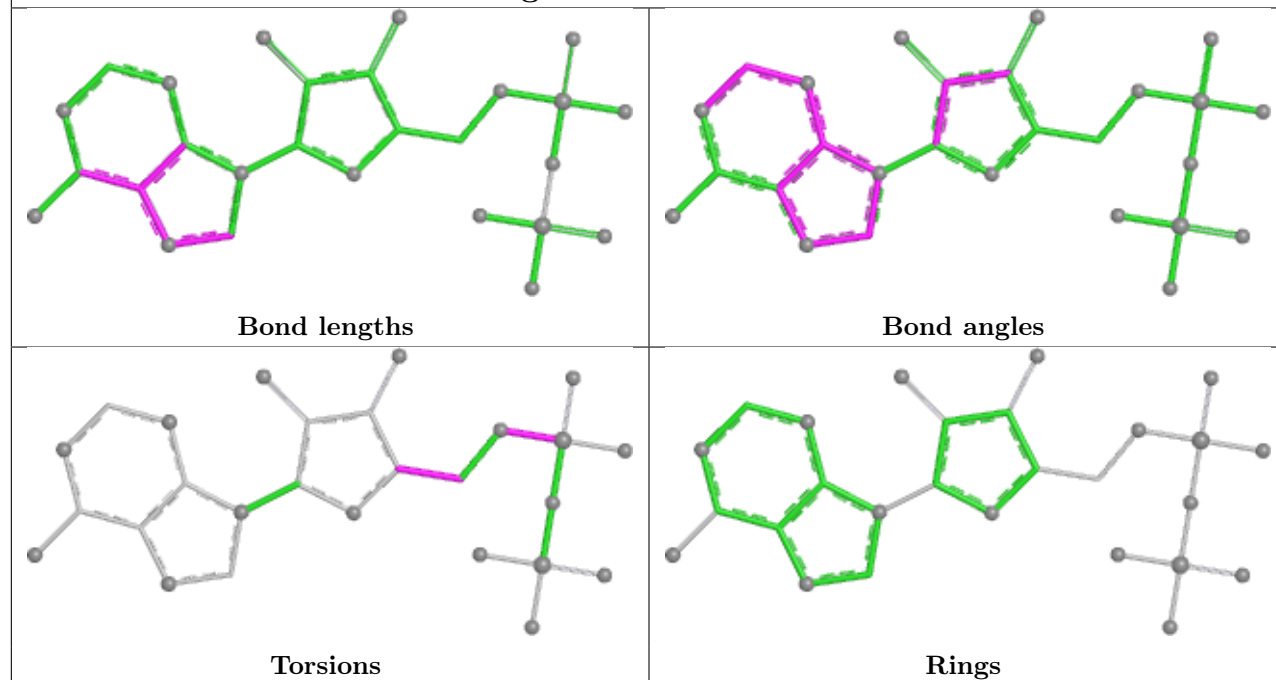
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



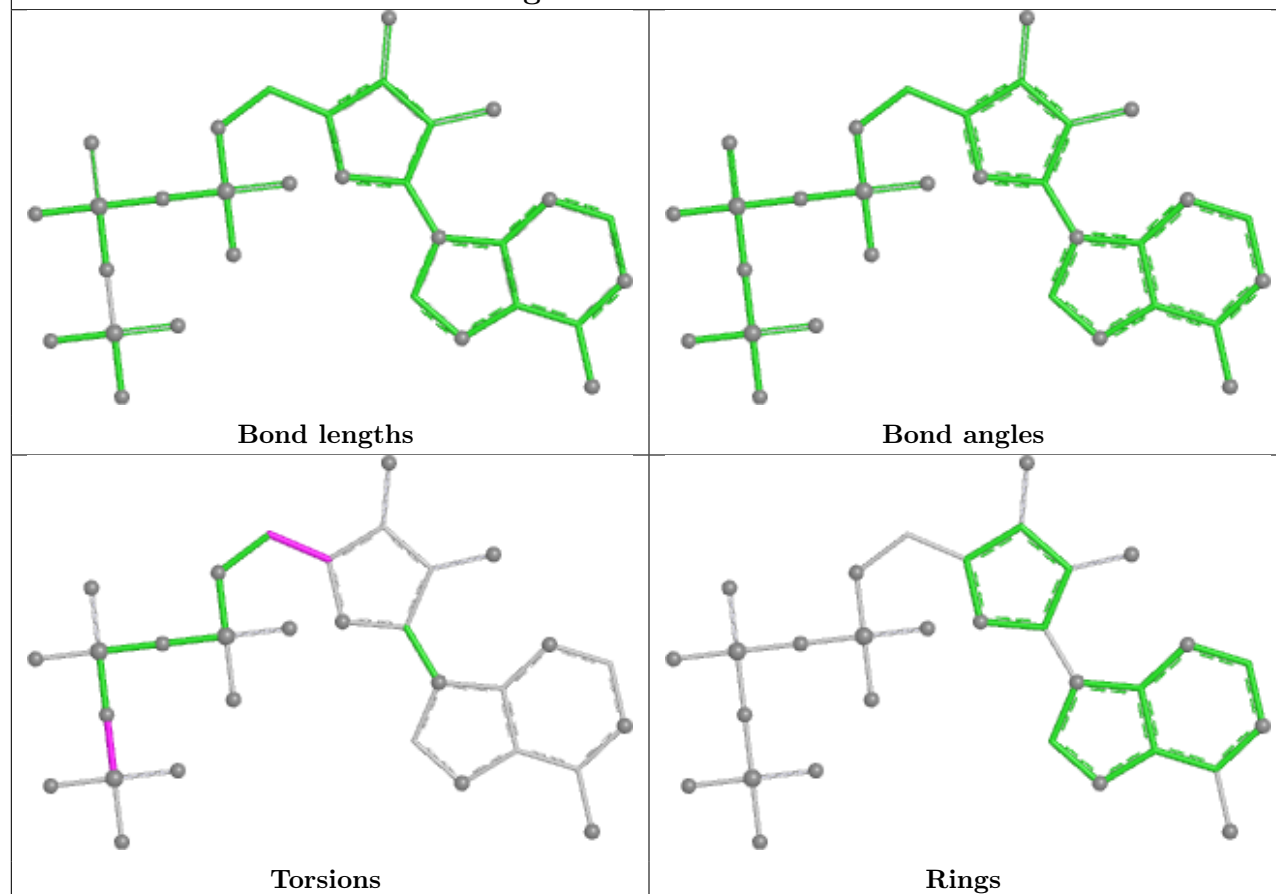


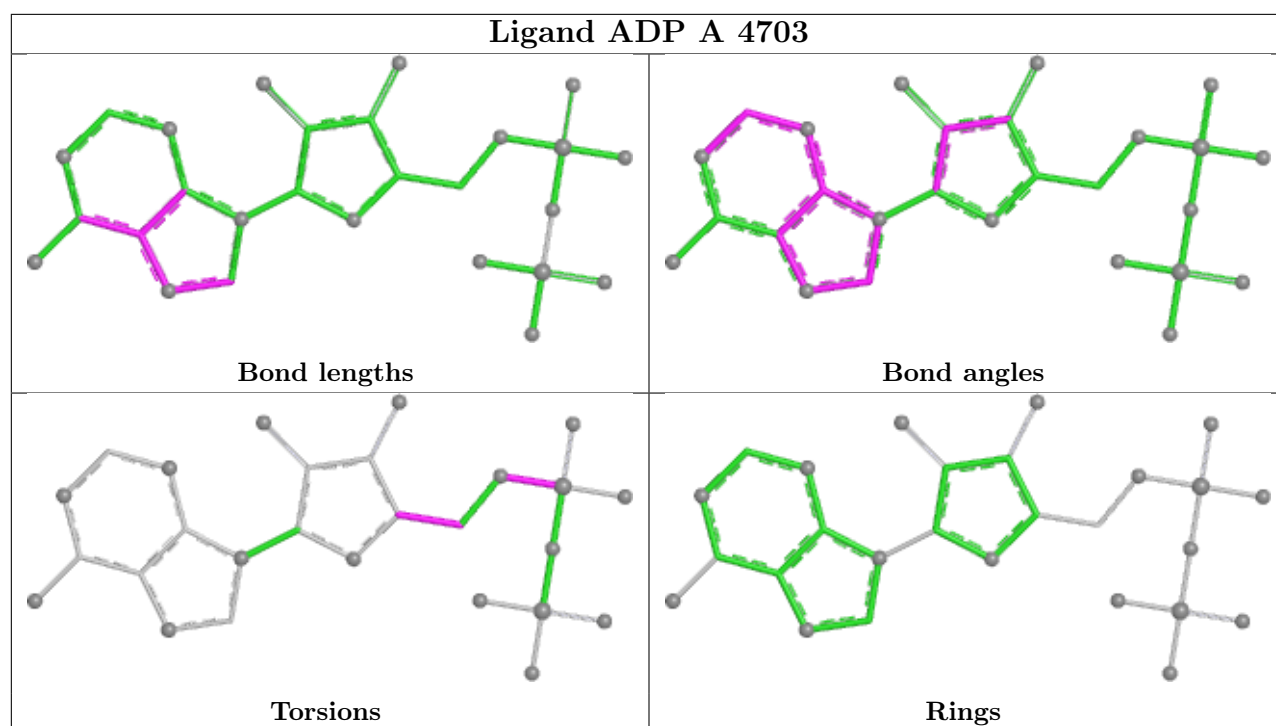


Ligand ADP B 4703



Ligand ATP A 4702





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1394:MET	C	1395:LYS	N	8.85
1	A	1394:MET	C	1395:LYS	N	3.62

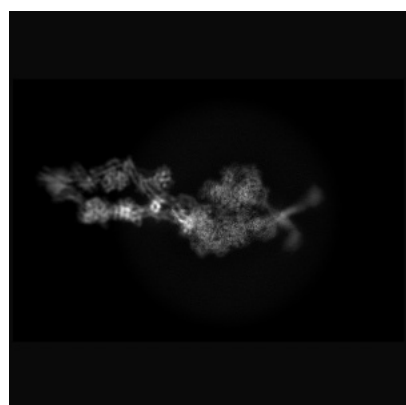
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47383. These allow visual inspection of the internal detail of the map and identification of artifacts.

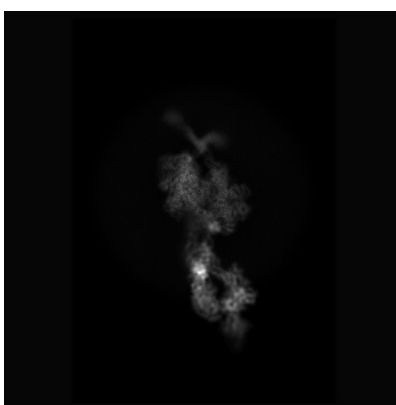
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

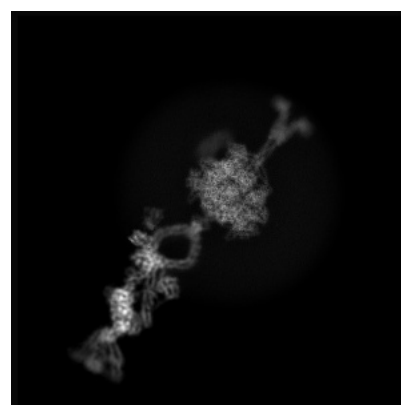
6.1.1 Primary map



X



Y

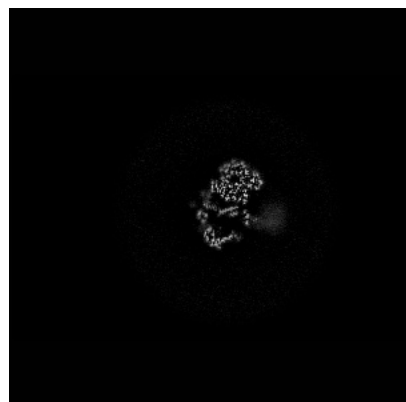


Z

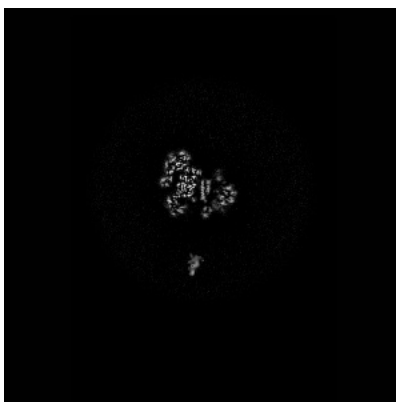
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

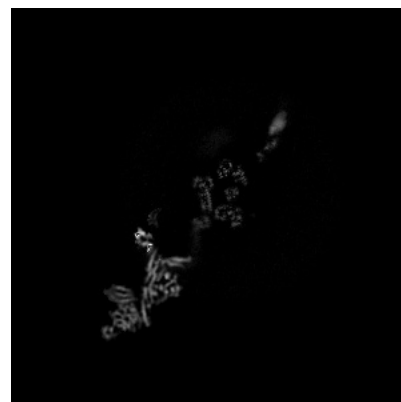
6.2.1 Primary map



X Index: 210



Y Index: 210

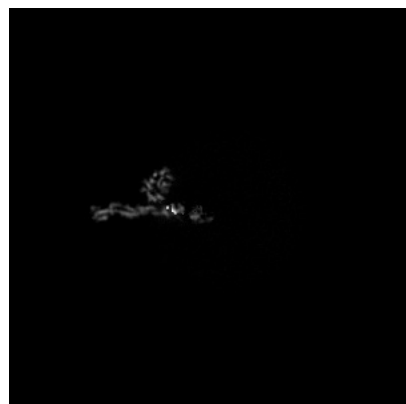


Z Index: 210

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

6.3 Largest variance slices [i](#)

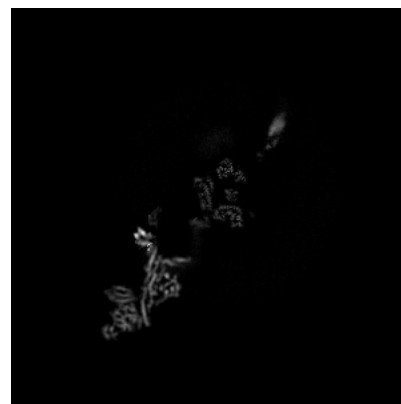
6.3.1 Primary map



X Index: 144



Y Index: 156

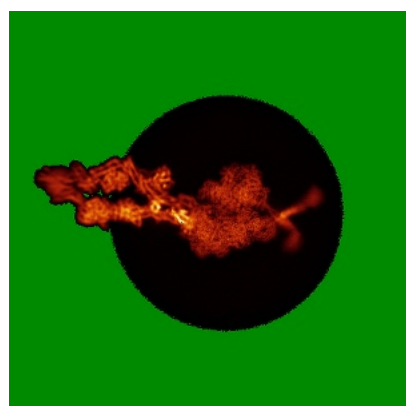


Z Index: 209

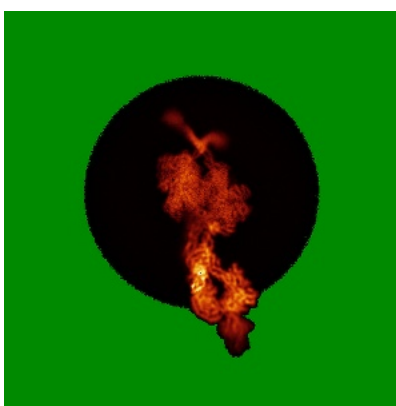
The images above show the largest variance slices of the map in three orthogonal directions.

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

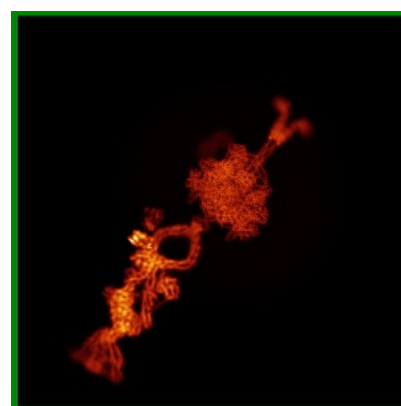
6.4.1 Primary map



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 [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.

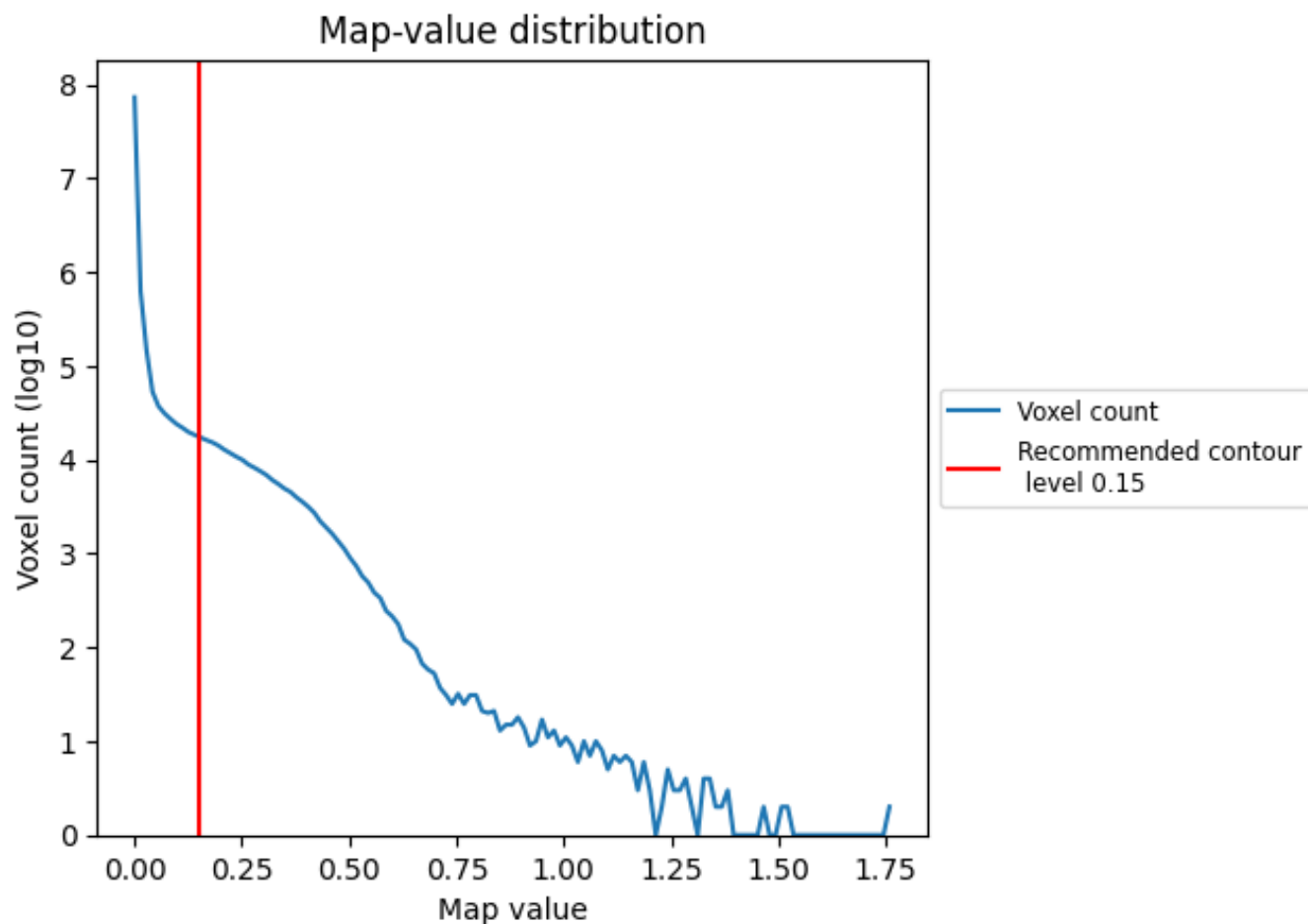
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

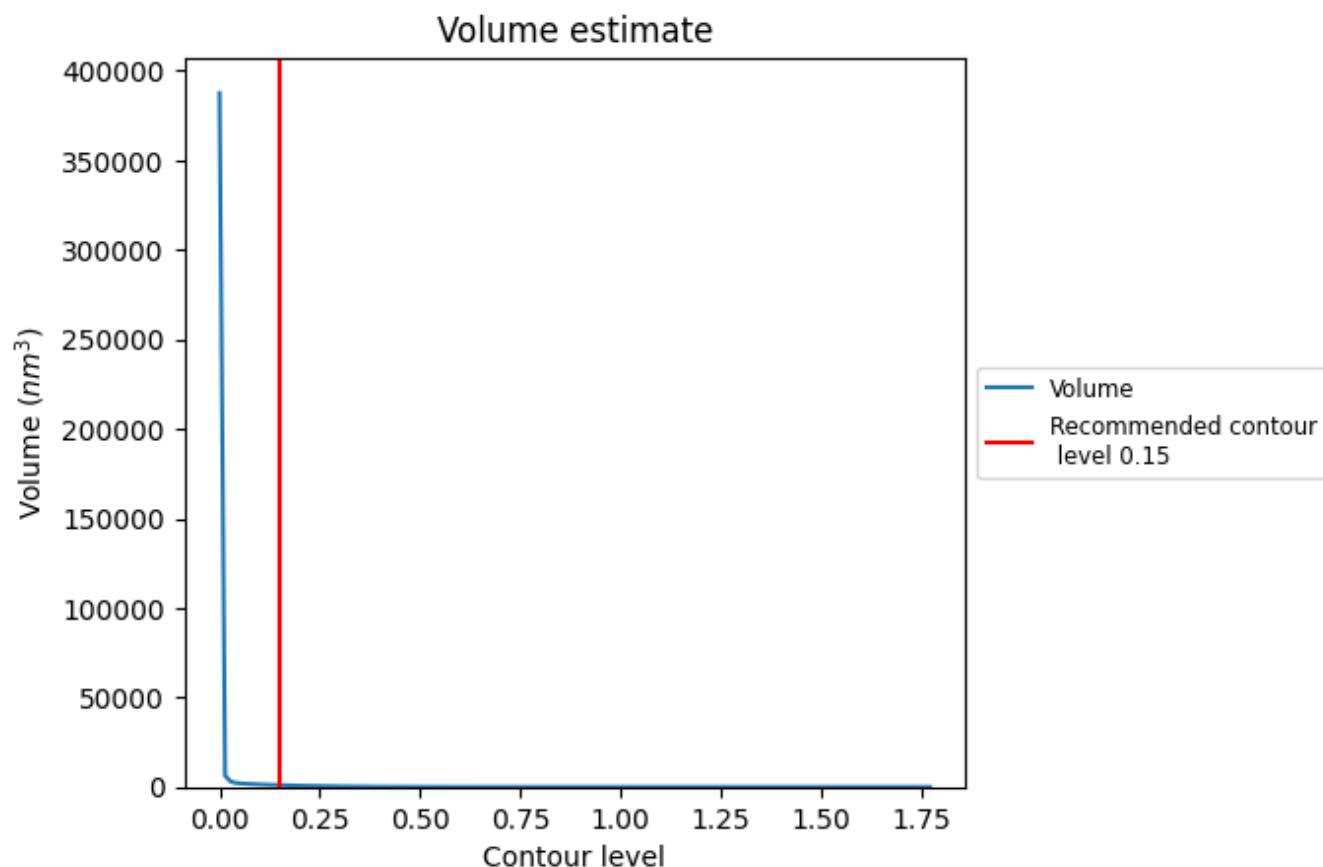
This section contains the results of statistical analysis of the map.

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.

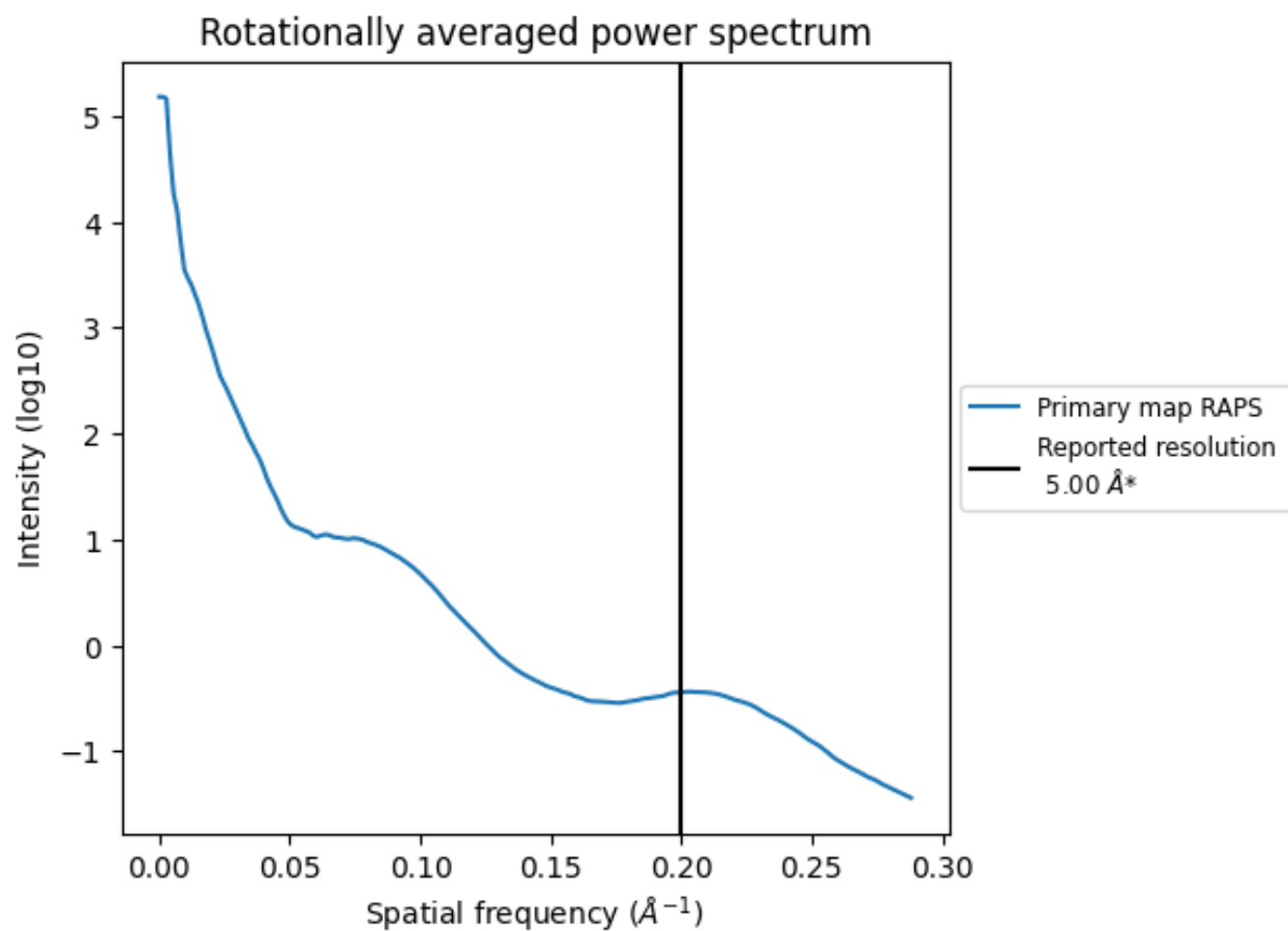
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1005 nm^3 ; this corresponds to an approximate mass of 908 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 0.200 Å⁻¹

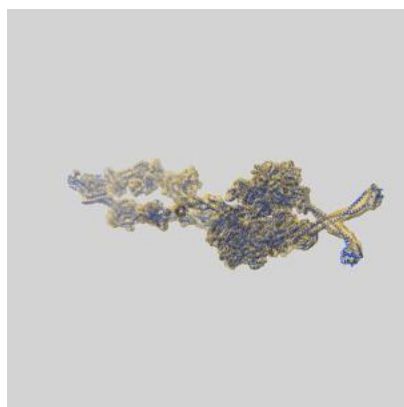
8 Fourier-Shell correlation

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

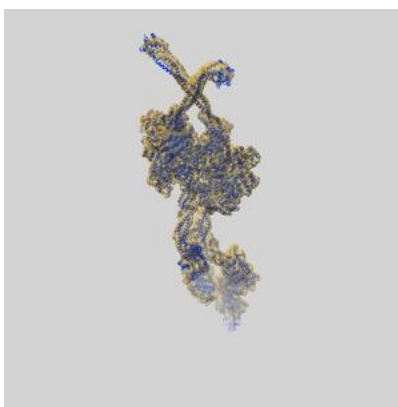
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47383 and PDB model 9E14. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

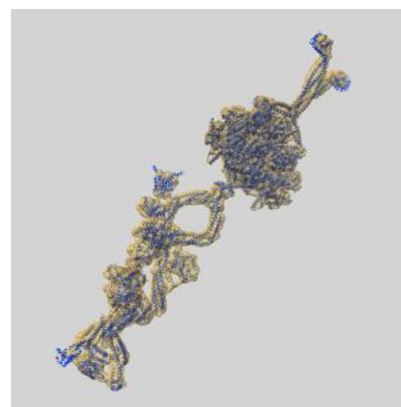
9.1 Map-model overlay [i](#)



X



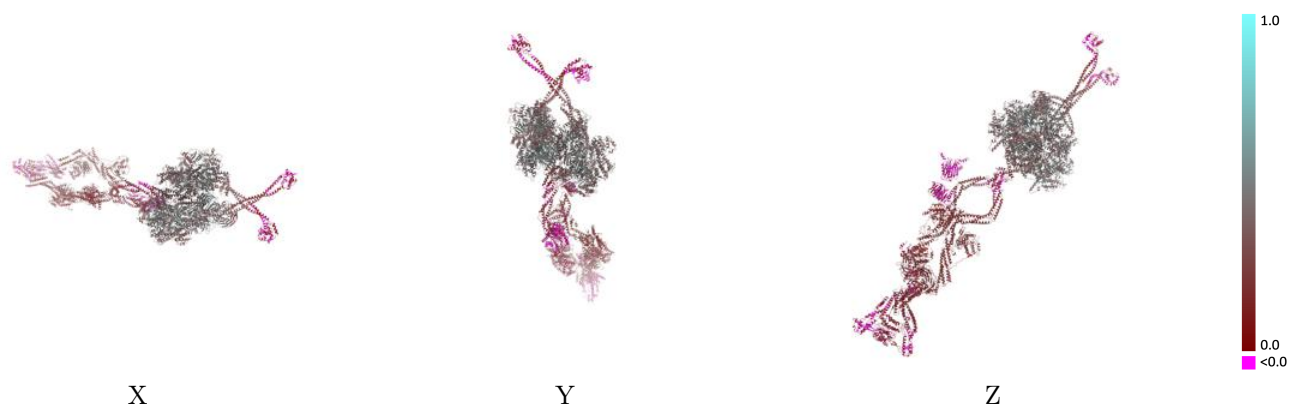
Y



Z

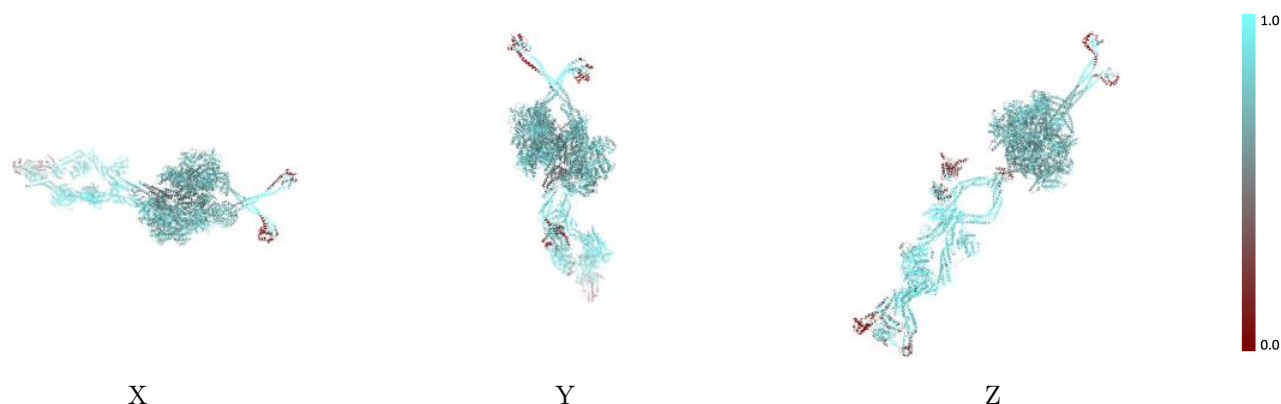
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



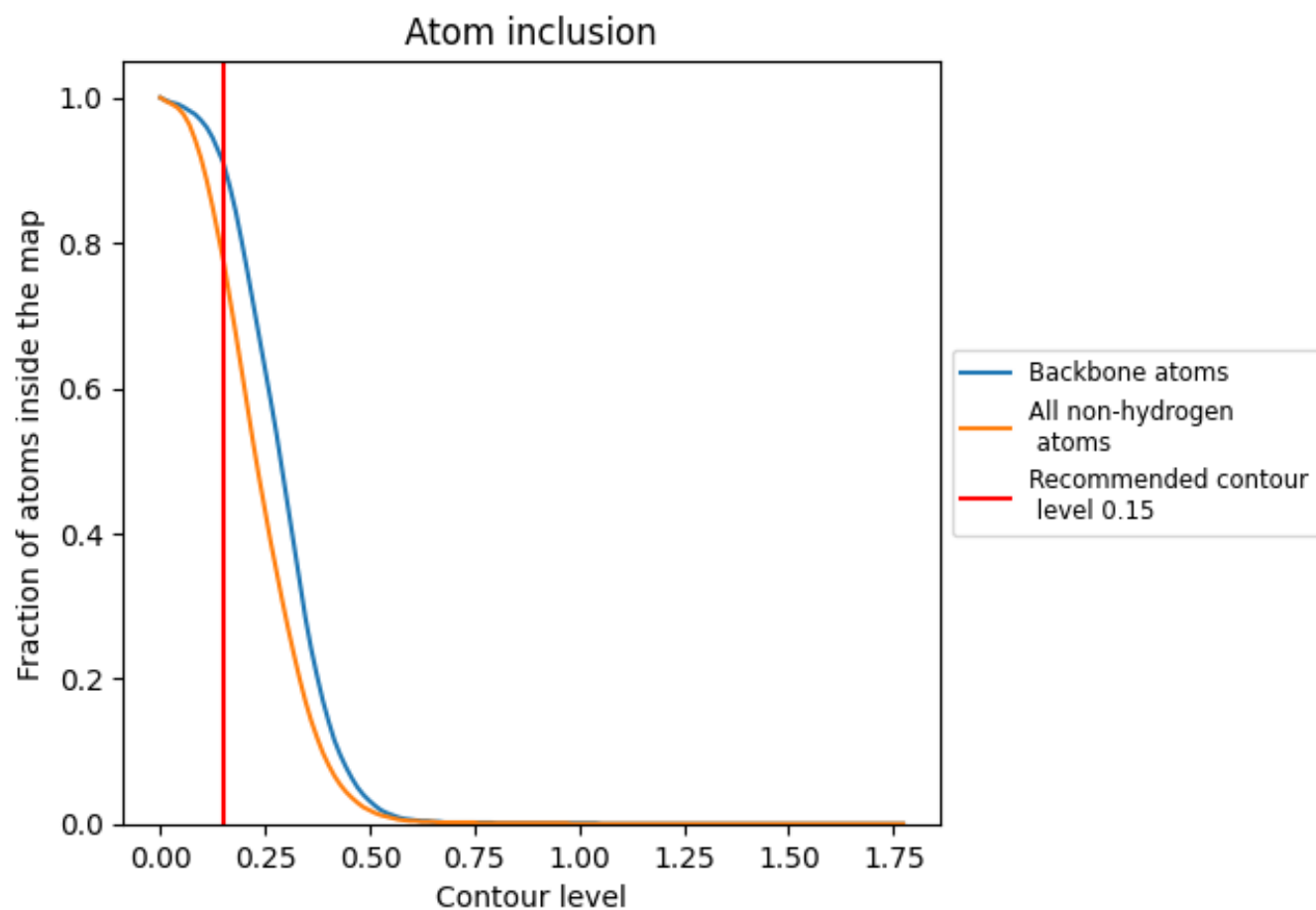
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% of all backbone atoms, 78% 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	<div></div> 0.7770	<div></div> 0.3020
A	<div></div> 0.7410	<div></div> 0.3160
B	<div></div> 0.7900	<div></div> 0.3320
C	<div></div> 0.9210	<div></div> 0.2070
D	<div></div> 0.9250	<div></div> 0.1850
E	<div></div> 0.9320	<div></div> 0.2040
F	<div></div> 0.9220	<div></div> 0.1970
G	<div></div> 0.7570	<div></div> 0.1070
H	<div></div> 0.8730	<div></div> 0.1490
I	<div></div> 0.7660	<div></div> 0.0700
J	<div></div> 0.6230	<div></div> 0.0360
K	<div></div> 0.3560	<div></div> 0.0150
L	<div></div> 0.3330	<div></div> 0.0080
O	<div></div> 0.8120	<div></div> 0.4860
P	<div></div> 0.7490	<div></div> 0.3860

