



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:37 AM UTC

PDB ID : 8PTK / pdb_00008ptk
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:

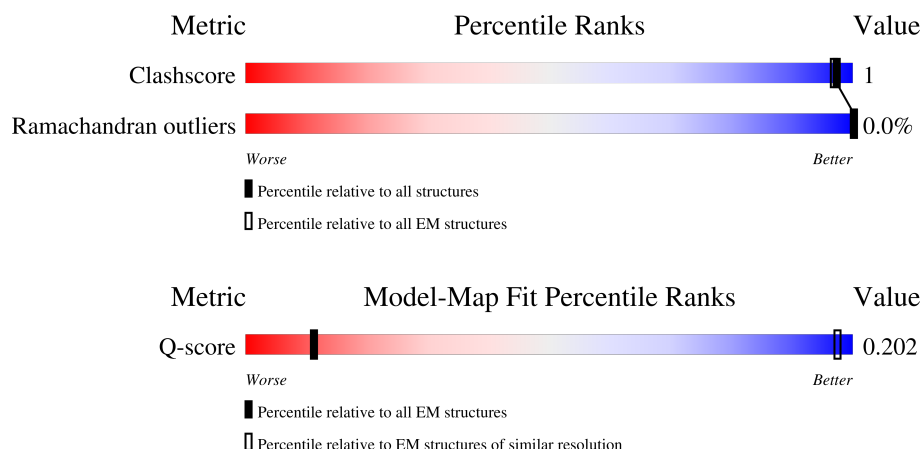
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



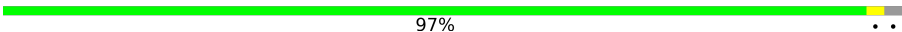
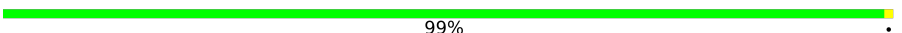
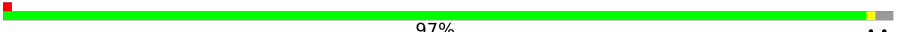
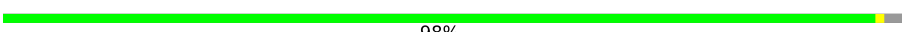
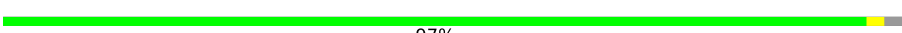
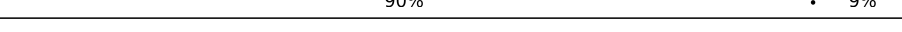
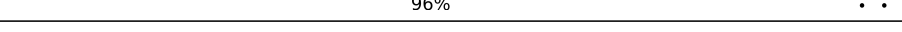
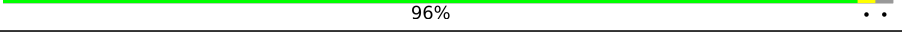
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	147 (9.50 - 10.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	410	96%
1	2	410	95%
1	3	410	78% 21%
1	4	410	77% 21%
2	A	376	98%

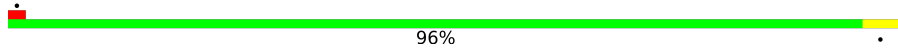
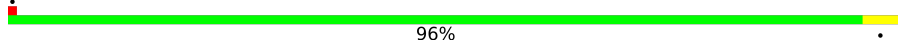
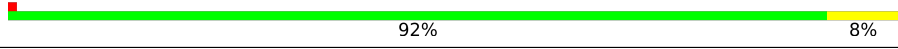
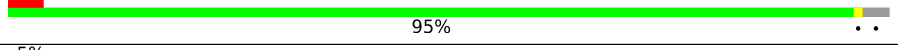
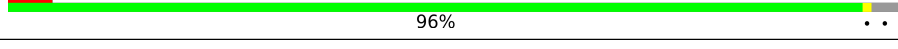
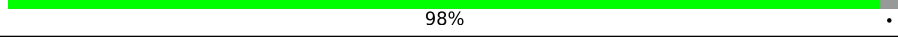
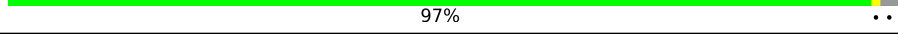
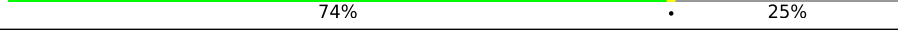
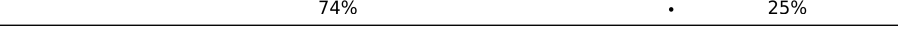
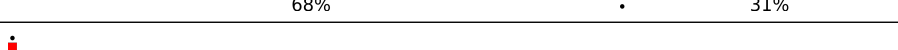
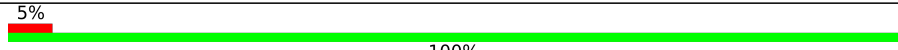
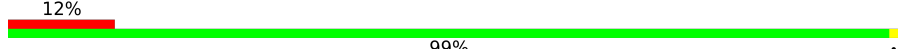
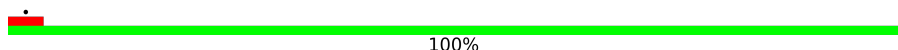
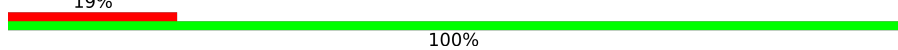
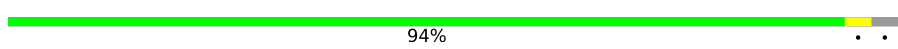
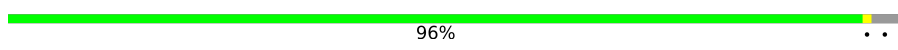
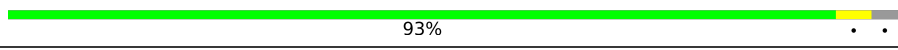
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Mol	Chain	Length	Quality of chain
2	B	376	 97% ..
2	C	376	 99% .
2	D	376	 97% ..
2	E	376	 98% ..
2	F	376	 97% ..
2	G	376	 98% ..
2	I	376	 97% ..
3	H	375	 97% ..
4	J	417	 88% . 9%
5	K	286	 96% ..
6	L	272	 98% ..
7	M	405	 77% . 22%
7	N	405	 65% 35%
7	P	405	 86% . 13%
7	Q	405	 80% . 19%
8	O	186	 90% . 9%
8	R	186	 96% ..
9	S	1281	 55% . 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% 48% 51%
13	Y	467	 78% . 20%
14	a	89	 97% .

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Mol	Chain	Length	Quality of chain
14	b	89	
14	d	89	
14	i	89	
15	e	4646	
15	f	4646	
15	m	4646	
15	n	4646	
16	g	612	
16	h	612	
16	o	612	
16	p	612	
17	j	492	
17	q	492	
17	r	492	
17	u	492	
18	k	113	
18	l	113	
18	v	113	
18	y	113	
19	s	96	
19	t	96	
19	w	96	
19	z	96	

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	C	N	O	0	0
			1988	1184	402	402		
1	2	402	Total	C	N	O	0	0
			1988	1184	402	402		
1	3	322	Total	C	N	O	0	0
			1590	946	322	322		
1	4	322	Total	C	N	O	0	0
			1590	946	322	322		

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

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

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

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

- Molecule 4 is a protein called Arp11.

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

- 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	C	N	O	0	0
			1378	822	278	278		

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

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

- Molecule 7 is a protein called Dynactin subunit 2.

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

- Molecule 8 is a protein called Dynactin subunit 3.

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

- Molecule 9 is a protein called Dynactin subunit 1.

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

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

- Molecule 10 is a protein called Dynactin 6.

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

- Molecule 11 is a protein called Dynactin subunit 5.

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

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

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

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	C	N	O	0	0
			441	263	89	89		

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

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

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	C	N	O	0	0
			2275	1355	460	460		
16	h	462	Total	C	N	O	0	0
			2284	1360	462	462		
16	o	425	Total	C	N	O	0	0
			2100	1250	425	425		
16	p	432	Total	C	N	O	0	0
			2134	1270	432	432		

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	C	N	O	0	0
			1605	957	324	324		
17	q	318	Total	C	N	O	0	0
			1574	938	318	318		
17	r	319	Total	C	N	O	0	0
			1581	943	319	319		
17	u	298	Total	C	N	O	0	0
			1473	877	298	298		

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

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

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

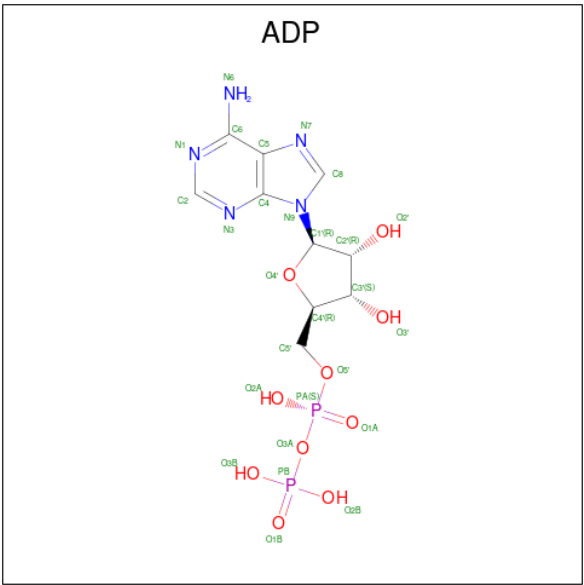
Mol	Chain	Residues	Atoms				AltConf	Trace
19	s	93	Total	C	N	O	0	0
			462	276	93	93		
19	t	93	Total	C	N	O	0	0
			462	276	93	93		
19	w	93	Total	C	N	O	0	0
			462	276	93	93		

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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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



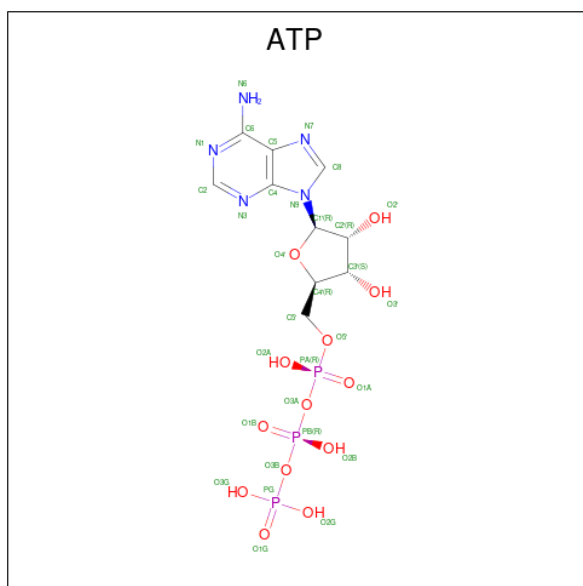
Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	G	1	Total	C	N	O	P	0
			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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
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	

Continued on next page...

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

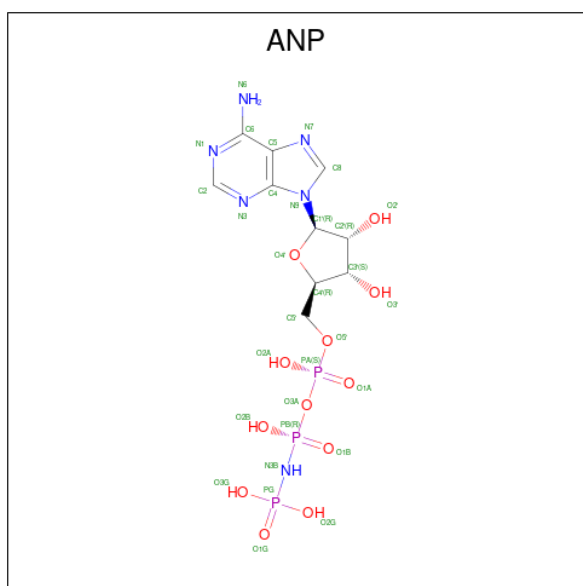
- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 23 is MAGNESIUM ION (CCD ID: 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 (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).

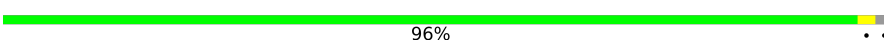


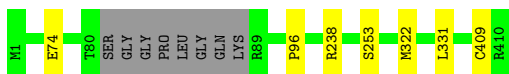
Mol	Chain	Residues	Atoms					AltConf
24	m	1	Total 31	C 10	N 6	O 12	P 3	0
24	m	1	Total 31	C 10	N 6	O 12	P 3	0
24	n	1	Total 31	C 10	N 6	O 12	P 3	0
24	n	1	Total 31	C 10	N 6	O 12	P 3	0

3 Residue-property plots [i](#)

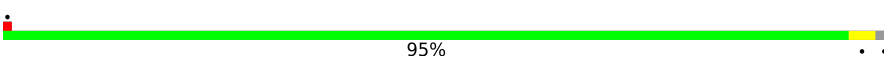
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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:  96%



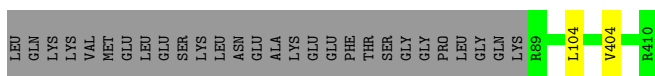
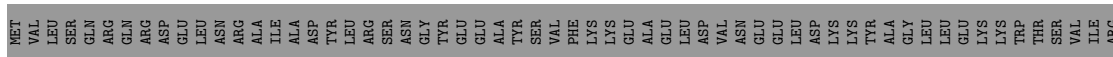
- Molecule 1: Platelet-activating factor acetylhydrolase IB subunit beta

Chain 2:  95%



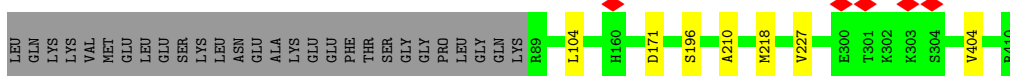
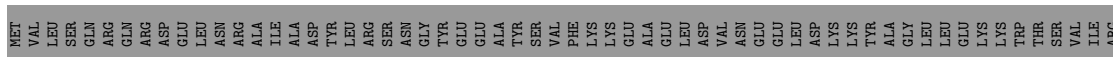
- Molecule 1: Platelet-activating factor acetylhydrolase IB subunit beta

Chain 3:  78% 21%

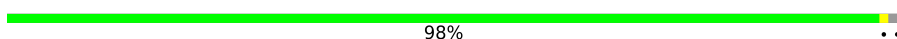


- Molecule 1: Platelet-activating factor acetylhydrolase IB subunit beta

Chain 4:  77% 21%



- Molecule 2: ARP1 actin related protein 1 homolog A

Chain A:  98%



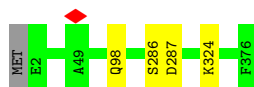
- Molecule 2: ARP1 actin related protein 1 homolog A

Chain B: 97%



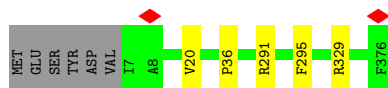
- Molecule 2: ARP1 actin related protein 1 homolog A

Chain C: 99%



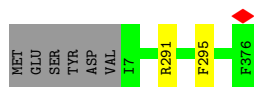
- Molecule 2: ARP1 actin related protein 1 homolog A

Chain D: 97%



- Molecule 2: ARP1 actin related protein 1 homolog A

Chain E: 98%



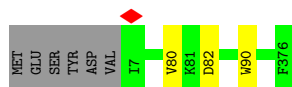
- Molecule 2: ARP1 actin related protein 1 homolog A

Chain F: 97%

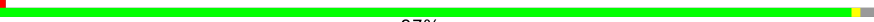


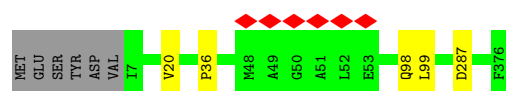
- Molecule 2: ARP1 actin related protein 1 homolog A

Chain G: 98%

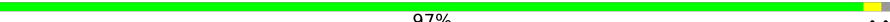


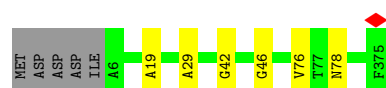
- Molecule 2: ARP1 actin related protein 1 homolog A

Chain I:  97%



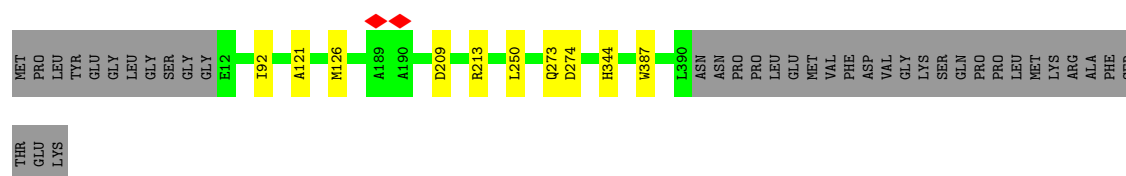
- Molecule 3: Actin, cytoplasmic 1

Chain H:  97%



- Molecule 4: Arp11

Chain J:  88% 9%

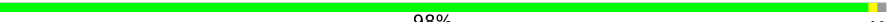


- Molecule 5: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K:  96%



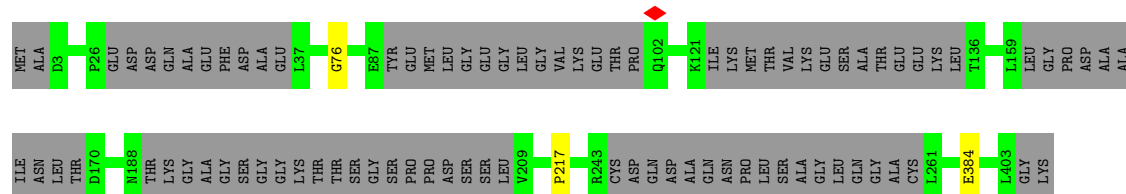
- Molecule 6: F-actin-capping protein subunit beta

Chain L:  98%



- Molecule 7: Dynactin subunit 2

Chain M:  77% 22%



- Molecule 7: Dynactin subunit 2

Chain N:  65% 35%

MET ALA D3 P26 GLU ASP ASP GLN ALA ALA GLU PHE ASP ALA LEU GLU GLU THR THR THR VAL GLU HIS ILE VAL ASN ASN PRO ASN ALA ALA TYR LYS ASP LYS PHE LYS ASP LYS ARG VAL GLY THR LYS GLY LEU ASP PHE SER ASP ARG ILE GLY LYS THR LYS ARG THR

GLY TYR SER GLU TYR LYS MET GLU SER GLY GLU LEU VAL GLU THR PRO G103 T117 E120 K121 I122 K123 M124 T125 VAL LYS GLU SER ALA THR GLU LYS LEU THR P137 H138 L156 E157 K158 LEU LEU PRO ASP ALA ILE ASN THR ASP

P171 T186 LYS THR LYS GLY ALA GLY GLY LYS THR THR VAL SER PRO ASP SER LEU V209 V242 ARG CYS ASP GLN ASP ALA ALA ASN PRO LEU SER GLY ALA GLN GLY THR GLY ALA C260 L403 GLY LYS

• Molecule 7: Dynactin subunit 2

Chain P:  86% 13%

MET ALA D3 D24 E27 D28 D29 Q30 A31 F71 S72 I75 GLY LYS THR LYS ARG THR GLY TYR GLU SER GLY TYR MET LEU GLU GLY LEU GLY VAL K98 E128 T131 E132 E133 T189 K190 GLY ALA GLY SER GLY LYS THR THR GLY S202

C244 ASP GLN ALA ALA ASN PRO GLN LEU SER ALA ALA LEU GLN ALA C260 S303 R336 L337 L403 GLY LYS

• Molecule 7: Dynactin subunit 2

Chain Q:  80% 19%

H1 E21 P26 GLU ASP ASP GLN ALA ALA ASP ALA LEU GLU GLU THR THR THR HIS ILE VAL ASN ASN PRO ASN ALA TYR LYS ASP LYS PHE LYS ASP LYS ARG VAL GLY THR LYS GLY LEU ASP PHE SER ASP ARG ILE GLY LYS THR LYS ARG THR

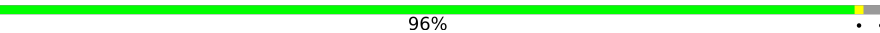
G82 G86 E132 K187 ASN THR LYS GLY ALA GLY SER THR THR THR THR THR SER S207 L231 L235 A259 L333 K401 K402 L403 GLY LYS

• Molecule 8: Dynactin subunit 3

Chain O:  90% 9%

MET ALA GLY V4 I78 M110 K117 G173 G180 LEU GLU ALA ALA LYS GLN VAL LYS PRO PRO ALA ALA GLU GLU

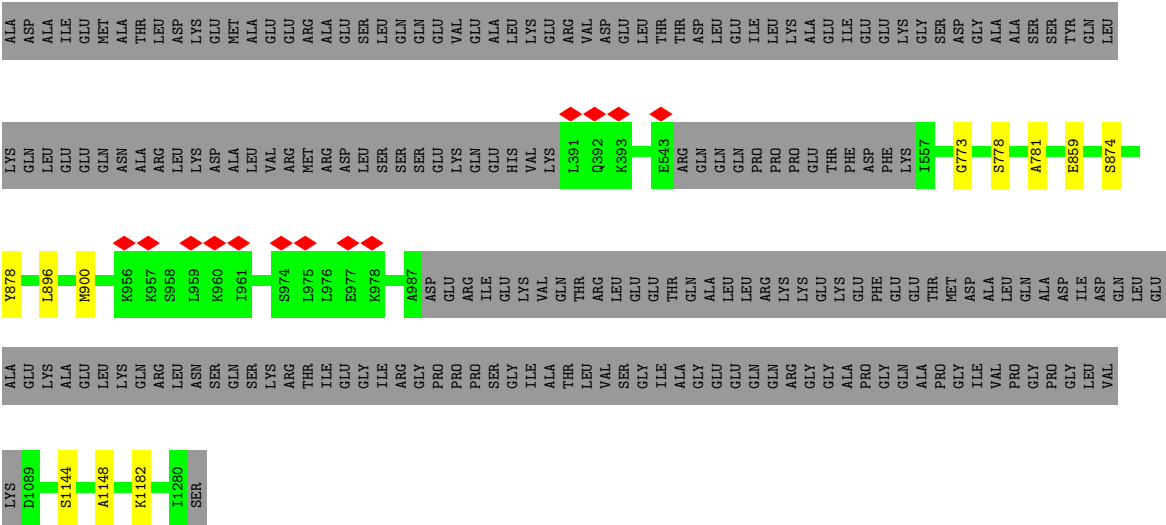
• Molecule 8: Dynactin subunit 3

Chain R:  96%

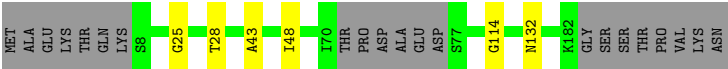
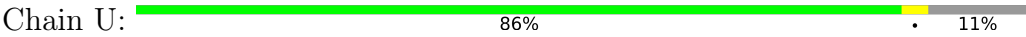
MET A2 V108 G180 VAL LYS PRO ALA GLU GLU

• Molecule 9: Dynactin subunit 1





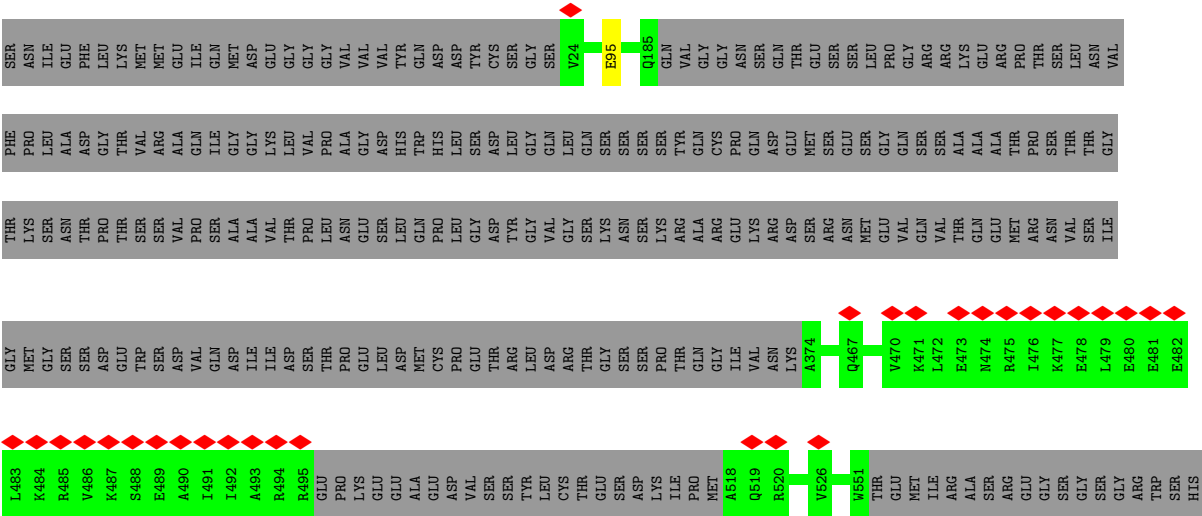
• Molecule 10: Dynactin 6

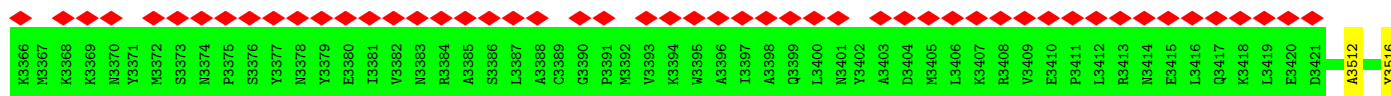


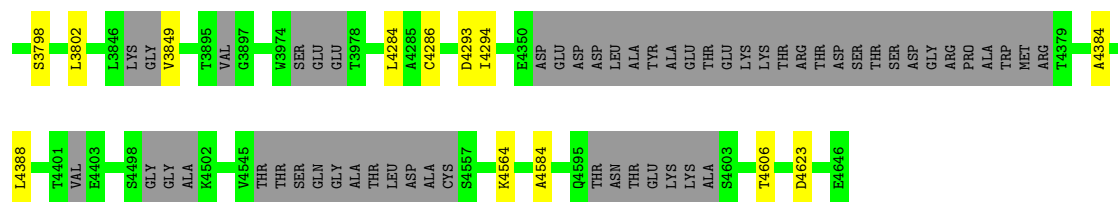
• Molecule 11: Dynactin subunit 5



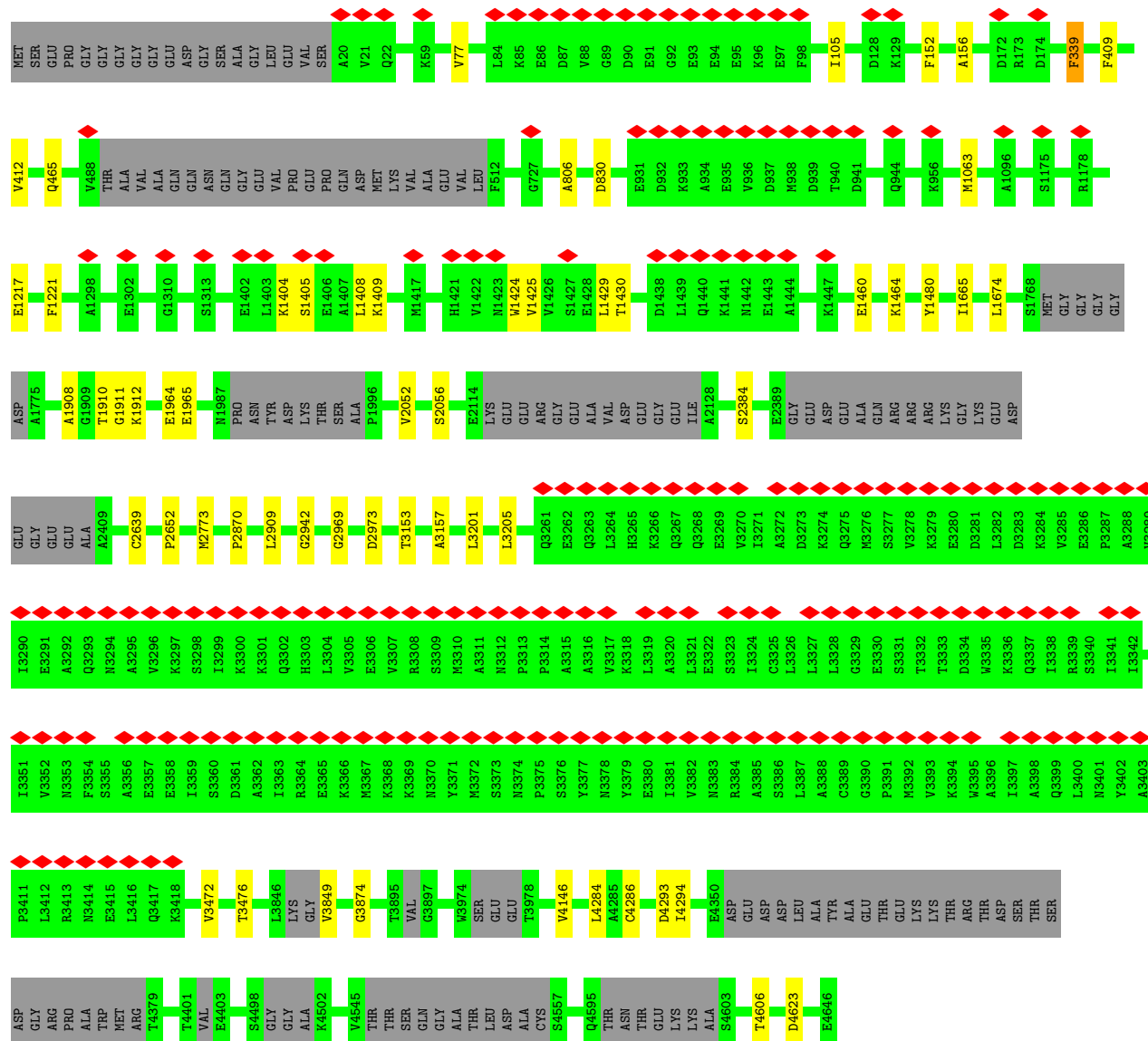
• Molecule 12: C-Jun-amino-terminal kinase-interacting protein 3





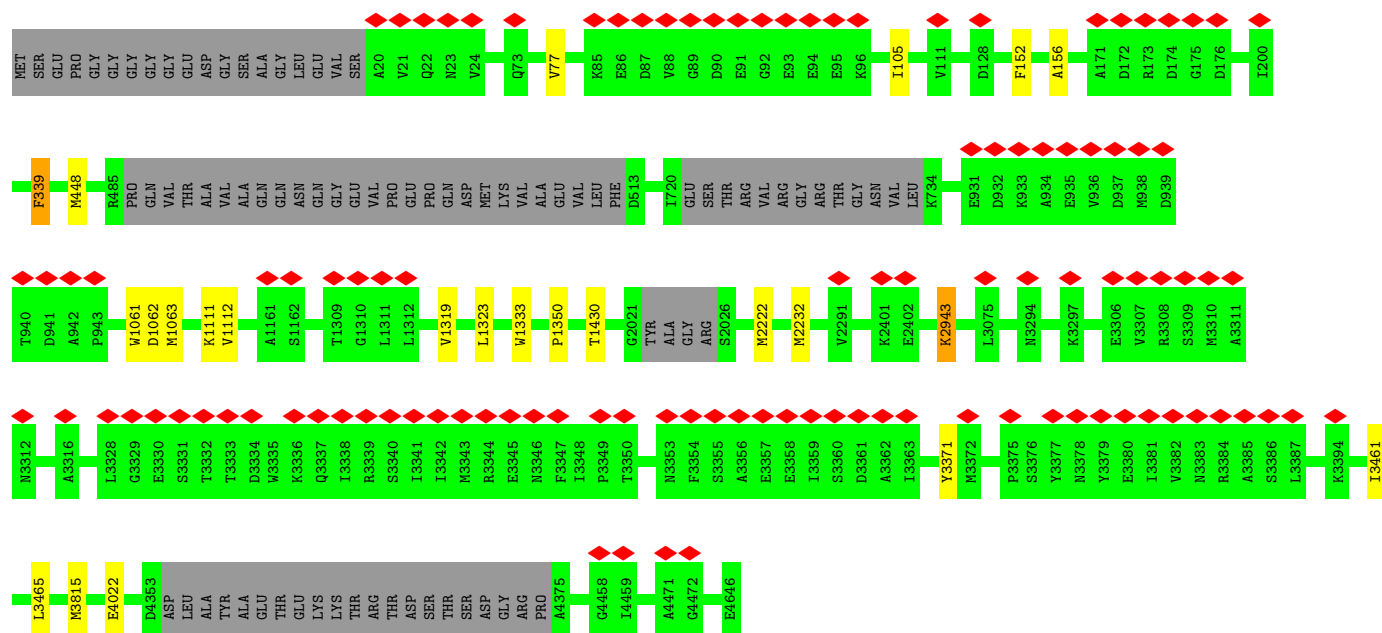


• Molecule 15: Cytoplasmic dynein 1 heavy chain 1

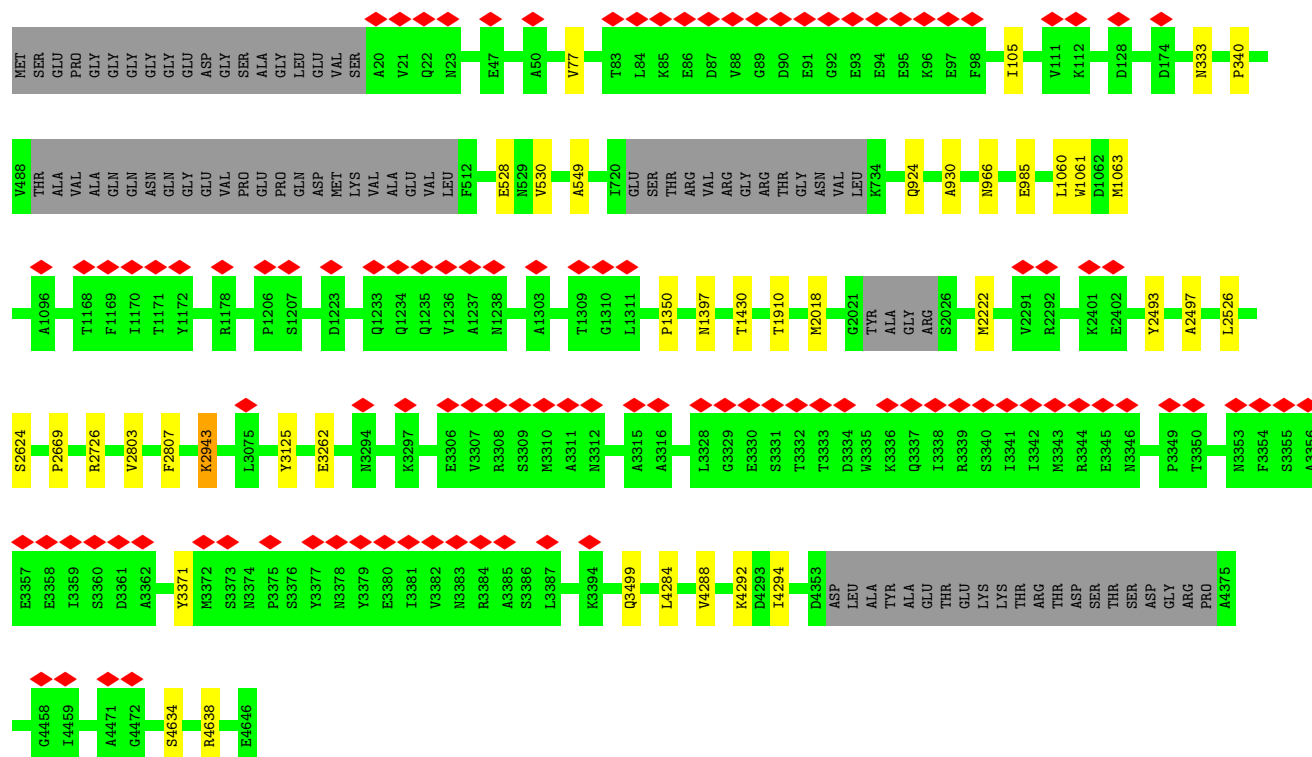


• Molecule 15: Cytoplasmic dynein 1 heavy chain 1



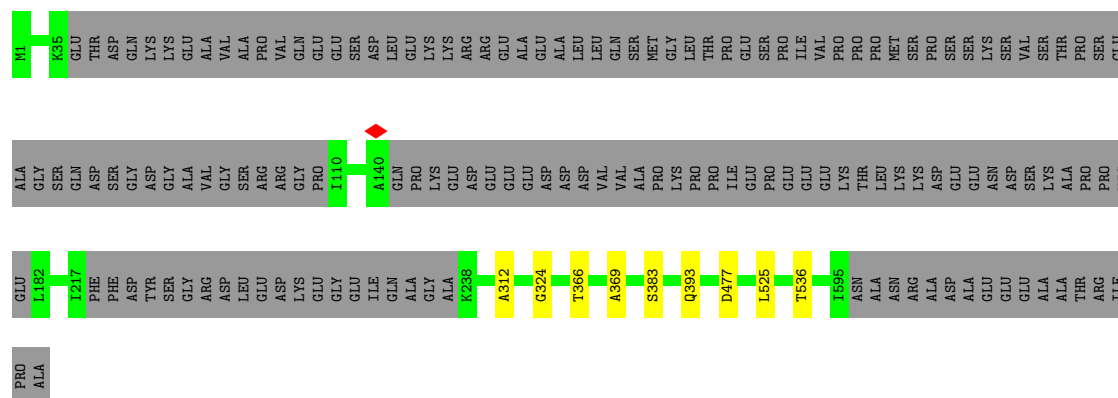


- Molecule 15: Cytoplasmic dynein 1 heavy chain 1



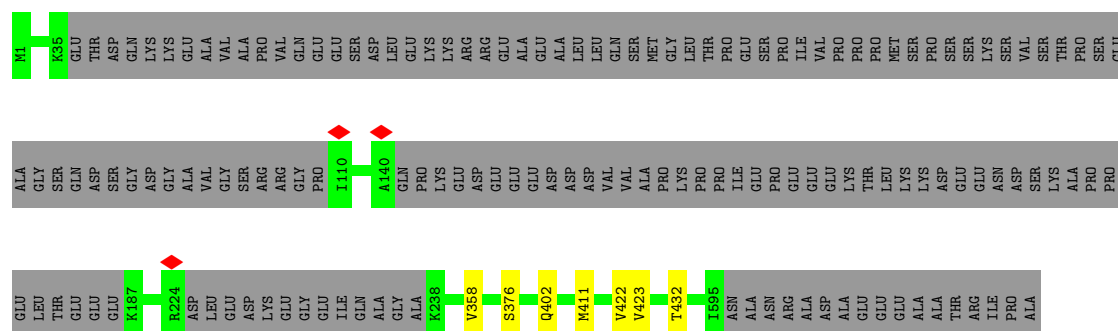
- Molecule 16: Cytoplasmic dynein 1 intermediate chain 2





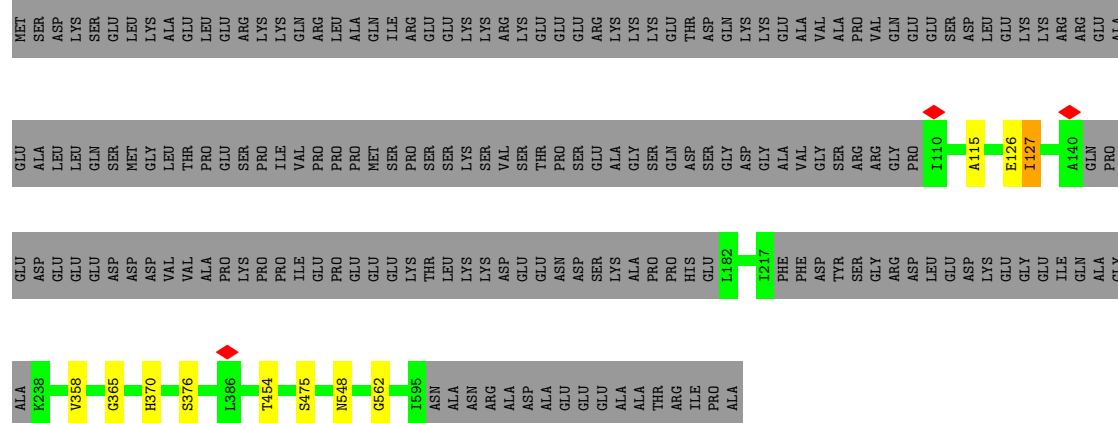
• Molecule 16: Cytoplasmic dynein 1 intermediate chain 2

Chain h: 74% 25%



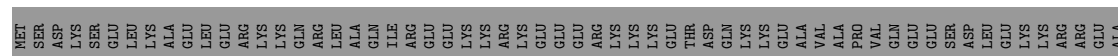
• Molecule 16: Cytoplasmic dynein 1 intermediate chain 2

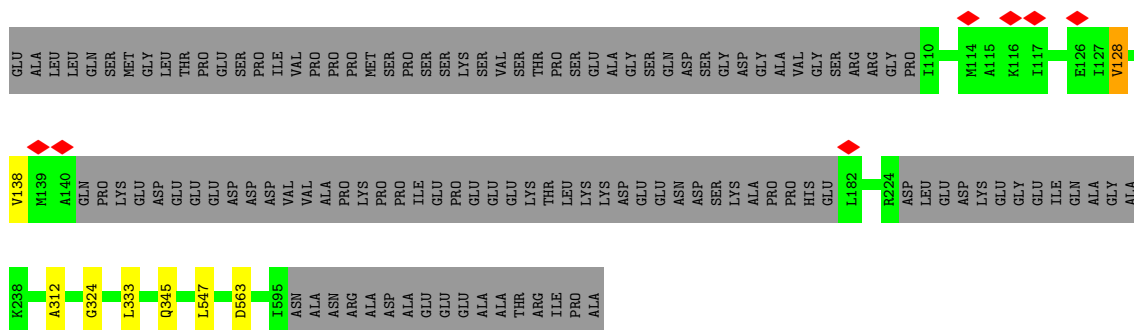
Chain o: 68% 31%



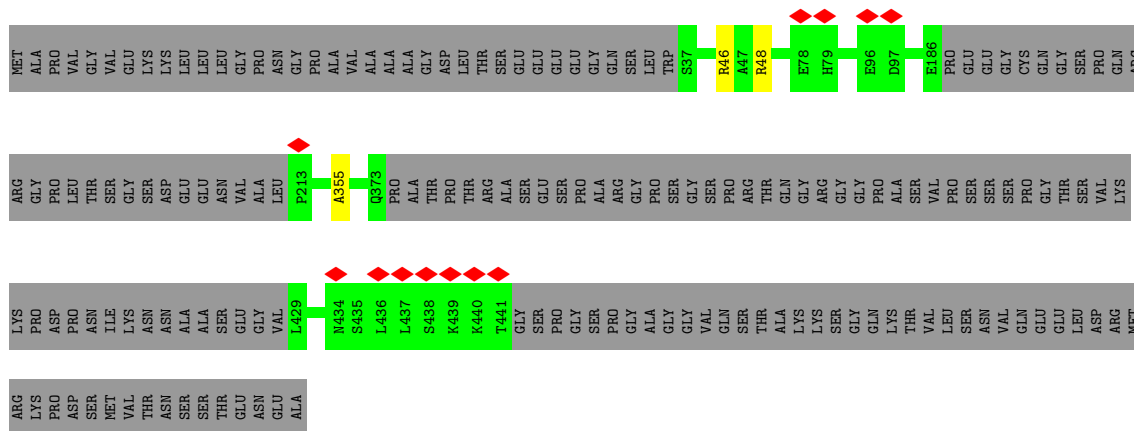
• Molecule 16: Cytoplasmic dynein 1 intermediate chain 2

Chain p: 69% 29%

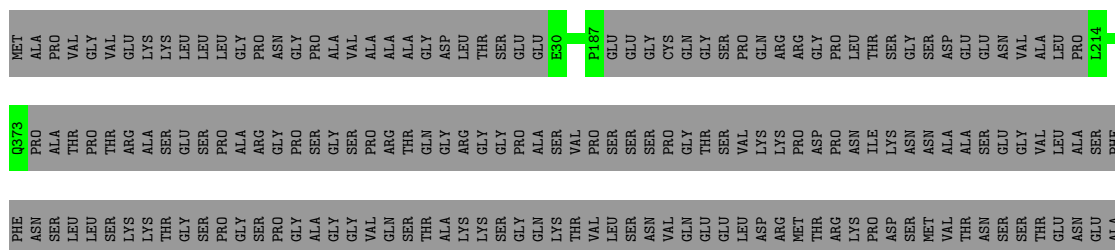




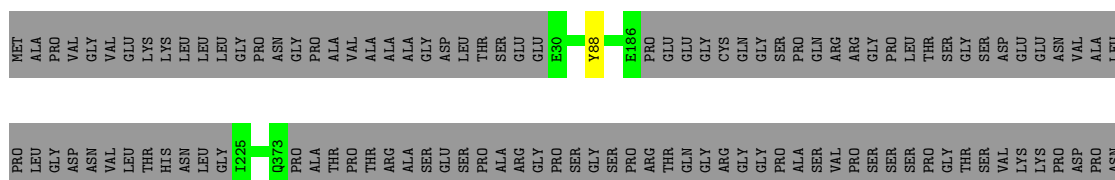
- Molecule 17: Cytoplasmic dynein 1 light intermediate chain 2

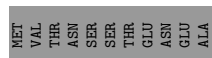


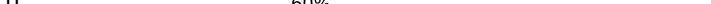
- Molecule 17: Cytoplasmic dynein 1 light intermediate chain 2

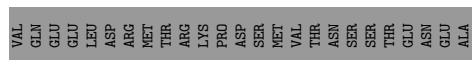
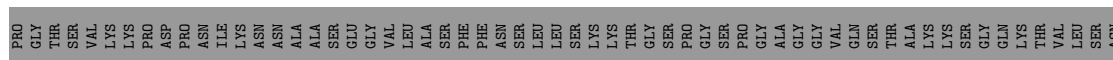


- Molecule 17: Cytoplasmic dynein 1 light intermediate chain 2



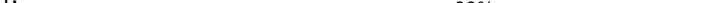


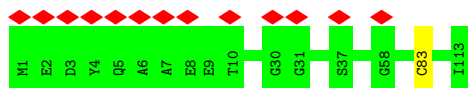
Chain u:  60% 39%

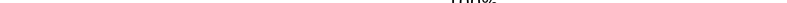


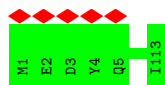
Chain k: 5% 100%



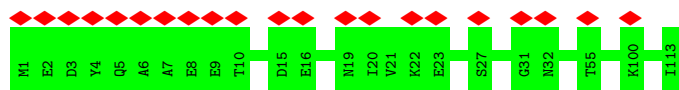
Chain 1:  12% 99%



Chain v: 

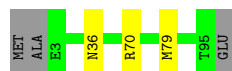


Chain γ : 19% 100%



- Molecule 19: Dynein light chain roadblock-type 1

Chain s: 94%



- Molecule 19: Dynein light chain roadblock-type 1

Chain t: 96%



- Molecule 19: Dynein light chain roadblock-type 1

Chain w: 93%



- Molecule 19: Dynein light chain roadblock-type 1

Chain z: 86% 10%



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ADP, ANP, 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	0.34	0/1986	0.81	1/2764 (0.0%)
1	2	0.33	0/1986	0.80	2/2764 (0.1%)
1	3	0.32	0/1589	0.80	0/2211
1	4	0.31	0/1589	0.80	2/2211 (0.1%)
2	A	0.31	0/1821	0.73	0/2531
2	B	0.35	0/1821	0.77	4/2531 (0.2%)
2	C	0.32	0/1846	0.79	4/2566 (0.2%)
2	D	0.32	0/1821	0.81	0/2531
2	E	0.33	0/1821	0.77	0/2531
2	F	0.33	0/1821	0.80	3/2531 (0.1%)
2	G	0.31	0/1821	0.76	0/2531
2	I	0.30	0/1821	0.75	4/2531 (0.2%)
3	H	0.33	0/1821	0.81	0/2531
4	J	0.30	0/1867	0.77	6/2596 (0.2%)
5	K	0.35	0/1377	0.82	2/1919 (0.1%)
6	L	0.32	0/1326	0.67	0/1844
7	M	0.48	0/1563	1.00	4/2171 (0.2%)
7	N	0.49	0/1304	0.91	1/1813 (0.1%)
7	P	0.56	2/1753 (0.1%)	0.95	3/2443 (0.1%)
7	Q	0.55	1/1629 (0.1%)	0.94	4/2268 (0.2%)
8	O	0.59	1/843 (0.1%)	1.06	0/1175
8	R	0.41	0/887	0.81	0/1236
9	S	0.52	1/3558 (0.0%)	0.95	8/4955 (0.2%)
9	T	0.39	0/3847	0.77	0/5363
10	U	0.32	0/830	0.79	0/1151
11	W	0.32	0/880	0.81	0/1222
12	X	0.42	0/1575	0.76	1/2193 (0.0%)
12	x	0.46	0/1400	0.84	1/1951 (0.1%)
13	Y	0.29	0/1858	0.70	0/2586
14	a	0.35	0/440	0.94	0/612
14	b	0.37	0/440	0.86	0/612
14	d	0.37	0/440	0.93	4/612 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	i	0.35	0/440	0.88	2/612 (0.3%)
15	e	0.37	0/22223	0.81	29/30973 (0.1%)
15	f	0.32	0/22304	0.75	21/31088 (0.1%)
15	m	0.31	0/22603	0.72	5/31515 (0.0%)
15	n	0.38	1/22623 (0.0%)	0.79	15/31543 (0.0%)
16	g	0.29	0/2271	0.67	2/3158 (0.1%)
16	h	0.27	0/2280	0.67	0/3170
16	o	0.31	0/2097	0.73	4/2916 (0.1%)
16	p	0.30	0/2131	0.72	2/2963 (0.1%)
17	j	0.32	0/1602	0.69	1/2229 (0.0%)
17	q	0.31	0/1572	0.75	0/2188
17	r	0.33	0/1578	0.76	0/2196
17	u	0.31	0/1470	0.76	0/2043
18	k	0.27	0/557	0.65	0/774
18	l	0.26	0/557	0.62	0/774
18	v	0.26	0/557	0.59	0/774
18	y	0.30	0/557	0.59	0/774
19	s	0.50	1/461 (0.2%)	0.79	0/642
19	t	0.37	0/461	0.85	2/642 (0.3%)
19	w	0.23	0/461	0.54	0/642
19	z	0.23	0/461	0.47	0/642
All	All	0.36	7/160647 (0.0%)	0.78	137/223744 (0.1%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	333	LEU	C-N	-10.01	1.23	1.34
7	P	336	ARG	CA-C	-9.73	1.40	1.52
7	P	337	LEU	N-CA	-9.21	1.35	1.46
9	S	853	ALA	C-N	8.70	1.40	1.33
8	O	117	LYS	C-N	7.90	1.46	1.33
19	s	36	ASN	C-N	7.37	1.42	1.34
15	n	2526	LEU	C-N	5.19	1.40	1.33

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	1127	PRO	CA-C-N	8.64	128.27	118.85
9	S	1127	PRO	C-N-CA	8.64	128.27	118.85
15	e	1692	ILE	N-CA-C	-8.29	104.63	112.83
15	e	3347	PHE	CA-C-N	8.02	125.29	120.24
15	e	3347	PHE	C-N-CA	8.02	125.29	120.24
15	n	966	ASN	CA-C-N	7.54	133.10	122.46
15	n	966	ASN	C-N-CA	7.54	133.10	122.46
15	f	1429	LEU	CA-C-N	7.47	131.17	120.79
15	f	1429	LEU	C-N-CA	7.47	131.17	120.79
9	S	1118	GLN	N-CA-CB	7.19	122.11	110.40
15	e	1437	VAL	CA-C-N	7.18	132.01	121.31
15	e	1437	VAL	C-N-CA	7.18	132.01	121.31
7	Q	132	GLU	N-CA-CB	7.17	122.45	110.41
9	S	1136	LEU	CA-C-N	7.08	127.67	120.38
9	S	1136	LEU	C-N-CA	7.08	127.67	120.38
15	f	339	PHE	CB-CA-C	7.06	118.83	109.65
7	P	336	ARG	O-C-N	7.01	129.29	122.07
15	e	639	ARG	CA-C-N	6.53	134.02	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	639	ARG	C-N-CA	6.53	134.02	121.54
15	e	892	SER	N-CA-C	6.53	118.55	110.91
4	J	274	ASP	CA-C-N	6.38	131.47	122.08
4	J	274	ASP	C-N-CA	6.38	131.47	122.08
19	t	35	ASP	CA-C-N	6.14	128.69	120.58
19	t	35	ASP	C-N-CA	6.14	128.69	120.58
7	M	76	GLY	N-CA-C	6.12	120.37	112.54
15	n	528	GLU	N-CA-CB	6.04	120.57	110.41
15	e	793	GLU	N-CA-CB	5.96	120.11	110.40
12	X	95	GLU	N-CA-CB	5.88	120.15	110.39
2	C	324	LYS	CA-C-N	5.87	132.75	121.54
2	C	324	LYS	C-N-CA	5.87	132.75	121.54
15	f	412	VAL	CA-C-N	-5.87	111.76	122.38
15	f	412	VAL	C-N-CA	-5.87	111.76	122.38
2	I	99	LEU	CA-C-N	5.85	131.28	122.68
2	I	99	LEU	C-N-CA	5.85	131.28	122.68
15	n	3125	TYR	CA-C-N	5.84	132.03	120.94
15	n	3125	TYR	C-N-CA	5.84	132.03	120.94
7	P	24	ASP	CA-C-N	5.83	129.54	120.68
7	P	24	ASP	C-N-CA	5.83	129.54	120.68
2	I	98	GLN	CA-C-N	5.82	132.66	121.54
2	I	98	GLN	C-N-CA	5.82	132.66	121.54
1	l	74	GLU	N-CA-CB	5.79	120.14	110.41
16	p	128	VAL	CA-C-N	5.76	132.54	121.54
16	p	128	VAL	C-N-CA	5.76	132.54	121.54
15	f	465	GLN	N-CA-CB	5.75	119.94	110.39
9	S	1137	PRO	N-CA-CB	5.73	108.64	103.08
15	e	2668	LEU	N-CA-C	5.63	122.25	109.81
15	f	830	ASP	N-CA-C	5.60	122.19	109.81
2	F	91	GLN	N-CA-CB	5.58	119.50	110.40
16	o	127	ILE	CA-C-N	5.54	128.85	120.77
16	o	127	ILE	C-N-CA	5.54	128.85	120.77
15	e	366	LYS	CB-CA-C	5.51	119.60	111.06
5	K	148	ILE	CA-C-N	5.50	132.03	121.54
5	K	148	ILE	C-N-CA	5.50	132.03	121.54
15	m	2222	MET	CB-CA-C	5.49	118.61	111.42
15	e	2859	PRO	CA-C-N	5.47	130.17	122.46
15	e	2859	PRO	C-N-CA	5.47	130.17	122.46
15	e	1480	TYR	CA-C-N	5.46	129.88	122.07
15	e	1480	TYR	C-N-CA	5.46	129.88	122.07
15	e	2373	MET	N-CA-CB	-5.41	101.89	110.28
15	e	2384	SER	CA-C-N	5.40	132.11	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	2384	SER	C-N-CA	5.40	132.11	122.13
15	m	2943	LYS	CA-C-N	5.39	134.51	125.02
15	m	2943	LYS	C-N-CA	5.39	134.51	125.02
14	i	52	PRO	CA-C-N	5.38	131.38	121.70
14	i	52	PRO	C-N-CA	5.38	131.38	121.70
15	e	1438	ASP	N-CA-C	5.37	117.86	110.35
15	e	3849	VAL	CA-C-N	5.36	129.96	122.08
15	e	3849	VAL	C-N-CA	5.36	129.96	122.08
4	J	273	GLN	CA-C-N	5.36	130.02	122.46
4	J	273	GLN	C-N-CA	5.36	130.02	122.46
1	2	171	ASP	CA-C-N	5.35	131.66	123.47
1	2	171	ASP	C-N-CA	5.35	131.66	123.47
15	e	2870	PRO	CA-C-N	5.35	131.60	121.97
15	e	2870	PRO	C-N-CA	5.35	131.60	121.97
15	f	1480	TYR	CA-C-N	5.35	129.72	122.07
15	f	1480	TYR	C-N-CA	5.35	129.72	122.07
15	n	2943	LYS	CA-C-N	5.35	134.43	125.02
15	n	2943	LYS	C-N-CA	5.35	134.43	125.02
7	M	384	GLU	N-CA-CB	5.34	118.53	110.30
9	S	612	MET	CB-CA-C	5.34	120.70	110.17
15	n	2726	ARG	CA-C-N	5.33	129.61	120.71
15	n	2726	ARG	C-N-CA	5.33	129.61	120.71
7	Q	333	LEU	O-C-N	-5.32	116.29	122.03
15	f	3849	VAL	CA-C-N	5.30	129.87	122.08
15	f	3849	VAL	C-N-CA	5.30	129.87	122.08
15	e	1861	MET	N-CA-C	-5.28	102.34	109.95
15	f	1404	LYS	CA-C-N	5.28	131.63	121.54
15	f	1404	LYS	C-N-CA	5.28	131.63	121.54
15	f	1430	THR	N-CA-C	5.28	117.46	111.02
15	n	333	ASN	N-CA-C	5.28	119.92	112.75
15	m	339	PHE	CB-CA-C	5.27	116.30	108.87
2	C	98	GLN	CA-C-N	5.26	131.59	121.54
2	C	98	GLN	C-N-CA	5.26	131.59	121.54
15	n	3499	GLN	N-CA-CB	5.26	118.48	110.44
14	d	52	PRO	CA-C-N	5.24	131.13	121.70
14	d	52	PRO	C-N-CA	5.24	131.13	121.70
2	F	324	LYS	CA-C-N	5.24	129.78	122.08
2	F	324	LYS	C-N-CA	5.24	129.78	122.08
15	f	409	PHE	CA-C-N	5.23	127.25	120.44
15	f	409	PHE	C-N-CA	5.23	127.25	120.44
15	n	2222	MET	CB-CA-C	5.23	118.27	111.42
15	f	1908	ALA	N-CA-C	-5.23	103.50	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	2870	PRO	CA-C-N	5.21	131.34	121.97
15	f	2870	PRO	C-N-CA	5.21	131.34	121.97
7	N	137	PRO	N-CA-CB	5.20	108.72	103.00
9	S	1127	PRO	N-CA-CB	5.18	108.10	103.08
15	m	4022	GLU	CB-CA-C	5.18	118.08	111.40
16	o	126	GLU	CA-C-N	5.17	131.27	121.97
16	o	126	GLU	C-N-CA	5.17	131.27	121.97
15	f	2384	SER	CA-C-N	5.17	131.69	122.13
15	f	2384	SER	C-N-CA	5.17	131.69	122.13
15	n	3262	GLU	N-CA-CB	5.16	118.96	110.39
2	B	324	LYS	CA-C-N	5.14	129.43	122.07
2	B	324	LYS	C-N-CA	5.14	129.43	122.07
7	Q	86	GLY	CA-C-N	5.14	129.42	122.07
7	Q	86	GLY	C-N-CA	5.14	129.42	122.07
15	n	1060	LEU	CA-C-N	-5.12	115.02	122.86
15	n	1060	LEU	C-N-CA	-5.12	115.02	122.86
1	4	171	ASP	CA-C-N	5.10	132.82	124.31
1	4	171	ASP	C-N-CA	5.10	132.82	124.31
2	B	98	GLN	CA-C-N	5.10	131.27	121.54
2	B	98	GLN	C-N-CA	5.10	131.27	121.54
4	J	250	LEU	CA-C-N	5.09	131.26	121.54
4	J	250	LEU	C-N-CA	5.09	131.26	121.54
15	e	1862	ALA	CA-C-N	5.08	131.24	121.54
15	e	1862	ALA	C-N-CA	5.08	131.24	121.54
12	x	133	THR	N-CA-CB	5.08	117.34	109.98
15	e	1964	GLU	CA-C-N	5.06	131.21	121.54
15	e	1964	GLU	C-N-CA	5.06	131.21	121.54
16	g	477	ASP	CA-C-N	5.03	132.71	124.31
16	g	477	ASP	C-N-CA	5.03	132.71	124.31
15	e	89	GLY	N-CA-C	5.02	120.23	114.16
17	j	48	ARG	N-CA-C	5.02	117.00	110.43
14	d	12	ASP	CA-C-N	5.01	130.82	122.20
14	d	12	ASP	C-N-CA	5.01	130.82	122.20
7	M	76	GLY	CA-C-N	5.00	129.23	122.07
7	M	76	GLY	C-N-CA	5.00	129.23	122.07

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

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Mol	Chain	Res	Type	Group
2	C	287	ASP	Peptide
2	F	287	ASP	Peptide
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

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Mol	Chain	Res	Type	Group
15	n	1061	TRP	Peptide
15	n	1063	MET	Peptide
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	U	832	0	371	3	0
11	W	881	0	379	2	0
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	1	0
14	b	441	0	204	2	0
14	d	441	0	204	2	0
14	i	441	0	204	3	0
15	e	22238	0	9837	21	0
15	f	22318	0	9878	23	0
15	m	22608	0	10040	6	0
15	n	22628	0	10047	12	0
16	g	2275	0	1017	4	0
16	h	2284	0	1022	3	0
16	o	2100	0	939	5	0
16	p	2134	0	954	3	0
17	j	1605	0	703	1	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	1	0
18	v	558	0	261	0	0
18	y	558	0	261	0	0
19	s	462	0	192	1	0
19	t	462	0	192	0	0
19	w	462	0	192	2	0
19	z	462	0	192	5	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	4	0
20	f	81	0	36	6	0
20	m	27	0	12	0	0
20	n	27	0	12	1	0
21	H	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	J	31	0	12	0	0
21	e	31	0	12	1	0
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	2	0
24	n	62	0	26	2	0
All	All	161538	0	71942	137	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 (137) 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)
15:e:1909:GLY:N	20:e:4801:ADP:O2A	2.23	0.71
15:e:2231:SER:CB	21:e:4803:ATP:O2B	2.39	0.70
15:m:152:PHE:O	15:m:156:ALA:HB3	2.00	0.61
15:e:2942:GLY:HA2	20:e:4806:ADP:O2A	2.02	0.58
19:w:68:PHE:HA	19:w:81:ALA:HA	1.88	0.55
15:f:2909:LEU:HA	20:f:4806:ADP:C2	2.42	0.55
15:e:2909:LEU:HA	20:e:4806:ADP:C2	2.42	0.54
15:f:1911:GLY:HA2	20:f:4801:ADP:H5'1	1.90	0.54
19:z:23:VAL:HA	19:z:29:PRO:HA	1.90	0.53
15:e:4286:CYS:HA	15:e:4293:ASP:HA	1.89	0.53
15:f:1910:THR:O	20:f:4801:ADP:H8	1.91	0.53
15:f:4286:CYS:HA	15:f:4293:ASP:HA	1.93	0.51
16:h:411:MET:HA	16:h:423:VAL:HA	1.93	0.51
19:w:72:ARG:HA	19:w:77:GLU:HA	1.93	0.51
15:f:4606:THR:HA	15:f:4623:ASP:HA	1.93	0.50
16:h:358:VAL:HA	16:h:376:SER:HA	1.93	0.50
2:I:20:VAL:HA	2:I:36:PRO:HA	1.93	0.50
15:n:2624:SER:HA	15:n:2669:PRO:HA	1.94	0.50
15:f:1911:GLY:N	20:f:4801:ADP:H5'1	2.27	0.50
19:z:76:ASN:HA	19:z:93:ASN:HA	1.94	0.50
2:B:20:VAL:HA	2:B:36:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:54:TRP:HA	14:b:87:LYS:HA	1.93	0.49
16:o:358:VAL:HA	16:o:376:SER:HA	1.94	0.49
14:d:59:GLY:HA3	14:i:62:PHE:HA	1.95	0.49
14:i:54:TRP:HA	14:i:87:LYS:HA	1.95	0.49
13:Y:433:LYS:HA	13:Y:450:GLU:HA	1.95	0.49
15:e:4606:THR:HA	15:e:4623:ASP:HA	1.94	0.49
2:D:20:VAL:HA	2:D:36:PRO:HA	1.95	0.48
15:f:1911:GLY:CA	20:f:4801:ADP:H5'1	2.44	0.48
2:D:291:ARG:O	2:D:295:PHE:N	2.44	0.47
15:e:1350:PRO:HA	15:e:1430:THR:HA	1.95	0.47
15:f:2942:GLY:HA2	20:f:4806:ADP:O2A	2.14	0.47
19:s:70:ARG:HA	19:s:79:MET:HA	1.96	0.47
5:K:153:THR:HA	5:K:180:THR:HA	1.97	0.47
15:f:77:VAL:HA	15:f:105:ILE:HA	1.97	0.47
2:E:291:ARG:O	2:E:295:PHE:N	2.45	0.47
15:e:1099:LYS:HA	15:e:1108:ASP:HA	1.97	0.47
15:f:1217:GLU:O	15:f:1221:PHE:N	2.47	0.47
15:m:1350:PRO:HA	15:m:1430:THR:HA	1.97	0.46
15:n:4284:LEU:N	15:n:4294:ILE:O	2.47	0.46
15:f:1665:ILE:O	15:f:1674:LEU:N	2.48	0.46
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
15:e:1213:ASN:O	15:e:1217:GLU:CB	2.64	0.45
15:n:1350:PRO:HA	15:n:1430:THR:HA	1.97	0.45
1:2:218:MET:O	1:2:227:VAL:N	2.49	0.45
15:f:2969:GLY:O	15:f:2973:ASP:N	2.49	0.45
15:e:3512:ALA:O	15:e:3516:TYR:CB	2.65	0.45
11:W:58:GLY:HA3	11:W:89:ASP:HA	1.99	0.45
15:f:1460:GLU:O	15:f:1464:LYS:N	2.44	0.45
15:m:3461:ILE:O	15:m:3465:LEU:N	2.50	0.45
15:n:530:VAL:HA	15:n:549:ALA:HB1	1.98	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
15:e:1409:LYS:O	15:e:1413:TRP:N	2.45	0.44
15:e:4564:LYS:HA	15:e:4584:ALA:HA	1.97	0.44
2:F:155:GLY:N	2:F:170:ILE:O	2.51	0.44
19:z:22:VAL:HA	19:z:88:LEU:HA	1.98	0.44
4:J:344:HIS:HA	13:Y:228:ALA:HA	1.99	0.44
14:b:52:PRO:HA	14:b:53:THR:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:m:77:VAL:HA	15:m:105:ILE:HA	1.99	0.44
14:d:62:PHE:HA	14:i:59:GLY:HA3	1.98	0.44
9:T:896:LEU:O	9:T:900:MET:CB	2.66	0.44
15:f:152:PHE:O	15:f:156:ALA:HB3	2.16	0.44
15:m:2943:LYS:O	24:m:4705:ANP:O2A	2.35	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
18:l:83:CYS:H	16:o:115:ALA:HB3	1.83	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
24:n:4705:ANP:O1G	24:n:4705:ANP:O2B	2.36	0.43
1:1:238:ARG:H	1:1:253:SER:HA	1.84	0.43
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
15:e:1479:ASN:HA	15:e:1485:ARG:HA	2.01	0.43
6:L:225:ARG:O	6:L:229:ASN:CB	2.67	0.43
16:p:312:ALA:HA	16:p:324:GLY:HA2	2.00	0.43
1:3:104:LEU:N	1:3:404:VAL:O	2.48	0.43
15:e:581:MET:O	15:e:585:PHE:CB	2.66	0.43
16:h:422:VAL:HA	16:h:432:THR:HA	2.01	0.43
9:T:874:SER:O	9:T:878:TYR:CB	2.67	0.43
16:g:525:LEU:O	16:g:536:THR:N	2.51	0.43
16:g:366:THR:N	16:g:369:ALA:O	2.52	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
24:m:4705:ANP:O2B	24:m:4705:ANP:O1G	2.37	0.42
10:U:114:GLY:HA3	10:U:132:ASN:HA	2.01	0.42
15:m:1319:VAL:O	15:m:1323:LEU:N	2.44	0.42
15:e:4284:LEU:N	15:e:4294:ILE:O	2.47	0.42
15:n:77:VAL:HA	15:n:105:ILE:HA	2.01	0.42
14:a:54:TRP:HA	14:a:87:LYS:HA	2.01	0.42
1:2:104:LEU:N	1:2:404:VAL:O	2.47	0.42
15:e:303:ILE:O	15:e:307:GLY:N	2.46	0.42
1:1:322:MET:O	1:1:331:LEU:N	2.49	0.42
15:n:924:GLN:O	15:n:930:ALA:N	2.52	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
15:n:2943:LYS:O	24:n:4705:ANP:O2A	2.37	0.42
15:n:4634:SER:O	15:n:4638:ARG:CB	2.68	0.42
15:f:2052:VAL:O	15:f:2056:SER:N	2.52	0.42
1:2:96:PRO:HA	1:2:409:CYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:1911:GLY:O	15:f:1912:LYS:C	2.63	0.42
16:g:383:SER:O	16:g:393:GLN:N	2.52	0.42
13:Y:435:LEU:H	13:Y:449:ALA:HB1	1.85	0.41
15:n:2803:VAL:O	15:n:2807:PHE:CB	2.68	0.41
16:o:365:GLY:HA3	16:o:370:HIS:HA	2.01	0.41
2:B:290:LEU:O	2:B:294:LEU:N	2.49	0.41
15:e:342:ASN:O	15:e:346:SER:CB	2.67	0.41
15:f:3874:GLY:HA2	15:f:4146:VAL:H	1.84	0.41
15:n:1910:THR:N	20:n:4701:ADP:O1B	2.53	0.41
16:p:333:LEU:N	16:p:345:GLN:O	2.52	0.41
19:z:77:GLU:N	19:z:92:GLN:O	2.54	0.41
3:H:19:ALA:HB3	3:H:29:ALA:HB3	2.01	0.41
15:f:806:ALA:HB1	17:j:355:ALA:HA	2.02	0.41
16:p:547:LEU:HA	16:p:563:ASP:HA	2.02	0.41
10:U:28:THR:N	10:U:48:ILE:O	2.53	0.41
15:f:3472:VAL:O	15:f:3476:THR:N	2.53	0.41
15:f:4284:LEU:N	15:f:4294:ILE:O	2.48	0.41
15:e:1232:ILE:O	15:e:1236:VAL:CB	2.68	0.41
15:e:3798:SER:O	15:e:3802:LEU:CB	2.68	0.41
15:f:3201:LEU:O	15:f:3205:LEU:N	2.47	0.41
15:n:4288:VAL:N	15:n:4292:LYS:O	2.51	0.41
16:o:548:ASN:N	16:o:562:GLY:O	2.53	0.41
11:W:147:SER:O	11:W:152:LEU:N	2.52	0.41
15:e:4384:ALA:O	15:e:4388:LEU:CB	2.68	0.41
19:z:70:ARG:HA	19:z:79:MET:HA	2.03	0.41
9:S:731:TYR:O	9:S:736:ALA:N	2.54	0.40
15:f:3153:THR:O	15:f:3157:ALA:N	2.53	0.40
15:e:1909:GLY:CA	20:e:4801:ADP:O2A	2.68	0.40
15:f:2639:CYS:HA	15:f:2652:PRO:HA	2.03	0.40
16:g:312:ALA:HA	16:g:324:GLY:HA2	2.03	0.40
15:n:2493:TYR:O	15:n:2497:ALA:HB2	2.22	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
16:o:454:THR:H	16:o:475:SER:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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%)	36	72
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%)	36	72
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%)	48	83
9	T	770/1281 (60%)	748 (97%)	21 (3%)	1 (0%)	48	83
10	U	165/190 (87%)	149 (90%)	16 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	11	46
15	e	4456/4646 (96%)	4310 (97%)	144 (3%)	2 (0%)	100	100
15	f	4474/4646 (96%)	4330 (97%)	140 (3%)	4 (0%)	48	83
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%)	43	78
16	p	426/612 (70%)	408 (96%)	17 (4%)	1 (0%)	43	78
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
14	i	51	ASN

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	n	4702	23	32,33,33	1.03	2 (6%)	48,52,52	0.52	0
20	ADP	e	4806	-	28,29,29	1.41	4 (14%)	43,45,45	1.89	8 (18%)
20	ADP	f	4805	-	28,29,29	1.40	4 (14%)	43,45,45	1.94	8 (18%)
21	ATP	e	4803	23	32,33,33	0.36	0	48,52,52	0.33	0
24	ANP	m	4705	-	33,33,33	0.90	3 (9%)	45,52,52	0.82	1 (2%)
20	ADP	e	4801	23	28,29,29	1.43	5 (17%)	43,45,45	1.80	9 (20%)
20	ADP	A	800	-	28,29,29	1.42	4 (14%)	43,45,45	1.90	12 (27%)
21	ATP	m	4702	23	32,33,33	1.40	2 (6%)	48,52,52	0.66	0
20	ADP	f	4801	23	28,29,29	1.43	5 (17%)	43,45,45	1.80	9 (20%)
20	ADP	C	800	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	10 (23%)
20	ADP	f	4806	-	28,29,29	1.39	4 (14%)	43,45,45	1.88	8 (18%)
20	ADP	F	800	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	10 (23%)
21	ATP	H	401	-	32,33,33	0.36	0	48,52,52	0.44	0
20	ADP	G	800	-	28,29,29	1.42	4 (14%)	43,45,45	1.86	11 (25%)
21	ATP	J	800	-	32,33,33	0.43	0	48,52,52	0.51	0
20	ADP	E	800	-	28,29,29	1.42	4 (14%)	43,45,45	1.83	10 (23%)
20	ADP	n	4701	-	28,29,29	1.45	5 (17%)	43,45,45	1.80	10 (23%)
24	ANP	n	4705	-	33,33,33	0.90	3 (9%)	45,52,52	0.89	2 (4%)
20	ADP	e	4805	-	28,29,29	1.41	4 (14%)	43,45,45	1.96	8 (18%)
20	ADP	B	800	-	28,29,29	1.42	4 (14%)	43,45,45	1.86	11 (25%)
20	ADP	I	800	-	28,29,29	1.41	4 (14%)	43,45,45	1.87	10 (23%)
24	ANP	n	4704	-	33,33,33	0.94	4 (12%)	45,52,52	0.71	2 (4%)
21	ATP	f	4803	23	32,33,33	0.36	0	48,52,52	0.33	0
24	ANP	m	4704	-	33,33,33	0.98	4 (12%)	45,52,52	0.56	0
20	ADP	D	800	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	8 (18%)
20	ADP	m	4701	-	28,29,29	1.46	4 (14%)	43,45,45	1.78	9 (20%)

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	n	4702	23	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	ADP	e	4806	-	-	2/16/32/32	0/3/3/3
20	ADP	f	4805	-	-	0/16/32/32	0/3/3/3
21	ATP	e	4803	23	-	2/22/38/38	0/3/3/3
24	ANP	m	4705	-	-	3/18/38/38	0/3/3/3
20	ADP	e	4801	23	-	3/16/32/32	0/3/3/3
20	ADP	A	800	-	-	1/16/32/32	0/3/3/3
21	ATP	m	4702	23	-	7/22/38/38	0/3/3/3
20	ADP	f	4801	23	-	3/16/32/32	0/3/3/3
20	ADP	C	800	-	-	2/16/32/32	0/3/3/3
20	ADP	f	4806	-	-	2/16/32/32	0/3/3/3
20	ADP	F	800	-	-	2/16/32/32	0/3/3/3
21	ATP	H	401	-	-	8/22/38/38	0/3/3/3
20	ADP	G	800	-	-	4/16/32/32	0/3/3/3
21	ATP	J	800	-	-	8/22/38/38	0/3/3/3
20	ADP	E	800	-	-	5/16/32/32	0/3/3/3
20	ADP	n	4701	-	-	7/16/32/32	0/3/3/3
24	ANP	n	4705	-	-	3/18/38/38	0/3/3/3
20	ADP	e	4805	-	-	0/16/32/32	0/3/3/3
20	ADP	B	800	-	-	2/16/32/32	0/3/3/3
20	ADP	I	800	-	-	3/16/32/32	0/3/3/3
24	ANP	n	4704	-	-	6/18/38/38	0/3/3/3
21	ATP	f	4803	23	-	2/22/38/38	0/3/3/3
24	ANP	m	4704	-	-	5/18/38/38	0/3/3/3
20	ADP	D	800	-	-	2/16/32/32	0/3/3/3
20	ADP	m	4701	-	-	3/16/32/32	0/3/3/3

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	m	4702	ATP	PB-O3B	-5.98	1.53	1.59
20	m	4701	ADP	C5-C4	4.91	1.47	1.39
20	C	800	ADP	C5-C4	4.84	1.47	1.39
20	E	800	ADP	C5-C4	4.82	1.47	1.39
20	D	800	ADP	C5-C4	4.82	1.47	1.39
20	n	4701	ADP	C5-C4	4.82	1.47	1.39
21	m	4702	ATP	PA-O3A	-4.81	1.54	1.59
20	I	800	ADP	C5-C4	4.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	800	ADP	C5-C4	4.75	1.47	1.39
20	e	4806	ADP	C5-C4	4.74	1.47	1.39
20	F	800	ADP	C5-C4	4.73	1.47	1.39
20	B	800	ADP	C5-C4	4.73	1.47	1.39
20	f	4806	ADP	C5-C4	4.70	1.47	1.39
20	A	800	ADP	C5-C4	4.70	1.47	1.39
21	n	4702	ATP	PB-O3B	-4.69	1.54	1.59
20	f	4805	ADP	C5-C4	4.69	1.47	1.39
20	e	4801	ADP	C5-C4	4.68	1.47	1.39
20	e	4805	ADP	C5-C4	4.67	1.47	1.39
20	f	4801	ADP	C5-C4	4.65	1.47	1.39
24	m	4704	ANP	PB-O3A	-3.14	1.55	1.59
20	D	800	ADP	C5-C6	2.80	1.48	1.41
20	G	800	ADP	C5-C6	2.79	1.48	1.41
20	A	800	ADP	C5-C6	2.79	1.48	1.41
20	n	4701	ADP	C5-C6	2.79	1.48	1.41
20	B	800	ADP	C5-C6	2.78	1.48	1.41
20	E	800	ADP	C5-C6	2.77	1.48	1.41
20	I	800	ADP	C5-C6	2.76	1.48	1.41
20	C	800	ADP	C5-C6	2.76	1.48	1.41
20	m	4701	ADP	C5-C6	2.75	1.48	1.41
20	e	4805	ADP	C5-C6	2.75	1.48	1.41
20	F	800	ADP	C5-C6	2.75	1.48	1.41
20	f	4806	ADP	C5-C6	2.74	1.48	1.41
20	e	4806	ADP	C5-C6	2.73	1.48	1.41
24	n	4704	ANP	PB-O3A	-2.71	1.55	1.59
20	f	4805	ADP	C5-C6	2.71	1.48	1.41
20	e	4801	ADP	C5-C6	2.64	1.48	1.41
20	f	4801	ADP	C5-C6	2.61	1.48	1.41
24	m	4705	ANP	PG-O1G	2.58	1.50	1.46
24	n	4705	ANP	PG-O1G	2.58	1.50	1.46
24	n	4704	ANP	PG-O1G	2.55	1.50	1.46
24	n	4705	ANP	PG-N3B	2.52	1.70	1.63
20	E	800	ADP	C5-N7	-2.51	1.34	1.39
20	e	4801	ADP	C5-N7	-2.51	1.34	1.39
20	f	4801	ADP	C5-N7	-2.49	1.34	1.39
24	m	4704	ANP	PG-O1G	2.47	1.49	1.46
24	m	4705	ANP	PG-N3B	2.45	1.69	1.63
24	n	4705	ANP	PB-O3A	-2.43	1.56	1.59
21	n	4702	ATP	PA-O3A	-2.41	1.56	1.59
24	m	4705	ANP	PB-O3A	-2.39	1.56	1.59
20	C	800	ADP	C5-N7	-2.39	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	800	ADP	C5-N7	-2.38	1.34	1.39
20	m	4701	ADP	C5-N7	-2.38	1.34	1.39
20	G	800	ADP	C8-N7	2.36	1.36	1.31
20	f	4806	ADP	C5-N7	-2.36	1.34	1.39
20	e	4806	ADP	C5-N7	-2.35	1.34	1.39
20	D	800	ADP	C5-N7	-2.35	1.34	1.39
20	e	4805	ADP	C5-N7	-2.34	1.34	1.39
20	D	800	ADP	C8-N7	2.33	1.36	1.31
20	F	800	ADP	C8-N7	2.33	1.36	1.31
20	f	4805	ADP	C5-N7	-2.31	1.34	1.39
20	I	800	ADP	C5-N7	-2.31	1.34	1.39
20	A	800	ADP	C5-N7	-2.30	1.34	1.39
20	I	800	ADP	C8-N7	2.30	1.36	1.31
20	F	800	ADP	C5-N7	-2.29	1.34	1.39
20	G	800	ADP	C5-N7	-2.29	1.34	1.39
20	A	800	ADP	C8-N7	2.28	1.36	1.31
20	n	4701	ADP	C5-N7	-2.28	1.34	1.39
20	n	4701	ADP	C8-N7	2.27	1.36	1.31
20	B	800	ADP	C8-N7	2.26	1.36	1.31
20	f	4801	ADP	C8-N7	2.26	1.36	1.31
20	f	4805	ADP	C8-N7	2.26	1.36	1.31
20	C	800	ADP	C8-N7	2.26	1.36	1.31
20	e	4805	ADP	C8-N7	2.26	1.36	1.31
24	n	4704	ANP	PG-N3B	2.24	1.69	1.63
20	e	4806	ADP	C8-N7	2.23	1.36	1.31
20	m	4701	ADP	C8-N7	2.22	1.35	1.31
24	m	4704	ANP	PG-N3B	2.20	1.69	1.63
20	e	4801	ADP	C8-N7	2.20	1.35	1.31
20	f	4806	ADP	C8-N7	2.19	1.35	1.31
20	E	800	ADP	C8-N7	2.18	1.35	1.31
24	n	4704	ANP	PB-O1B	2.13	1.49	1.46
24	m	4704	ANP	PB-O1B	2.12	1.49	1.46
20	e	4801	ADP	PA-O3A	2.11	1.61	1.59
20	f	4801	ADP	PA-O3A	2.08	1.61	1.59
20	n	4701	ADP	C4-N9	-2.07	1.33	1.37

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	e	4805	ADP	C5-C4-N3	-6.46	117.83	126.72
20	f	4805	ADP	C5-C4-N3	-6.44	117.85	126.72
20	e	4806	ADP	C5-C4-N3	-6.15	118.25	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	f	4806	ADP	C5-C4-N3	-6.13	118.28	126.72
20	D	800	ADP	C5-C4-N3	-5.92	118.56	126.72
20	E	800	ADP	C5-C4-N3	-5.90	118.60	126.72
20	f	4801	ADP	C5-C4-N3	-5.81	118.71	126.72
20	e	4801	ADP	C5-C4-N3	-5.79	118.75	126.72
20	I	800	ADP	C5-C4-N3	-5.77	118.78	126.72
20	C	800	ADP	C5-C4-N3	-5.75	118.80	126.72
20	G	800	ADP	C5-C4-N3	-5.71	118.86	126.72
20	B	800	ADP	C5-C4-N3	-5.68	118.89	126.72
20	F	800	ADP	C5-C4-N3	-5.68	118.90	126.72
20	m	4701	ADP	C5-C4-N3	-5.57	119.04	126.72
20	A	800	ADP	C5-C4-N3	-5.57	119.04	126.72
20	n	4701	ADP	C5-C4-N3	-5.40	119.28	126.72
20	e	4805	ADP	N3-C4-N9	5.32	136.21	127.17
20	f	4805	ADP	N3-C4-N9	5.31	136.19	127.17
20	e	4806	ADP	N3-C4-N9	4.95	135.58	127.17
20	f	4806	ADP	N3-C4-N9	4.90	135.50	127.17
20	D	800	ADP	N3-C4-N9	4.75	135.24	127.17
20	I	800	ADP	N3-C4-N9	4.65	135.08	127.17
20	e	4801	ADP	N3-C4-N9	4.65	135.07	127.17
20	E	800	ADP	N3-C4-N9	4.64	135.06	127.17
20	f	4801	ADP	N3-C4-N9	4.62	135.03	127.17
20	C	800	ADP	N3-C4-N9	4.59	134.97	127.17
20	F	800	ADP	N3-C4-N9	4.58	134.96	127.17
20	B	800	ADP	N3-C4-N9	4.57	134.95	127.17
20	m	4701	ADP	N3-C4-N9	4.57	134.94	127.17
20	G	800	ADP	N3-C4-N9	4.56	134.93	127.17
20	A	800	ADP	N3-C4-N9	4.47	134.77	127.17
20	n	4701	ADP	N3-C4-N9	4.38	134.61	127.17
24	n	4705	ANP	O1B-PB-N3B	-4.21	105.57	111.77
20	f	4805	ADP	C2-N3-C4	4.14	121.93	111.83
20	e	4805	ADP	C2-N3-C4	4.13	121.92	111.83
20	e	4806	ADP	C2-N3-C4	3.85	121.24	111.83
20	f	4806	ADP	C2-N3-C4	3.85	121.23	111.83
20	D	800	ADP	C2-N3-C4	3.85	121.22	111.83
20	G	800	ADP	C2-N3-C4	3.78	121.05	111.83
20	m	4701	ADP	N3-C2-N1	-3.77	122.87	128.58
20	m	4701	ADP	C2-N3-C4	3.76	121.00	111.83
20	E	800	ADP	C2-N3-C4	3.75	121.00	111.83
20	n	4701	ADP	C2-N3-C4	3.75	120.99	111.83
20	I	800	ADP	C2-N3-C4	3.75	120.98	111.83
20	B	800	ADP	C2-N3-C4	3.74	120.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	800	ADP	C2-N3-C4	3.73	120.93	111.83
20	C	800	ADP	C2-N3-C4	3.72	120.92	111.83
20	A	800	ADP	C2-N3-C4	3.70	120.86	111.83
20	n	4701	ADP	N3-C2-N1	-3.67	123.02	128.58
24	m	4705	ANP	O1B-PB-N3B	-3.64	106.40	111.77
20	e	4801	ADP	C2-N3-C4	3.63	120.70	111.83
20	f	4801	ADP	C2-N3-C4	3.63	120.70	111.83
20	f	4805	ADP	N3-C2-N1	-3.59	123.15	128.58
20	e	4805	ADP	N3-C2-N1	-3.58	123.16	128.58
20	E	800	ADP	C4-C5-N7	-3.46	106.62	110.58
20	A	800	ADP	C4-C5-N7	-3.46	106.62	110.58
20	G	800	ADP	C4-C5-N7	-3.42	106.67	110.58
20	B	800	ADP	C4-C5-N7	-3.42	106.67	110.58
20	G	800	ADP	N3-C2-N1	-3.42	123.41	128.58
20	D	800	ADP	N3-C2-N1	-3.39	123.46	128.58
20	f	4806	ADP	N3-C2-N1	-3.36	123.49	128.58
20	f	4806	ADP	C4-C5-N7	-3.36	106.74	110.58
20	f	4801	ADP	N3-C2-N1	-3.35	123.50	128.58
20	D	800	ADP	C4-C5-N7	-3.35	106.75	110.58
20	F	800	ADP	C4-C5-N7	-3.35	106.75	110.58
20	B	800	ADP	N3-C2-N1	-3.35	123.52	128.58
20	e	4806	ADP	N3-C2-N1	-3.34	123.52	128.58
20	C	800	ADP	C4-C5-N7	-3.34	106.77	110.58
20	e	4806	ADP	C4-C5-N7	-3.33	106.77	110.58
20	e	4801	ADP	N3-C2-N1	-3.33	123.53	128.58
20	A	800	ADP	N3-C2-N1	-3.32	123.56	128.58
20	F	800	ADP	N3-C2-N1	-3.32	123.56	128.58
20	e	4801	ADP	C4-C5-N7	-3.31	106.79	110.58
20	f	4801	ADP	C4-C5-N7	-3.31	106.79	110.58
20	I	800	ADP	N3-C2-N1	-3.31	123.57	128.58
20	I	800	ADP	C4-C5-N7	-3.29	106.82	110.58
20	n	4701	ADP	C4-C5-N7	-3.29	106.82	110.58
20	C	800	ADP	N3-C2-N1	-3.26	123.65	128.58
20	E	800	ADP	N3-C2-N1	-3.22	123.71	128.58
20	m	4701	ADP	C4-C5-N7	-3.18	106.94	110.58
20	f	4805	ADP	C4-C5-N7	-3.15	106.98	110.58
20	e	4805	ADP	C4-C5-N7	-3.11	107.02	110.58
20	A	800	ADP	C2'-C1'-N9	-2.91	106.08	113.30
20	A	800	ADP	O4'-C1'-N9	2.90	113.66	108.09
20	A	800	ADP	C4-N9-C8	2.81	108.69	105.74
20	e	4806	ADP	C3'-C2'-C1'	2.74	106.64	101.46
20	F	800	ADP	C4-N9-C8	2.73	108.60	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	800	ADP	C4-N9-C8	2.72	108.59	105.74
20	f	4806	ADP	C3'-C2'-C1'	2.71	106.60	101.46
20	B	800	ADP	C4-N9-C8	2.71	108.59	105.74
20	n	4701	ADP	C4-N9-C8	2.71	108.58	105.74
20	f	4805	ADP	C3'-C2'-C1'	2.65	106.48	101.46
20	e	4805	ADP	C3'-C2'-C1'	2.63	106.44	101.46
20	A	800	ADP	C5-N7-C8	2.60	107.53	103.45
20	I	800	ADP	C4-N9-C8	2.58	108.44	105.74
20	B	800	ADP	C5-N7-C8	2.56	107.48	103.45
20	E	800	ADP	C5-N7-C8	2.56	107.48	103.45
20	G	800	ADP	C5-N7-C8	2.55	107.46	103.45
20	F	800	ADP	C5-N7-C8	2.50	107.37	103.45
20	D	800	ADP	C4-N9-C8	2.50	108.36	105.74
20	D	800	ADP	C5-N7-C8	2.49	107.37	103.45
20	f	4805	ADP	C4-N9-C8	2.48	108.34	105.74
20	C	800	ADP	C3'-C2'-C1'	2.47	106.14	101.46
20	B	800	ADP	C3'-C2'-C1'	2.46	106.11	101.46
20	e	4805	ADP	C4-N9-C8	2.45	108.31	105.74
20	I	800	ADP	C5-N7-C8	2.45	107.30	103.45
20	f	4805	ADP	C5-N7-C8	2.44	107.28	103.45
20	f	4806	ADP	C5-N7-C8	2.44	107.28	103.45
20	m	4701	ADP	C4-N9-C8	2.44	108.30	105.74
20	C	800	ADP	C5-N7-C8	2.43	107.27	103.45
20	e	4806	ADP	C4-N9-C8	2.42	108.28	105.74
20	e	4801	ADP	C5-N7-C8	2.42	107.25	103.45
20	C	800	ADP	C4-N9-C8	2.42	108.28	105.74
20	e	4806	ADP	C5-N7-C8	2.42	107.25	103.45
20	m	4701	ADP	C2-N1-C6	2.42	122.70	118.73
20	I	800	ADP	C3'-C2'-C1'	2.41	106.02	101.46
20	e	4805	ADP	C5-N7-C8	2.41	107.23	103.45
20	F	800	ADP	C3'-C2'-C1'	2.39	105.99	101.46
20	e	4801	ADP	C4-N9-C8	2.38	108.23	105.74
20	n	4701	ADP	C6-C5-N7	2.37	136.66	132.09
20	f	4801	ADP	C5-N7-C8	2.37	107.17	103.45
20	f	4801	ADP	C4-N9-C8	2.36	108.22	105.74
20	f	4806	ADP	C4-N9-C8	2.35	108.20	105.74
20	A	800	ADP	C6-C5-N7	2.31	136.53	132.09
24	n	4704	ANP	O1B-PB-N3B	-2.29	108.39	111.77
20	E	800	ADP	C4-N9-C8	2.28	108.14	105.74
20	G	800	ADP	C6-C5-N7	2.26	136.46	132.09
20	E	800	ADP	C2'-C1'-N9	-2.26	107.68	113.30
20	B	800	ADP	C6-C5-N7	2.23	136.40	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	I	800	ADP	C2'-C1'-N9	-2.23	107.77	113.30
20	F	800	ADP	C6-C5-N7	2.23	136.39	132.09
20	n	4701	ADP	C5-N7-C8	2.22	106.94	103.45
20	m	4701	ADP	C5-N7-C8	2.21	106.93	103.45
20	G	800	ADP	C3'-C2'-C1'	2.21	105.65	101.46
20	E	800	ADP	C3'-C2'-C1'	2.21	105.64	101.46
20	n	4701	ADP	O3B-PB-O2B	2.17	115.94	107.80
20	C	800	ADP	C6-C5-N7	2.17	136.27	132.09
20	D	800	ADP	C6-C5-N7	2.16	136.25	132.09
20	E	800	ADP	C6-C5-N7	2.16	136.25	132.09
20	n	4701	ADP	C2-N1-C6	2.16	122.27	118.73
20	I	800	ADP	C6-C5-N7	2.15	136.23	132.09
20	G	800	ADP	C2'-C1'-N9	-2.14	107.98	113.30
20	f	4801	ADP	C2-N1-C6	2.14	122.24	118.73
20	e	4801	ADP	C2-N1-C6	2.13	122.23	118.73
20	F	800	ADP	C2'-C1'-N9	-2.10	108.08	113.30
20	e	4801	ADP	C2'-C3'-C4'	2.10	106.67	102.61
20	A	800	ADP	N9-C8-N7	-2.10	110.96	113.94
20	f	4801	ADP	C2'-C3'-C4'	2.08	106.63	102.61
20	m	4701	ADP	C6-C5-N7	2.08	136.10	132.09
20	C	800	ADP	C2'-C1'-N9	-2.07	108.15	113.30
20	A	800	ADP	C3'-C2'-C1'	2.07	105.37	101.46
24	n	4705	ANP	O3A-PB-N3B	2.06	112.30	106.59
20	G	800	ADP	N9-C8-N7	-2.03	111.06	113.94
20	B	800	ADP	C2'-C1'-N9	-2.03	108.27	113.30
24	n	4704	ANP	O1G-PG-N3B	-2.01	108.81	111.77
20	B	800	ADP	N9-C8-N7	-2.00	111.10	113.94

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	C	800	ADP	C5'-O5'-PA-O2A
20	C	800	ADP	C5'-O5'-PA-O3A
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	G	800	ADP	C5'-O5'-PA-O3A
20	I	800	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
20	I	800	ADP	C5'-O5'-PA-O2A
20	I	800	ADP	C5'-O5'-PA-O3A
20	n	4701	ADP	C5'-O5'-PA-O1A
20	n	4701	ADP	C5'-O5'-PA-O2A
20	n	4701	ADP	C5'-O5'-PA-O3A
21	H	401	ATP	C5'-O5'-PA-O1A
21	H	401	ATP	C5'-O5'-PA-O2A
21	H	401	ATP	C5'-O5'-PA-O3A
21	J	800	ATP	PB-O3B-PG-O2G
21	J	800	ATP	C5'-O5'-PA-O2A
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	C5'-O5'-PA-O3A
21	m	4702	ATP	O4'-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	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	D	800	ADP	C3'-C4'-C5'-O5'
21	H	401	ATP	C3'-C4'-C5'-O5'
21	m	4702	ATP	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	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	B	800	ADP	O4'-C4'-C5'-O5'
20	F	800	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
20	F	800	ADP	C3'-C4'-C5'-O5'
20	B	800	ADP	C3'-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	A	800	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
20	m	4701	ADP	PB-O3A-PA-O1A
20	e	4801	ADP	C5'-O5'-PA-O1A
20	f	4801	ADP	C5'-O5'-PA-O1A
21	J	800	ATP	C5'-O5'-PA-O1A
21	J	800	ATP	C5'-O5'-PA-O3A
24	m	4704	ANP	C5'-O5'-PA-O3A
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
20	m	4701	ADP	O4'-C4'-C5'-O5'
20	e	4801	ADP	O4'-C4'-C5'-O5'
20	f	4801	ADP	O4'-C4'-C5'-O5'
21	e	4803	ATP	O4'-C4'-C5'-O5'
21	f	4803	ATP	O4'-C4'-C5'-O5'
20	n	4701	ADP	PB-O3A-PA-O1A
20	n	4701	ADP	O4'-C4'-C5'-O5'
20	n	4701	ADP	PB-O3A-PA-O2A
21	e	4803	ATP	C3'-C4'-C5'-O5'
21	f	4803	ATP	C3'-C4'-C5'-O5'
24	m	4705	ANP	O4'-C4'-C5'-O5'
24	n	4705	ANP	O4'-C4'-C5'-O5'
21	J	800	ATP	C2'-C1'-N9-C8
21	H	401	ATP	PA-O3A-PB-O1B
20	n	4701	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 16 short contacts:

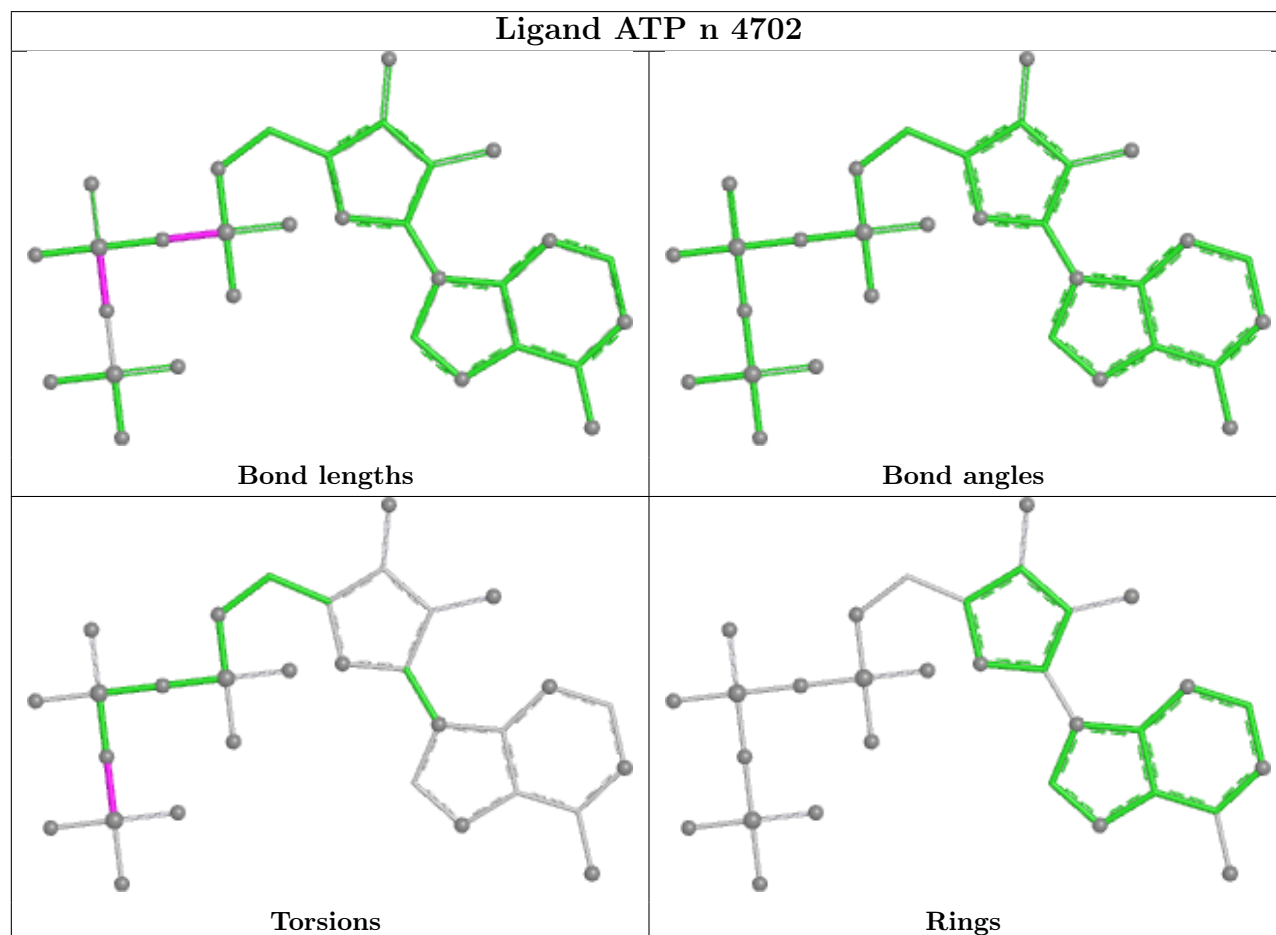
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	e	4806	ADP	2	0
21	e	4803	ATP	1	0

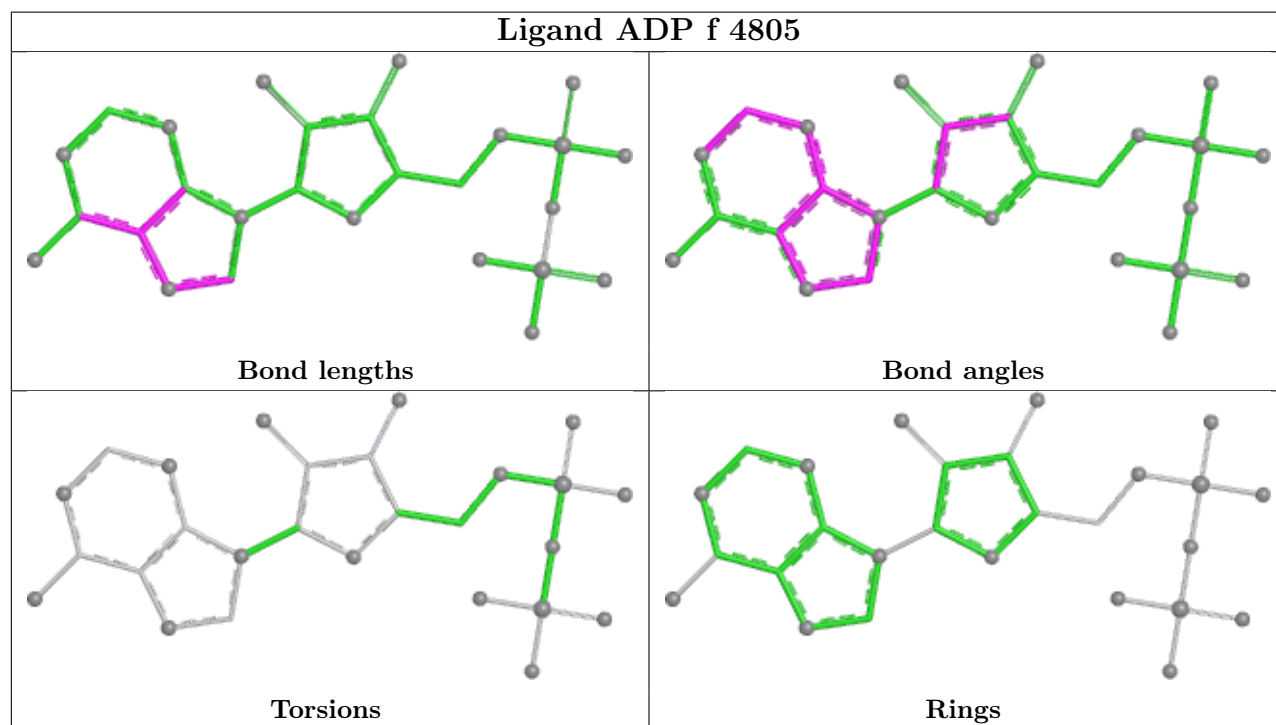
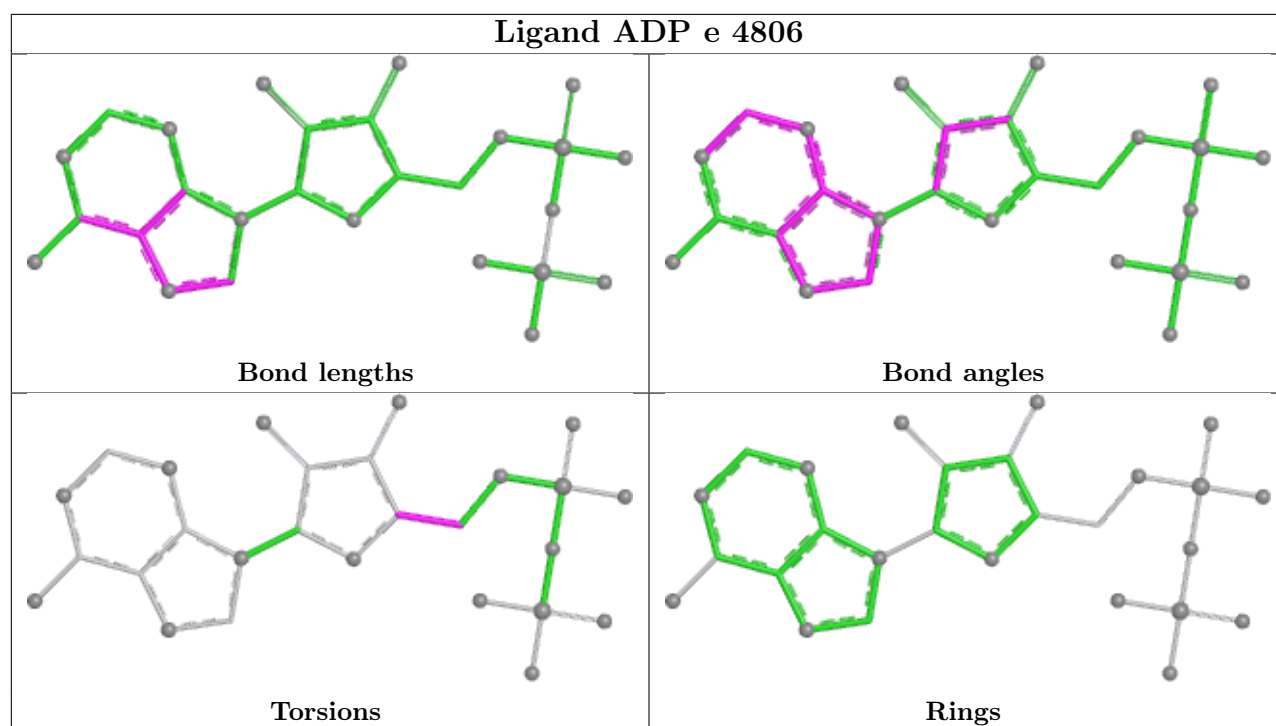
Continued on next page...

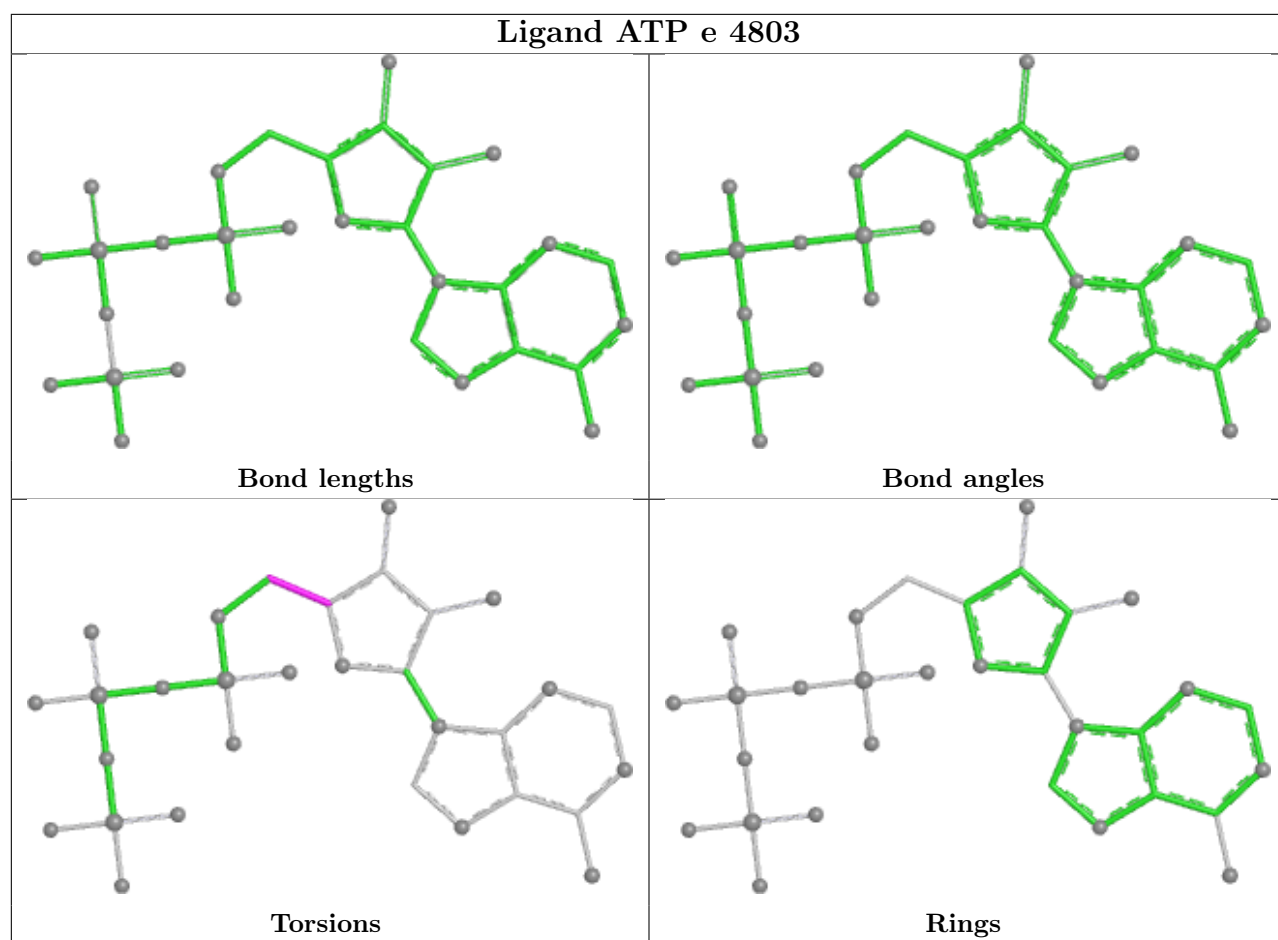
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	m	4705	ANP	2	0
20	e	4801	ADP	2	0
20	f	4801	ADP	4	0
20	f	4806	ADP	2	0
20	n	4701	ADP	1	0
24	n	4705	ANP	2	0

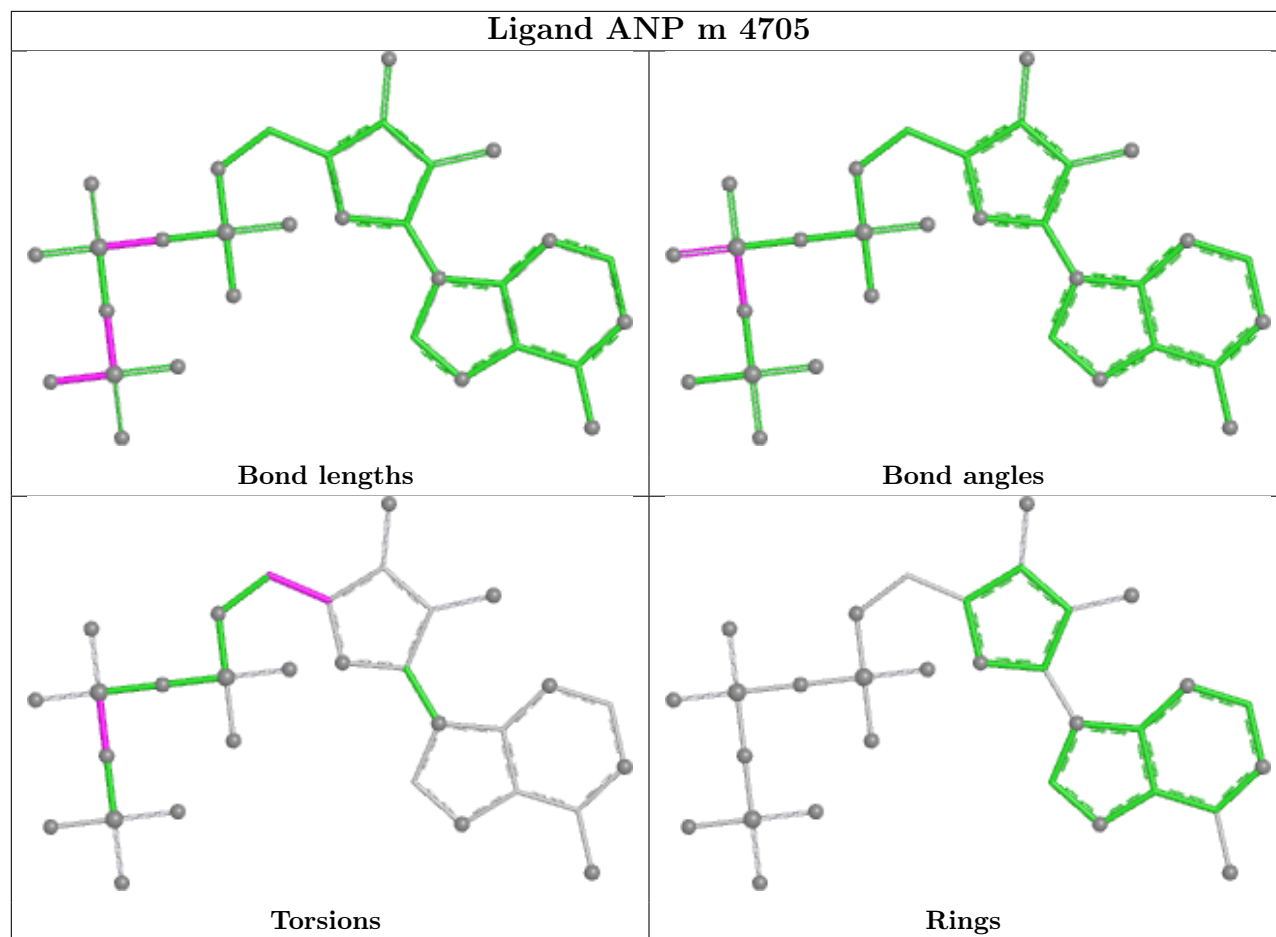
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



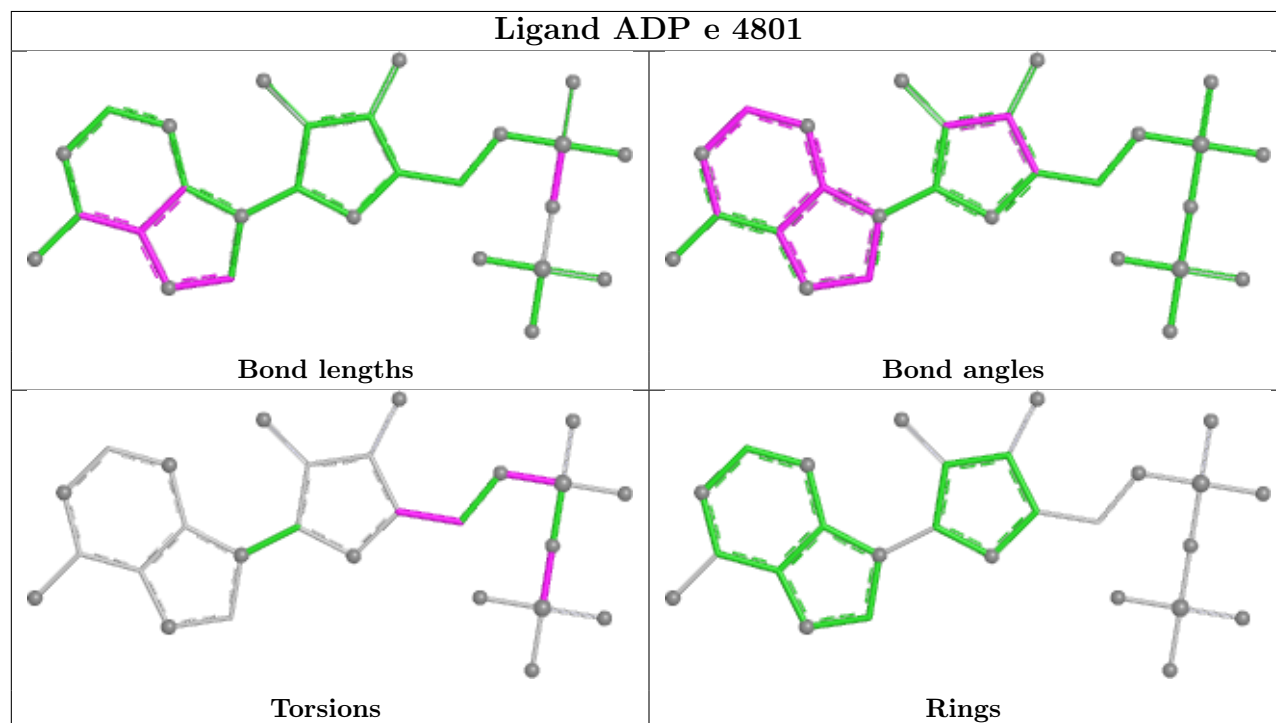


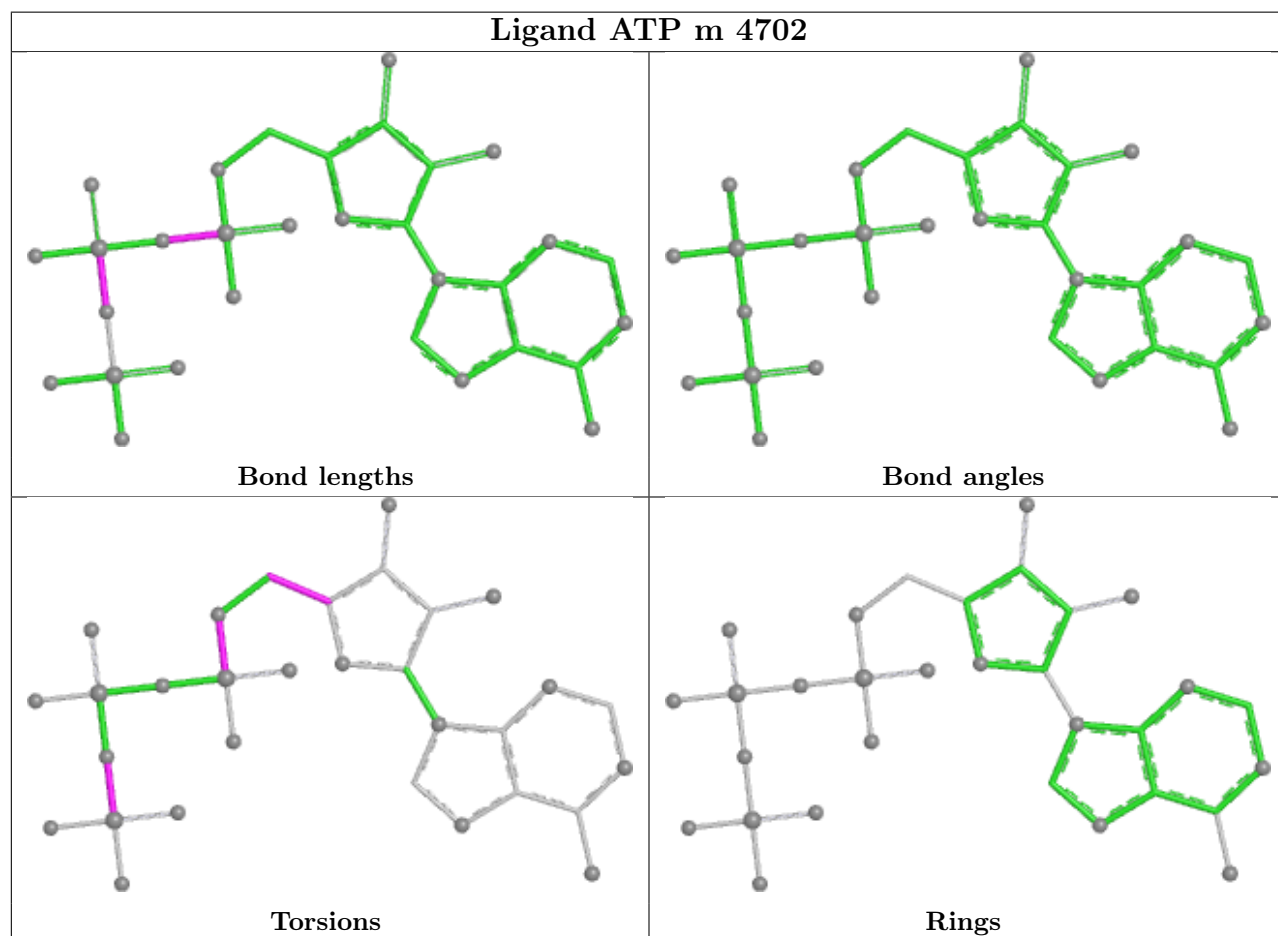
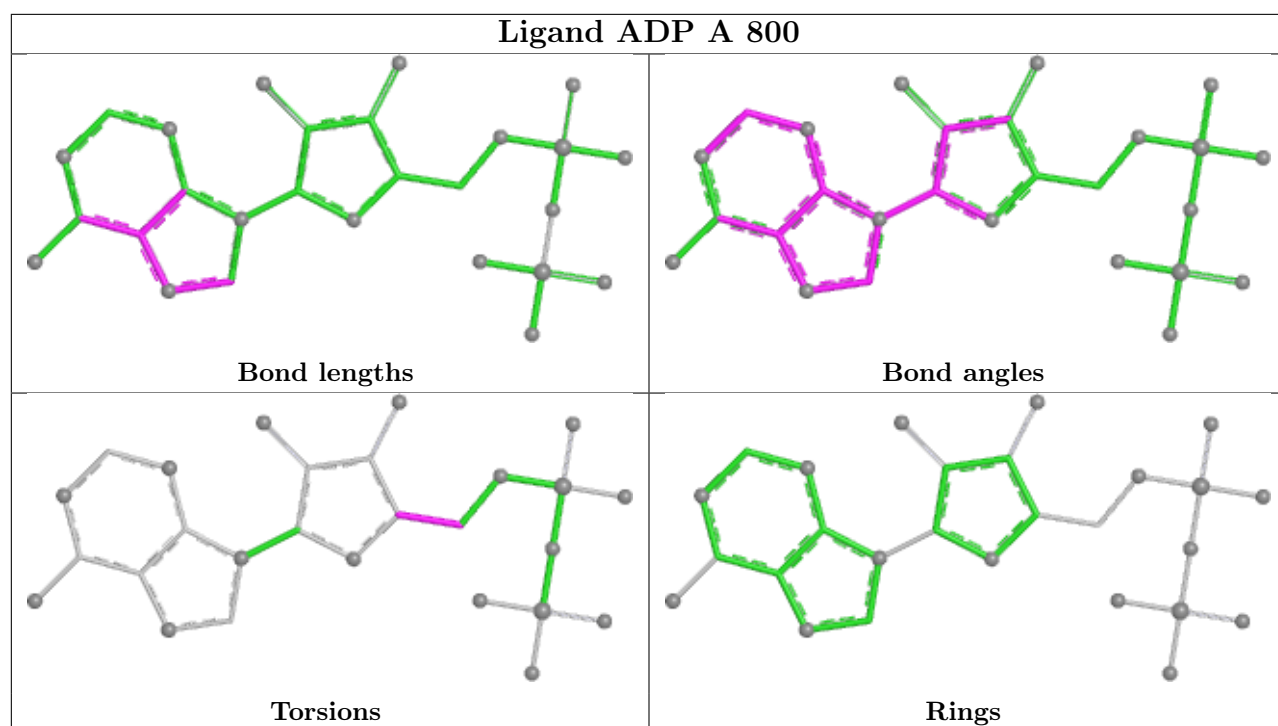


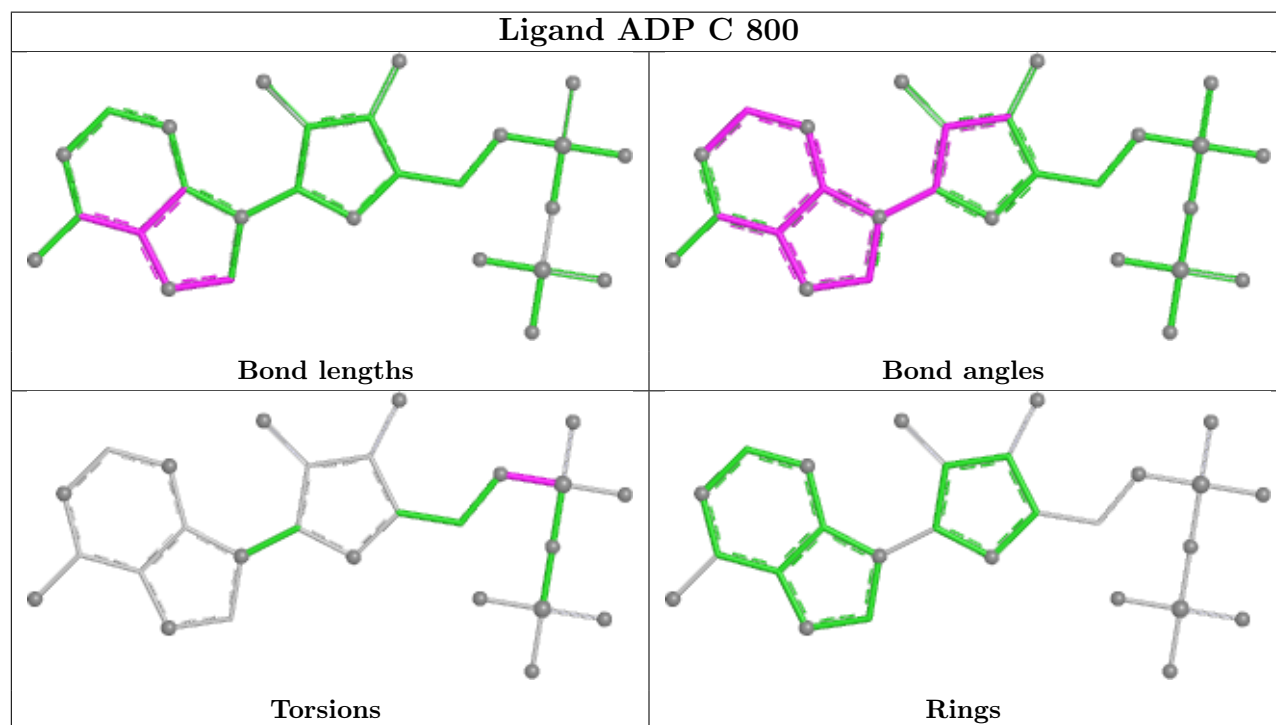
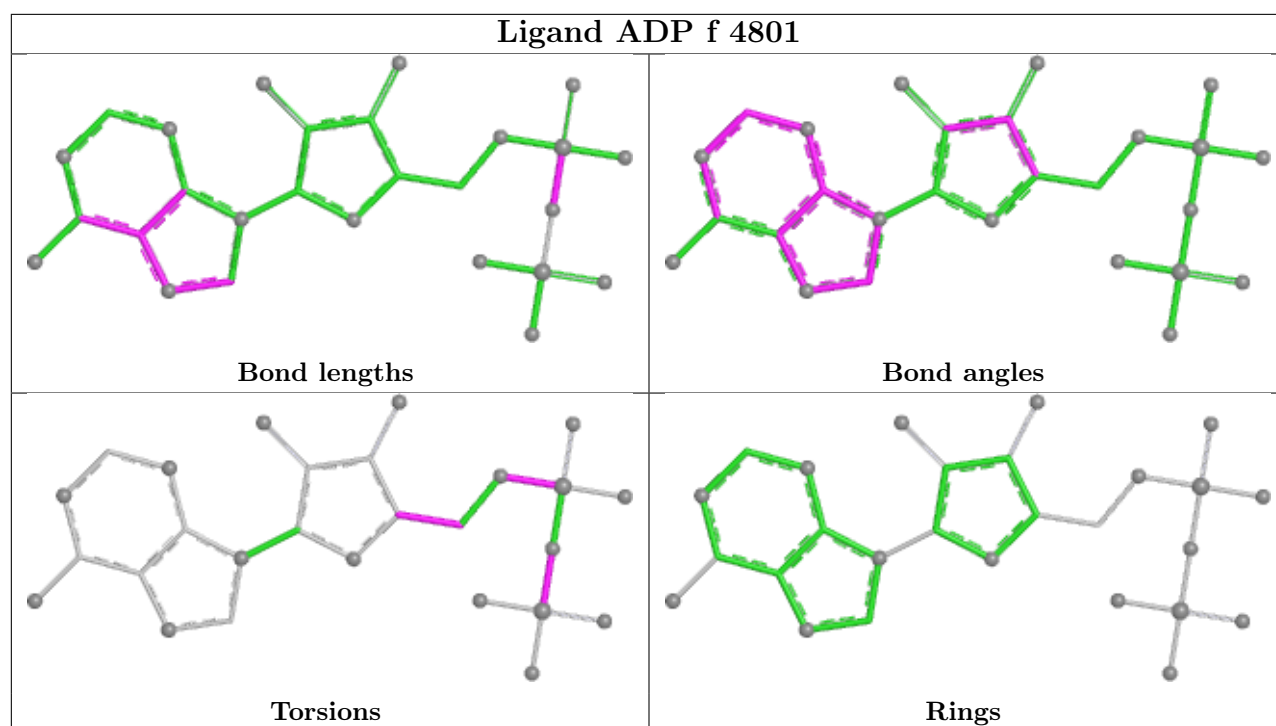
Ligand ANP m 4705

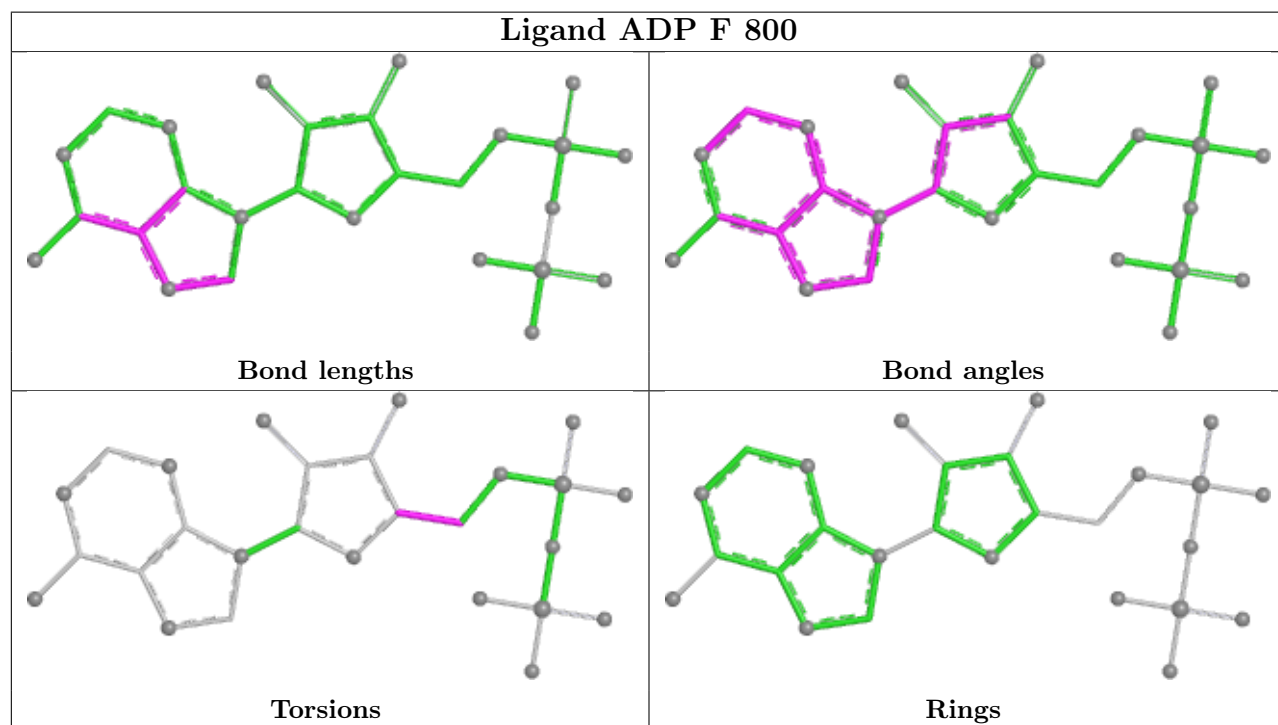
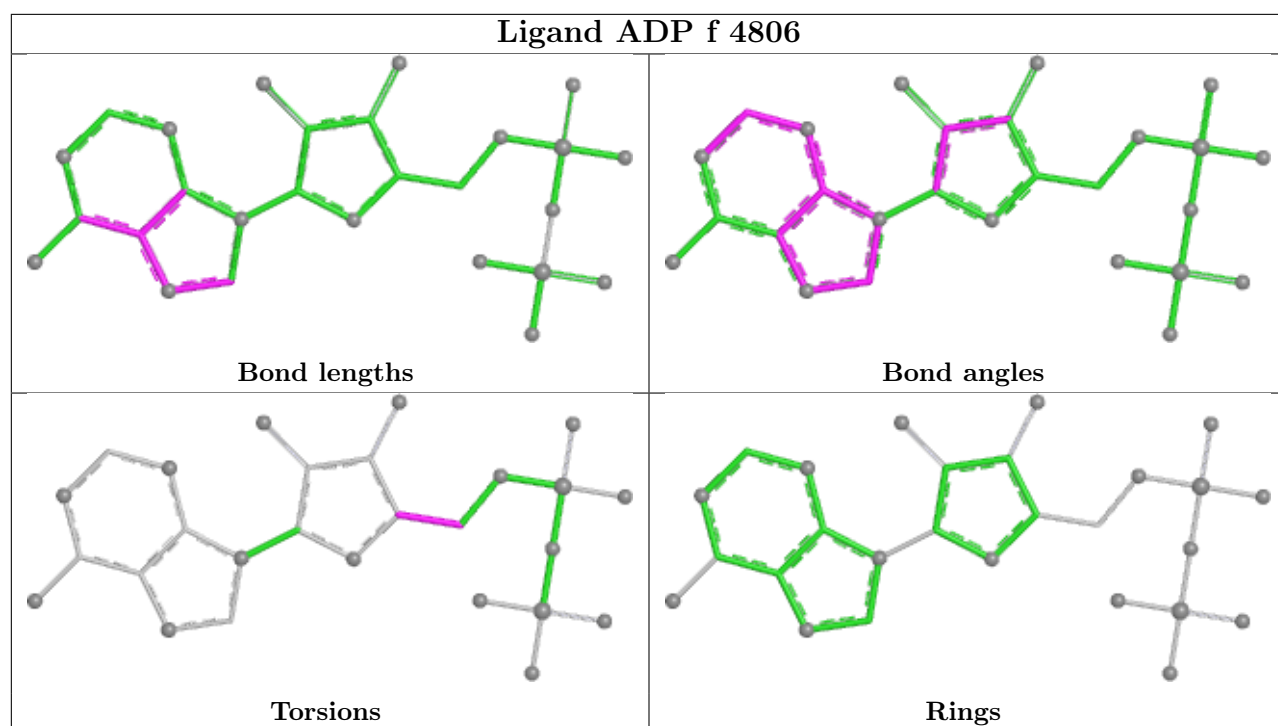


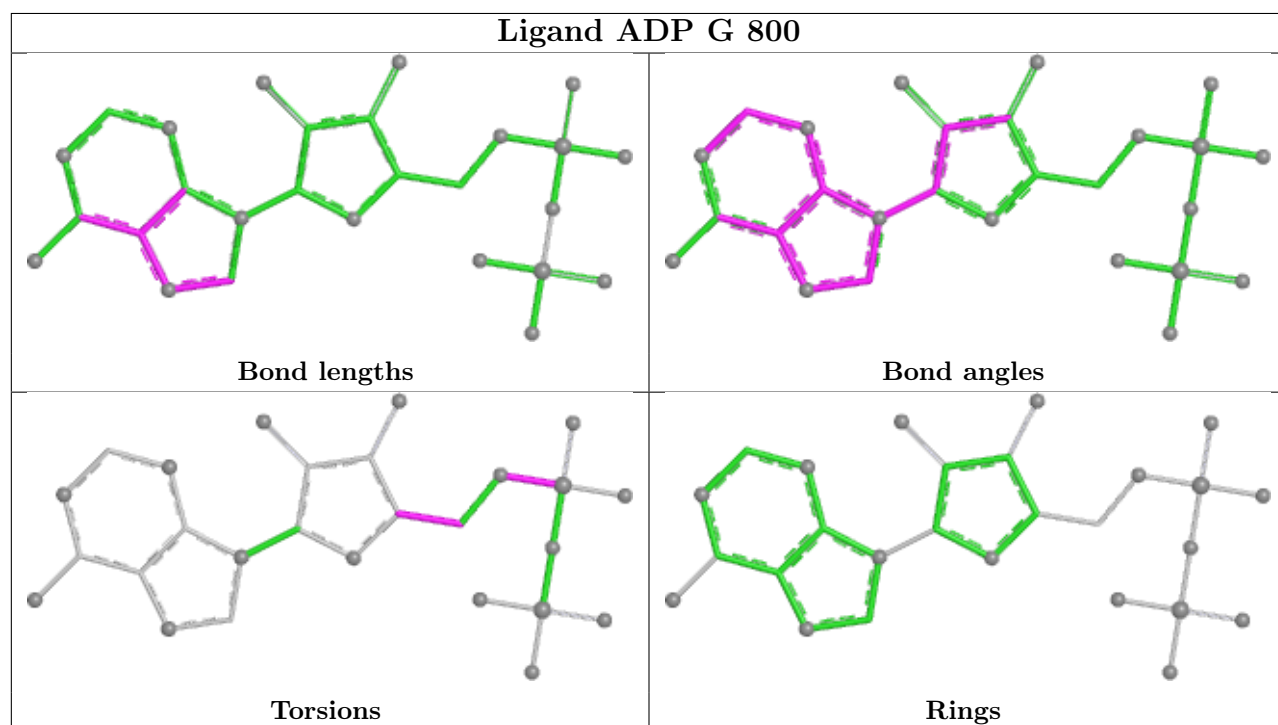
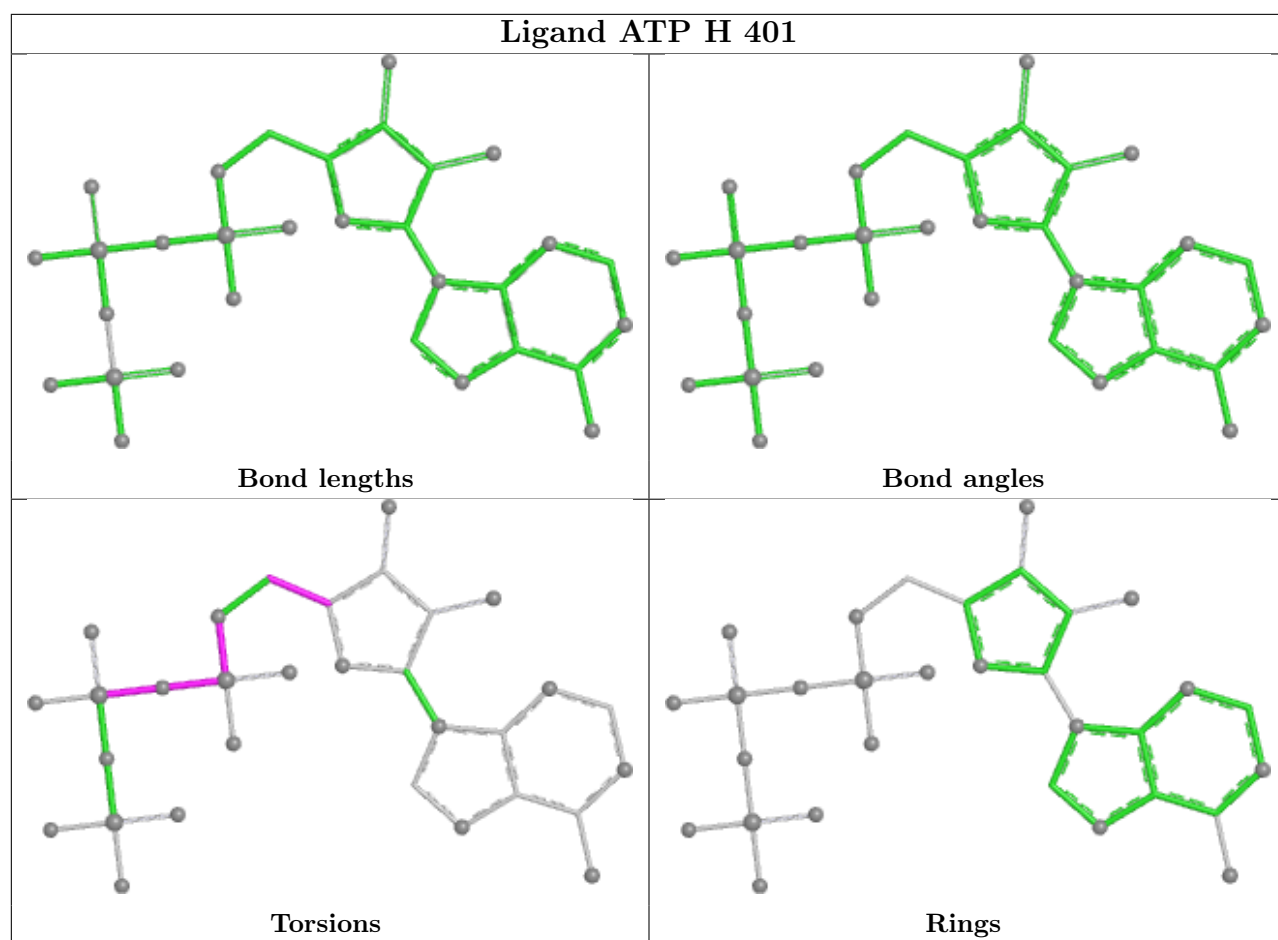
Ligand ADP e 4801

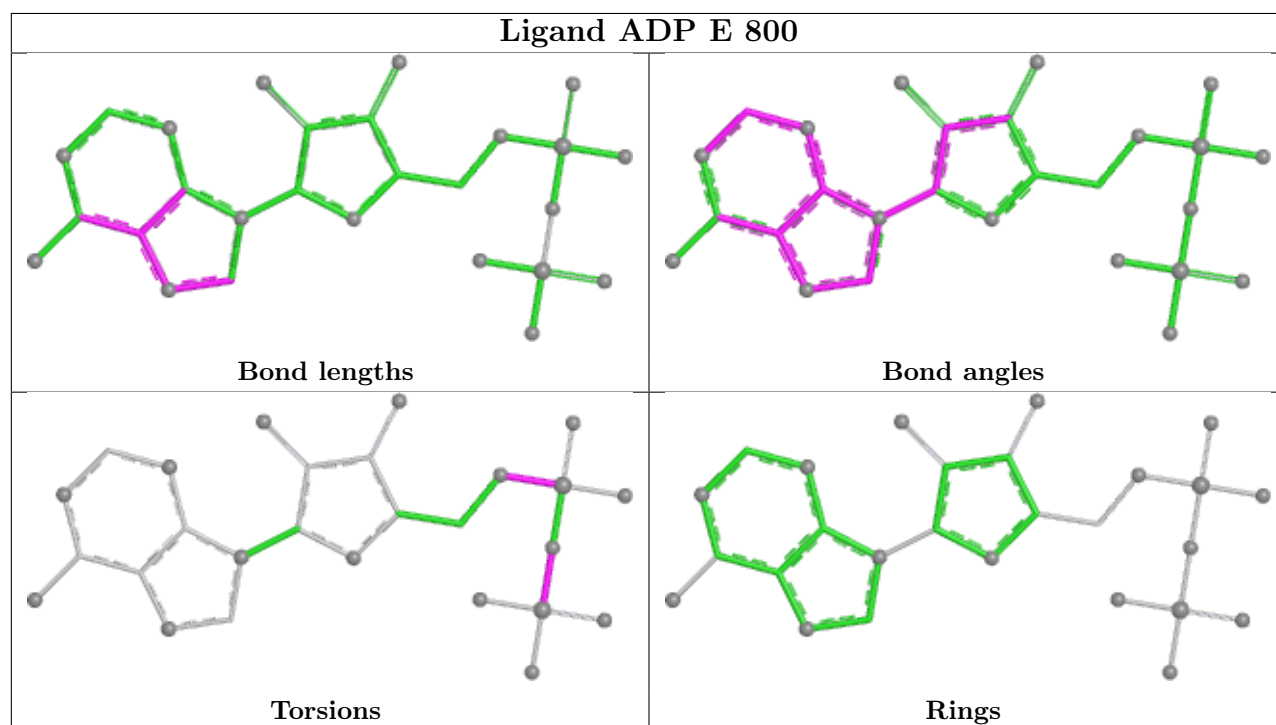
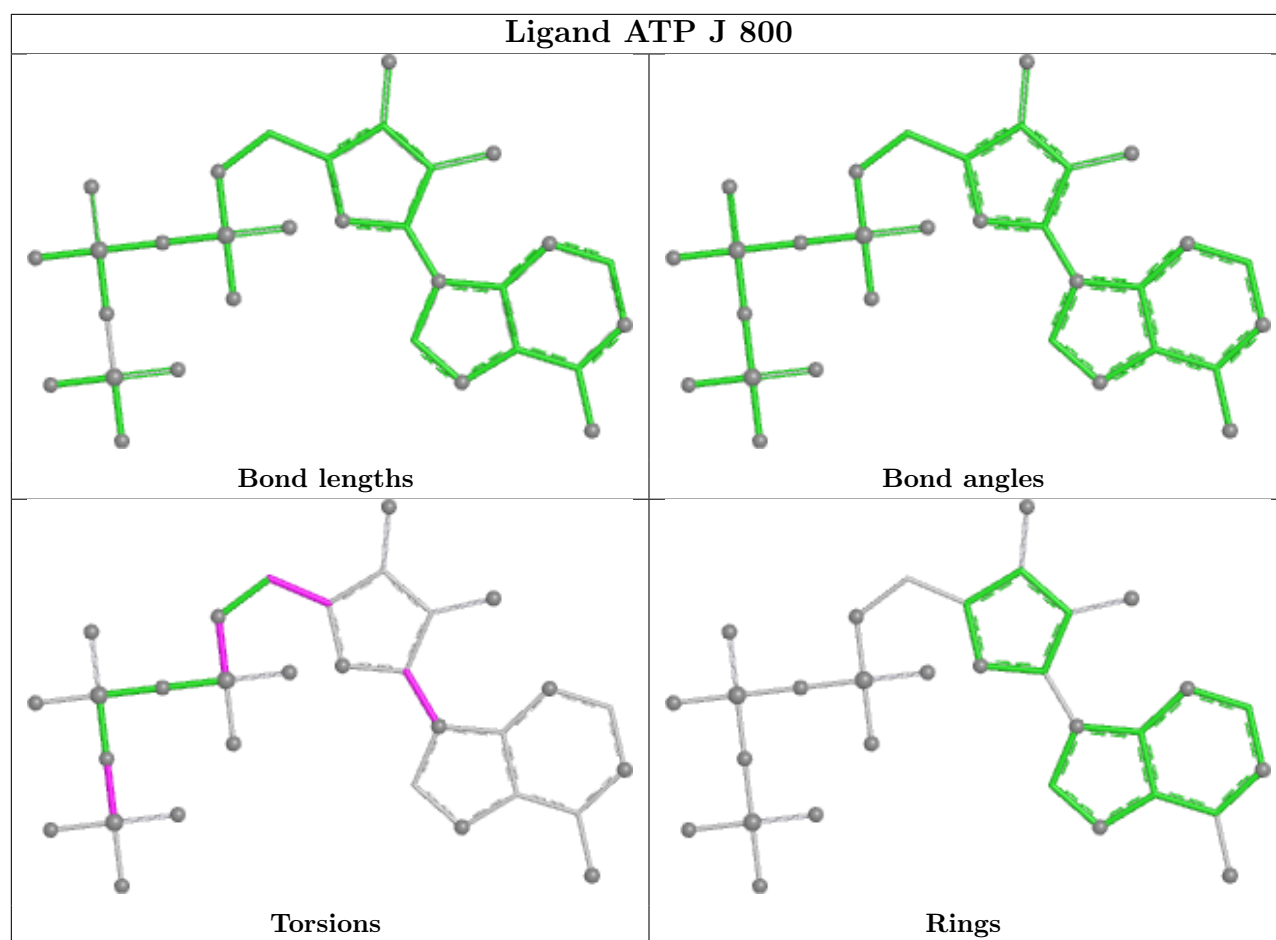


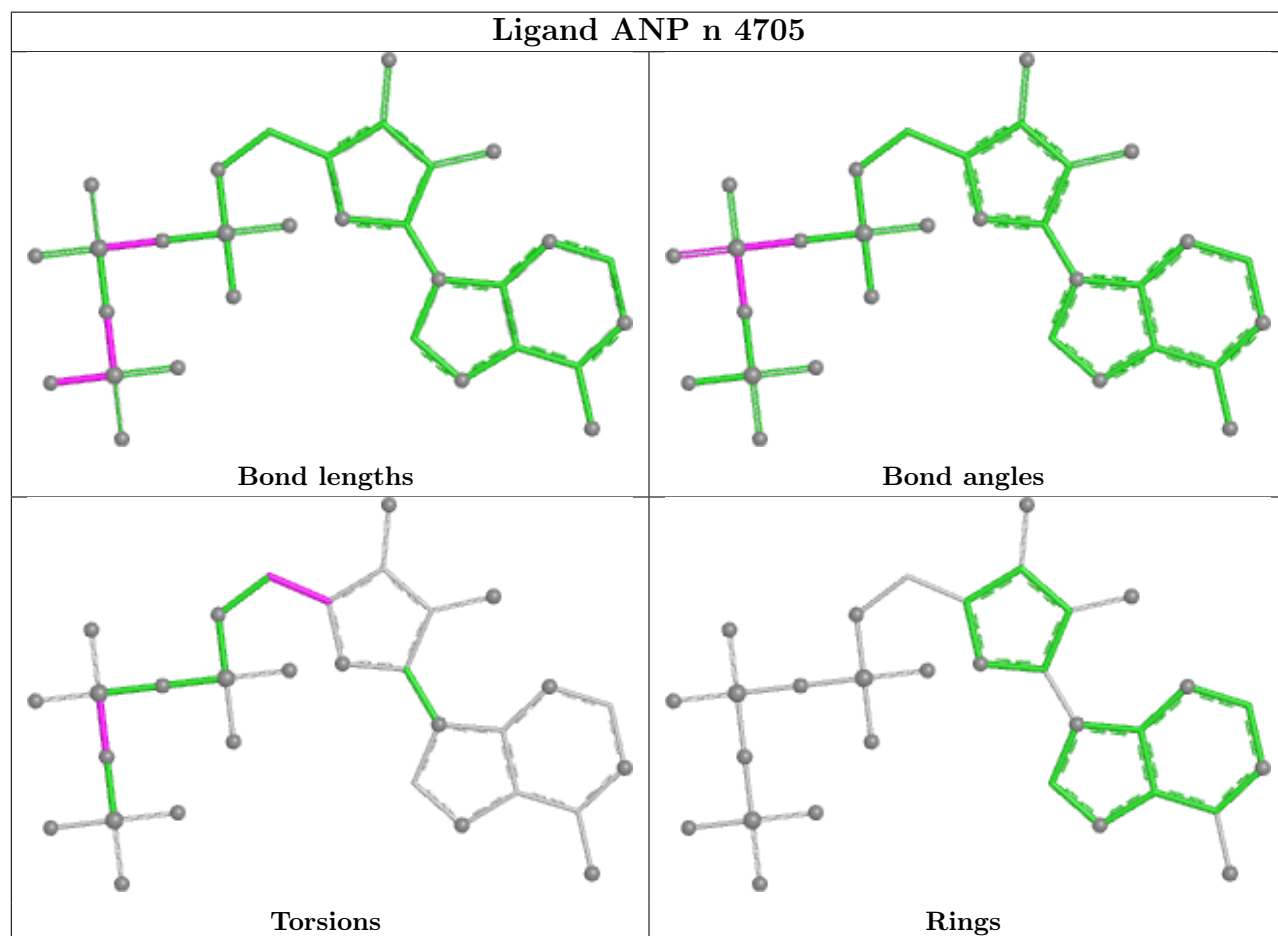
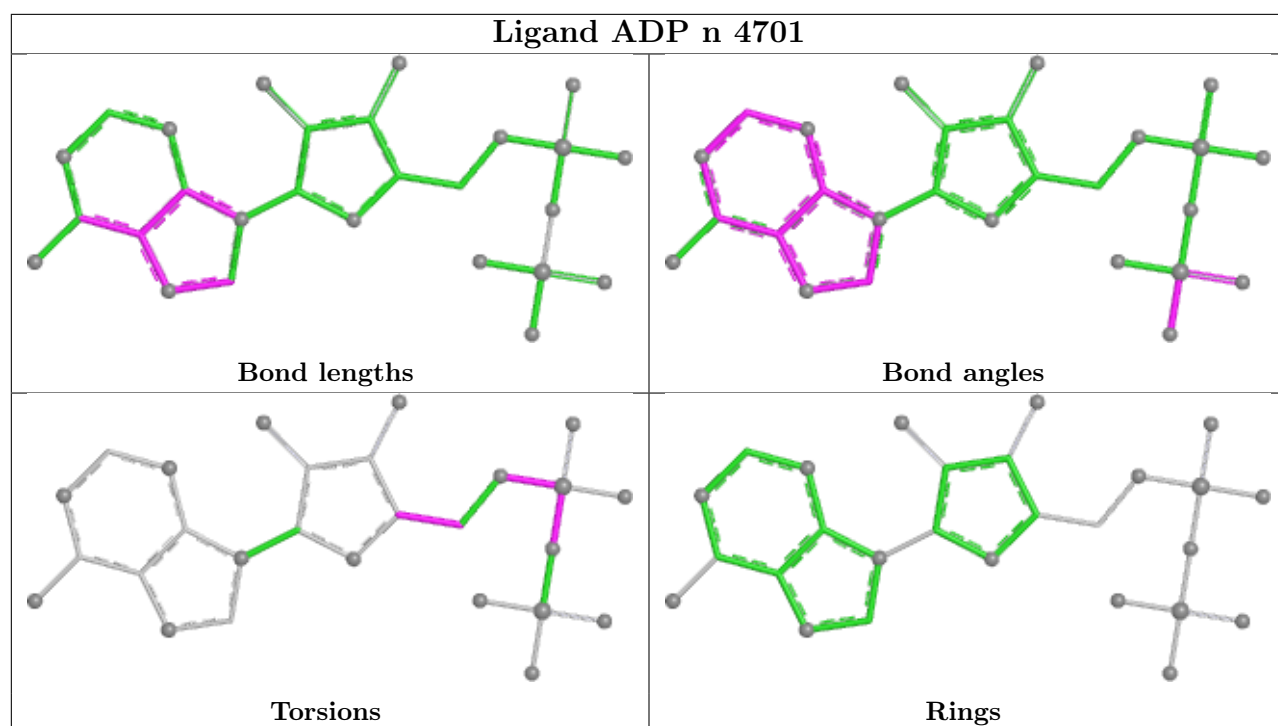


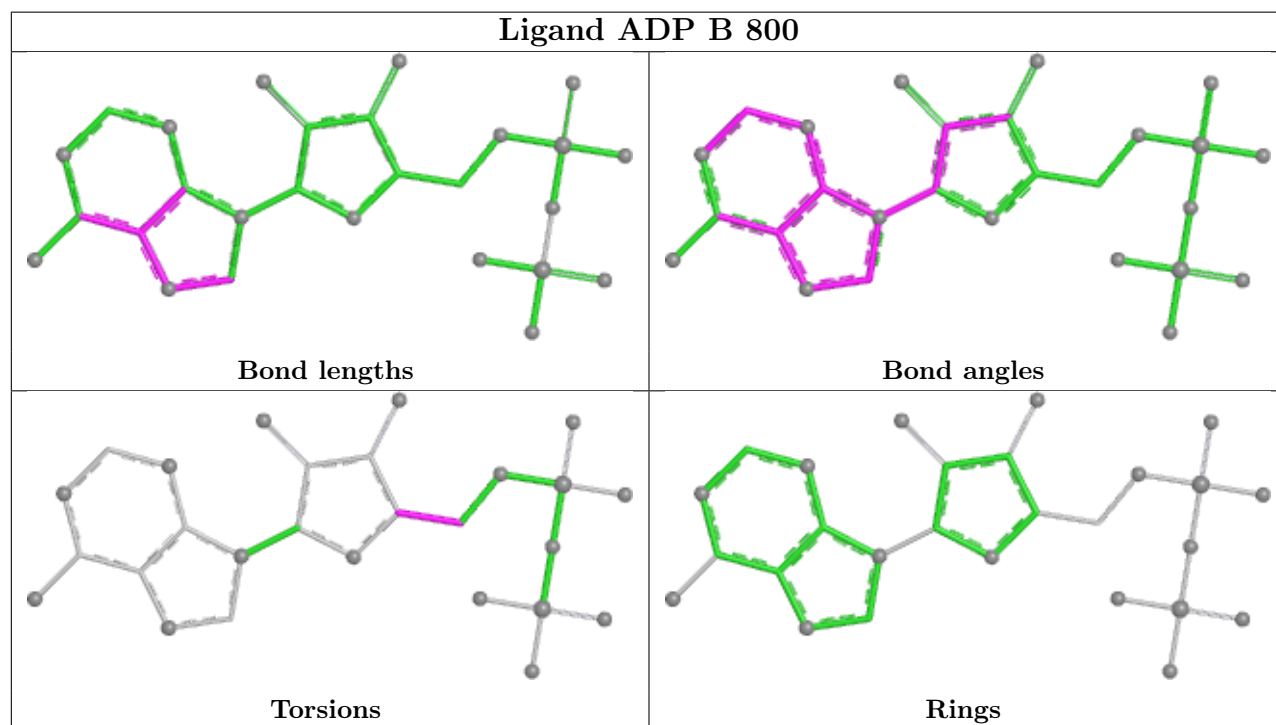
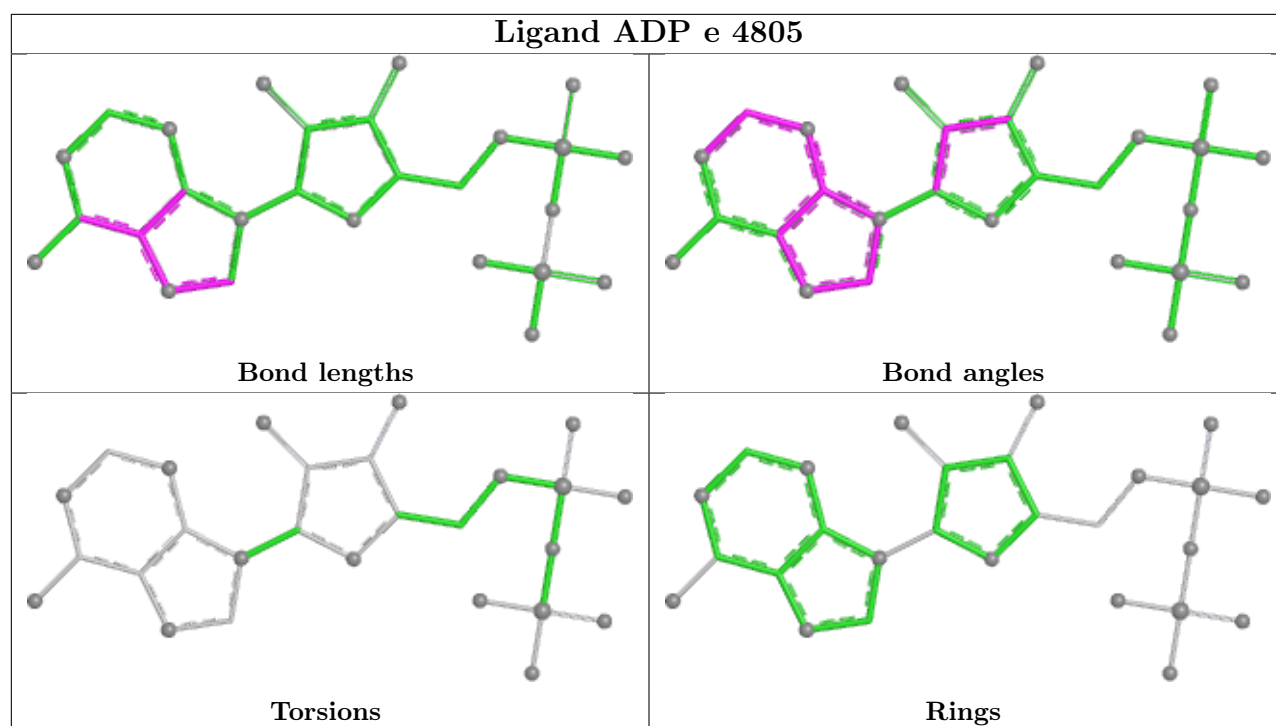


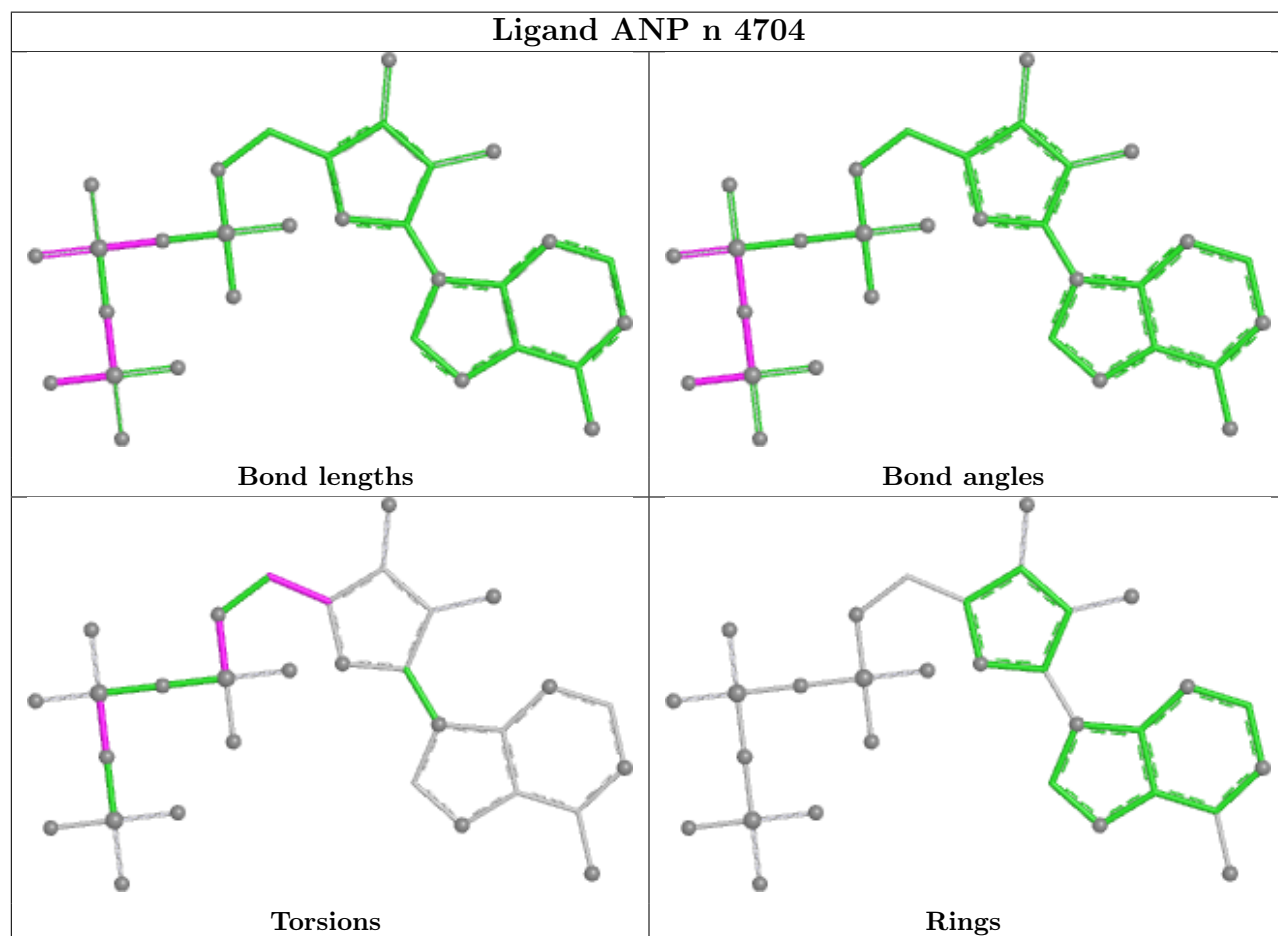
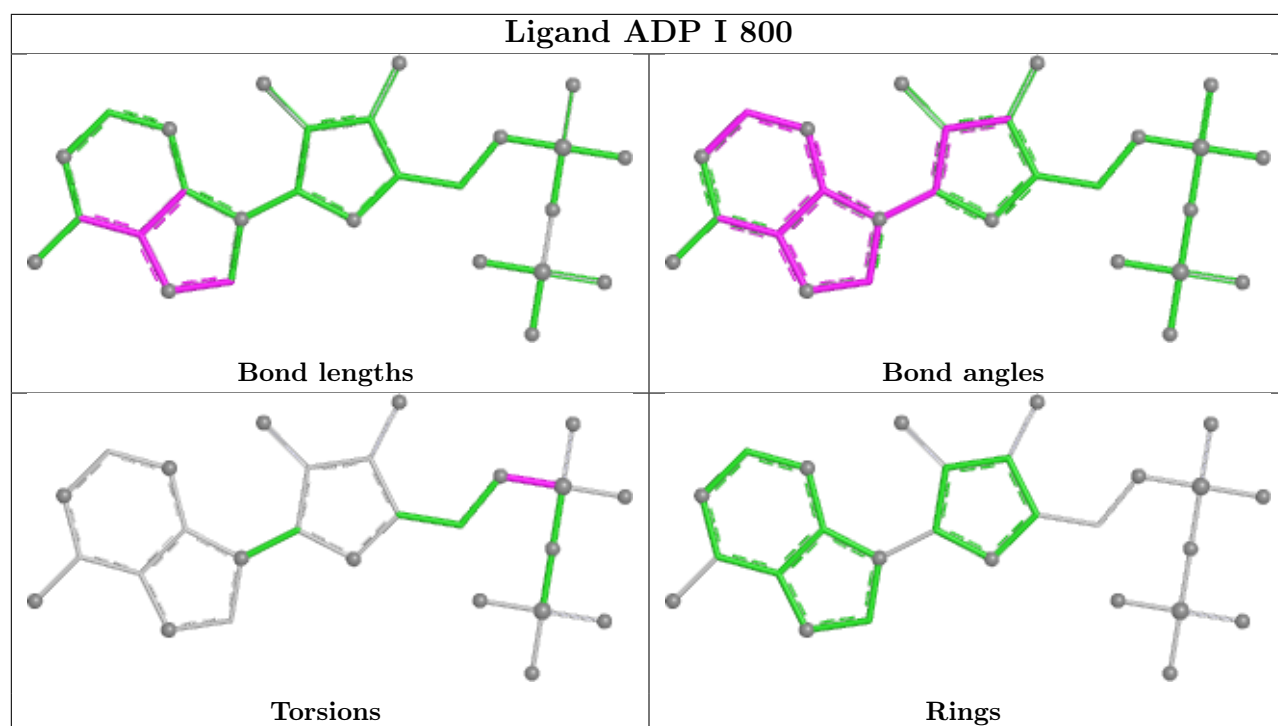


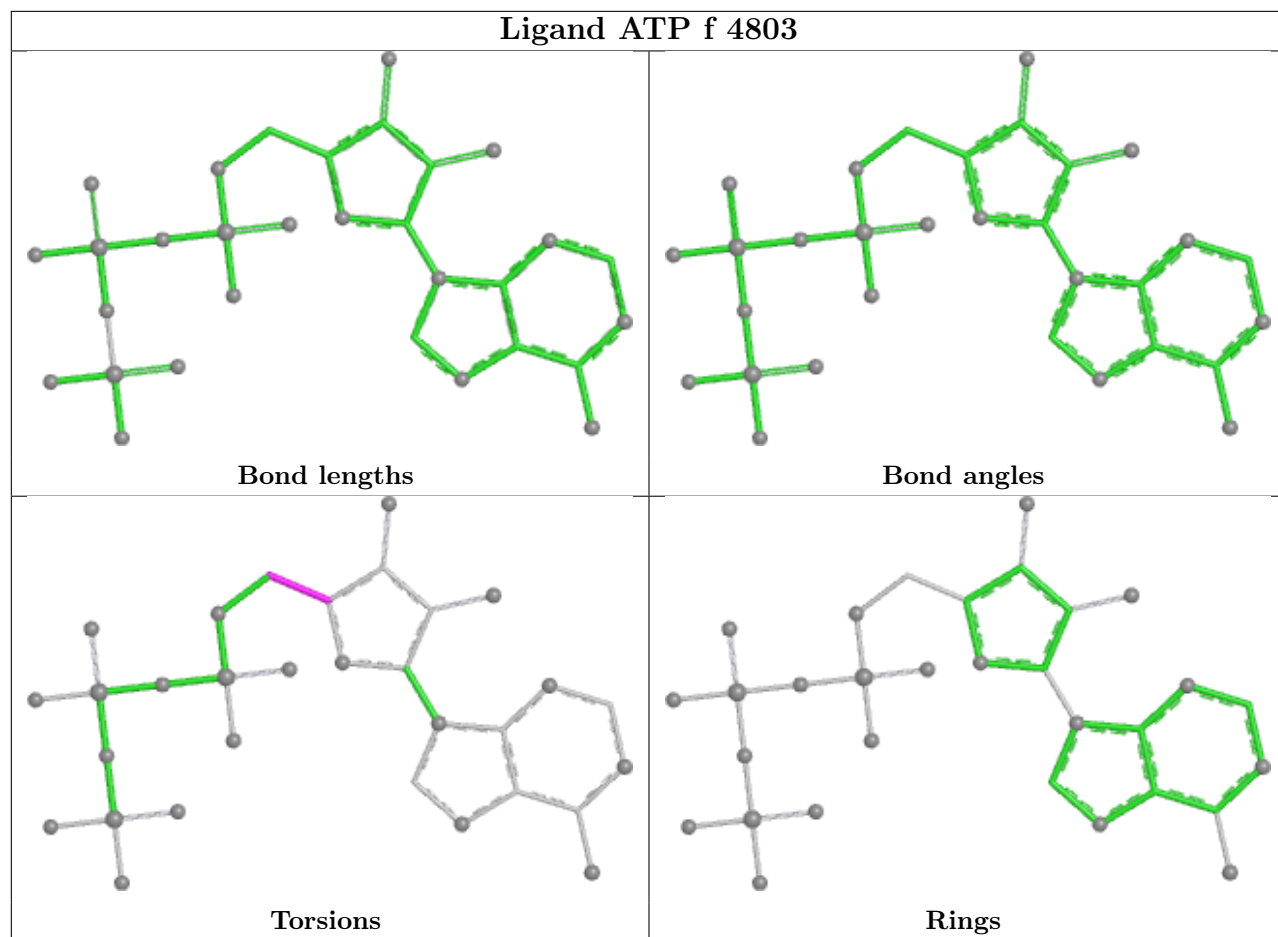




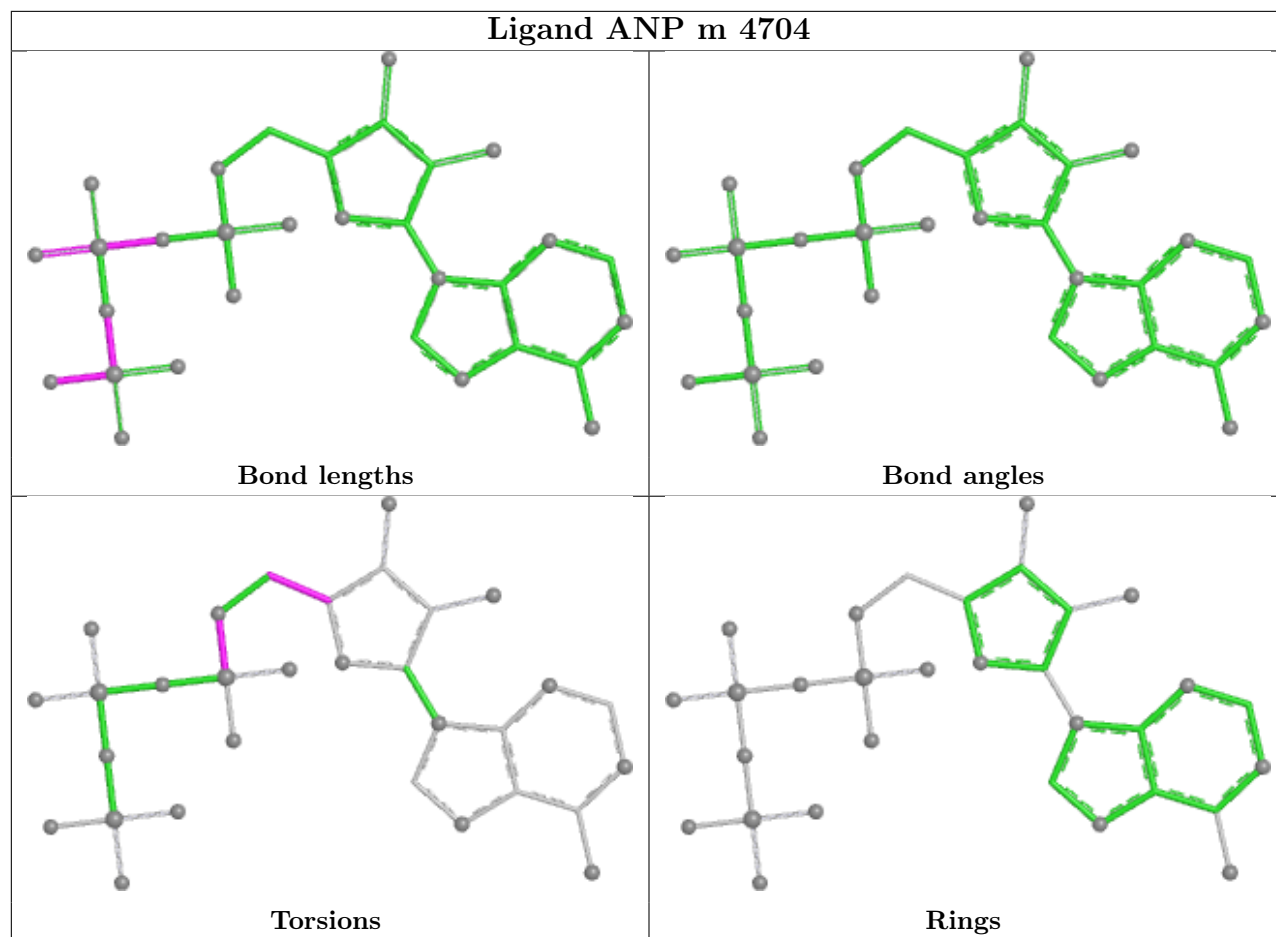




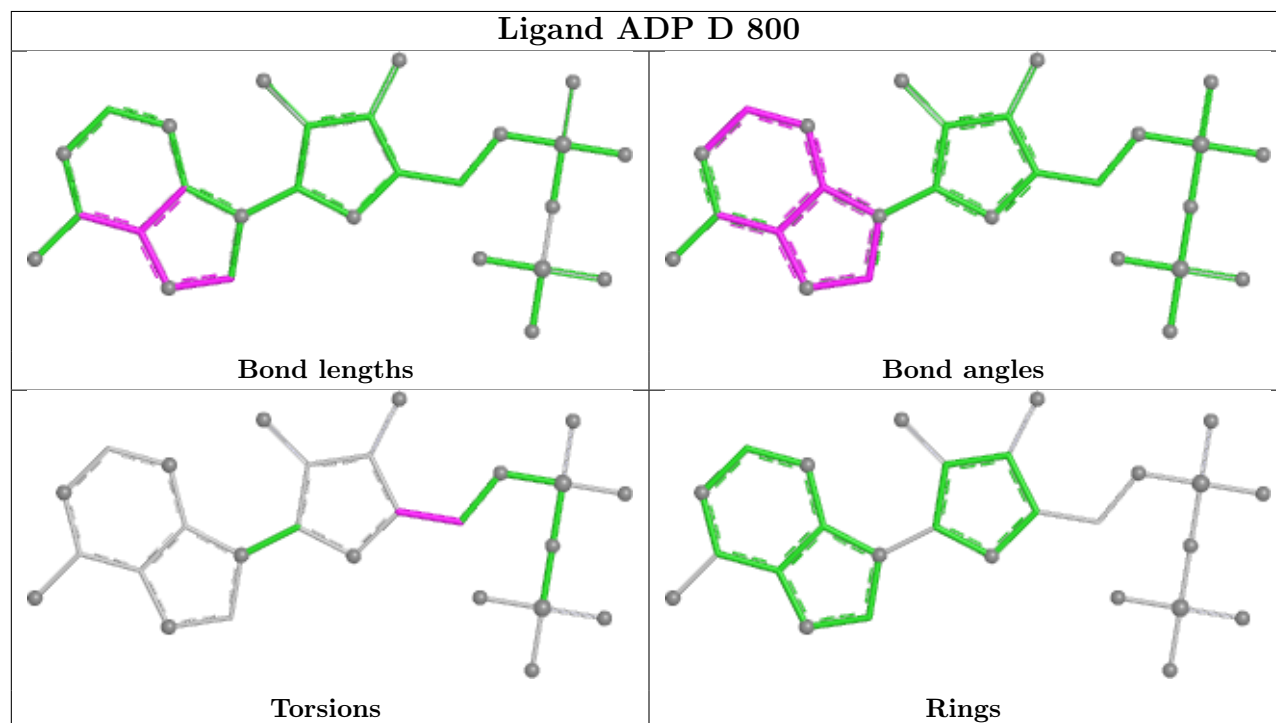


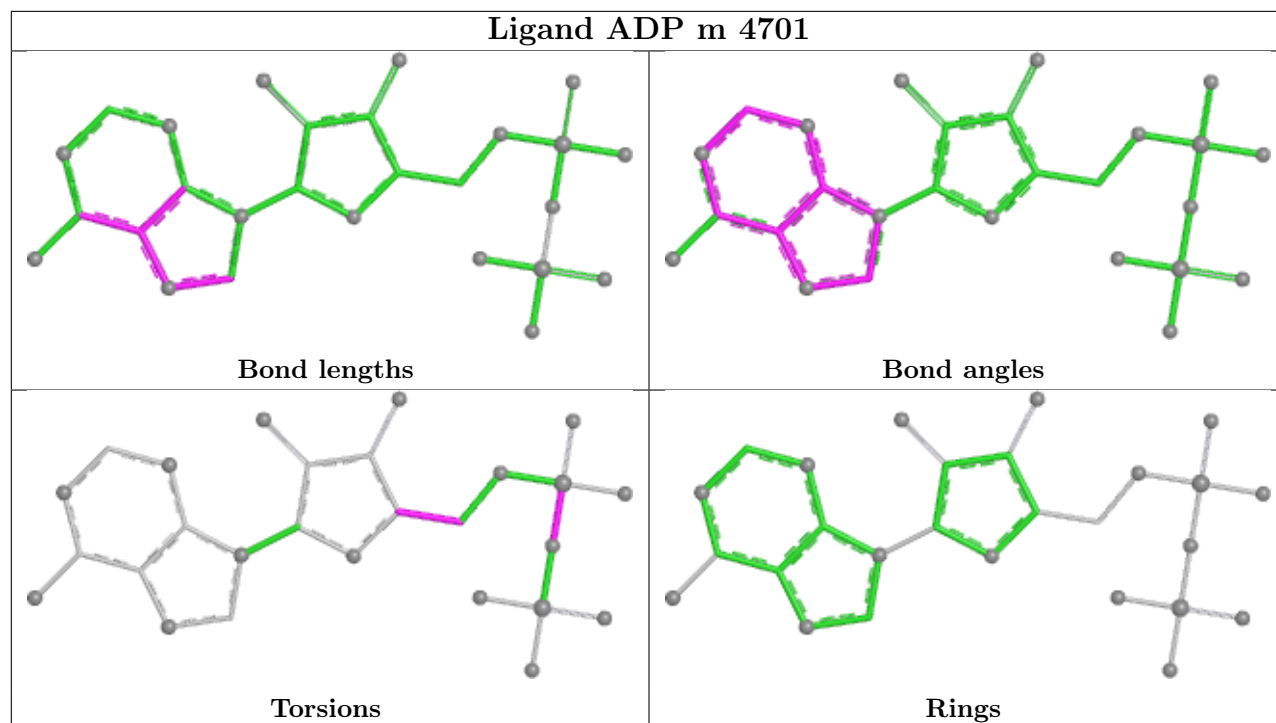


Ligand ANP m 4704



Ligand ADP D 800





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.

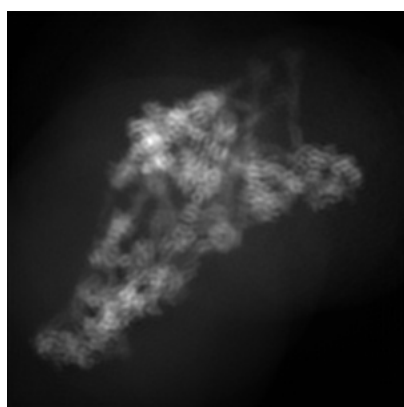
6 Map visualisation [i](#)

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.

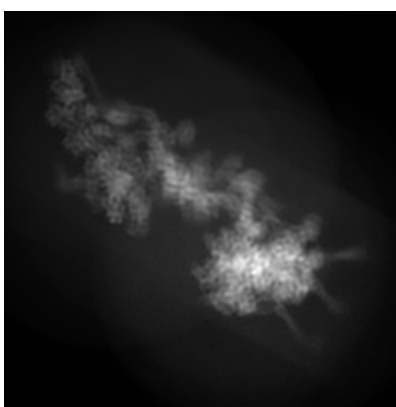
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

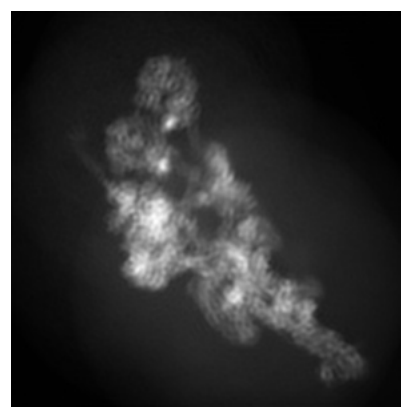
6.1.1 Primary map



X



Y

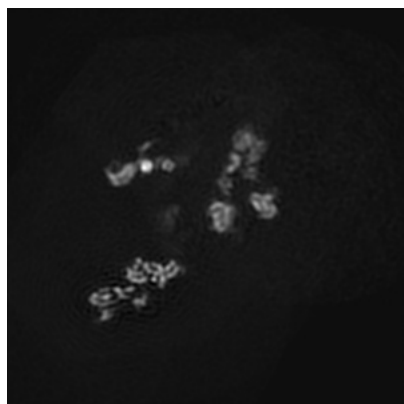


Z

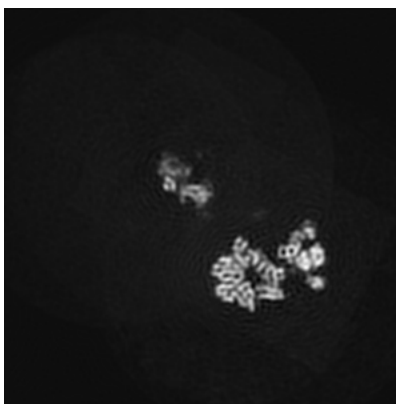
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

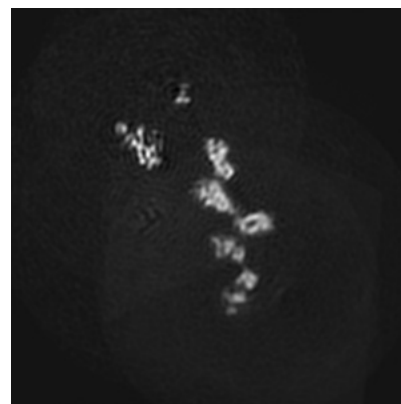
6.2.1 Primary map



X Index: 320



Y Index: 320

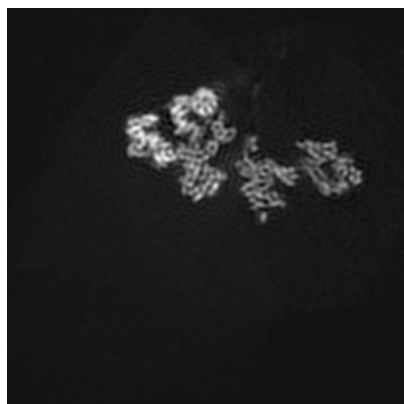


Z Index: 320

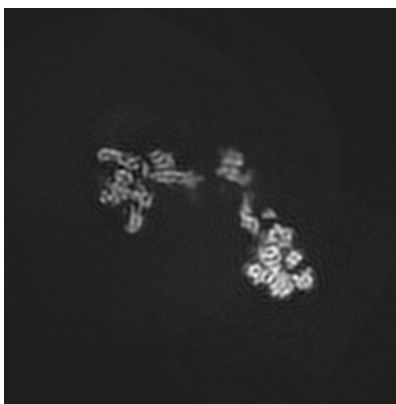
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

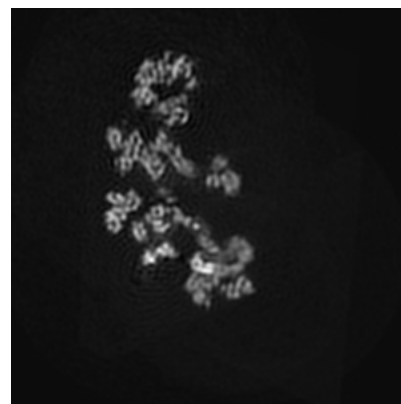
6.3.1 Primary map



X Index: 232



Y Index: 231

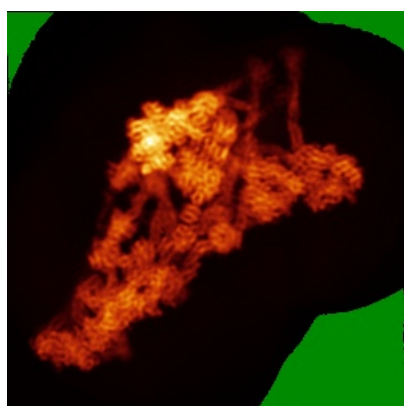


Z Index: 389

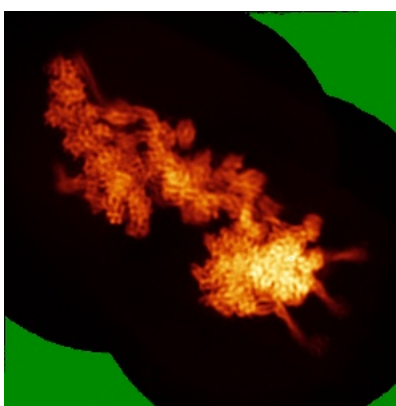
The images above show the largest variance slices of the map in three orthogonal directions.

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

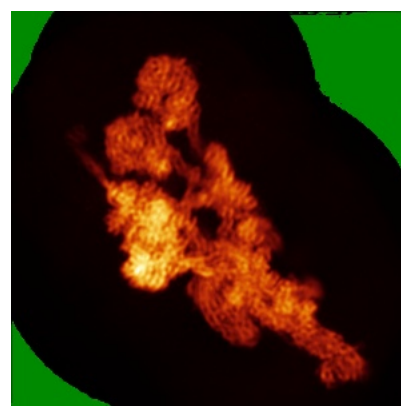
6.4.1 Primary map



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



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.

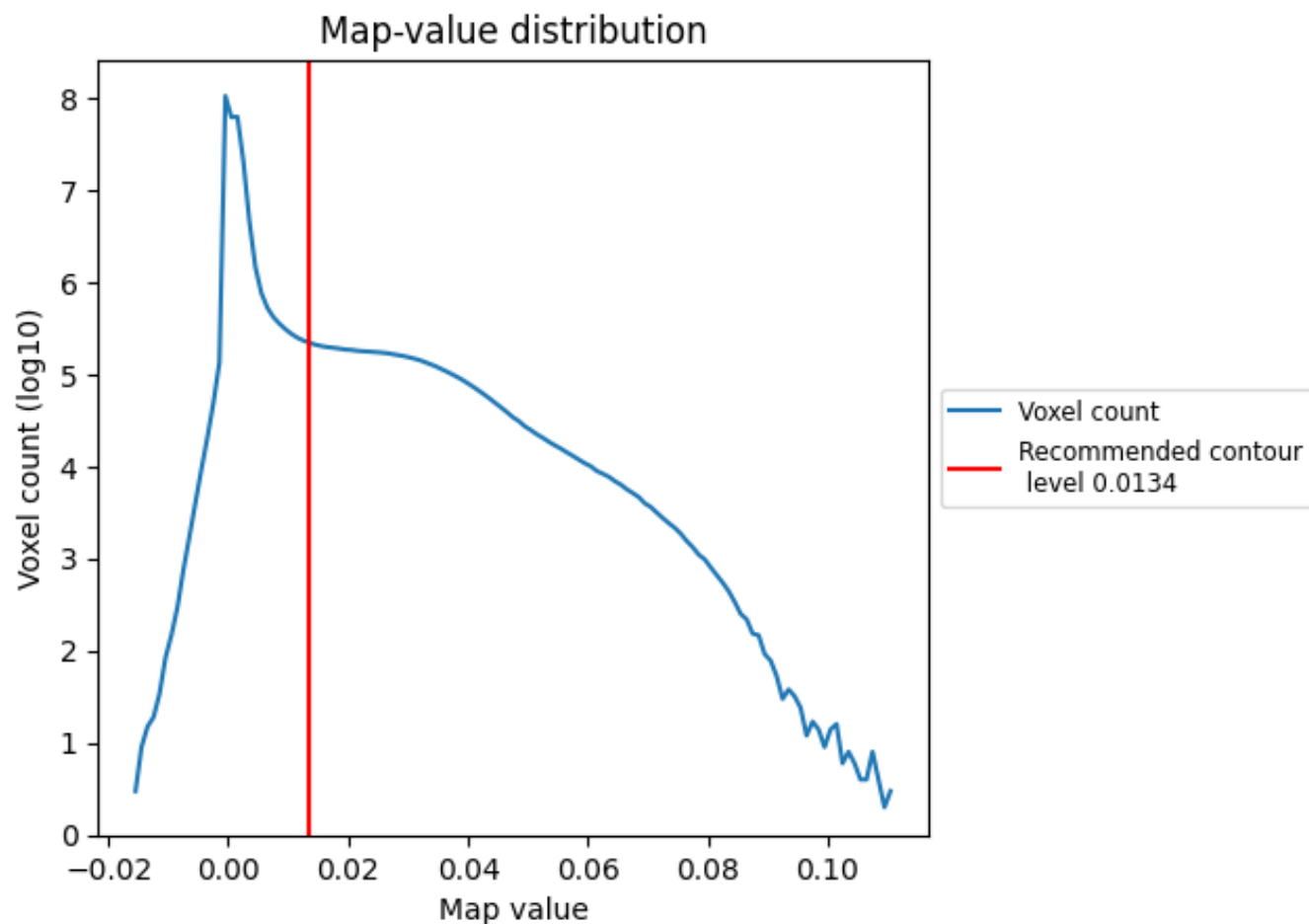
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

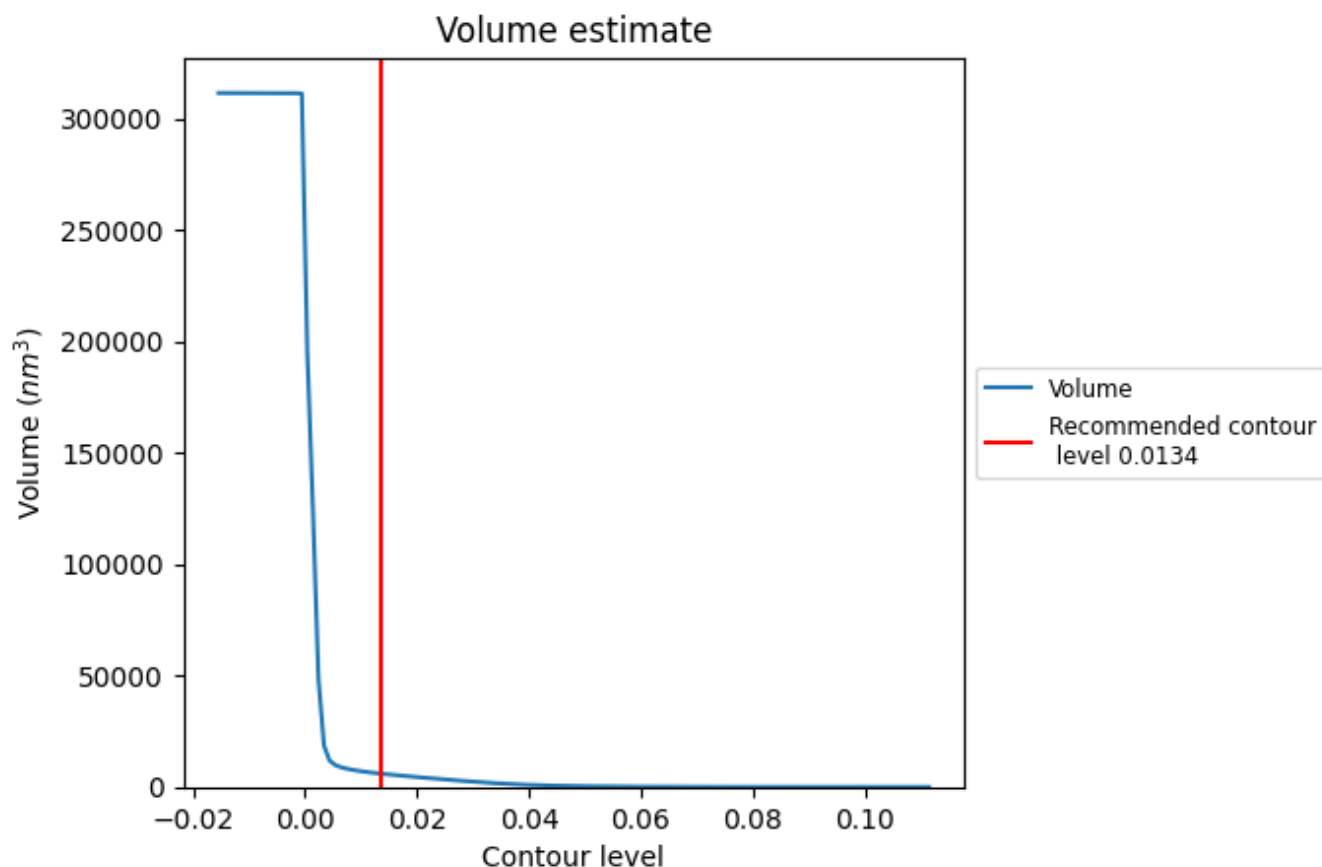
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

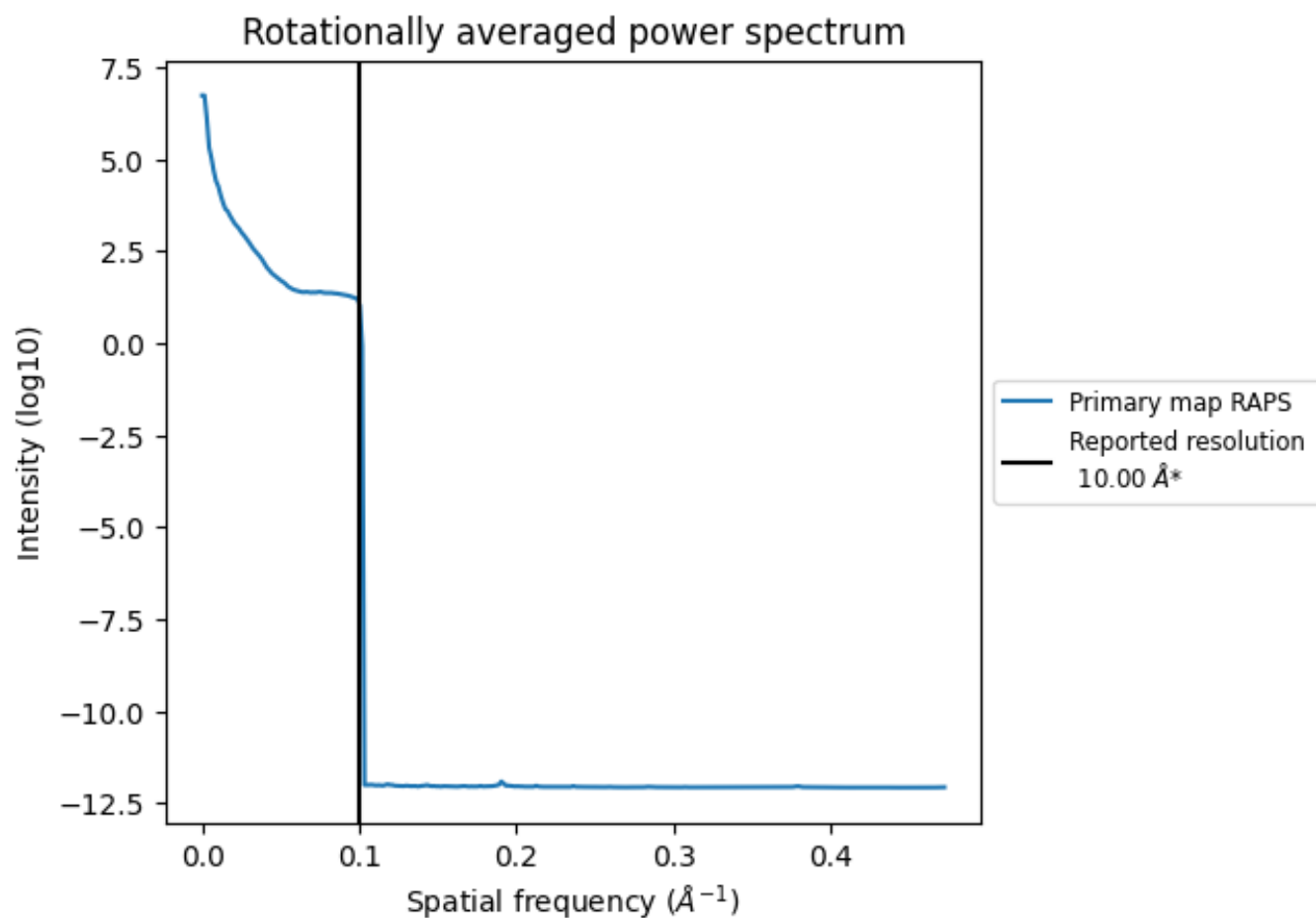
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

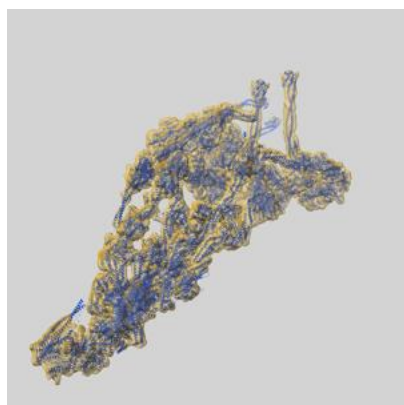
8 Fourier-Shell correlation

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

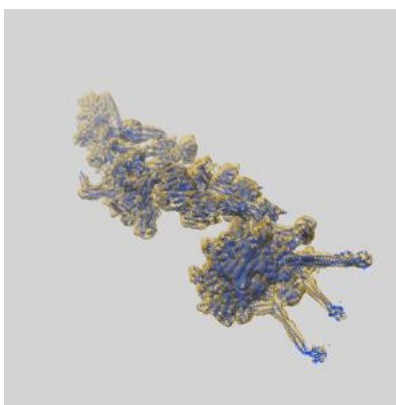
9 Map-model fit [i](#)

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

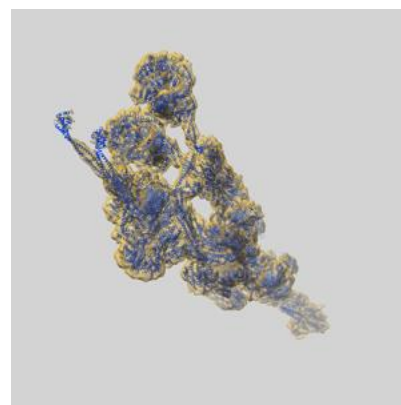
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0134 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](#)

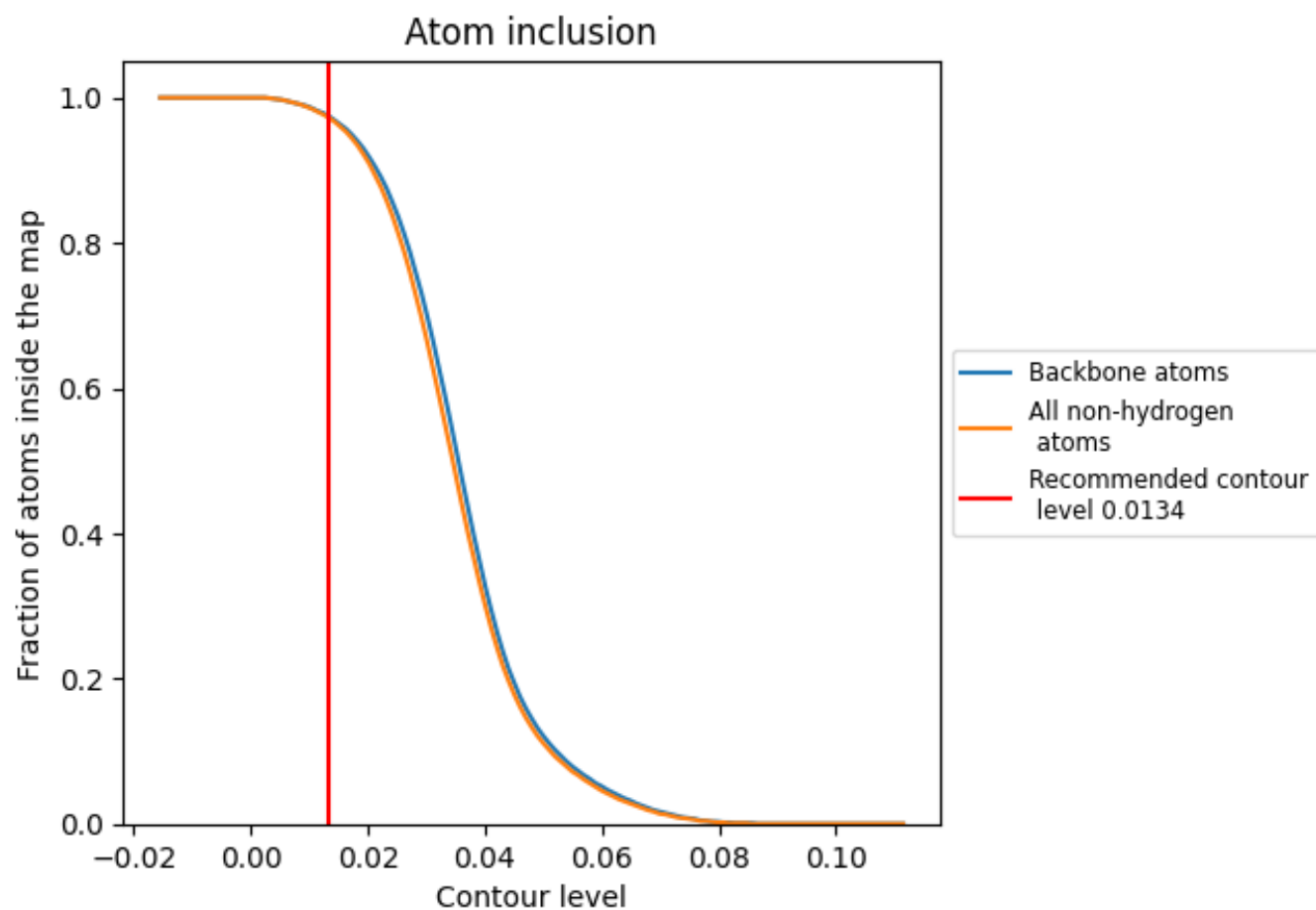


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

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