Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 08:21 pm GMT

PDB ID	:	6ZNL
EMDB ID	:	EMD-11313
Title	:	Cryo-EM structure of the dynactin complex
Authors	:	Lau, C.K.; Lacey, S.E.; Carter, A.P.
Deposited on	:	2020-07-06
Resolution	:	3.80 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

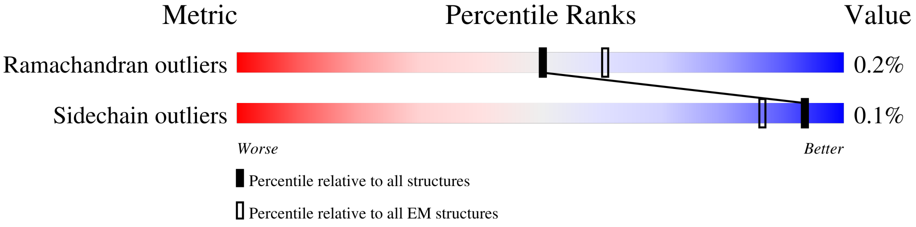
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

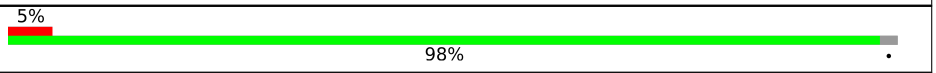
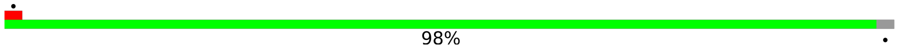
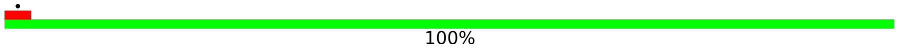
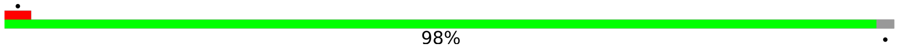
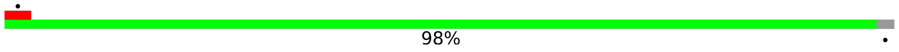
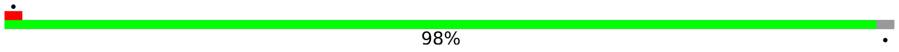
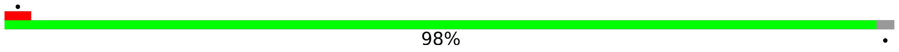
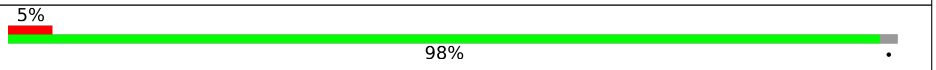
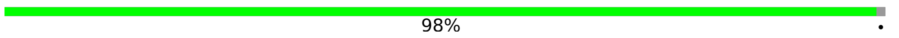
The reported resolution of this entry is 3.80 Å.

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	376	
1	B	376	
1	C	376	
1	D	376	
1	E	376	
1	F	376	
1	G	376	
1	I	376	
2	H	375	

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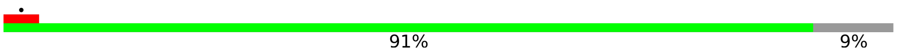
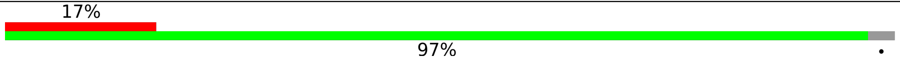
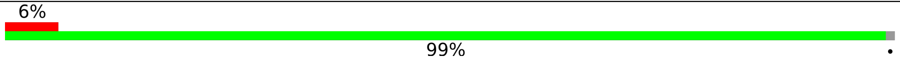
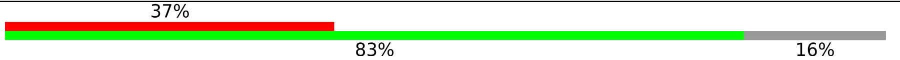
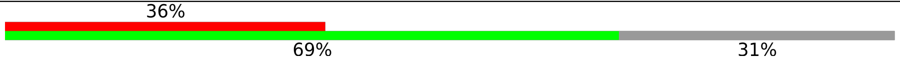
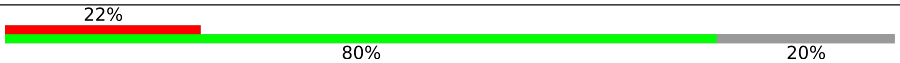
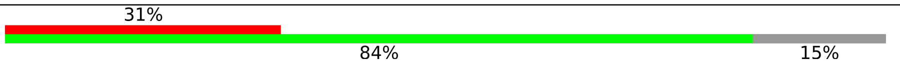
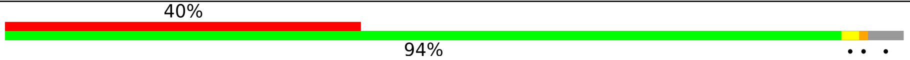
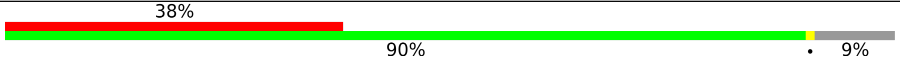
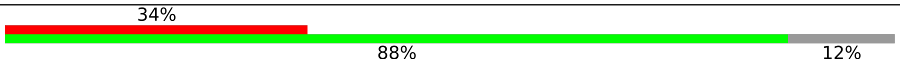
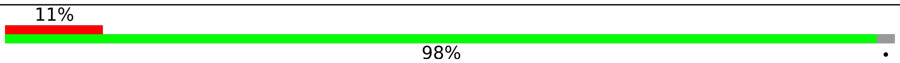
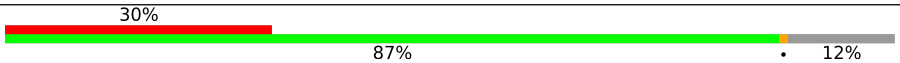
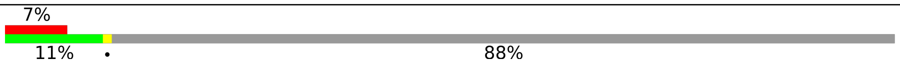
Mol	Chain	Length	Quality of chain
3	J	417	
4	K	286	
5	L	272	
6	M	405	
6	N	405	
6	m	405	
6	n	405	
7	O	186	
7	o	186	
8	U	190	
9	V	182	
10	Y	467	
11	Z	1286	
11	z	1286	

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 52864 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 ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total 2944	C 1886	N 509	O 539	S 10	0	0
1	B	370	Total 2956	C 1892	N 509	O 545	S 10	0	0
1	C	375	Total 2998	C 1918	N 514	O 556	S 10	0	0
1	D	370	Total 2956	C 1892	N 509	O 545	S 10	0	0
1	E	370	Total 2956	C 1892	N 509	O 545	S 10	0	0
1	F	370	Total 2956	C 1892	N 509	O 545	S 10	0	0
1	G	370	Total 2956	C 1892	N 509	O 545	S 10	0	0
1	I	370	Total 2941	C 1885	N 509	O 537	S 10	0	0

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	370	Total 2885	C 1827	N 486	O 550	S 22	0	0

- Molecule 3 is a protein called Arp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	379	Total 2932	C 1888	N 496	O 532	S 16	0	0

- Molecule 4 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	278	Total 2264	C 1428	N 396	O 434	S 6	0	0

- Molecule 5 is a protein called F-actin capping protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	269	Total 2122	C 1323	N 370	O 418	S 11	0	0

- Molecule 6 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	340	Total 2238	C 1382	N 408	O 443	S 5	0	0
6	N	280	Total 1767	C 1089	N 327	O 346	S 5	0	0
6	m	325	Total 2262	C 1413	N 397	O 446	S 6	0	0
6	n	343	Total 2349	C 1471	N 423	O 451	S 4	0	0

- Molecule 7 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	179	Total 1183	C 736	N 210	O 233	S 4	0	0
7	o	170	Total 1082	C 679	N 208	O 194	S 1	0	0

- Molecule 8 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	167	Total 1224	C 771	N 212	O 231	S 10	0	0

- Molecule 9 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	179	Total 1260	C 818	N 222	O 211	S 9	0	0

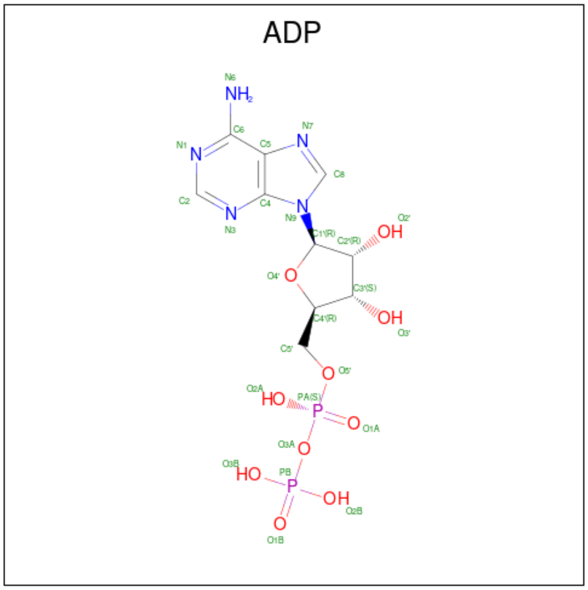
- Molecule 10 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Y	410	2960	1868	543	529	20	0	0

- Molecule 11 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Z	192	1444	904	262	275	3	0	0
11	z	155	952	583	189	177	3	0	0

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	A	1	27	10	5	10	2	0
12	B	1	27	10	5	10	2	0
12	C	1	27	10	5	10	2	0
12	D	1	27	10	5	10	2	0
12	E	1	27	10	5	10	2	0
12	F	1	27	10	5	10	2	0

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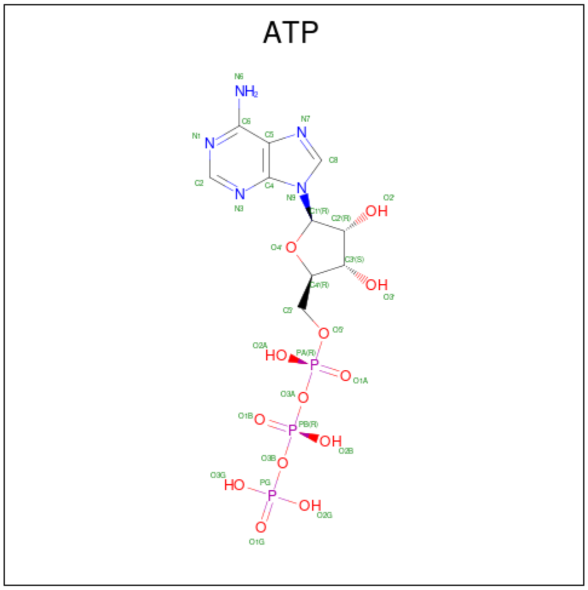
Mol	Chain	Residues	Atoms	AltConf
12	G	1	Total C N O P 27 10 5 10 2	0
12	I	1	Total C N O P 27 10 5 10 2	0
12	J	1	Total C N O P 27 10 5 10 2	0

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

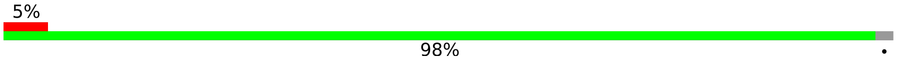
Mol	Chain	Residues	Atoms	AltConf
14	Y	3	Total Zn 3 3	0

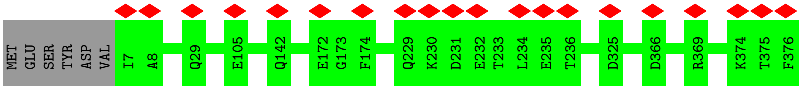
3 Residue-property plots ⓘ

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

- Molecule 1: ARP1 actin related protein 1 homolog A

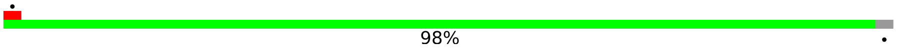
Chain A:

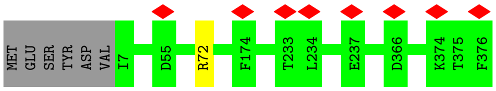




- Molecule 1: ARP1 actin related protein 1 homolog A

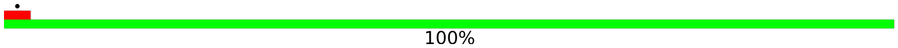
Chain B:

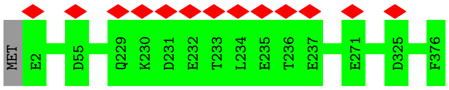




- Molecule 1: ARP1 actin related protein 1 homolog A

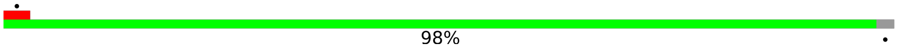
Chain C:

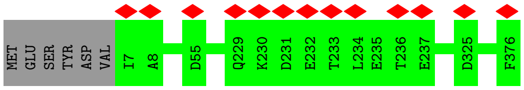




- Molecule 1: ARP1 actin related protein 1 homolog A

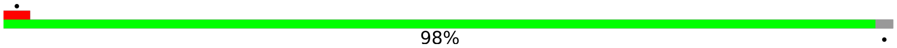
Chain D:

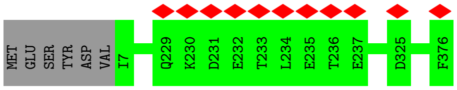




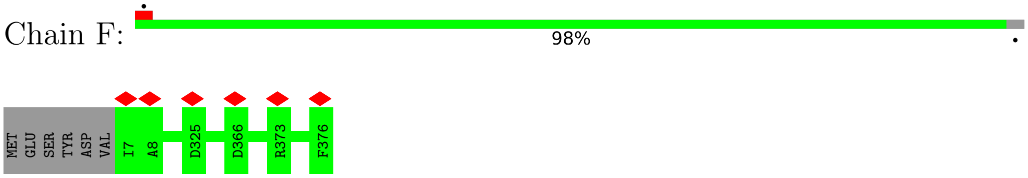
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain E:

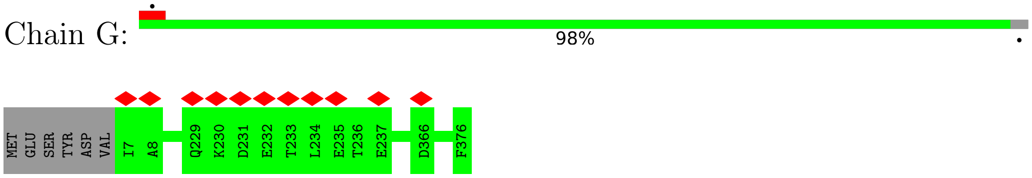




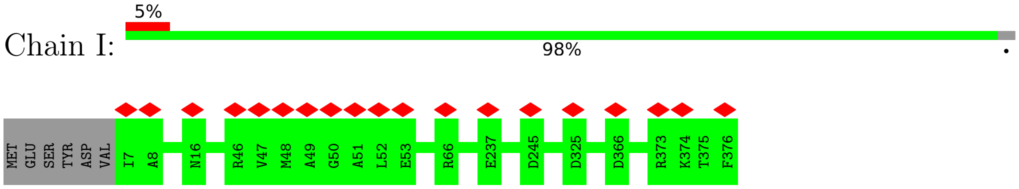
- Molecule 1: ARP1 actin related protein 1 homolog A



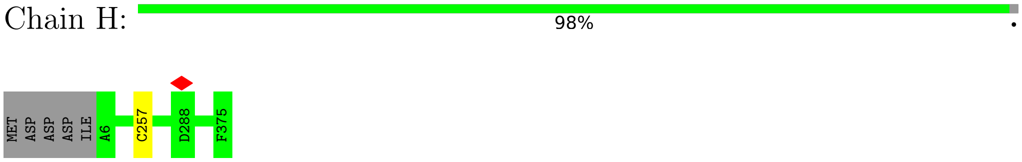
- Molecule 1: ARP1 actin related protein 1 homolog A



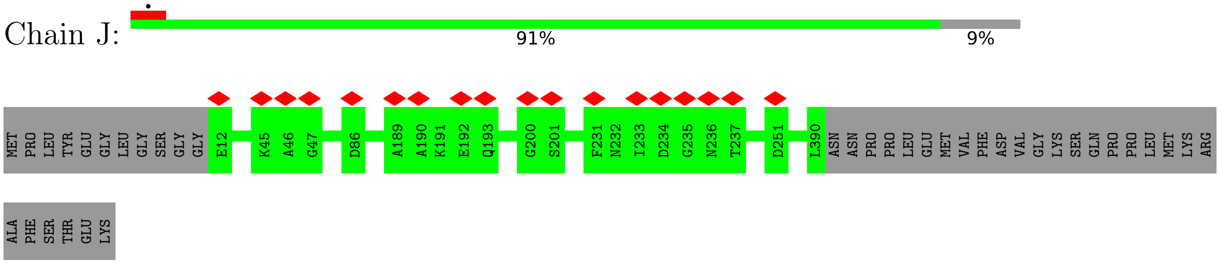
- Molecule 1: ARP1 actin related protein 1 homolog A



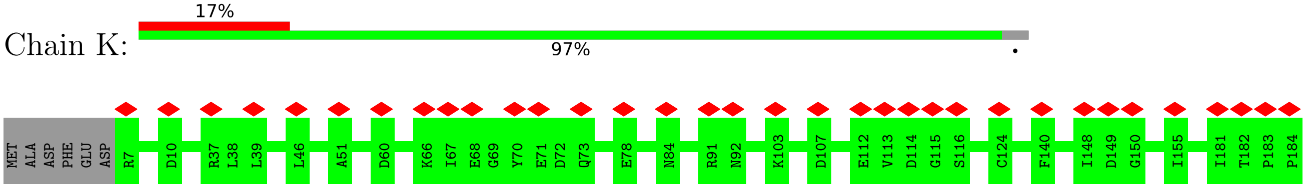
- Molecule 2: Actin, cytoplasmic 1

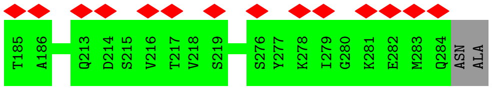


- Molecule 3: Arp11



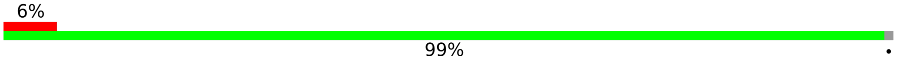
- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1

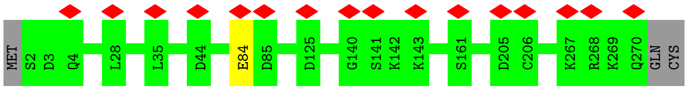




- Molecule 5: F-actin capping protein beta subunit

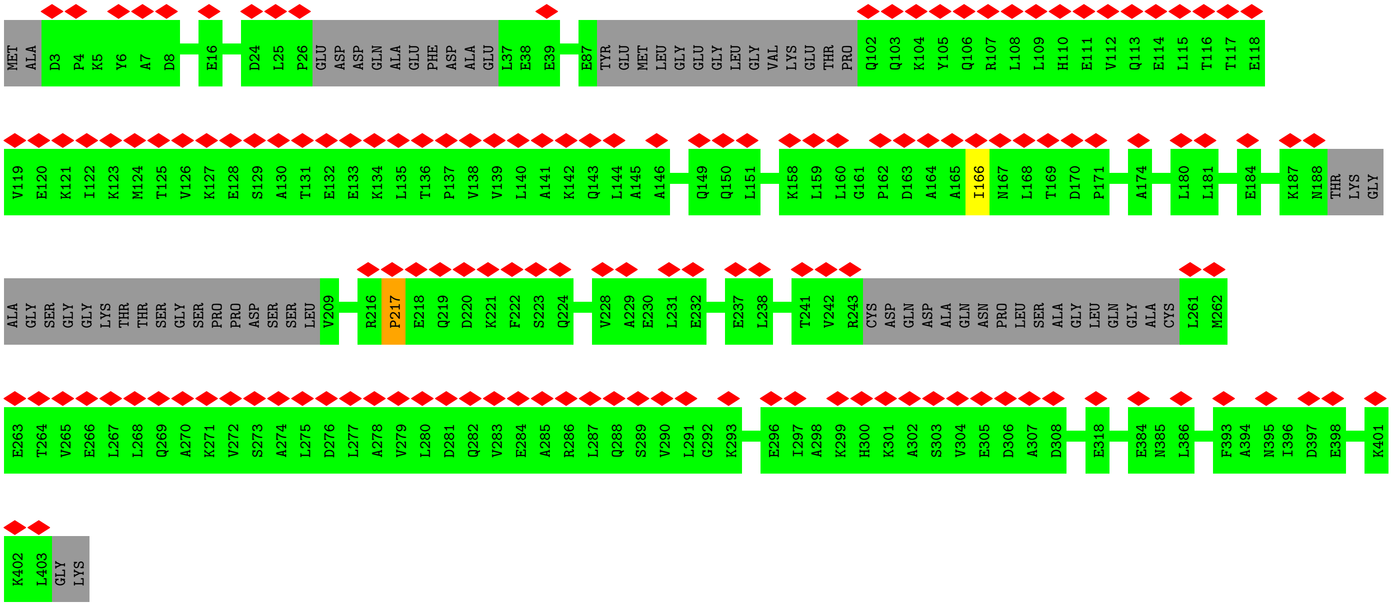
Chain L:





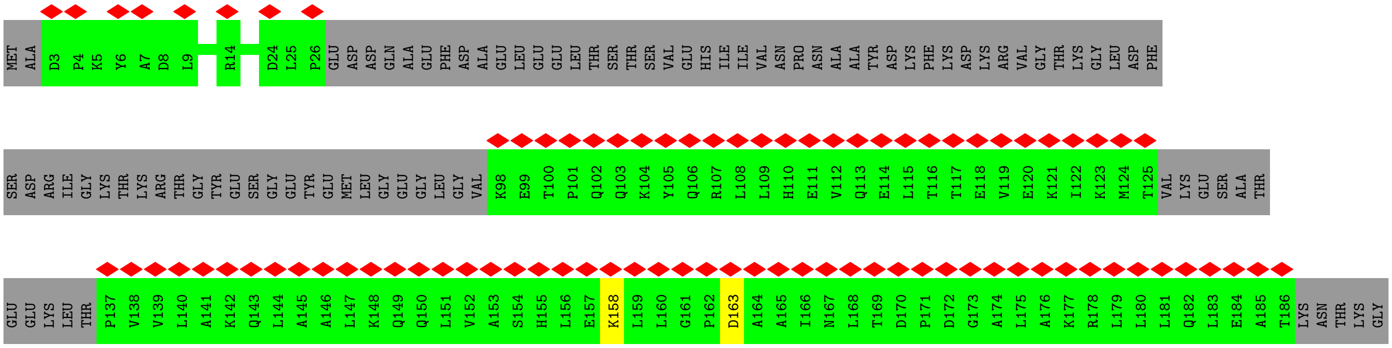
- Molecule 6: Dynactin subunit 2

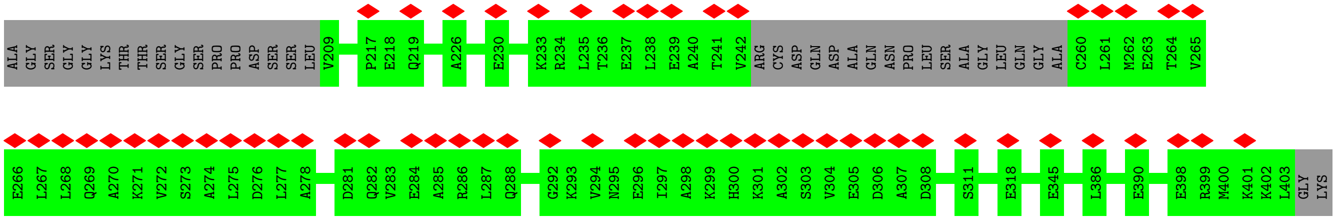
Chain M:



- Molecule 6: Dynactin subunit 2

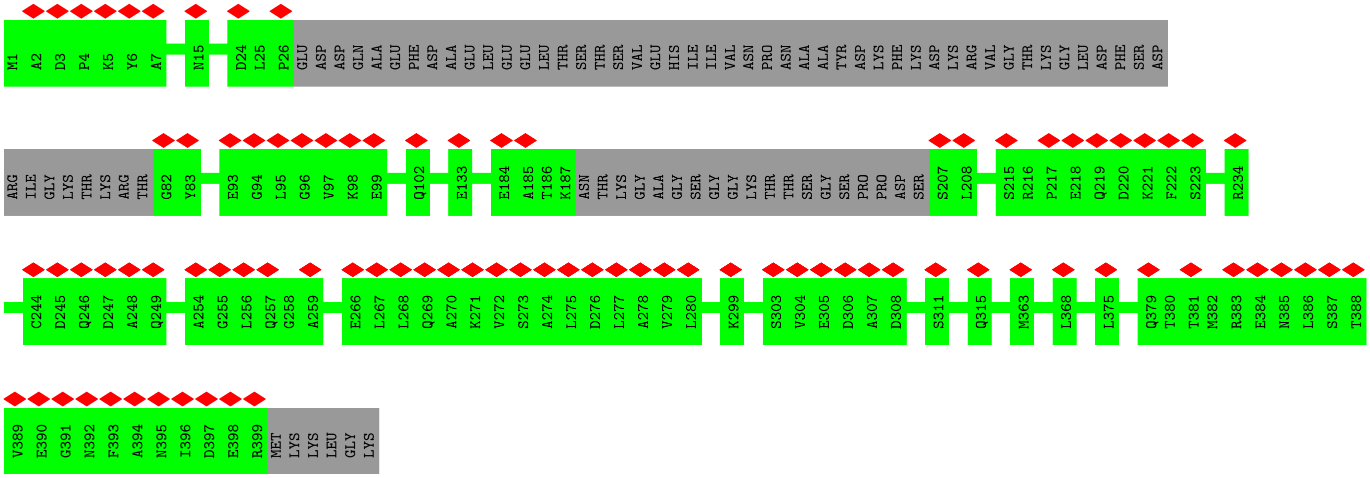
Chain N:





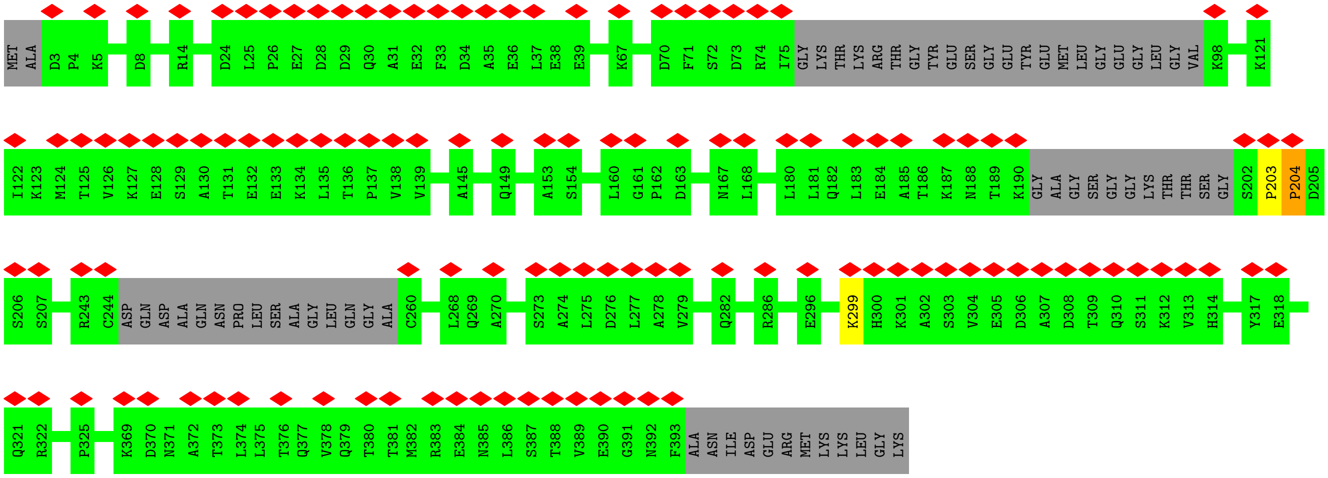
- Molecule 6: Dynactin subunit 2

Chain m:



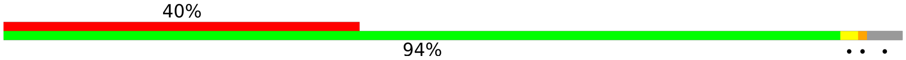
- Molecule 6: Dynactin subunit 2

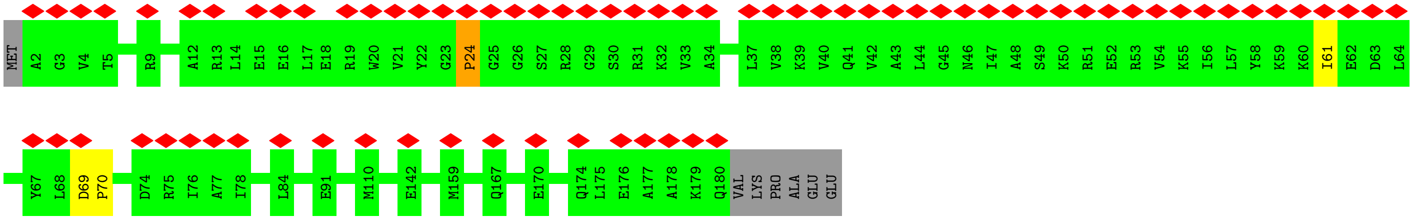
Chain n:



- Molecule 7: Dynactin subunit 3

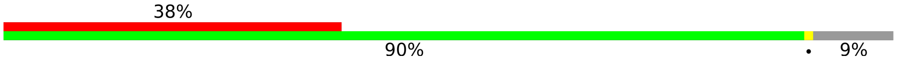
Chain O:

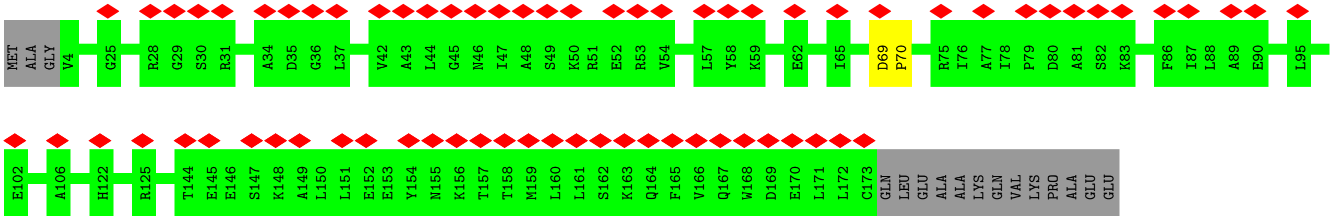




- Molecule 7: Dynactin subunit 3

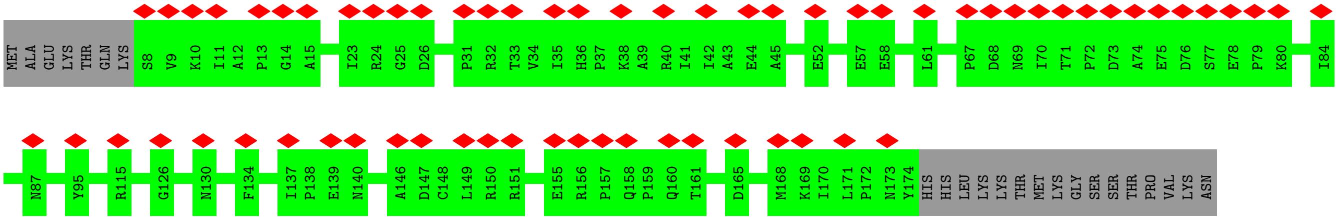
Chain o:





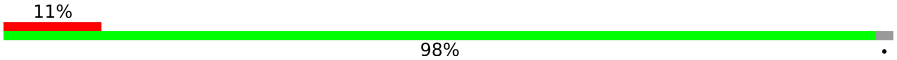
- Molecule 8: Dynactin 6

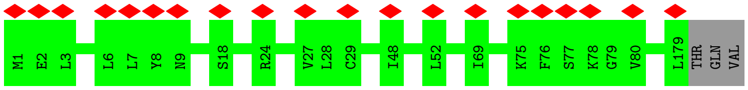
Chain U:



- Molecule 9: Dynactin subunit 5

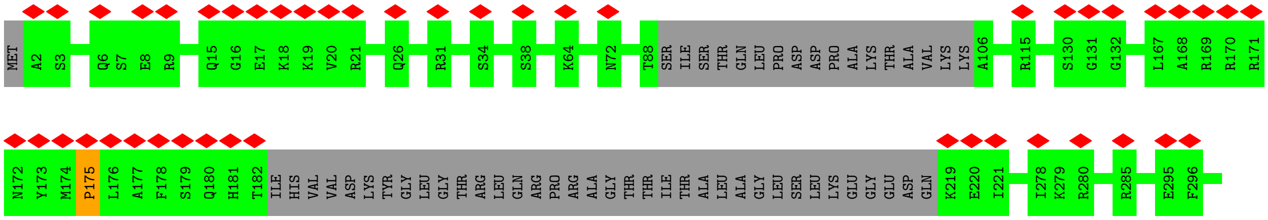
Chain V:

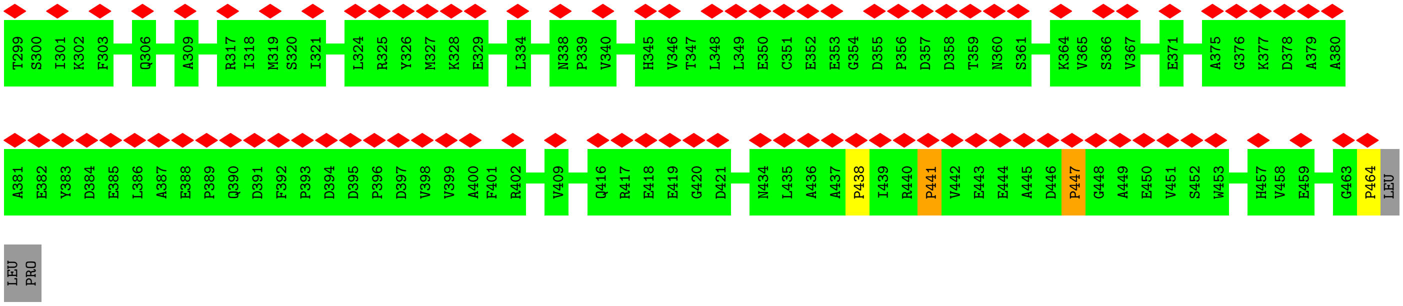




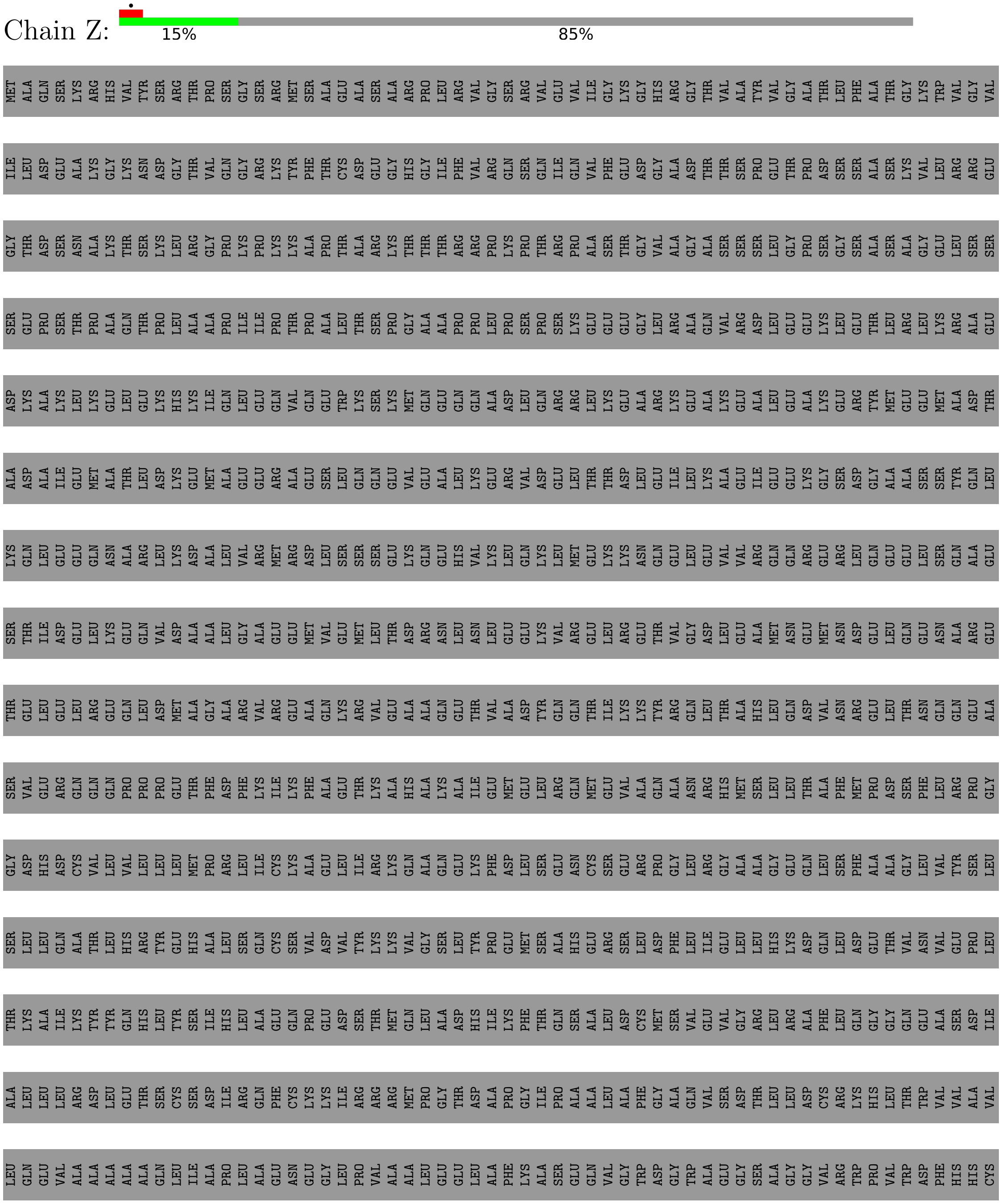
- Molecule 10: Dynactin subunit 4

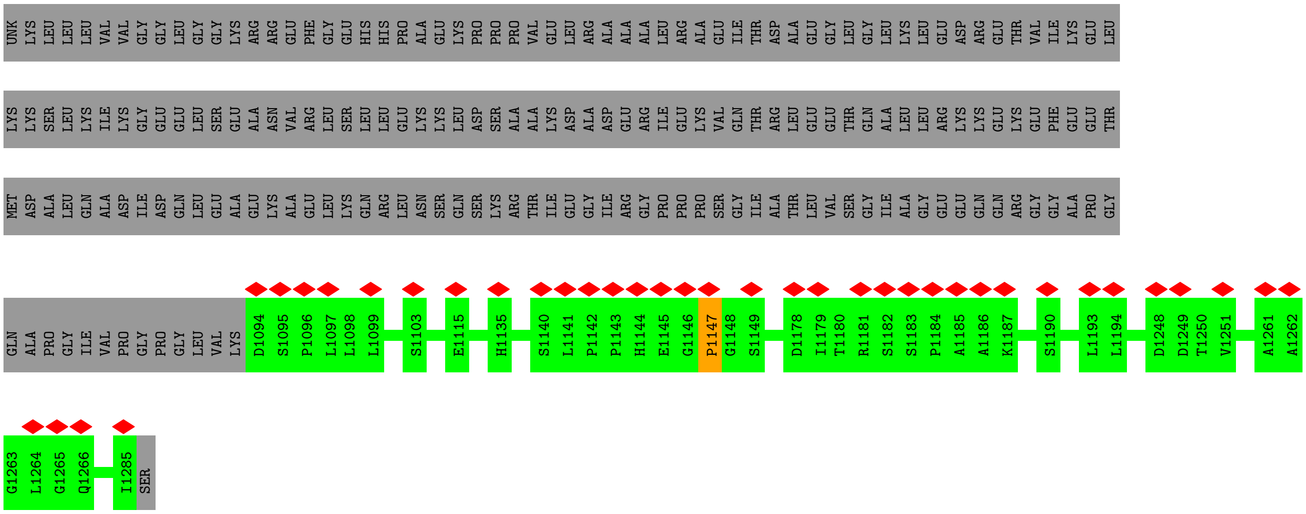
Chain Y:



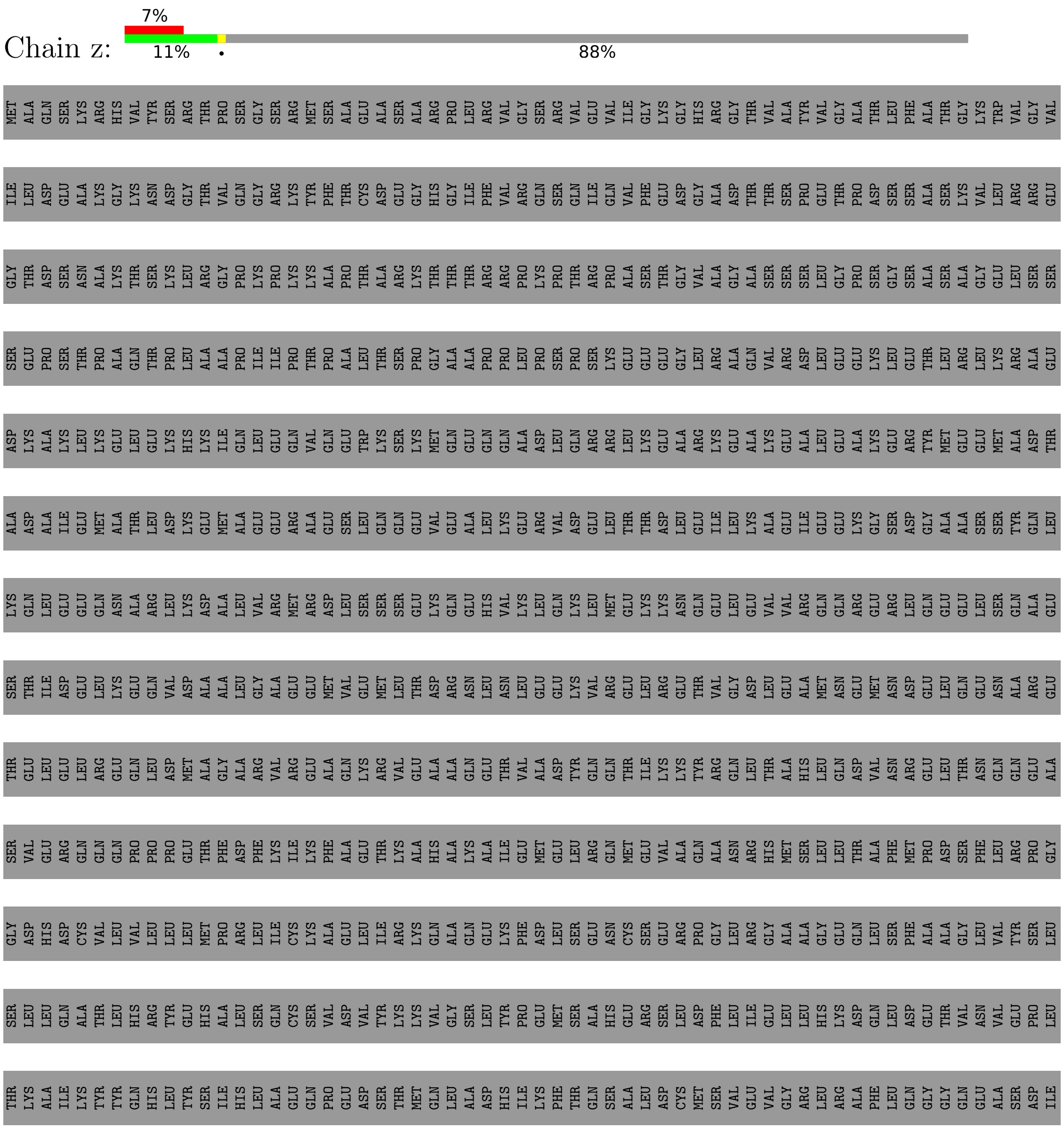


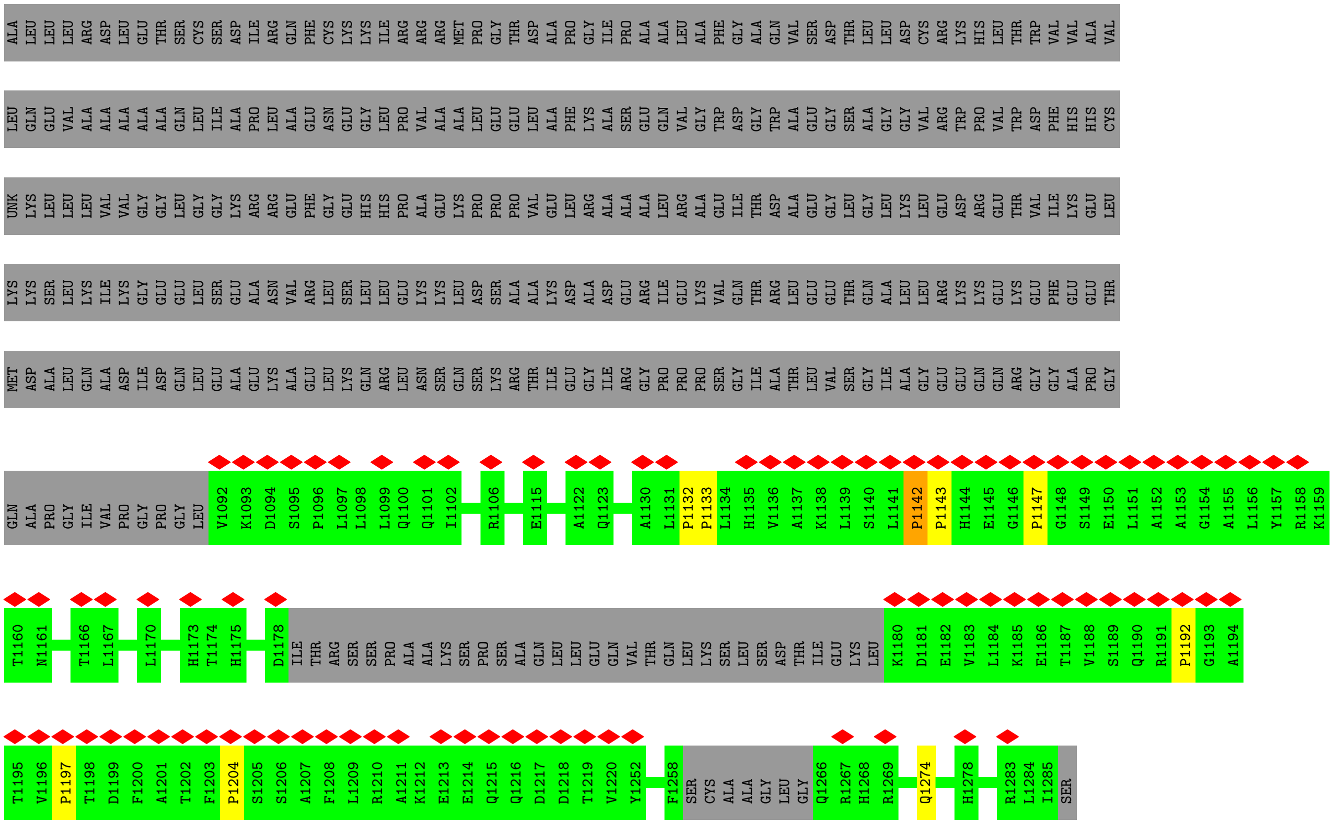
- Molecule 11: Dynactin subunit 1





- Molecule 11: Dynactin subunit 1




ALA LEU LEU LEU ARG ASP LEU GLU THR SER CYS SER ASP ILE ARG GLN PHE CYS LYS LYS ILE ARG ARG ARG MET PRO GLY THR ASP ALA PRO GLY ILE PRO ALA ALA LEU ALA PHE GLY ALA GLN VAL SER ASP THR LEU LEU ASP CYS ARG LYS HIS LEU THR TRP VAL VAL ALA VAL
LEU GLN GLU VAL ALA ALA ALA ALA ALA GLN LEU ILE ALA PRO LEU ALA GLU ASN GLU GLY LEU PRO VAL ALA ALA LEU GLU GLU LEU ALA PHE LYS ALA SER GLU GLN VAL GLY TRP ASP GLY TRP ALA GLU GLY SER ALA GLY GLY VAL ARG TRP PRO VAL TRP ASP PHE HIS HIS CYS
UNK LYS LEU LEU LEU VAL VAL GLY GLY LEU GLY GLY LYS ARG ARG GLU PHE GLY GLU HIS HIS PRO ALA GLU LYS PRO PRO PRO VAL GLU LEU ARG ALA ALA ALA LEU ARG ALA GLU ILE THR ASP ALA GLU GLY LEU GLY LEU LYS LEU GLU ASP ARG GLU THR VAL ILE LYS GLU LEU
LYS LYS SER LEU LYS ILE LYS GLY GLU GLU LEU SER GLU ALA ASN VAL ARG LEU SER LEU LEU GLU LYS LYS LEU ASP SER ALA ALA LYS ASP ALA ASP GLU ARG ILE GLU LYS VAL GLN THR ARG LEU GLU GLU THR GLN ALA LEU LEU ARG LYS LYS GLU LYS GLU PHE GLU GLU THR
MET ASP ALA LEU GLN ALA ASP ILE ASP GLN LEU GLU ALA GLU LYS ALA GLU LEU LYS GLN ARG LEU ASN SER GLN SER LYS ARG THR ILE GLU GLY ILE ARG GLY PRO PRO PRO SER GLY ILE ALA THR LEU VAL SER GLY ILE ALA GLY GLU GLU GLN GLN ARG GLY GLY ALA PRO GLY
GLN ALA PRO GLY ILE VAL PRO GLY PRO GLY LEU V1092 K1093 D1094 S1095 P1096 L1097 L1098 L1099 Q1100 Q1101 I1102 R1106 E1115 A1122 Q1123 A1130 L1131 P1132 P1133 L1134 H1135 V1136 A1137 K1138 L1139 S1140 L1141 P1142 P1143 H1144 E1145 G1146 P1147 G1148 S1149 E1150 L1151 A1152 A1153 G1154 A1155 L1156 Y1157 R1158 K1159
T1160 N1161 T1166 L1167 L1170 H1173 T1174 H1175 D1178 ILE THR ARG SER SER PRO ALA ALA LYS SER PRO SER ALA GLN LEU LEU GLU GLN VAL THR GLN LEU LYS SER LEU SER ASP THR ILE GLU LYS LEU K1180 D1181 E1182 V1183 L1184 K1185 E1186 T1187 V1188 S1189 Q1190 R1191 P1192 G1193 A1194
T1195 V1196 P1197 T1198 D1199 F1200 A1201 T1202 F1203 P1204 S1205 S1206 A1207 F1208 L1209 R1210 A1211 K1212 E1213 E1214 Q1215 Q1216 D1217 D1218 T1219 V1220 Y1252 F1258 SER CYS ALA ALA GLY LEU GLY Q1266 R1267 H1268 R1269 Q1274 H1278 R1283 L1284 I1285 SER

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	336972	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.184	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.053	Depositor
Map size (Å)	578.88, 578.88, 578.88	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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, ZN, 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	0.67	0/3013	0.77	0/4070
1	B	0.67	0/3025	0.79	0/4085
1	C	0.67	0/3068	0.78	0/4144
1	D	0.66	0/3025	0.78	0/4085
1	E	0.67	0/3025	0.78	0/4085
1	F	0.68	0/3025	0.78	0/4085
1	G	0.67	0/3025	0.77	0/4085
1	I	0.67	0/3010	0.75	0/4066
2	H	0.68	0/2948	0.73	0/3991
3	J	0.68	0/2994	0.75	0/4066
4	K	0.68	0/2316	0.75	0/3135
5	L	0.69	0/2156	0.76	0/2906
6	M	0.77	0/2259	0.81	1/3090 (0.0%)
6	N	0.79	0/1783	0.82	0/2451
6	m	0.73	0/2287	0.77	0/3119
6	n	0.74	0/2375	0.80	2/3246 (0.1%)
7	O	0.77	0/1194	0.81	2/1631 (0.1%)
7	o	0.79	0/1093	0.81	1/1498 (0.1%)
8	U	0.71	0/1241	0.79	0/1691
9	V	0.71	0/1286	0.78	0/1757
10	Y	0.71	0/3020	0.81	5/4119 (0.1%)
11	Z	0.70	0/1467	0.77	1/1992 (0.1%)
11	z	0.80	0/955	0.95	8/1302 (0.6%)
All	All	0.70	0/53590	0.78	20/72699 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(^{o})**	**Ideal(^{o})**
11	z	1133	PRO	N-CA-CB	6.13	110.65	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Z	1147	PRO	N-CA-CB	6.06	110.58	103.30
11	z	1197	PRO	N-CA-CB	6.01	110.51	103.30
11	z	1132	PRO	N-CA-CB	6.00	110.50	103.30
11	z	1147	PRO	N-CA-CB	5.85	110.32	103.30
11	z	1143	PRO	N-CA-CB	5.82	110.29	103.30
6	n	204	PRO	N-CA-CB	5.77	110.22	103.30
7	O	70	PRO	N-CA-CB	5.76	110.21	103.30
11	z	1192	PRO	N-CA-CB	5.71	110.15	103.30
10	Y	447	PRO	N-CA-CB	5.70	110.14	103.30
10	Y	438	PRO	N-CA-CB	5.65	110.08	103.30
10	Y	441	PRO	N-CA-CB	5.65	110.08	103.30
10	Y	464	PRO	N-CA-CB	5.62	110.04	103.30
11	z	1204	PRO	N-CA-CB	5.60	110.02	103.30
7	O	24	PRO	N-CA-CB	5.47	109.87	103.30
6	M	217	PRO	N-CA-CB	5.46	109.85	103.30
7	o	70	PRO	N-CA-CB	5.41	109.79	103.30
11	z	1142	PRO	N-CA-CB	5.33	109.69	103.30
10	Y	175	PRO	N-CA-CB	5.29	109.65	103.30
6	n	203	PRO	N-CA-CB	5.21	109.56	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	368/376 (98%)	353 (96%)	15 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	C	373/376 (99%)	364 (98%)	9 (2%)	0	100	100
1	D	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	E	368/376 (98%)	358 (97%)	10 (3%)	0	100	100
1	F	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
1	G	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
1	I	368/376 (98%)	347 (94%)	21 (6%)	0	100	100
2	H	368/375 (98%)	352 (96%)	16 (4%)	0	100	100
3	J	377/417 (90%)	347 (92%)	30 (8%)	0	100	100
4	K	276/286 (96%)	259 (94%)	17 (6%)	0	100	100
5	L	267/272 (98%)	258 (97%)	9 (3%)	0	100	100
6	M	330/405 (82%)	299 (91%)	29 (9%)	2 (1%)	25	62
6	N	270/405 (67%)	258 (96%)	10 (4%)	2 (1%)	22	60
6	m	319/405 (79%)	301 (94%)	18 (6%)	0	100	100
6	n	335/405 (83%)	305 (91%)	28 (8%)	2 (1%)	25	62
7	O	177/186 (95%)	159 (90%)	15 (8%)	3 (2%)	9	43
7	o	168/186 (90%)	154 (92%)	13 (8%)	1 (1%)	25	62
8	U	165/190 (87%)	141 (86%)	24 (14%)	0	100	100
9	V	177/182 (97%)	161 (91%)	16 (9%)	0	100	100
10	Y	404/467 (86%)	355 (88%)	46 (11%)	3 (1%)	22	60
11	Z	190/1286 (15%)	176 (93%)	13 (7%)	1 (0%)	29	66
11	z	147/1286 (11%)	139 (95%)	7 (5%)	1 (1%)	22	60
All	All	6919/9761 (71%)	6504 (94%)	400 (6%)	15 (0%)	50	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	217	PRO
7	O	24	PRO
10	Y	175	PRO
10	Y	441	PRO
6	n	204	PRO
11	z	1142	PRO
6	n	299	LYS

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Mol	Chain	Res	Type
6	N	158	LYS
6	N	163	ASP
7	O	61	ILE
7	O	69	ASP
7	o	69	ASP
10	Y	447	PRO
6	M	166	ILE
11	Z	1147	PRO

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	315/324 (97%)	315 (100%)	0	100	100
1	B	318/324 (98%)	317 (100%)	1 (0%)	92	96
1	C	323/324 (100%)	323 (100%)	0	100	100
1	D	318/324 (98%)	318 (100%)	0	100	100
1	E	318/324 (98%)	318 (100%)	0	100	100
1	F	318/324 (98%)	318 (100%)	0	100	100
1	G	318/324 (98%)	318 (100%)	0	100	100
1	I	314/324 (97%)	314 (100%)	0	100	100
2	H	313/318 (98%)	312 (100%)	1 (0%)	92	96
3	J	323/363 (89%)	323 (100%)	0	100	100
4	K	247/254 (97%)	247 (100%)	0	100	100
5	L	238/241 (99%)	237 (100%)	1 (0%)	91	95
6	M	164/346 (47%)	164 (100%)	0	100	100
6	N	112/346 (32%)	112 (100%)	0	100	100
6	m	197/346 (57%)	197 (100%)	0	100	100
6	n	192/346 (56%)	192 (100%)	0	100	100
7	O	87/160 (54%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	o	67/160 (42%)	67 (100%)	0	100	100
8	U	129/163 (79%)	129 (100%)	0	100	100
9	V	121/163 (74%)	121 (100%)	0	100	100
10	Y	274/416 (66%)	274 (100%)	0	100	100
11	Z	154/1074 (14%)	154 (100%)	0	100	100
11	z	53/1074 (5%)	52 (98%)	1 (2%)	57	76
All	All	5213/8362 (62%)	5209 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	72	ARG
2	H	257	CYS
5	L	84	GLU
11	z	1274	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
12	ADP	C	800	-	24,29,29	0.66	0	29,45,45	0.72	1 (3%)
12	ADP	G	800	-	24,29,29	0.64	0	29,45,45	0.69	1 (3%)
12	ADP	J	800	-	24,29,29	0.67	0	29,45,45	0.77	1 (3%)
12	ADP	I	800	-	24,29,29	0.65	0	29,45,45	0.71	1 (3%)
12	ADP	F	800	-	24,29,29	0.64	0	29,45,45	0.70	1 (3%)
12	ADP	A	800	-	24,29,29	0.65	0	29,45,45	0.70	1 (3%)
13	ATP	H	401	-	26,33,33	0.66	0	31,52,52	0.79	1 (3%)
12	ADP	B	800	-	24,29,29	0.66	0	29,45,45	0.71	1 (3%)
12	ADP	E	800	-	24,29,29	0.65	0	29,45,45	0.72	1 (3%)
12	ADP	D	800	-	24,29,29	0.65	0	29,45,45	0.71	1 (3%)

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
12	ADP	C	800	-	-	4/12/32/32	0/3/3/3
12	ADP	G	800	-	-	4/12/32/32	0/3/3/3
12	ADP	J	800	-	-	4/12/32/32	0/3/3/3
12	ADP	I	800	-	-	4/12/32/32	0/3/3/3
12	ADP	F	800	-	-	3/12/32/32	0/3/3/3
12	ADP	A	800	-	-	5/12/32/32	0/3/3/3
13	ATP	H	401	-	-	6/18/38/38	0/3/3/3
12	ADP	B	800	-	-	3/12/32/32	0/3/3/3
12	ADP	E	800	-	-	4/12/32/32	0/3/3/3
12	ADP	D	800	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H	401	ATP	C5-C6-N6	2.26	123.79	120.35
12	A	800	ADP	C5-C6-N6	2.25	123.77	120.35
12	I	800	ADP	C5-C6-N6	2.25	123.77	120.35
12	D	800	ADP	C5-C6-N6	2.24	123.75	120.35
12	F	800	ADP	C5-C6-N6	2.20	123.70	120.35
12	E	800	ADP	C5-C6-N6	2.18	123.66	120.35
12	G	800	ADP	C5-C6-N6	2.17	123.65	120.35
12	B	800	ADP	C5-C6-N6	2.17	123.65	120.35
12	C	800	ADP	C5-C6-N6	2.15	123.62	120.35
12	J	800	ADP	C5-C6-N6	2.14	123.61	120.35

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	800	ADP	PA-O3A-PB-O3B
12	B	800	ADP	C5'-O5'-PA-O1A
12	C	800	ADP	C5'-O5'-PA-O1A
12	D	800	ADP	C5'-O5'-PA-O3A
12	D	800	ADP	C3'-C4'-C5'-O5'
12	E	800	ADP	C5'-O5'-PA-O3A
12	E	800	ADP	C3'-C4'-C5'-O5'
12	G	800	ADP	C5'-O5'-PA-O2A
12	G	800	ADP	C5'-O5'-PA-O3A
12	I	800	ADP	C5'-O5'-PA-O3A
13	H	401	ATP	PB-O3A-PA-O5'
13	H	401	ATP	C5'-O5'-PA-O1A
13	H	401	ATP	C5'-O5'-PA-O3A
12	F	800	ADP	C3'-C4'-C5'-O5'
12	G	800	ADP	C3'-C4'-C5'-O5'
12	C	800	ADP	C3'-C4'-C5'-O5'
12	A	800	ADP	C3'-C4'-C5'-O5'
12	B	800	ADP	C3'-C4'-C5'-O5'
12	D	800	ADP	O4'-C4'-C5'-O5'
12	I	800	ADP	C3'-C4'-C5'-O5'
12	E	800	ADP	O4'-C4'-C5'-O5'
12	F	800	ADP	O4'-C4'-C5'-O5'
12	G	800	ADP	O4'-C4'-C5'-O5'
12	C	800	ADP	O4'-C4'-C5'-O5'
12	A	800	ADP	O4'-C4'-C5'-O5'
12	B	800	ADP	O4'-C4'-C5'-O5'
12	J	800	ADP	PB-O3A-PA-O2A
13	H	401	ATP	PA-O3A-PB-O2B

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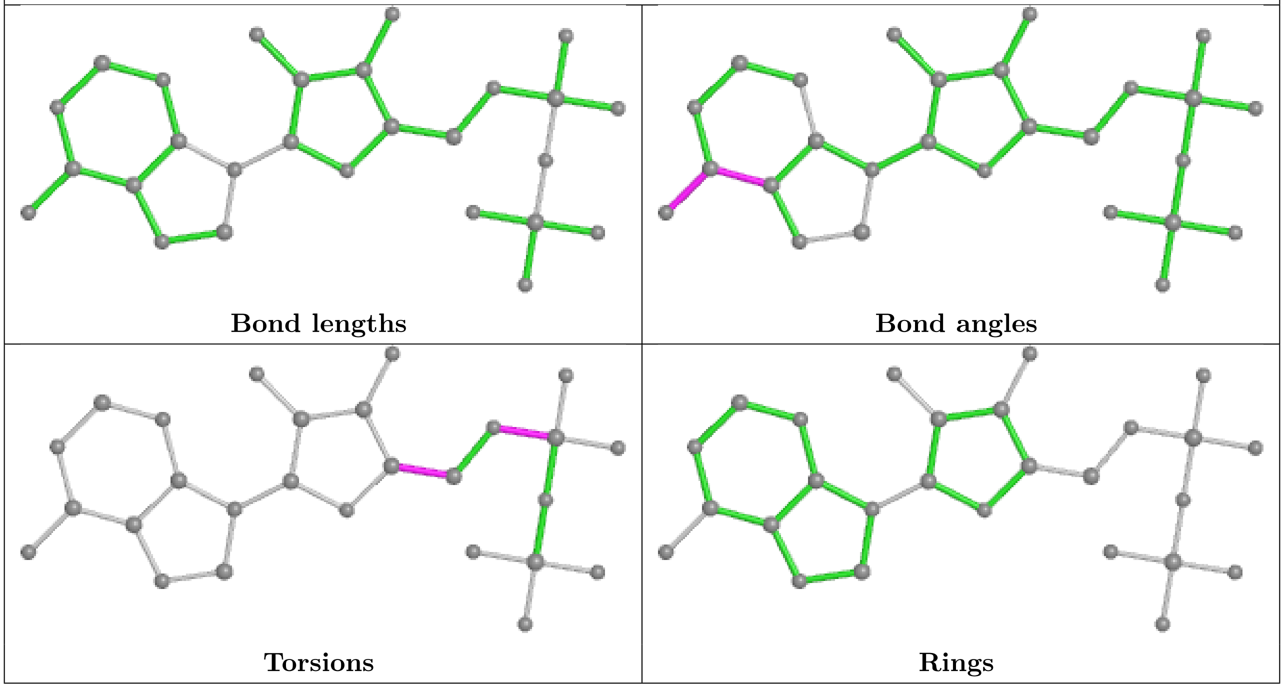
Mol	Chain	Res	Type	Atoms
12	A	800	ADP	C5'-O5'-PA-O2A
12	D	800	ADP	C5'-O5'-PA-O2A
12	E	800	ADP	C5'-O5'-PA-O2A
12	I	800	ADP	C5'-O5'-PA-O2A
12	I	800	ADP	O4'-C4'-C5'-O5'
13	H	401	ATP	PG-O3B-PB-O2B
12	A	800	ADP	C5'-O5'-PA-O3A
12	C	800	ADP	C5'-O5'-PA-O3A
12	F	800	ADP	C5'-O5'-PA-O3A
13	H	401	ATP	O4'-C4'-C5'-O5'
12	J	800	ADP	PB-O3A-PA-O1A
12	J	800	ADP	C5'-O5'-PA-O1A
12	J	800	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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 C 800



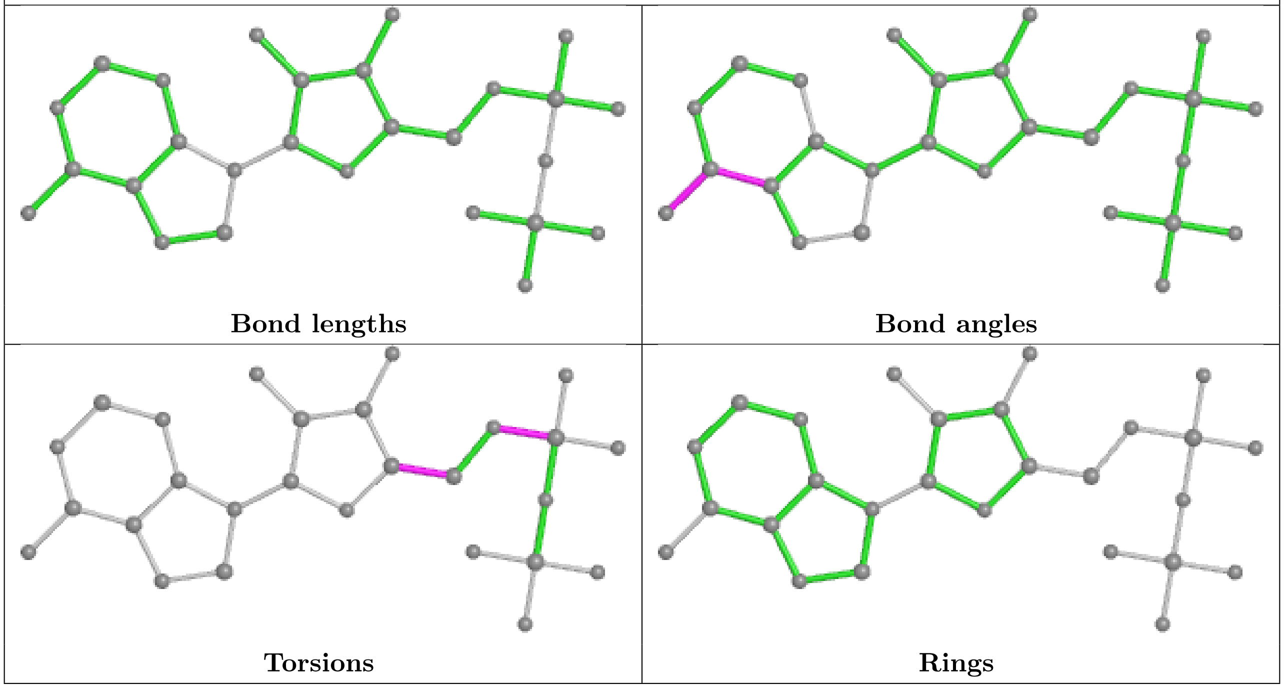
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP G 800



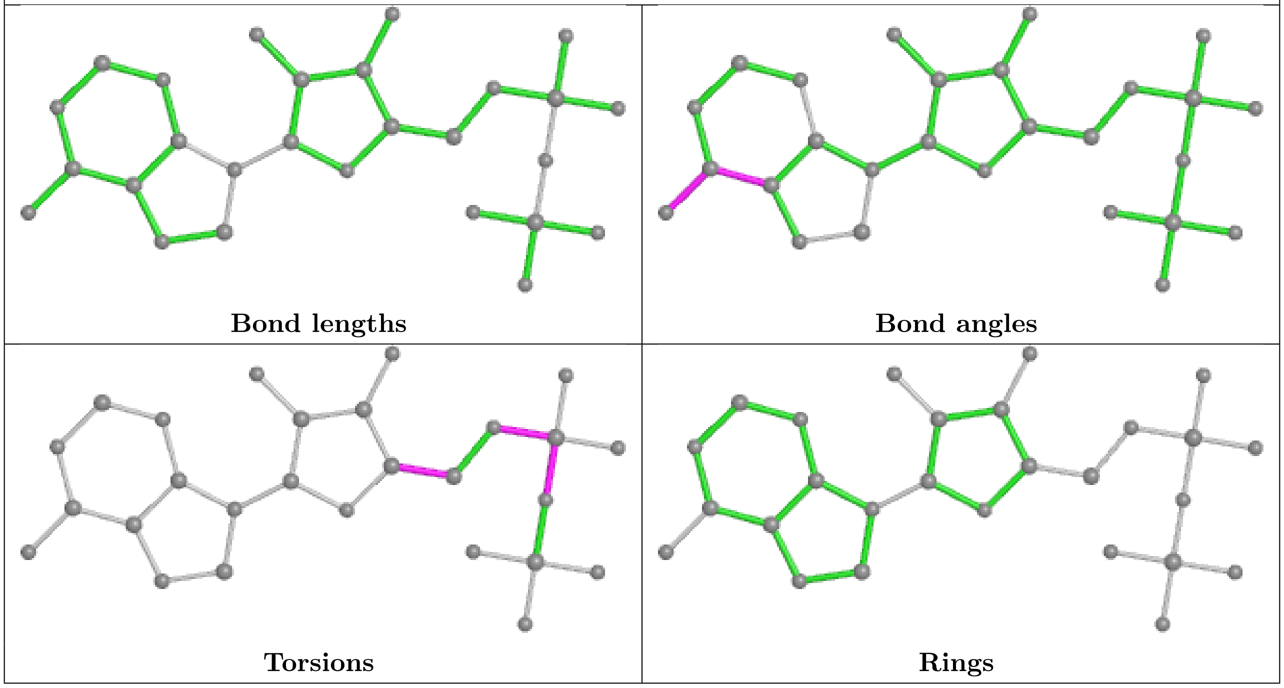
Bond lengths

Bond angles

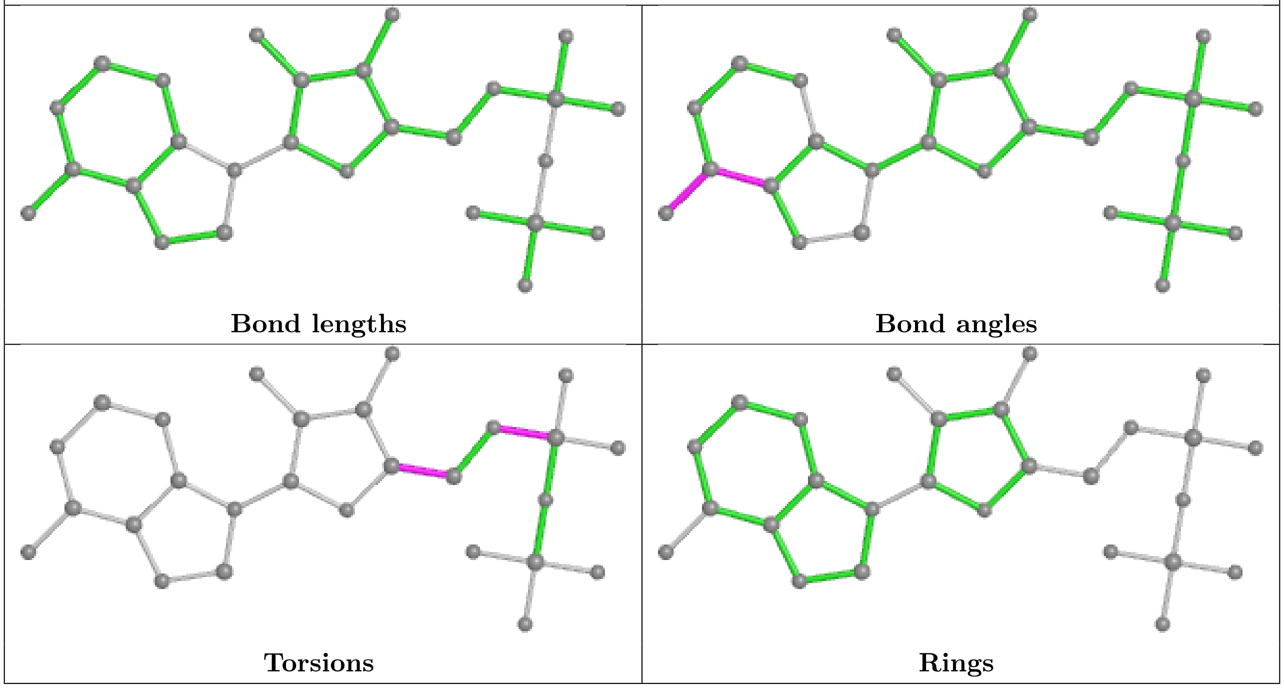
Torsions

Rings

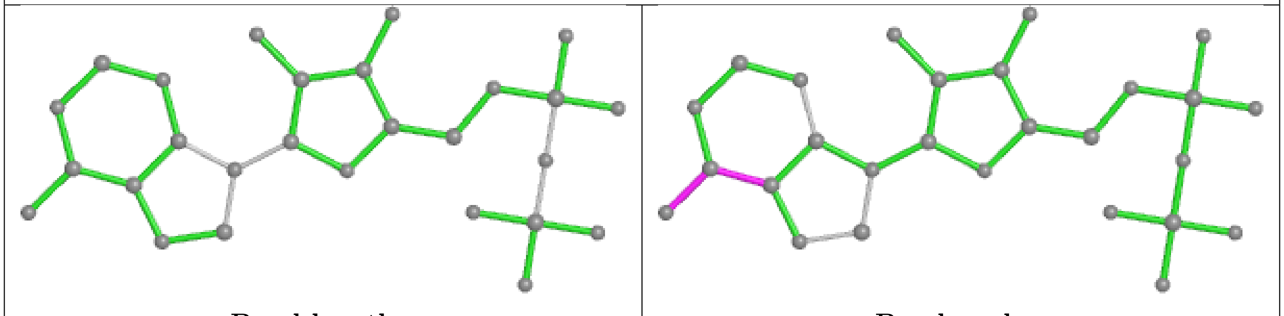
Ligand ADP J 800



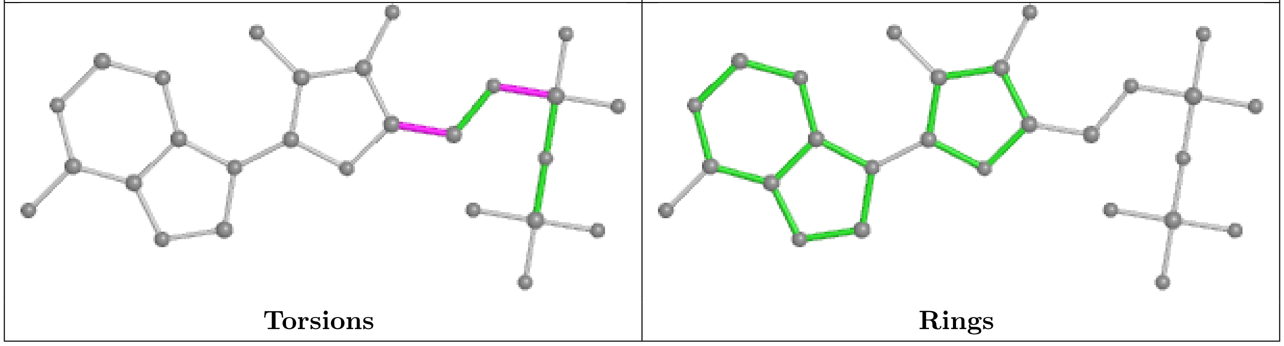
Ligand ADP I 800



Ligand ADP F 800

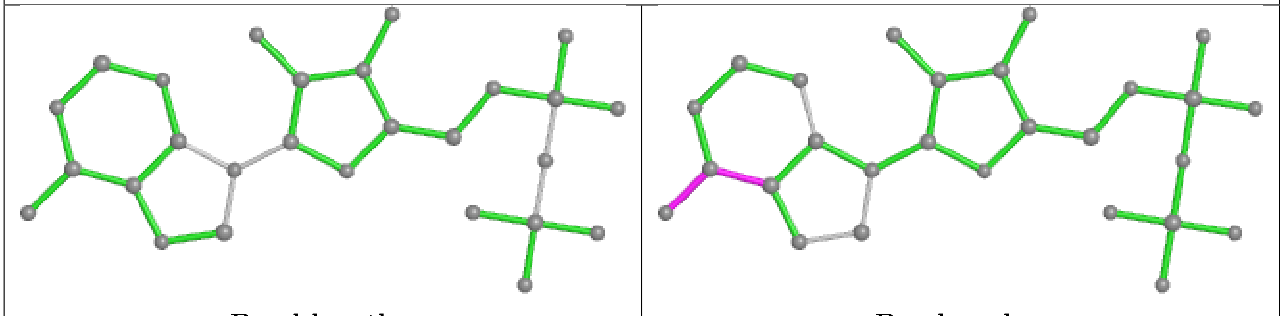


Bond lengths Bond angles

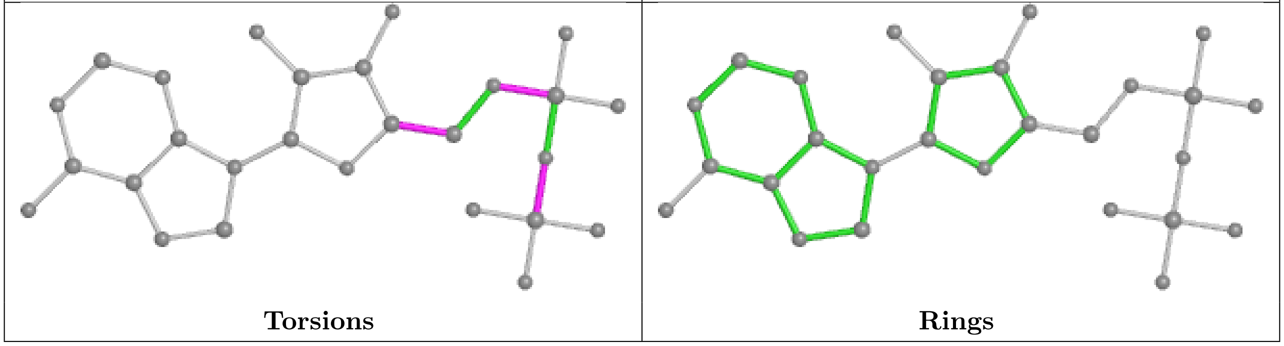


Torsions Rings

Ligand ADP A 800

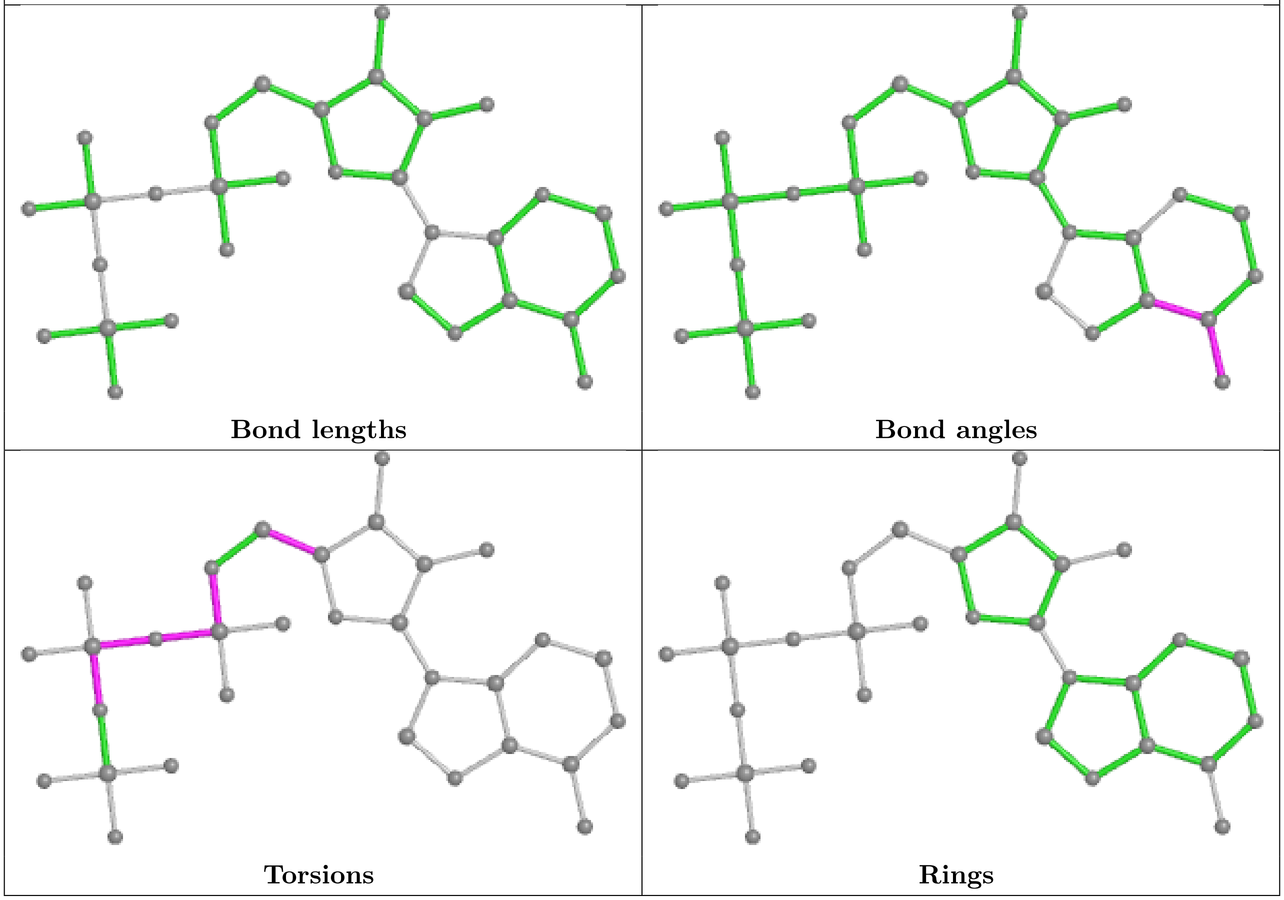


Bond lengths Bond angles

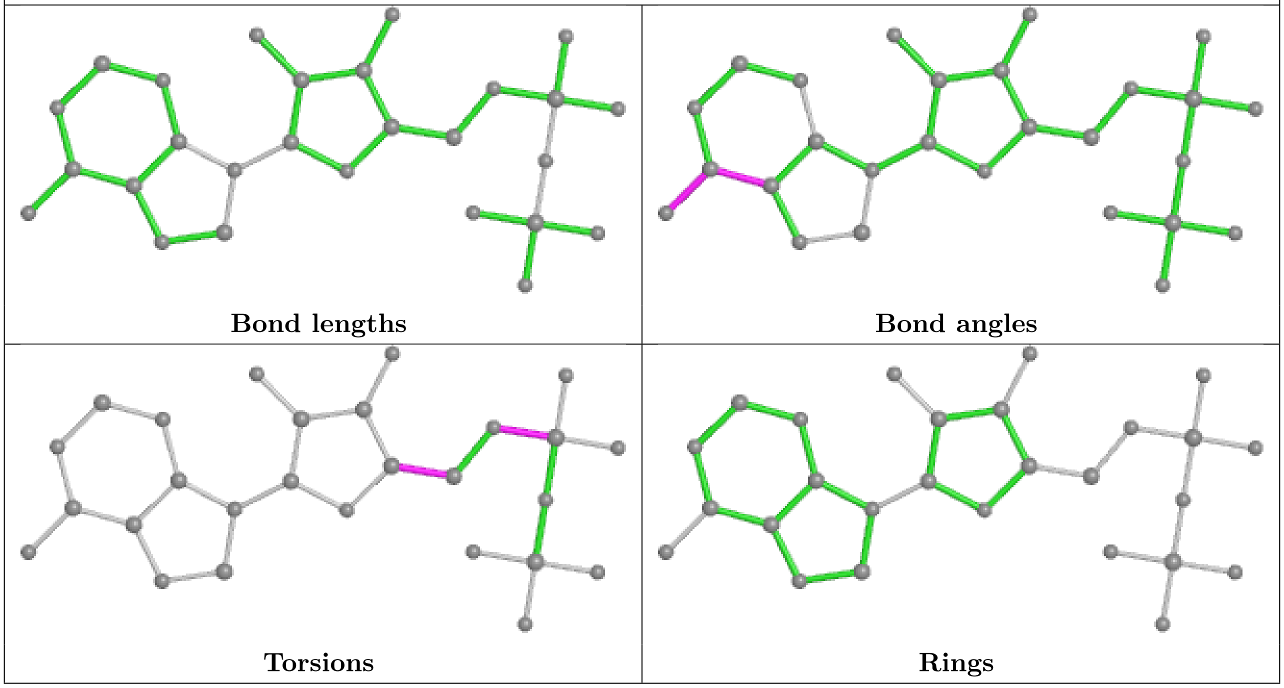


Torsions Rings

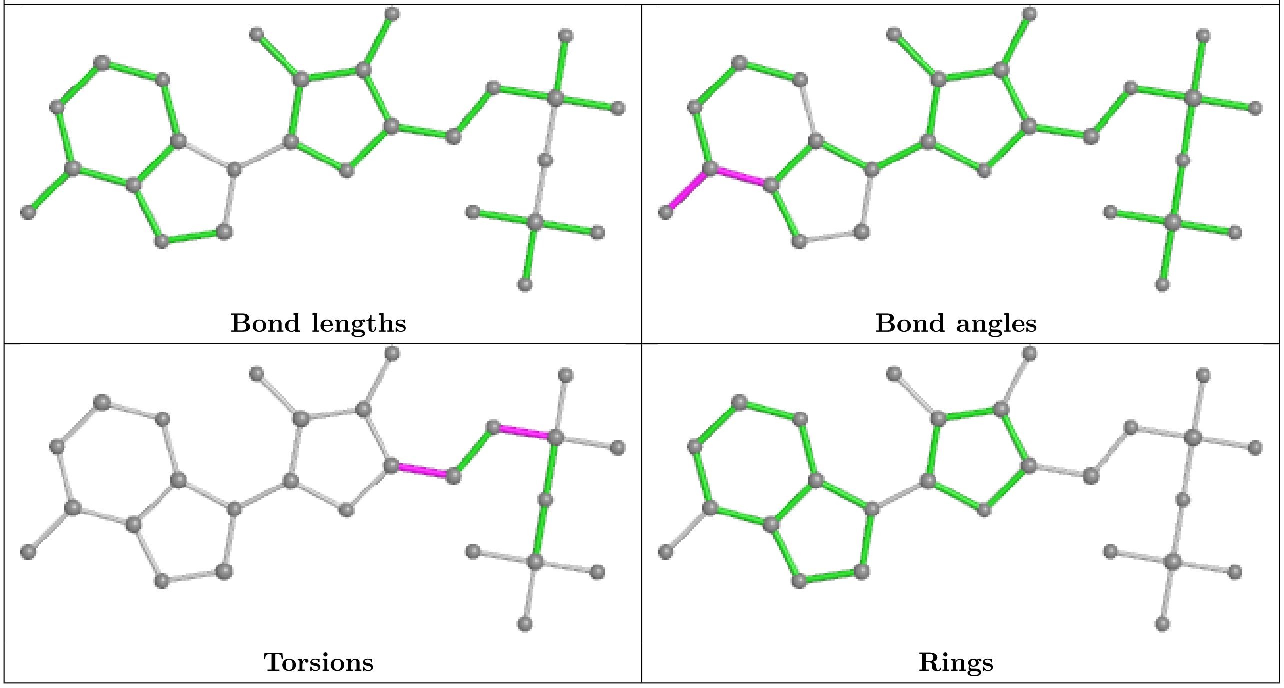
Ligand ATP H 401



Ligand ADP B 800



Ligand ADP E 800



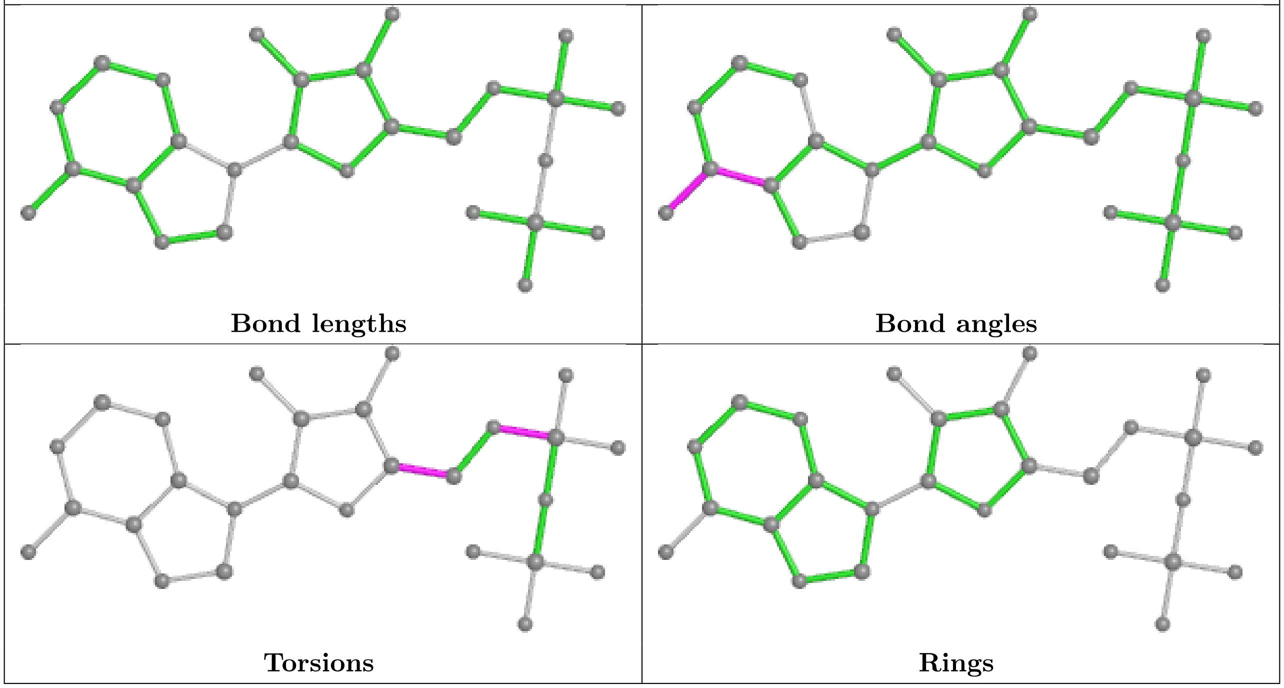
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 800



Bond lengths

Bond angles

Torsions

Rings

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
11	z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	1220:VAL	C	1252:TYR	N	34.09

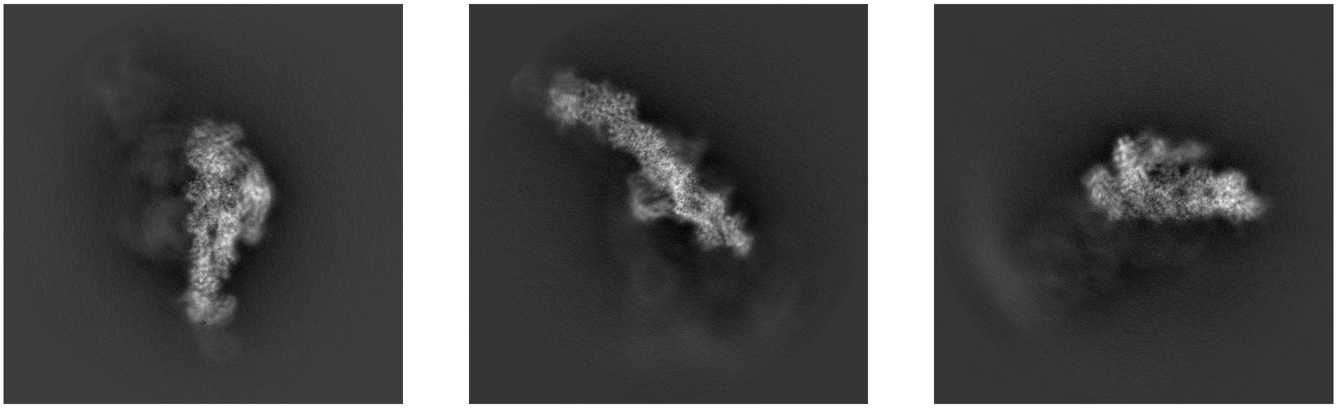
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11313. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

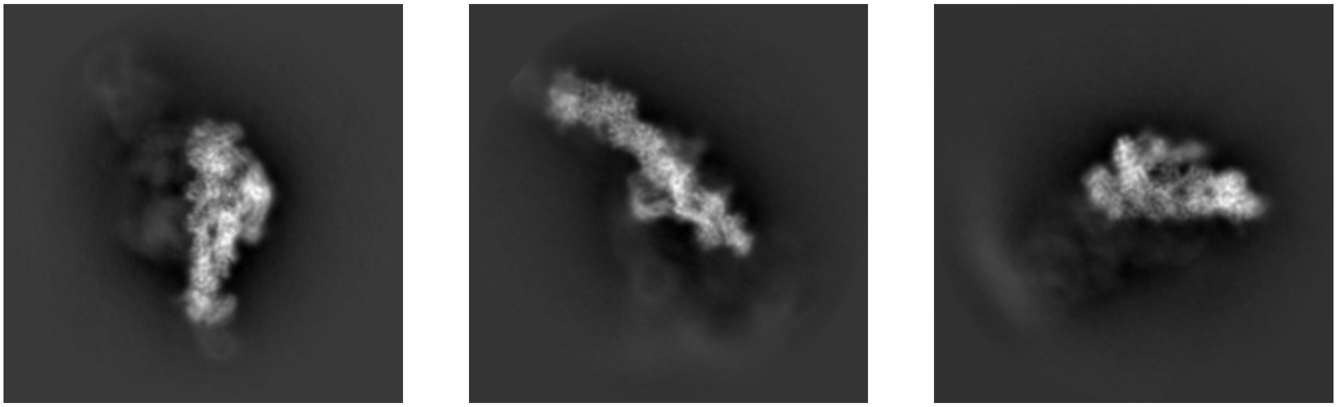
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

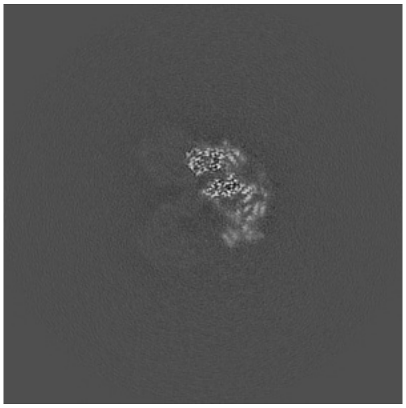


X Y Z

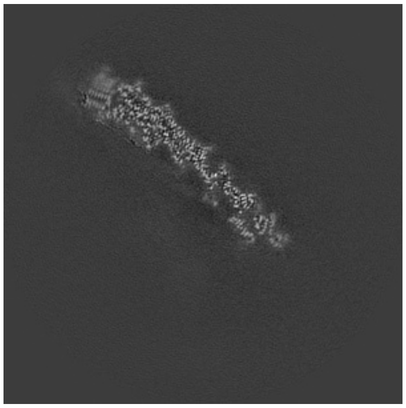
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

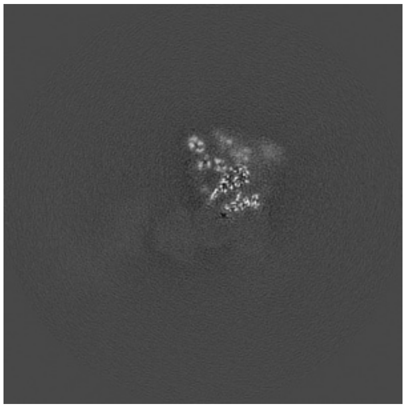
6.2.1 Primary map



X Index: 216

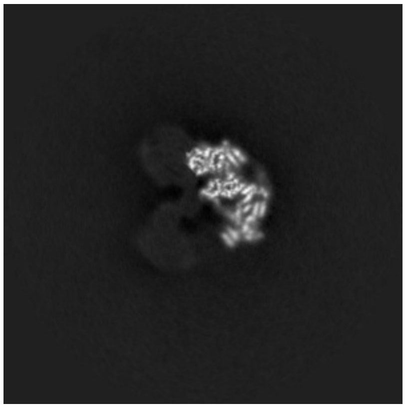


Y Index: 216

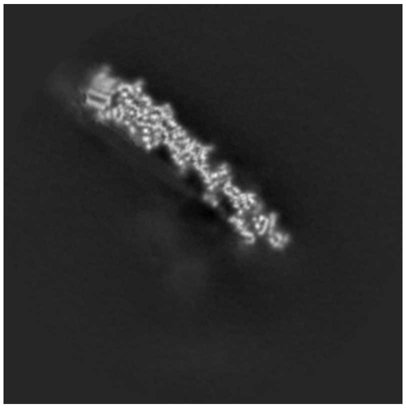


Z Index: 216

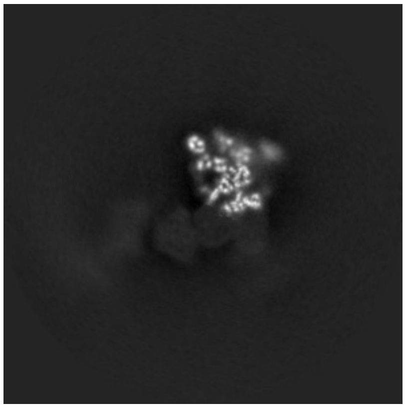
6.2.2 Raw map



X Index: 216



Y Index: 216

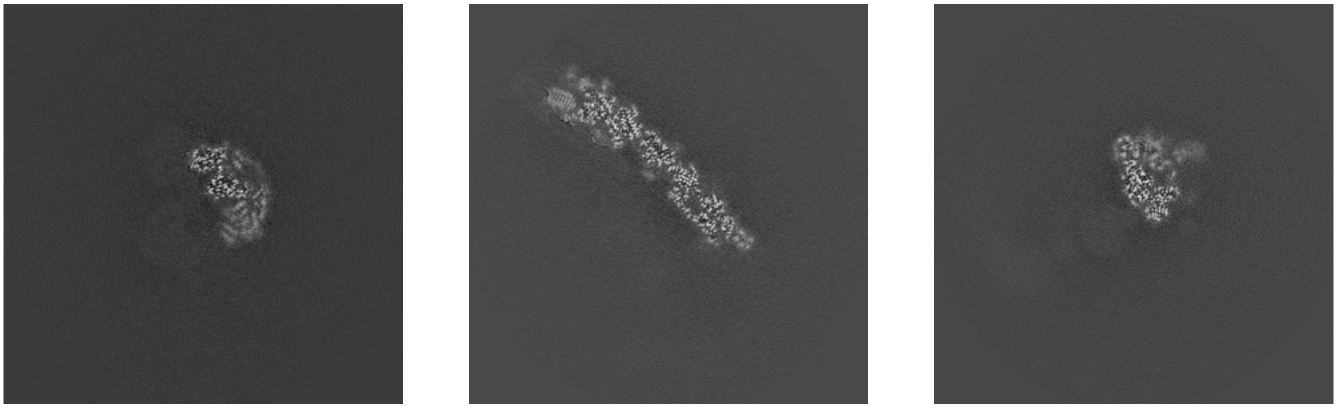


Z Index: 216

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

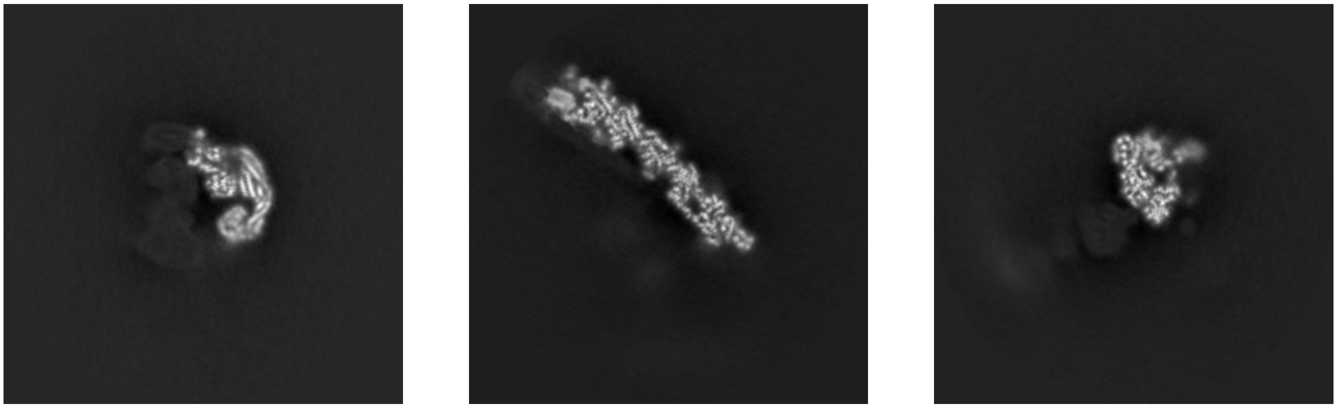
6.3 Largest variance slices ⓘ

6.3.1 Primary map



X Index: 212 Y Index: 220 Z Index: 228

6.3.2 Raw map



X Index: 205 Y Index: 220 Z Index: 229

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.053. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

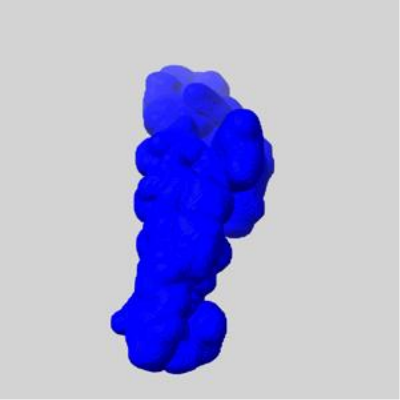
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

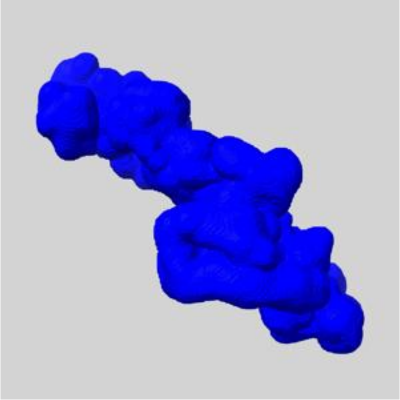
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

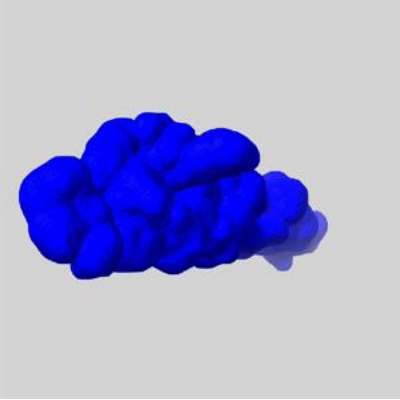
6.5.1 emd_11313_msk_1.map



X



Y

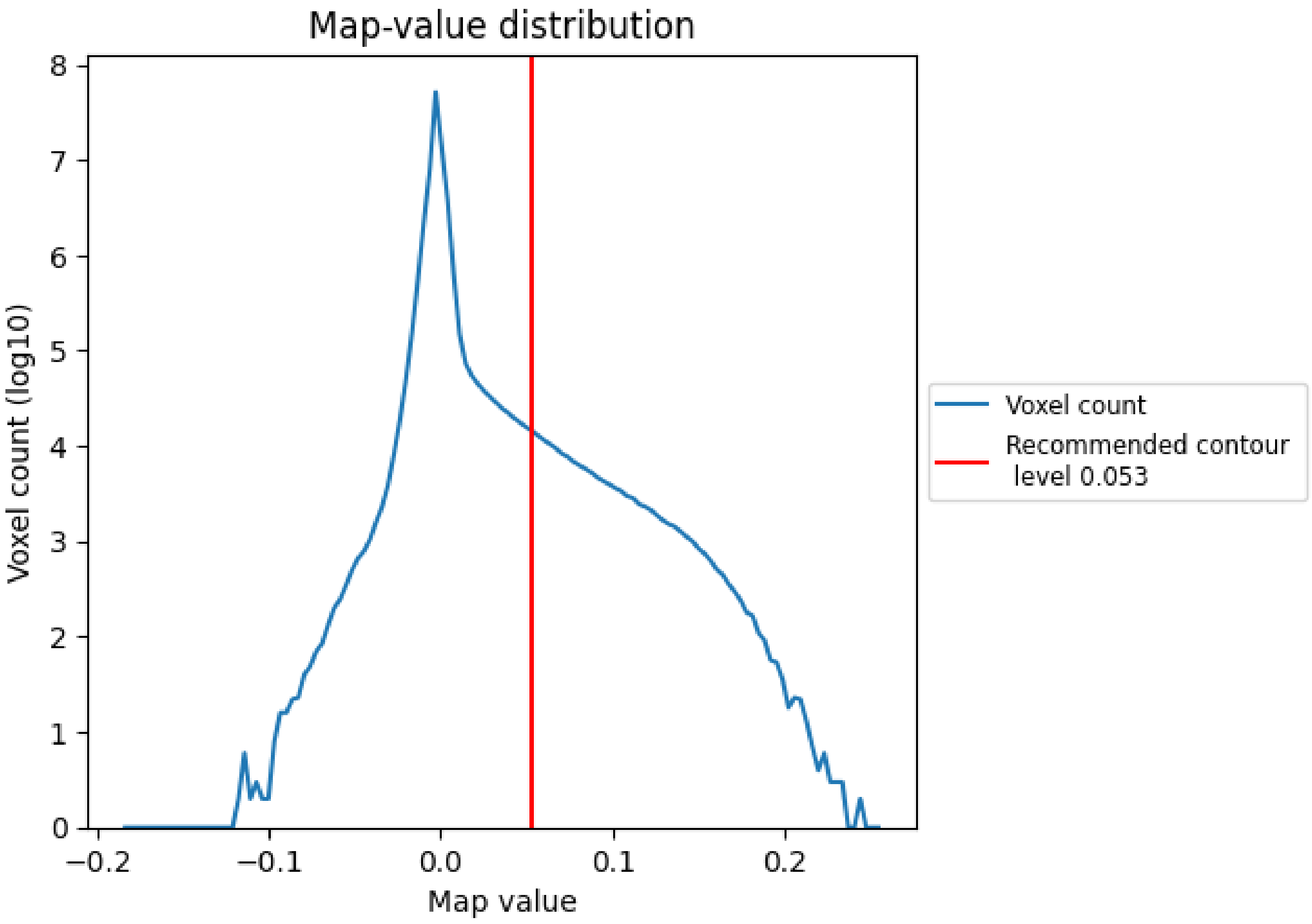


Z

7 Map analysis ⓘ

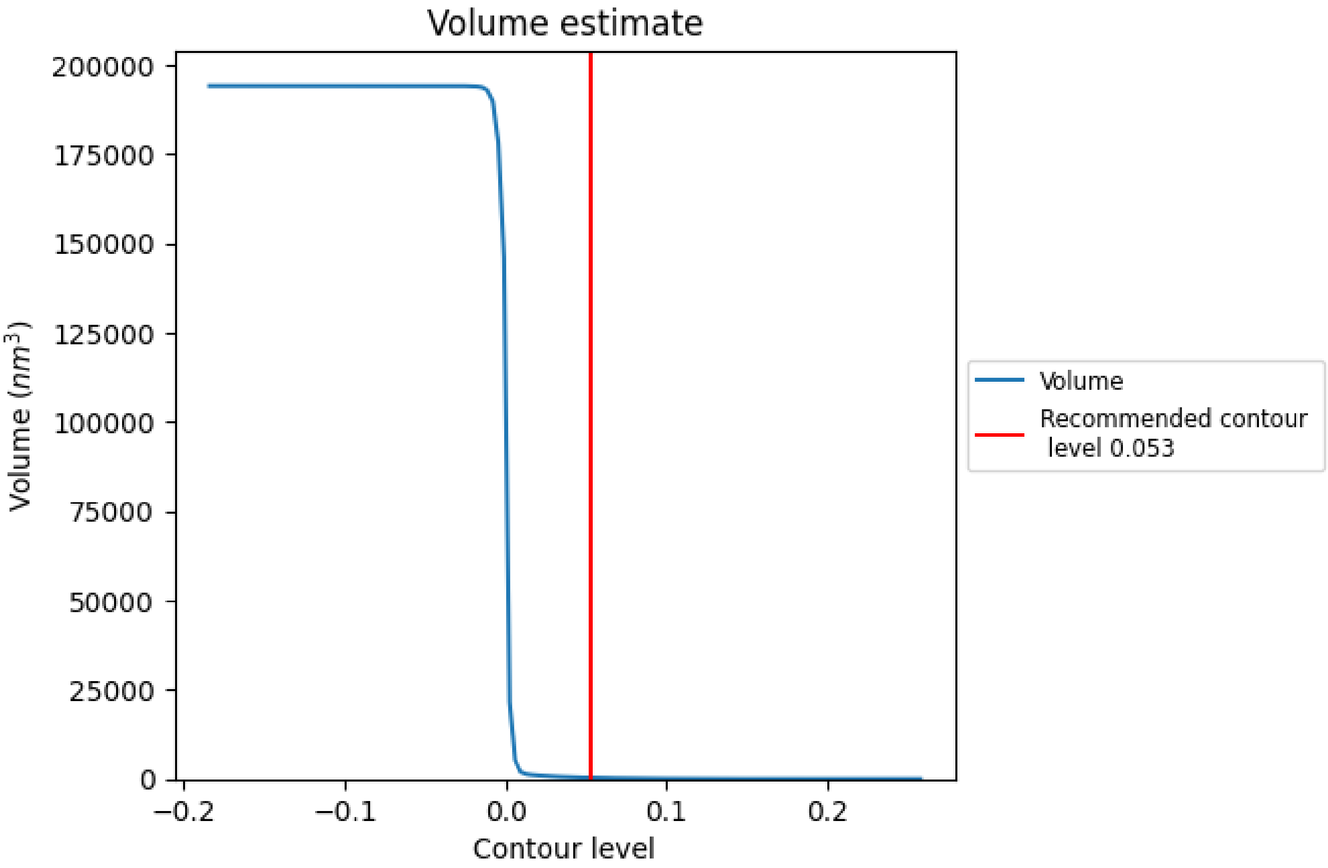
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

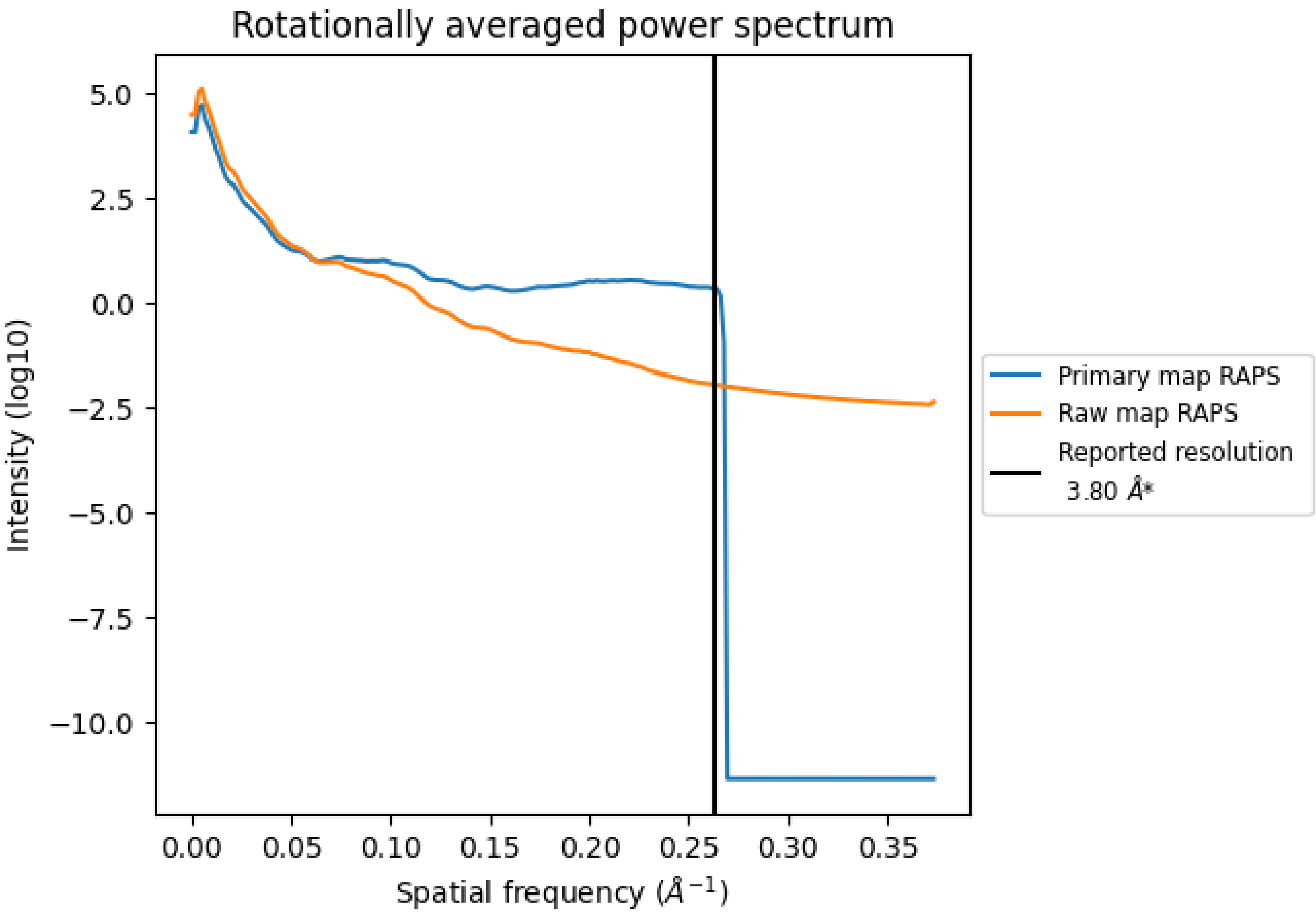
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 353 nm^3; this corresponds to an approximate mass of 318 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 ⓘ

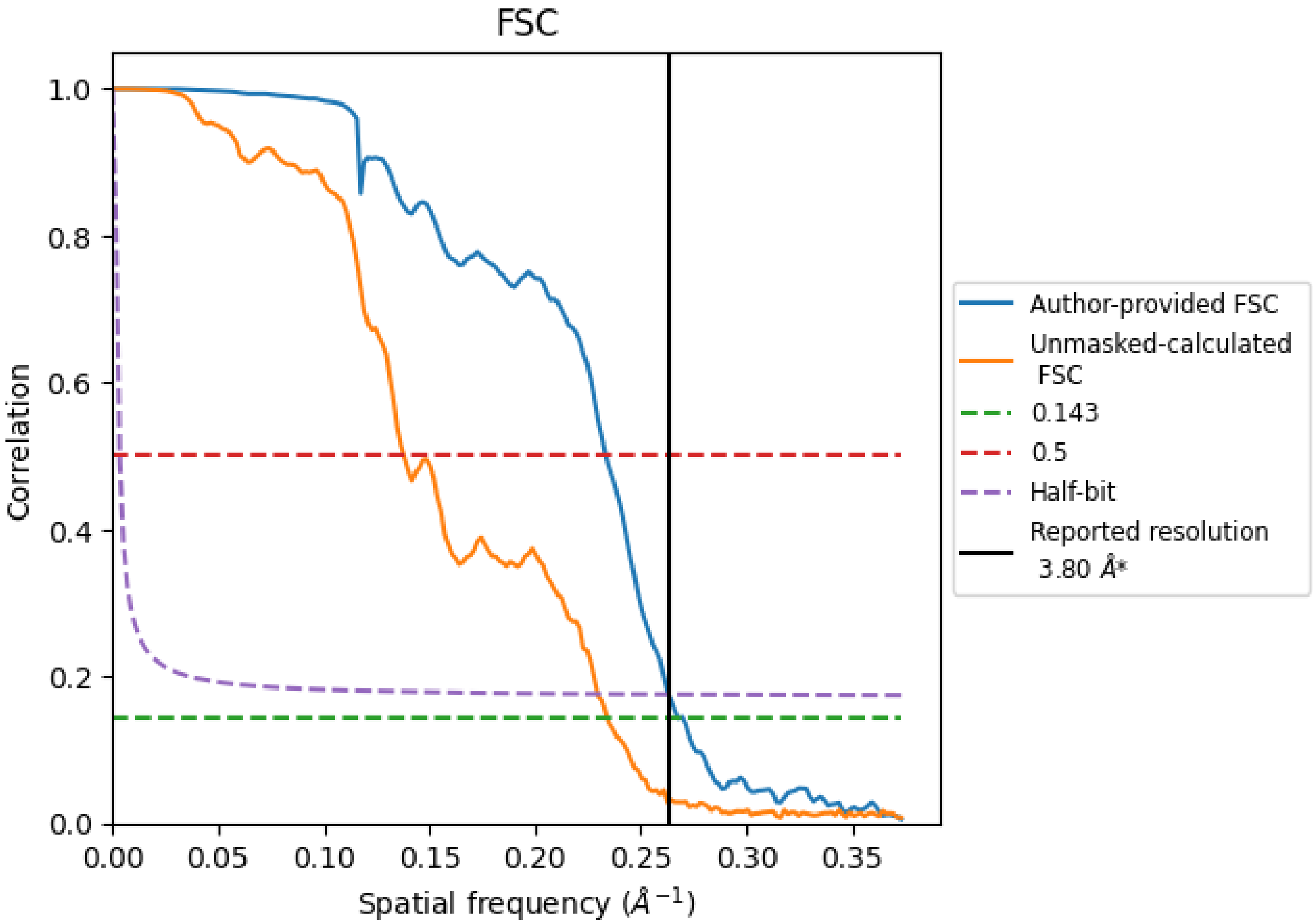


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates ⓘ

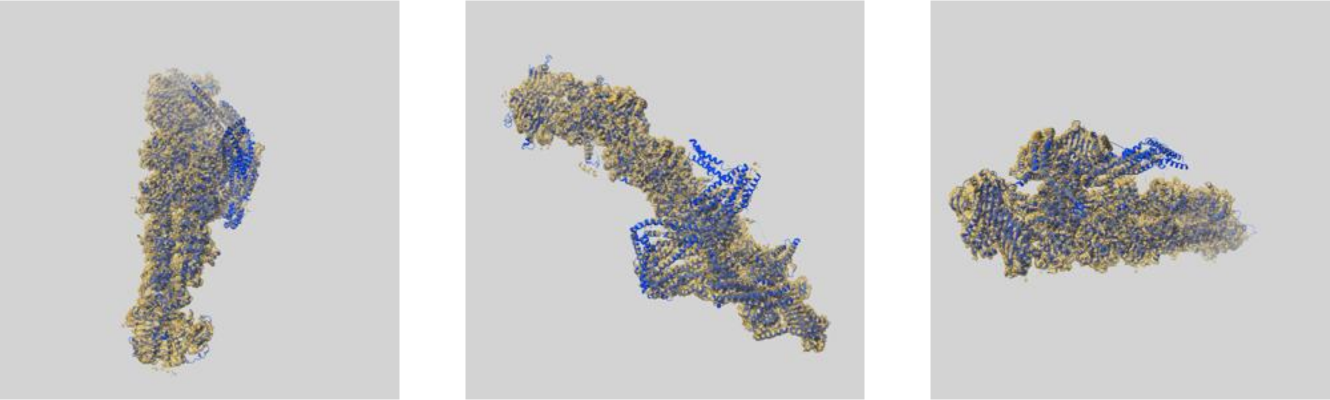
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.74	4.28	3.80
Unmasked-calculated*	4.27	7.25	4.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.8 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-11313 and PDB model 6ZNL. Per-residue inclusion information can be found in section 3 on page 8.

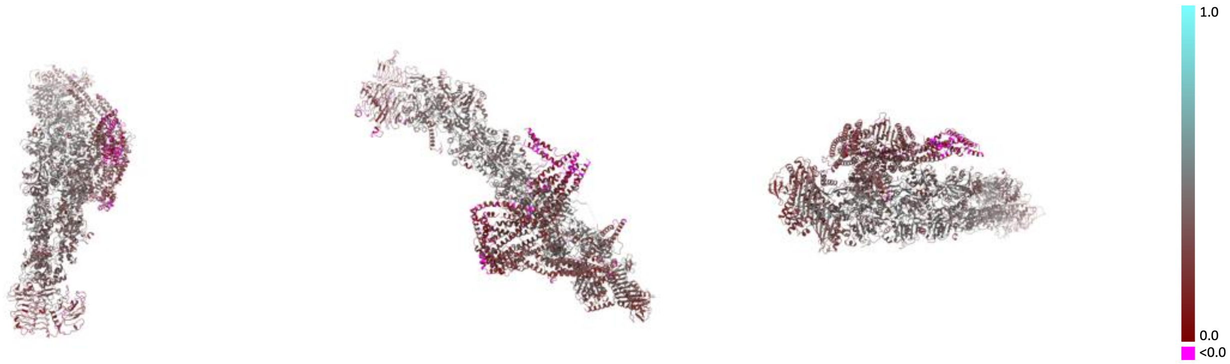
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.053 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.

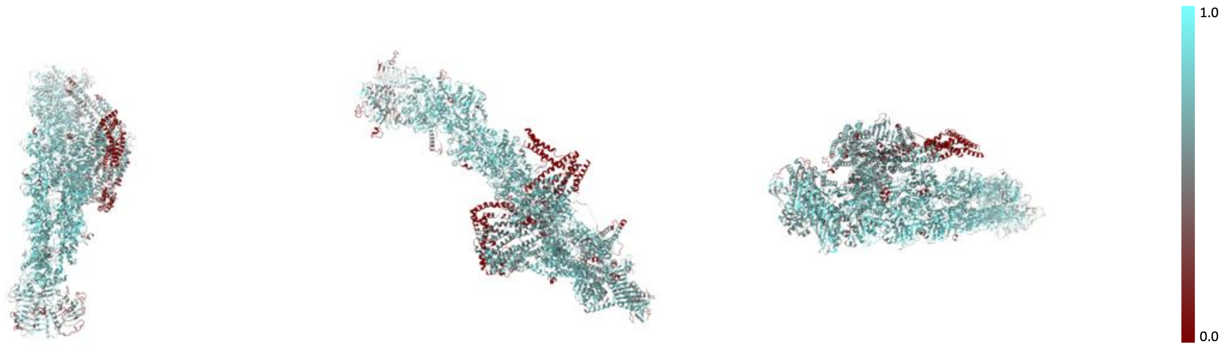
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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.

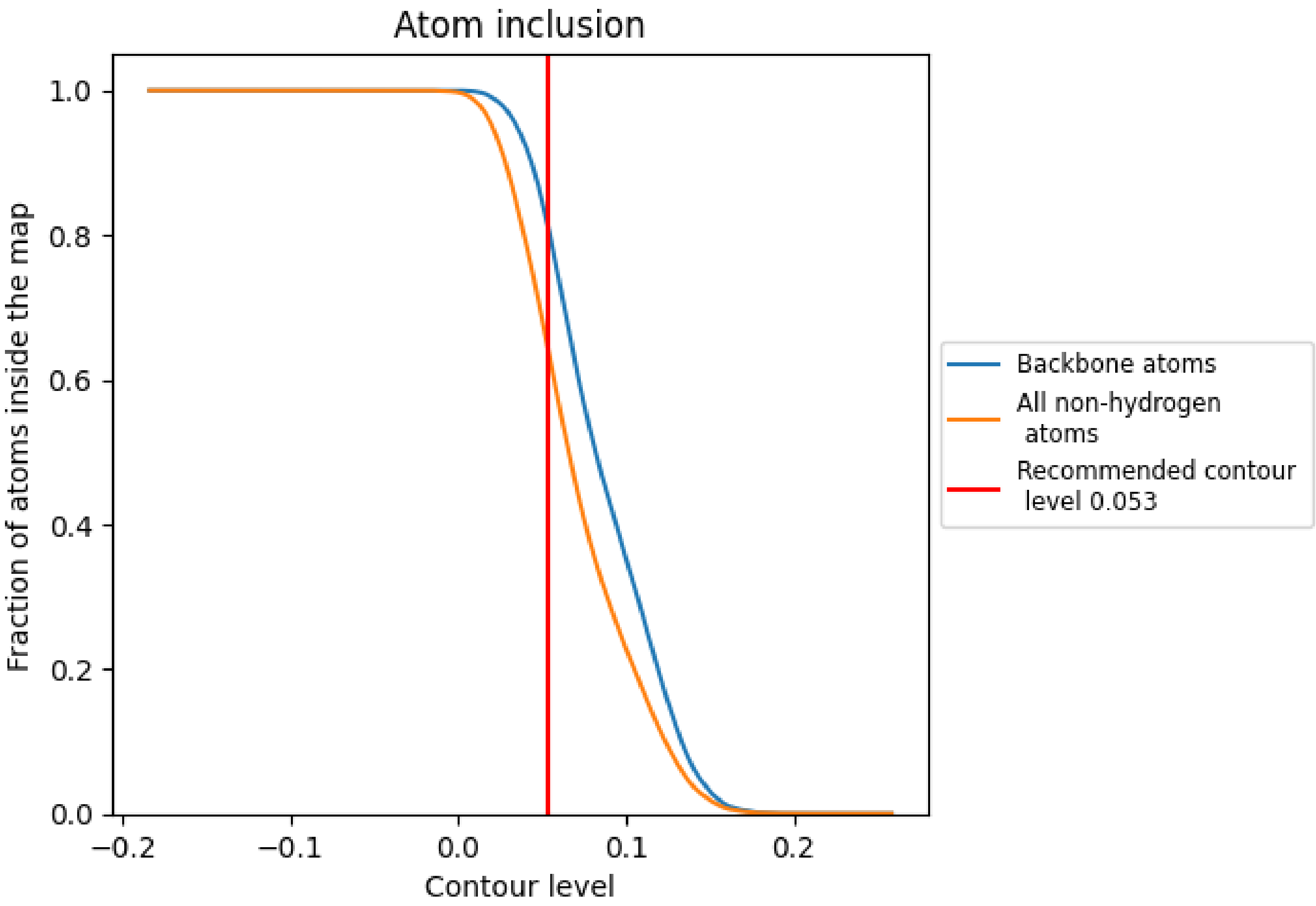
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 (0.053).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 65% 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 (0.053) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	▬ 0.6492	▬ 0.3520
A	▬ 0.6962	▬ 0.3760
B	▬ 0.7527	▬ 0.4130
C	▬ 0.7395	▬ 0.4330
D	▬ 0.7516	▬ 0.4250
E	▬ 0.7372	▬ 0.4250
F	▬ 0.7578	▬ 0.4170
G	▬ 0.7533	▬ 0.4200
H	▬ 0.7760	▬ 0.4280
I	▬ 0.7297	▬ 0.3940
J	▬ 0.7342	▬ 0.3990
K	▬ 0.5984	▬ 0.2980
L	▬ 0.6684	▬ 0.3360
M	▬ 0.4817	▬ 0.2560
N	▬ 0.4183	▬ 0.2070
O	▬ 0.4681	▬ 0.2370
U	▬ 0.4701	▬ 0.2040
V	▬ 0.6289	▬ 0.3070
Y	▬ 0.5322	▬ 0.2750
Z	▬ 0.5919	▬ 0.3100
m	▬ 0.5464	▬ 0.2950
n	▬ 0.5013	▬ 0.2860
o	▬ 0.4953	▬ 0.2540
z	▬ 0.3750	▬ 0.1970