wwPDB EM Validation Summary Report

Oct 8, 2022 – 05:54 pm BST

PDB ID	:	7Z8F
EMDB ID	:	EMD-14549
Title	:	Composite structure of dynein-dynactin-BICDR on microtubules
Authors	:	Chaaban, S.; Carter, A.P.
Deposited on	:	2022-03-17
Resolution	:	20.00 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:

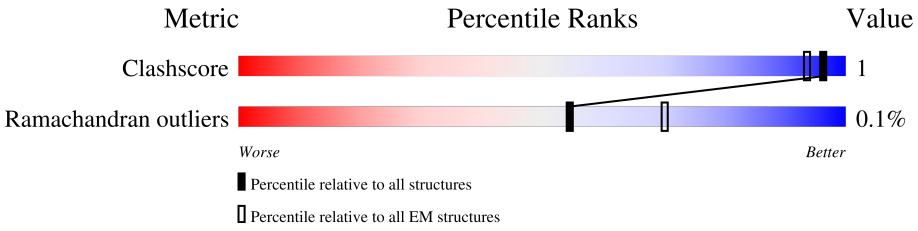
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 20.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	98%
1	B	376	97%
1	C	376	100%
1	D	376	98%
1	E	376	97%
1	F	376	98%
1	G	376	98%
1	I	376	98%
2	H	375	99%

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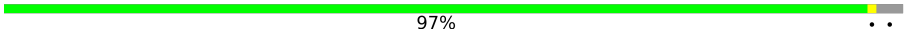
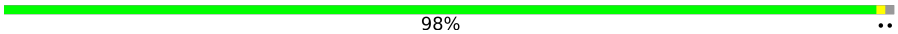
Mol	Chain	Length	Quality of chain
3	J	417	
4	K	286	
5	L	272	
6	M	405	
6	N	405	
6	P	405	
6	Q	405	
7	O	186	
7	R	186	
8	S	1281	
8	T	1281	
9	U	190	
10	V	182	
11	W	577	
11	X	577	
11	w	577	
11	x	577	
12	Y	467	
13	e	4646	
13	f	4646	
13	m	4646	
13	n	4646	
14	g	638	
14	h	638	
14	o	638	

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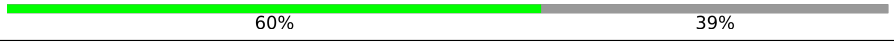
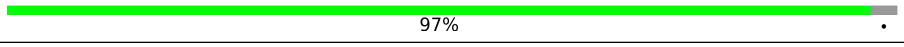
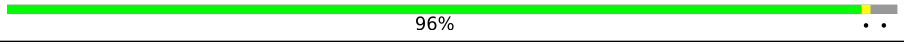
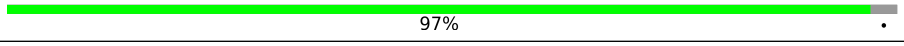
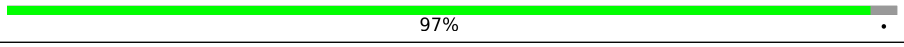
Mol	Chain	Length	Quality of chain
14	p	638	
15	i	492	
15	j	492	
15	q	492	
15	r	492	
16	k	96	
16	l	96	
16	s	96	
16	t	96	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 118408 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 1480	C 740	N 370	O 370	0	0
1	B	370	Total 1480	C 740	N 370	O 370	0	0
1	C	375	Total 1500	C 750	N 375	O 375	0	0
1	D	370	Total 1480	C 740	N 370	O 370	0	0
1	E	370	Total 1480	C 740	N 370	O 370	0	0
1	F	370	Total 1480	C 740	N 370	O 370	0	0
1	G	369	Total 1476	C 738	N 369	O 369	0	0
1	I	370	Total 1480	C 740	N 370	O 370	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	372	Total 1489	C 744	N 372	O 373	0	0

- Molecule 3 is a protein called Arp11.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	379	Total 1516	C 758	N 379	O 379	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 1112	C 556	N 278	O 278	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	269	Total 1076	C 538	N 269	O 269	0	0

- Molecule 6 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	340	Total 1360	C 680	N 340	O 340	0	0
6	N	280	Total 1120	C 560	N 280	O 280	0	0
6	P	343	Total 1372	C 686	N 343	O 343	0	0
6	Q	325	Total 1300	C 650	N 325	O 325	0	0

- Molecule 7 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	170	Total 680	C 340	N 170	O 170	0	0
7	R	179	Total 716	C 358	N 179	O 179	0	0

- Molecule 8 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	155	Total 620	C 310	N 155	O 155	0	0
8	T	192	Total 768	C 384	N 192	O 192	0	0

- Molecule 9 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	178	Total 712	C 356	N 178	O 178	0	0

- Molecule 10 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	182	Total	C	N	O	0	0
			728	364	182	182		

- Molecule 11 is a protein called BICD family-like cargo adapter 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	207	Total	C	N	O	0	0
			828	414	207	207		
11	X	269	Total	C	N	O	0	0
			1076	538	269	269		
11	w	207	Total	C	N	O	0	0
			828	414	207	207		
11	x	240	Total	C	N	O	0	0
			960	480	240	240		

- Molecule 12 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Y	383	Total	C	N	O	0	0
			1532	766	383	383		

- Molecule 13 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	4579	Total	C	N	O	0	0
			18317	9158	4579	4580		
13	f	4579	Total	C	N	O	0	0
			18317	9158	4579	4580		
13	m	4562	Total	C	N	O	0	0
			18249	9124	4562	4563		
13	n	4566	Total	C	N	O	0	0
			18265	9132	4566	4567		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	1567	GLU	ARG	conflict	UNP Q14204
e	1610	GLU	LYS	conflict	UNP Q14204
f	1567	GLU	ARG	conflict	UNP Q14204
f	1610	GLU	LYS	conflict	UNP Q14204
m	1567	GLU	ARG	conflict	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
m	1610	GLU	LYS	conflict	UNP Q14204
n	1567	GLU	ARG	conflict	UNP Q14204
n	1610	GLU	LYS	conflict	UNP Q14204

- Molecule 14 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	g	394	Total	C	N	O	0	0
			1576	788	394	394		
14	h	396	Total	C	N	O	0	0
			1584	792	396	396		
14	o	394	Total	C	N	O	0	0
			1576	788	394	394		
14	p	401	Total	C	N	O	0	0
			1604	802	401	401		

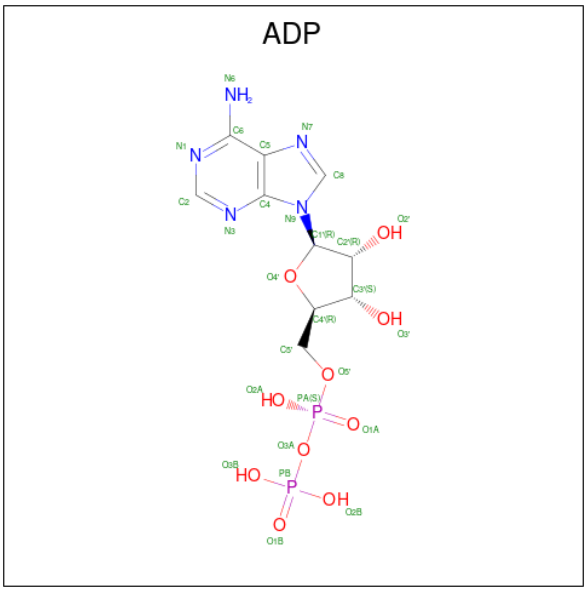
- Molecule 15 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	i	299	Total	C	N	O	0	0
			1196	598	299	299		
15	j	330	Total	C	N	O	0	0
			1320	660	330	330		
15	q	325	Total	C	N	O	0	0
			1300	650	325	325		
15	r	299	Total	C	N	O	0	0
			1196	598	299	299		

- Molecule 16 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	k	93	Total	C	N	O	0	0
			372	186	93	93		
16	l	93	Total	C	N	O	0	0
			372	186	93	93		
16	s	93	Total	C	N	O	0	0
			372	186	93	93		
16	t	93	Total	C	N	O	0	0
			372	186	93	93		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

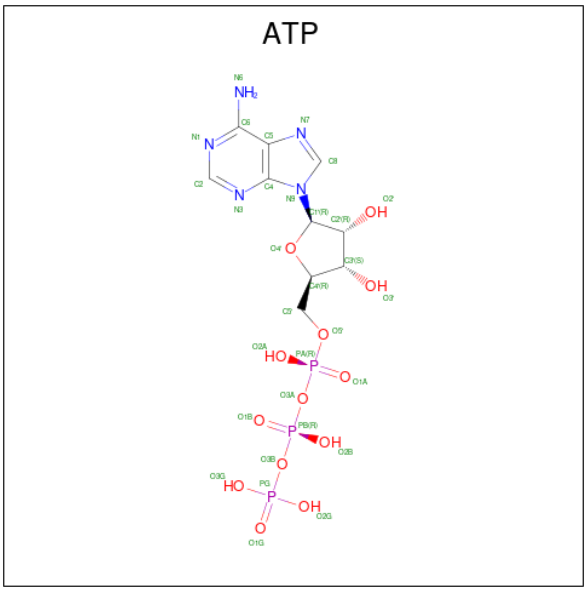


Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	f	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	m	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	n	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total Mg 1 1	0
18	B	1	Total Mg 1 1	0
18	C	1	Total Mg 1 1	0
18	D	1	Total Mg 1 1	0
18	E	1	Total Mg 1 1	0
18	F	1	Total Mg 1 1	0
18	G	1	Total Mg 1 1	0
18	H	1	Total Mg 1 1	0
18	I	1	Total Mg 1 1	0
18	J	1	Total Mg 1 1	0
18	e	1	Total Mg 1 1	0
18	f	1	Total Mg 1 1	0
18	m	1	Total Mg 1 1	0
18	n	1	Total Mg 1 1	0

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

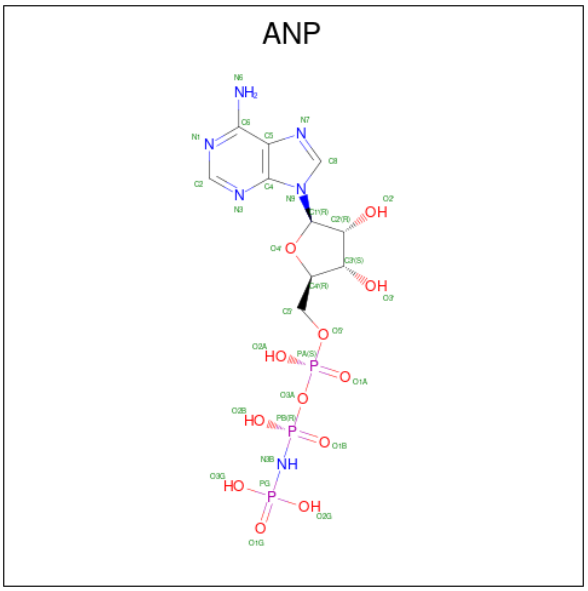


Mol	Chain	Residues	Atoms					AltConf
19	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	e	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	f	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	m	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	n	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 21 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



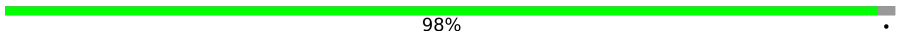
Mol	Chain	Residues	Atoms					AltConf
21	e	1	Total	C	N	O	P	0
			62	20	12	24	6	
21	e	1	Total	C	N	O	P	0
			62	20	12	24	6	
21	f	1	Total	C	N	O	P	0
			62	20	12	24	6	
21	f	1	Total	C	N	O	P	0
			62	20	12	24	6	
21	m	1	Total	C	N	O	P	0
			62	20	12	24	6	
21	m	1	Total	C	N	O	P	0
			62	20	12	24	6	
21	n	1	Total	C	N	O	P	0
			62	20	12	24	6	
21	n	1	Total	C	N	O	P	0
			62	20	12	24	6	

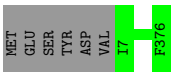
3 Residue-property plots (i)

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

• Molecule 1: ARP1 actin related protein 1 homolog A

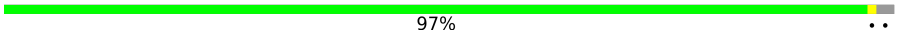
Chain A:

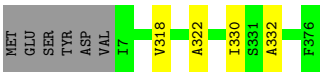




• Molecule 1: ARP1 actin related protein 1 homolog A

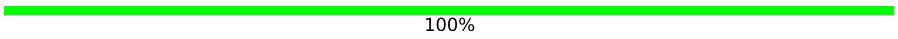
Chain B:





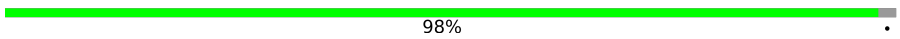
• Molecule 1: ARP1 actin related protein 1 homolog A

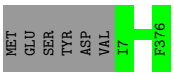
Chain C:



• Molecule 1: ARP1 actin related protein 1 homolog A

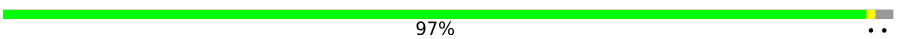
Chain D:





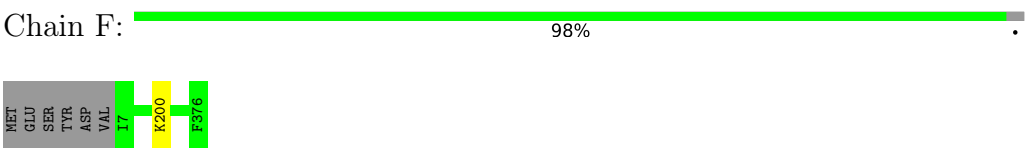
• Molecule 1: ARP1 actin related protein 1 homolog A

Chain E:



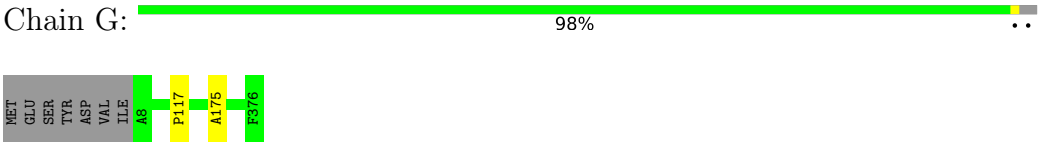
• Molecule 1: ARP1 actin related protein 1 homolog A

Chain F:



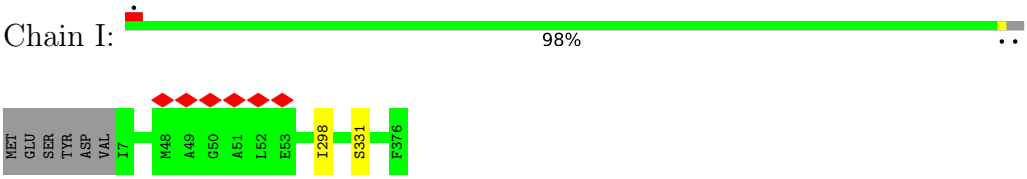
• Molecule 1: ARP1 actin related protein 1 homolog A

Chain G:



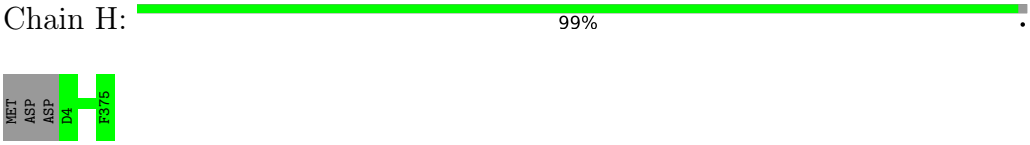
• Molecule 1: ARP1 actin related protein 1 homolog A

Chain I:



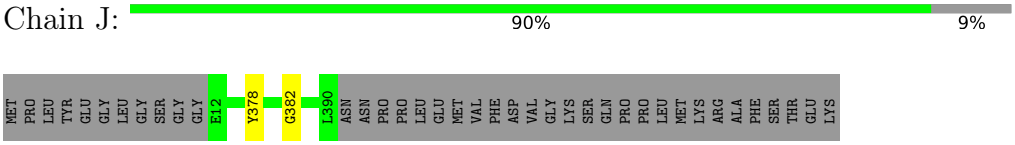
• Molecule 2: Actin, cytoplasmic 1

Chain H:



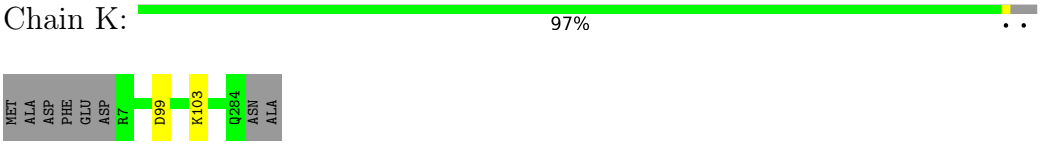
• Molecule 3: Arp11

Chain J:



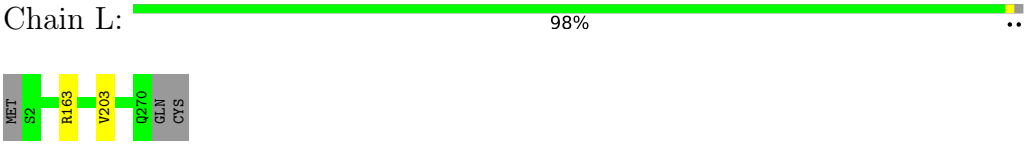
• Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K:



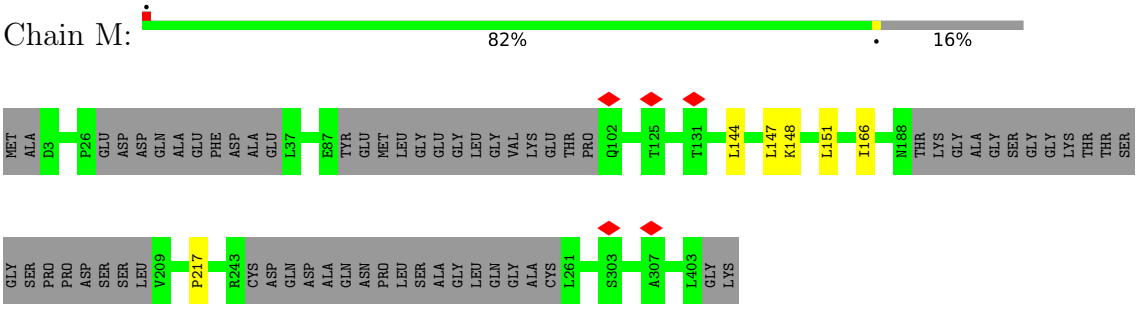
• Molecule 5: F-actin capping protein beta subunit

Chain L:



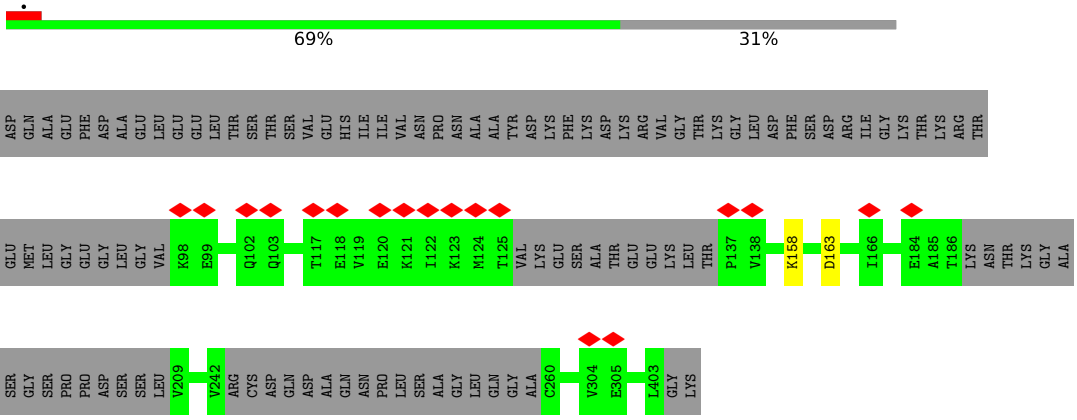
• Molecule 6: Dynactin subunit 2

Chain M:



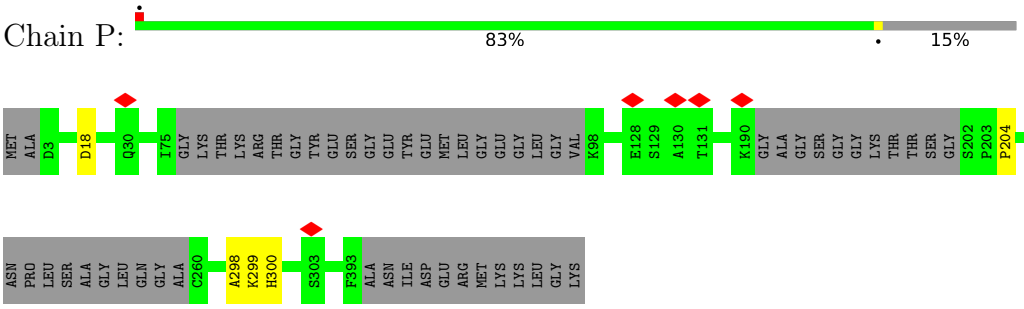
• Molecule 6: Dynactin subunit 2

Chain N:



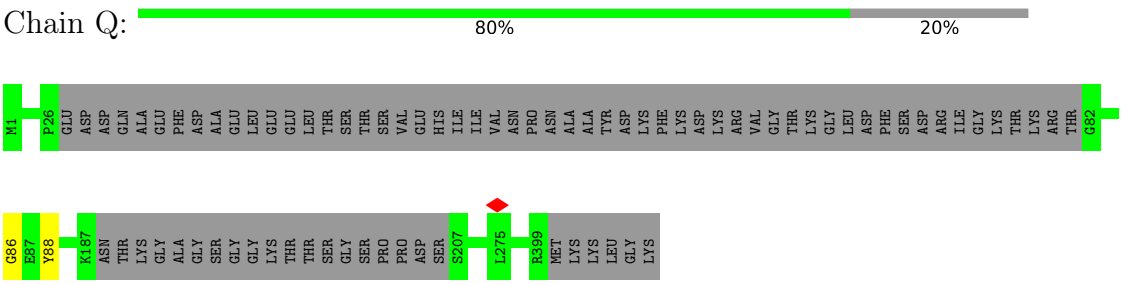
• Molecule 6: Dynactin subunit 2

Chain P:



• Molecule 6: Dynactin subunit 2

Chain Q:



• Molecule 7: Dynactin subunit 3

Chain O:

MET ALA GLY V4 G25 D69 C173 GLN LEU GLU ALA ALA LYS GLN VAL LYS PRO ALA GLU GLU

• Molecule 7: Dynactin subunit 3

Chain R: 91% 5% •

MET A2 P24 G36 V40 I61 D69 Q85 A89 C173 A177 Q180 VAL LYS PRO ALA GLU GLU

• Molecule 8: Dynactin subunit 1

Chain S: 12% 88%

MET ALA GLN SER LYS ARG HIS VAL TYR SER ARG THR PRO SER GLY SER ARG MET SER ALA GLU ALA SER ALA ARG PRO LEU ARG VAL GLY SER ARG VAL GLU VAL ILE GLY LYS GLY HIS ARG GLY THR VAL ALA TYR VAL GLY ALA THR LEU PHE ALA THR GLY LYS TRP VAL GLY VAL

ILE LEU ASP GLU ALA LYS GLY LYS ASN ASP GLY THR VAL GLN GLY ARG LYS TYR PHE THR CYS ASP GLU GLY HIS GLY ILE PHE VAL ARG GLN SER GLN ILE GLN VAL PHE GLU ASP GLY ALA ASP THR THR SER PRO GLU THR PRO ASP SER SER ALA SER LYS VAL LEU ARG ARG GLU

GLY THR ASP SER ASN ALA LYS THR SER LYS LEU ARG GLY PRO LYS PRO LYS LYS ALA PRO THR ALA ARG LYS THR THR THR ARG ARG PRO LYS PRO THR ARG PRO ALA SER THR GLY VAL ALA GLY ALA SER SER SER LEU GLY PRO SER GLY SER ALA SER ALA GLY GLU LEU SER SER

SER GLU PRO SER THR PRO ALA GLN THR PRO LEU ALA ALA PRO ILE ILE PRO THR PRO ALA LEU THR SER PRO GLY ALA ALA PRO PRO LEU PRO SER PRO SER LYS GLU GLU GLU GLY LEU ARG ALA GLN VAL ARG ASP LEU GLU GLU LYS LEU GLU THR LEU ARG LEU LYS ARG ALA GLU

ASP LYS ALA LYS LEU LYS GLU LEU GLU LYS HIS LYS ILE GLN LEU GLU GLN VAL GLN GLU TRP LYS SER LYS MET GLN GLU GLN GLN ALA ASP LEU GLN ARG ARG LEU LYS GLU ALA ARG LYS GLU ALA LYS GLU ALA LEU GLU ALA LYS GLU ARG TYR MET GLU GLU MET ALA ASP THR

ALA ASP ALA ILE GLU MET ALA THR LEU ASP LYS GLU MET ALA GLU GLU ARG ALA GLU SER LEU GLN GLN GLU VAL GLU ALA LEU LYS GLU ARG VAL ASP GLU LEU THR THR ASP LEU GLU ILE LEU LYS ALA GLU ILE GLU GLU LYS GLY SER ASP GLY ALA ALA SER SER TYR GLN LEU

LYS GLN LEU GLU GLU GLN ASN ALA ARG LEU LYS ASP ALA LEU VAL ARG MET ARG ASP LEU SER SER SER GLU LYS GLN GLU HIS VAL LYS LEU GLN LYS LEU MET GLU LYS LYS ASN GLN GLU LEU GLU VAL VAL ARG GLN GLN ARG GLU ARG LEU GLN GLU GLU LEU SER GLN ALA GLU

SER THR ILE ASP GLU LEU LYS GLU GLN VAL ASP ALA ALA LEU GLY ALA GLU GLU MET VAL GLU MET LEU THR ASP ARG ASN LEU ASN LEU GLU GLU LYS VAL ARG GLU LEU ARG GLU THR VAL GLY ASP LEU GLU ALA MET ASN GLU MET ASN ASP GLU LEU GLN GLU ASN ALA ARG GLU

THR GLU LEU GLU LEU ARG GLU GLN LEU ASP MET ALA GLY ALA ARG VAL ARG GLU ALA GLN LYS ARG VAL GLU ALA ALA GLN GLU THR VAL ALA ASP TYR GLN GLN THR ILE LYS LYS TYR ARG GLN LEU THR ALA HIS LEU GLN ASP VAL ASN ARG GLU LEU THR ASN GLN GLU ALA

SER VAL GLU ARG GLN GLN GLN PRO PRO PRO GLU THR PHE ASP PHE LYS ILE LYS PHE ALA GLU THR LYS ALA HIS ALA LYS ALA ILE GLU MET GLU LEU ARG GLN MET GLU VAL ALA GLN ALA ASN ARG HIS MET SER LEU LEU THR ALA PHE MET PRO ASP SER PHE LEU ARG PRO GLY

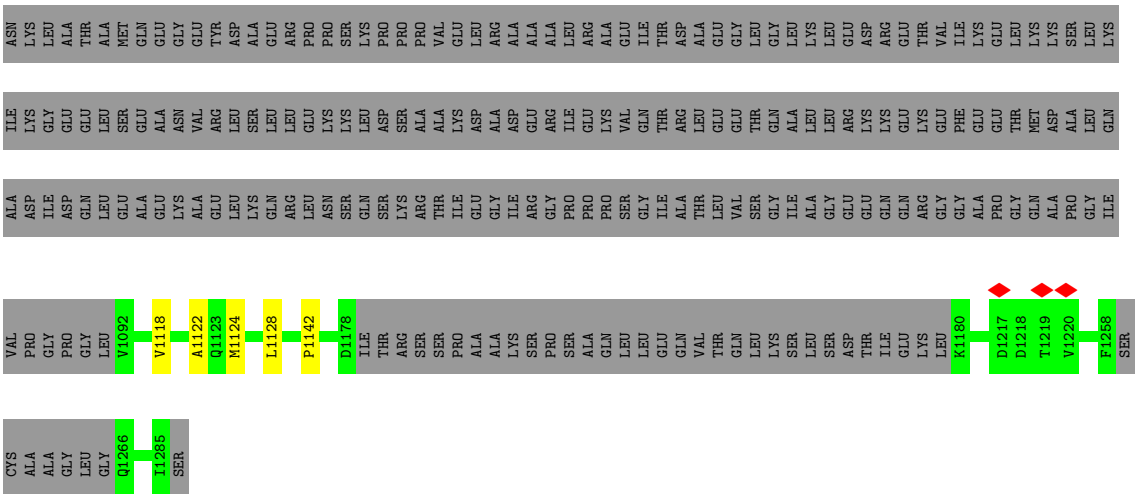
GLY ASP HIS ASP CYS VAL LEU VAL LEU LEU LEU MET PRO ARG LEU ILE CYS LYS ALA GLU LEU ILE ARG LYS GLN ALA GLN GLU LYS PHE ASP LEU SER GLU ASN CYS SER GLU ARG PRO GLY LEU ARG GLY ALA ALA GLY GLU GLN LEU SER PHE ALA ALA GLY LEU VAL TYR SER LEU

SER LEU LEU GLN ALA THR LEU HIS ARG TYR GLU HIS ALA LEU SER GLN CYS SER VAL ASP VAL TYR LYS LYS VAL GLY SER LEU TYR PRO GLU MET SER ALA HIS GLU ARG SER LEU ASP PHE LEU ILE GLU LEU LEU HIS LYS ASP GLN LEU ASP GLU THR VAL ASN VAL GLU PRO LEU

THR LYS ALA ILE LYS TYR TYR GLN HIS LEU TYR SER ILE HIS LEU ALA GLU GLN PRO GLU ASP SER THR MET GLN LEU ALA ASP HIS ILE LYS PHE THR GLN SER ALA LEU ASP CYS MET SER VAL GLU VAL GLY ARG LEU ARG ALA PHE LEU GLN GLY GLY GLN GLU ALA SER ASP ILE

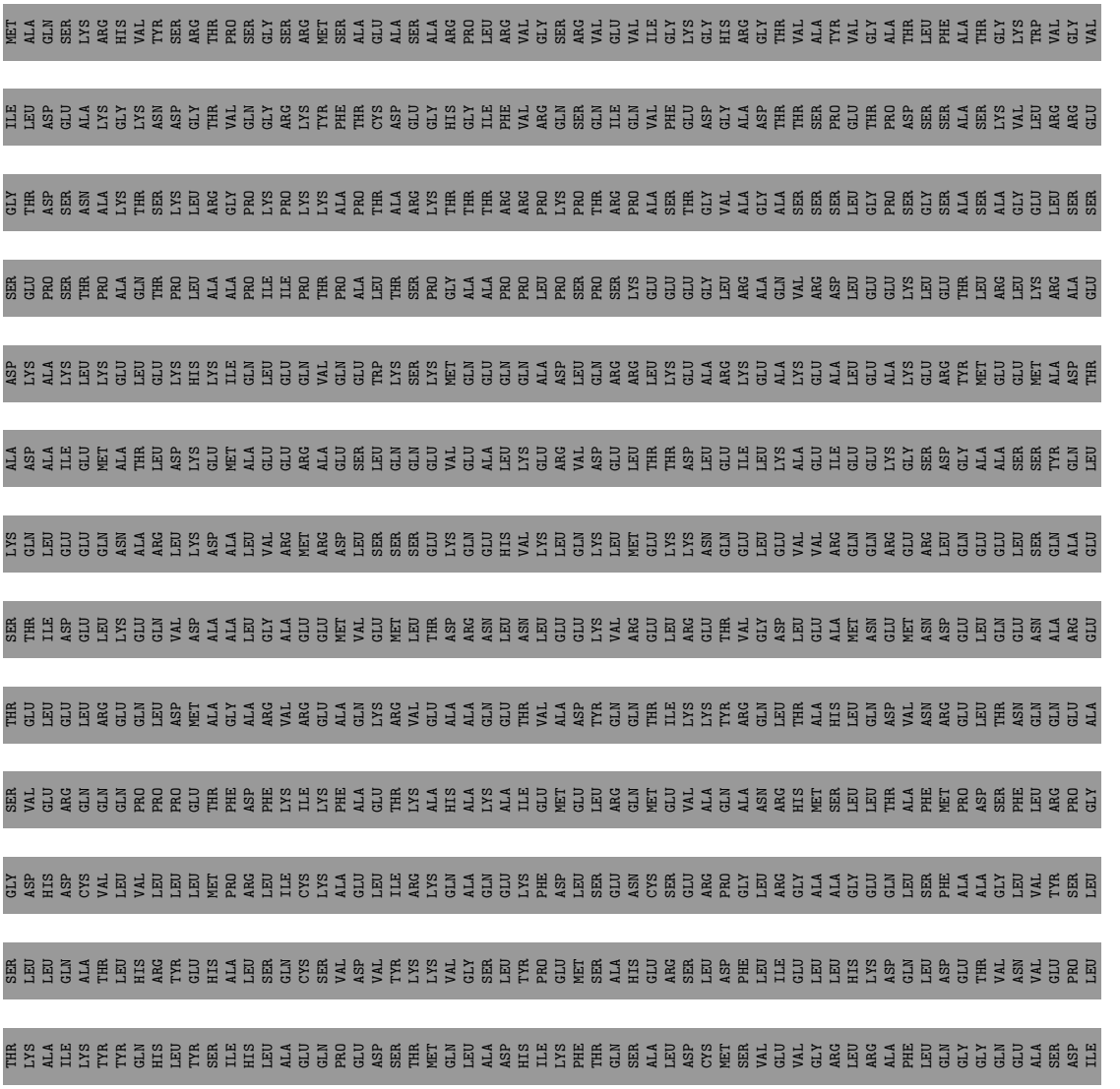
ALA LEU LEU LEU ARG ASP LEU GLU THR SER CYS SER ASP ILE ARG GLN PHE CYS LYS LYS ILE ARG ARG ARG MET PRO GLY THR ASP ALA PRO GLY ILE PRO ALA ALA LEU ALA PHE GLY ALA GLN VAL SER ASP THR LEU LEU ASP CYS ARG LYS HIS LEU THR TRP VAL VAL ALA VAL

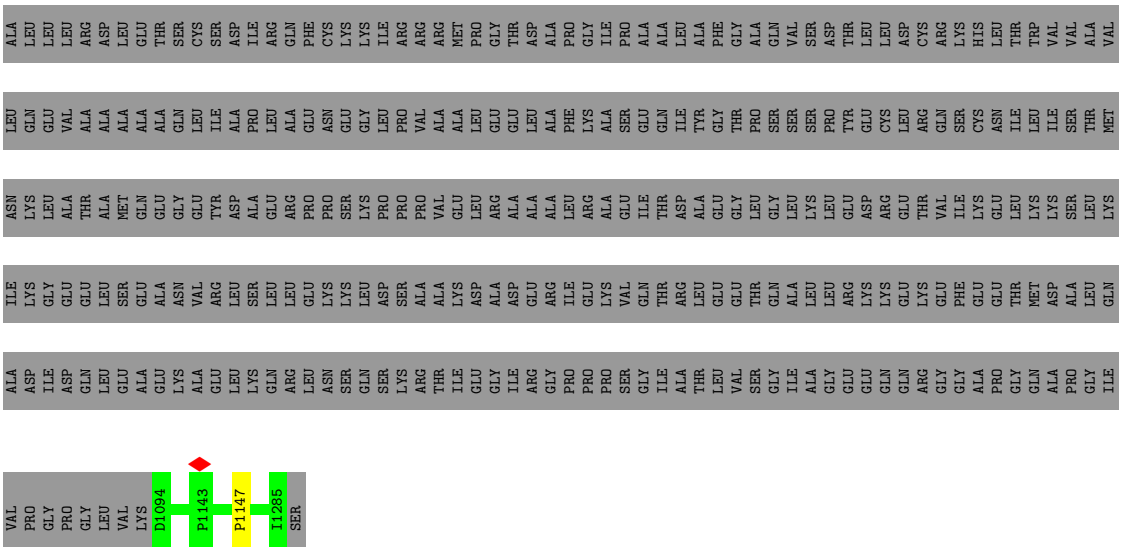
LEU GLN GLU VAL ALA ALA ALA ALA ALA GLN LEU ILE ALA PRO LEU ALA GLU ASN GLU GLY LEU PRO VAL ALA ALA LEU GLU GLU LEU ALA PHE LYS ALA SER GLU GLN ILE TYR GLY THR PRO SER SER SER PRO TYR GLU CYS LEU ARG GLN SER CYS ASN ILE LEU ILE SER THR MET



• Molecule 8: Dynactin subunit 1

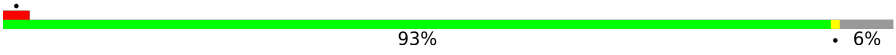
Chain T:

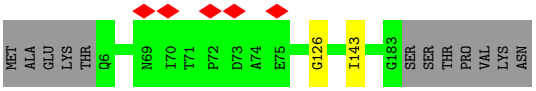




• Molecule 9: Dynactin 6

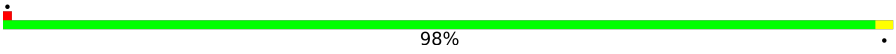
Chain U:





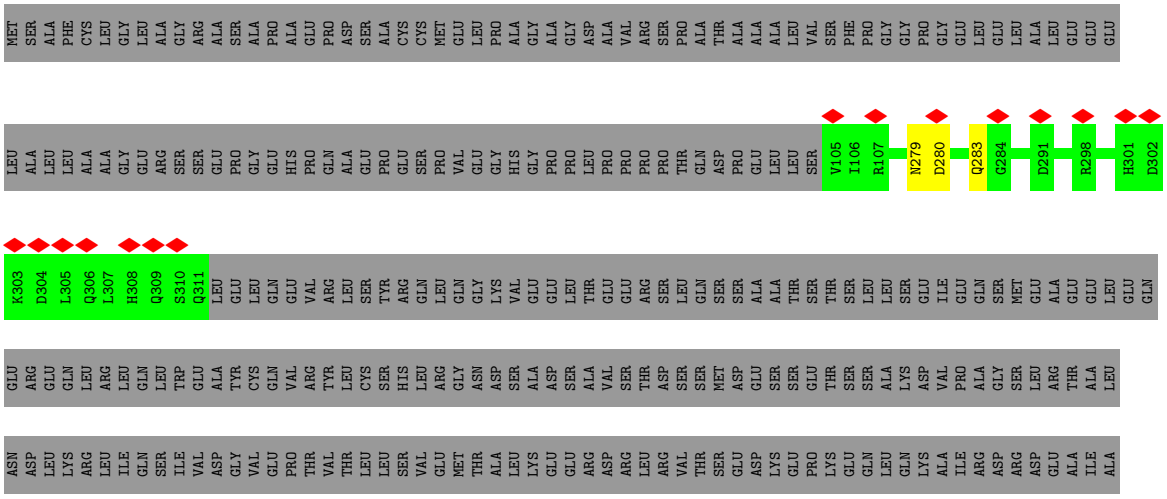
• Molecule 10: Dynactin subunit 5

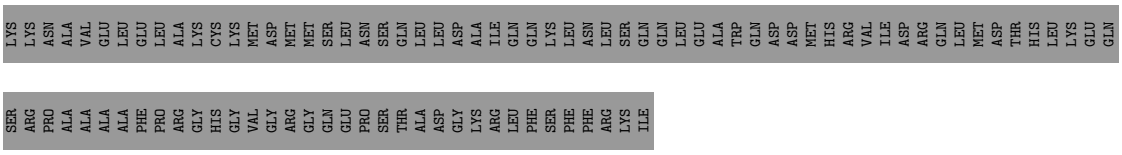
Chain V:



• Molecule 11: BICD family-like cargo adapter 1

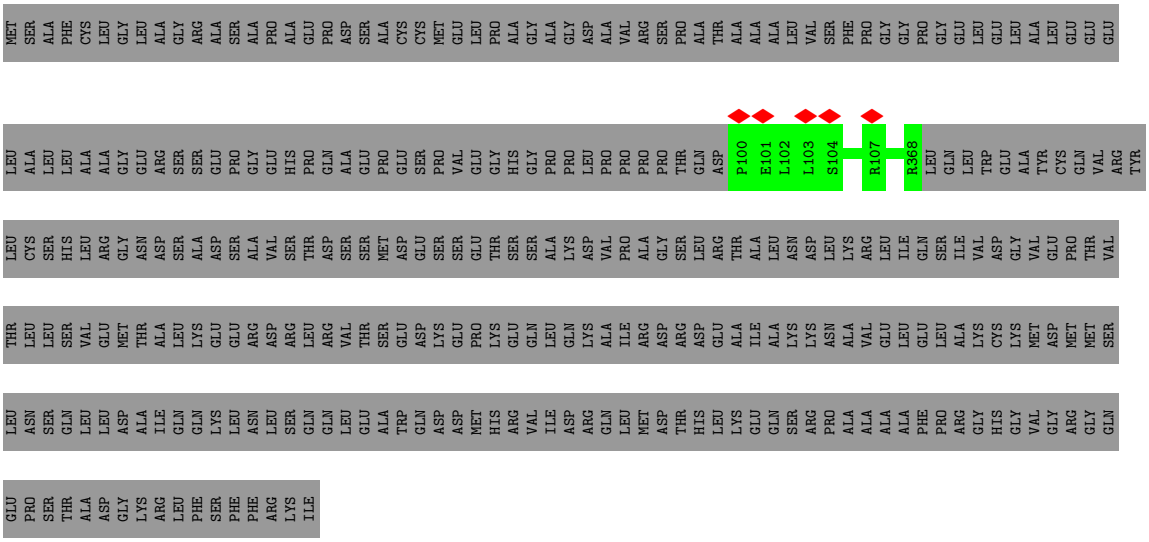
Chain W:





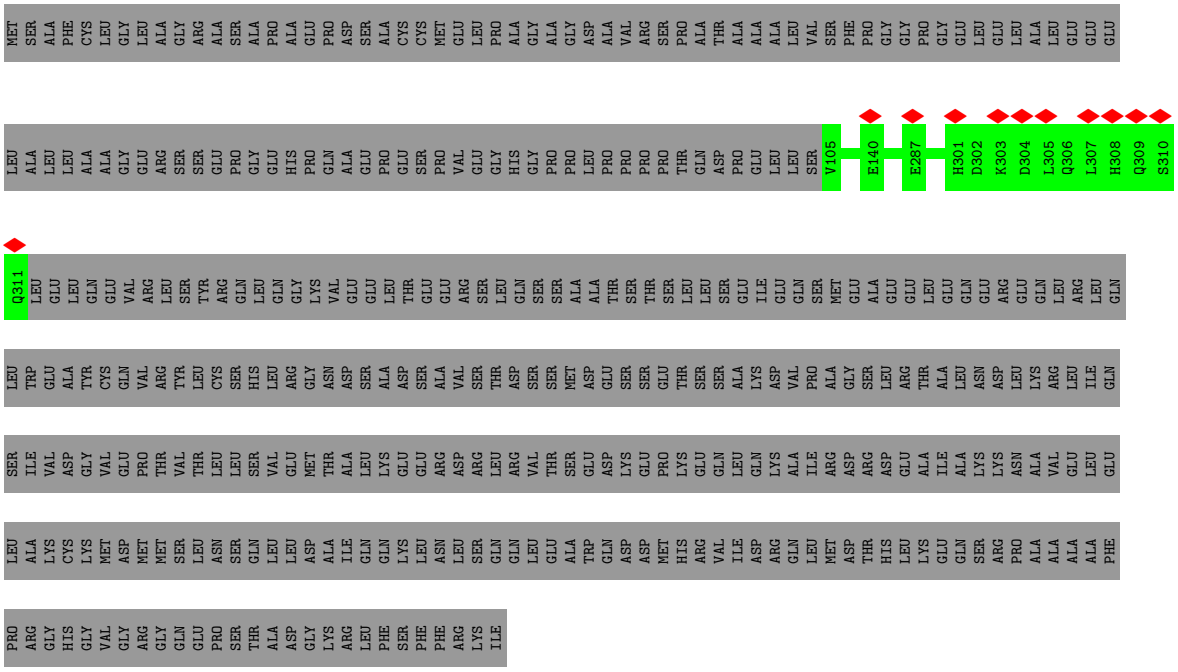
• Molecule 11: BICD family-like cargo adapter 1

Chain X:



• Molecule 11: BICD family-like cargo adapter 1

Chain w:

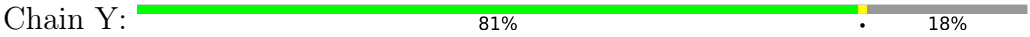


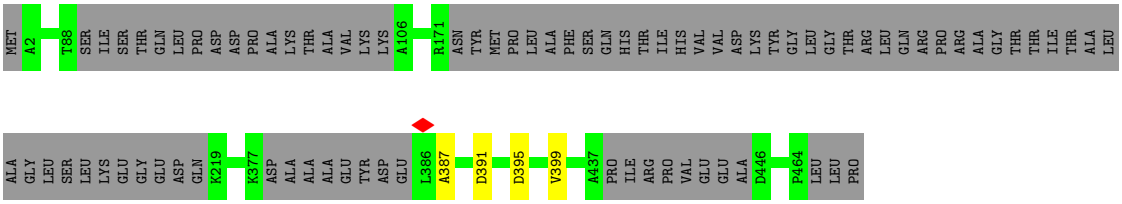
• Molecule 11: BICD family-like cargo adapter 1

Chain x:

• Molecule 12: Dynactin subunit 4

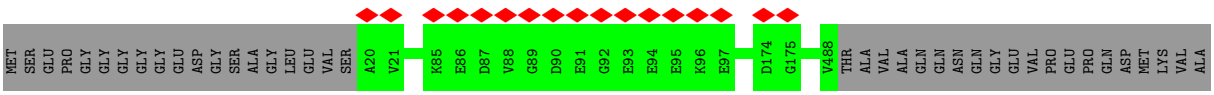
Chain Y:

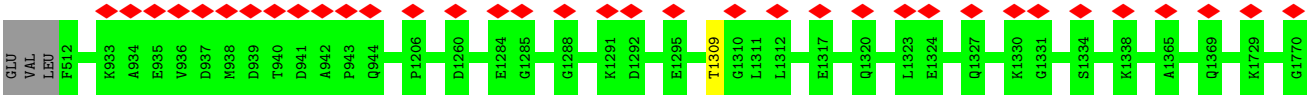


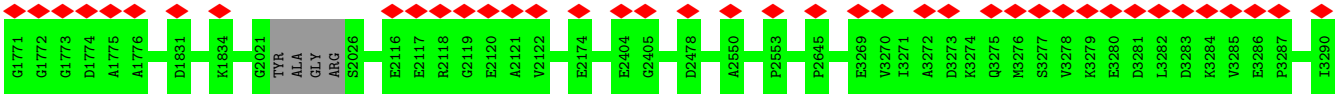


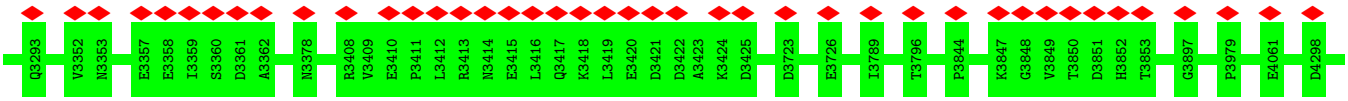
• Molecule 13: Cytoplasmic dynein 1 heavy chain 1

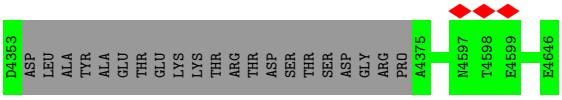
Chain e:





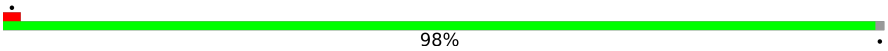


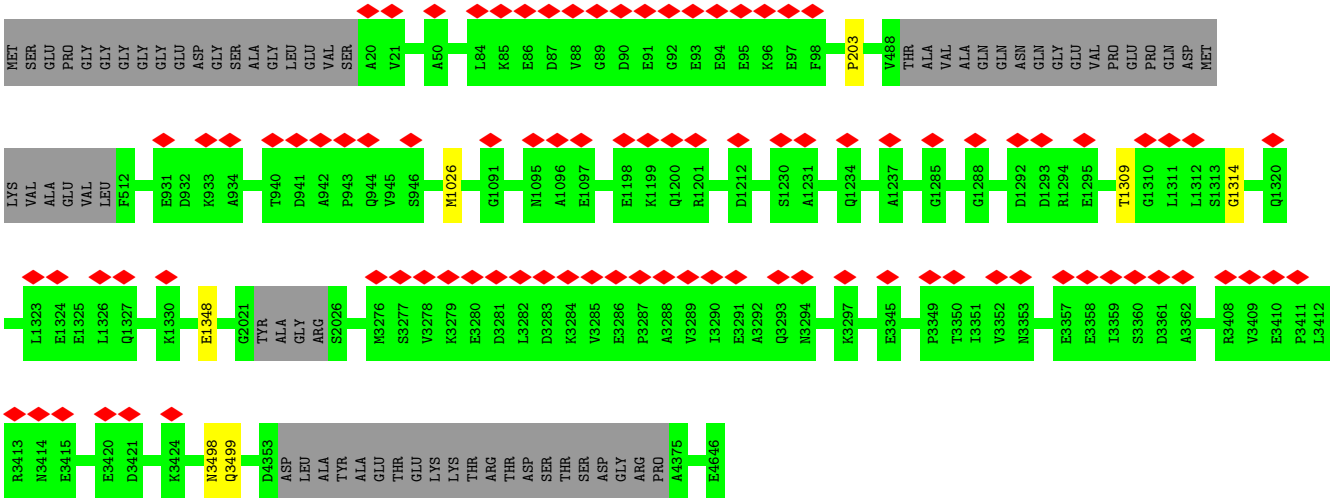




• Molecule 13: Cytoplasmic dynein 1 heavy chain 1

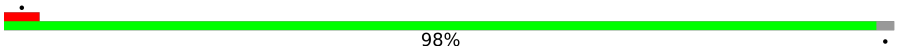
Chain f:

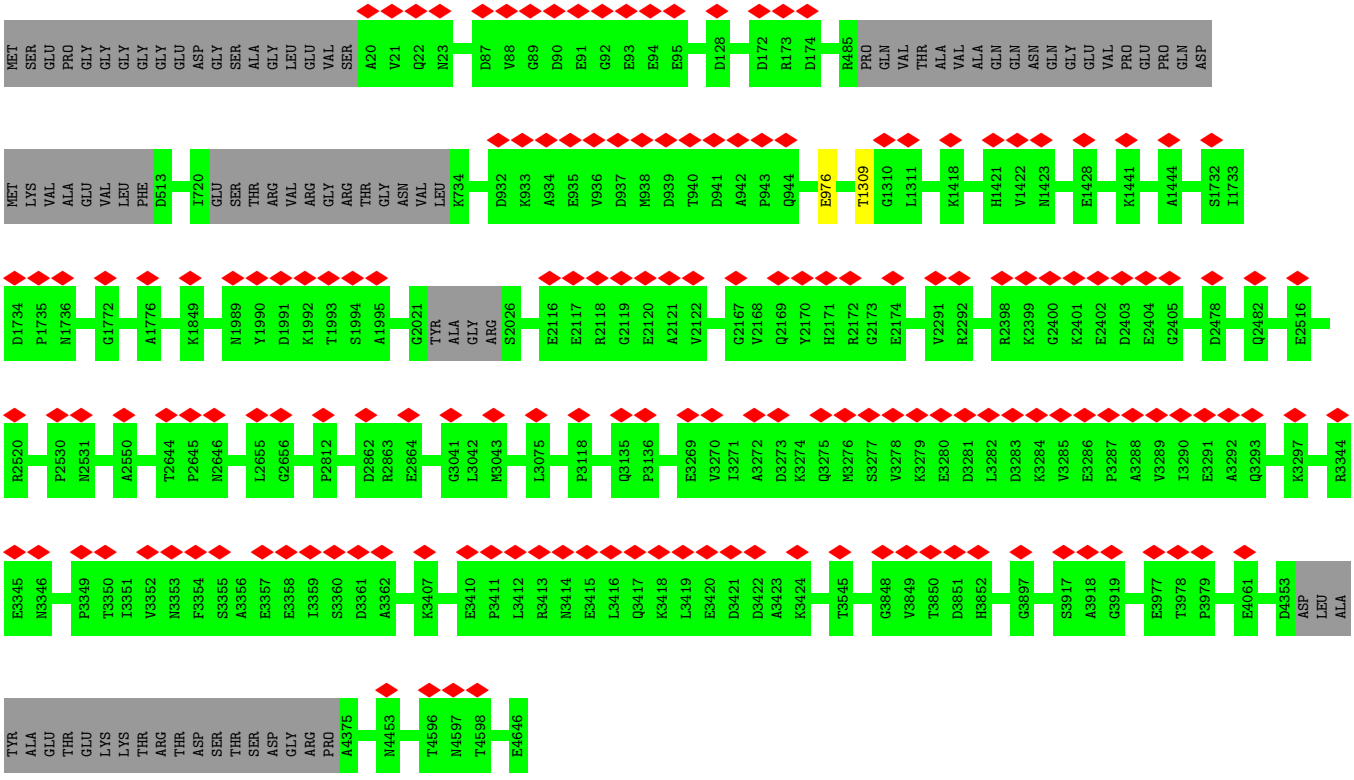




• Molecule 13: Cytoplasmic dynein 1 heavy chain 1

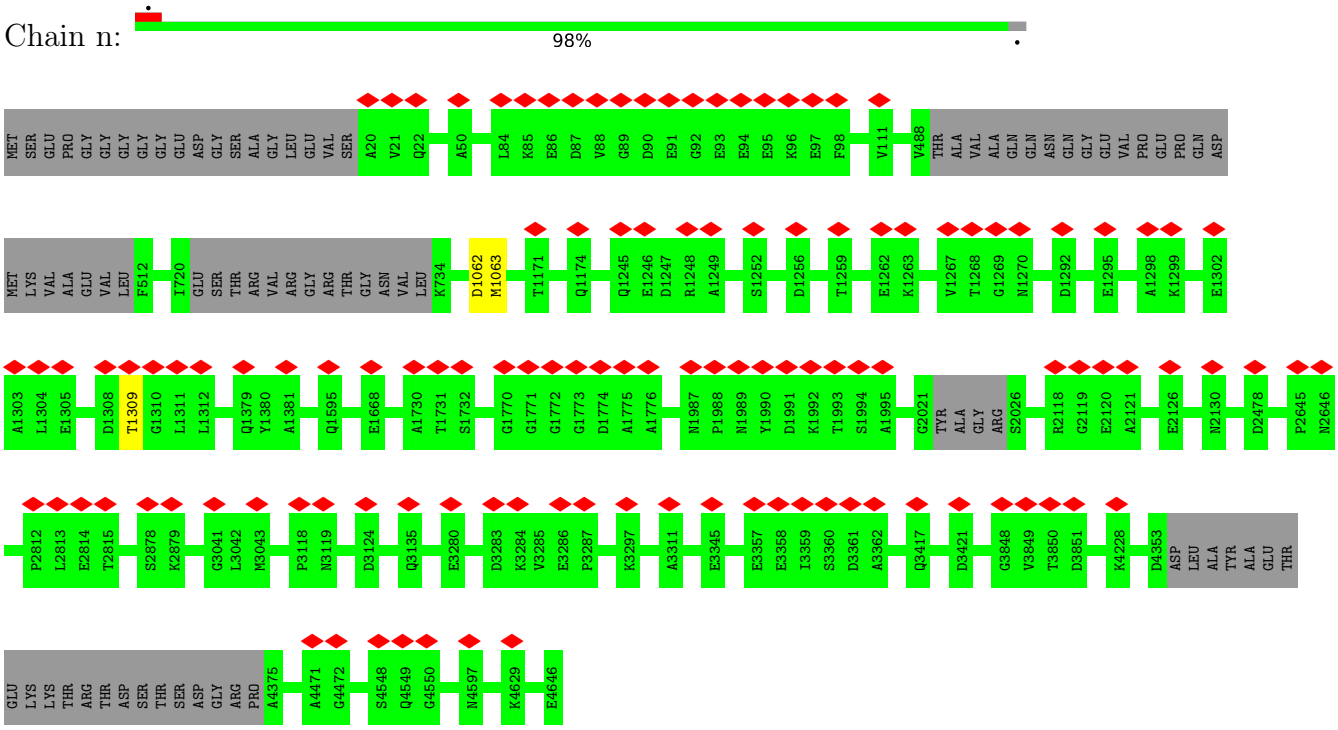
Chain m:





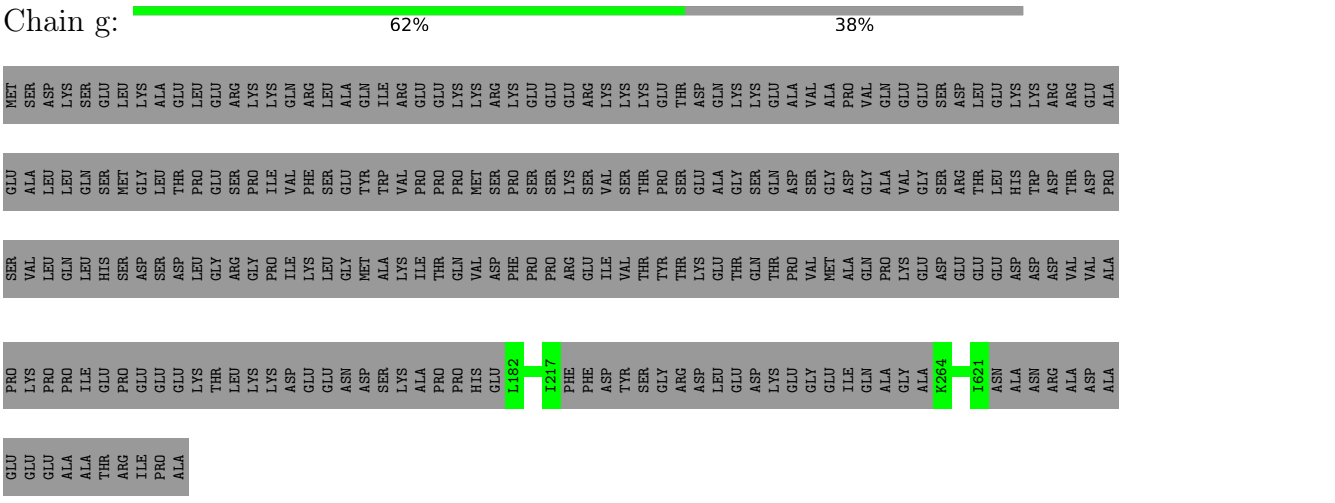
• Molecule 13: Cytoplasmic dynein 1 heavy chain 1

Chain n:



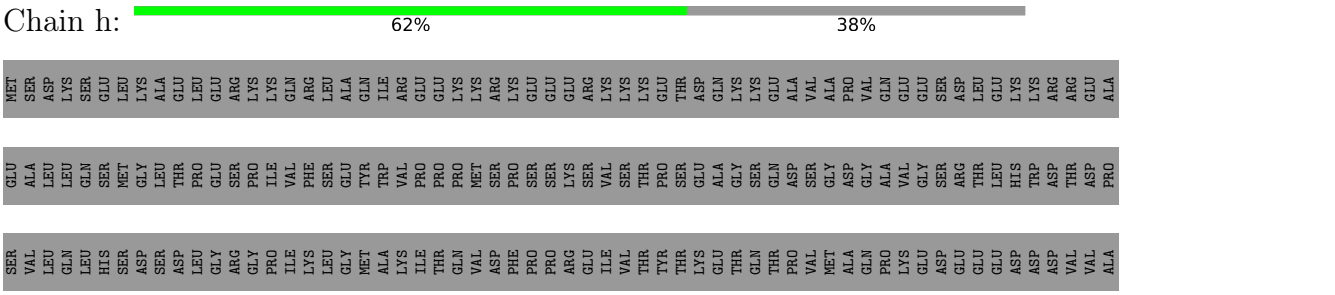
• Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

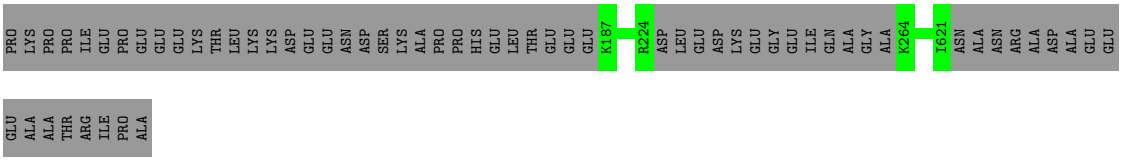
Chain g:



• Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

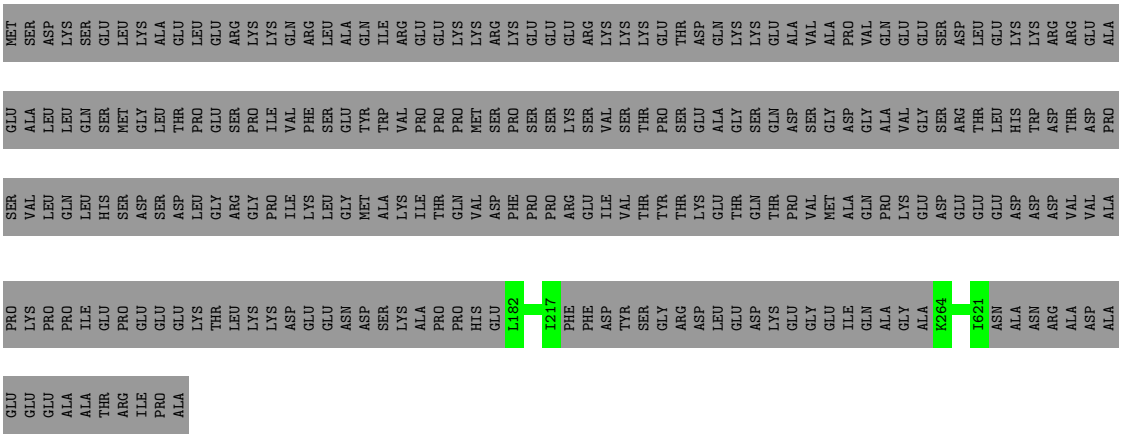
Chain h:





• Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

Chain o:

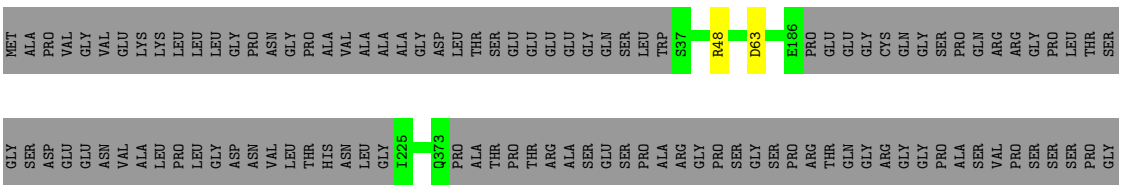


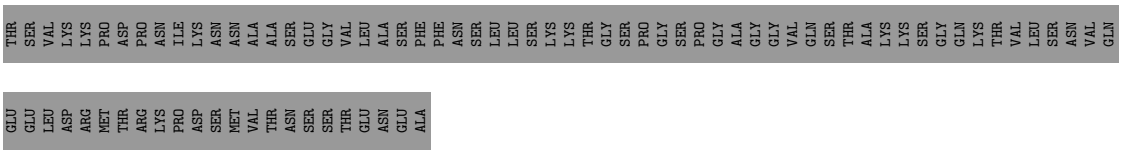
• Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

Chain p:

• Molecule 15: Cytoplasmic dynein 1 light intermediate chain 2

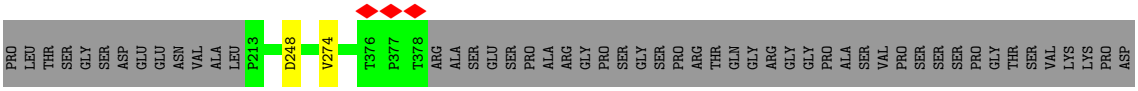
Chain i:





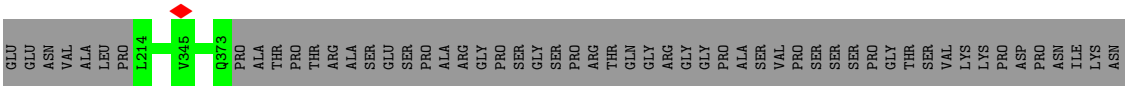
• Molecule 15: Cytoplasmic dynein 1 light intermediate chain 2

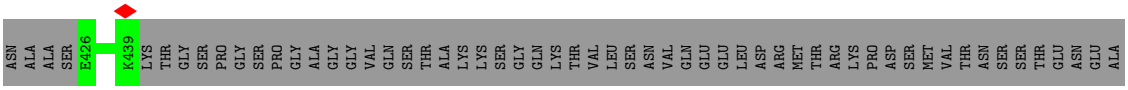
Chain j:



• Molecule 15: Cytoplasmic dynein 1 light intermediate chain 2

Chain q:



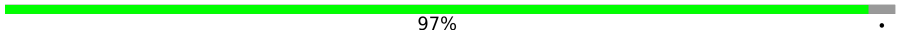


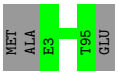
• Molecule 15: Cytoplasmic dynein 1 light intermediate chain 2

Chain r:

• Molecule 16: Dynein light chain roadblock-type 1

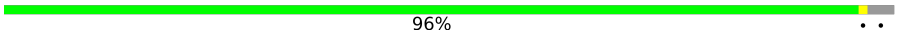
Chain k:





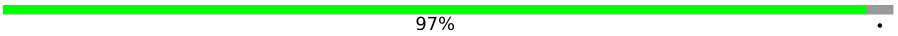
• Molecule 16: Dynein light chain roadblock-type 1

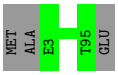
Chain l:



• Molecule 16: Dynein light chain roadblock-type 1

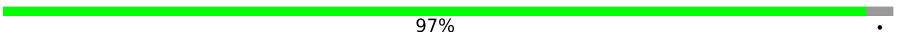
Chain s:

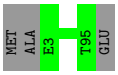




• Molecule 16: Dynein light chain roadblock-type 1

Chain t:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	628033	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.478	Depositor
Minimum map value	-0.203	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0851	Depositor
Map size (Å)	955.776, 955.776, 955.776	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.489, 2.489, 2.489	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, 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	0.23	0/1479	0.49	0/1847
1	B	0.24	0/1479	0.51	0/1847
1	C	0.24	0/1499	0.51	0/1872
1	D	0.24	0/1479	0.51	0/1847
1	E	0.23	0/1479	0.51	0/1847
1	F	1.08	0/1479	1.10	0/1847
1	G	0.24	0/1475	0.49	0/1842
1	I	0.24	0/1479	0.50	0/1847
2	H	0.24	0/1488	0.49	0/1857
3	J	0.23	0/1515	0.50	0/1892
4	K	0.24	0/1111	0.52	0/1387
5	L	0.24	0/1075	0.50	0/1342
6	M	0.90	0/1355	0.95	0/1685
6	N	0.92	0/1115	0.97	0/1385
6	P	0.89	0/1368	0.96	0/1703
6	Q	0.91	0/1297	0.94	0/1616
7	O	0.87	0/679	0.94	0/847
7	R	0.91	0/715	0.97	0/892
8	S	0.90	0/616	0.97	0/763
8	T	0.92	0/767	0.94	0/957
9	U	0.28	0/711	0.56	0/887
10	V	0.32	0/727	0.60	0/907
11	W	0.77	0/827	0.88	0/1032
11	X	0.65	0/1075	0.72	0/1342
11	w	0.82	0/827	0.82	0/1032
11	x	0.60	0/959	0.73	0/1197
12	Y	0.24	0/1527	0.51	0/1900
13	e	0.44	0/18313	0.57	0/22883
13	f	0.65	1/18313 (0.0%)	0.68	0/22883
13	m	0.46	0/18244	0.58	0/22795
13	n	0.50	1/18260 (0.0%)	0.60	1/22815 (0.0%)
14	g	0.32	0/1574	0.57	0/1964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	h	0.32	0/1582	0.57	0/1974
14	o	0.31	0/1574	0.55	0/1964
14	p	0.34	0/1602	0.56	0/1999
15	i	0.55	1/1194 (0.1%)	0.65	0/1489
15	j	0.95	5/1317 (0.4%)	0.87	1/1641 (0.1%)
15	q	0.87	0/1297	0.87	0/1616
15	r	0.50	0/1194	0.71	2/1489 (0.1%)
16	k	0.72	0/371	0.85	0/462
16	l	0.69	0/371	0.78	0/462
16	s	0.68	0/371	0.67	0/462
16	t	0.67	0/371	0.69	0/462
All	All	0.54	8/117550 (0.0%)	0.65	4/146779 (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
15	q	0	1
15	r	0	2
All	All	0	3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1026	MET	C-N	-5.56	1.23	1.34
15	i	63	ASP	C-N	-5.54	1.23	1.33
15	j	141	ARG	C-N	-5.29	1.24	1.34
15	j	95	ASP	C-N	-5.28	1.22	1.34
13	n	1063	MET	C-O	5.28	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	r	79	HIS	C-N-CA	-6.43	108.80	122.30
13	n	1062	ASP	C-N-CA	5.97	136.63	121.70
15	j	48	ARG	O-C-N	5.14	130.92	122.70
15	r	79	HIS	CA-C-N	-5.02	106.17	116.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	q	44	SER	Mainchain
15	r	37	SER	Mainchain
15	r	80	GLY	Mainchain

5.2 Too-close contacts (i)

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	1480	0	406	0	0
1	B	1480	0	406	4	0
1	C	1500	0	411	0	0
1	D	1480	0	406	0	0
1	E	1480	0	406	3	0
1	F	1480	0	406	1	0
1	G	1476	0	405	2	0
1	I	1480	0	406	1	0
2	H	1489	0	408	0	0
3	J	1516	0	408	1	0
4	K	1112	0	291	1	0
5	L	1076	0	295	1	0
6	M	1360	0	346	2	0
6	N	1120	0	277	0	0
6	P	1372	0	341	2	0
6	Q	1300	0	339	3	0
7	O	680	0	176	0	0
7	R	716	0	187	3	0
8	S	620	0	154	2	0
8	T	768	0	196	0	0
9	U	712	0	193	1	0
10	V	728	0	202	1	0
11	W	828	0	216	2	0
11	X	1076	0	280	0	0
11	w	828	0	216	0	0
11	x	960	0	251	0	0
12	Y	1532	0	375	2	0
13	e	18317	0	4801	0	0
13	f	18317	0	4801	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	18249	0	4780	0	0
13	n	18265	0	4783	0	0
14	g	1576	0	421	0	0
14	h	1584	0	425	0	0
14	o	1576	0	421	0	0
14	p	1604	0	430	0	0
15	i	1196	0	312	0	0
15	j	1320	0	345	0	0
15	q	1300	0	342	0	0
15	r	1196	0	312	0	0
16	k	372	0	93	0	0
16	l	372	0	93	0	0
16	s	372	0	93	0	0
16	t	372	0	93	0	0
17	A	27	0	12	0	0
17	B	27	0	12	0	0
17	C	27	0	12	0	0
17	D	27	0	12	0	0
17	E	27	0	12	0	0
17	F	27	0	12	0	0
17	G	27	0	12	0	0
17	H	27	0	12	0	0
17	I	27	0	12	0	0
17	e	27	0	12	0	0
17	f	27	0	12	0	0
17	m	27	0	12	0	0
17	n	27	0	12	0	0
18	A	1	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	D	1	0	0	0	0
18	E	1	0	0	0	0
18	F	1	0	0	0	0
18	G	1	0	0	0	0
18	H	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	e	1	0	0	0	0
18	f	1	0	0	0	0
18	m	1	0	0	0	0
18	n	1	0	0	0	0
19	J	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	e	31	0	12	0	0
19	f	31	0	12	0	0
19	m	31	0	12	0	0
19	n	31	0	12	0	0
20	Y	3	0	0	0	0
21	e	62	0	26	0	0
21	f	62	0	26	0	0
21	m	62	0	26	0	0
21	n	62	0	26	0	0
All	All	118408	0	31268	26	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 1.

The worst 5 of 26 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)
5:L:163:ARG:O	5:L:203:VAL:N	2.25	0.70
7:R:36:GLY:O	7:R:40:VAL:N	2.35	0.59
6:P:298:ALA:O	6:P:300:HIS:N	2.38	0.57
6:M:144:LEU:O	6:M:148:LYS:N	2.41	0.52
11:W:279:ASN:O	11:W:283:GLN:N	2.86	0.50

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	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	B	368/376 (98%)	359 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	373/376 (99%)	362 (97%)	11 (3%)	0	100	100
1	D	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	E	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	F	368/376 (98%)	358 (97%)	10 (3%)	0	100	100
1	G	367/376 (98%)	356 (97%)	11 (3%)	0	100	100
1	I	368/376 (98%)	354 (96%)	14 (4%)	0	100	100
2	H	370/375 (99%)	364 (98%)	6 (2%)	0	100	100
3	J	377/417 (90%)	361 (96%)	16 (4%)	0	100	100
4	K	276/286 (96%)	264 (96%)	12 (4%)	0	100	100
5	L	267/272 (98%)	260 (97%)	7 (3%)	0	100	100
6	M	330/405 (82%)	298 (90%)	30 (9%)	2 (1%)	25	66
6	N	270/405 (67%)	258 (96%)	10 (4%)	2 (1%)	22	63
6	P	335/405 (83%)	305 (91%)	28 (8%)	2 (1%)	25	66
6	Q	319/405 (79%)	302 (95%)	17 (5%)	0	100	100
7	O	168/186 (90%)	154 (92%)	13 (8%)	1 (1%)	25	66
7	R	177/186 (95%)	159 (90%)	15 (8%)	3 (2%)	9	42
8	S	147/1281 (12%)	139 (95%)	7 (5%)	1 (1%)	22	63
8	T	190/1281 (15%)	176 (93%)	13 (7%)	1 (0%)	29	69
9	U	176/190 (93%)	161 (92%)	15 (8%)	0	100	100
10	V	180/182 (99%)	175 (97%)	3 (2%)	2 (1%)	14	52
11	W	205/577 (36%)	205 (100%)	0	0	100	100
11	X	267/577 (46%)	265 (99%)	2 (1%)	0	100	100
11	w	205/577 (36%)	204 (100%)	1 (0%)	0	100	100
11	x	238/577 (41%)	238 (100%)	0	0	100	100
12	Y	373/467 (80%)	352 (94%)	21 (6%)	0	100	100
13	e	4571/4646 (98%)	4476 (98%)	94 (2%)	1 (0%)	100	100
13	f	4571/4646 (98%)	4500 (98%)	65 (1%)	6 (0%)	51	86
13	m	4552/4646 (98%)	4458 (98%)	92 (2%)	2 (0%)	100	100
13	n	4556/4646 (98%)	4464 (98%)	91 (2%)	1 (0%)	100	100
14	g	390/638 (61%)	384 (98%)	6 (2%)	0	100	100
14	h	392/638 (61%)	383 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	o	390/638 (61%)	382 (98%)	8 (2%)	0	100	100
14	p	397/638 (62%)	391 (98%)	6 (2%)	0	100	100
15	i	295/492 (60%)	281 (95%)	13 (4%)	1 (0%)	41	77
15	j	324/492 (66%)	318 (98%)	6 (2%)	0	100	100
15	q	319/492 (65%)	310 (97%)	9 (3%)	0	100	100
15	r	295/492 (60%)	281 (95%)	14 (5%)	0	100	100
16	k	91/96 (95%)	79 (87%)	12 (13%)	0	100	100
16	l	91/96 (95%)	81 (89%)	9 (10%)	1 (1%)	14	52
16	s	91/96 (95%)	84 (92%)	7 (8%)	0	100	100
16	t	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
All	All	29234/35547 (82%)	28458 (97%)	750 (3%)	26 (0%)	54	86

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	217	PRO
6	P	204	PRO
7	R	24	PRO
8	S	1142	PRO
10	V	80	VAL

5.3.2 Protein sidechains (i)

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 17 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
17	ADP	f	4701	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	5 (17%)
17	ADP	C	800	18	24,29,29	0.90	1 (4%)	29,45,45	1.49	4 (13%)
17	ADP	e	4701	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)
21	ANP	n	4704	-	29,33,33	1.07	4 (13%)	31,52,52	1.12	2 (6%)
21	ANP	m	4705	-	29,33,33	1.07	4 (13%)	31,52,52	1.16	2 (6%)
17	ADP	n	4701	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)
17	ADP	G	800	18	24,29,29	0.74	0	29,45,45	0.83	1 (3%)
19	ATP	e	4702	18	26,33,33	0.64	0	31,52,52	1.09	1 (3%)
21	ANP	f	4705	-	29,33,33	1.06	3 (10%)	31,52,52	1.12	2 (6%)
17	ADP	F	802	18	24,29,29	0.74	0	29,45,45	0.83	1 (3%)
17	ADP	E	800	18	24,29,29	0.91	1 (4%)	29,45,45	1.47	4 (13%)
17	ADP	m	4701	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	5 (17%)
17	ADP	A	800	18	24,29,29	0.91	1 (4%)	29,45,45	1.51	4 (13%)
17	ADP	H	800	18	24,29,29	0.72	0	29,45,45	0.84	1 (3%)
21	ANP	f	4703	-	29,33,33	0.96	2 (6%)	31,52,52	1.25	4 (12%)
19	ATP	f	4702	18	26,33,33	0.85	0	31,52,52	1.01	2 (6%)
21	ANP	e	4705	-	29,33,33	1.07	4 (13%)	31,52,52	1.16	2 (6%)
19	ATP	J	800	18	26,33,33	0.73	0	31,52,52	0.86	2 (6%)
17	ADP	B	800	18	24,29,29	0.90	1 (4%)	29,45,45	1.51	4 (13%)
19	ATP	m	4702	18	26,33,33	0.65	0	31,52,52	1.09	1 (3%)
21	ANP	n	4705	-	29,33,33	1.07	4 (13%)	31,52,52	1.17	2 (6%)
21	ANP	m	4704	-	29,33,33	1.07	4 (13%)	31,52,52	1.12	2 (6%)
21	ANP	e	4704	-	29,33,33	1.06	4 (13%)	31,52,52	1.12	2 (6%)
17	ADP	I	800	18	24,29,29	0.71	0	29,45,45	0.88	2 (6%)
17	ADP	D	800	18	24,29,29	0.91	1 (4%)	29,45,45	1.51	4 (13%)
19	ATP	n	4702	18	26,33,33	0.64	0	31,52,52	1.09	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
17	ADP	f	4701	-	-	6/12/32/32	0/3/3/3
17	ADP	C	800	18	-	3/12/32/32	0/3/3/3
17	ADP	e	4701	-	-	6/12/32/32	0/3/3/3
21	ANP	n	4704	-	-	7/14/38/38	0/3/3/3
21	ANP	m	4705	-	-	5/14/38/38	0/3/3/3
17	ADP	n	4701	-	-	6/12/32/32	0/3/3/3
17	ADP	G	800	18	-	0/12/32/32	0/3/3/3
19	ATP	e	4702	18	-	2/18/38/38	0/3/3/3
21	ANP	f	4705	-	-	7/14/38/38	0/3/3/3
17	ADP	F	802	18	-	0/12/32/32	0/3/3/3
17	ADP	E	800	18	-	3/12/32/32	0/3/3/3
17	ADP	m	4701	-	-	6/12/32/32	0/3/3/3
17	ADP	A	800	18	-	0/12/32/32	0/3/3/3
17	ADP	H	800	18	-	0/12/32/32	0/3/3/3
21	ANP	f	4703	-	-	5/14/38/38	0/3/3/3
19	ATP	f	4702	18	-	2/18/38/38	0/3/3/3
21	ANP	e	4705	-	-	5/14/38/38	0/3/3/3
19	ATP	J	800	18	-	2/18/38/38	0/3/3/3
17	ADP	B	800	18	-	0/12/32/32	0/3/3/3
19	ATP	m	4702	18	-	2/18/38/38	0/3/3/3
21	ANP	n	4705	-	-	5/14/38/38	0/3/3/3
21	ANP	m	4704	-	-	7/14/38/38	0/3/3/3
21	ANP	e	4704	-	-	7/14/38/38	0/3/3/3
17	ADP	I	800	18	-	0/12/32/32	0/3/3/3
17	ADP	D	800	18	-	3/12/32/32	0/3/3/3
19	ATP	n	4702	18	-	2/18/38/38	0/3/3/3

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	f	4703	ANP	PG-O1G	2.60	1.50	1.46
21	n	4704	ANP	PB-O3A	-2.57	1.55	1.59
21	m	4704	ANP	PB-O3A	-2.56	1.55	1.59
21	e	4704	ANP	PB-O3A	-2.56	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	f	4705	ANP	PB-O3A	-2.53	1.55	1.59

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	n	4705	ANP	PB-O3A-PA	-4.02	118.47	132.62
21	m	4705	ANP	PB-O3A-PA	-4.00	118.52	132.62
21	e	4705	ANP	PB-O3A-PA	-3.99	118.55	132.62
21	f	4703	ANP	PB-O3A-PA	-3.93	118.78	132.62
17	n	4701	ADP	N3-C2-N1	-3.66	122.95	128.68

There are no chirality outliers.

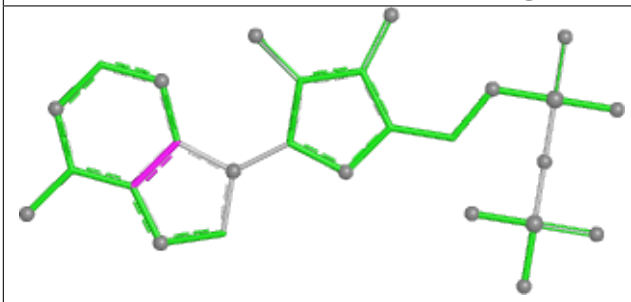
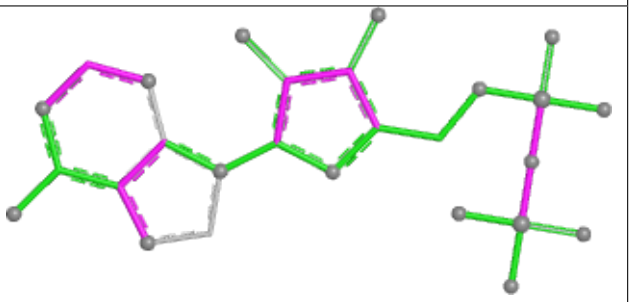
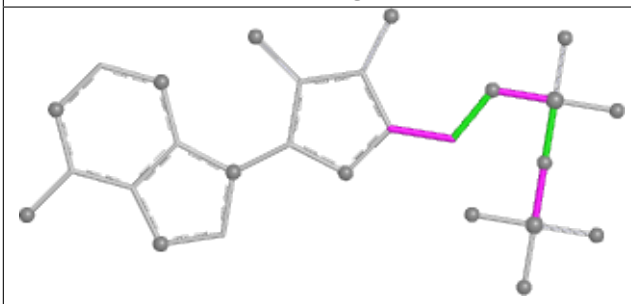
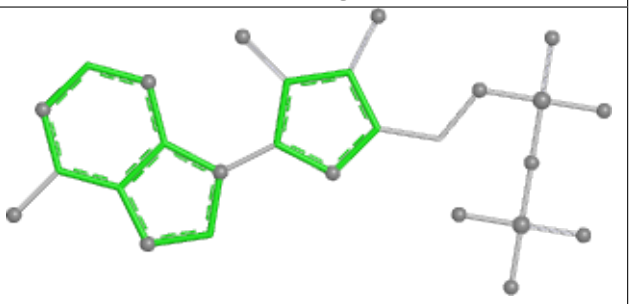
5 of 91 torsion outliers are listed below:

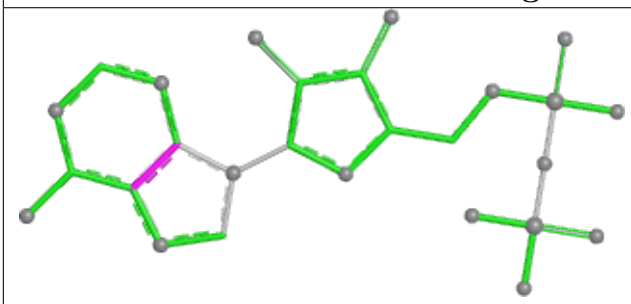
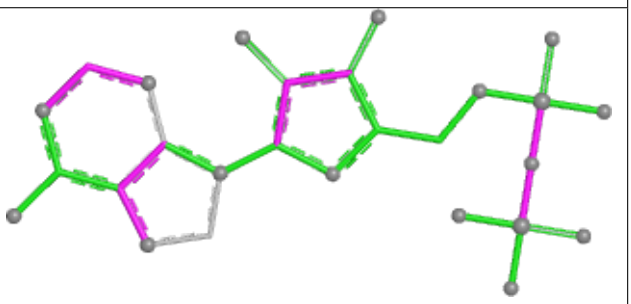
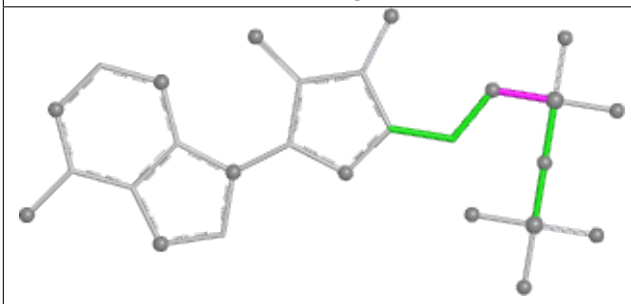
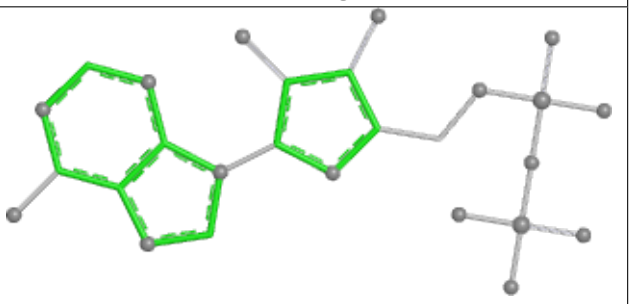
Mol	Chain	Res	Type	Atoms
17	C	800	ADP	C5'-O5'-PA-O1A
17	D	800	ADP	C5'-O5'-PA-O1A
17	E	800	ADP	C5'-O5'-PA-O1A
17	E	800	ADP	C5'-O5'-PA-O2A
17	e	4701	ADP	PA-O3A-PB-O2B

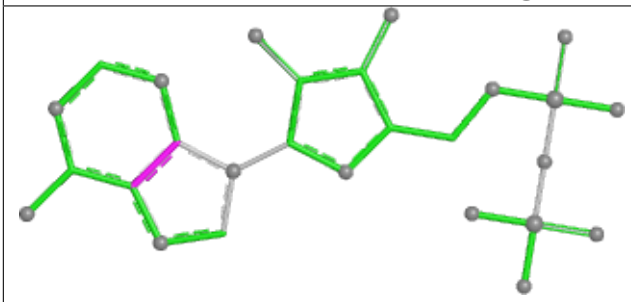
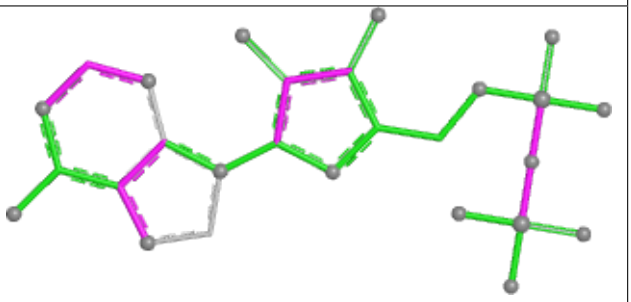
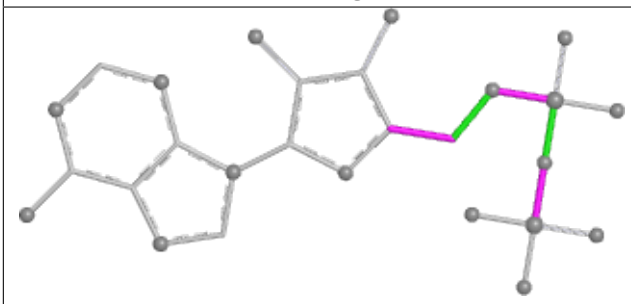
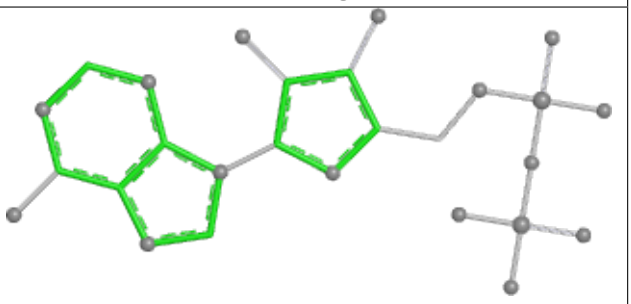
There are no ring outliers.

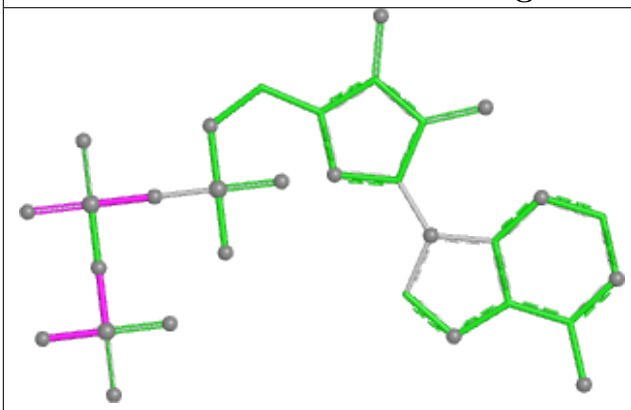
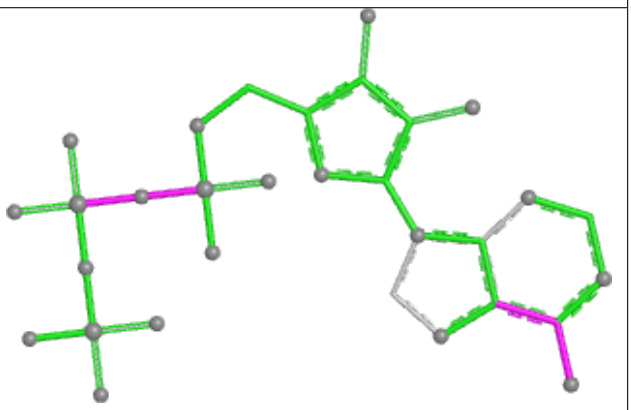
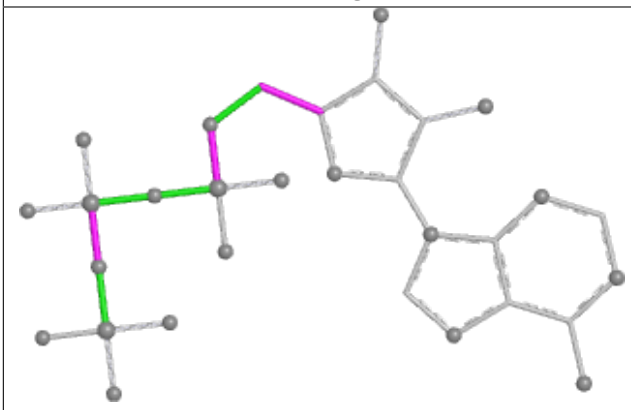
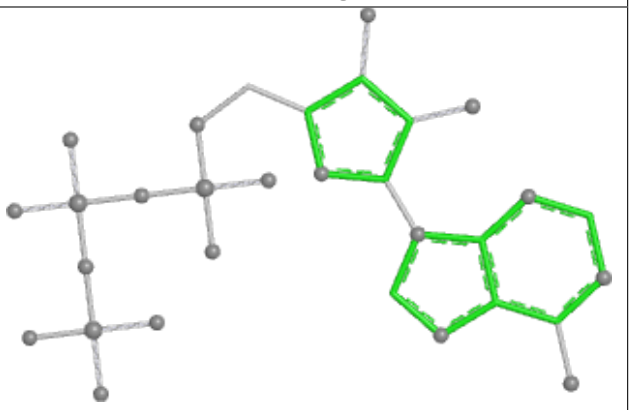
No monomer is involved in short contacts.

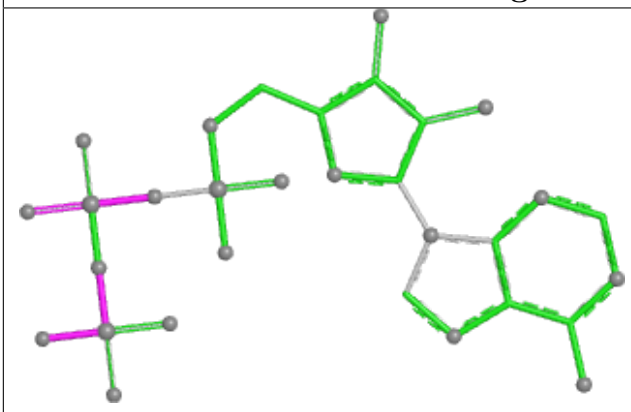
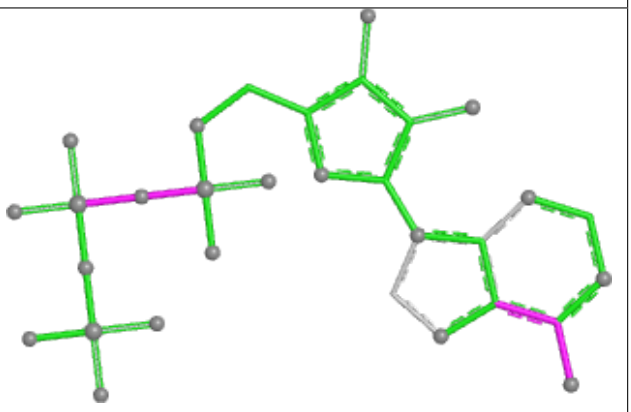
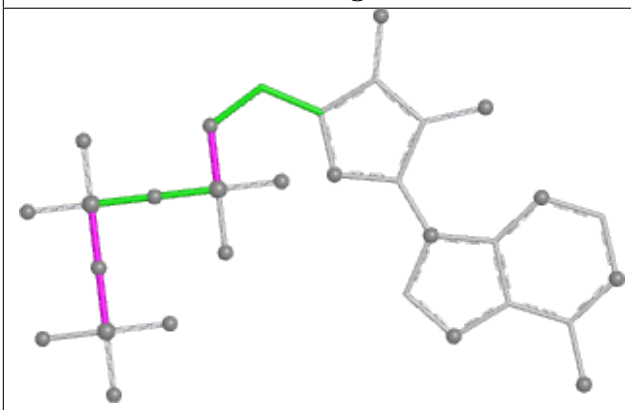
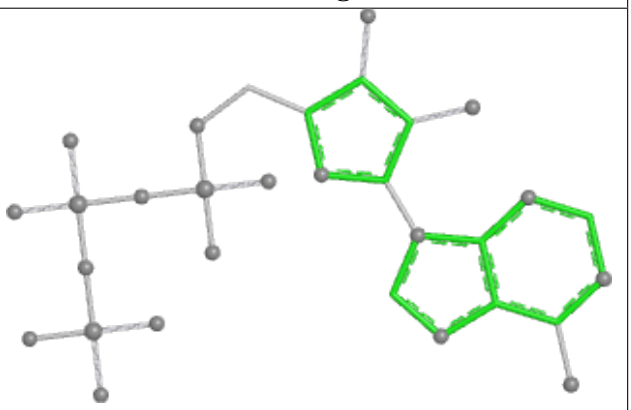
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

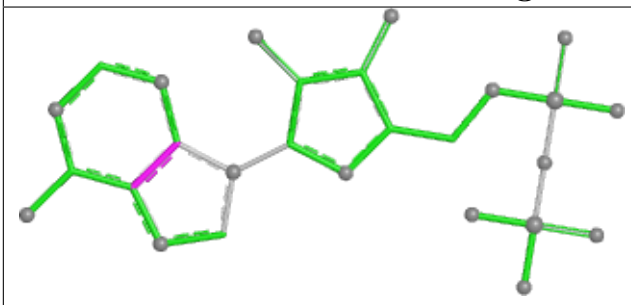
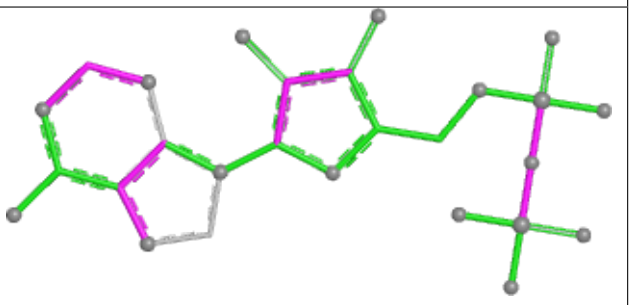
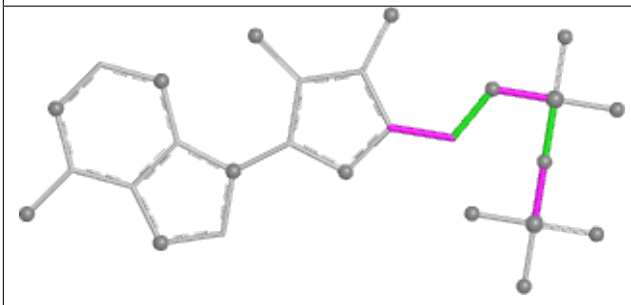
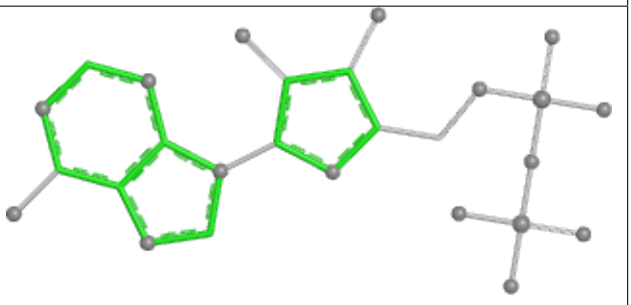
Ligand ADP f 4701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

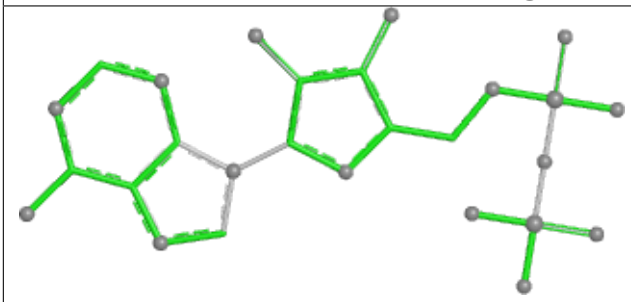
Ligand ADP e 4701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP n 4704	
 Bond lengths	 Bond angles
 Torsions	 Rings

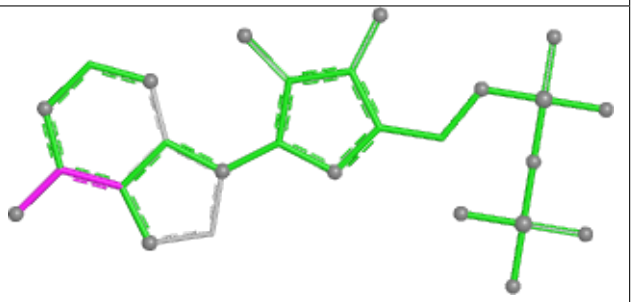
Ligand ANP m 4705	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP n 4701	
 Bond lengths	 Bond angles
 Torsions	 Rings

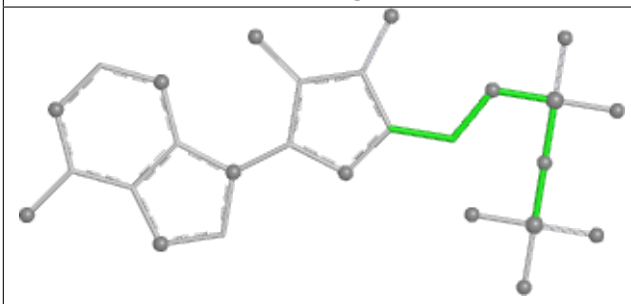
Ligand ADP G 800



Bond lengths



Bond angles



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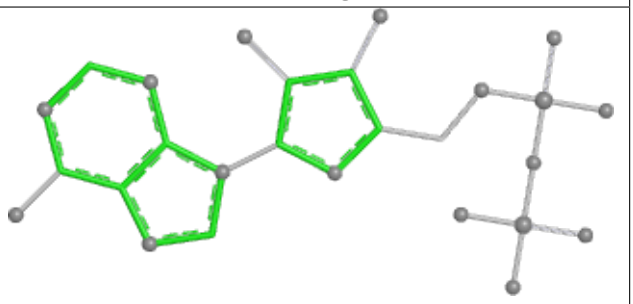
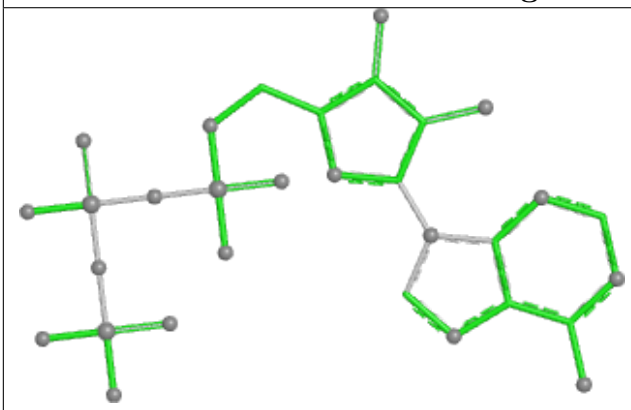


Rings

Ligand ATP e 4702



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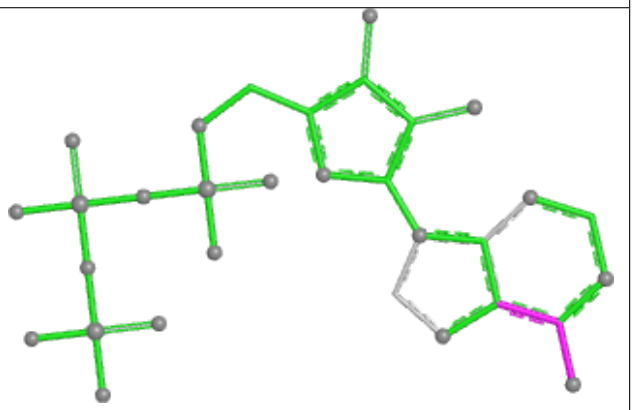
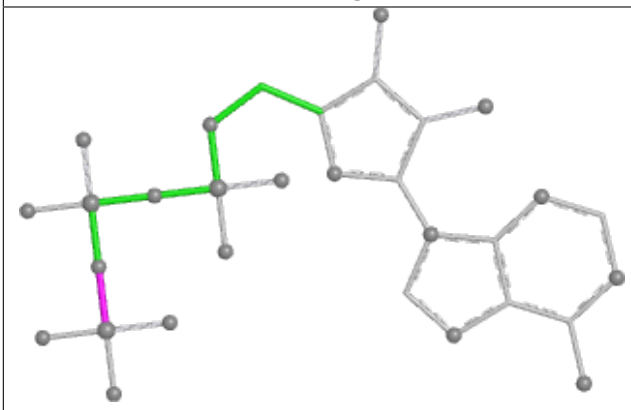
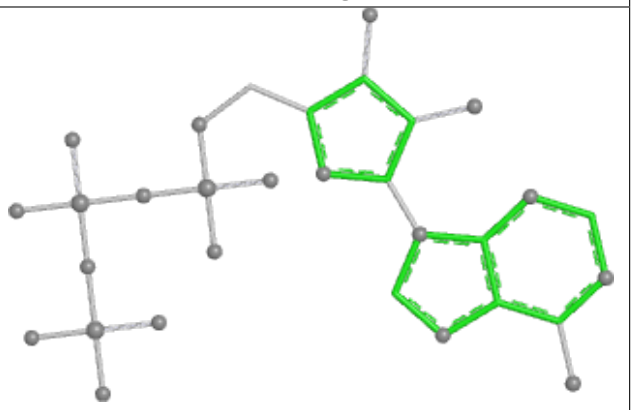


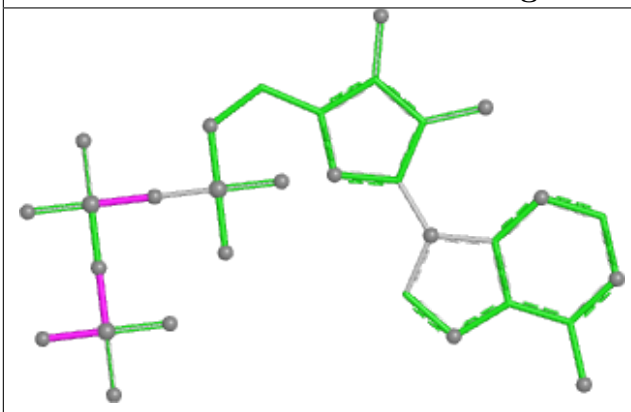
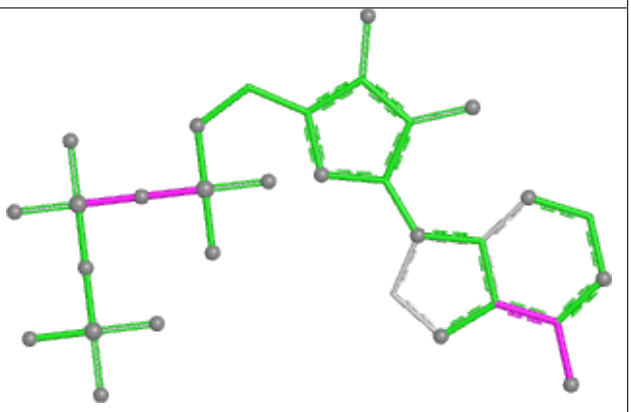
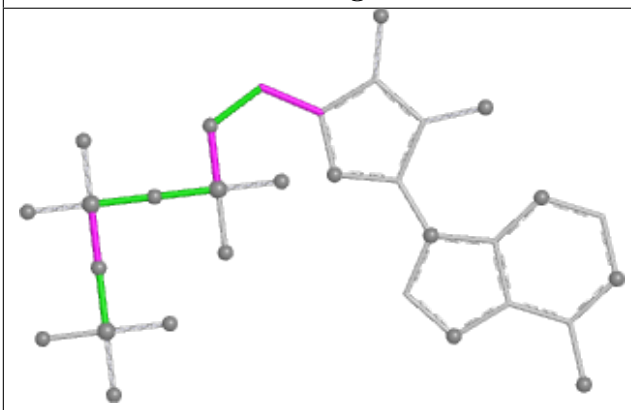
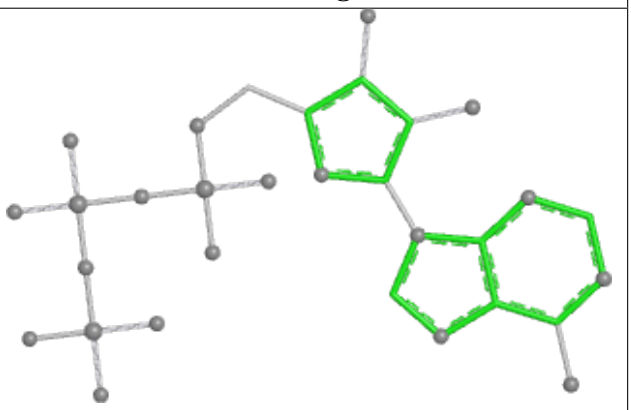
Bond angles

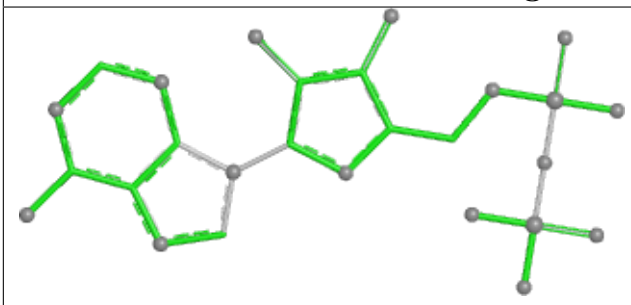
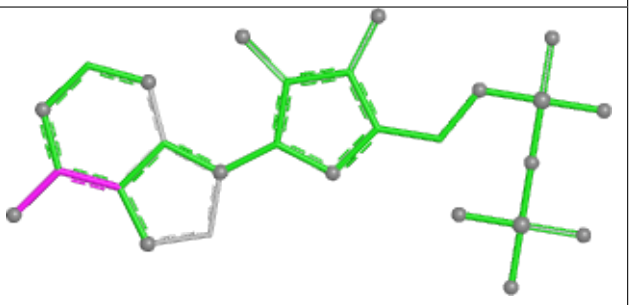
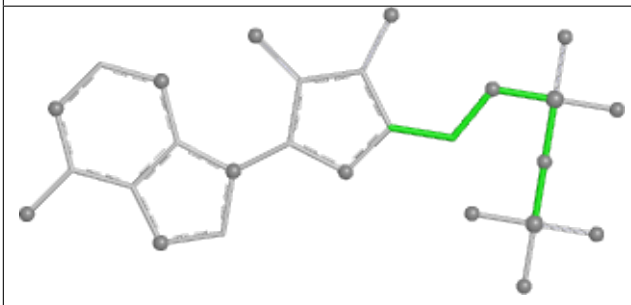
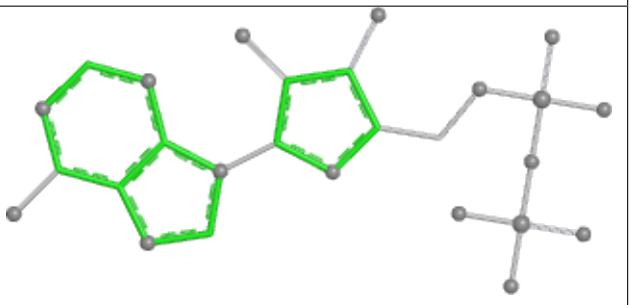


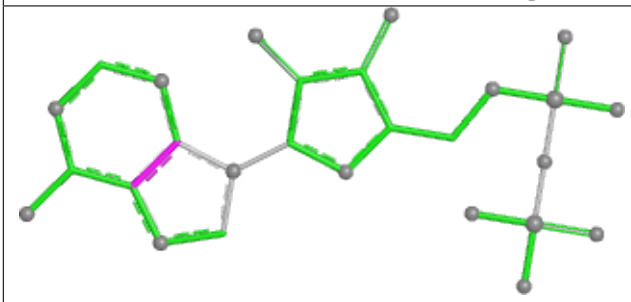
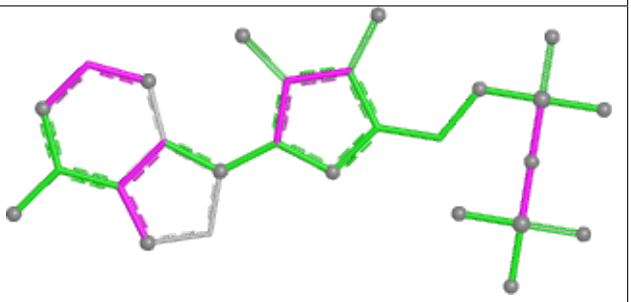
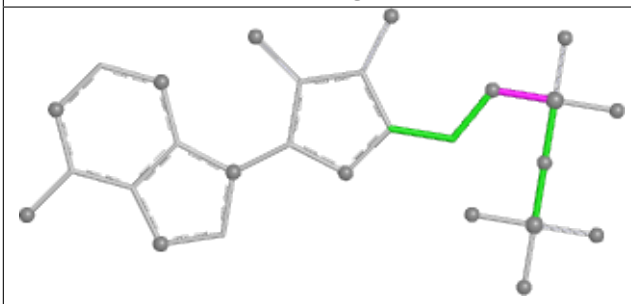
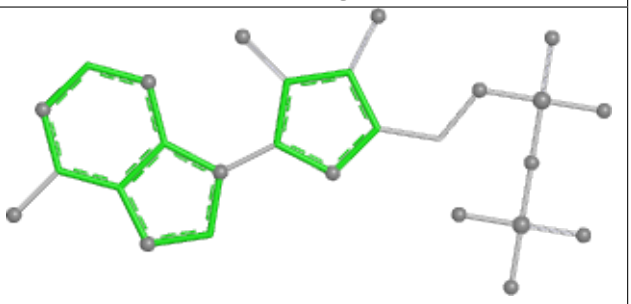
Torsions

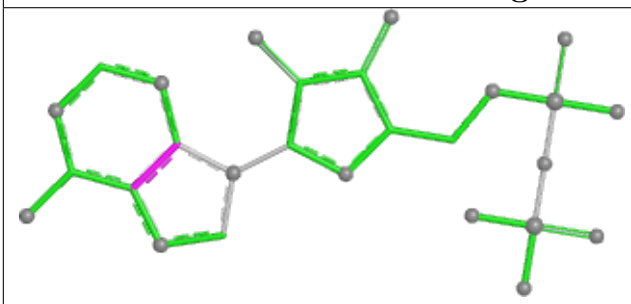
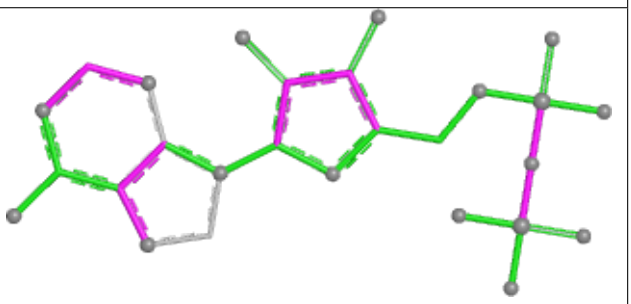
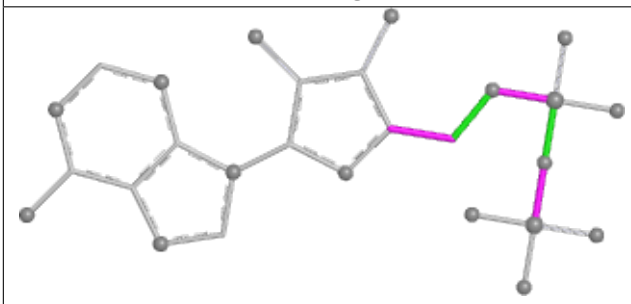
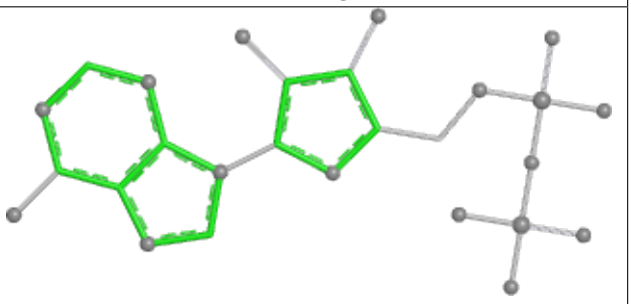


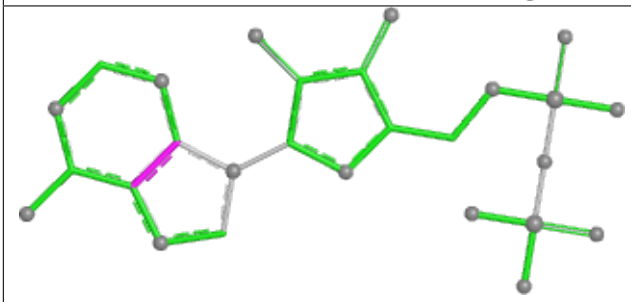
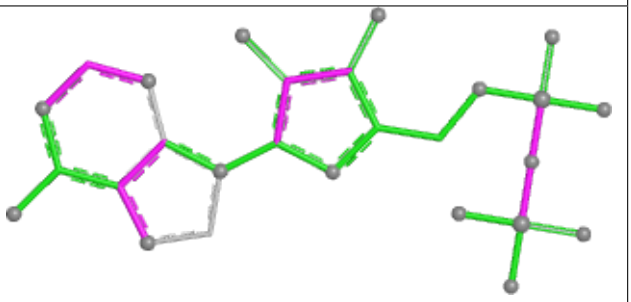
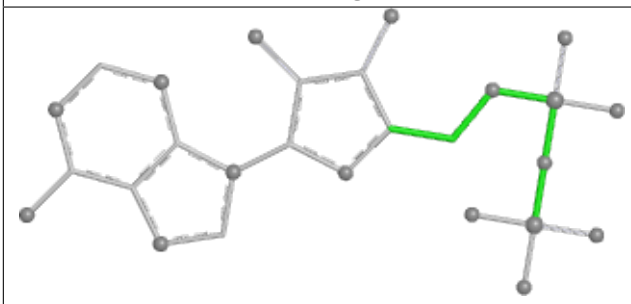
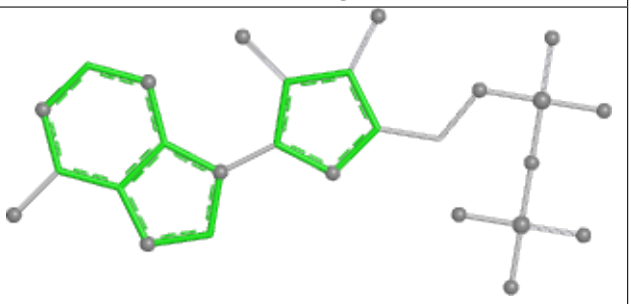
Rings

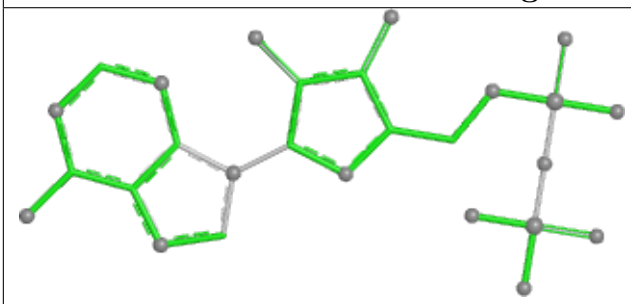
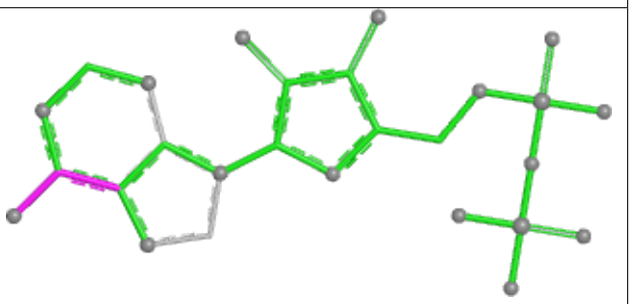
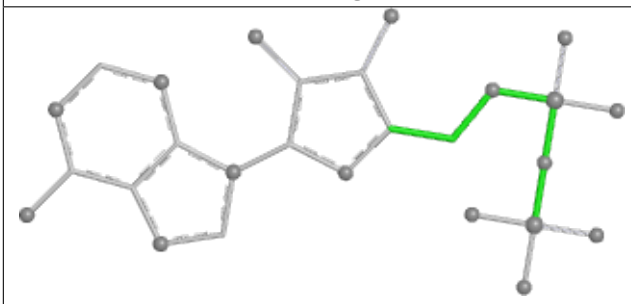
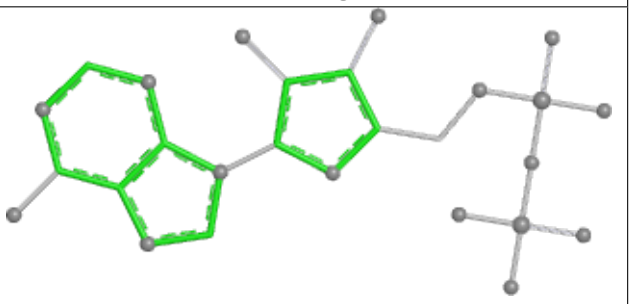
Ligand ANP f 4705	
 Bond lengths	 Bond angles
 Torsions	 Rings

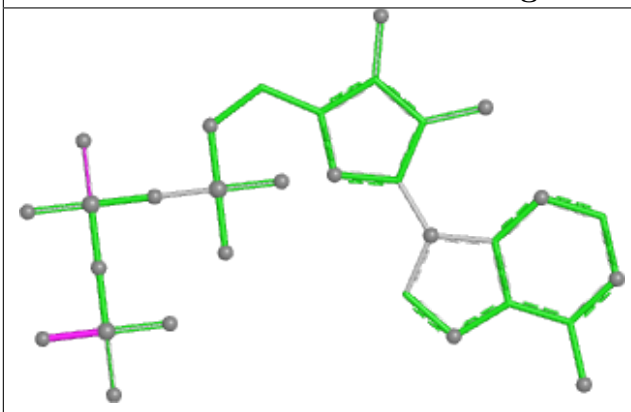
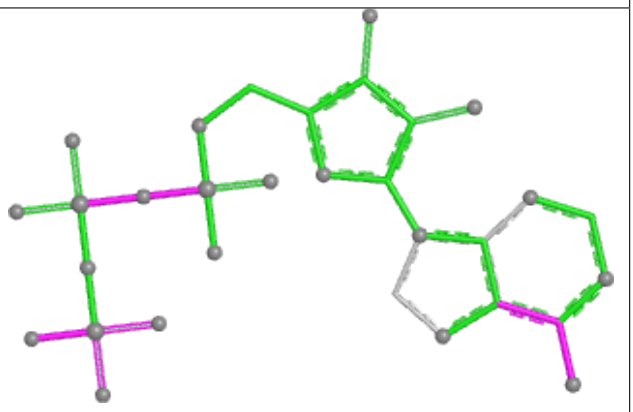
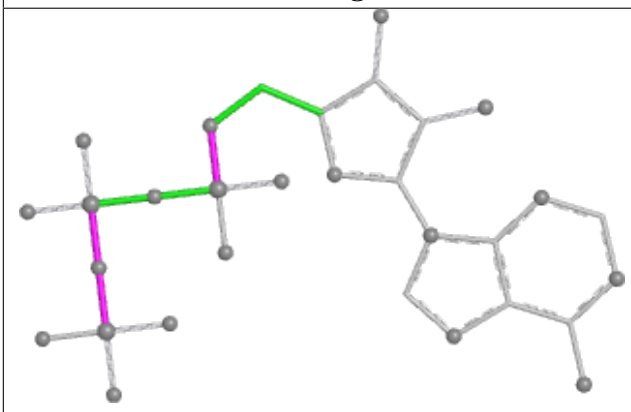
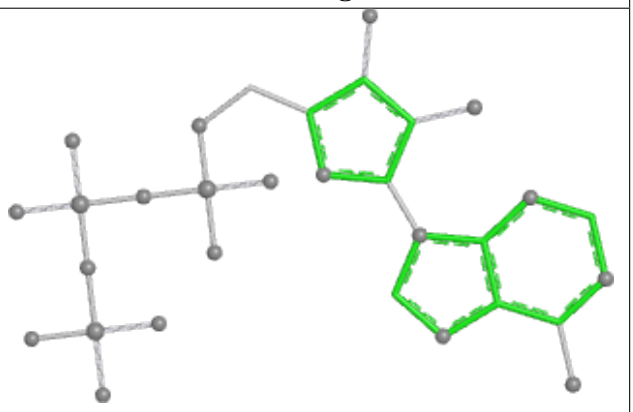
Ligand ADP F 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP m 4701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP H 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP f 4703	
 Bond lengths	 Bond angles
 Torsions	 Rings

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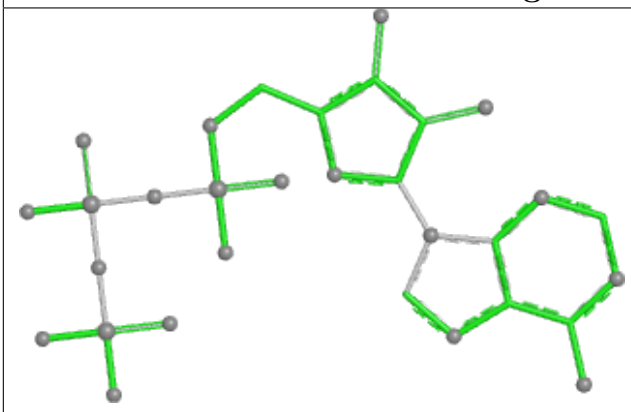
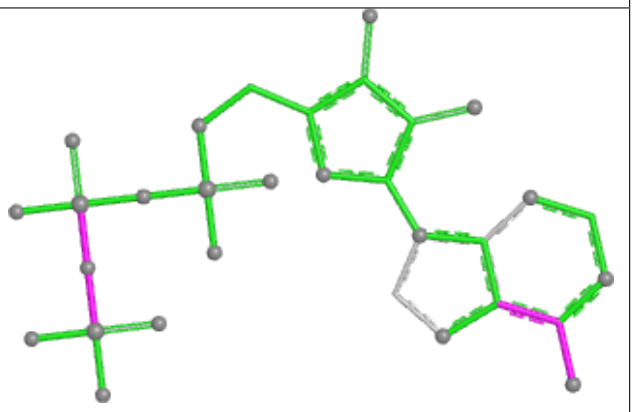
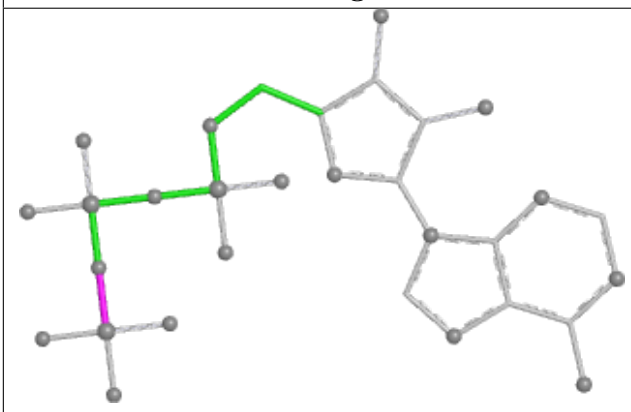
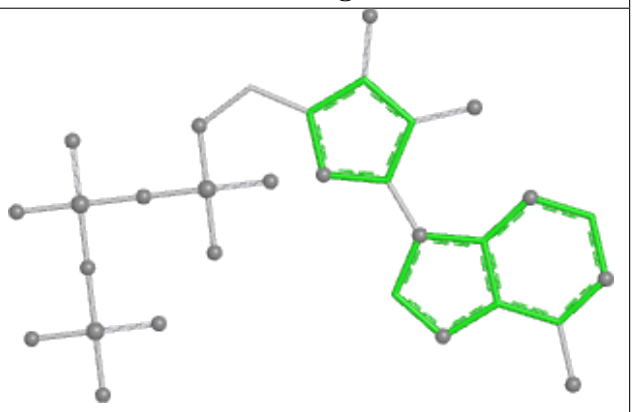
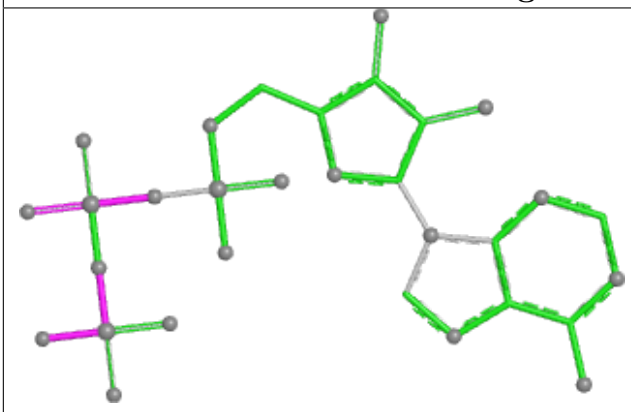
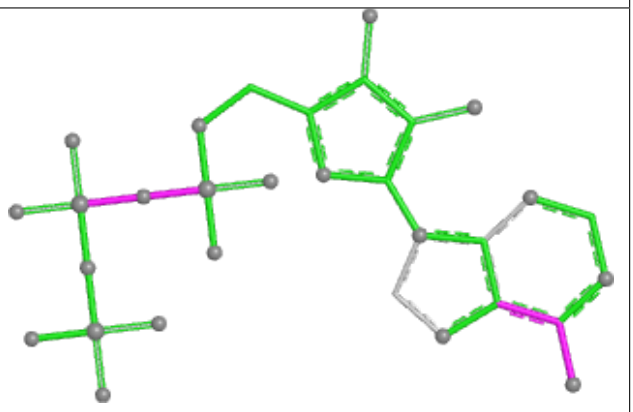
 Bond lengths	 Bond angles
 Torsions	 Rings

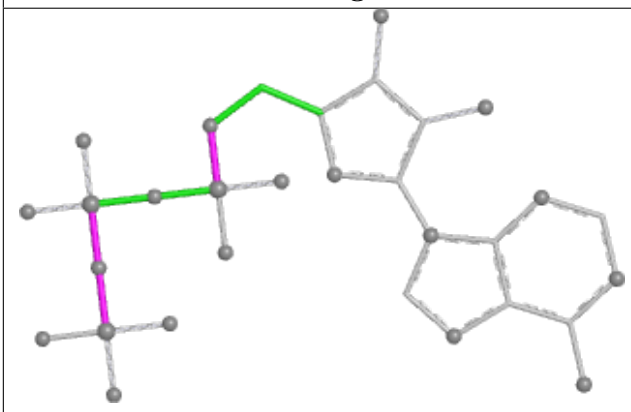
Ligand ANP e 4705



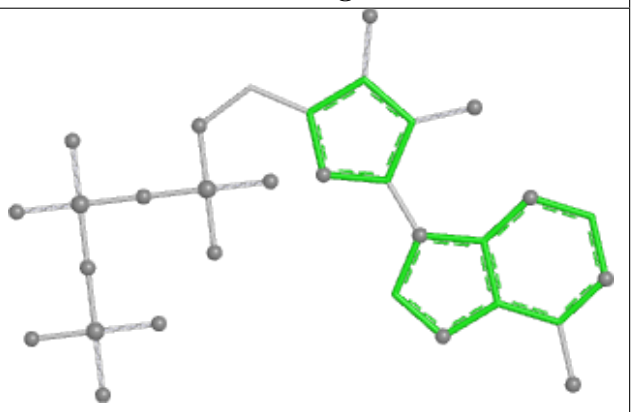
Bond lengths



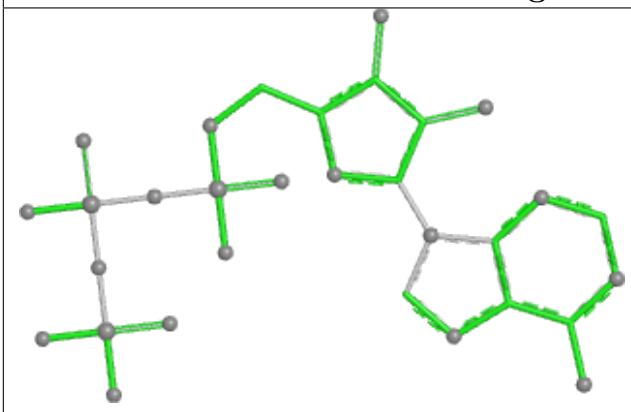
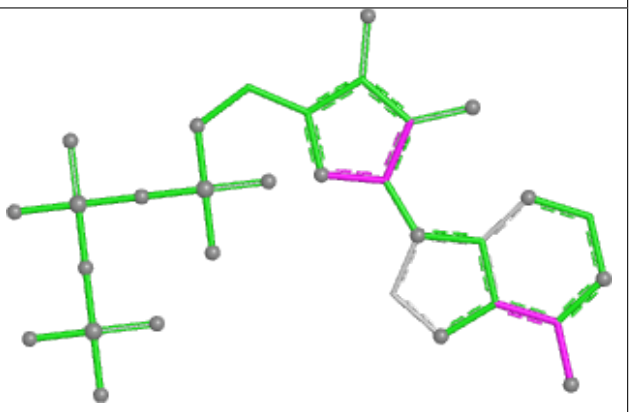
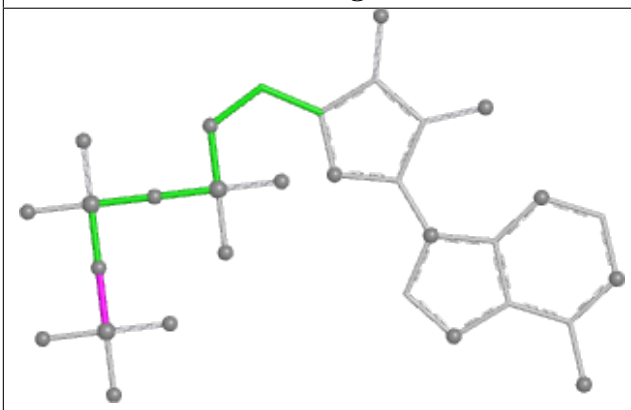
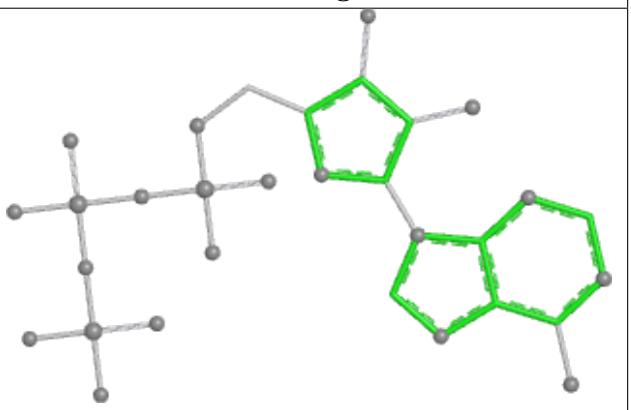
Bond angles

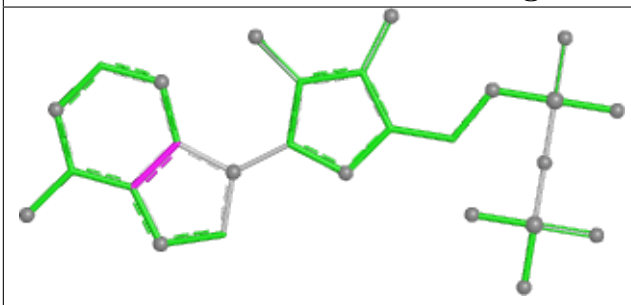
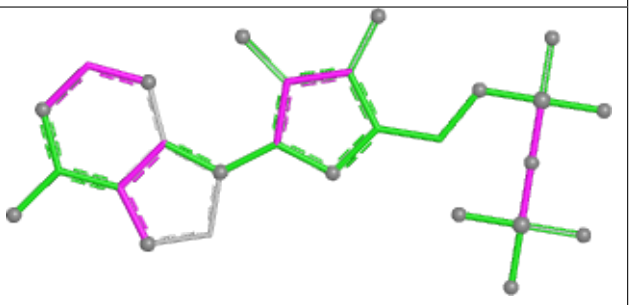
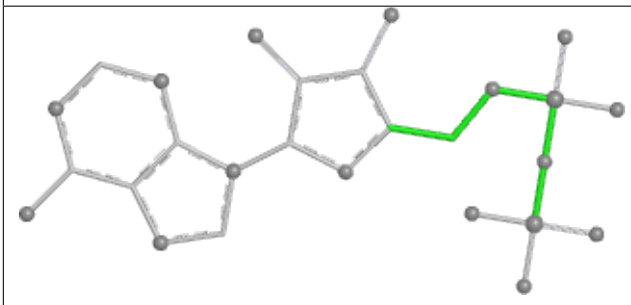
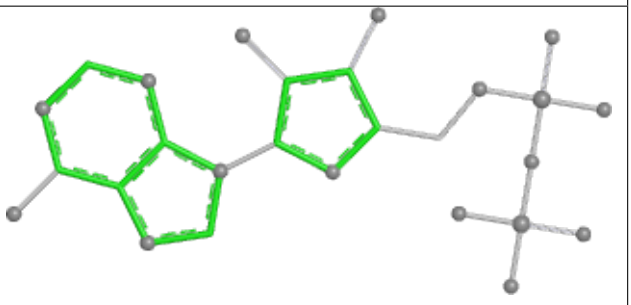


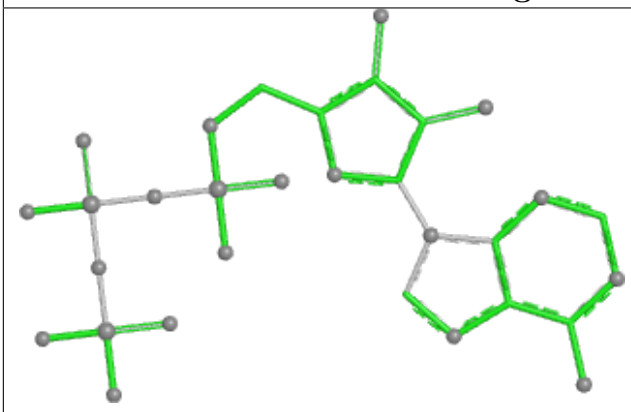
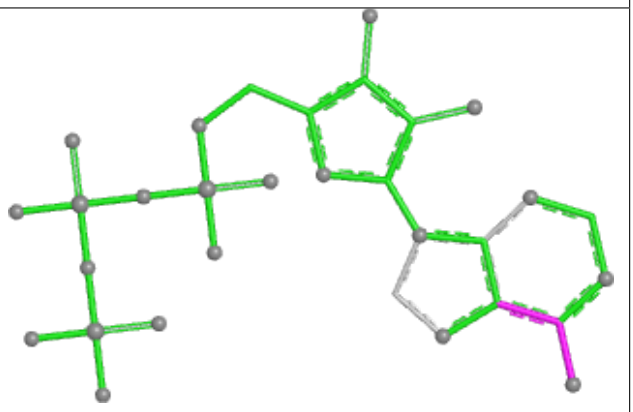
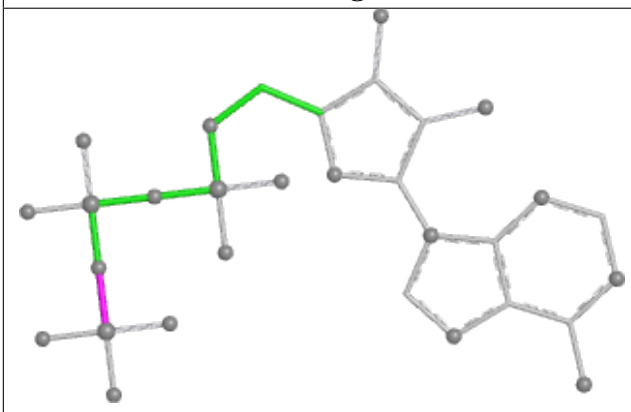
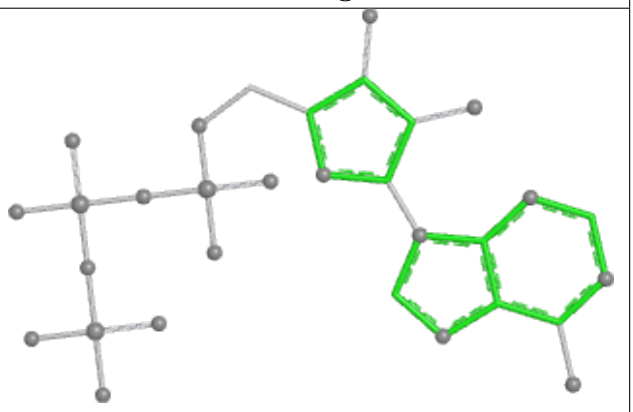
Torsions

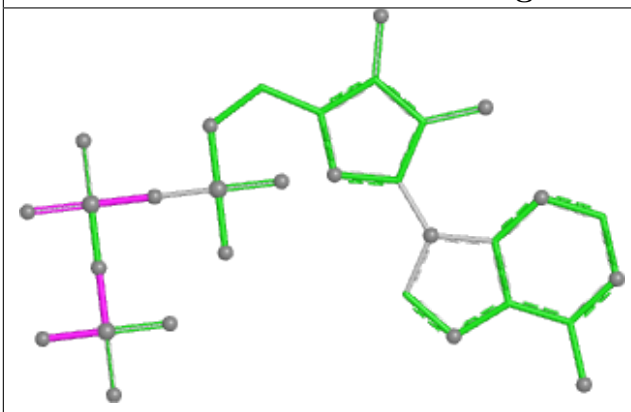
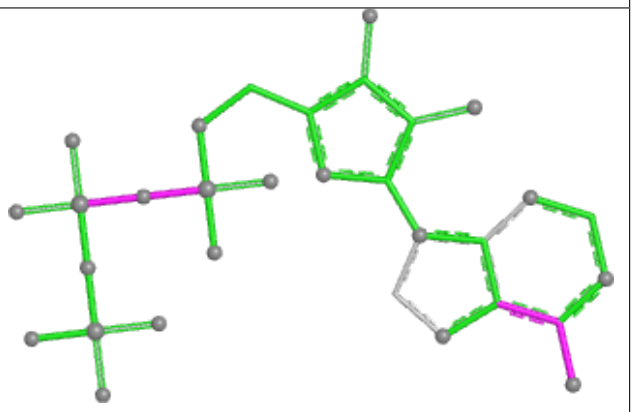
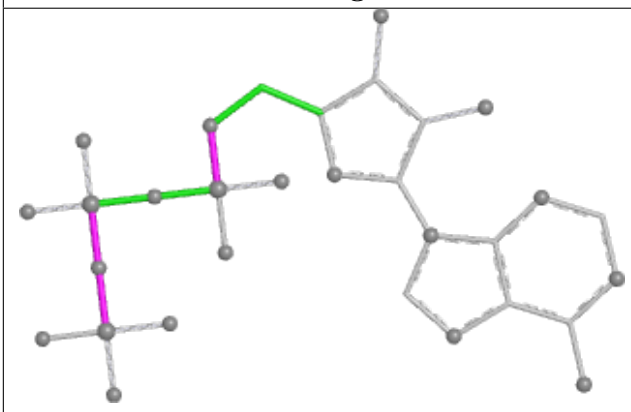
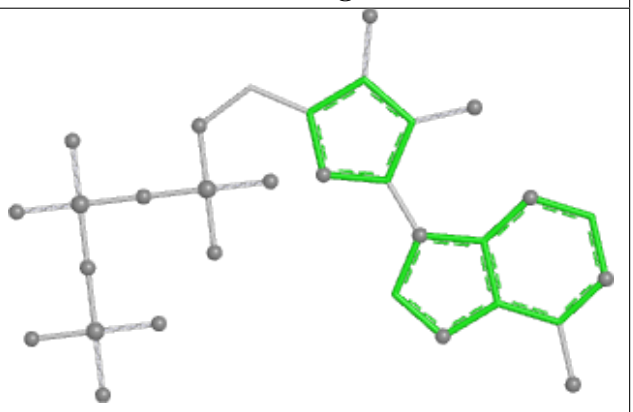


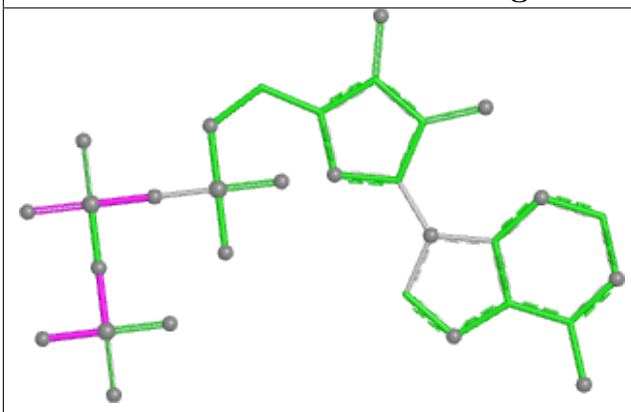
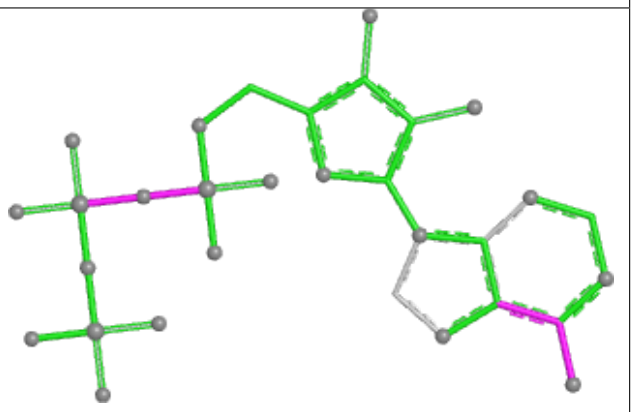
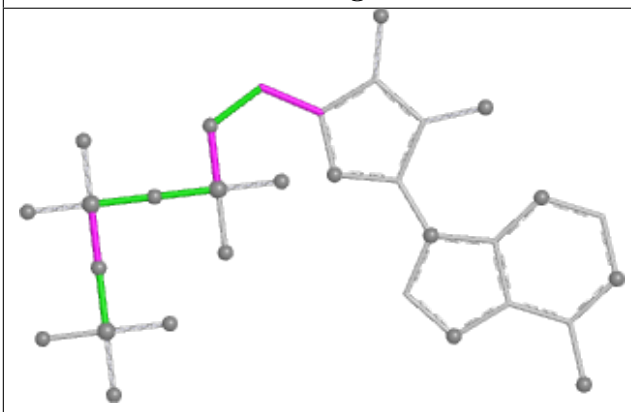
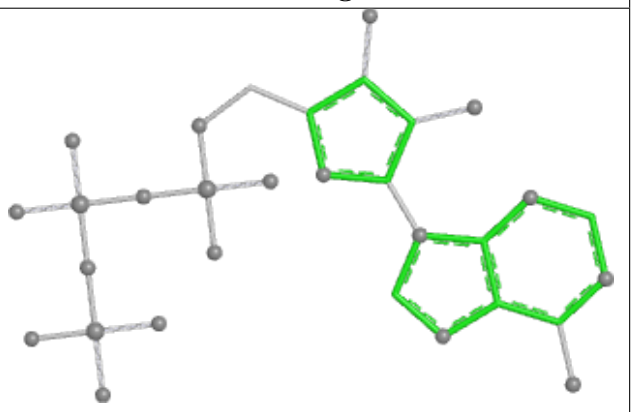
Rings

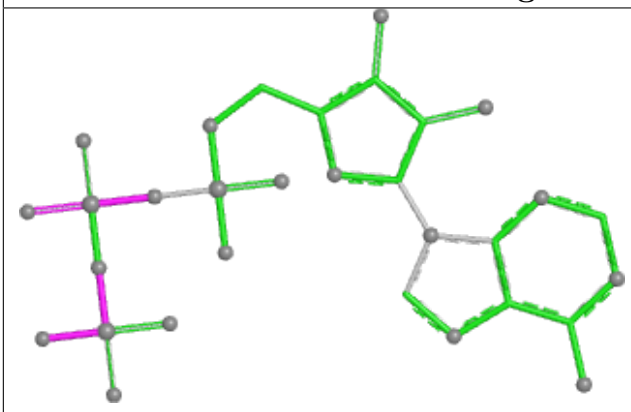
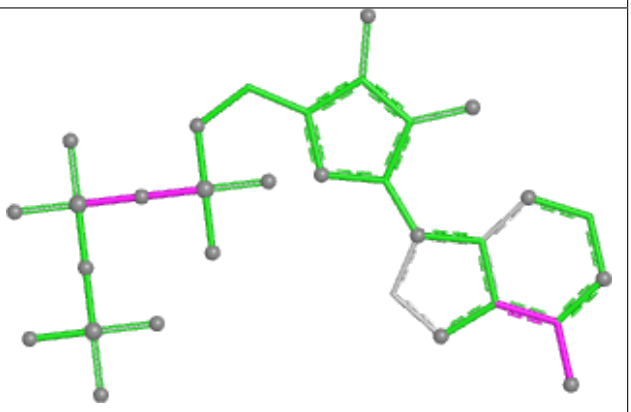
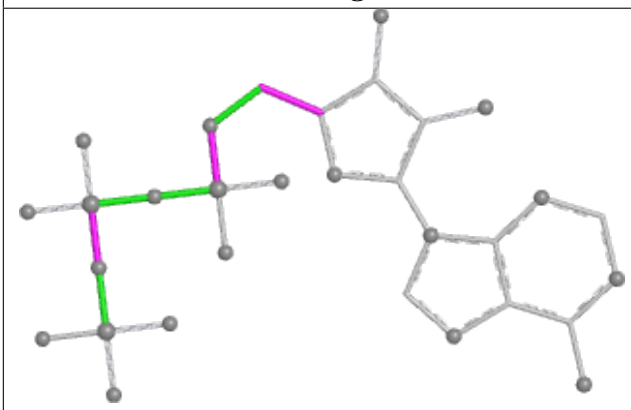
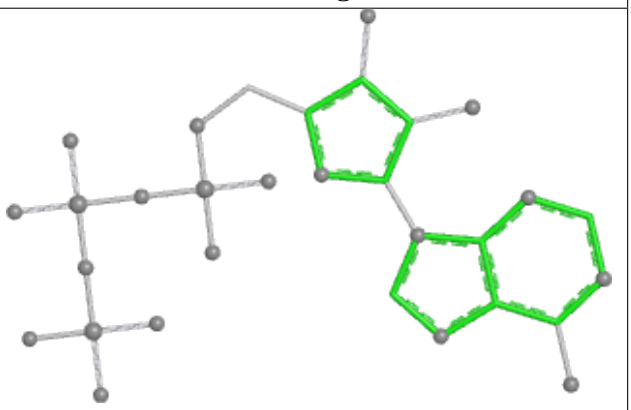
Ligand ATP J 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

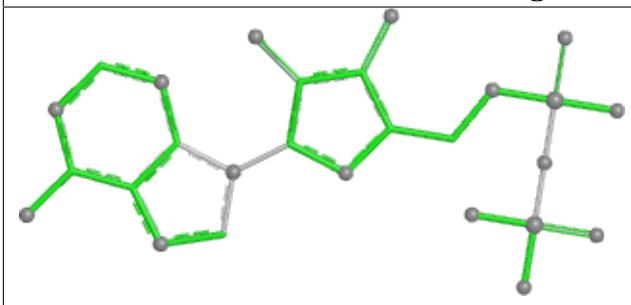
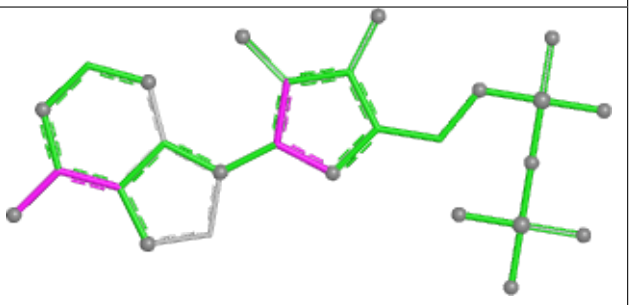
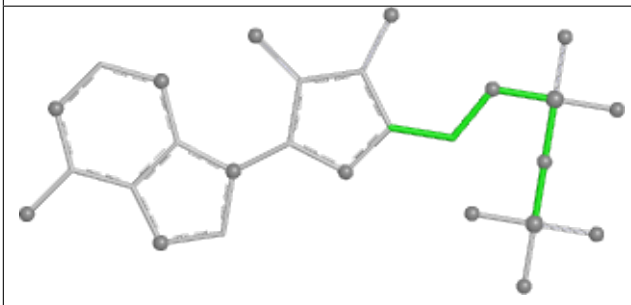
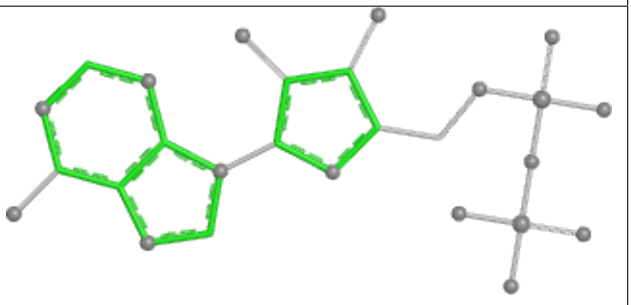
Ligand ADP B 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

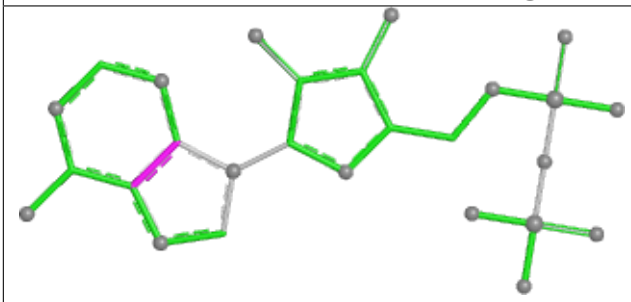
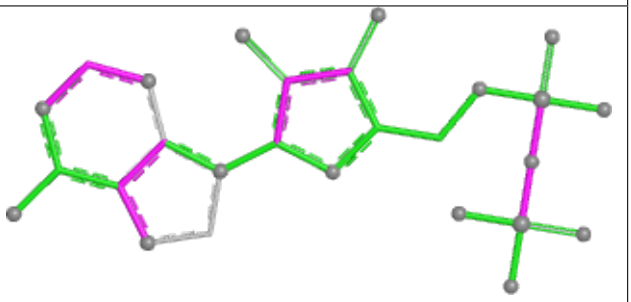
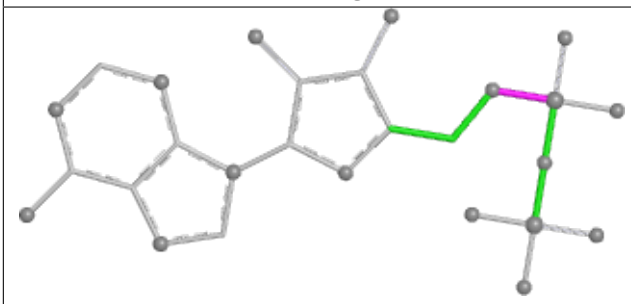
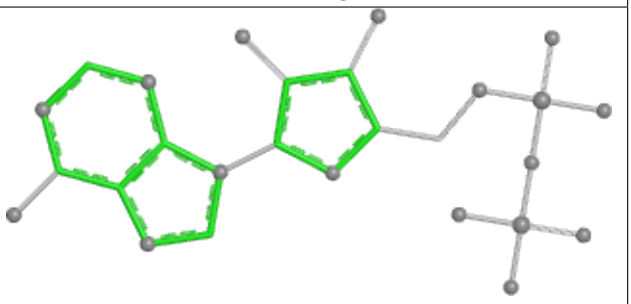
Ligand ATP m 4702	
 Bond lengths	 Bond angles
 Torsions	 Rings

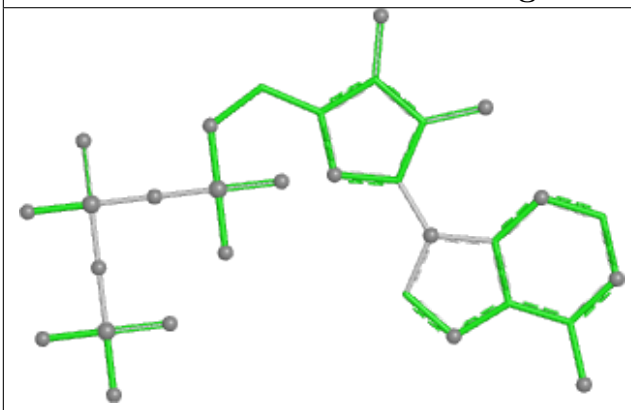
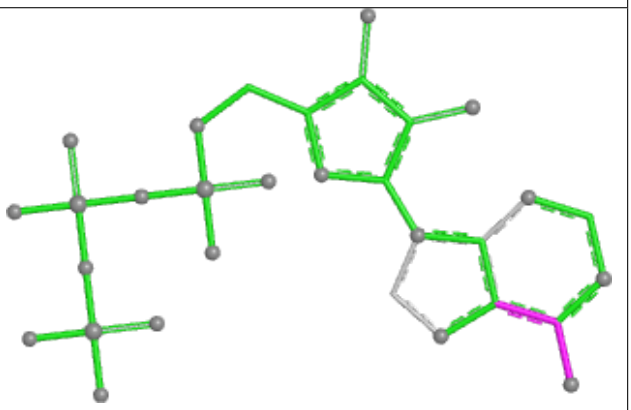
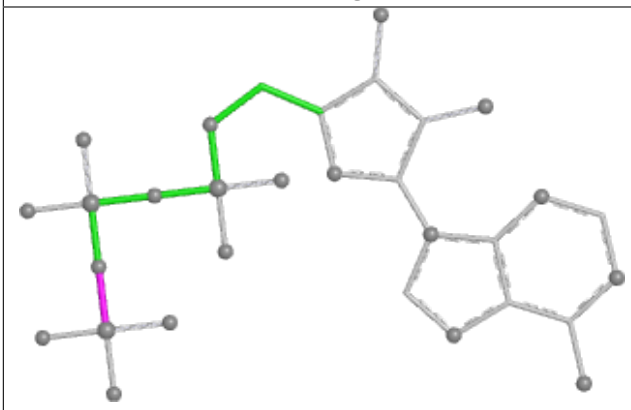
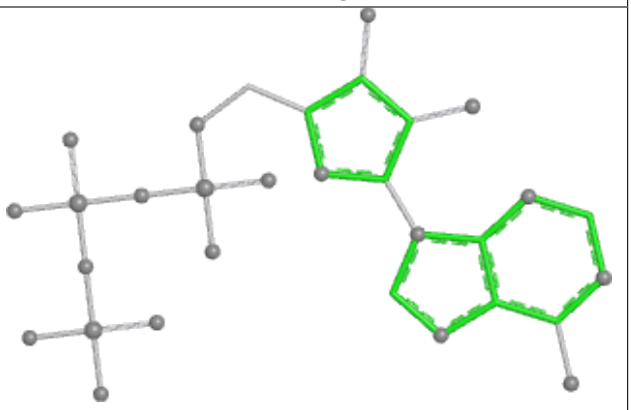
Ligand ANP n 4705	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP m 4704	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP e 4704	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP I 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP n 4702	
 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
8	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	1220:VAL	C	1252:TYR	N	34.20

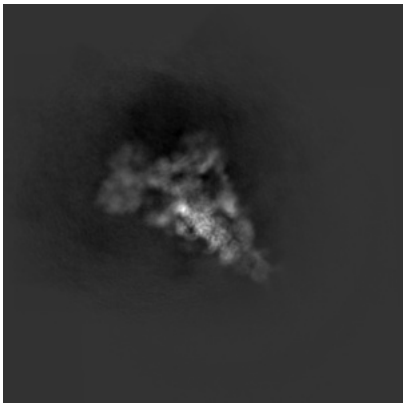
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14549. These allow visual inspection of the internal detail of the map and identification of artifacts.

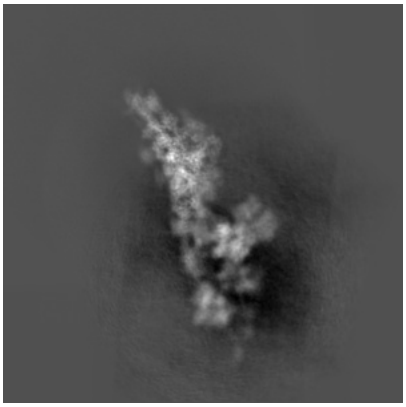
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

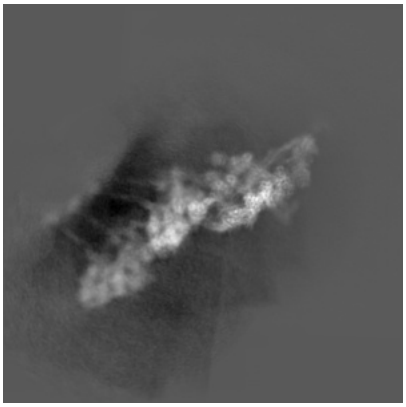
6.1.1 Primary map



X



Y

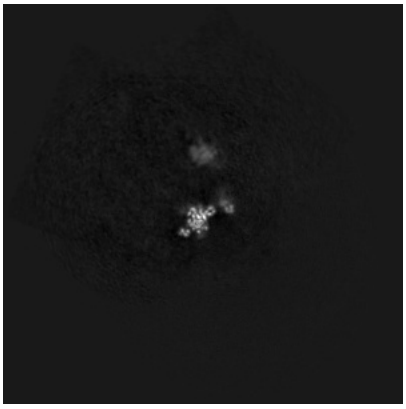


Z

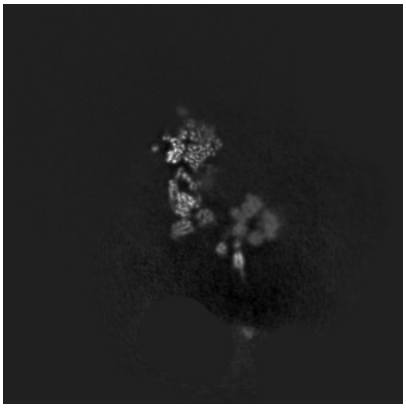
The images above show the map projected in three orthogonal directions.

6.2 Central slices

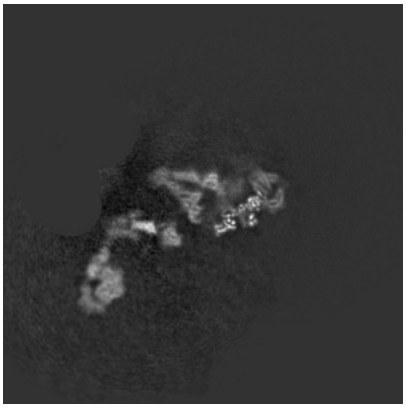
6.2.1 Primary map



X Index: 192



Y Index: 192

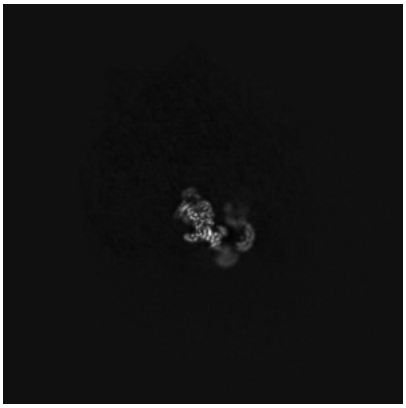


Z Index: 192

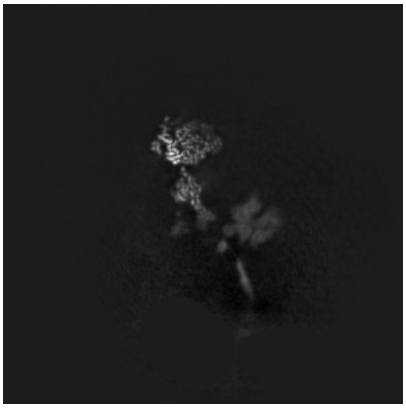
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

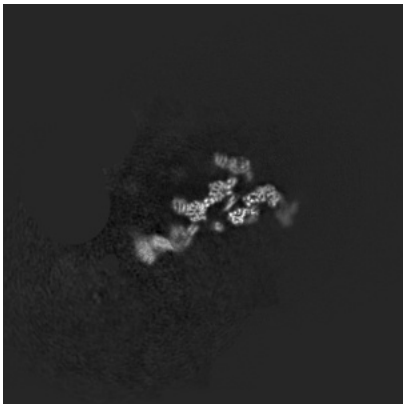
6.3.1 Primary map



X Index: 236



Y Index: 197



Z Index: 175

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0851. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

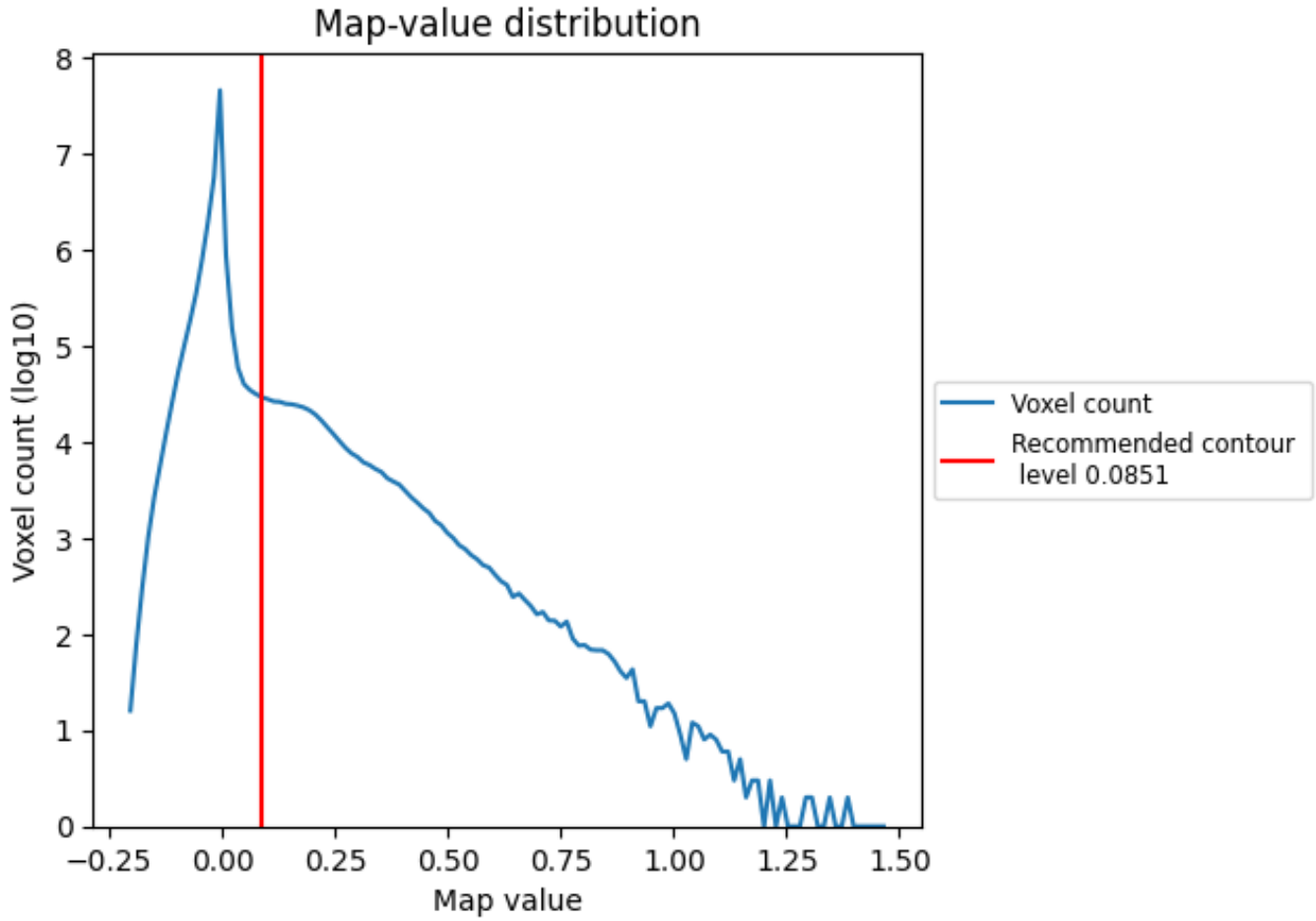
6.5 Mask visualisation (i)

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

7 Map analysis

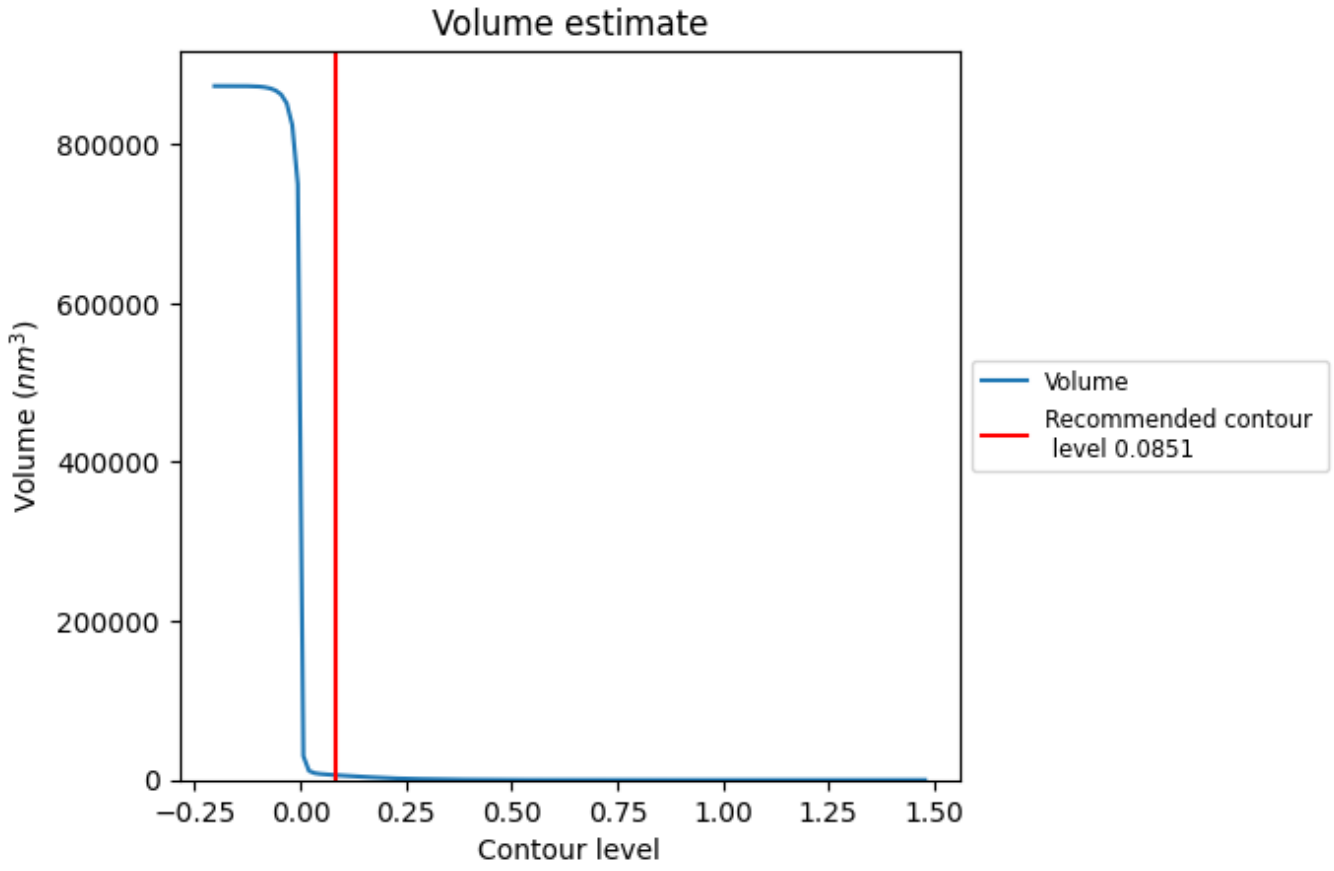
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

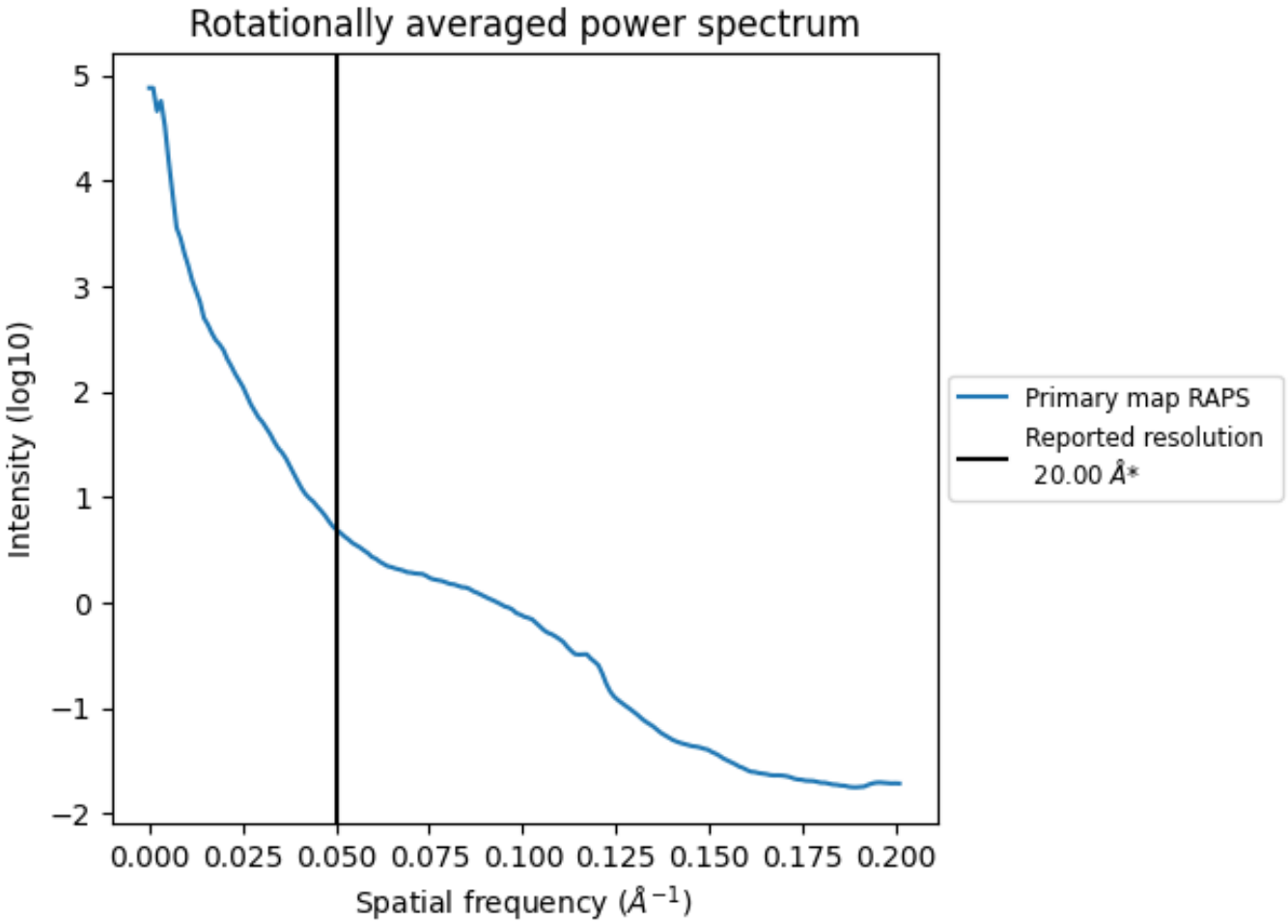
7.2 Volume estimate



The volume at the recommended contour level is 5991 nm^3; this corresponds to an approximate mass of 5412 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.050 Å^{-1}

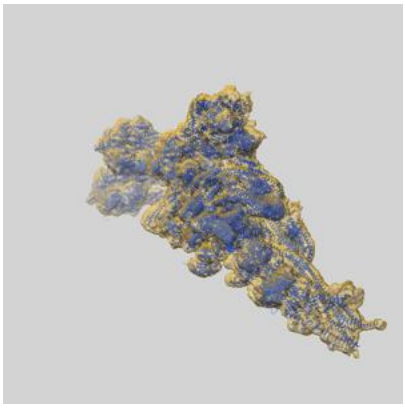
8 Fourier-Shell correlation (i)

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

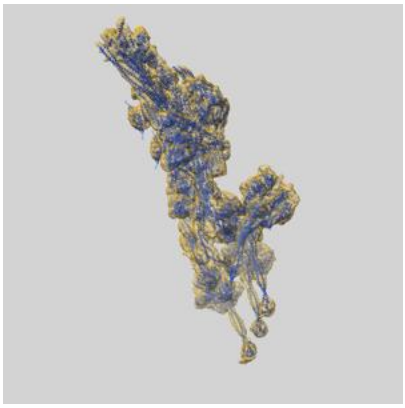
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14549 and PDB model 7Z8F. Per-residue inclusion information can be found in section 3 on page 13.

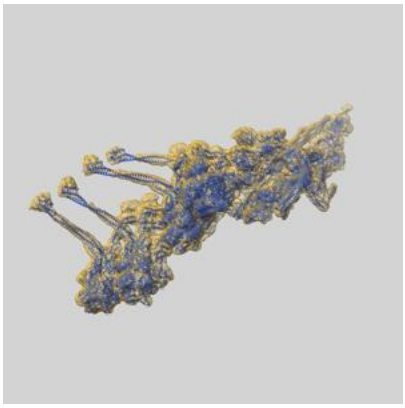
9.1 Map-model overlay



X



Y



Z

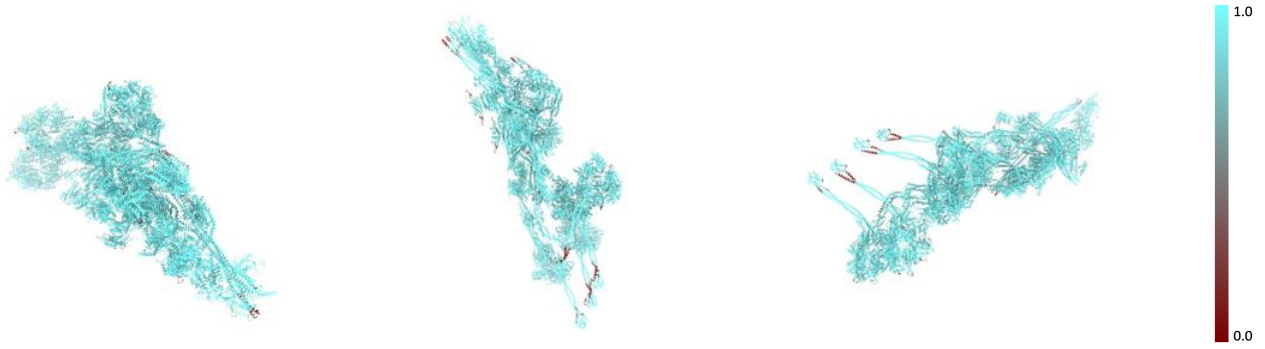
The images above show the 3D surface view of the map at the recommended contour level 0.0851 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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.

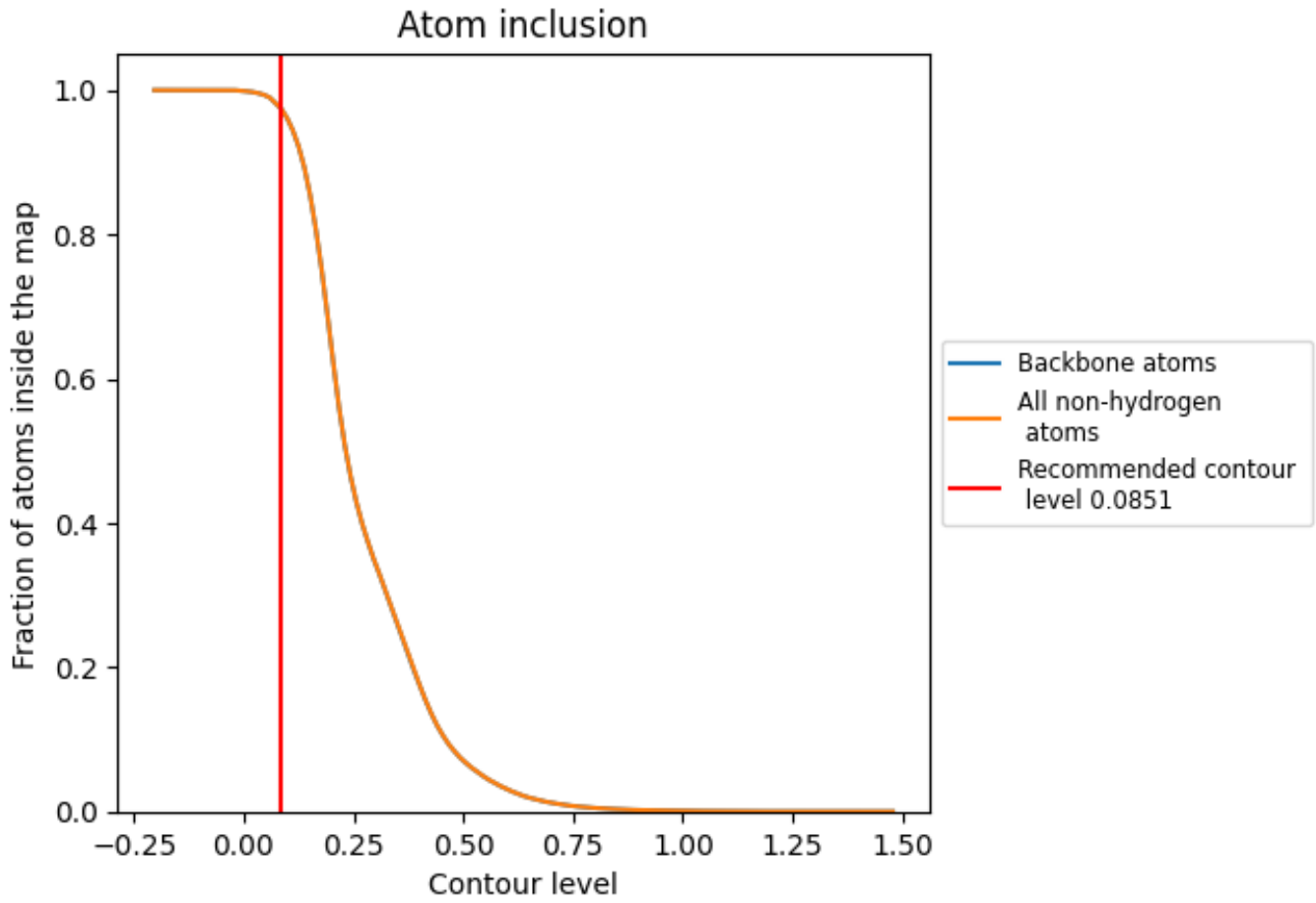
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0851).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.0851) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9747	0.2150
A	0.9973	0.3320
B	1.0000	0.3610
C	1.0000	0.3660
D	1.0000	0.3570
E	1.0000	0.3460
F	0.9987	0.3370
G	0.9987	0.3310
H	1.0000	0.3300
I	0.9821	0.3350
J	0.9955	0.3520
K	0.9991	0.3250
L	1.0000	0.3360
M	0.9735	0.2620
N	0.9286	0.2250
O	0.9912	0.2500
P	0.9796	0.2830
Q	0.9946	0.2850
R	1.0000	0.2690
S	0.9758	0.2410
T	0.9948	0.3050
U	0.9635	0.3190
V	0.9890	0.3350
W	0.9118	0.2270
X	0.9796	0.2620
Y	0.9961	0.3200
e	0.9625	0.1650
f	0.9773	0.2590
g	1.0000	0.2600
h	1.0000	0.2840
i	1.0000	0.2370
j	0.9795	0.2030
k	1.0000	0.1580
l	1.0000	0.1940
m	0.9565	0.1370

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Chain	Atom inclusion	Q-score
n	0.9687	0.1260
o	1.0000	0.3580
p	0.9794	0.1810
q	0.9908	0.1620
r	0.9975	0.0950
s	0.9946	0.2170
t	1.0000	0.2590
w	0.9372	0.2010
x	0.9729	0.2600