Full wwPDB EM Validation Report ⓘ

Apr 3, 2024 – 12:41 am BST

PDB ID	:	8PTK
EMDB ID	:	EMD-17873
Title	:	Composite structure of Dynein-Dynactin-JIP3-LIS1
Authors	:	Singh, K.; Lau, C.K.; Manigrasso, G.; Gassmann, R.; Carter, A.P.
Deposited on	:	2023-07-14
Resolution	:	10.00 Å(reported)
Based on initial model	:	7Z8G

This is a Full wwPDB EM Validation 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:

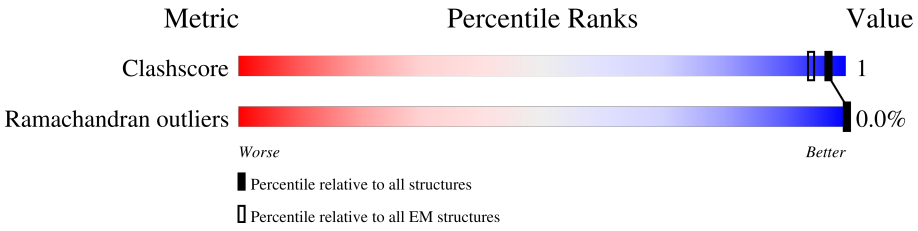
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 10.00 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	1	410	96%
1	2	410	96%
1	3	410	78% 21%
1	4	410	77% 21%
2	A	376	98%
2	B	376	97%
2	C	376	99%
2	D	376	97%
2	E	376	98%

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Mol	Chain	Length	Quality of chain
2	F	376	97%
2	G	376	98%
2	I	376	98%
3	H	375	97%
4	J	417	89% 9%
5	K	286	97%
6	L	272	98%
7	M	405	78% 22%
7	N	405	65% 35%
7	P	405	87% 13%
7	Q	405	80% 19%
8	O	186	90% 9%
8	R	186	96%
9	S	1281	56% 44%
9	T	1281	60% 39%
10	U	190	86% 11%
11	W	182	96%
12	X	581	5% 55% 45%
12	x	581	5% 49% 51%
13	Y	467	78% 20%
14	a	89	99%
14	b	89	100%
14	d	89	100%
14	i	89	98%
15	e	4646	96%

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Mol	Chain	Length	Quality of chain
15	f	4646	5% 97%
15	m	4646	98%
15	n	4646	98%
16	g	612	75% 25%
16	h	612	75% 25%
16	o	612	69% 31%
16	p	612	70% 29%
17	j	492	66% 34%
17	q	492	65% 35%
17	r	492	65% 35%
17	u	492	60% 39%
18	k	113	5% 100%
18	l	113	12% 100%
18	v	113	100%
18	y	113	19% 100%
19	s	96	97%
19	t	96	97%
19	w	96	97%
19	z	96	97%

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 161538 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 Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	402	Total 1988	C 1184	N 402	O 402	0	0
1	2	402	Total 1988	C 1184	N 402	O 402	0	0
1	3	322	Total 1590	C 946	N 322	O 322	0	0
1	4	322	Total 1590	C 946	N 322	O 322	0	0

- Molecule 2 is a protein called ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	370	Total 1822	C 1082	N 370	O 370	0	0
2	B	370	Total 1822	C 1082	N 370	O 370	0	0
2	C	375	Total 1847	C 1097	N 375	O 375	0	0
2	D	370	Total 1822	C 1082	N 370	O 370	0	0
2	E	370	Total 1822	C 1082	N 370	O 370	0	0
2	F	370	Total 1822	C 1082	N 370	O 370	0	0
2	G	370	Total 1822	C 1082	N 370	O 370	0	0
2	I	370	Total 1822	C 1082	N 370	O 370	0	0

- Molecule 3 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	370	Total 1822	C 1082	N 370	O 370	0	0

- Molecule 4 is a protein called Arp11.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	379	Total 1868	C 1110	N 379	O 379	0	0

- Molecule 5 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	278	Total 1378	C 822	N 278	O 278	0	0

- Molecule 6 is a protein called F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	269	Total 1327	C 789	N 269	O 269	0	0

- Molecule 7 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	316	Total 1570	C 938	N 316	O 316	0	0
7	N	263	Total 1310	C 784	N 263	O 263	0	0
7	P	353	Total 1757	C 1051	N 353	O 353	0	0
7	Q	329	Total 1632	C 974	N 329	O 329	0	0

- Molecule 8 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	170	Total 844	C 504	N 170	O 170	0	0
8	R	179	Total 888	C 530	N 179	O 179	0	0

- Molecule 9 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	S	718	Total 3565	C 2129	N 718	O 718	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	T	776	Total 3850	C 2298	N 776	O 776	0	0

- Molecule 10 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	169	Total 832	C 494	N 169	O 169	0	0

- Molecule 11 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	179	Total 881	C 523	N 179	O 179	0	0

- Molecule 12 is a protein called C-Jun-amino-terminal kinase-interacting protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	318	Total 1578	C 942	N 318	O 318	0	0
12	x	282	Total 1403	C 839	N 282	O 282	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-6	SER	-	expression tag	UNP Q9UPT6
X	-5	ASN	-	expression tag	UNP Q9UPT6
X	-4	ILE	-	expression tag	UNP Q9UPT6
X	-3	GLU	-	expression tag	UNP Q9UPT6
X	-2	PHE	-	expression tag	UNP Q9UPT6
X	-1	LEU	-	expression tag	UNP Q9UPT6
X	0	LYS	-	expression tag	UNP Q9UPT6
X	561	GLY	-	expression tag	UNP Q9UPT6
X	562	SER	-	expression tag	UNP Q9UPT6
X	563	GLY	-	expression tag	UNP Q9UPT6
X	564	SER	-	expression tag	UNP Q9UPT6
X	565	GLY	-	expression tag	UNP Q9UPT6
X	566	ARG	-	expression tag	UNP Q9UPT6
X	567	TRP	-	expression tag	UNP Q9UPT6
X	568	SER	-	expression tag	UNP Q9UPT6
X	569	HIS	-	expression tag	UNP Q9UPT6

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Chain	Residue	Modelled	Actual	Comment	Reference
X	570	PRO	-	expression tag	UNP Q9UPT6
X	571	GLN	-	expression tag	UNP Q9UPT6
X	572	PHE	-	expression tag	UNP Q9UPT6
X	573	GLU	-	expression tag	UNP Q9UPT6
X	574	LYS	-	expression tag	UNP Q9UPT6
x	-6	SER	-	expression tag	UNP Q9UPT6
x	-5	ASN	-	expression tag	UNP Q9UPT6
x	-4	ILE	-	expression tag	UNP Q9UPT6
x	-3	GLU	-	expression tag	UNP Q9UPT6
x	-2	PHE	-	expression tag	UNP Q9UPT6
x	-1	LEU	-	expression tag	UNP Q9UPT6
x	0	LYS	-	expression tag	UNP Q9UPT6
x	561	GLY	-	expression tag	UNP Q9UPT6
x	562	SER	-	expression tag	UNP Q9UPT6
x	563	GLY	-	expression tag	UNP Q9UPT6
x	564	SER	-	expression tag	UNP Q9UPT6
x	565	GLY	-	expression tag	UNP Q9UPT6
x	566	ARG	-	expression tag	UNP Q9UPT6
x	567	TRP	-	expression tag	UNP Q9UPT6
x	568	SER	-	expression tag	UNP Q9UPT6
x	569	HIS	-	expression tag	UNP Q9UPT6
x	570	PRO	-	expression tag	UNP Q9UPT6
x	571	GLN	-	expression tag	UNP Q9UPT6
x	572	PHE	-	expression tag	UNP Q9UPT6
x	573	GLU	-	expression tag	UNP Q9UPT6
x	574	LYS	-	expression tag	UNP Q9UPT6

- Molecule 13 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Y	375	Total	C	N	O	0	0
			1863	1113	375	375		

- Molecule 14 is a protein called Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	a	89	Total	C	N	O	0	0
			441	263	89	89		
14	b	89	Total	C	N	O	0	0
			441	263	89	89		
14	d	89	Total	C	N	O	0	0
			441	263	89	89		

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Mol	Chain	Residues	Atoms				AltConf	Trace
14	i	89	Total 441	C 263	N 89	O 89	0	0

- Molecule 15 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	e	4486	Total 22238	C 13266	N 4486	O 4486	0	0
15	f	4502	Total 22318	C 13314	N 4502	O 4502	0	0
15	m	4562	Total 22608	C 13484	N 4562	O 4562	0	0
15	n	4566	Total 22628	C 13496	N 4566	O 4566	0	0

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 16 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	g	460	Total 2275	C 1355	N 460	O 460	0	0
16	h	462	Total 2284	C 1360	N 462	O 462	0	0
16	o	425	Total 2100	C 1250	N 425	O 425	0	0
16	p	432	Total 2134	C 1270	N 432	O 432	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	484	SER	THR	conflict	UNP Q13409
g	499	GLY	ASP	conflict	UNP Q13409
h	484	SER	THR	conflict	UNP Q13409
h	499	GLY	ASP	conflict	UNP Q13409
o	484	SER	THR	conflict	UNP Q13409
o	499	GLY	ASP	conflict	UNP Q13409
p	484	SER	THR	conflict	UNP Q13409
p	499	GLY	ASP	conflict	UNP Q13409

- Molecule 17 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	j	324	Total 1605	C 957	N 324	O 324	0	0
17	q	318	Total 1574	C 938	N 318	O 318	0	0
17	r	319	Total 1581	C 943	N 319	O 319	0	0
17	u	298	Total 1473	C 877	N 298	O 298	0	0

- Molecule 18 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	k	113	Total 558	C 332	N 113	O 113	0	0
18	l	113	Total 558	C 332	N 113	O 113	0	0
18	v	113	Total 558	C 332	N 113	O 113	0	0
18	y	113	Total 558	C 332	N 113	O 113	0	0

- Molecule 19 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	s	93	Total 462	C 276	N 93	O 93	0	0
19	t	93	Total 462	C 276	N 93	O 93	0	0
19	w	93	Total 462	C 276	N 93	O 93	0	0

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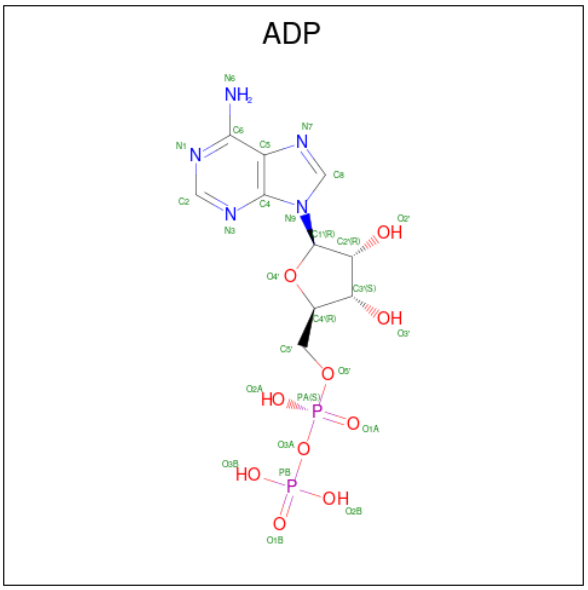
Mol	Chain	Residues	Atoms				AltConf	Trace
19	z	93	Total	C	N	O	0	0
			462	276	93	93		

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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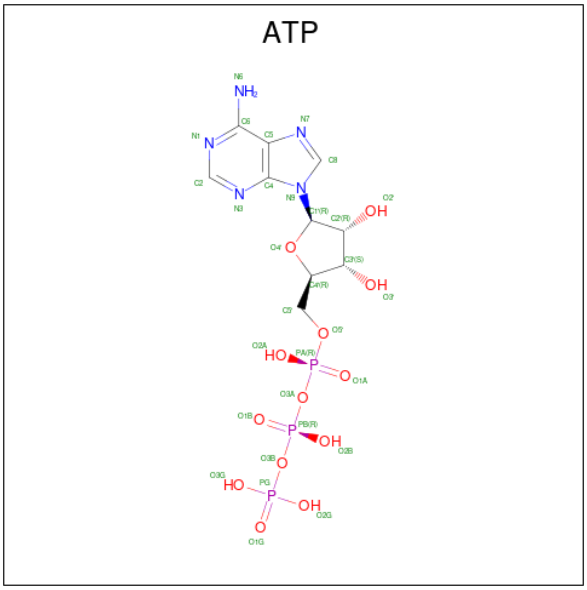
Mol	Chain	Residues	Atoms					AltConf
20	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	f	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	f	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	f	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	m	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	n	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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

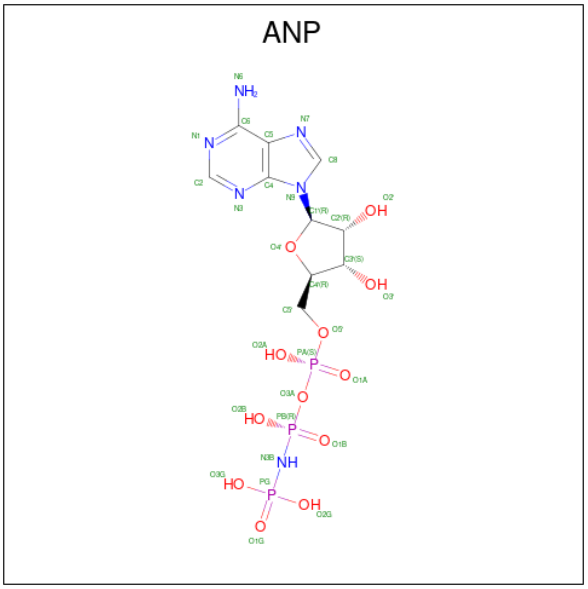
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
23	e	2	Total	Mg	0
			2	2	
23	f	2	Total	Mg	0
			2	2	
23	m	1	Total	Mg	0
			1	1	
23	n	1	Total	Mg	0
			1	1	

- Molecule 24 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



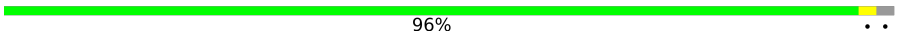
Mol	Chain	Residues	Atoms					AltConf
24	m	1	Total	C	N	O	P	0
			31	10	6	12	3	
24	m	1	Total	C	N	O	P	0
			31	10	6	12	3	
24	n	1	Total	C	N	O	P	0
			31	10	6	12	3	
24	n	1	Total	C	N	O	P	0
			31	10	6	12	3	

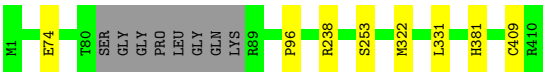
3 Residue-property plots (i)

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: Platelet-activating factor acetylhydrolase IB subunit beta

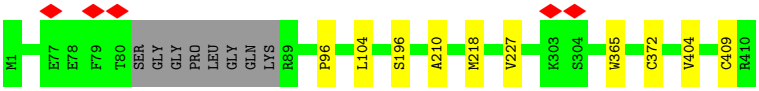
Chain 1:





• Molecule 1: Platelet-activating factor acetylhydrolase IB subunit beta

Chain 2:

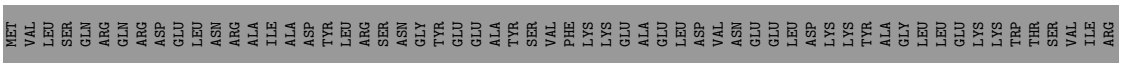


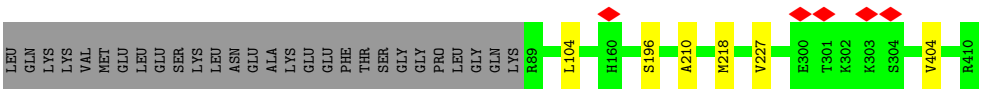
• Molecule 1: Platelet-activating factor acetylhydrolase IB subunit beta

Chain 3:

• Molecule 1: Platelet-activating factor acetylhydrolase IB subunit beta

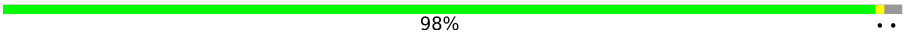
Chain 4:

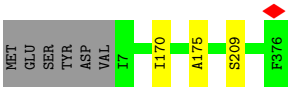




• Molecule 2: ARP1 actin related protein 1 homolog A

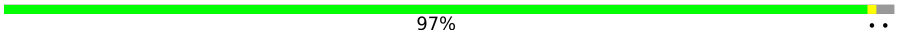
Chain A:

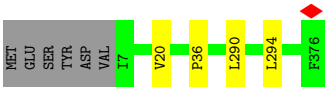




• Molecule 2: ARP1 actin related protein 1 homolog A

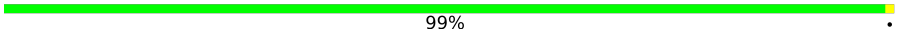
Chain B:

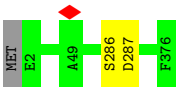




• Molecule 2: ARP1 actin related protein 1 homolog A

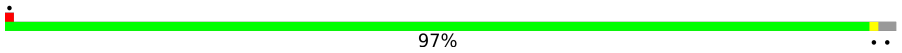
Chain C:

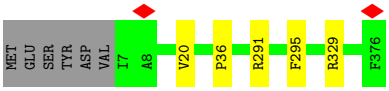




• Molecule 2: ARP1 actin related protein 1 homolog A

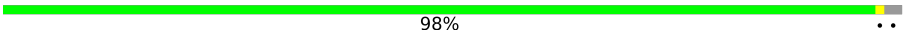
Chain D:

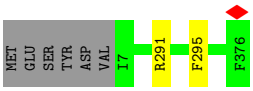




• Molecule 2: ARP1 actin related protein 1 homolog A

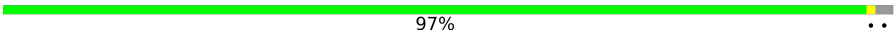
Chain E:

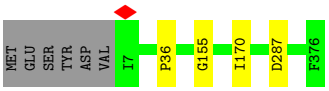




• Molecule 2: ARP1 actin related protein 1 homolog A

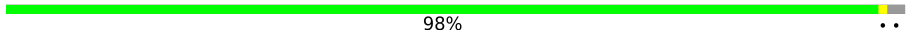
Chain F:

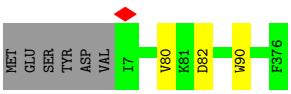




• Molecule 2: ARP1 actin related protein 1 homolog A

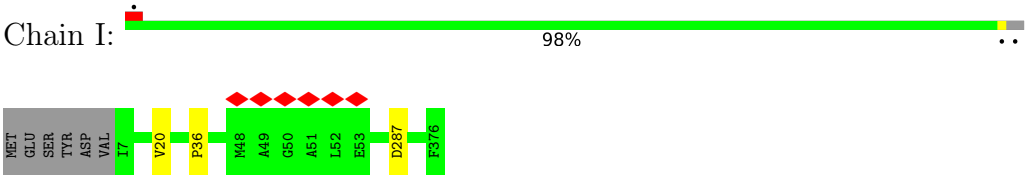
Chain G:





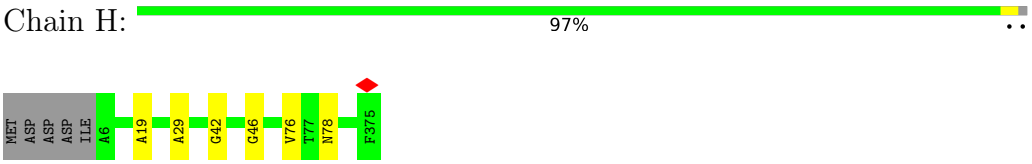
• Molecule 2: ARP1 actin related protein 1 homolog A

Chain I:



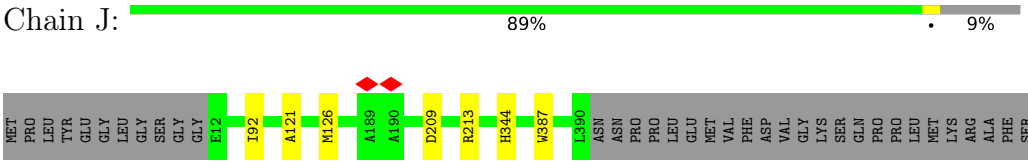
• Molecule 3: Actin, cytoplasmic 1

Chain H:



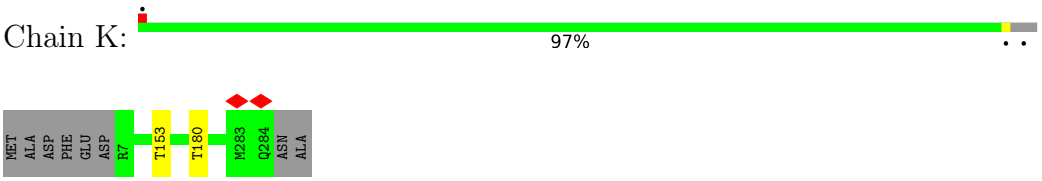
• Molecule 4: Arp11

Chain J:



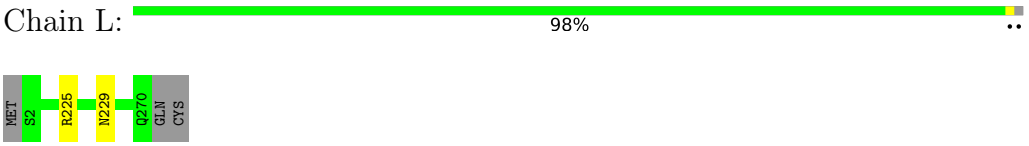
• Molecule 5: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K:



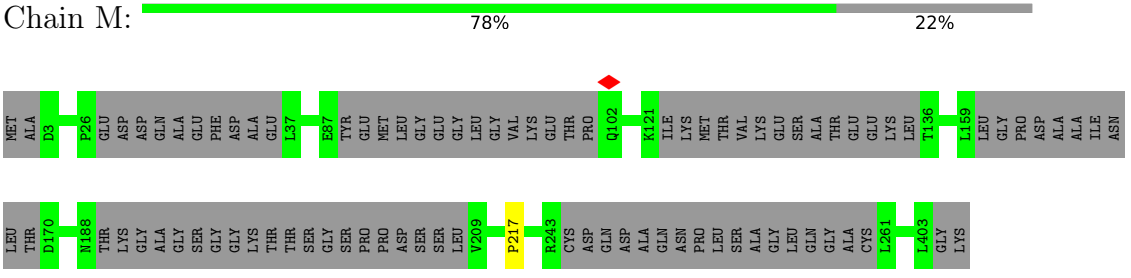
• Molecule 6: F-actin-capping protein subunit beta

Chain L:



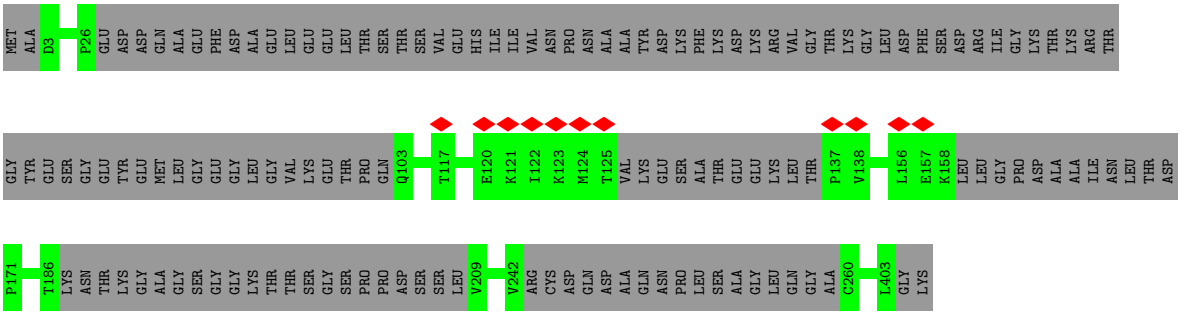
• Molecule 7: Dynactin subunit 2

Chain M:



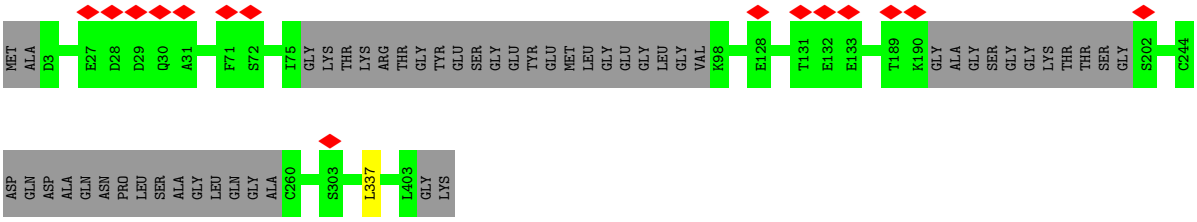
• Molecule 7: Dynactin subunit 2

Chain N:



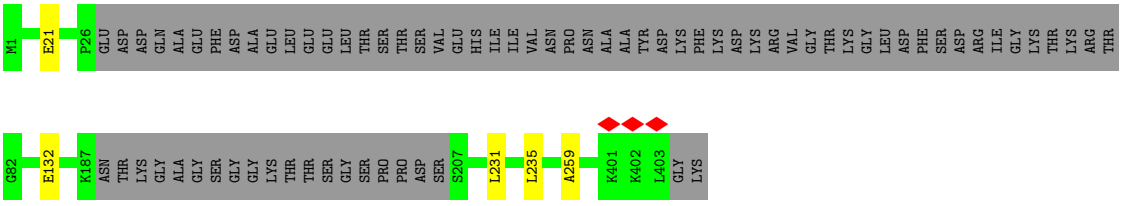
• Molecule 7: Dynactin subunit 2

Chain P:



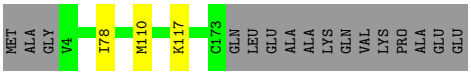
• Molecule 7: Dynactin subunit 2

Chain Q:



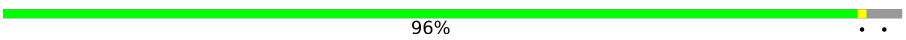
• Molecule 8: Dynactin subunit 3

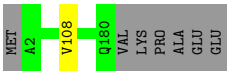
Chain O:



• Molecule 8: Dynactin subunit 3

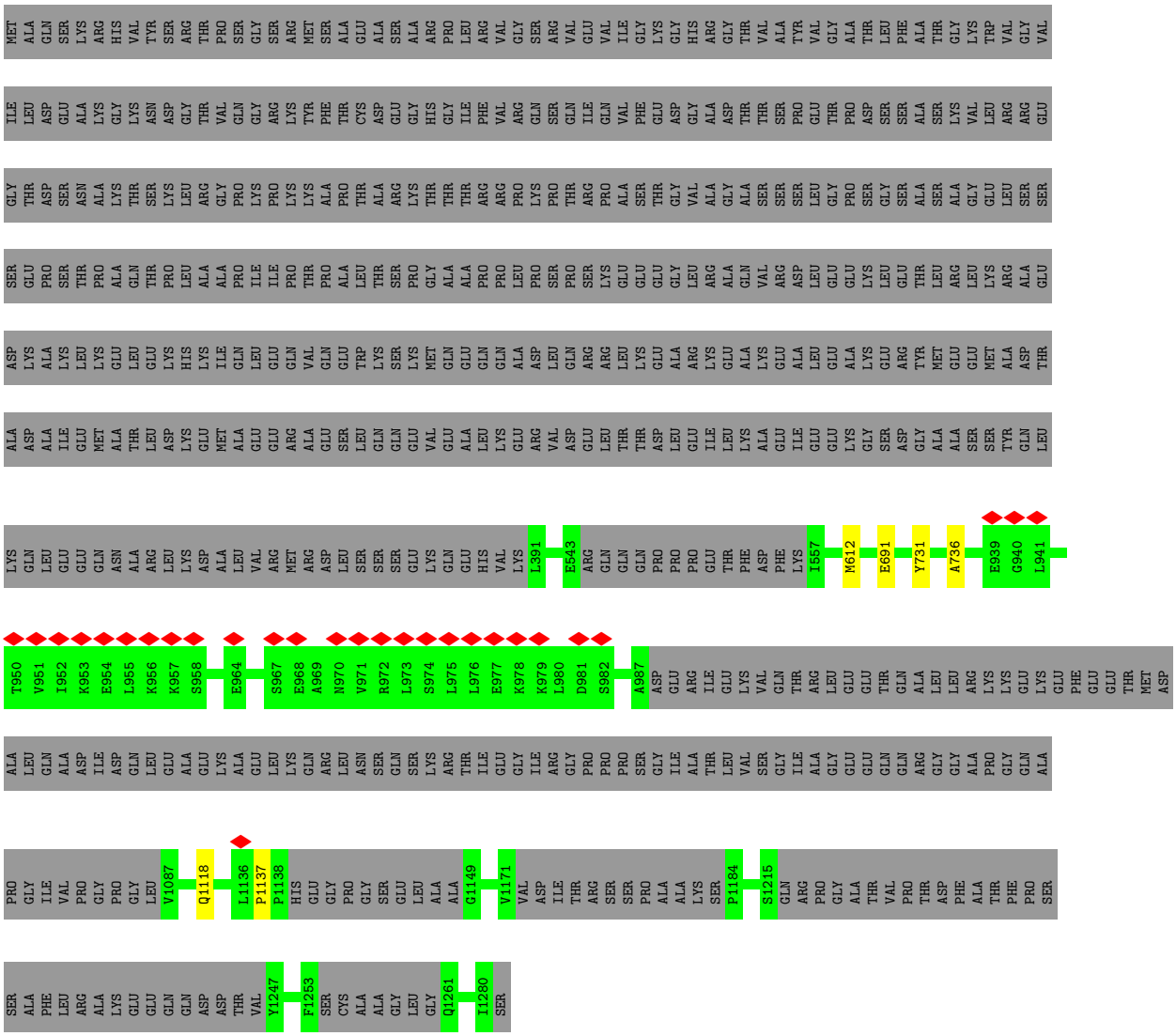
Chain R:





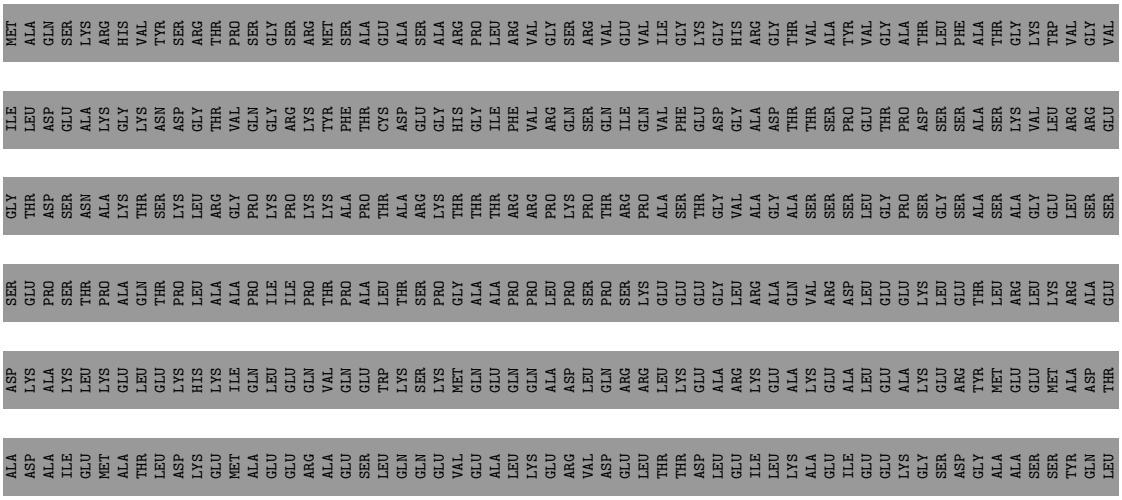
• Molecule 9: Dynactin subunit 1

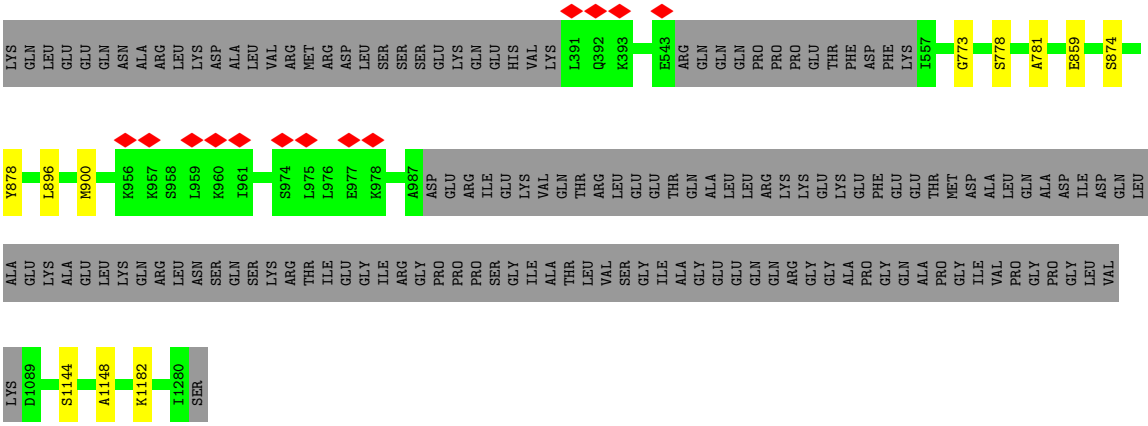
Chain S:



• Molecule 9: Dynactin subunit 1

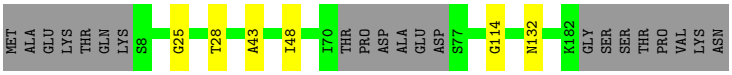
Chain T:





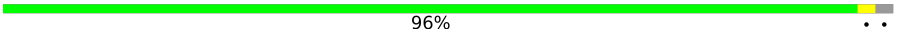
• Molecule 10: Dynactin 6

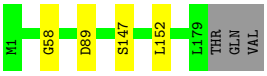
Chain U:



• Molecule 11: Dynactin subunit 5

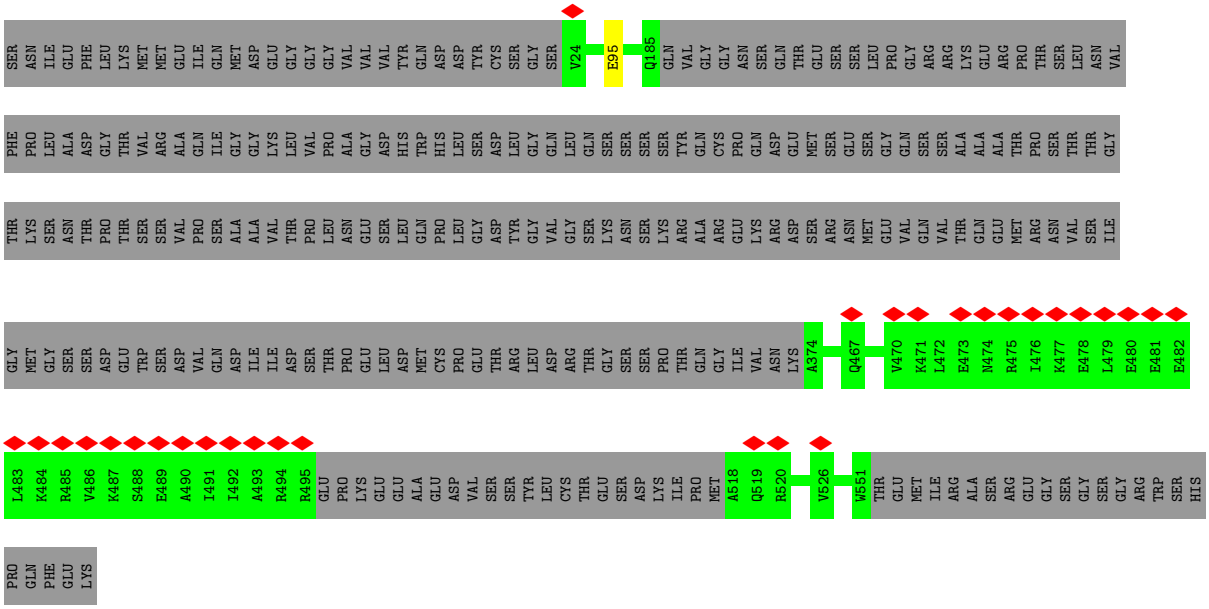
Chain W:





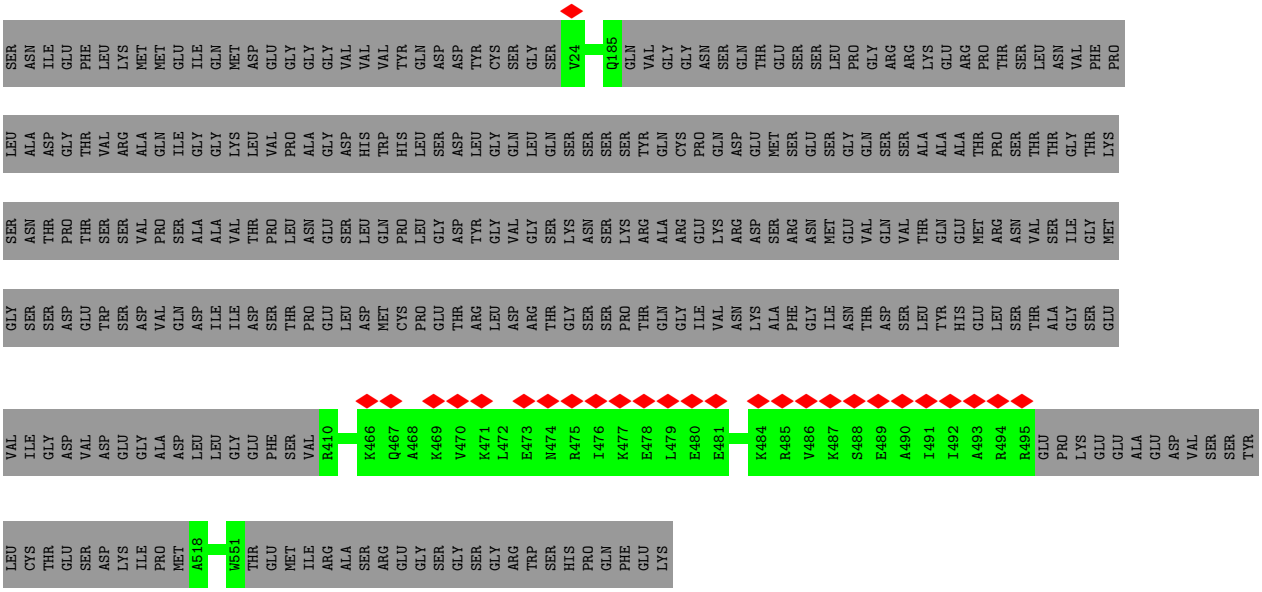
• Molecule 12: C-Jun-amino-terminal kinase-interacting protein 3

Chain X:



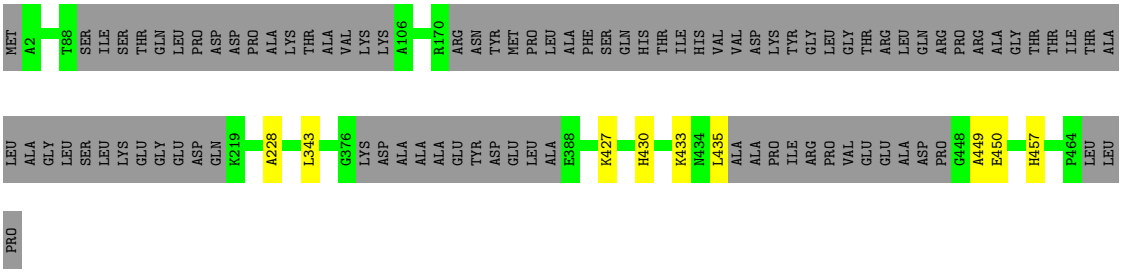
• Molecule 12: C-Jun-amino-terminal kinase-interacting protein 3

Chain x:



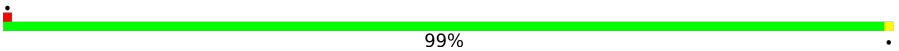
• Molecule 13: Dynactin subunit 4

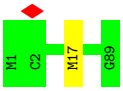
Chain Y:



• Molecule 14: Dynein light chain 1, cytoplasmic

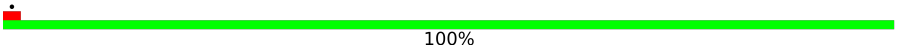
Chain a:





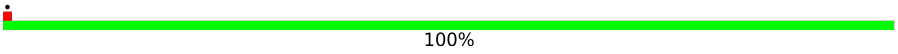
• Molecule 14: Dynein light chain 1, cytoplasmic

Chain b:



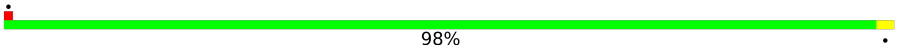
• Molecule 14: Dynein light chain 1, cytoplasmic

Chain d:



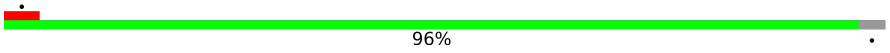
• Molecule 14: Dynein light chain 1, cytoplasmic

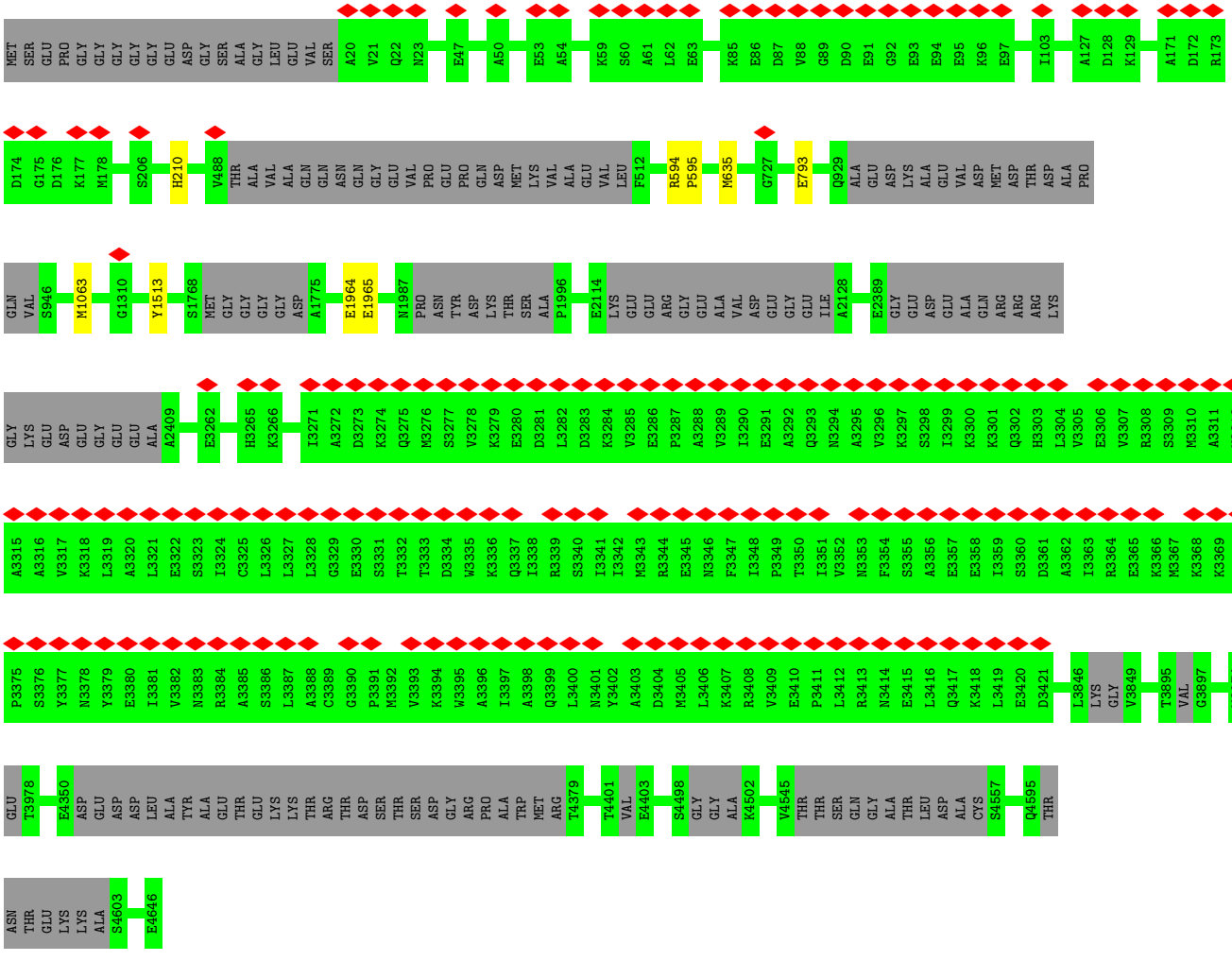
Chain i:



• Molecule 15: Cytoplasmic dynein 1 heavy chain 1

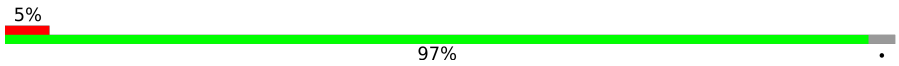
Chain e:

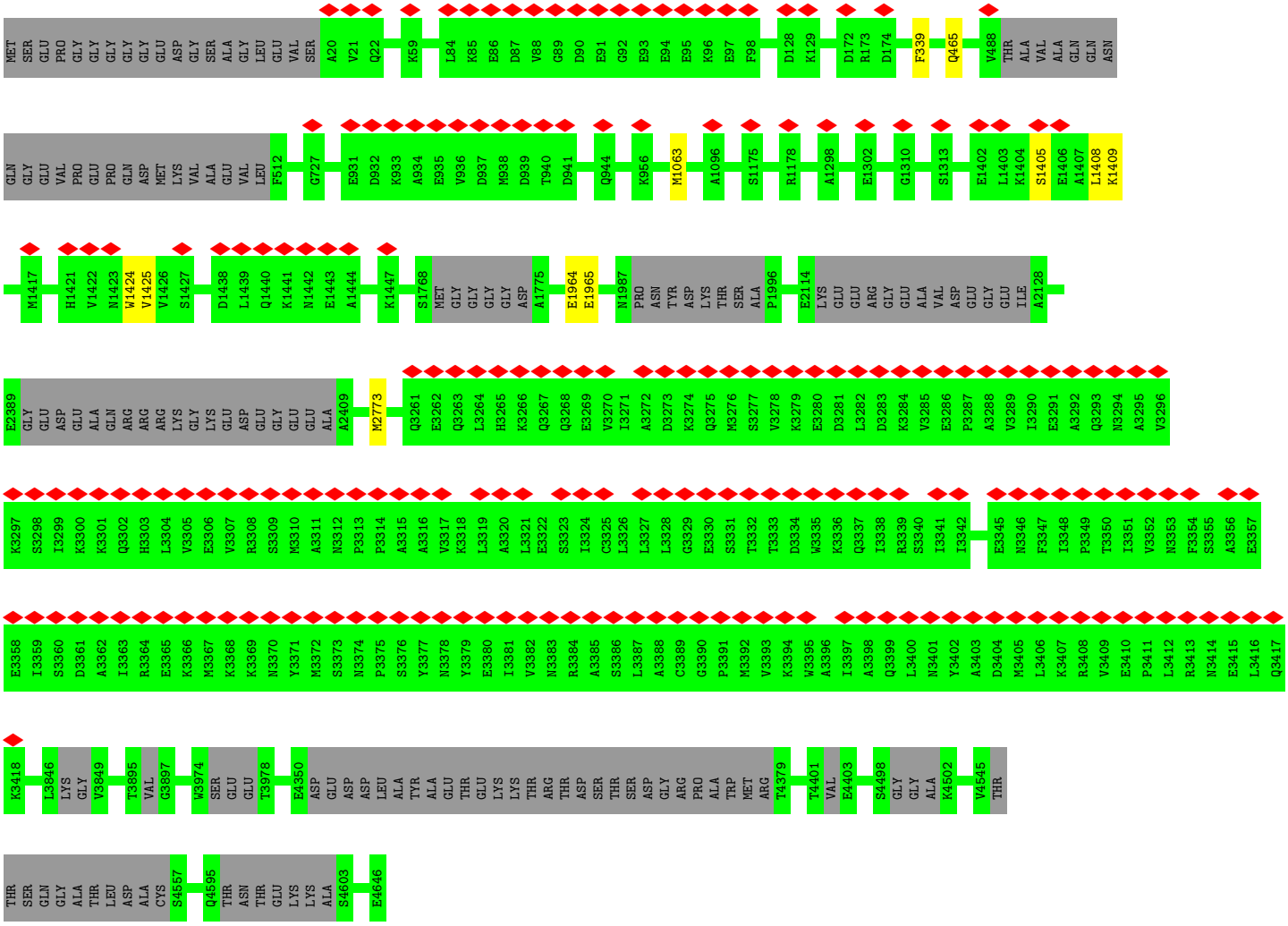




• Molecule 15: Cytoplasmic dynein 1 heavy chain 1

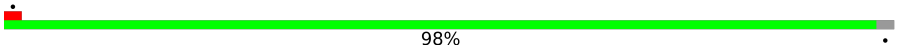
Chain f:

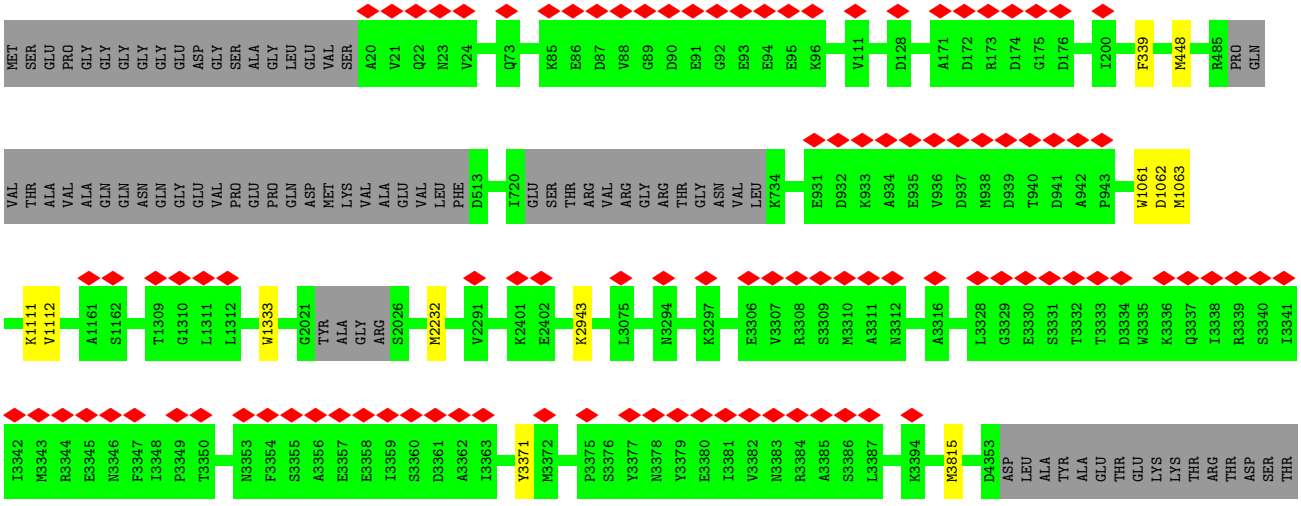


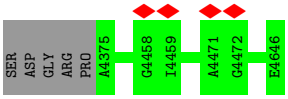


• Molecule 15: Cytoplasmic dynein 1 heavy chain 1

Chain m:

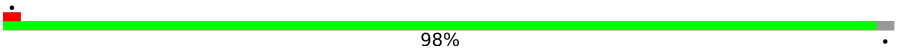


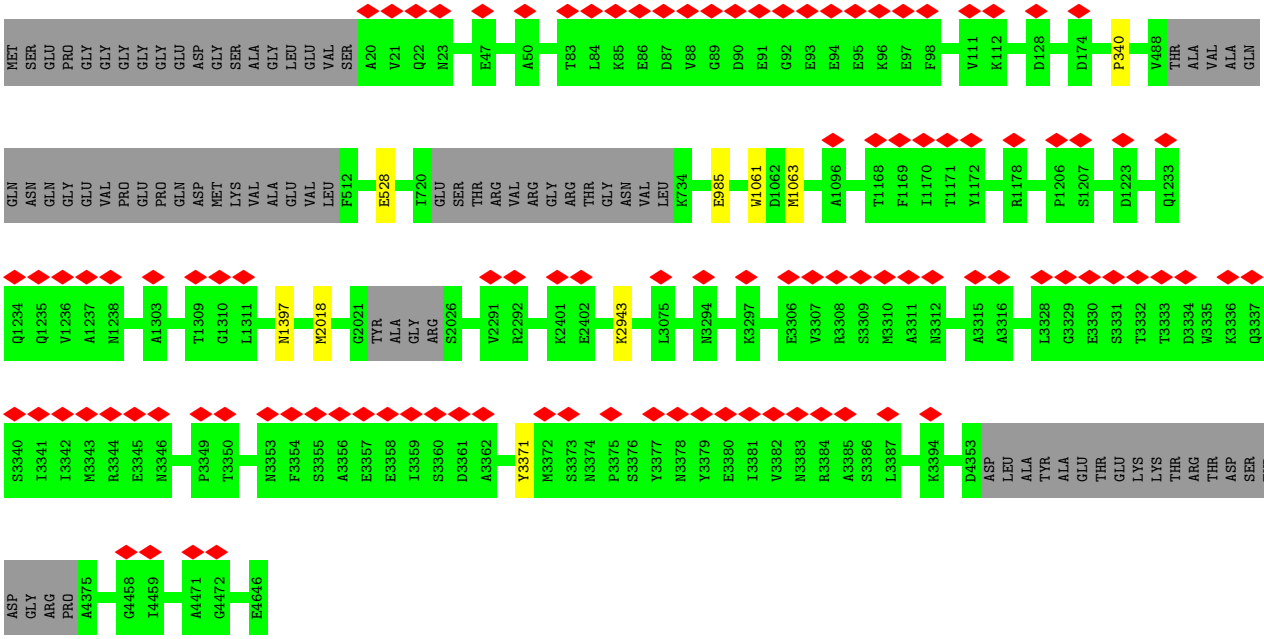




• Molecule 15: Cytoplasmic dynein 1 heavy chain 1

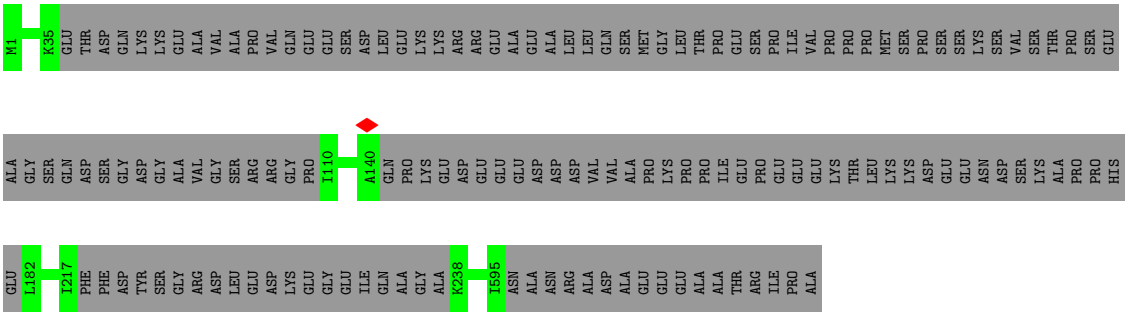
Chain n:





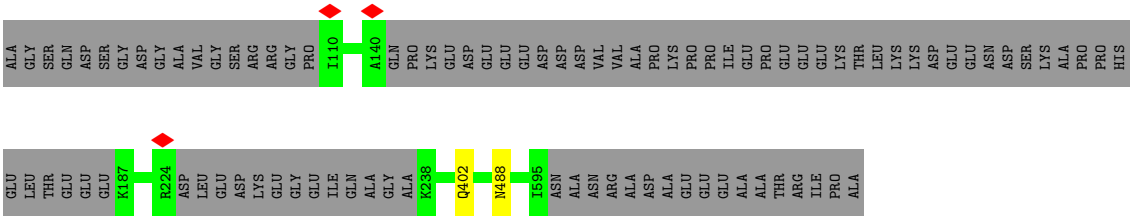
• Molecule 16: Cytoplasmic dynein 1 intermediate chain 2

Chain g:



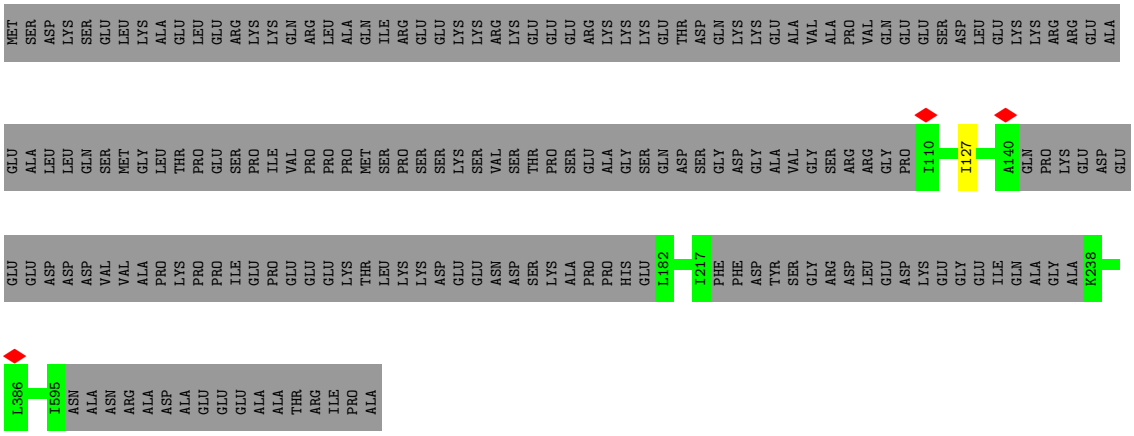
• Molecule 16: Cytoplasmic dynein 1 intermediate chain 2

Chain h:



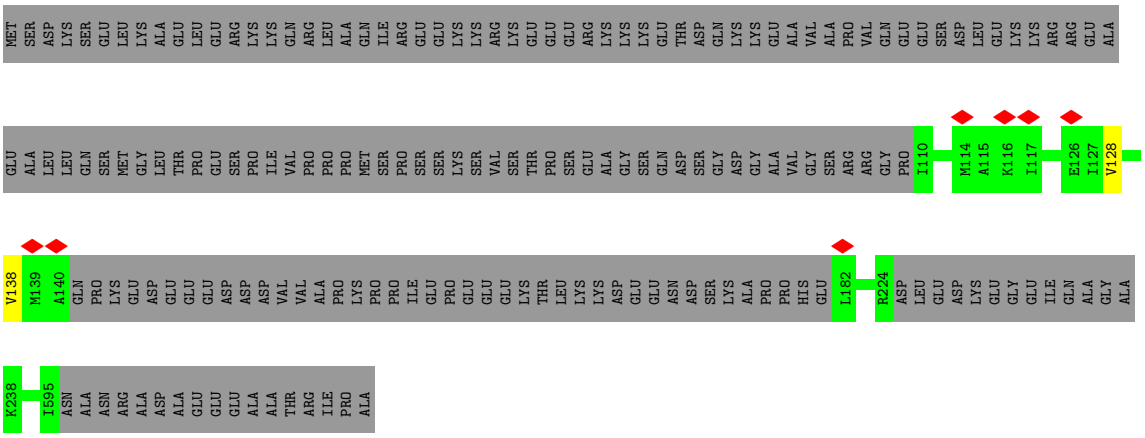
• Molecule 16: Cytoplasmic dynein 1 intermediate chain 2

Chain o:



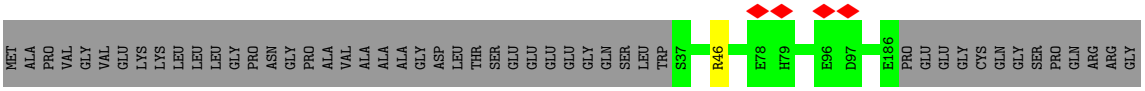
• Molecule 16: Cytoplasmic dynein 1 intermediate chain 2

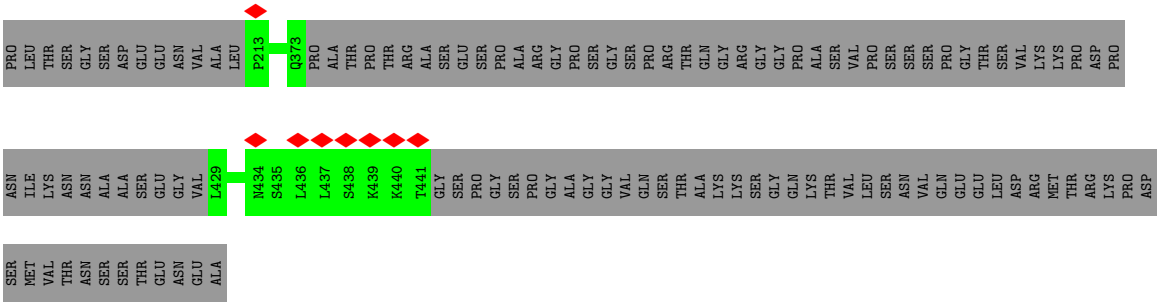
Chain p:



• Molecule 17: Cytoplasmic dynein 1 light intermediate chain 2

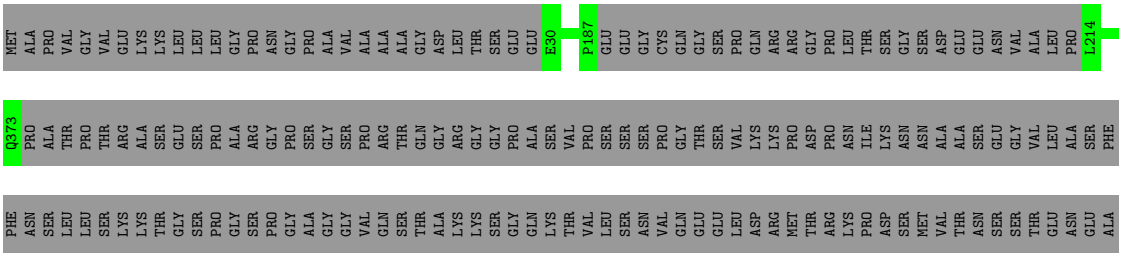
Chain j:





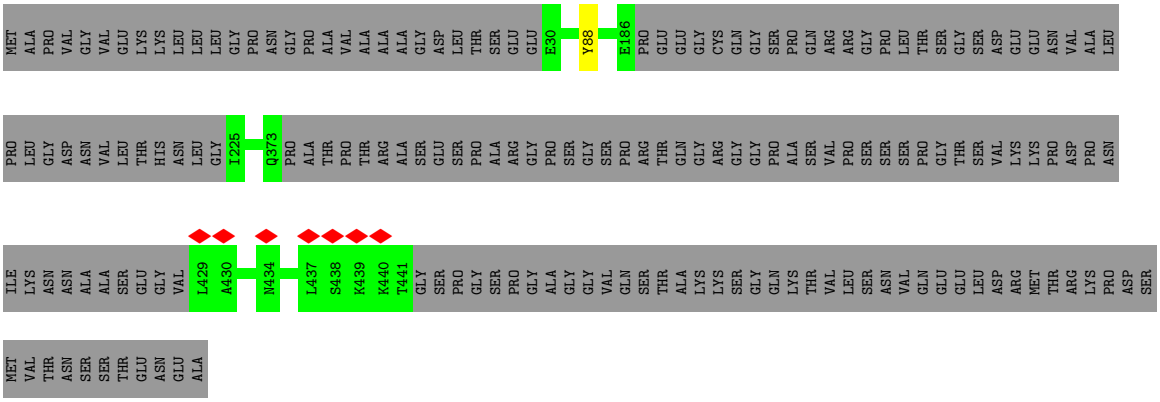
• Molecule 17: Cytoplasmic dynein 1 light intermediate chain 2

Chain q:



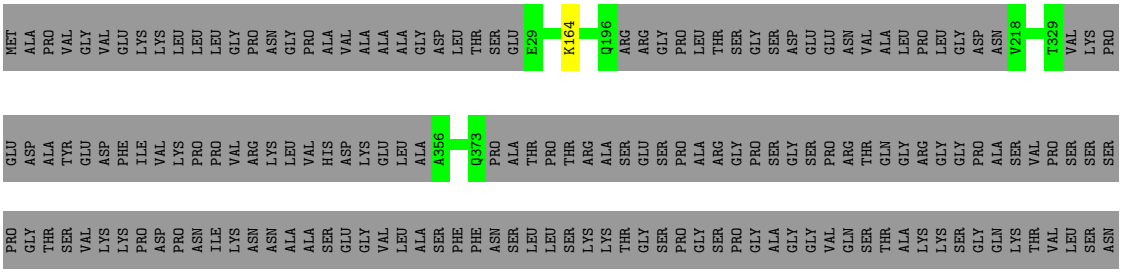
• Molecule 17: Cytoplasmic dynein 1 light intermediate chain 2

Chain r:



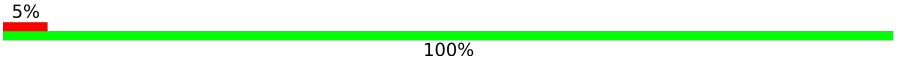
• Molecule 17: Cytoplasmic dynein 1 light intermediate chain 2

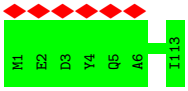
Chain u:



• Molecule 18: Dynein light chain Tctex-type 1

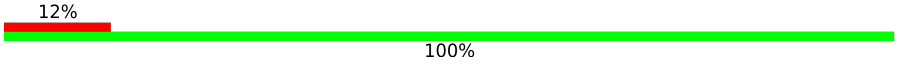
Chain k:

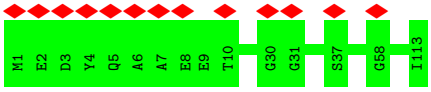




• Molecule 18: Dynein light chain Tctex-type 1

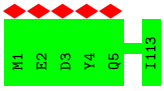
Chain l:





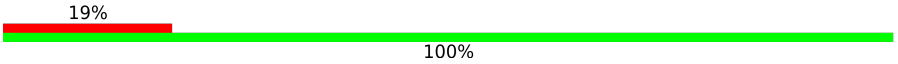
• Molecule 18: Dynein light chain Tctex-type 1

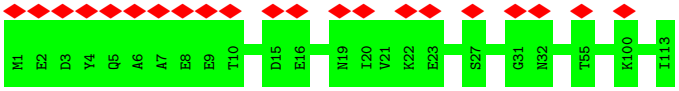
Chain v:



• Molecule 18: Dynein light chain Tctex-type 1

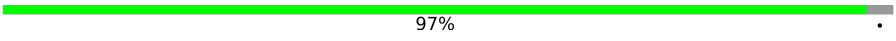
Chain y:

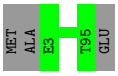




• Molecule 19: Dynein light chain roadblock-type 1

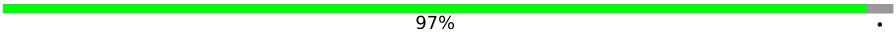
Chain s:

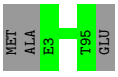




• Molecule 19: Dynein light chain roadblock-type 1

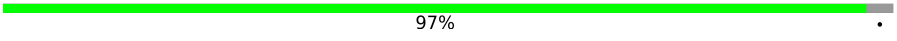
Chain t:

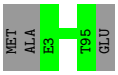




• Molecule 19: Dynein light chain roadblock-type 1

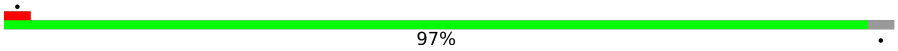
Chain w:

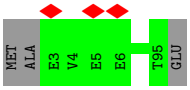




• Molecule 19: Dynein light chain roadblock-type 1

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	700290	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)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0134	Depositor
Map size (Å)	677.76, 677.76, 677.76	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ANP, ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.31	0/1986	0.66	2/2764 (0.1%)
1	2	0.30	0/1986	0.63	0/2764
1	3	0.30	0/1589	0.67	1/2211 (0.0%)
1	4	0.29	0/1589	0.64	0/2211
2	A	0.29	0/1821	0.54	0/2531
2	B	0.31	0/1821	0.58	0/2531
2	C	0.30	0/1846	0.59	0/2566
2	D	0.29	0/1821	0.57	0/2531
2	E	0.30	0/1821	0.56	0/2531
2	F	0.30	0/1821	0.57	0/2531
2	G	0.29	0/1821	0.54	0/2531
2	I	0.28	0/1821	0.55	0/2531
3	H	0.29	0/1821	0.58	0/2531
4	J	0.30	0/1867	0.59	0/2596
5	K	0.32	0/1377	0.57	0/1919
6	L	0.30	0/1326	0.51	0/1844
7	M	0.35	0/1563	0.61	0/2171
7	N	0.36	0/1304	0.53	0/1813
7	P	0.38	1/1753 (0.1%)	0.63	0/2443
7	Q	0.37	0/1629	0.63	1/2268 (0.0%)
8	O	0.38	1/843 (0.1%)	0.62	0/1175
8	R	0.33	0/887	0.51	0/1236
9	S	0.37	0/3558	0.61	2/4955 (0.0%)
9	T	0.33	0/3847	0.51	0/5363
10	U	0.30	0/830	0.67	0/1151
11	W	0.30	0/880	0.62	0/1222
12	X	0.33	0/1575	0.55	1/2193 (0.0%)
12	x	0.34	0/1400	0.55	0/1951
13	Y	0.30	0/1858	0.57	0/2586
14	a	0.30	0/440	0.68	0/612
14	b	0.31	0/440	0.67	0/612
14	d	0.31	0/440	0.68	0/612

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	i	0.31	0/440	0.68	0/612
15	e	0.32	0/22223	0.56	1/30973 (0.0%)
15	f	0.29	0/22304	0.53	1/31088 (0.0%)
15	m	0.28	0/22603	0.52	1/31515 (0.0%)
15	n	0.32	0/22623	0.55	2/31543 (0.0%)
16	g	0.28	0/2271	0.57	0/3158
16	h	0.28	0/2280	0.57	1/3170 (0.0%)
16	o	0.29	0/2097	0.61	0/2916
16	p	0.29	0/2131	0.58	0/2963
17	j	0.29	0/1602	0.54	0/2229
17	q	0.29	0/1572	0.53	0/2188
17	r	0.29	0/1578	0.55	0/2196
17	u	0.29	0/1470	0.59	0/2043
18	k	0.27	0/557	0.53	0/774
18	l	0.26	0/557	0.53	0/774
18	v	0.27	0/557	0.51	0/774
18	y	0.28	0/557	0.54	0/774
19	s	0.36	0/461	0.60	0/642
19	t	0.29	0/461	0.63	0/642
19	w	0.25	0/461	0.46	0/642
19	z	0.25	0/461	0.47	0/642
All	All	0.30	2/160647 (0.0%)	0.56	13/223744 (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
2	A	0	1
2	C	0	2
2	F	0	2
2	G	0	3
2	I	0	1
3	H	0	3
4	J	0	1
8	O	0	2
8	R	0	1
9	S	0	1
14	a	0	1
14	i	0	1
15	e	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	f	0	6
15	m	0	11
15	n	0	6
16	h	0	1
16	p	0	1
17	j	0	1
17	r	0	1
17	u	0	1
All	All	0	53

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	337	LEU	N-CA	-5.57	1.35	1.46
8	O	117	LYS	C-N	5.36	1.46	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	132	GLU	N-CA-CB	6.58	122.45	110.60
9	S	1118	GLN	N-CA-CB	6.40	122.11	110.60
15	n	528	GLU	N-CA-CB	5.54	120.57	110.60
1	1	381	HIS	CB-CA-C	5.44	121.28	110.40
1	3	381	HIS	CB-CA-C	5.44	121.28	110.40
12	X	95	GLU	N-CA-CB	5.30	120.15	110.60
1	1	74	GLU	N-CA-CB	5.30	120.14	110.60
15	e	793	GLU	N-CA-CB	5.28	120.11	110.60
15	f	465	GLN	N-CA-CB	5.19	119.94	110.60
16	h	488	ASN	C-N-CA	5.16	134.61	121.70
9	S	612	MET	CB-CA-C	5.15	120.70	110.40
15	m	2943	LYS	C-N-CA	5.12	134.51	121.70
15	n	2943	LYS	C-N-CA	5.09	134.43	121.70

There are no chirality outliers.

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	209	SER	Peptide
2	C	286	SER	Peptide
2	C	287	ASP	Peptide
2	F	287	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	F	36	PRO	Peptide
2	G	80	VAL	Peptide
2	G	82	ASP	Peptide
2	G	90	TRP	Peptide
3	H	46	GLY	Peptide
3	H	76	VAL	Peptide
3	H	78	ASN	Peptide
2	I	287	ASP	Peptide
4	J	126	MET	Peptide
8	O	110	MET	Peptide
8	O	78	ILE	Peptide
8	R	108	VAL	Peptide
9	S	691	GLU	Peptide
14	a	17	MET	Peptide
15	e	1063	MET	Peptide
15	e	1513	TYR	Peptide
15	e	1964	GLU	Peptide
15	e	210	HIS	Peptide
15	e	594	ARG	Peptide
15	e	635	MET	Peptide
15	f	1063	MET	Peptide
15	f	1408	LEU	Peptide
15	f	1424	TRP	Peptide
15	f	1964	GLU	Peptide
15	f	2773	MET	Peptide
15	f	339	PHE	Mainchain
16	h	402	GLN	Peptide
14	i	64	SER	Peptide
17	j	46	ARG	Peptide
15	m	1061	TRP	Peptide
15	m	1062	ASP	Peptide
15	m	1063	MET	Peptide
15	m	1111	LYS	Peptide
15	m	1112	VAL	Peptide
15	m	1333	TRP	Peptide
15	m	2232	MET	Peptide
15	m	3371	TYR	Peptide
15	m	339	PHE	Mainchain
15	m	3815	MET	Peptide
15	m	448	MET	Peptide
15	n	1061	TRP	Peptide
15	n	1063	MET	Peptide

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Mol	Chain	Res	Type	Group
15	n	1397	ASN	Peptide
15	n	2018	MET	Peptide
15	n	3371	TYR	Peptide
15	n	985	GLU	Peptide
16	p	128	VAL	Peptide
17	r	88	TYR	Peptide
17	u	164	LYS	Peptide

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	1	1988	0	878	3	0
1	2	1988	0	878	5	0
1	3	1590	0	696	1	0
1	4	1590	0	696	3	0
2	A	1822	0	820	1	0
2	B	1822	0	820	2	0
2	C	1847	0	830	0	0
2	D	1822	0	820	3	0
2	E	1822	0	820	1	0
2	F	1822	0	820	1	0
2	G	1822	0	820	0	0
2	I	1822	0	820	1	0
3	H	1822	0	835	2	0
4	J	1868	0	823	4	0
5	K	1378	0	611	1	0
6	L	1327	0	585	1	0
7	M	1570	0	706	0	0
7	N	1310	0	593	0	0
7	P	1757	0	792	0	0
7	Q	1632	0	755	2	0
8	O	844	0	385	0	0
8	R	888	0	413	0	0
9	S	3565	0	1652	1	0
9	T	3850	0	1801	5	0
10	U	832	0	371	3	0
11	W	881	0	379	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X	1578	0	704	0	0
12	x	1403	0	618	0	0
13	Y	1863	0	794	5	0
14	a	441	0	204	0	0
14	b	441	0	204	0	0
14	d	441	0	204	0	0
14	i	441	0	204	0	0
15	e	22238	0	9837	0	0
15	f	22318	0	9878	0	0
15	m	22608	0	10040	0	0
15	n	22628	0	10047	0	0
16	g	2275	0	1017	0	0
16	h	2284	0	1022	0	0
16	o	2100	0	939	0	0
16	p	2134	0	954	0	0
17	j	1605	0	703	0	0
17	q	1574	0	689	0	0
17	r	1581	0	692	0	0
17	u	1473	0	645	0	0
18	k	558	0	261	0	0
18	l	558	0	261	0	0
18	v	558	0	261	0	0
18	y	558	0	261	0	0
19	s	462	0	192	0	0
19	t	462	0	192	0	0
19	w	462	0	192	0	0
19	z	462	0	192	0	0
20	A	27	0	12	0	0
20	B	27	0	12	0	0
20	C	27	0	12	0	0
20	D	27	0	12	0	0
20	E	27	0	12	0	0
20	F	27	0	12	0	0
20	G	27	0	12	0	0
20	I	27	0	12	0	0
20	e	81	0	36	0	0
20	f	81	0	36	0	0
20	m	27	0	12	0	0
20	n	27	0	12	0	0
21	H	31	0	12	0	0
21	J	31	0	12	0	0
21	e	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	f	31	0	12	0	0
21	m	31	0	12	0	0
21	n	31	0	12	0	0
22	Y	3	0	0	0	0
23	e	2	0	0	0	0
23	f	2	0	0	0	0
23	m	1	0	0	0	0
23	n	1	0	0	0	0
24	m	62	0	26	0	0
24	n	62	0	26	0	0
All	All	161538	0	71942	44	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.

All (44) 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)
2:I:20:VAL:HA	2:I:36:PRO:HA	1.93	0.50
2:B:20:VAL:HA	2:B:36:PRO:HA	1.93	0.49
13:Y:433:LYS:HA	13:Y:450:GLU:HA	1.95	0.49
2:D:20:VAL:HA	2:D:36:PRO:HA	1.95	0.48
2:D:291:ARG:O	2:D:295:PHE:N	2.44	0.47
5:K:153:THR:HA	5:K:180:THR:HA	1.97	0.47
2:E:291:ARG:O	2:E:295:PHE:N	2.45	0.47
1:2:196:SER:N	1:2:210:ALA:O	2.47	0.46
10:U:25:GLY:HA3	10:U:43:ALA:HB3	1.98	0.46
2:D:329:ARG:HA	7:Q:21:GLU:HA	1.98	0.45
1:2:218:MET:O	1:2:227:VAL:N	2.49	0.45
11:W:58:GLY:HA3	11:W:89:ASP:HA	1.99	0.45
2:A:170:ILE:HA	2:A:175:ALA:HA	1.98	0.45
9:T:778:SER:H	9:T:781:ALA:HB3	1.82	0.44
13:Y:343:LEU:HA	13:Y:430:HIS:HA	2.00	0.44
2:F:155:GLY:N	2:F:170:ILE:O	2.51	0.44
4:J:344:HIS:HA	13:Y:228:ALA:HA	1.99	0.44
9:T:896:LEU:O	9:T:900:MET:CB	2.66	0.44
1:4:196:SER:N	1:4:210:ALA:O	2.48	0.44
1:4:218:MET:O	1:4:227:VAL:N	2.50	0.44
4:J:209:ASP:O	4:J:213:ARG:CB	2.66	0.43
9:T:773:GLY:H	9:T:859:GLU:HA	1.82	0.43
1:1:238:ARG:H	1:1:253:SER:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:231:LEU:O	7:Q:235:LEU:CB	2.65	0.43
1:4:104:LEU:N	1:4:404:VAL:O	2.49	0.43
6:L:225:ARG:O	6:L:229:ASN:CB	2.67	0.43
1:3:104:LEU:N	1:3:404:VAL:O	2.48	0.43
9:T:874:SER:O	9:T:878:TYR:CB	2.67	0.43
4:J:92:ILE:HA	4:J:121:ALA:HB3	2.01	0.42
13:Y:427:LYS:HA	13:Y:457:HIS:HA	2.01	0.42
10:U:114:GLY:HA3	10:U:132:ASN:HA	2.01	0.42
1:2:104:LEU:N	1:2:404:VAL:O	2.47	0.42
1:1:322:MET:O	1:1:331:LEU:N	2.49	0.42
1:1:96:PRO:HA	1:1:409:CYS:HA	2.02	0.42
9:T:1144:SER:O	9:T:1148:ALA:HB2	2.20	0.42
1:2:96:PRO:HA	1:2:409:CYS:HA	2.02	0.42
13:Y:435:LEU:H	13:Y:449:ALA:HB1	1.85	0.41
2:B:290:LEU:O	2:B:294:LEU:N	2.49	0.41
3:H:19:ALA:HB3	3:H:29:ALA:HB3	2.01	0.41
10:U:28:THR:N	10:U:48:ILE:O	2.53	0.41
11:W:147:SER:O	11:W:152:LEU:N	2.52	0.41
9:S:731:TYR:O	9:S:736:ALA:N	2.54	0.40
3:H:42:GLY:HA3	4:J:387:TRP:HA	2.03	0.40
1:2:365:TRP:HA	1:2:372:CYS:HA	2.04	0.40

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	1	398/410 (97%)	379 (95%)	19 (5%)	0	100	100
1	2	398/410 (97%)	376 (94%)	22 (6%)	0	100	100
1	3	320/410 (78%)	298 (93%)	22 (7%)	0	100	100
1	4	320/410 (78%)	298 (93%)	22 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	368/376 (98%)	352 (96%)	16 (4%)	0	100	100
2	B	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
2	C	373/376 (99%)	359 (96%)	14 (4%)	0	100	100
2	D	368/376 (98%)	352 (96%)	16 (4%)	0	100	100
2	E	368/376 (98%)	354 (96%)	14 (4%)	0	100	100
2	F	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
2	G	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
2	I	368/376 (98%)	352 (96%)	16 (4%)	0	100	100
3	H	368/375 (98%)	355 (96%)	13 (4%)	0	100	100
4	J	377/417 (90%)	358 (95%)	19 (5%)	0	100	100
5	K	276/286 (96%)	255 (92%)	21 (8%)	0	100	100
6	L	267/272 (98%)	262 (98%)	5 (2%)	0	100	100
7	M	302/405 (75%)	294 (97%)	7 (2%)	1 (0%)	41	77
7	N	251/405 (62%)	245 (98%)	6 (2%)	0	100	100
7	P	345/405 (85%)	327 (95%)	18 (5%)	0	100	100
7	Q	323/405 (80%)	313 (97%)	9 (3%)	1 (0%)	41	77
8	O	168/186 (90%)	159 (95%)	9 (5%)	0	100	100
8	R	177/186 (95%)	163 (92%)	14 (8%)	0	100	100
9	S	704/1281 (55%)	689 (98%)	14 (2%)	1 (0%)	51	86
9	T	770/1281 (60%)	748 (97%)	21 (3%)	1 (0%)	51	86
10	U	165/190 (87%)	149 (90%)	16 (10%)	0	100	100
11	W	177/182 (97%)	160 (90%)	17 (10%)	0	100	100
12	X	312/581 (54%)	305 (98%)	7 (2%)	0	100	100
12	x	276/581 (48%)	273 (99%)	3 (1%)	0	100	100
13	Y	365/467 (78%)	337 (92%)	28 (8%)	0	100	100
14	a	87/89 (98%)	82 (94%)	5 (6%)	0	100	100
14	b	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
14	d	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
14	i	87/89 (98%)	84 (97%)	2 (2%)	1 (1%)	14	52
15	e	4456/4646 (96%)	4310 (97%)	144 (3%)	2 (0%)	100	100
15	f	4474/4646 (96%)	4330 (97%)	140 (3%)	4 (0%)	51	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	m	4552/4646 (98%)	4435 (97%)	117 (3%)	0	100	100
15	n	4556/4646 (98%)	4432 (97%)	123 (3%)	1 (0%)	100	100
16	g	452/612 (74%)	439 (97%)	13 (3%)	0	100	100
16	h	454/612 (74%)	438 (96%)	16 (4%)	0	100	100
16	o	419/612 (68%)	397 (95%)	21 (5%)	1 (0%)	47	81
16	p	426/612 (70%)	408 (96%)	17 (4%)	1 (0%)	47	81
17	j	318/492 (65%)	312 (98%)	6 (2%)	0	100	100
17	q	314/492 (64%)	306 (98%)	8 (2%)	0	100	100
17	r	313/492 (64%)	306 (98%)	7 (2%)	0	100	100
17	u	292/492 (59%)	271 (93%)	21 (7%)	0	100	100
18	k	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
18	l	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
18	v	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
18	y	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
19	s	91/96 (95%)	78 (86%)	13 (14%)	0	100	100
19	t	91/96 (95%)	84 (92%)	7 (8%)	0	100	100
19	w	91/96 (95%)	80 (88%)	11 (12%)	0	100	100
19	z	91/96 (95%)	75 (82%)	16 (18%)	0	100	100
All	All	32190/36745 (88%)	31037 (96%)	1139 (4%)	14 (0%)	100	100

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	M	217	PRO
9	S	1137	PRO
16	o	127	ILE
15	f	1405	SER
15	f	1425	VAL
16	p	138	VAL
15	f	1409	LYS
9	T	1182	LYS
15	e	1965	GLU
7	Q	259	ALA
15	f	1965	GLU
15	n	340	PRO
15	e	595	PRO

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Mol	Chain	Res	Type
14	i	51	ASN

5.3.2 Protein sidechains

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

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 35 ligands modelled in this entry, 9 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	$\#\|Z\| > 2$
21	ATP	H	401	-	26,33,33	0.57	0	31,52,52	0.81	2 (6%)
21	ATP	e	4803	23	26,33,33	0.61	0	31,52,52	0.76	1 (3%)
24	ANP	m	4705	-	29,33,33	1.04	3 (10%)	31,52,52	1.39	3 (9%)
20	ADP	f	4806	-	24,29,29	0.94	1 (4%)	29,45,45	1.57	4 (13%)
20	ADP	B	800	-	24,29,29	0.96	1 (4%)	29,45,45	1.44	4 (13%)
20	ADP	D	800	-	24,29,29	1.01	1 (4%)	29,45,45	1.41	4 (13%)
20	ADP	e	4801	23	24,29,29	0.99	1 (4%)	29,45,45	1.45	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	ADP	C	800	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
24	ANP	m	4704	-	29,33,33	1.09	4 (13%)	31,52,52	1.10	2 (6%)
20	ADP	e	4805	-	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
21	ATP	n	4702	23	26,33,33	0.69	0	31,52,52	0.88	1 (3%)
20	ADP	I	800	-	24,29,29	0.97	1 (4%)	29,45,45	1.53	4 (13%)
21	ATP	m	4702	23	26,33,33	0.59	0	31,52,52	0.93	1 (3%)
20	ADP	f	4801	23	24,29,29	0.99	1 (4%)	29,45,45	1.45	6 (20%)
20	ADP	F	800	-	24,29,29	0.95	1 (4%)	29,45,45	1.42	4 (13%)
20	ADP	A	800	-	24,29,29	0.97	1 (4%)	29,45,45	1.43	4 (13%)
20	ADP	f	4805	-	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
20	ADP	G	800	-	24,29,29	0.98	1 (4%)	29,45,45	1.44	4 (13%)
24	ANP	n	4704	-	29,33,33	1.08	4 (13%)	31,52,52	1.27	4 (12%)
20	ADP	e	4806	-	24,29,29	0.95	1 (4%)	29,45,45	1.57	4 (13%)
20	ADP	E	800	-	24,29,29	0.97	1 (4%)	29,45,45	1.40	4 (13%)
21	ATP	J	800	-	26,33,33	0.61	0	31,52,52	0.88	1 (3%)
21	ATP	f	4803	23	26,33,33	0.61	0	31,52,52	0.76	1 (3%)
20	ADP	n	4701	-	24,29,29	1.00	1 (4%)	29,45,45	1.41	6 (20%)
20	ADP	m	4701	-	24,29,29	1.01	1 (4%)	29,45,45	1.38	4 (13%)
24	ANP	n	4705	-	29,33,33	1.05	3 (10%)	31,52,52	1.42	4 (12%)

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
21	ATP	H	401	-	-	7/18/38/38	0/3/3/3
21	ATP	e	4803	23	-	2/18/38/38	0/3/3/3
24	ANP	m	4705	-	-	2/14/38/38	0/3/3/3
20	ADP	f	4806	-	-	2/12/32/32	0/3/3/3
20	ADP	B	800	-	-	2/12/32/32	0/3/3/3
20	ADP	D	800	-	-	4/12/32/32	0/3/3/3
20	ADP	e	4801	23	-	3/12/32/32	0/3/3/3
20	ADP	C	800	-	-	2/12/32/32	0/3/3/3
24	ANP	m	4704	-	-	5/14/38/38	0/3/3/3
20	ADP	e	4805	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	ATP	n	4702	23	-	2/18/38/38	0/3/3/3
20	ADP	I	800	-	-	3/12/32/32	0/3/3/3
21	ATP	m	4702	23	-	7/18/38/38	0/3/3/3
20	ADP	f	4801	23	-	3/12/32/32	0/3/3/3
20	ADP	F	800	-	-	2/12/32/32	0/3/3/3
20	ADP	A	800	-	-	1/12/32/32	0/3/3/3
20	ADP	f	4805	-	-	1/12/32/32	0/3/3/3
20	ADP	G	800	-	-	4/12/32/32	0/3/3/3
24	ANP	n	4704	-	-	6/14/38/38	0/3/3/3
20	ADP	e	4806	-	-	2/12/32/32	0/3/3/3
20	ADP	E	800	-	-	5/12/32/32	0/3/3/3
21	ATP	J	800	-	-	7/18/38/38	0/3/3/3
21	ATP	f	4803	23	-	2/18/38/38	0/3/3/3
20	ADP	n	4701	-	-	7/12/32/32	0/3/3/3
20	ADP	m	4701	-	-	3/12/32/32	0/3/3/3
24	ANP	n	4705	-	-	2/14/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	m	4704	ANP	PB-O3A	-3.09	1.55	1.59
24	n	4704	ANP	PB-O3A	-2.67	1.55	1.59
20	m	4701	ADP	C5-C4	2.61	1.47	1.40
20	C	800	ADP	C5-C4	2.56	1.47	1.40
20	E	800	ADP	C5-C4	2.56	1.47	1.40
20	D	800	ADP	C5-C4	2.56	1.47	1.40
20	n	4701	ADP	C5-C4	2.56	1.47	1.40
24	n	4705	ANP	PG-N3B	2.52	1.70	1.63
20	I	800	ADP	C5-C4	2.52	1.47	1.40
20	G	800	ADP	C5-C4	2.51	1.47	1.40
20	e	4806	ADP	C5-C4	2.50	1.47	1.40
20	F	800	ADP	C5-C4	2.49	1.47	1.40
20	B	800	ADP	C5-C4	2.49	1.47	1.40
24	m	4705	ANP	PG-O1G	2.49	1.50	1.46
24	n	4705	ANP	PG-O1G	2.48	1.50	1.46
20	f	4806	ADP	C5-C4	2.47	1.47	1.40
20	A	800	ADP	C5-C4	2.47	1.47	1.40
20	f	4805	ADP	C5-C4	2.46	1.47	1.40
20	e	4801	ADP	C5-C4	2.46	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	4704	ANP	PG-O1G	2.45	1.50	1.46
20	e	4805	ADP	C5-C4	2.45	1.47	1.40
24	m	4705	ANP	PG-N3B	2.45	1.69	1.63
20	f	4801	ADP	C5-C4	2.44	1.47	1.40
24	n	4705	ANP	PB-O3A	-2.39	1.56	1.59
24	m	4704	ANP	PG-O1G	2.38	1.49	1.46
24	m	4705	ANP	PB-O3A	-2.35	1.56	1.59
24	n	4704	ANP	PG-N3B	2.24	1.69	1.63
24	m	4704	ANP	PG-N3B	2.20	1.69	1.63
24	n	4704	ANP	PB-O1B	2.05	1.49	1.46
24	m	4704	ANP	PB-O1B	2.05	1.49	1.46

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	m	4705	ANP	PB-O3A-PA	-4.66	116.20	132.62
24	n	4704	ANP	PB-O3A-PA	-4.63	116.30	132.62
24	n	4705	ANP	PB-O3A-PA	-4.49	116.81	132.62
24	n	4705	ANP	O1B-PB-N3B	-4.21	105.57	111.77
24	m	4704	ANP	PB-O3A-PA	-3.97	118.64	132.62
20	e	4806	ADP	PA-O3A-PB	-3.96	119.24	132.83
20	f	4806	ADP	PA-O3A-PB	-3.96	119.25	132.83
20	I	800	ADP	PA-O3A-PB	-3.87	119.53	132.83
20	e	4806	ADP	C3'-C2'-C1'	3.76	106.64	100.98
20	f	4806	ADP	C3'-C2'-C1'	3.73	106.60	100.98
20	m	4701	ADP	N3-C2-N1	-3.72	122.87	128.68
20	f	4805	ADP	C3'-C2'-C1'	3.65	106.48	100.98
24	m	4705	ANP	O1B-PB-N3B	-3.64	106.40	111.77
20	e	4805	ADP	C3'-C2'-C1'	3.63	106.44	100.98
20	n	4701	ADP	N3-C2-N1	-3.62	123.02	128.68
20	f	4805	ADP	N3-C2-N1	-3.53	123.15	128.68
20	e	4805	ADP	N3-C2-N1	-3.53	123.16	128.68
20	e	4801	ADP	PA-O3A-PB	-3.46	120.96	132.83
20	f	4801	ADP	PA-O3A-PB	-3.44	121.02	132.83
20	C	800	ADP	C3'-C2'-C1'	3.43	106.14	100.98
20	G	800	ADP	PA-O3A-PB	-3.42	121.09	132.83
20	E	800	ADP	PA-O3A-PB	-3.42	121.10	132.83
20	B	800	ADP	C3'-C2'-C1'	3.41	106.11	100.98
20	G	800	ADP	N3-C2-N1	-3.37	123.41	128.68
20	I	800	ADP	C3'-C2'-C1'	3.35	106.02	100.98
20	D	800	ADP	PA-O3A-PB	-3.34	121.35	132.83
20	D	800	ADP	N3-C2-N1	-3.34	123.46	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	800	ADP	C3'-C2'-C1'	3.33	105.99	100.98
20	F	800	ADP	PA-O3A-PB	-3.33	121.42	132.83
20	A	800	ADP	PA-O3A-PB	-3.32	121.42	132.83
20	f	4806	ADP	N3-C2-N1	-3.32	123.49	128.68
20	f	4801	ADP	N3-C2-N1	-3.31	123.50	128.68
20	B	800	ADP	N3-C2-N1	-3.30	123.52	128.68
20	e	4806	ADP	N3-C2-N1	-3.30	123.52	128.68
20	e	4801	ADP	N3-C2-N1	-3.29	123.53	128.68
20	A	800	ADP	N3-C2-N1	-3.28	123.56	128.68
20	F	800	ADP	N3-C2-N1	-3.27	123.56	128.68
20	I	800	ADP	N3-C2-N1	-3.27	123.57	128.68
20	C	800	ADP	N3-C2-N1	-3.22	123.65	128.68
20	E	800	ADP	N3-C2-N1	-3.18	123.71	128.68
20	n	4701	ADP	PA-O3A-PB	-3.14	122.04	132.83
20	e	4805	ADP	PA-O3A-PB	-3.14	122.04	132.83
20	f	4805	ADP	PA-O3A-PB	-3.14	122.05	132.83
20	G	800	ADP	C3'-C2'-C1'	3.10	105.65	100.98
20	E	800	ADP	C3'-C2'-C1'	3.10	105.64	100.98
20	C	800	ADP	PA-O3A-PB	-3.09	122.23	132.83
20	B	800	ADP	PA-O3A-PB	-3.02	122.45	132.83
20	A	800	ADP	C3'-C2'-C1'	2.92	105.37	100.98
20	m	4701	ADP	PA-O3A-PB	-2.83	123.12	132.83
20	E	800	ADP	C4-C5-N7	-2.67	106.62	109.40
20	A	800	ADP	C4-C5-N7	-2.66	106.62	109.40
20	G	800	ADP	C4-C5-N7	-2.62	106.67	109.40
20	B	800	ADP	C4-C5-N7	-2.62	106.67	109.40
20	f	4801	ADP	C3'-C2'-C1'	2.59	104.88	100.98
20	D	800	ADP	C3'-C2'-C1'	2.57	104.84	100.98
20	e	4801	ADP	C3'-C2'-C1'	2.57	104.84	100.98
20	f	4806	ADP	C4-C5-N7	-2.55	106.74	109.40
20	D	800	ADP	C4-C5-N7	-2.54	106.75	109.40
20	F	800	ADP	C4-C5-N7	-2.54	106.75	109.40
20	C	800	ADP	C4-C5-N7	-2.53	106.77	109.40
20	e	4806	ADP	C4-C5-N7	-2.52	106.77	109.40
20	e	4801	ADP	C4-C5-N7	-2.50	106.79	109.40
20	f	4801	ADP	C4-C5-N7	-2.50	106.79	109.40
20	I	800	ADP	C4-C5-N7	-2.48	106.82	109.40
20	n	4701	ADP	C4-C5-N7	-2.47	106.82	109.40
20	m	4701	ADP	C4-C5-N7	-2.35	106.94	109.40
20	f	4805	ADP	C4-C5-N7	-2.32	106.98	109.40
20	m	4701	ADP	C2-N1-C6	2.31	122.70	118.75
24	n	4704	ANP	O1B-PB-N3B	-2.29	108.39	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	e	4803	ATP	C5-C6-N6	2.29	123.83	120.35
20	e	4805	ADP	C4-C5-N7	-2.28	107.02	109.40
21	f	4803	ATP	C5-C6-N6	2.27	123.81	120.35
21	m	4702	ATP	C5-C6-N6	2.26	123.79	120.35
24	m	4705	ANP	C5-C6-N6	2.25	123.78	120.35
21	n	4702	ATP	C5-C6-N6	2.25	123.77	120.35
24	m	4704	ANP	C5-C6-N6	2.25	123.77	120.35
21	H	401	ATP	C5-C6-N6	2.24	123.75	120.35
21	J	800	ATP	C5-C6-N6	2.19	123.68	120.35
20	n	4701	ADP	O3B-PB-O2B	2.17	115.94	107.64
24	n	4704	ANP	C5-C6-N6	2.14	123.60	120.35
21	H	401	ATP	PB-O3B-PG	2.10	140.05	132.83
24	n	4705	ANP	C5-C6-N6	2.09	123.53	120.35
20	e	4801	ADP	C2'-C3'-C4'	2.07	106.67	102.64
20	n	4701	ADP	C3'-C2'-C1'	2.06	104.09	100.98
24	n	4705	ANP	O3A-PB-N3B	2.06	112.30	106.59
20	n	4701	ADP	C2-N1-C6	2.06	122.27	118.75
20	f	4801	ADP	C2'-C3'-C4'	2.05	106.63	102.64
20	f	4801	ADP	C2-N1-C6	2.04	122.24	118.75
20	e	4801	ADP	C2-N1-C6	2.03	122.23	118.75
24	n	4704	ANP	O1G-PG-N3B	-2.01	108.81	111.77

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	B	800	ADP	O4'-C4'-C5'-O5'
20	C	800	ADP	C5'-O5'-PA-O2A
20	C	800	ADP	C5'-O5'-PA-O3A
20	D	800	ADP	C3'-C4'-C5'-O5'
20	E	800	ADP	PA-O3A-PB-O3B
20	E	800	ADP	C5'-O5'-PA-O1A
20	E	800	ADP	C5'-O5'-PA-O2A
20	E	800	ADP	C5'-O5'-PA-O3A
20	G	800	ADP	C5'-O5'-PA-O1A
20	G	800	ADP	C5'-O5'-PA-O2A
20	I	800	ADP	C5'-O5'-PA-O1A
20	I	800	ADP	C5'-O5'-PA-O2A
20	n	4701	ADP	C5'-O5'-PA-O1A
20	n	4701	ADP	C5'-O5'-PA-O2A
21	H	401	ATP	C5'-O5'-PA-O1A
21	H	401	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
21	H	401	ATP	C3'-C4'-C5'-O5'
21	J	800	ATP	PB-O3B-PG-O2G
21	J	800	ATP	C5'-O5'-PA-O3A
21	J	800	ATP	O4'-C4'-C5'-O5'
21	J	800	ATP	C3'-C4'-C5'-O5'
21	m	4702	ATP	C5'-O5'-PA-O1A
21	m	4702	ATP	C5'-O5'-PA-O2A
21	m	4702	ATP	O4'-C4'-C5'-O5'
21	m	4702	ATP	C3'-C4'-C5'-O5'
21	n	4702	ATP	PB-O3B-PG-O3G
24	m	4704	ANP	C5'-O5'-PA-O1A
24	m	4704	ANP	C5'-O5'-PA-O2A
24	m	4704	ANP	C5'-O5'-PA-O3A
24	m	4705	ANP	PG-N3B-PB-O1B
24	m	4705	ANP	PG-N3B-PB-O3A
24	n	4704	ANP	PG-N3B-PB-O1B
24	n	4704	ANP	C5'-O5'-PA-O1A
24	n	4704	ANP	C5'-O5'-PA-O2A
24	n	4704	ANP	C5'-O5'-PA-O3A
24	n	4705	ANP	PG-N3B-PB-O1B
24	n	4705	ANP	PG-N3B-PB-O3A
20	D	800	ADP	O4'-C4'-C5'-O5'
20	F	800	ADP	O4'-C4'-C5'-O5'
24	m	4704	ANP	O4'-C4'-C5'-O5'
20	B	800	ADP	C3'-C4'-C5'-O5'
20	F	800	ADP	C3'-C4'-C5'-O5'
20	e	4806	ADP	O4'-C4'-C5'-O5'
20	f	4806	ADP	O4'-C4'-C5'-O5'
21	H	401	ATP	O4'-C4'-C5'-O5'
24	m	4704	ANP	C3'-C4'-C5'-O5'
24	n	4704	ANP	O4'-C4'-C5'-O5'
24	n	4704	ANP	C3'-C4'-C5'-O5'
20	e	4806	ADP	C3'-C4'-C5'-O5'
20	f	4806	ADP	C3'-C4'-C5'-O5'
20	A	800	ADP	O4'-C4'-C5'-O5'
21	J	800	ATP	PB-O3B-PG-O1G
21	m	4702	ATP	PB-O3B-PG-O1G
21	H	401	ATP	PB-O3A-PA-O5'
20	m	4701	ADP	O4'-C4'-C5'-O5'
20	E	800	ADP	PA-O3A-PB-O1B
21	n	4702	ATP	PB-O3B-PG-O1G
21	m	4702	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
20	D	800	ADP	C5'-O5'-PA-O3A
20	G	800	ADP	C5'-O5'-PA-O3A
20	e	4801	ADP	O4'-C4'-C5'-O5'
20	f	4801	ADP	O4'-C4'-C5'-O5'
20	m	4701	ADP	PB-O3A-PA-O1A
21	J	800	ATP	C5'-O5'-PA-O1A
21	J	800	ATP	C5'-O5'-PA-O2A
20	n	4701	ADP	O4'-C4'-C5'-O5'
20	e	4801	ADP	PA-O3A-PB-O1B
20	f	4801	ADP	PA-O3A-PB-O1B
20	G	800	ADP	C3'-C4'-C5'-O5'
20	m	4701	ADP	PB-O3A-PA-O2A
21	H	401	ATP	PA-O3A-PB-O2B
21	e	4803	ATP	O4'-C4'-C5'-O5'
21	f	4803	ATP	O4'-C4'-C5'-O5'
20	n	4701	ADP	PB-O3A-PA-O1A
21	e	4803	ATP	C3'-C4'-C5'-O5'
21	f	4803	ATP	C3'-C4'-C5'-O5'
20	n	4701	ADP	C3'-C4'-C5'-O5'
20	I	800	ADP	C5'-O5'-PA-O3A
20	n	4701	ADP	C5'-O5'-PA-O3A
21	H	401	ATP	C5'-O5'-PA-O3A
21	m	4702	ATP	C5'-O5'-PA-O3A
20	e	4805	ADP	O4'-C4'-C5'-O5'
20	f	4805	ADP	O4'-C4'-C5'-O5'
20	n	4701	ADP	PB-O3A-PA-O2A
20	D	800	ADP	C5'-O5'-PA-O1A
20	e	4801	ADP	C5'-O5'-PA-O1A
20	f	4801	ADP	C5'-O5'-PA-O1A

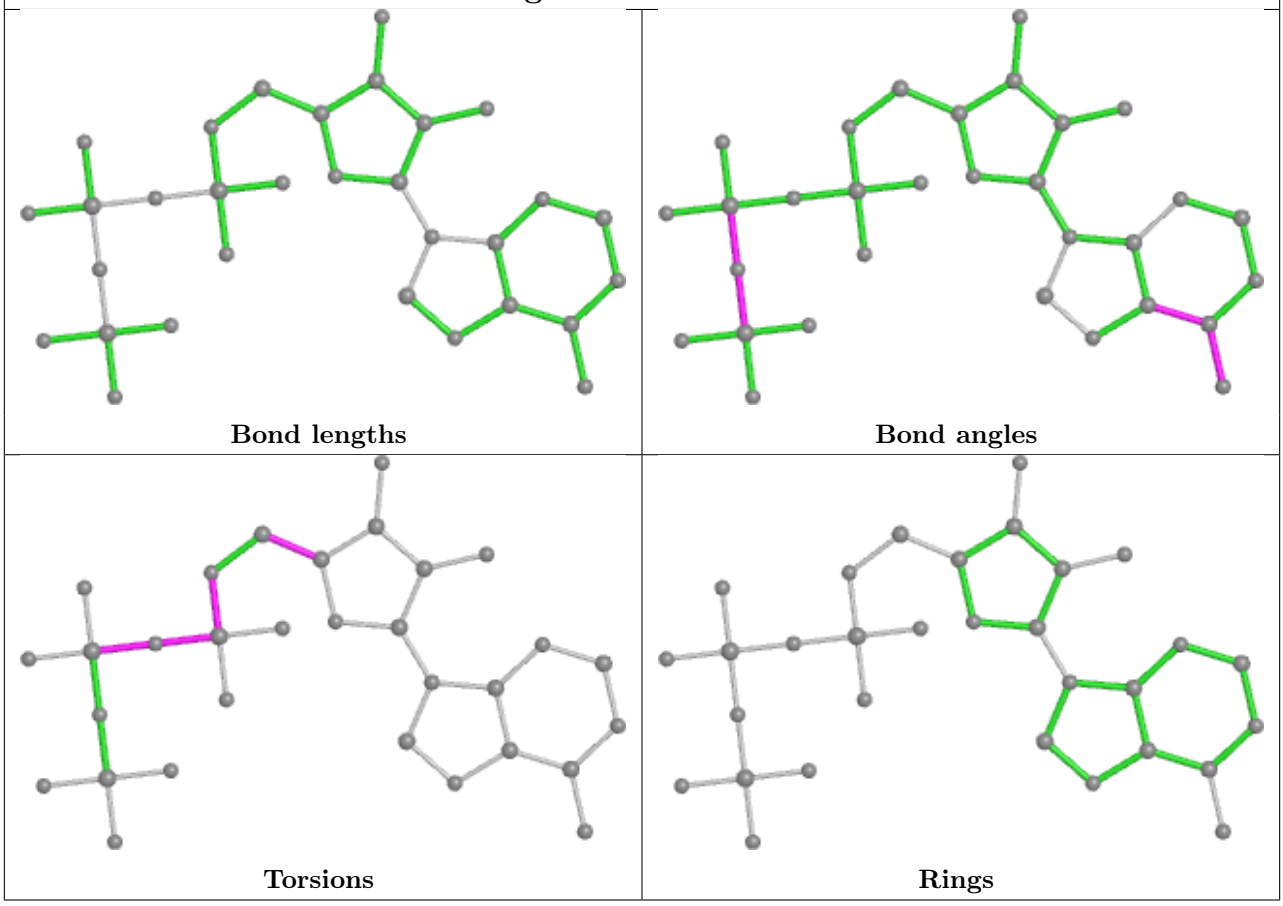
There are no ring outliers.

No monomer is involved in short contacts.

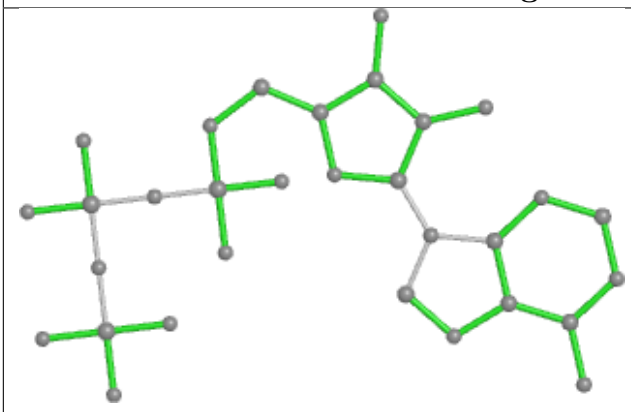
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

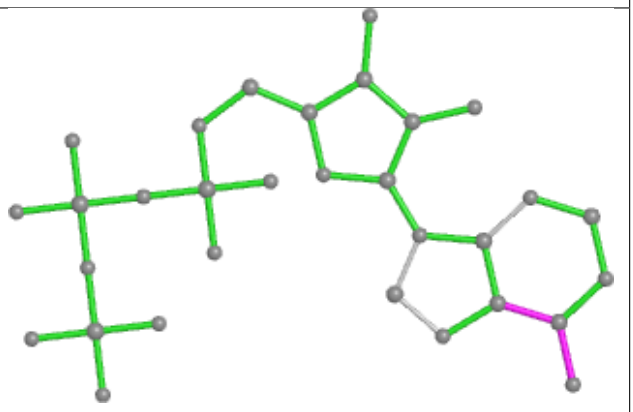
Ligand ATP H 401



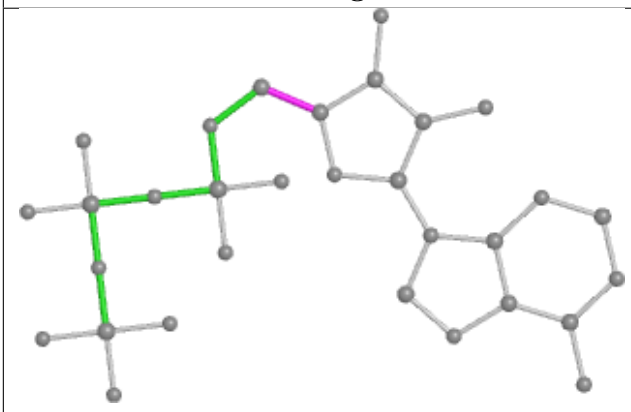
Ligand ATP e 4803



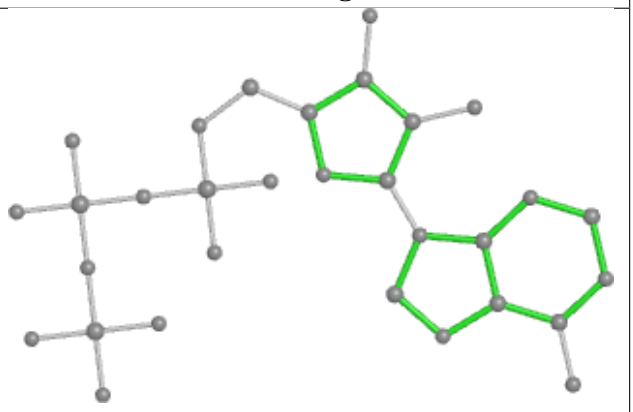
Bond lengths



Bond angles

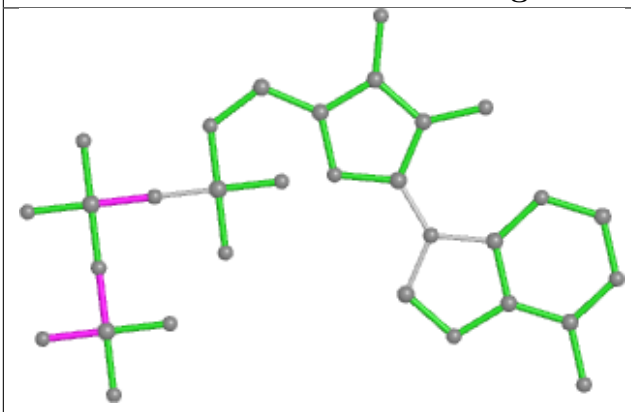


Torsions

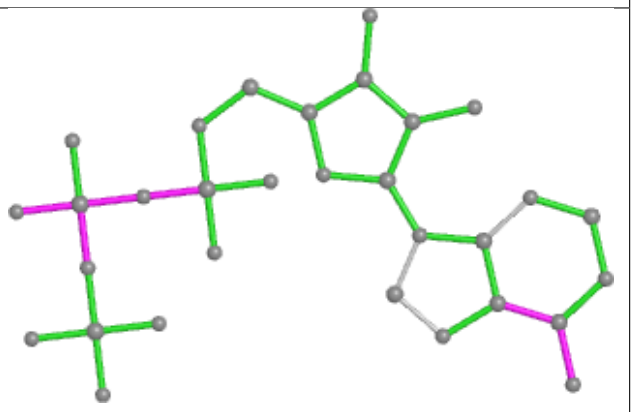


Rings

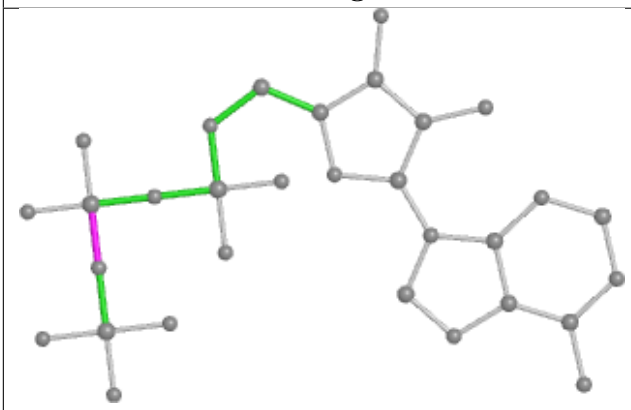
Ligand ANP m 4705



Bond lengths



Bond angles



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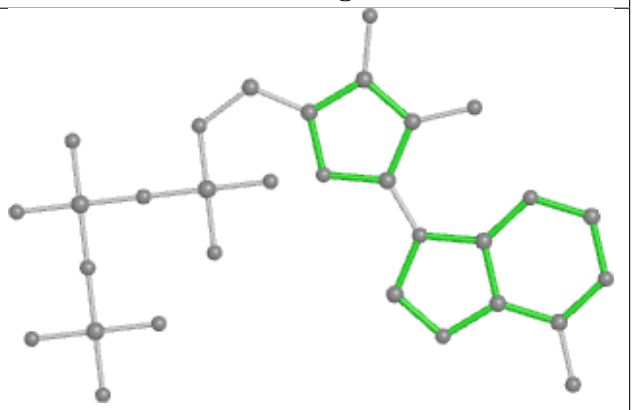
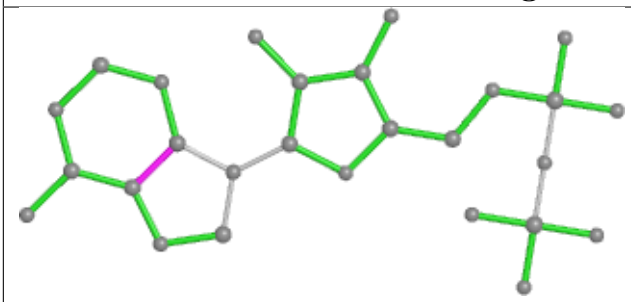
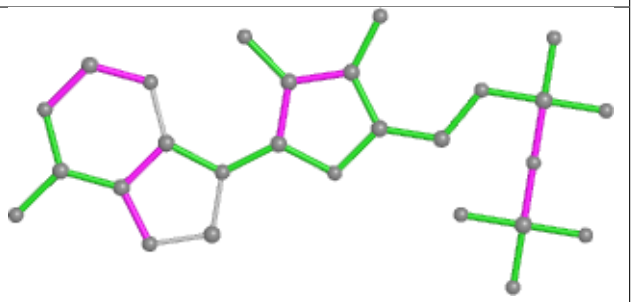


Rings

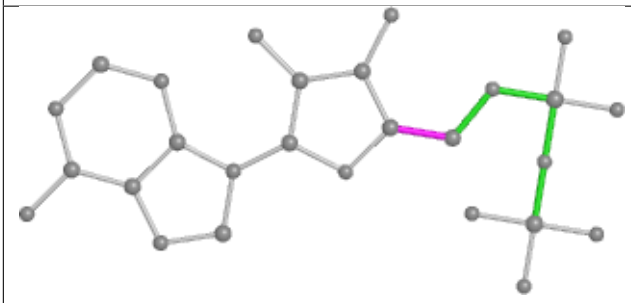
Ligand ADP f 4806



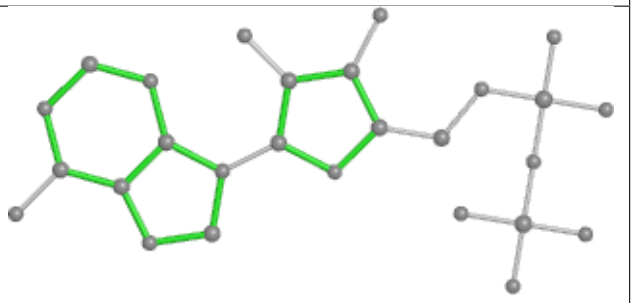
Bond lengths



Bond angles

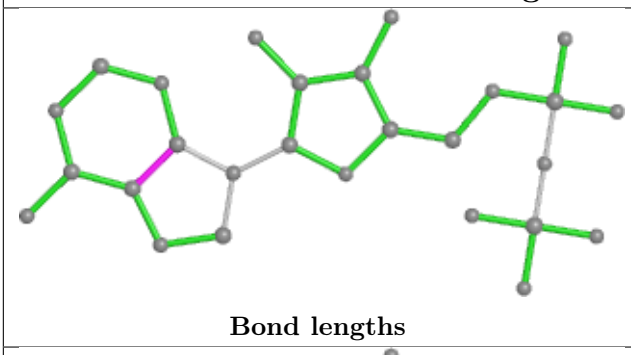


Torsions

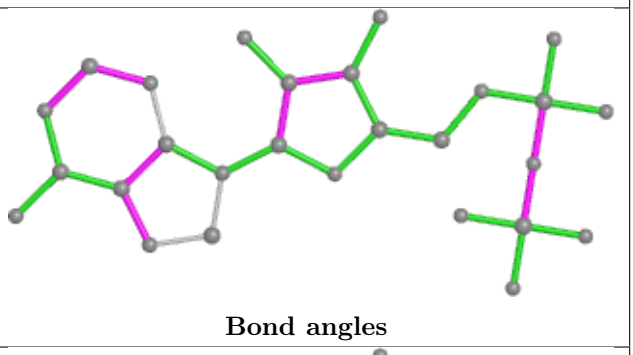


Rings

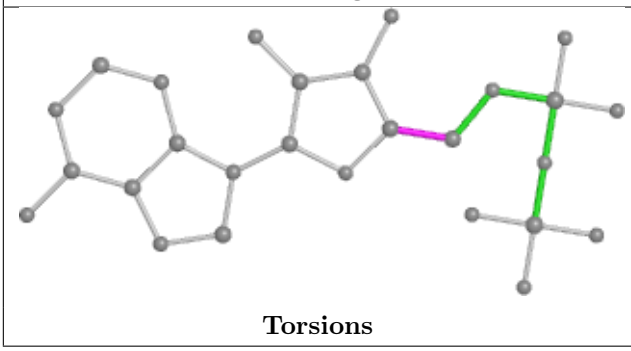
Ligand ADP B 800



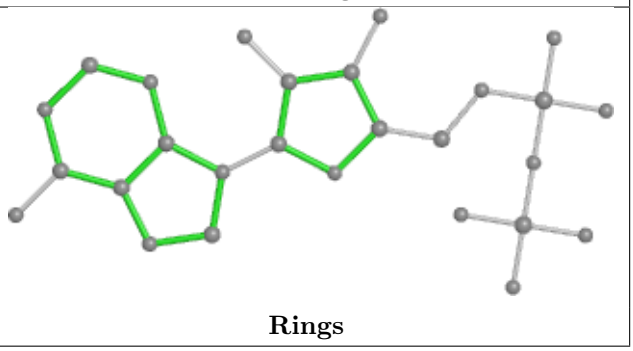
Bond lengths



Bond angles

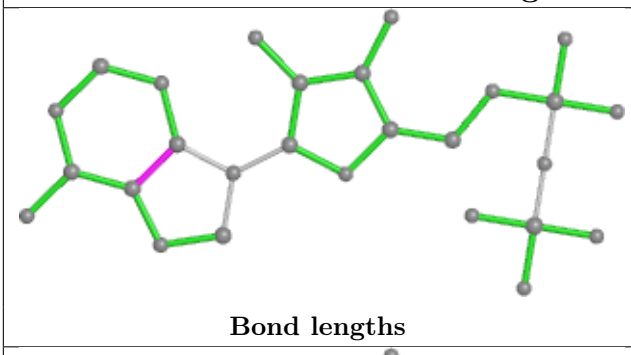


Torsions

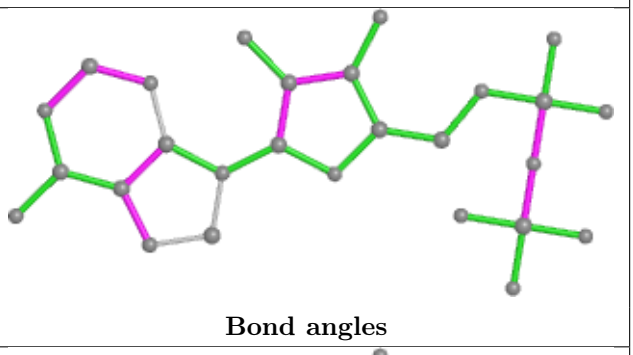


Rings

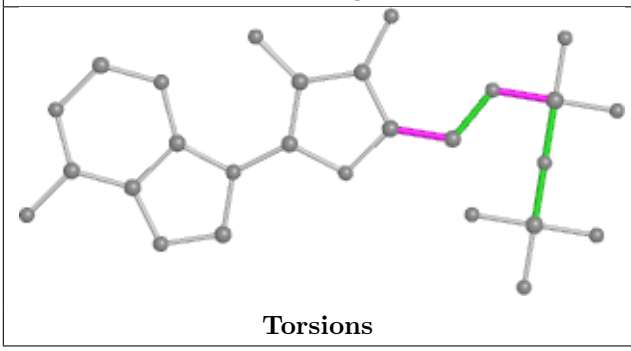
Ligand ADP D 800



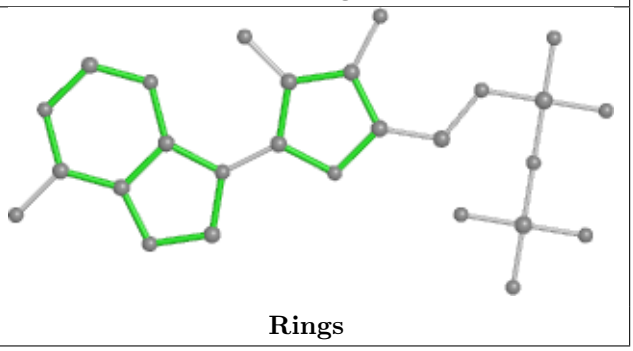
Bond lengths



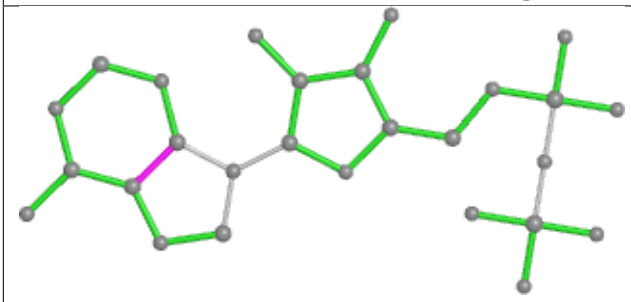
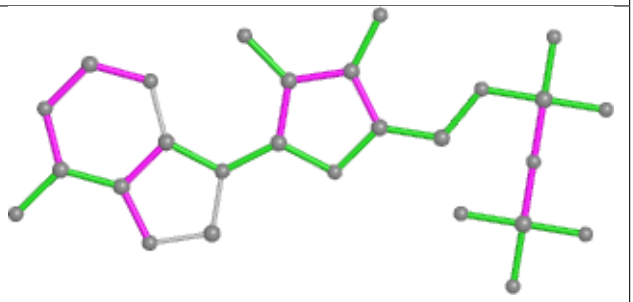
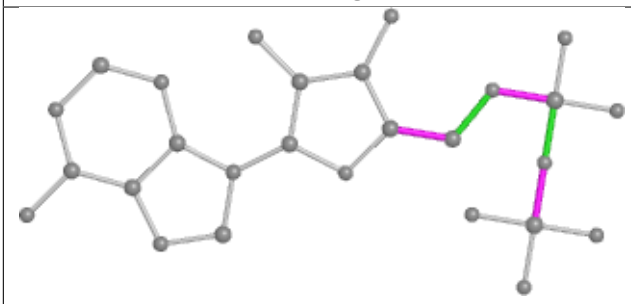
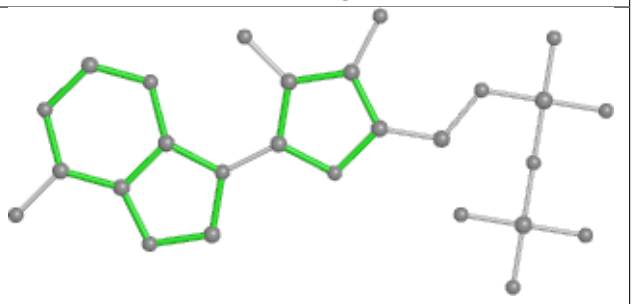
Bond angles

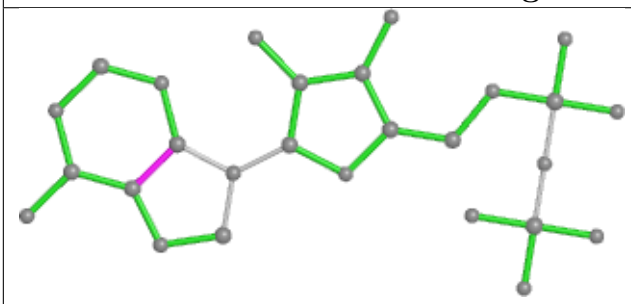
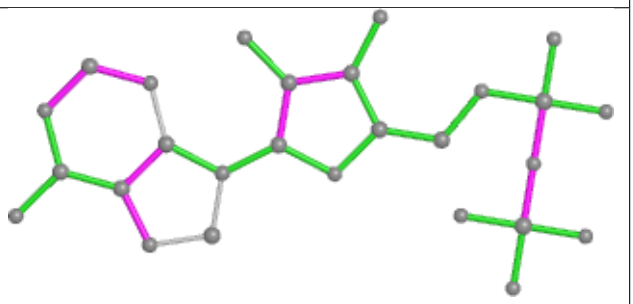
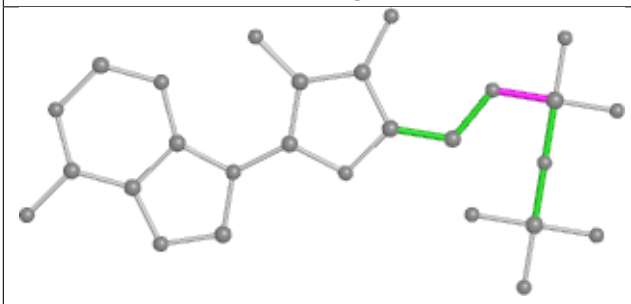
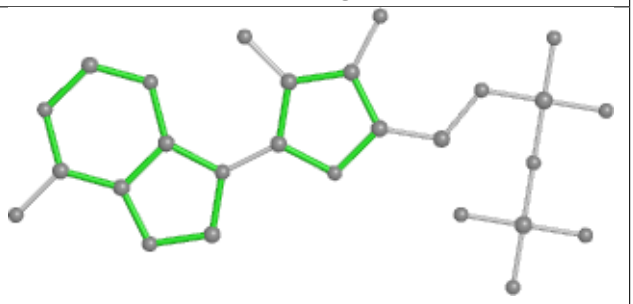


Torsions

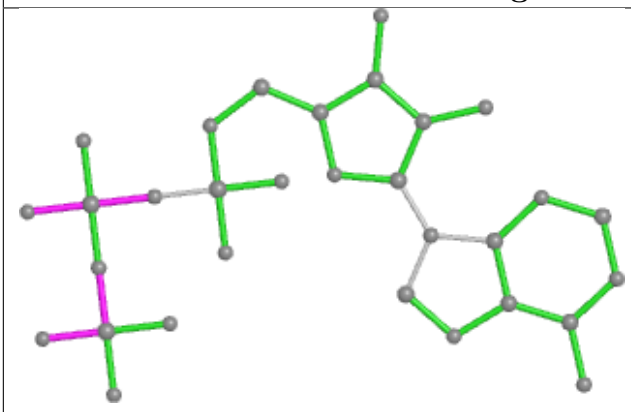


Rings

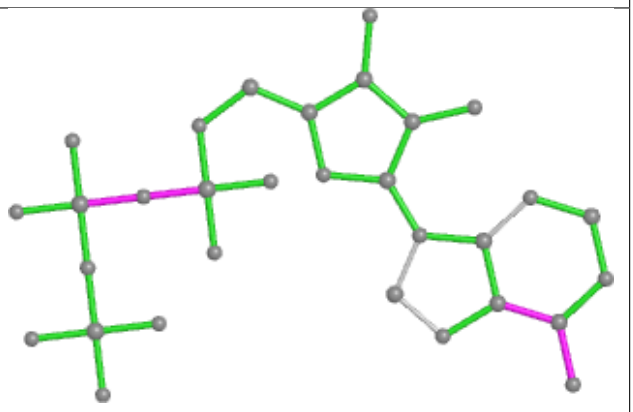
Ligand ADP e 4801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

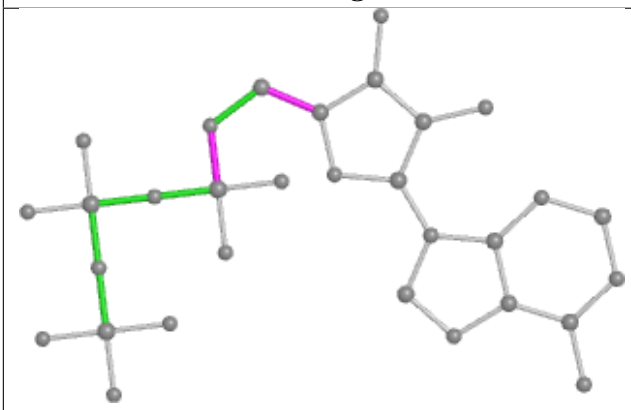
Ligand ANP m 4704



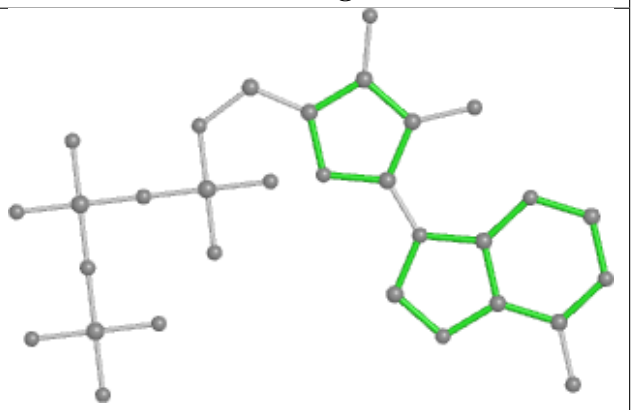
Bond lengths



Bond angles

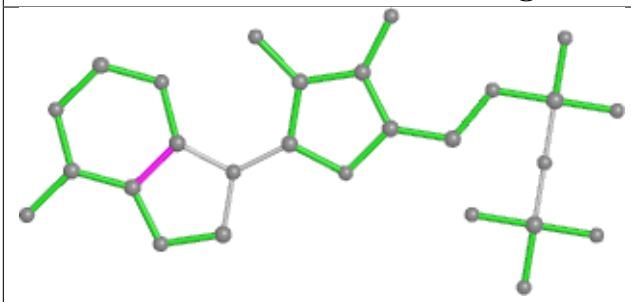


Torsions

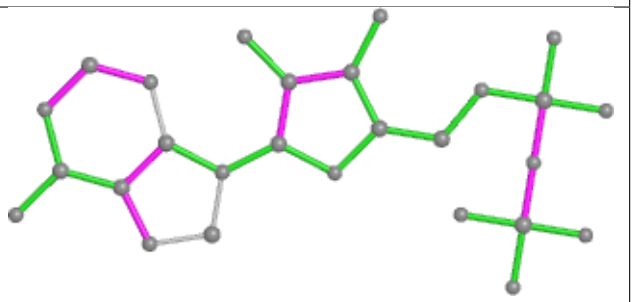


Rings

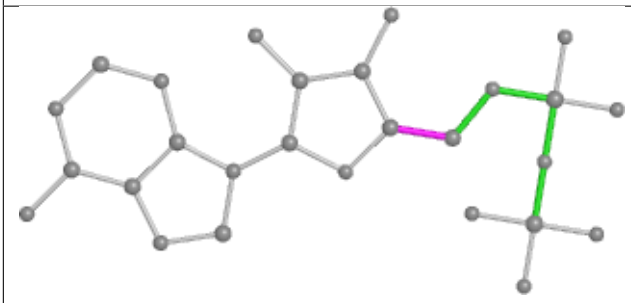
Ligand ADP e 4805



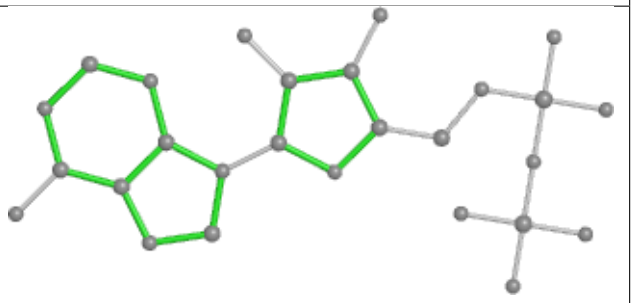
Bond lengths



Bond angles

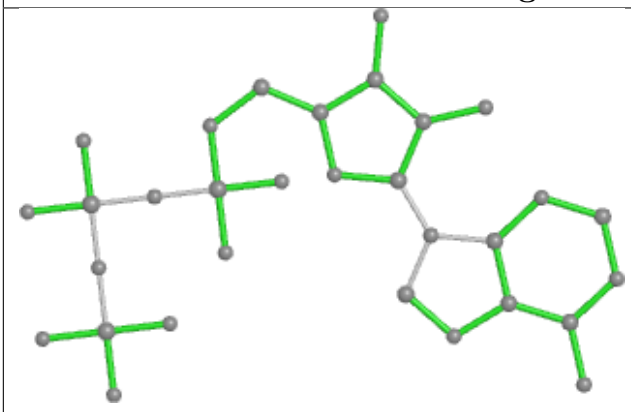


Torsions

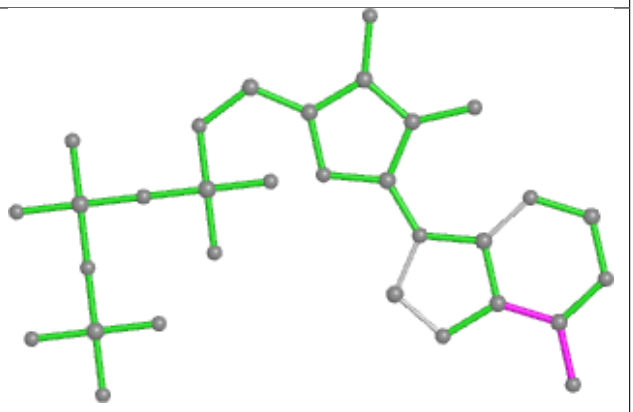


Rings

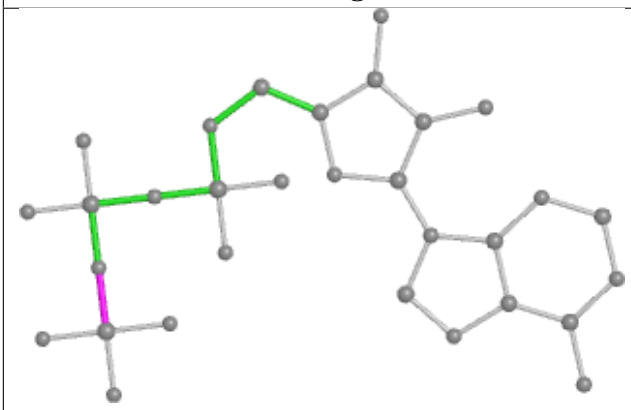
Ligand ATP n 4702



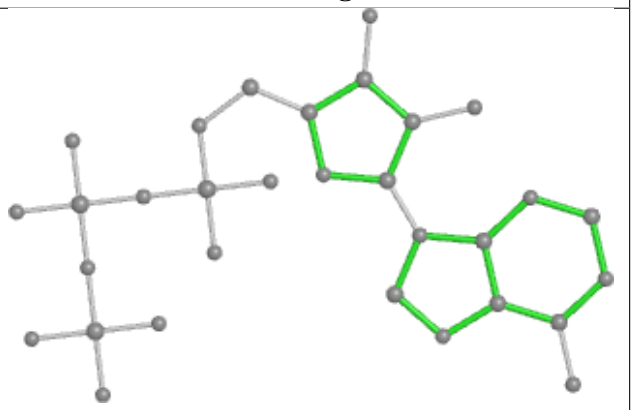
Bond lengths



Bond angles

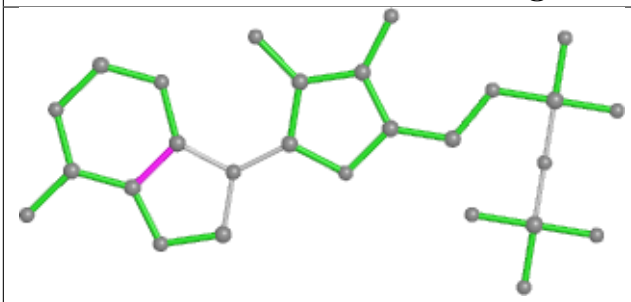


Torsions



Rings

Ligand ADP I 800



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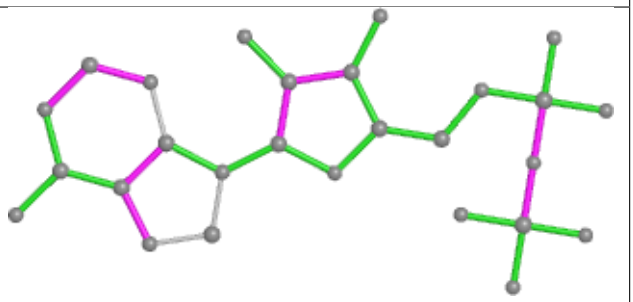
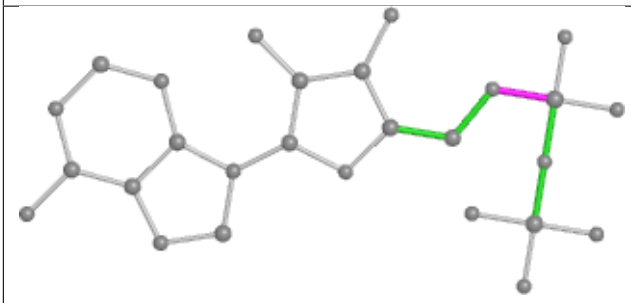
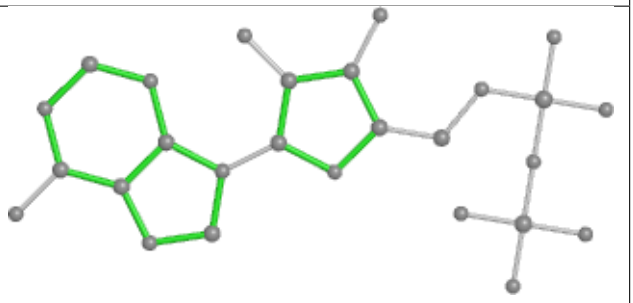


Bond angles

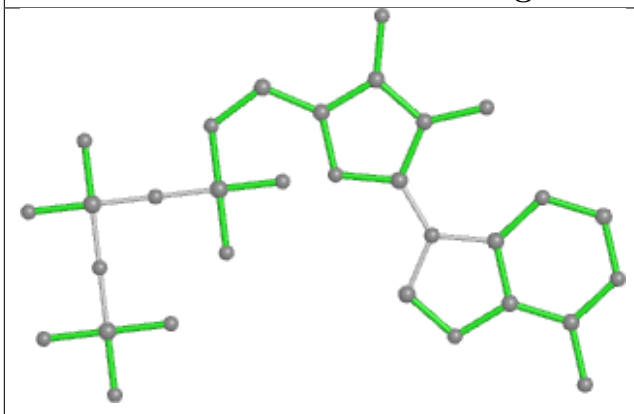


Torsions



Rings

Ligand ATP m 4702



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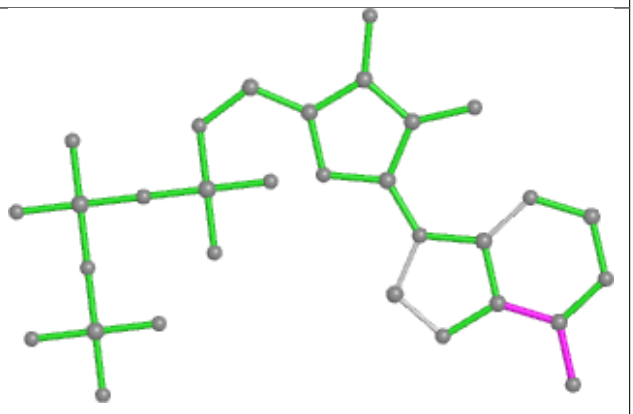
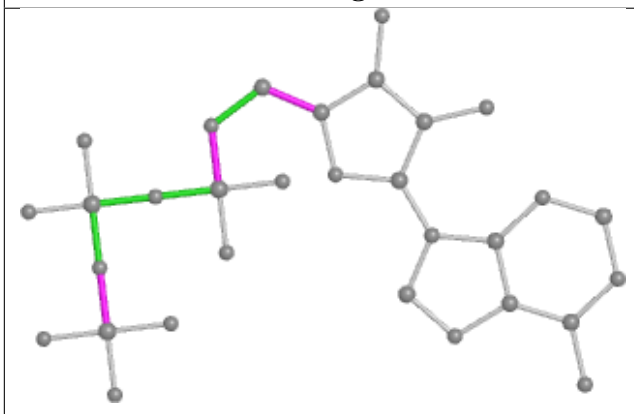


Bond angles



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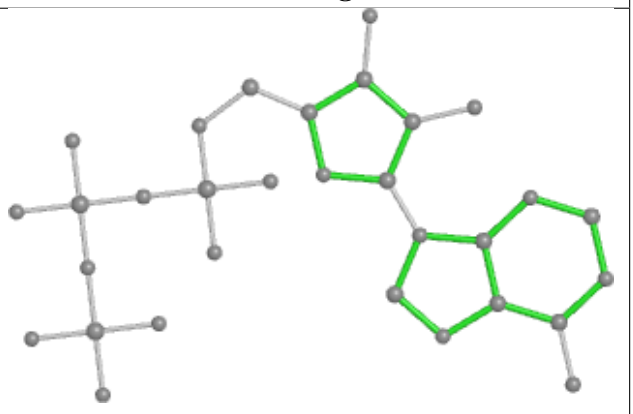
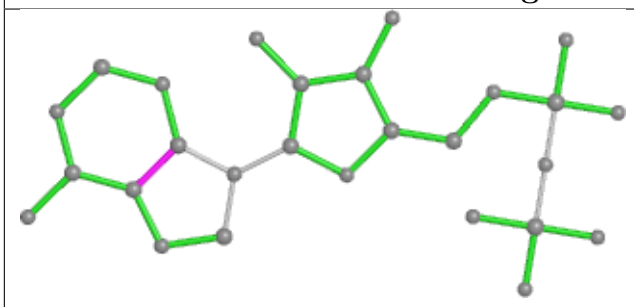


Rings

Ligand ADP f 4801



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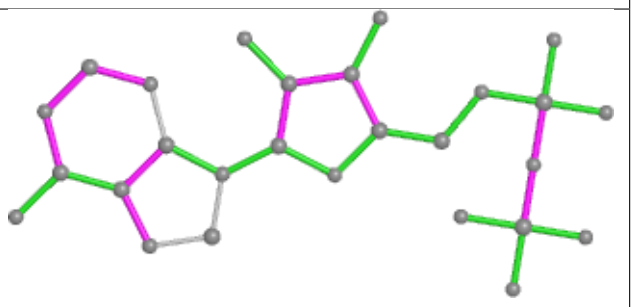
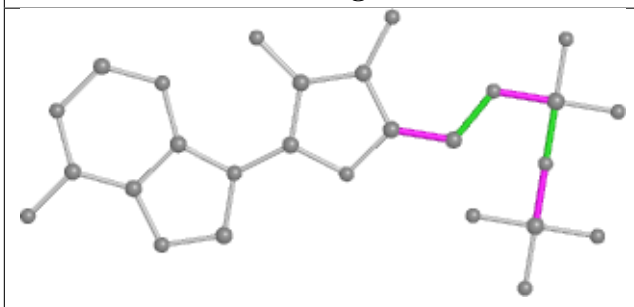


Bond angles



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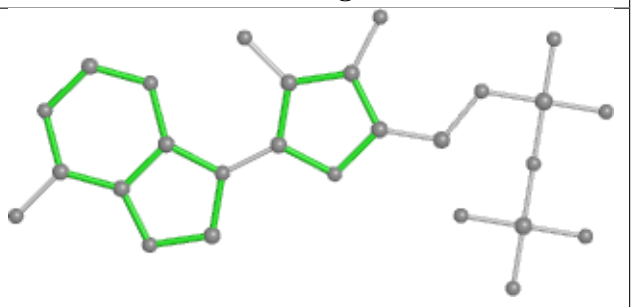
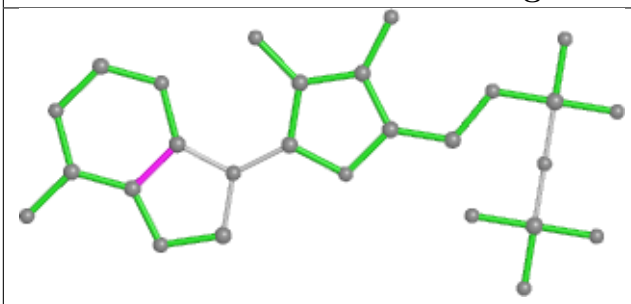


Rings

Ligand ADP F 800



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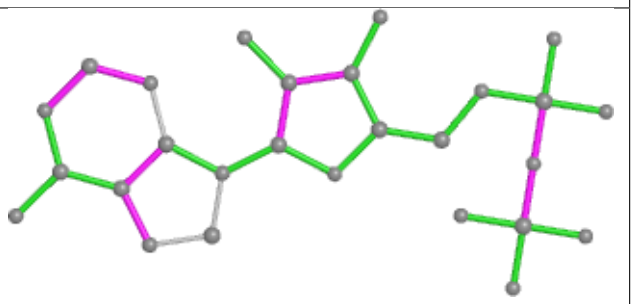
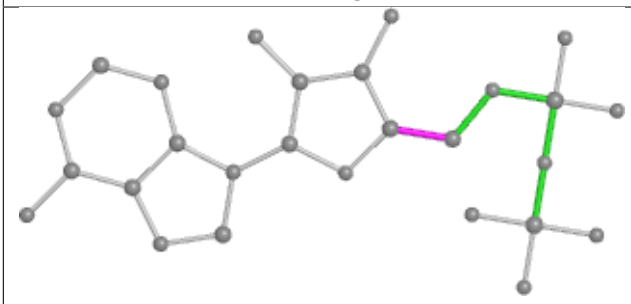
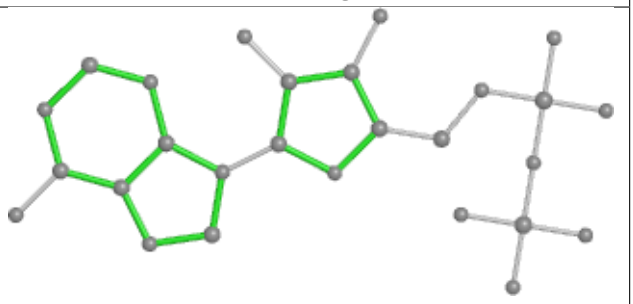


Bond angles

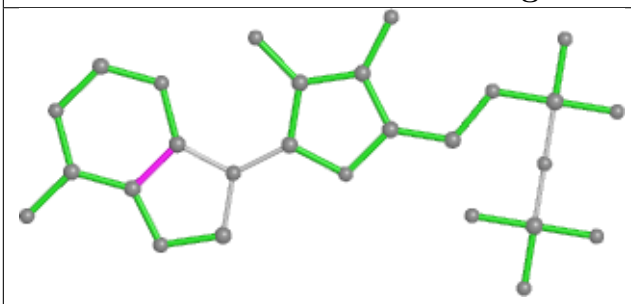


Torsions

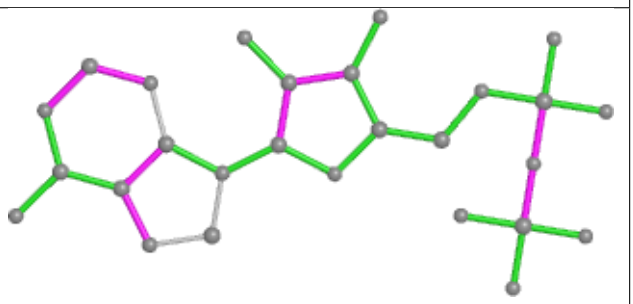


Rings

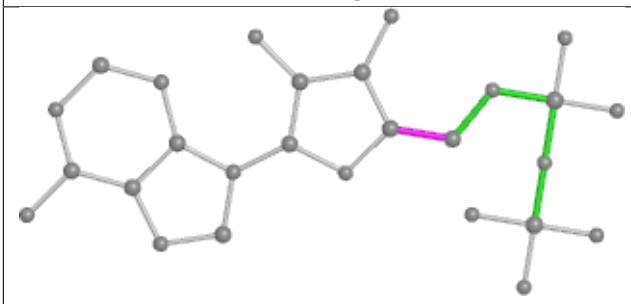
Ligand ADP A 800



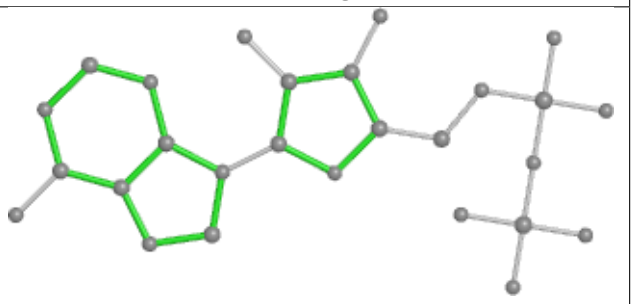
Bond lengths



Bond angles

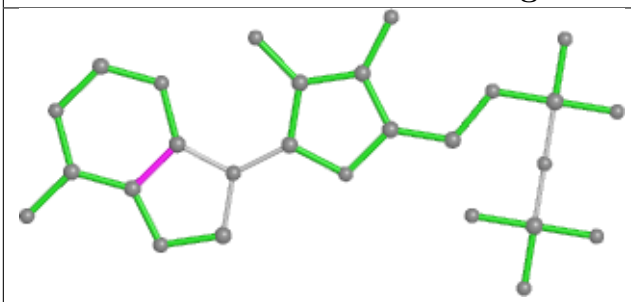


Torsions

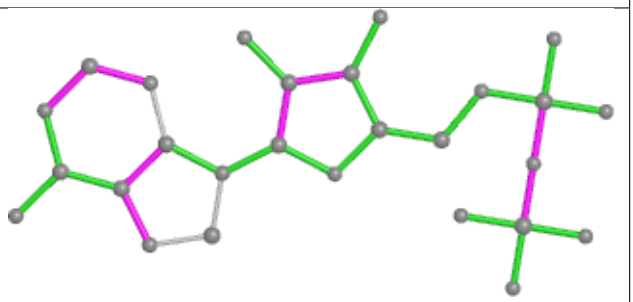


Rings

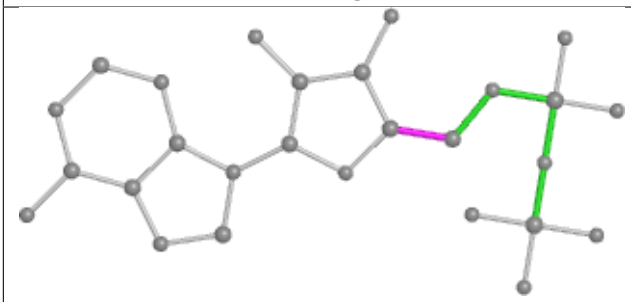
Ligand ADP f 4805



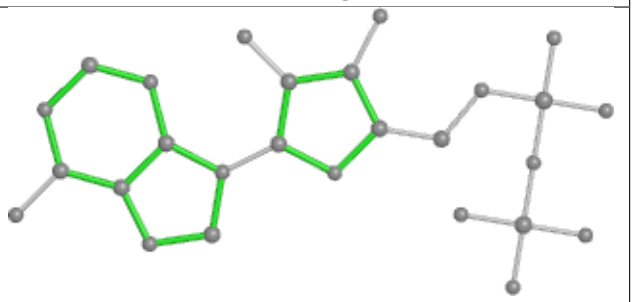
Bond lengths



Bond angles

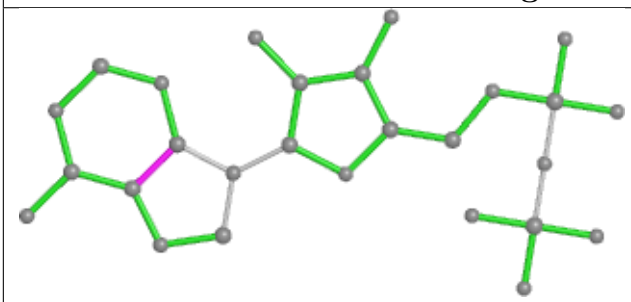


Torsions



Rings

Ligand ADP G 800



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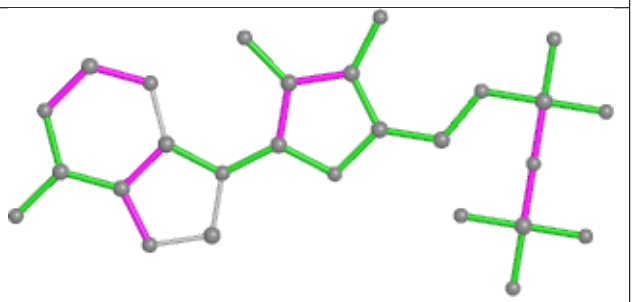
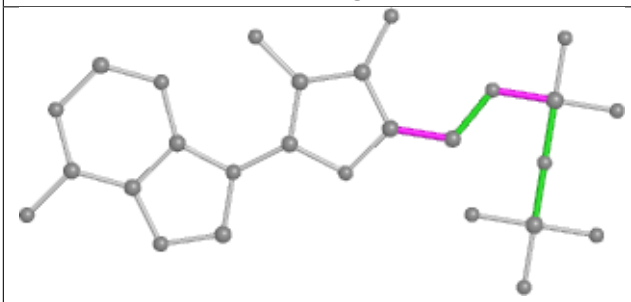
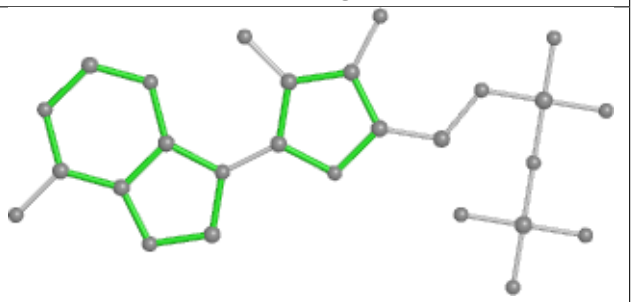


Bond angles

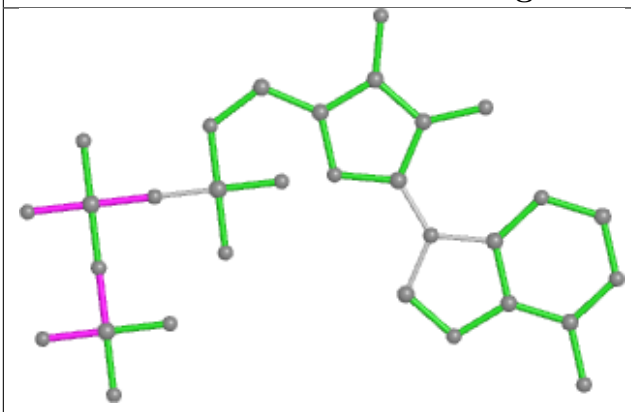


Torsions

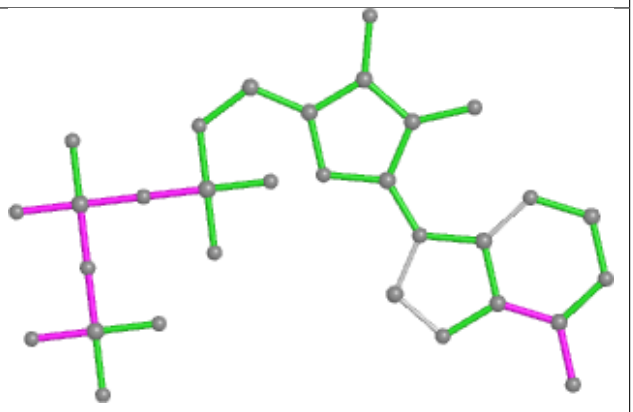


Rings

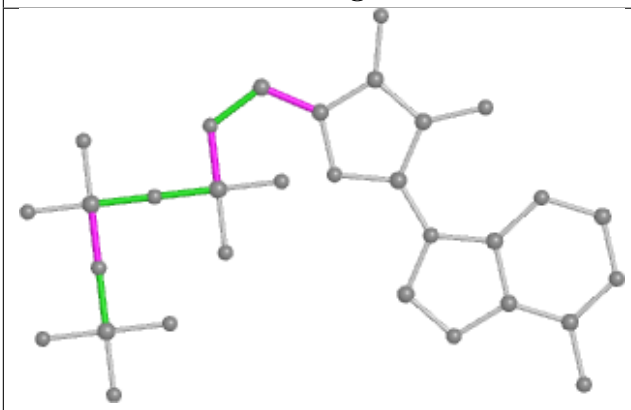
Ligand ANP n 4704



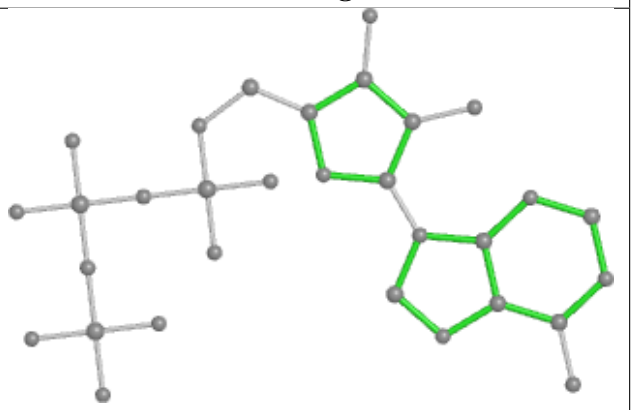
Bond lengths



Bond angles

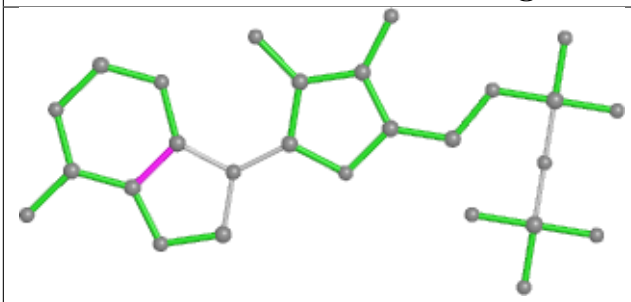


Torsions

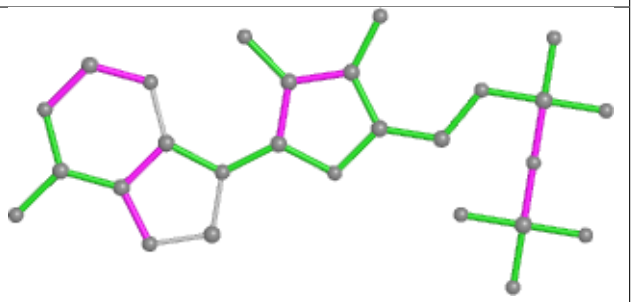


Rings

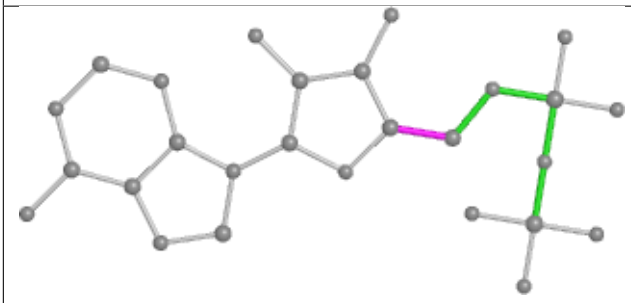
Ligand ADP e 4806



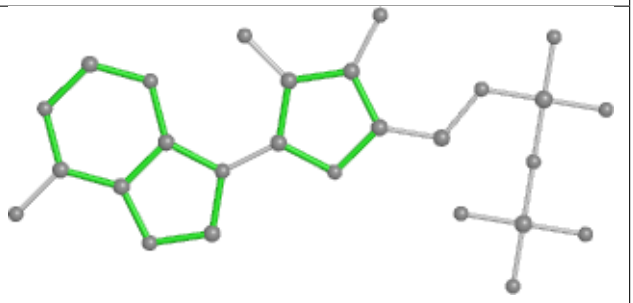
Bond lengths



Bond angles

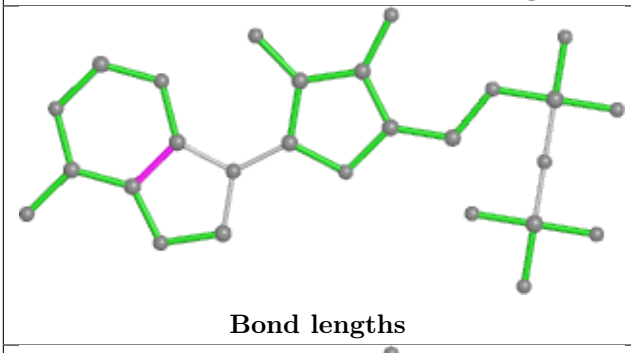


Torsions

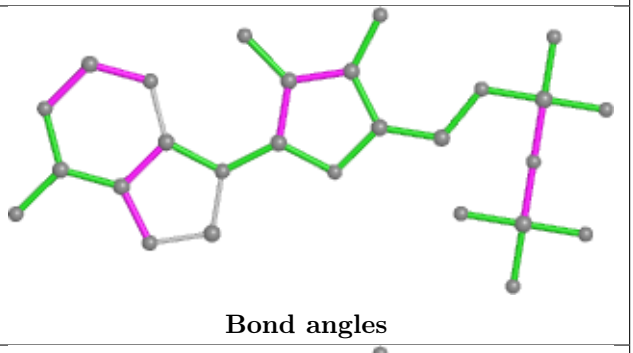


Rings

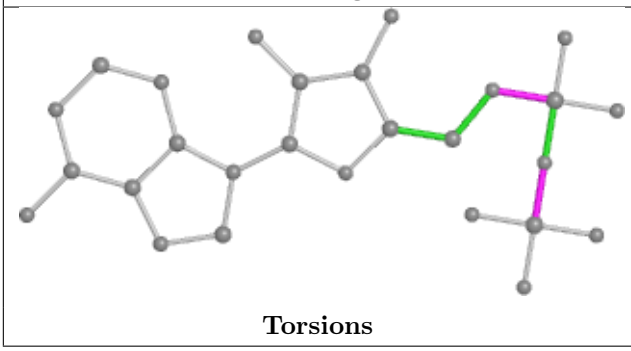
Ligand ADP E 800



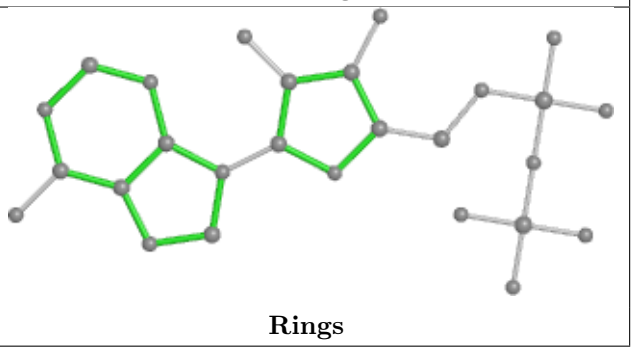
Bond lengths



Bond angles

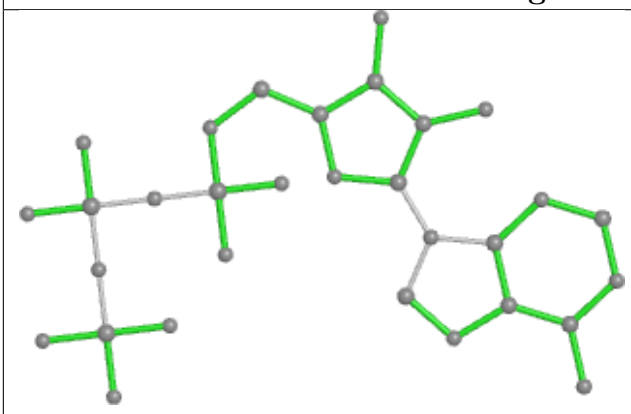


Torsions

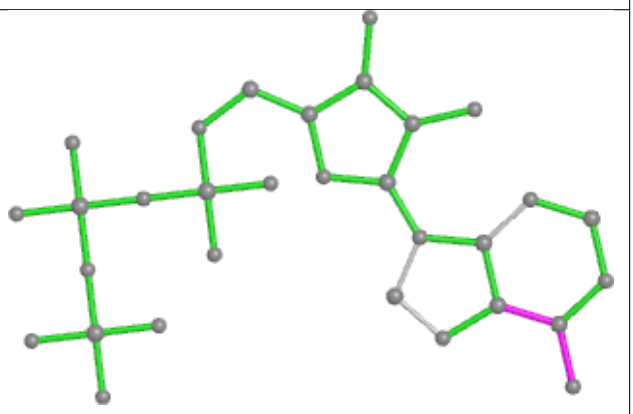


Rings

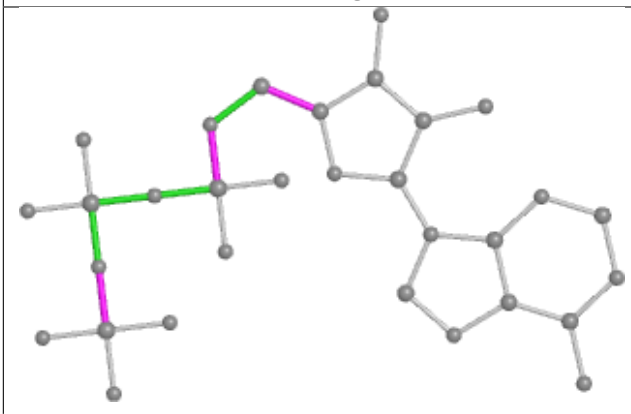
Ligand ATP J 800



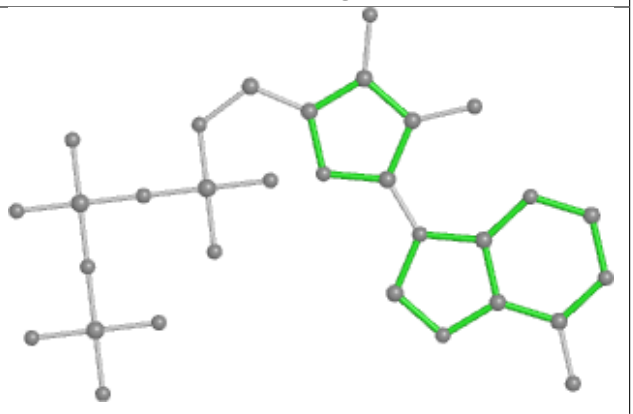
Bond lengths



Bond angles

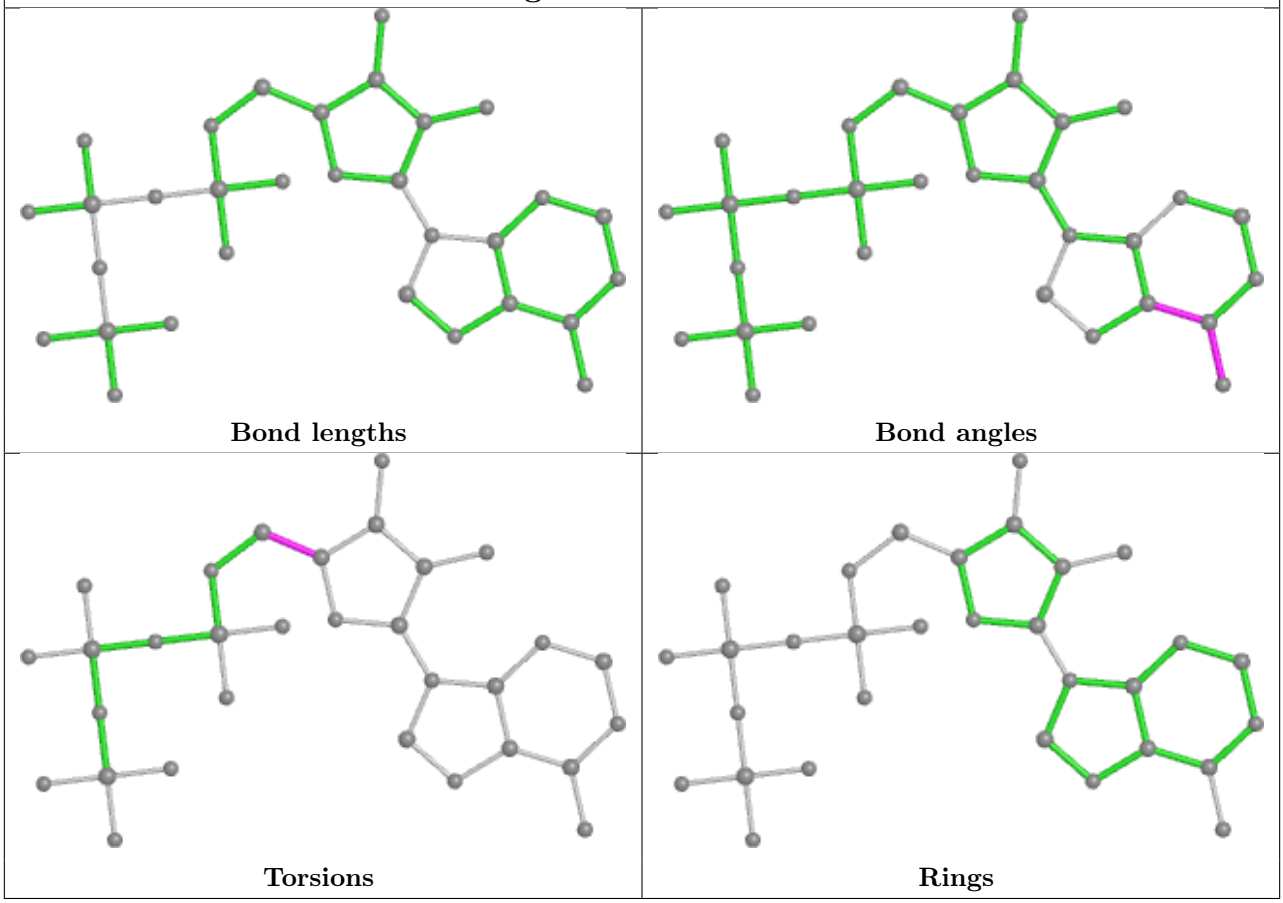


Torsions

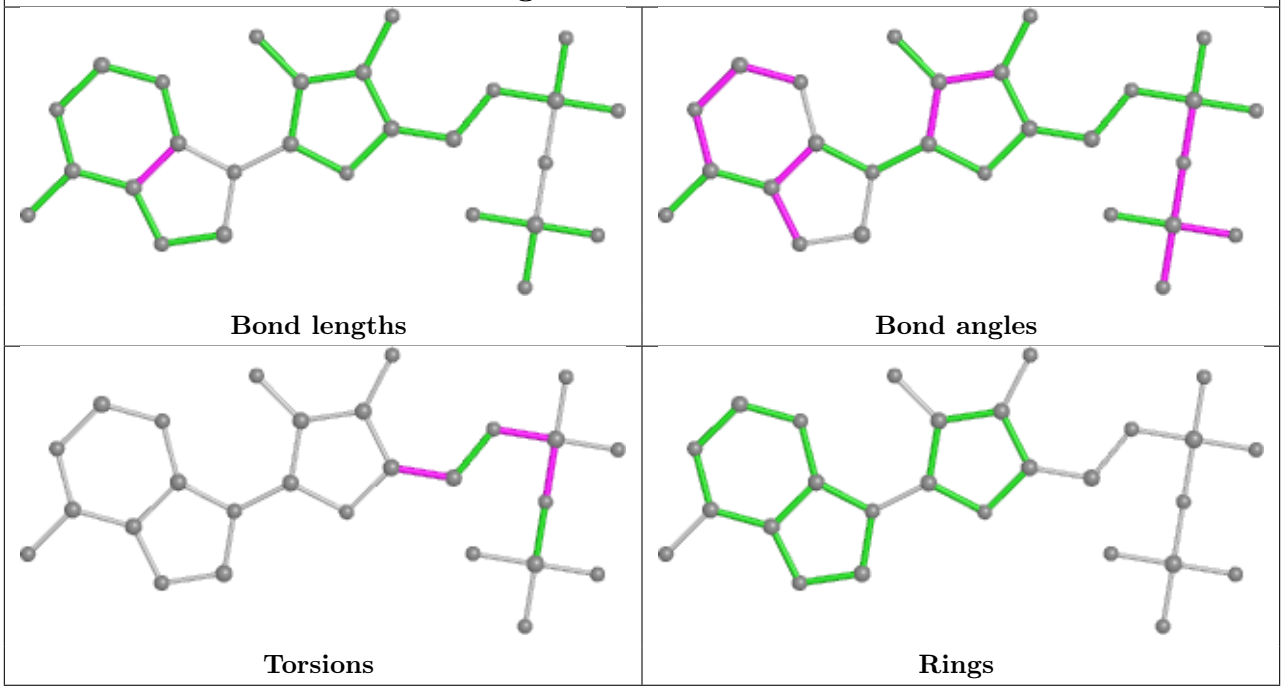


Rings

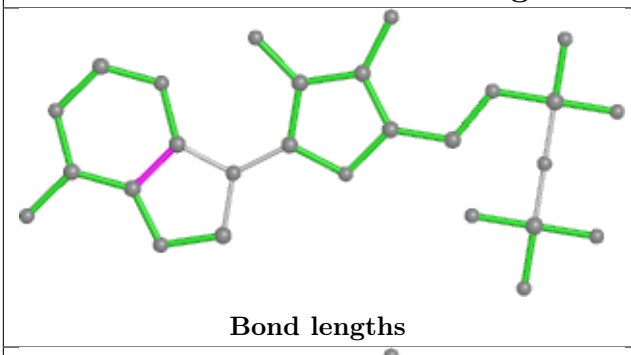
Ligand ATP f 4803



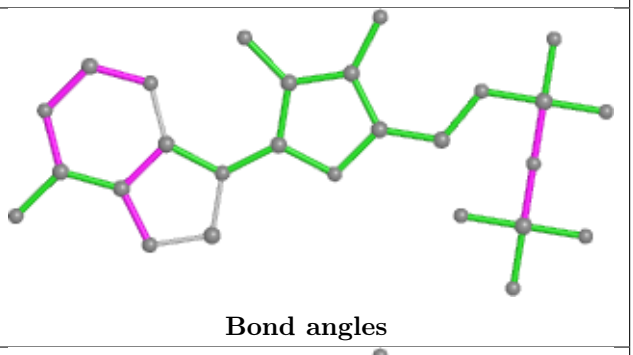
Ligand ADP n 4701



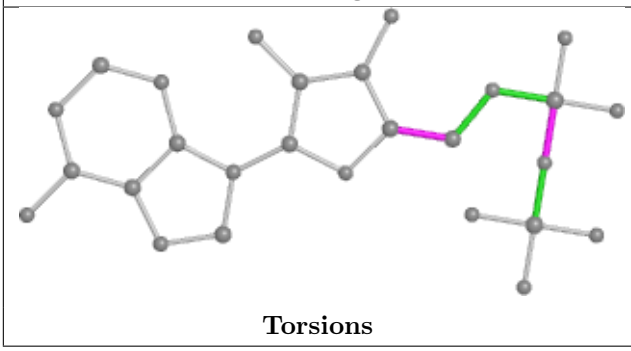
Ligand ADP m 4701



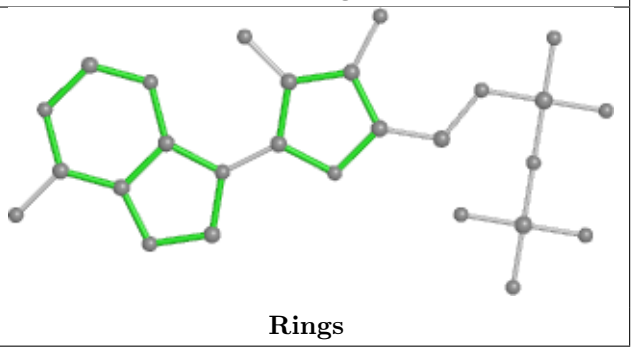
Bond lengths



Bond angles

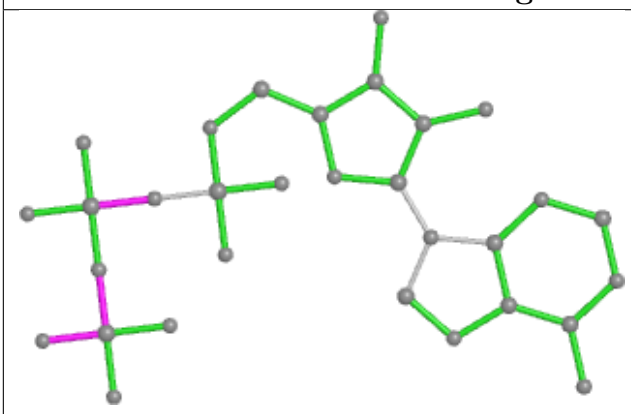


Torsions

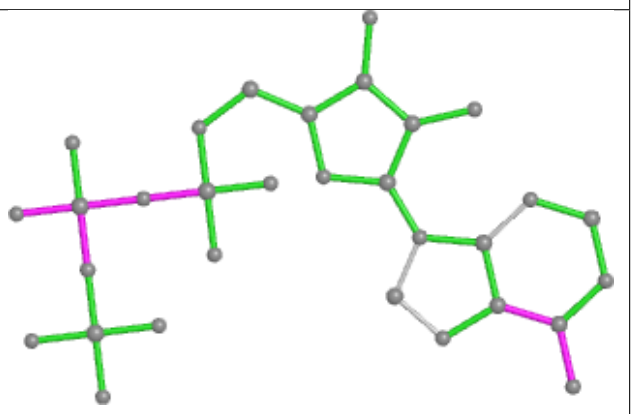


Rings

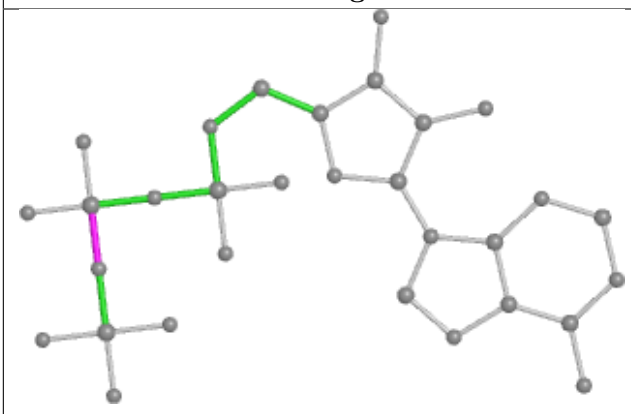
Ligand ANP n 4705



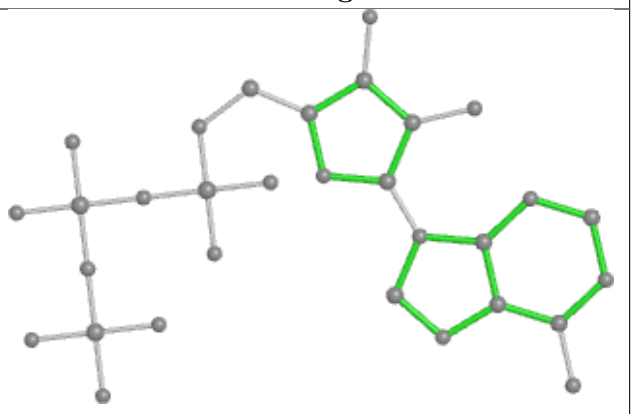
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

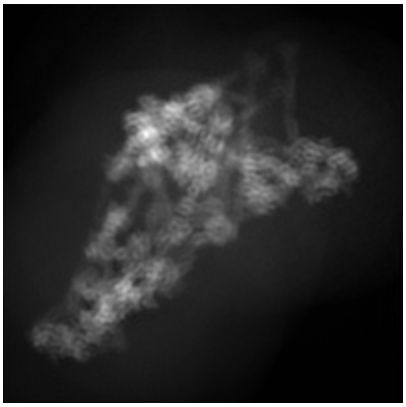
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17873. These allow visual inspection of the internal detail of the map and identification of artifacts.

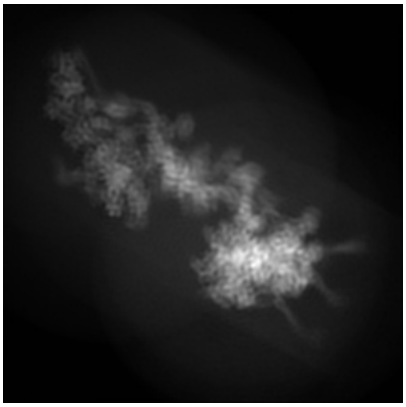
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

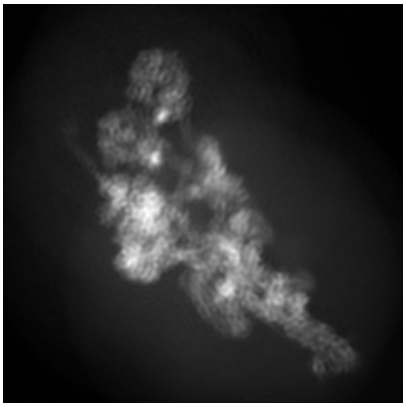
6.1.1 Primary map



X



Y

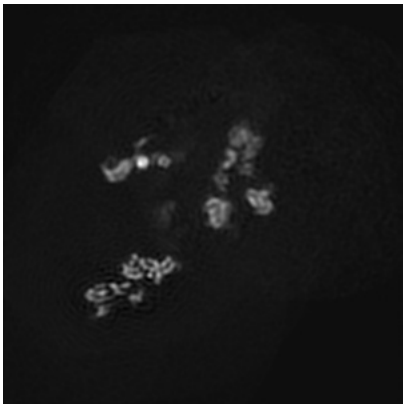


Z

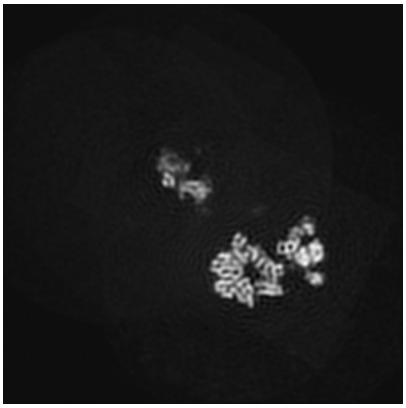
The images above show the map projected in three orthogonal directions.

6.2 Central slices

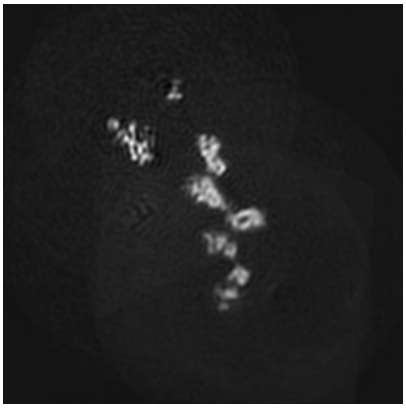
6.2.1 Primary map



X Index: 320



Y Index: 320

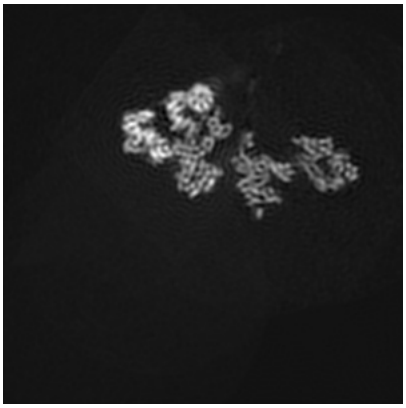


Z Index: 320

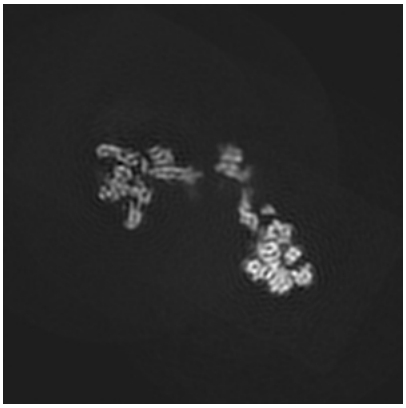
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

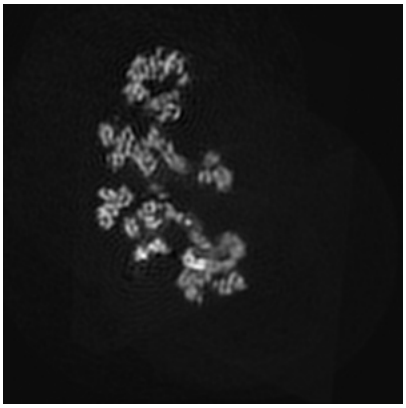
6.3.1 Primary map



X Index: 232



Y Index: 231

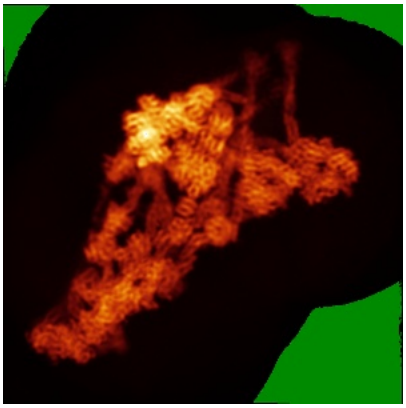


Z Index: 389

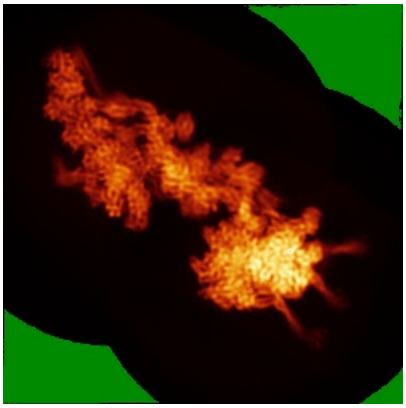
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

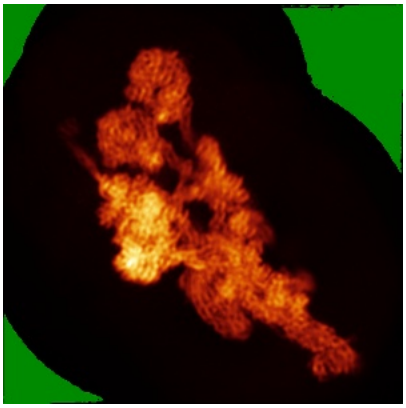
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0134. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

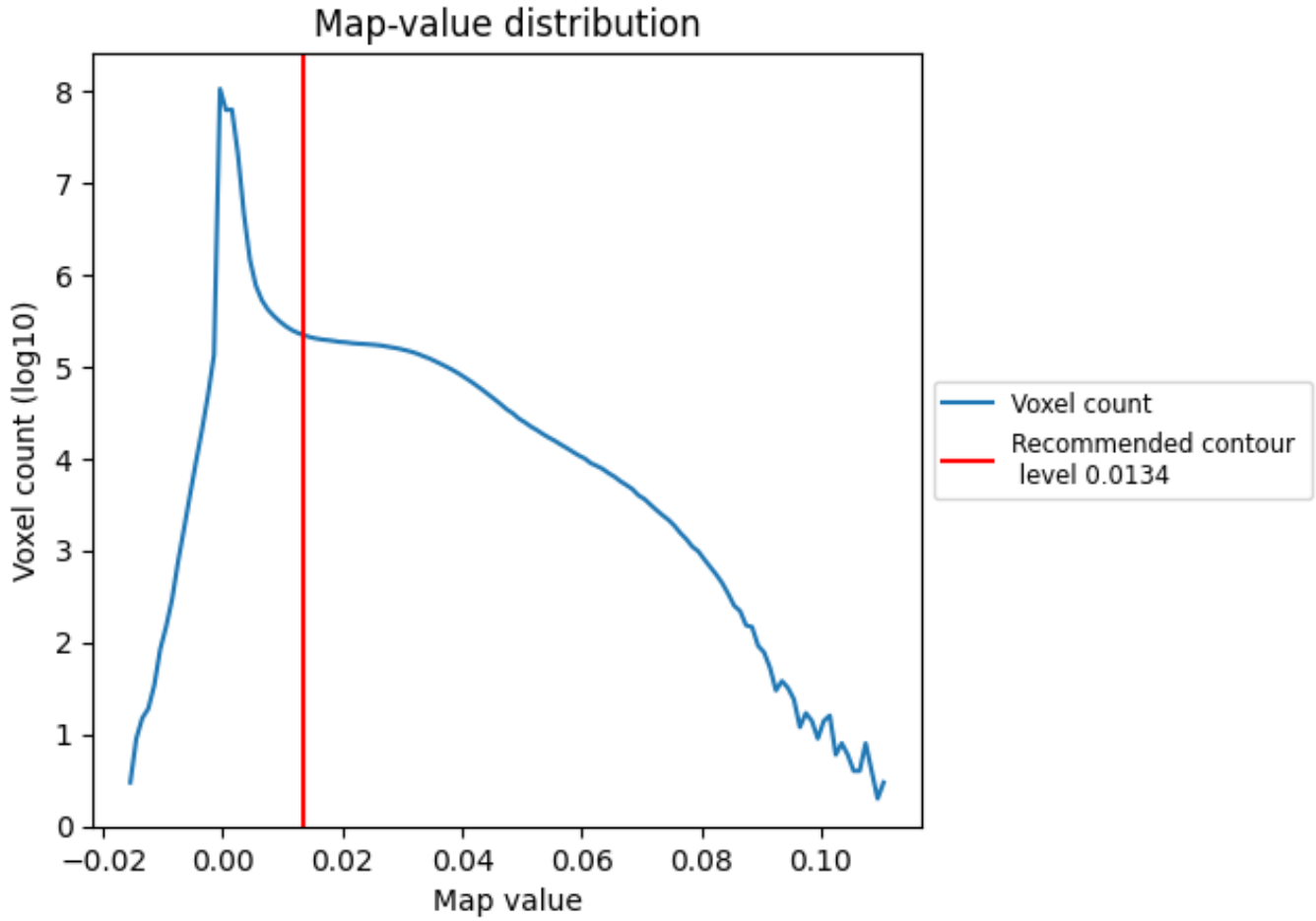
6.6 Mask visualisation (i)

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

7 Map analysis

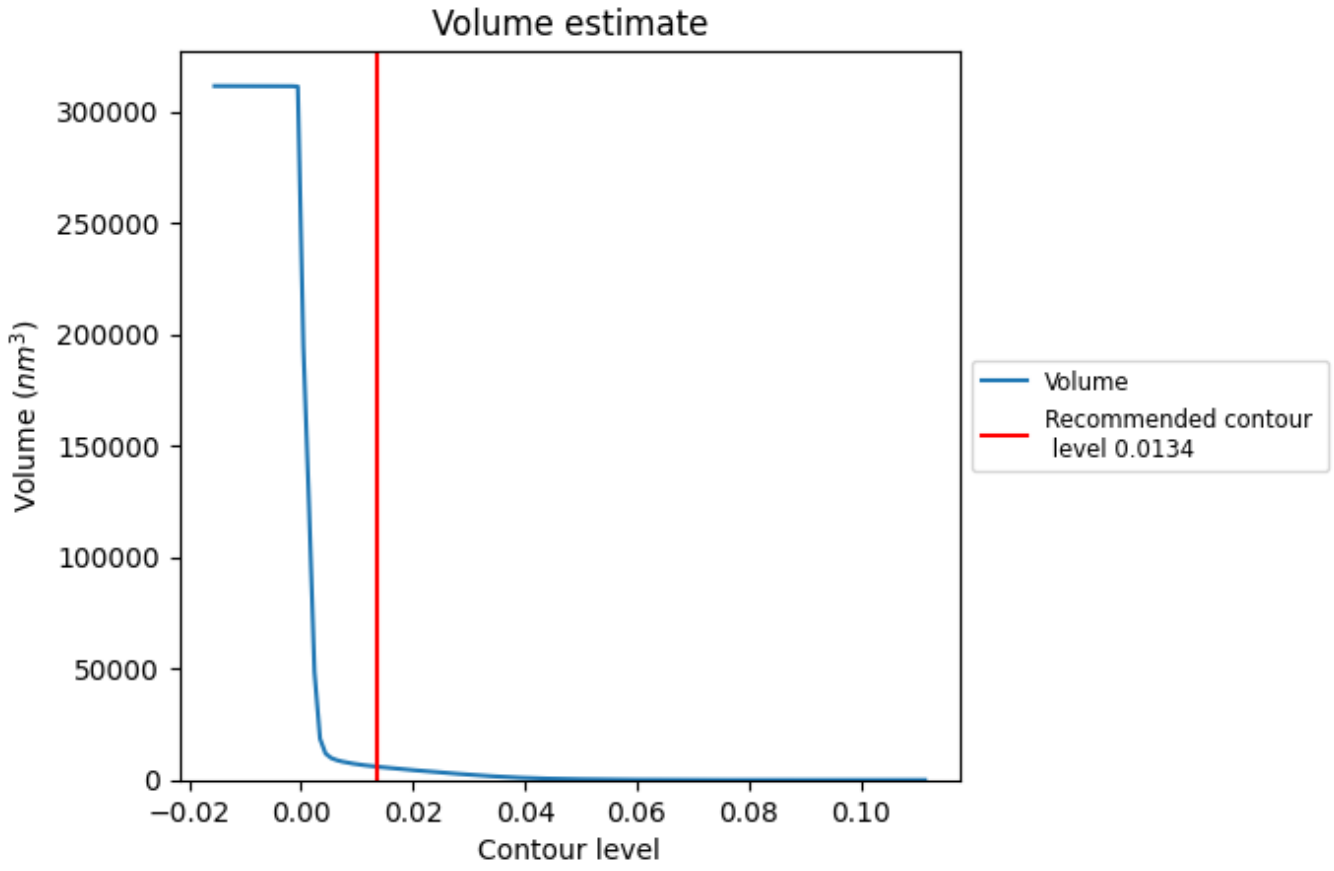
This section contains the results of statistical analysis of the map.

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.

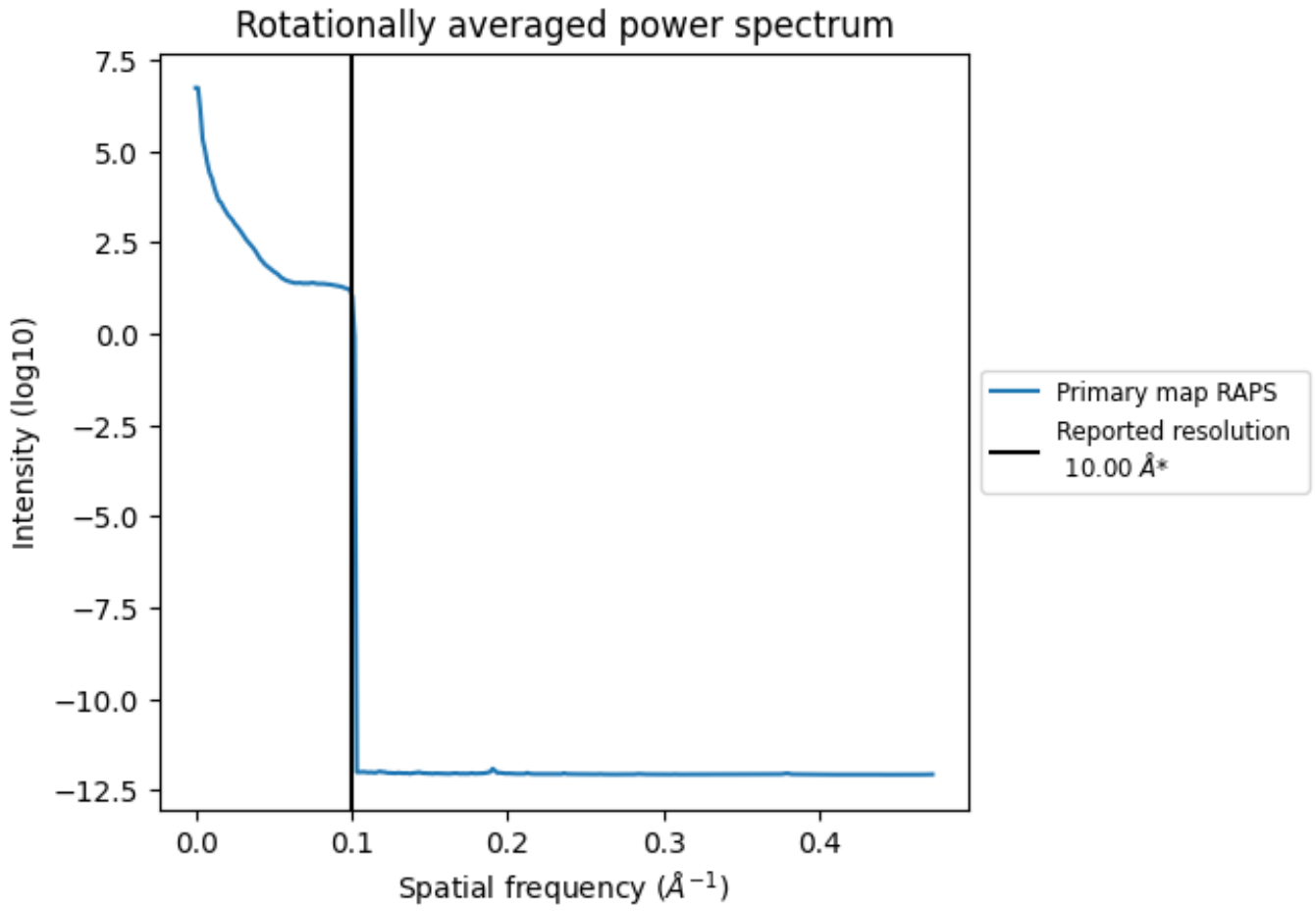
7.2 Volume estimate



The volume at the recommended contour level is 5997 nm^3; this corresponds to an approximate mass of 5417 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 0.100 $Å^{-1}$

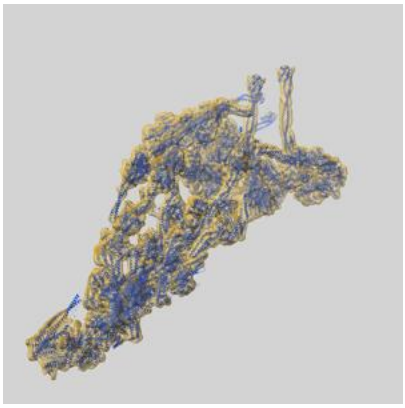
8 Fourier-Shell correlation (i)

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

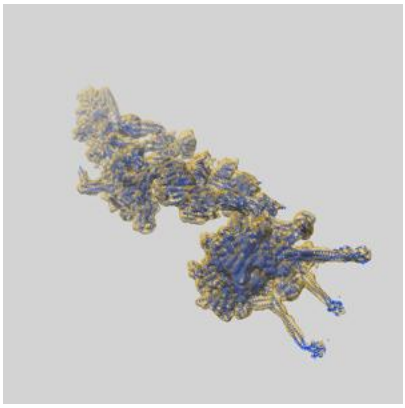
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17873 and PDB model 8PTK. Per-residue inclusion information can be found in section 3 on page 15.

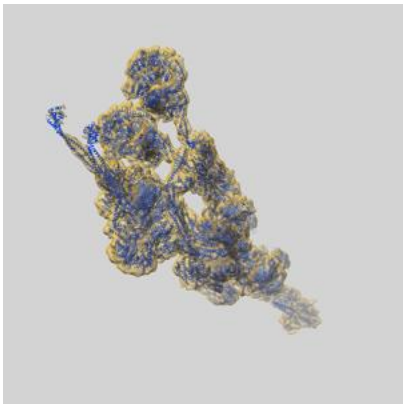
9.1 Map-model overlay



X



Y



Z

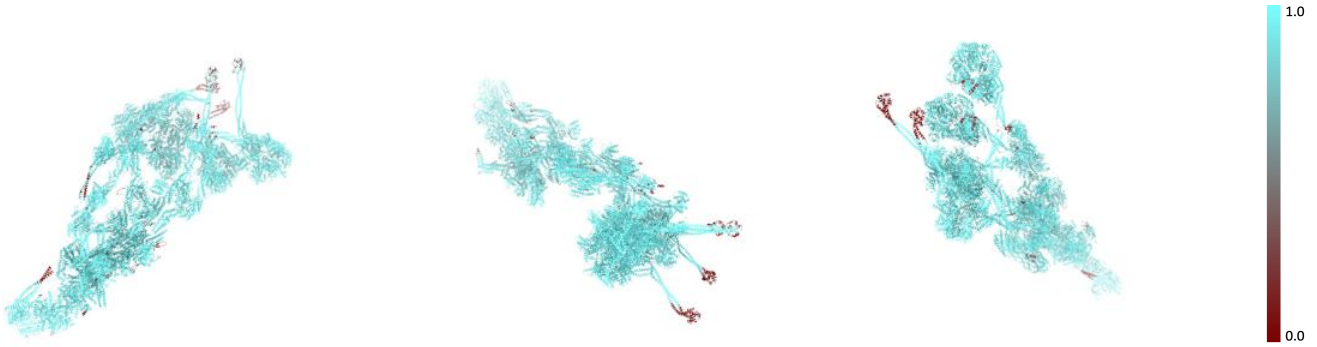
The images above show the 3D surface view of the map at the recommended contour level 0.0134 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

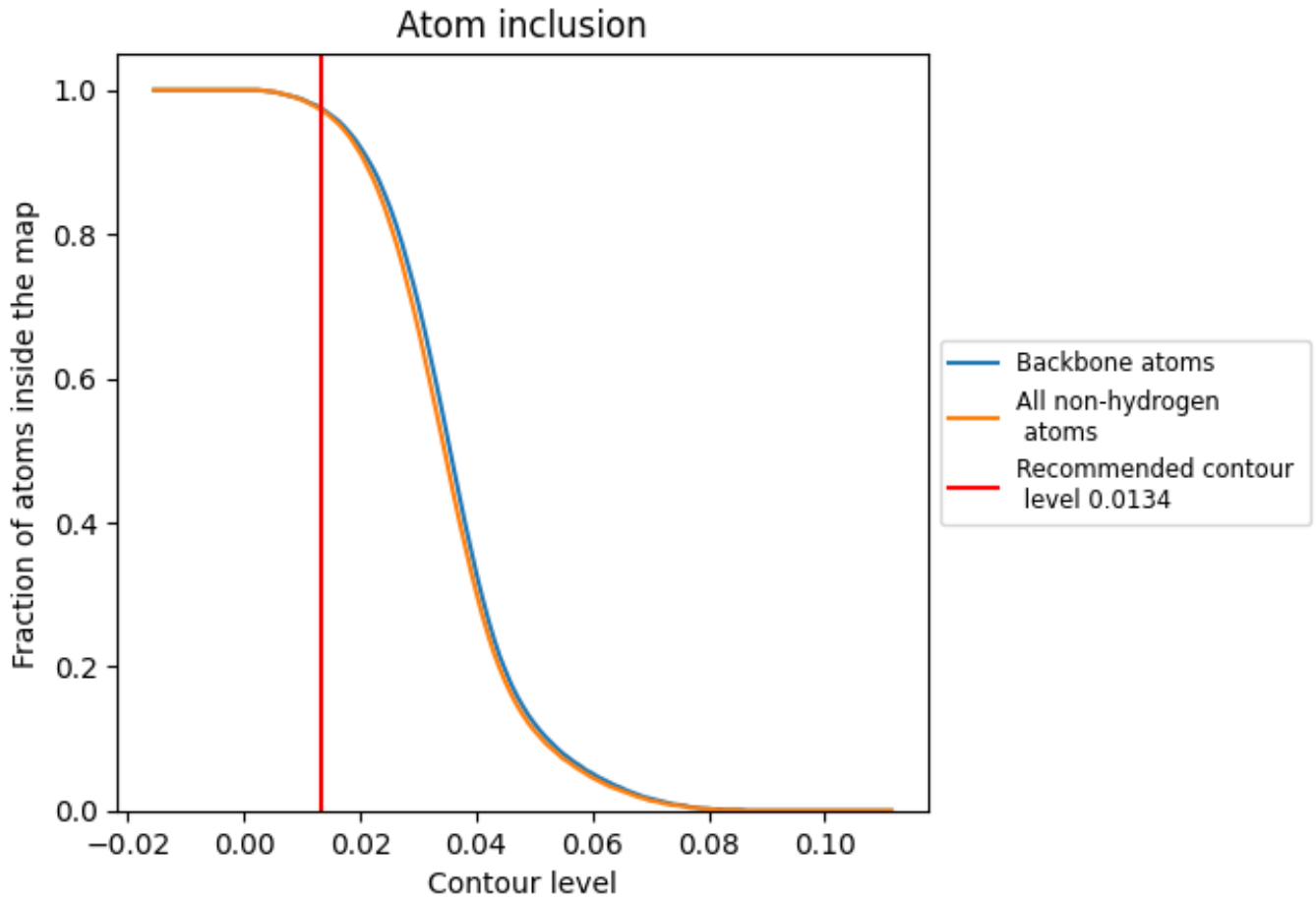
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0134).

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 (0.0134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9720	0.2020
1	0.9960	0.1730
2	0.9870	0.1850
3	0.9980	0.1640
4	0.9860	0.1860
A	0.9970	0.2160
B	0.9980	0.2100
C	0.9950	0.2000
D	0.9960	0.2100
E	0.9970	0.2050
F	0.9970	0.2070
G	0.9970	0.2070
H	0.9970	0.2060
I	0.9810	0.2110
J	0.9950	0.2010
K	0.9930	0.2290
L	1.0000	0.2250
M	0.9950	0.2450
N	0.9490	0.2230
O	1.0000	0.2380
P	0.9550	0.2300
Q	0.9930	0.2360
R	0.9990	0.2490
S	0.9570	0.1990
T	0.9810	0.2110
U	0.9980	0.2120
W	0.9980	0.2090
X	0.8920	0.2290
Y	0.9950	0.2100
a	0.9710	0.1080
b	0.9730	0.1220
d	0.9860	0.1370
e	0.9590	0.2090
f	0.9530	0.2030
g	0.9940	0.1670

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Chain	Atom inclusion	Q-score
h	0.9890	0.1820
i	0.9840	0.1590
j	0.9530	0.1810
k	0.9430	0.0860
l	0.8850	0.0860
m	0.9740	0.2100
n	0.9750	0.2080
o	0.9910	0.1790
p	0.9820	0.1590
q	0.9990	0.1830
r	0.9790	0.1840
s	0.9960	0.1700
t	1.0000	0.2070
u	0.9980	0.1320
v	0.9570	0.0940
w	1.0000	0.1360
x	0.8970	0.2380
y	0.7970	0.0840
z	0.9700	0.0990