



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:29 AM UTC

PDB ID : 7Z8F / pdb_00007z8f
EMDB ID : EMD-14549
Title : Composite structure of dynein-dynactin-BICDR on microtubules
Authors : Chaaban, S.; Carter, A.P.
Deposited on : 2022-03-17
Resolution : 20.00 Å(reported)

This is a 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:

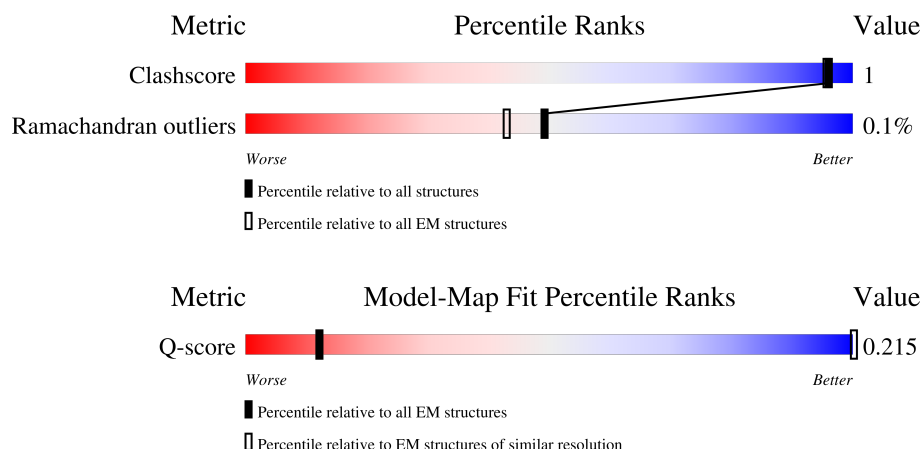
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 20.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



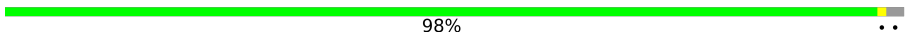
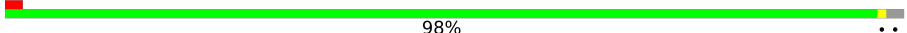
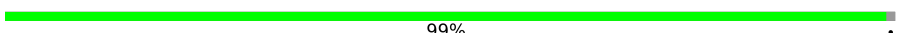
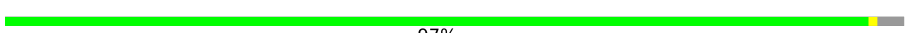
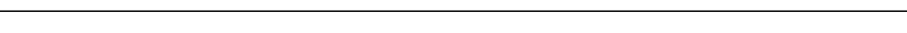
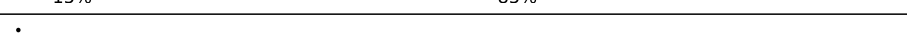
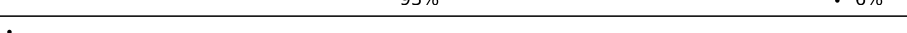
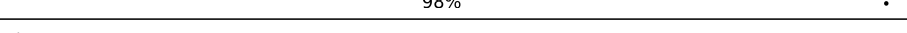
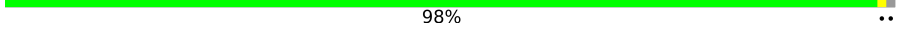
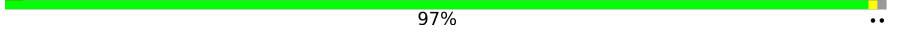
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	28 (19.50 - 20.50)

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

Mol	Chain	Length	Quality of chain
1	A	376	
1	B	376	
1	C	376	
1	D	376	
1	E	376	

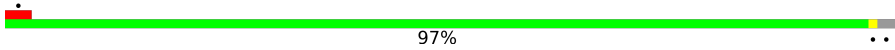
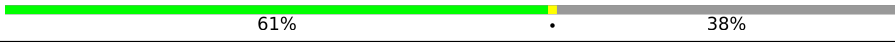
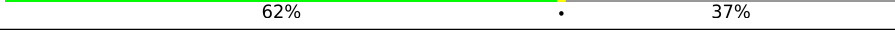
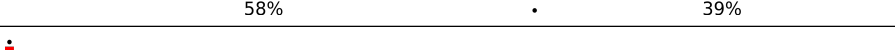
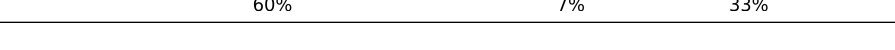
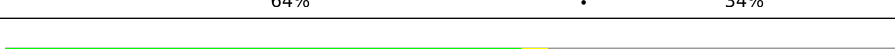
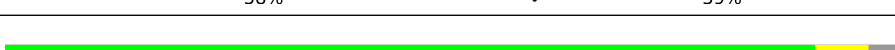
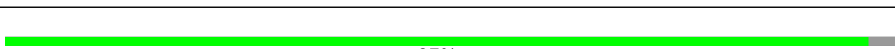
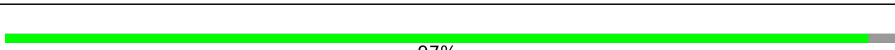
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	376	 88% 11%
1	G	376	 98%
1	I	376	 98%
2	H	375	 99%
3	J	417	 90% 9%
4	K	286	 97%
5	L	272	 98%
6	M	405	 82% 16%
6	N	405	 68% 31%
6	P	405	 82% 15%
6	Q	405	 80% 20%
7	O	186	 90% 9%
7	R	186	 90% 6%
8	S	1281	 11% 88%
8	T	1281	 15% 85%
9	U	190	 93% 6%
10	V	182	 98%
11	W	577	 35% 64%
11	X	577	 46% 53%
11	w	577	 35% 64%
11	x	577	 41% 58%
12	Y	467	 81% 18%
13	e	4646	 98%
13	f	4646	 97%
13	m	4646	 97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	n	4646	
14	g	638	
14	h	638	
14	o	638	
14	p	638	
15	i	492	
15	j	492	
15	q	492	
15	r	492	
16	k	96	
16	l	96	
16	s	96	
16	t	96	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 118408 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	370	Total	C	N	O	0	0
			1480	740	370	370		
1	B	370	Total	C	N	O	0	0
			1480	740	370	370		
1	C	375	Total	C	N	O	0	0
			1500	750	375	375		
1	D	370	Total	C	N	O	0	0
			1480	740	370	370		
1	E	370	Total	C	N	O	0	0
			1480	740	370	370		
1	F	370	Total	C	N	O	0	0
			1480	740	370	370		
1	G	369	Total	C	N	O	0	0
			1476	738	369	369		
1	I	370	Total	C	N	O	0	0
			1480	740	370	370		

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

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

- Molecule 3 is a protein called Arp11.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	278	Total	C	N	O	0	0
			1112	556	278	278		

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

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

- Molecule 6 is a protein called Dynactin subunit 2.

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

- Molecule 7 is a protein called Dynactin subunit 3.

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

- Molecule 8 is a protein called Dynactin subunit 1.

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

- Molecule 9 is a protein called Dynactin 6.

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

- Molecule 10 is a protein called Dynactin subunit 5.

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

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

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

- Molecule 12 is a protein called Dynactin subunit 4.

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

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

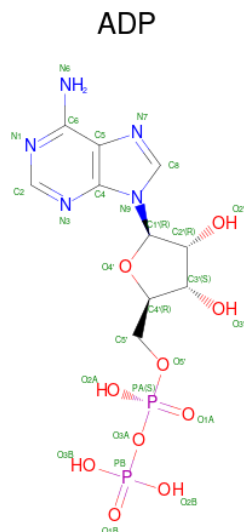
- Molecule 15 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

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

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

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

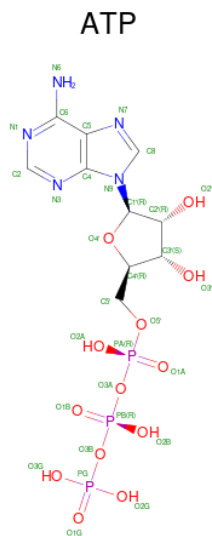
- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

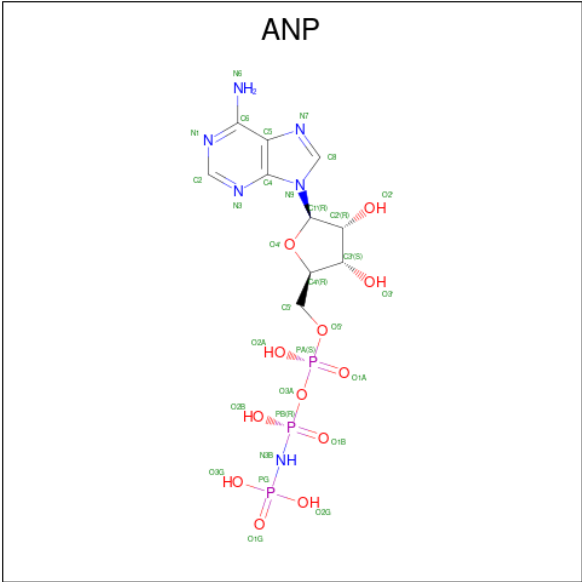


Mol	Chain	Residues	Atoms					AltConf
19	J	1	Total 31	C 10	N 5	O 13	P 3	0
19	e	1	Total 31	C 10	N 5	O 13	P 3	0
19	f	1	Total 31	C 10	N 5	O 13	P 3	0
19	m	1	Total 31	C 10	N 5	O 13	P 3	0
19	n	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 21 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



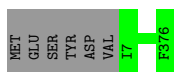
Mol	Chain	Residues	Atoms					AltConf
21	e	1	Total	C	N	O	P	0
			31	10	6	12	3	
21	e	1	Total	C	N	O	P	0
			31	10	6	12	3	
21	f	1	Total	C	N	O	P	0
			31	10	6	12	3	
21	f	1	Total	C	N	O	P	0
			31	10	6	12	3	
21	m	1	Total	C	N	O	P	0
			31	10	6	12	3	
21	m	1	Total	C	N	O	P	0
			31	10	6	12	3	
21	n	1	Total	C	N	O	P	0
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

3 Residue-property plots [i](#)

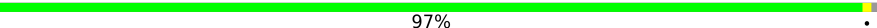
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

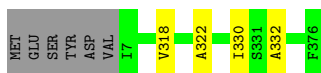
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain A:  98%

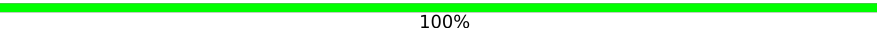


- Molecule 1: ARP1 actin related protein 1 homolog A

Chain B:  97%

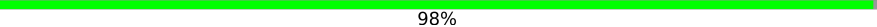


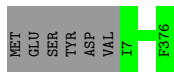
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain C:  100%

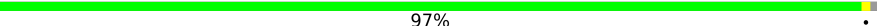


- Molecule 1: ARP1 actin related protein 1 homolog A

Chain D:  98%



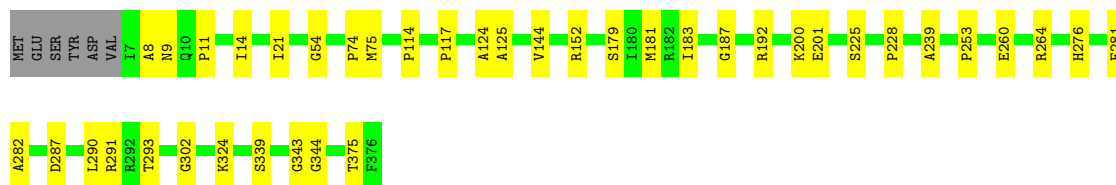
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain E:  97%

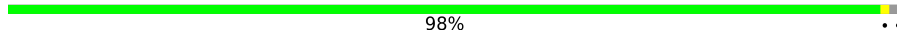


- Molecule 1: ARP1 actin related protein 1 homolog A

Chain F:  88% 11% .

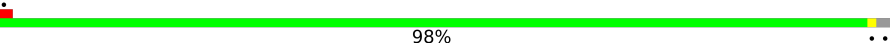


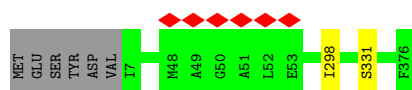
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain G:  98% ..



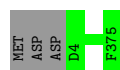
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain I:  98% ..



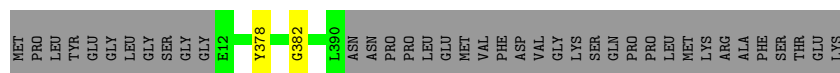
- Molecule 2: Actin, cytoplasmic 1

Chain H:  99% .

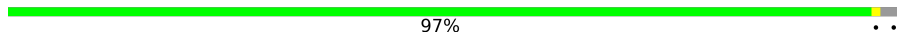


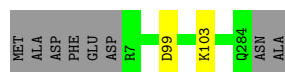
- Molecule 3: Arp11

Chain J:  90% 9%

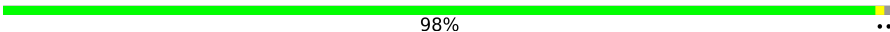


- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K:  97% ..



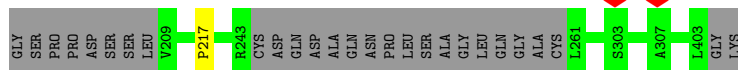
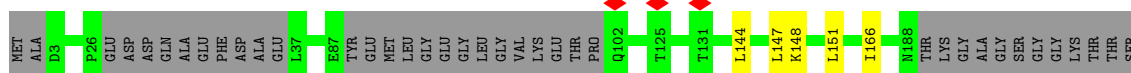
- Molecule 5: F-actin capping protein beta subunit

Chain L:  98% ..



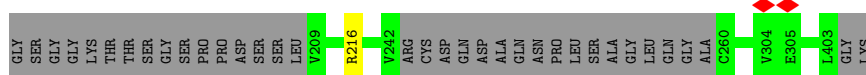
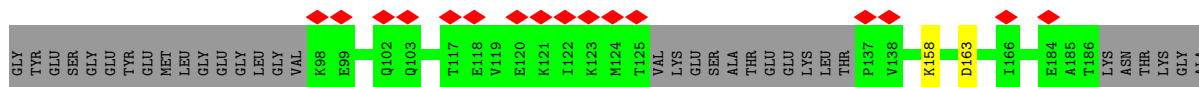
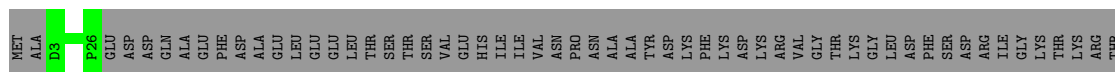
• Molecule 6: Dynactin subunit 2

Chain M: 82% 16%



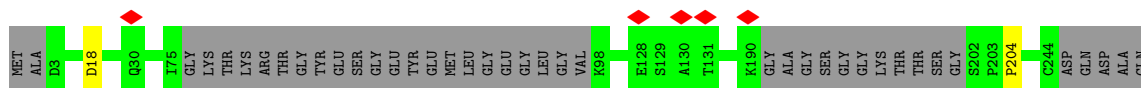
• Molecule 6: Dynactin subunit 2

Chain N: 68% 31%



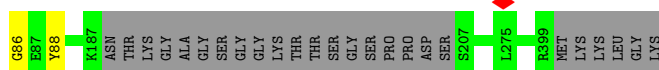
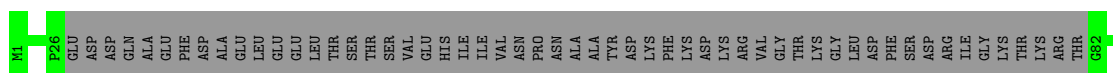
• Molecule 6: Dynactin subunit 2

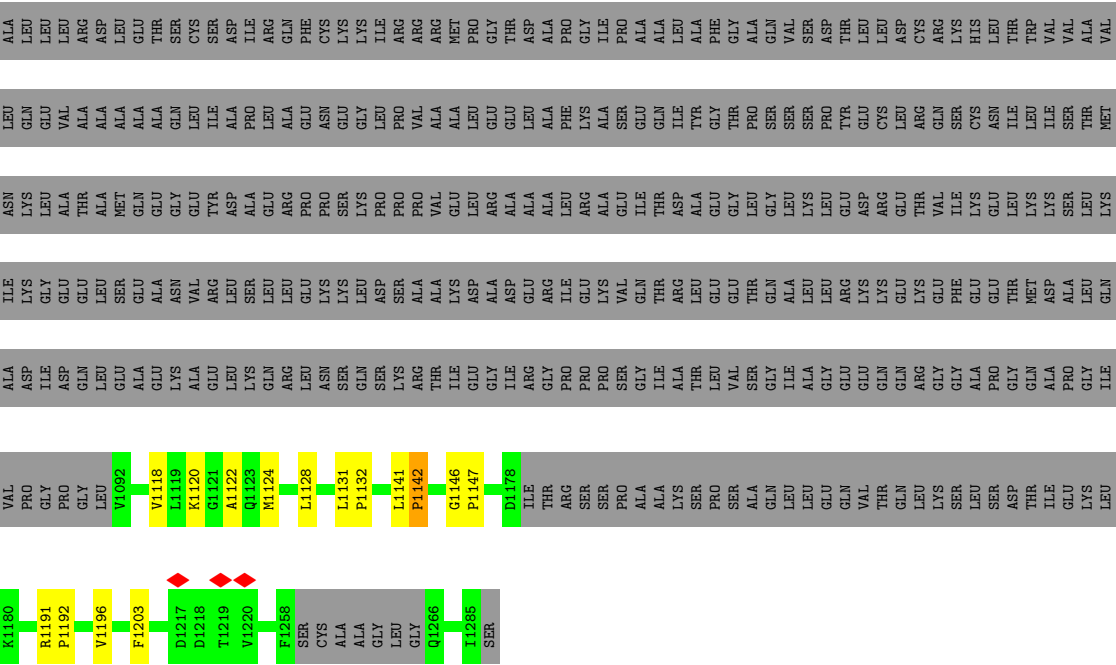
Chain P: 82% 15%



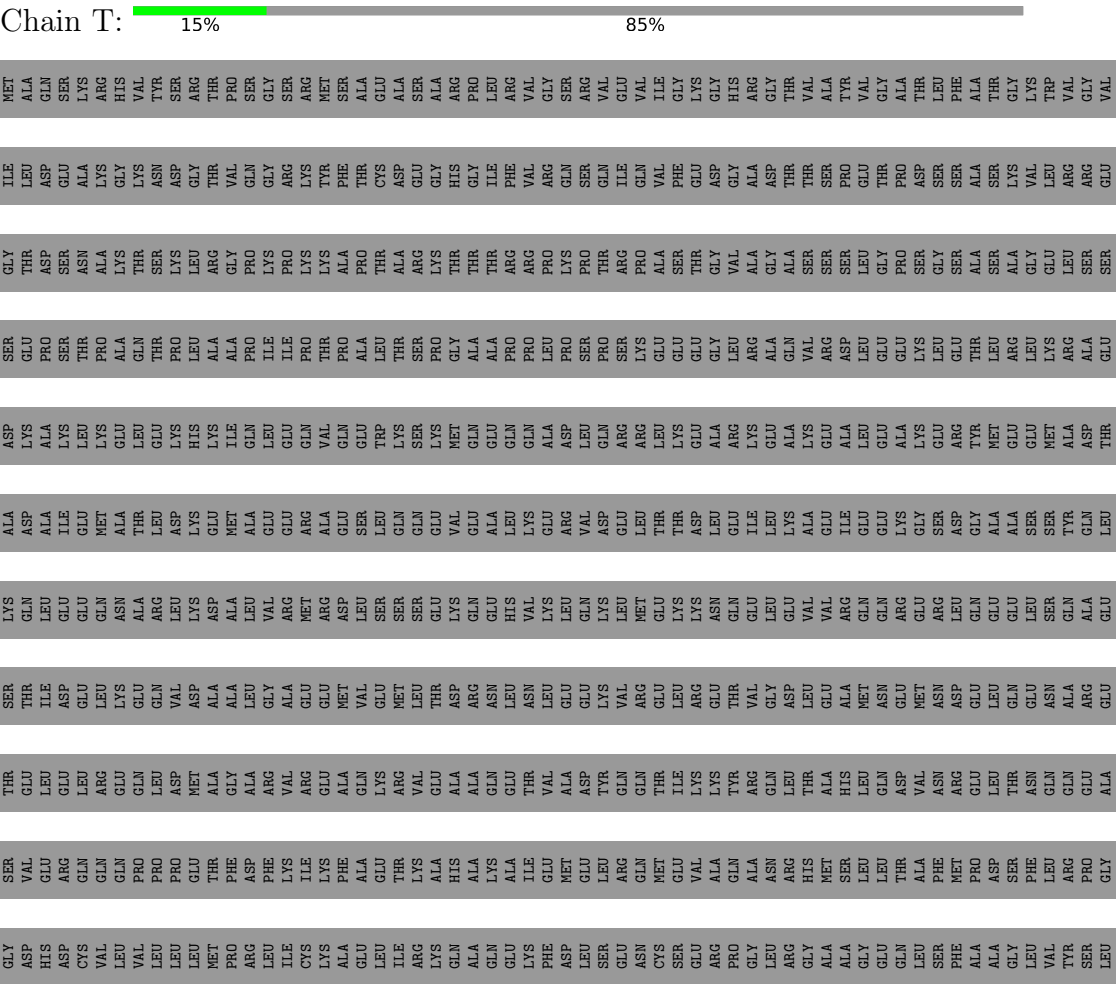
• Molecule 6: Dynactin subunit 2

Chain Q: 80% 20%



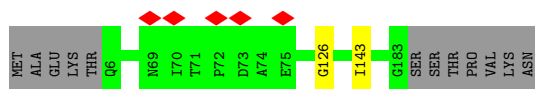


• Molecule 8: Dynactin subunit 1



VAL
PRO
GLY
PRO
GLY
LEU
VAL
LYS
D1094
P1143
P1147
I1285
SER

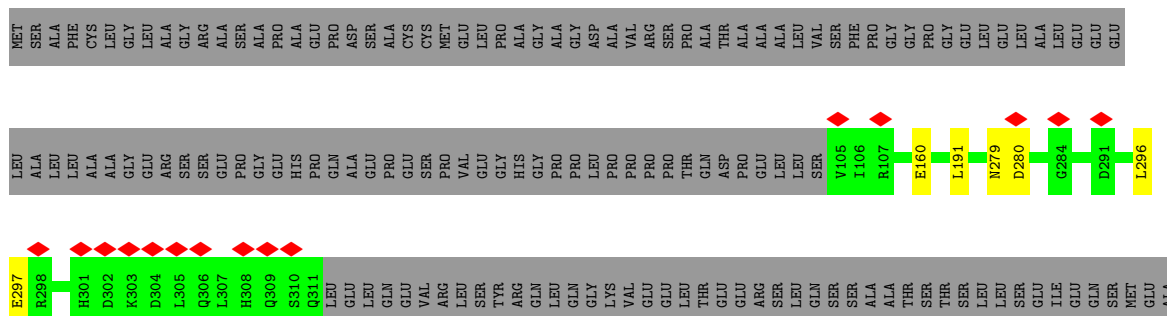
Chain U: 93% 6%



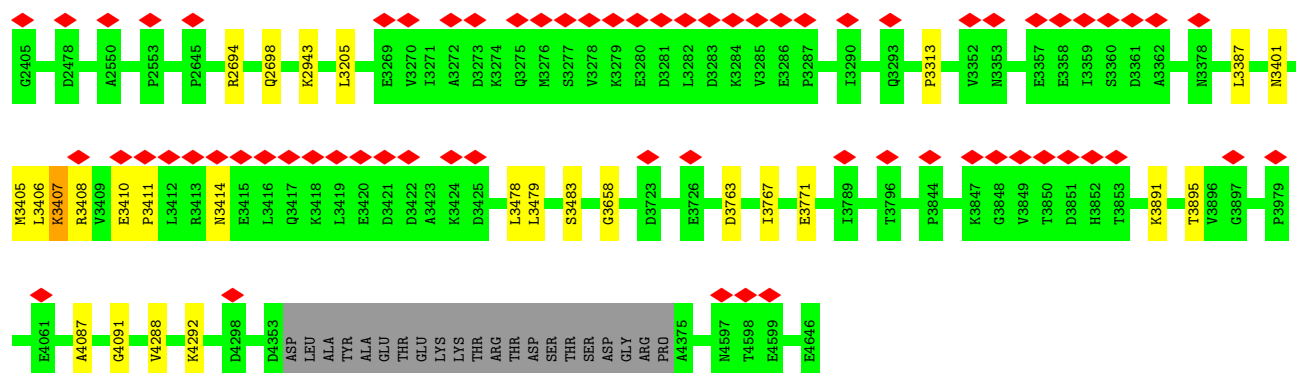
Chain V: 98%



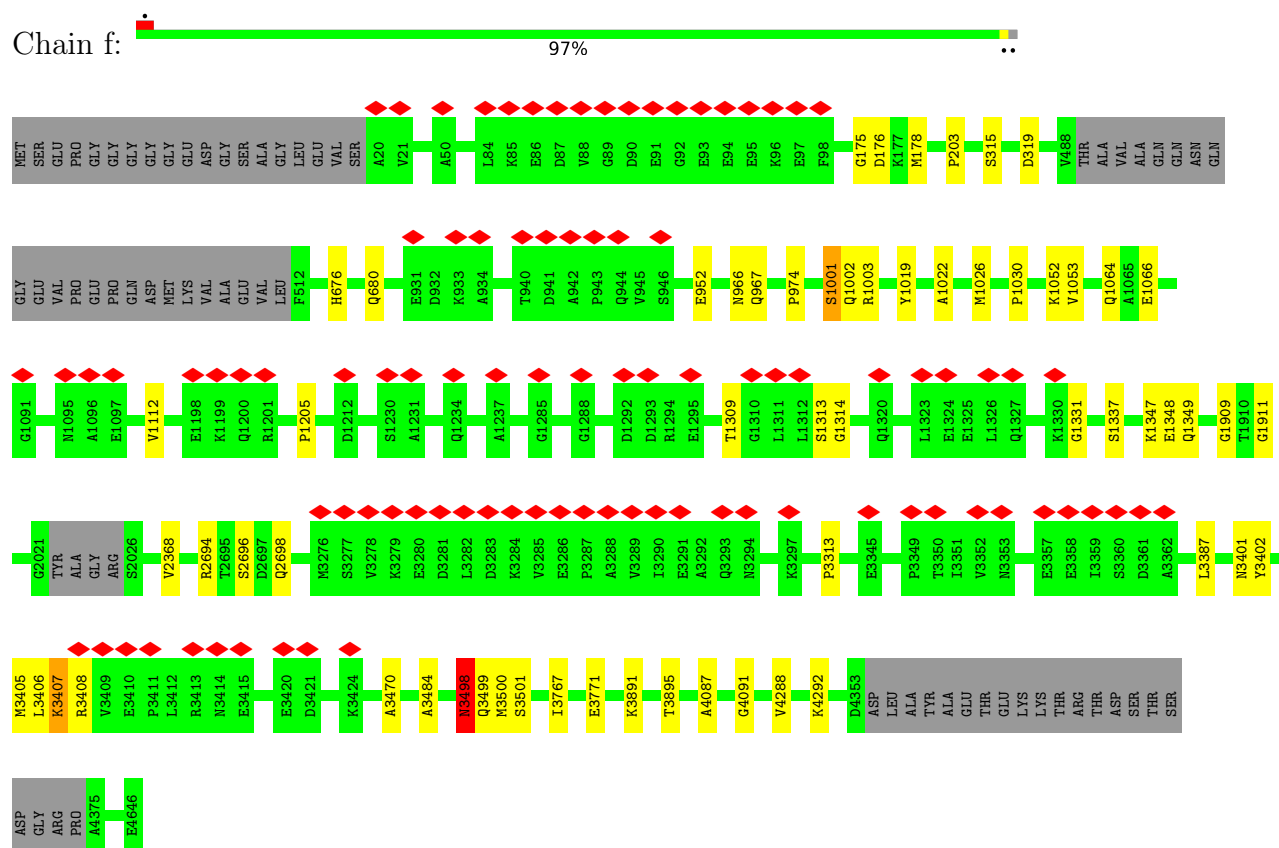
Chain W: 35% 64%



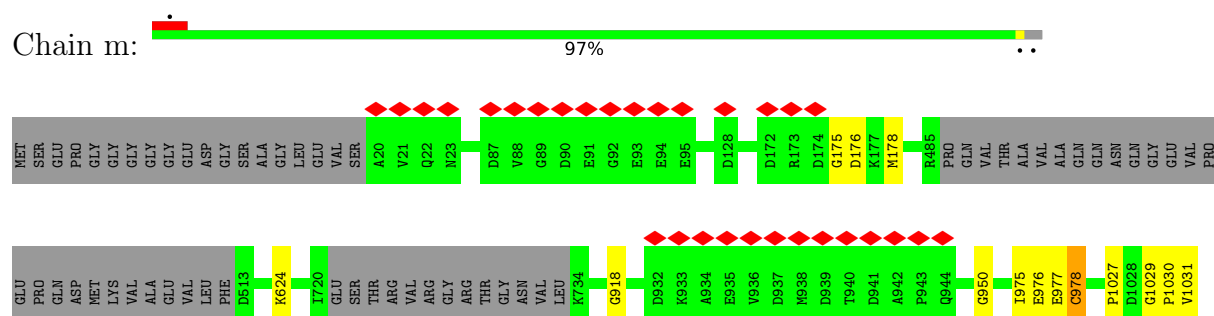


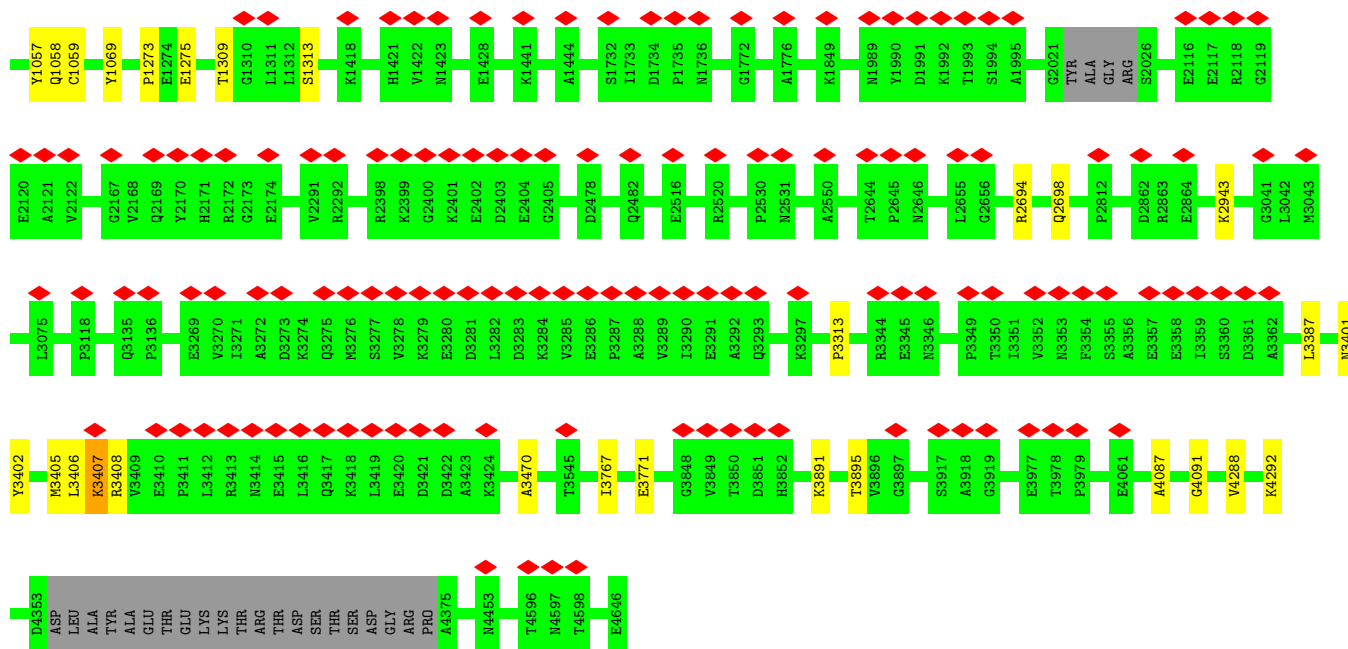


- Molecule 13: Cytoplasmic dynein 1 heavy chain 1



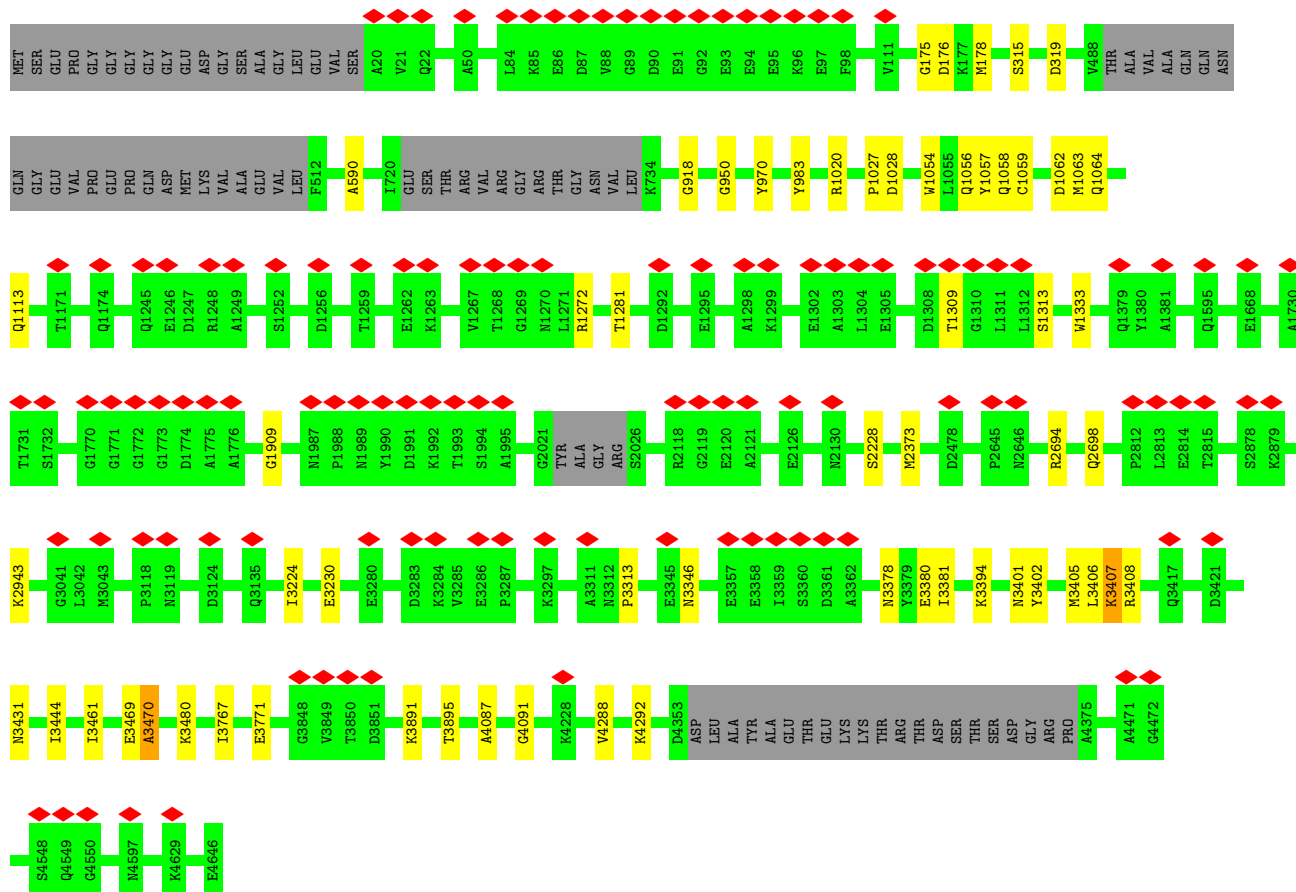
- Molecule 13: Cytoplasmic dynein 1 heavy chain 1



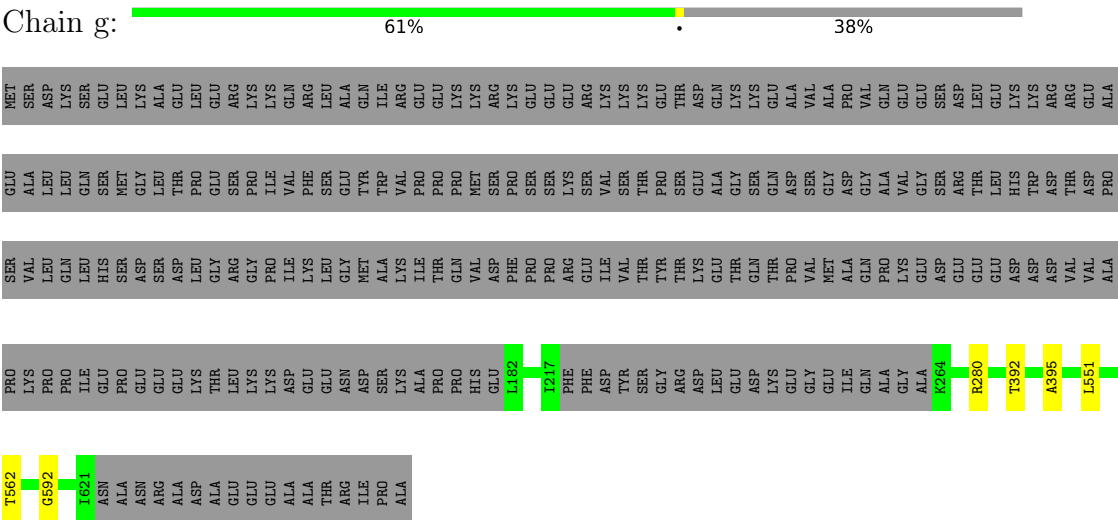


• Molecule 13: Cytoplasmic dynein 1 heavy chain 1

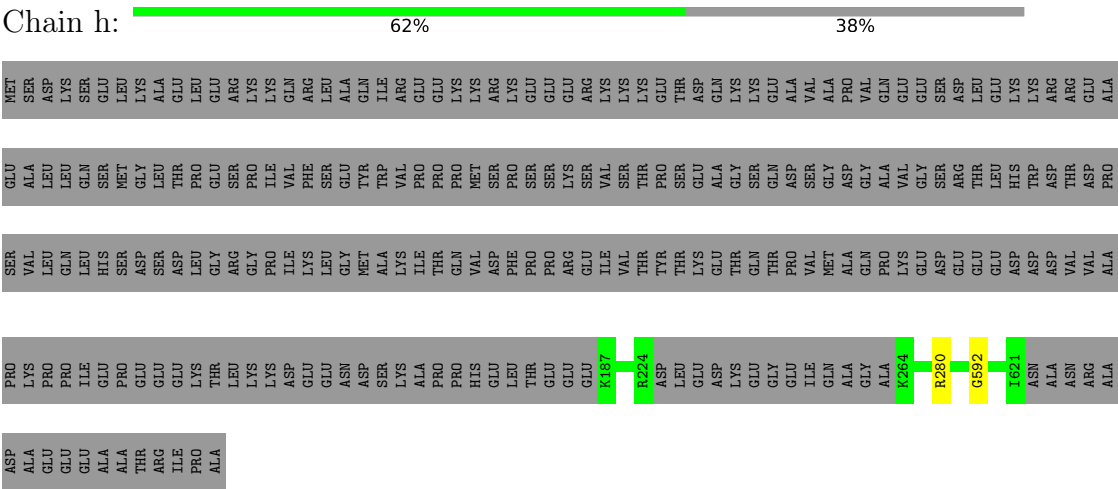
Chain n: 97%



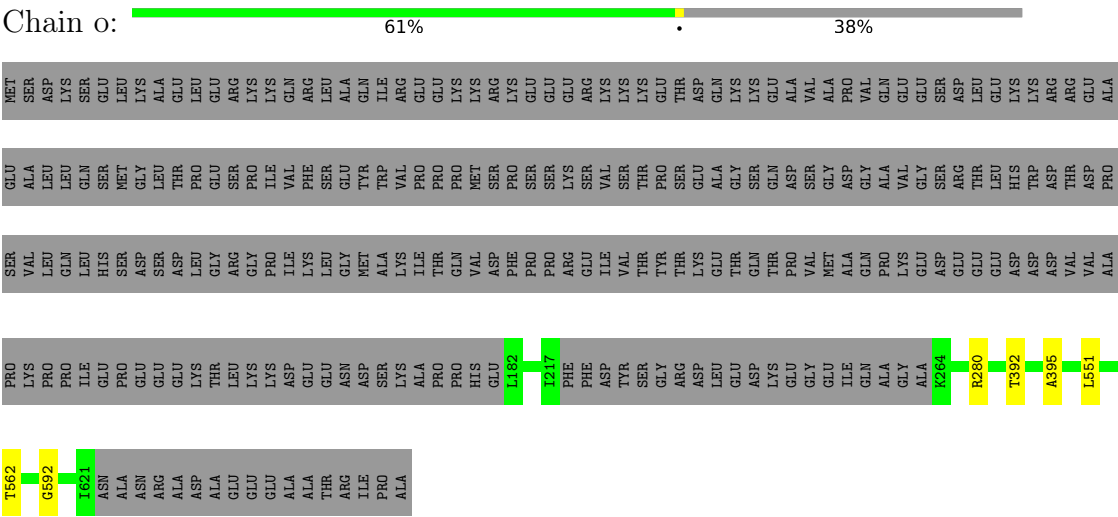
• Molecule 14: Cytoplasmic dynein 1 intermediate chain 2



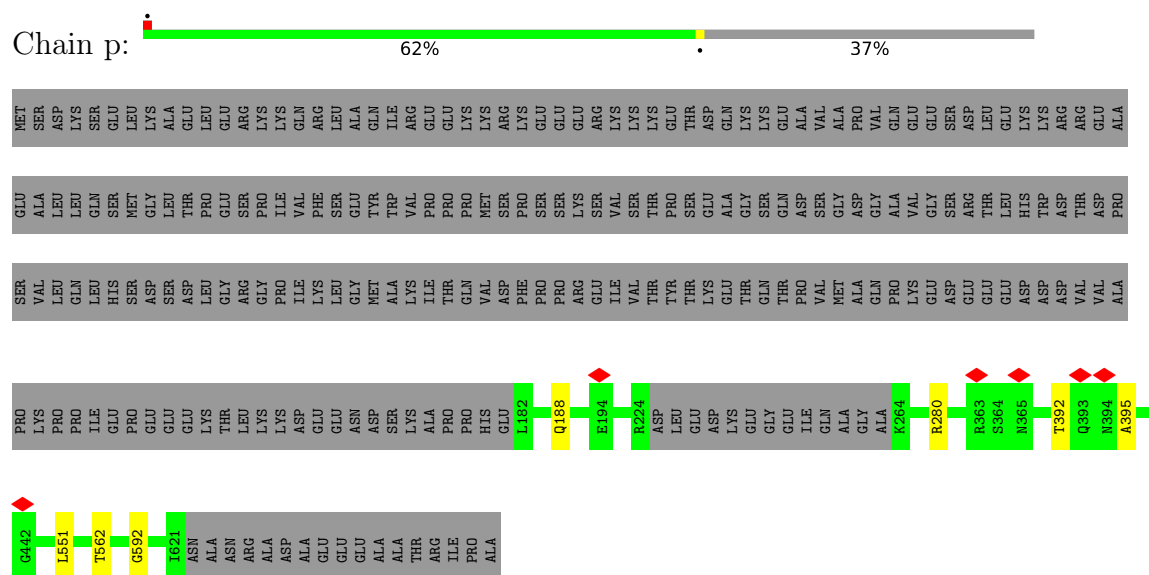
● Molecule 14: Cytoplasmic dynein 1 intermediate chain 2



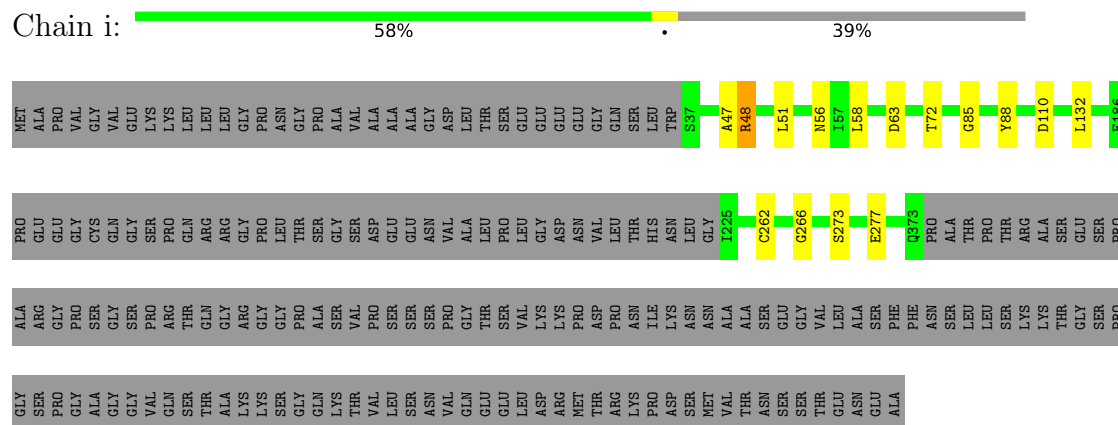
● Molecule 14: Cytoplasmic dynein 1 intermediate chain 2



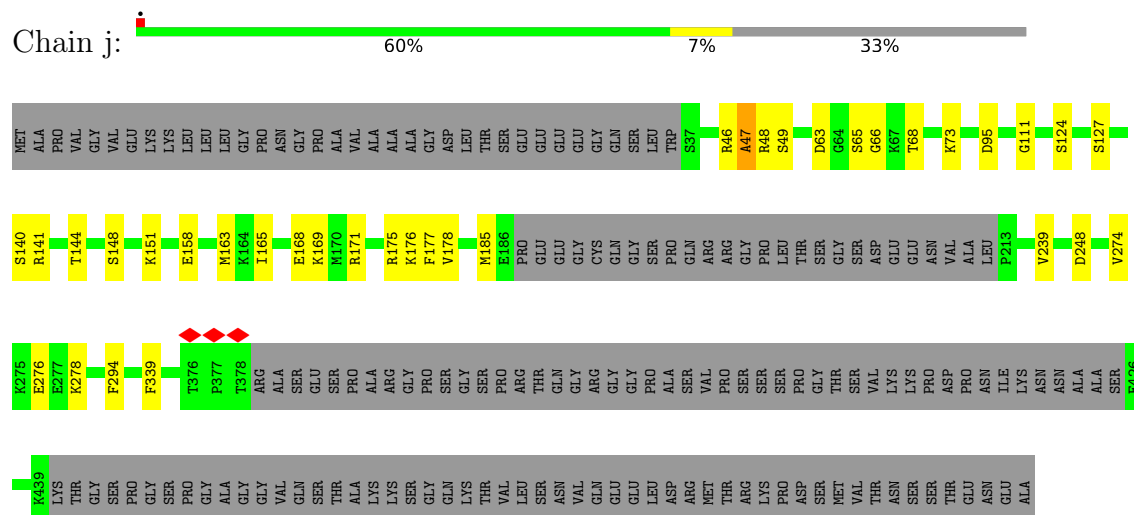
- Molecule 14: Cytoplasmic dynein 1 intermediate chain 2



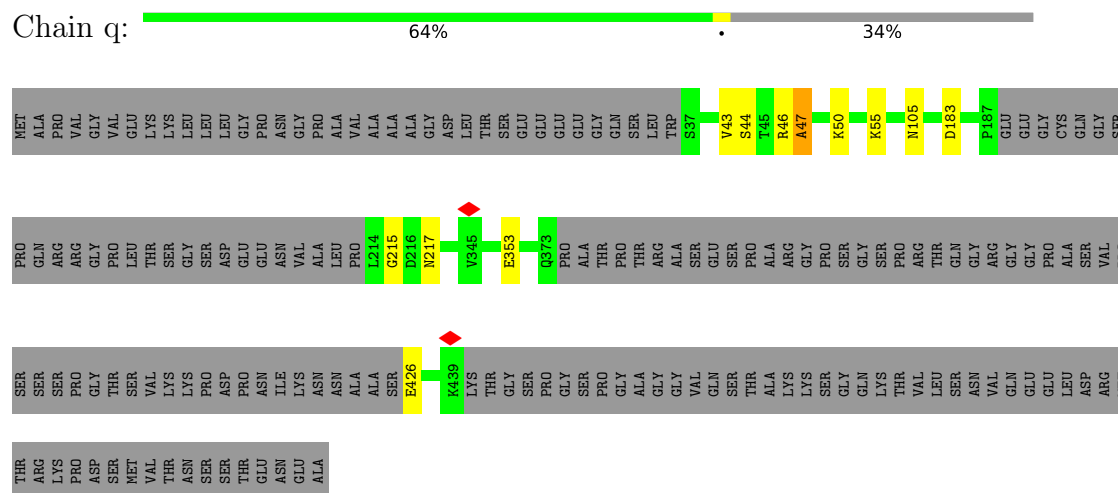
- Molecule 15: Cytoplasmic dynein 1 light intermediate chain 2



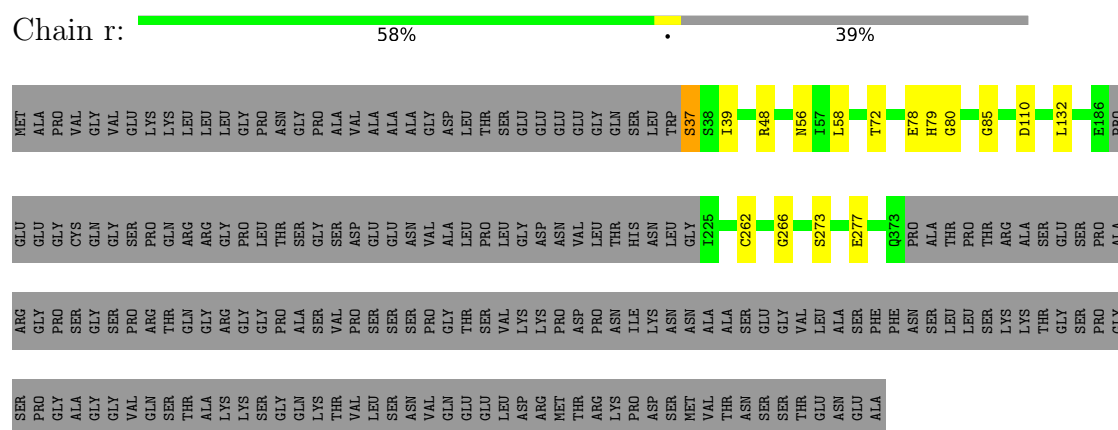
- Molecule 15: Cytoplasmic dynein 1 light intermediate chain 2



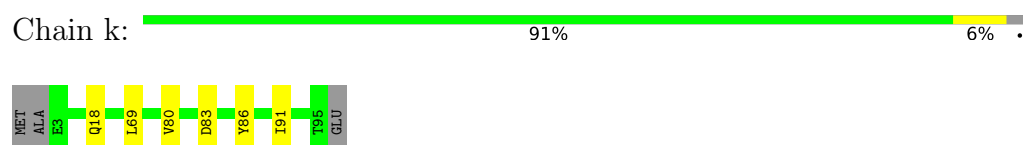
- Molecule 15: Cytoplasmic dynein 1 light intermediate chain 2



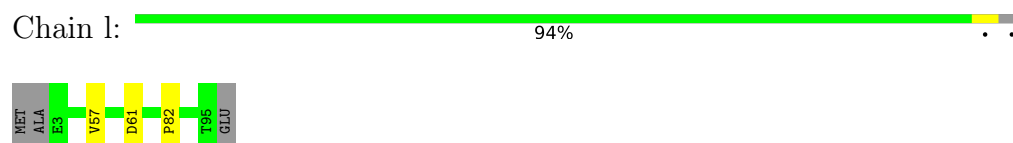
- Molecule 15: Cytoplasmic dynein 1 light intermediate chain 2



- Molecule 16: Dynein light chain roadblock-type 1



- Molecule 16: Dynein light chain roadblock-type 1

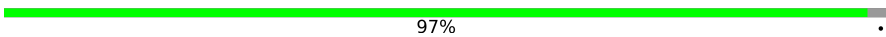


- Molecule 16: Dynein light chain roadblock-type 1





- Molecule 16: Dynein light chain roadblock-type 1

Chain t:  97%



4 Experimental information

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ZN, 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	A	0.17	0/1479	0.36	0/1847
1	B	0.16	0/1479	0.37	0/1847
1	C	0.17	0/1499	0.37	0/1872
1	D	0.16	0/1479	0.37	0/1847
1	E	0.15	0/1479	0.34	0/1847
1	F	1.83	25/1479 (1.7%)	2.31	27/1847 (1.5%)
1	G	0.16	0/1475	0.33	0/1842
1	I	0.17	0/1479	0.37	0/1847
2	H	0.16	0/1488	0.30	0/1857
3	J	0.17	0/1515	0.33	0/1892
4	K	0.19	0/1111	0.47	0/1387
5	L	0.16	0/1075	0.39	0/1342
6	M	1.36	0/1355	2.40	0/1685
6	N	1.43	1/1115 (0.1%)	2.53	0/1385
6	P	1.37	0/1368	2.34	3/1703 (0.2%)
6	Q	1.40	0/1297	2.39	0/1616
7	O	1.32	0/679	2.45	2/847 (0.2%)
7	R	1.37	0/715	2.55	6/892 (0.7%)
8	S	1.33	0/616	2.57	22/763 (2.9%)
8	T	1.41	0/767	2.30	0/957
9	U	0.27	0/711	0.46	0/887
10	V	0.36	0/727	0.48	0/907
11	W	1.26	0/827	2.12	4/1032 (0.4%)
11	X	1.03	0/1075	1.63	4/1342 (0.3%)
11	w	1.26	0/827	2.01	2/1032 (0.2%)
11	x	0.99	1/959 (0.1%)	1.65	4/1197 (0.3%)
12	Y	0.19	0/1527	0.36	0/1900
13	e	0.61	1/18313 (0.0%)	0.87	23/22883 (0.1%)
13	f	1.00	10/18313 (0.1%)	1.21	31/22883 (0.1%)
13	m	0.66	1/18244 (0.0%)	0.90	24/22795 (0.1%)
13	n	0.72	6/18260 (0.0%)	0.96	44/22815 (0.2%)
14	g	0.36	0/1574	0.59	0/1964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	h	0.36	0/1582	0.58	0/1974
14	o	0.35	0/1574	0.54	0/1964
14	p	0.40	0/1602	0.61	1/1999 (0.1%)
15	i	0.81	2/1194 (0.2%)	0.98	3/1489 (0.2%)
15	j	1.52	27/1317 (2.1%)	1.55	12/1641 (0.7%)
15	q	1.37	2/1297 (0.2%)	1.66	8/1616 (0.5%)
15	r	0.75	2/1194 (0.2%)	1.12	7/1489 (0.5%)
16	k	1.09	0/371	1.50	0/462
16	l	1.08	0/371	1.32	0/462
16	s	1.03	0/371	1.18	0/462
16	t	1.00	0/371	1.17	0/462
All	All	0.81	78/117550 (0.1%)	1.15	227/146779 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	q	0	1
15	r	0	2
All	All	0	3

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	j	248	ASP	C-N	-9.18	1.22	1.33
15	j	274	VAL	C-N	-8.75	1.22	1.33
15	j	95	ASP	C-N	-8.74	1.22	1.34
1	F	228	PRO	C-O	-8.38	1.14	1.24
1	F	117	PRO	C-O	-8.30	1.14	1.23
13	n	1063	MET	C-O	8.25	1.33	1.24
13	n	1062	ASP	C-O	-8.21	1.14	1.24
1	F	11	PRO	C-O	-8.05	1.15	1.23
1	F	152	ARG	C-O	-7.96	1.14	1.24
15	r	79	HIS	C-N	7.78	1.38	1.33
13	f	1026	MET	C-N	-7.58	1.23	1.34
15	j	141	ARG	C-N	-7.58	1.24	1.33
15	i	63	ASP	C-N	-7.47	1.23	1.33
6	N	216	ARG	N-CA	7.38	1.51	1.46
13	n	1020	ARG	C-O	-7.27	1.14	1.24
1	F	114	PRO	C-O	-7.22	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	j	176	LYS	C-N	-6.95	1.24	1.33
15	j	63	ASP	C-N	-6.89	1.23	1.33
1	F	179	SER	C-O	-6.82	1.14	1.23
13	f	1019	TYR	C-N	-6.77	1.24	1.34
13	f	3484	ALA	C-O	6.71	1.32	1.24
15	j	47	ALA	C-O	6.66	1.31	1.23
13	f	967	GLN	C-N	-6.57	1.25	1.33
13	e	3479	LEU	C-O	-6.54	1.16	1.24
13	n	1027	PRO	C-O	-6.52	1.16	1.24
15	j	127	SER	C-N	-6.46	1.24	1.33
1	F	21	ILE	C-O	-6.42	1.17	1.24
1	F	225	SER	C-O	-6.42	1.16	1.23
15	j	276	GLU	C-N	-6.31	1.25	1.33
1	F	287	ASP	C-O	-6.31	1.15	1.23
15	j	177	PHE	C-N	-6.29	1.25	1.33
15	j	151	LYS	C-N	-6.26	1.24	1.33
1	F	183	ILE	C-O	-6.26	1.17	1.24
13	f	966	ASN	C-N	6.24	1.42	1.33
15	j	239	VAL	C-N	-6.24	1.25	1.33
13	f	1022	ALA	C-N	-6.23	1.25	1.34
15	j	165	ILE	C-N	-6.19	1.26	1.33
1	F	239	ALA	C-O	-6.12	1.16	1.24
15	j	65	SER	C-N	-6.11	1.25	1.33
15	j	169	LYS	C-N	-6.10	1.25	1.33
13	n	3480	LYS	C-O	6.07	1.31	1.24
1	F	125	ALA	C-O	-6.01	1.17	1.24
15	j	294	PHE	C-N	-5.97	1.25	1.33
15	j	158	GLU	C-N	-5.90	1.25	1.33
13	f	1052	LYS	C-N	-5.90	1.26	1.33
13	f	1112	VAL	CA-C	-5.89	1.45	1.52
15	j	178	VAL	C-N	-5.86	1.26	1.33
15	j	124	SER	C-N	-5.86	1.26	1.34
13	m	1273	PRO	C-O	5.81	1.31	1.24
1	F	75	MET	C-O	-5.80	1.17	1.24
1	F	343	GLY	C-O	-5.75	1.16	1.23
15	j	144	THR	C-N	-5.74	1.26	1.33
11	x	195	ASP	C-O	-5.73	1.17	1.24
1	F	14	ILE	C-O	-5.63	1.17	1.24
1	F	276	HIS	C-O	-5.62	1.17	1.24
15	q	353	GLU	C-O	5.61	1.30	1.24
1	F	344	GLY	CA-C	-5.56	1.45	1.52
1	F	281	PHE	C-O	-5.56	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1053	VAL	C-N	-5.54	1.26	1.33
15	i	58	LEU	C-N	-5.51	1.26	1.33
1	F	253	PRO	C-O	-5.51	1.17	1.24
15	j	111	GLY	C-N	5.47	1.41	1.33
15	j	140	SER	C-N	-5.47	1.26	1.33
1	F	264	ARG	C-O	-5.46	1.18	1.24
15	j	148	SER	C-N	-5.45	1.26	1.33
15	j	49	SER	C-O	5.43	1.31	1.23
15	r	58	LEU	C-N	-5.39	1.26	1.33
1	F	181	MET	C-O	-5.32	1.18	1.24
1	F	282	ALA	C-O	-5.32	1.17	1.24
1	F	124	ALA	C-O	-5.29	1.18	1.24
1	F	339	SER	C-O	-5.25	1.17	1.24
15	q	43	VAL	C-O	-5.22	1.18	1.24
15	j	185	MET	C-N	-5.21	1.26	1.33
1	F	74	PRO	N-CA	-5.13	1.40	1.47
13	n	3381	ILE	C-O	-5.09	1.18	1.24
15	j	339	PHE	C-N	-5.07	1.27	1.33
15	j	68	THR	C-N	-5.04	1.27	1.33
13	f	1205	PRO	CA-C	5.04	1.54	1.51

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	r	79	HIS	CA-C-N	-14.10	108.80	122.20
15	r	79	HIS	C-N-CA	-14.10	108.80	122.20
13	m	1030	PRO	N-CA-C	-12.64	99.88	114.92
13	n	3407	LYS	N-CA-C	-10.61	99.72	111.07
13	e	3407	LYS	N-CA-C	-9.99	100.38	111.07
13	f	3407	LYS	N-CA-C	-9.96	100.41	111.07
13	m	3407	LYS	N-CA-C	-9.90	100.48	111.07
13	n	3470	ALA	N-CA-C	-9.15	100.12	111.11
13	n	1062	ASP	CA-C-N	9.02	136.63	122.74
13	n	1062	ASP	C-N-CA	9.02	136.63	122.74
13	f	3470	ALA	N-CA-C	-8.83	100.51	111.11
13	m	3470	ALA	N-CA-C	-8.75	100.61	111.11
13	m	1313	SER	CA-C-O	-8.10	112.96	121.55
13	n	1027	PRO	CA-C-N	-8.10	109.46	122.66
13	n	1027	PRO	C-N-CA	-8.10	109.46	122.66
13	f	1313	SER	CA-C-O	-8.05	112.34	121.19
15	j	171	ARG	O-C-N	7.90	130.50	122.12
13	f	974	PRO	N-CA-C	7.84	123.38	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	978	CYS	N-CA-C	-7.74	102.92	111.36
15	q	217	ASN	N-CA-C	-7.70	101.33	110.41
13	f	952	GLU	O-C-N	7.55	128.44	121.04
13	n	1313	SER	CA-C-O	-7.48	113.62	121.55
13	f	175	GLY	CA-C-N	-7.31	111.95	122.77
13	f	175	GLY	C-N-CA	-7.31	111.95	122.77
13	n	175	GLY	CA-C-N	-7.19	112.13	122.77
13	n	175	GLY	C-N-CA	-7.19	112.13	122.77
13	f	1112	VAL	CA-C-O	-7.17	113.25	120.85
13	m	175	GLY	CA-C-N	-7.15	112.19	122.77
13	m	175	GLY	C-N-CA	-7.15	112.19	122.77
13	e	175	GLY	CA-C-N	-7.09	112.27	122.77
13	e	175	GLY	C-N-CA	-7.09	112.27	122.77
15	q	215	GLY	CA-C-O	-6.96	115.52	121.57
13	f	1112	VAL	O-C-N	6.86	128.90	121.83
15	j	66	GLY	CA-C-N	6.80	129.29	120.44
15	j	66	GLY	C-N-CA	6.80	129.29	120.44
11	X	301	HIS	CA-C-O	-6.79	113.35	120.55
13	n	3405	MET	CA-C-O	-6.69	113.46	120.55
14	p	188	GLN	N-CA-C	6.69	118.57	111.28
11	W	297	GLU	N-CA-C	-6.65	104.98	113.23
13	f	1026	MET	CA-C-N	6.59	126.37	119.05
13	f	1026	MET	C-N-CA	6.59	126.37	119.05
1	F	54	GLY	CA-C-O	-6.58	116.75	121.88
13	n	1058	GLN	N-CA-C	-6.56	105.38	113.19
11	w	279	ASN	O-C-N	6.55	129.17	122.09
15	q	47	ALA	CA-C-N	6.54	130.44	120.82
15	q	47	ALA	C-N-CA	6.54	130.44	120.82
7	O	107	LEU	CA-C-N	6.52	124.35	120.24
7	O	107	LEU	C-N-CA	6.52	124.35	120.24
13	e	3478	LEU	N-CA-C	-6.51	104.18	111.28
13	e	3405	MET	CA-C-O	-6.47	112.79	120.10
11	W	296	LEU	N-CA-C	-6.43	105.59	113.50
13	n	3346	ASN	N-CA-C	-6.36	105.00	112.89
13	f	2368	VAL	N-CA-C	-6.34	106.62	112.96
13	e	1058	GLN	N-CA-C	-6.33	105.27	112.87
15	j	48	ARG	O-C-N	6.33	130.92	122.82
13	f	1030	PRO	CA-C-N	6.32	128.53	120.56
13	f	1030	PRO	C-N-CA	6.32	128.53	120.56
15	r	48	ARG	N-CA-C	-6.32	100.05	109.15
15	j	66	GLY	O-C-N	-6.29	115.50	122.55
13	m	3405	MET	CA-C-O	-6.27	113.02	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	j	175	ARG	O-C-N	6.21	129.23	122.15
13	f	1337	SER	N-CA-C	-6.19	103.12	112.04
11	w	299	GLN	N-CA-C	-6.15	104.57	111.28
11	X	301	HIS	CA-C-N	6.09	128.94	120.29
11	X	301	HIS	C-N-CA	6.09	128.94	120.29
8	S	1203	PHE	CA-C-N	6.09	125.81	119.05
8	S	1203	PHE	C-N-CA	6.09	125.81	119.05
13	f	1002	GLN	N-CA-C	-6.08	105.91	113.15
13	m	1058	GLN	N-CA-C	-6.08	104.97	113.37
13	n	3313	PRO	N-CA-C	6.06	118.10	110.70
1	F	343	GLY	CA-C-N	6.05	126.70	119.98
1	F	343	GLY	C-N-CA	6.05	126.70	119.98
13	m	1027	PRO	N-CA-C	6.01	121.88	113.53
13	f	3405	MET	CA-C-O	-6.00	113.31	120.10
13	n	1281	THR	N-CA-C	-6.00	104.11	112.45
13	e	1069	TYR	CA-C-O	-5.95	114.58	120.70
13	f	3498	ASN	CA-C-N	5.93	132.88	121.54
13	f	3498	ASN	C-N-CA	5.93	132.88	121.54
13	n	3405	MET	O-C-N	5.93	128.40	122.12
13	e	3313	PRO	N-CA-C	5.92	117.92	110.70
11	x	325	GLN	N-CA-C	-5.90	104.79	112.23
13	m	1069	TYR	CA-C-O	-5.89	114.83	120.90
13	e	3405	MET	N-CA-C	-5.89	104.94	111.71
13	m	3313	PRO	N-CA-C	5.88	117.88	110.70
8	S	1191	ARG	CA-C-N	5.88	125.26	118.85
8	S	1191	ARG	C-N-CA	5.88	125.26	118.85
13	f	3313	PRO	N-CA-C	5.87	117.86	110.70
8	S	1141	LEU	CA-C-N	5.86	126.42	120.38
8	S	1141	LEU	C-N-CA	5.86	126.42	120.38
13	n	3224	ILE	CA-C-O	-5.86	114.85	120.95
1	F	187	GLY	CA-C-O	-5.86	114.72	120.75
15	r	79	HIS	O-C-N	5.85	130.77	123.28
13	m	1275	GLU	CA-C-N	-5.83	110.94	121.14
13	m	1275	GLU	C-N-CA	-5.83	110.94	121.14
13	m	3405	MET	N-CA-C	-5.82	105.01	111.71
13	n	3394	LYS	N-CA-C	-5.81	104.94	111.28
15	q	183	ASP	N-CA-C	-5.78	106.56	113.21
1	F	152	ARG	CA-C-O	-5.78	114.11	120.36
13	m	624	LYS	N-CA-C	-5.78	105.06	111.36
1	F	201	GLU	N-CA-C	-5.73	105.55	112.54
13	e	3205	LEU	O-C-N	5.72	127.96	122.07
13	m	1273	PRO	CA-C-O	5.68	130.95	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	1132	PRO	CA-C-N	5.68	125.36	119.05
8	S	1132	PRO	C-N-CA	5.68	125.36	119.05
13	n	3402	TYR	CA-C-O	-5.67	114.54	120.55
13	f	3405	MET	N-CA-C	-5.66	105.20	111.71
15	i	88	TYR	N-CA-C	5.66	117.61	108.32
13	e	3401	ASN	N-CA-C	-5.65	105.12	111.28
13	f	1001	SER	N-CA-C	-5.65	106.93	113.88
7	R	2	ALA	CA-C-N	5.60	126.20	119.98
7	R	2	ALA	C-N-CA	5.60	126.20	119.98
8	S	1196	VAL	CA-C-N	5.60	125.26	119.05
8	S	1196	VAL	C-N-CA	5.60	125.26	119.05
1	F	324	LYS	CA-C-O	-5.58	114.92	121.16
11	X	341	ALA	CA-C-O	-5.56	114.98	120.82
13	n	3431	ASN	CA-C-O	-5.54	114.67	120.55
13	n	1063	MET	N-CA-C	-5.49	99.48	108.76
1	F	8	ALA	CA-C-O	-5.49	115.21	121.58
13	m	3401	ASN	N-CA-C	-5.49	105.30	111.28
13	e	1267	VAL	N-CA-C	-5.48	107.41	112.83
13	n	3407	LYS	CA-C-N	-5.48	112.94	120.28
13	n	3407	LYS	C-N-CA	-5.48	112.94	120.28
13	n	3406	LEU	CA-C-N	-5.47	113.33	120.44
13	n	3406	LEU	C-N-CA	-5.47	113.33	120.44
13	n	3401	ASN	N-CA-C	-5.46	105.33	111.28
1	F	225	SER	CA-C-O	-5.45	115.06	121.16
13	e	1106	VAL	CA-C-O	-5.45	117.89	122.63
13	e	1337	SER	N-CA-C	-5.42	104.92	112.45
13	n	1272	ARG	CA-C-O	-5.41	113.88	120.54
15	j	278	LYS	CA-C-N	5.41	131.55	123.05
15	j	278	LYS	C-N-CA	5.41	131.55	123.05
13	n	970	TYR	CA-C-N	-5.41	115.48	123.05
13	n	970	TYR	C-N-CA	-5.41	115.48	123.05
13	n	3401	ASN	O-C-N	5.40	127.84	122.12
13	e	1038	SER	N-CA-C	-5.39	105.56	111.82
13	f	3401	ASN	N-CA-C	-5.39	105.40	111.28
13	e	3405	MET	CA-C-N	5.39	127.94	120.29
13	e	3405	MET	C-N-CA	5.39	127.94	120.29
1	F	54	GLY	O-C-N	5.38	127.47	122.47
13	m	3405	MET	CA-C-N	5.36	127.91	120.29
13	m	3405	MET	C-N-CA	5.36	127.91	120.29
13	f	1331	GLY	CA-C-O	-5.36	115.21	121.00
11	x	325	GLN	CA-C-N	5.36	125.88	119.94
11	x	325	GLN	C-N-CA	5.36	125.88	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	n	3224	ILE	O-C-N	5.34	127.05	121.87
13	f	3405	MET	CA-C-N	5.32	127.84	120.29
13	f	3405	MET	C-N-CA	5.32	127.84	120.29
15	r	72	THR	O-C-N	5.31	127.75	122.12
13	n	1064	GLN	CA-C-N	5.31	127.65	120.38
13	n	1064	GLN	C-N-CA	5.31	127.65	120.38
13	f	3406	LEU	CA-C-N	-5.30	113.56	120.44
13	f	3406	LEU	C-N-CA	-5.30	113.56	120.44
13	n	3461	ILE	CA-C-O	-5.29	115.45	120.95
15	q	217	ASN	CA-C-O	-5.29	116.26	121.02
1	F	287	ASP	CA-C-O	-5.28	115.80	121.56
8	S	1120	LYS	CA-C-N	5.28	125.84	119.98
8	S	1120	LYS	C-N-CA	5.28	125.84	119.98
15	q	47	ALA	CA-C-O	-5.28	115.34	121.15
1	F	11	PRO	CA-C-O	-5.28	114.98	121.31
13	n	1333	TRP	N-CA-C	-5.28	106.71	112.72
13	m	3406	LEU	CA-C-N	-5.27	113.59	120.44
13	m	3406	LEU	C-N-CA	-5.27	113.59	120.44
13	e	3483	SER	N-CA-C	-5.27	105.45	111.14
13	e	3406	LEU	CA-C-N	-5.26	113.61	120.44
13	e	3406	LEU	C-N-CA	-5.26	113.61	120.44
13	n	983	TYR	N-CA-C	-5.25	105.73	111.82
15	r	78	GLU	CA-C-N	-5.24	114.63	122.39
15	r	78	GLU	C-N-CA	-5.24	114.63	122.39
8	S	1147	PRO	CA-C-N	5.24	125.65	119.94
8	S	1147	PRO	C-N-CA	5.24	125.65	119.94
1	F	192	ARG	CA-C-N	5.24	127.73	120.29
1	F	192	ARG	C-N-CA	5.24	127.73	120.29
15	j	163	MET	CA-C-N	5.23	129.79	122.36
15	j	163	MET	C-N-CA	5.23	129.79	122.36
13	n	1027	PRO	N-CA-C	5.23	120.80	113.53
13	n	1028	ASP	N-CA-C	-5.23	107.43	112.97
15	q	50	LYS	CA-C-O	-5.21	115.57	121.72
15	i	72	THR	O-C-N	5.21	127.64	122.12
1	F	282	ALA	CA-C-N	5.20	127.22	120.56
1	F	282	ALA	C-N-CA	5.20	127.22	120.56
7	R	35	ASP	CA-C-N	5.20	125.87	119.99
7	R	35	ASP	C-N-CA	5.20	125.87	119.99
1	F	302	GLY	CA-C-O	-5.18	118.66	122.23
7	R	44	LEU	CA-C-N	5.17	125.58	119.94
7	R	44	LEU	C-N-CA	5.17	125.58	119.94
13	n	3230	GLU	CA-C-O	-5.17	115.39	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	260	GLU	CA-C-N	5.17	127.47	120.38
1	F	260	GLU	C-N-CA	5.17	127.47	120.38
15	i	51	LEU	O-C-N	5.17	126.29	121.27
1	F	375	THR	N-CA-C	-5.16	105.81	112.68
8	S	1142	PRO	CA-C-N	5.15	125.31	119.90
8	S	1142	PRO	C-N-CA	5.15	125.31	119.90
13	f	2696	SER	CA-C-O	-5.15	115.41	120.82
13	n	3444	ILE	CA-C-O	-5.15	115.59	120.95
1	F	9	ASN	N-CA-C	5.14	116.74	111.03
13	n	3401	ASN	CA-C-O	-5.13	115.11	120.55
6	P	390	GLU	CA-C-N	5.13	125.64	120.00
6	P	390	GLU	C-N-CA	5.13	125.64	120.00
13	n	590	ALA	N-CA-C	-5.12	105.82	111.71
8	S	1192	PRO	CA-C-N	5.11	125.65	119.98
8	S	1192	PRO	C-N-CA	5.11	125.65	119.98
8	S	1146	GLY	CA-C-N	5.11	125.34	119.83
8	S	1146	GLY	C-N-CA	5.11	125.34	119.83
13	n	3461	ILE	O-C-N	5.11	126.82	121.87
1	F	293	THR	CA-C-N	5.10	127.54	120.29
1	F	293	THR	C-N-CA	5.10	127.54	120.29
13	f	3402	TYR	CA-C-O	-5.10	115.14	120.55
13	m	3402	TYR	CA-C-O	-5.09	115.16	120.55
13	e	3414	ASN	N-CA-C	-5.08	105.74	111.28
11	x	195	ASP	CA-C-O	-5.08	115.04	120.42
15	j	168	GLU	O-C-N	5.07	127.93	122.15
1	F	144	VAL	CA-C-N	5.07	127.49	120.29
1	F	144	VAL	C-N-CA	5.07	127.49	120.29
13	e	3763	ASP	N-CA-C	-5.07	106.01	113.61
13	e	3387	LEU	N-CA-C	-5.07	106.88	113.16
11	W	160	GLU	O-C-N	5.05	127.54	122.09
13	m	3387	LEU	N-CA-C	-5.05	106.90	113.16
13	n	3405	MET	N-CA-C	-5.05	105.78	111.28
13	n	1113	GLN	N-CA-C	-5.04	106.82	112.87
11	W	191	LEU	N-CA-C	-5.04	105.67	111.07
13	f	3387	LEU	N-CA-C	-5.04	106.91	113.16
1	F	281	PHE	CA-C-N	5.04	127.44	120.29
1	F	281	PHE	C-N-CA	5.04	127.44	120.29
6	P	301	LYS	N-CA-C	5.02	118.26	110.17
15	j	73	LYS	N-CA-C	-5.02	106.67	112.89
8	S	1131	LEU	CA-C-N	5.01	125.54	120.38
8	S	1131	LEU	C-N-CA	5.01	125.54	120.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1480	0	406	0	0
1	B	1480	0	406	4	0
1	C	1500	0	411	0	0
1	D	1480	0	406	0	0
1	E	1480	0	406	3	0
1	F	1480	0	406	2	0
1	G	1476	0	405	2	0
1	I	1480	0	406	1	0
2	H	1489	0	408	0	0
3	J	1516	0	408	1	0
4	K	1112	0	291	1	0
5	L	1076	0	295	2	0
6	M	1360	0	346	2	0
6	N	1120	0	277	0	0
6	P	1372	0	341	4	0
6	Q	1300	0	339	3	0
7	O	680	0	176	0	0
7	R	716	0	187	3	0
8	S	620	0	154	2	0
8	T	768	0	196	0	0
9	U	712	0	193	1	0
10	V	728	0	202	1	0
11	W	828	0	216	1	0
11	X	1076	0	280	0	0
11	w	828	0	216	1	0
11	x	960	0	251	0	0
12	Y	1532	0	375	2	0
13	e	18317	0	4801	19	0
13	f	18317	0	4801	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	18249	0	4780	16	0
13	n	18265	0	4783	21	0
14	g	1576	0	421	3	0
14	h	1584	0	425	1	0
14	o	1576	0	421	3	0
14	p	1604	0	430	3	0
15	i	1196	0	312	5	0
15	j	1320	0	346	1	0
15	q	1300	0	342	3	0
15	r	1196	0	312	5	0
16	k	372	0	93	3	0
16	l	372	0	93	1	0
16	s	372	0	93	0	0
16	t	372	0	93	0	0
17	A	27	0	12	0	0
17	B	27	0	12	0	0
17	C	27	0	12	0	0
17	D	27	0	12	0	0
17	E	27	0	12	0	0
17	F	27	0	12	0	0
17	G	27	0	12	0	0
17	H	27	0	12	0	0
17	I	27	0	12	0	0
17	e	27	0	12	1	0
17	f	27	0	12	2	0
17	m	27	0	12	0	0
17	n	27	0	12	1	0
18	A	1	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	D	1	0	0	0	0
18	E	1	0	0	0	0
18	F	1	0	0	0	0
18	G	1	0	0	0	0
18	H	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	e	1	0	0	0	0
18	f	1	0	0	0	0
18	m	1	0	0	0	0
18	n	1	0	0	0	0
19	J	31	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	e	31	0	12	1	0
19	f	31	0	12	0	0
19	m	31	0	12	0	0
19	n	31	0	12	2	0
20	Y	3	0	0	0	0
21	e	62	0	26	3	0
21	f	62	0	26	1	0
21	m	62	0	26	2	0
21	n	62	0	26	2	0
All	All	118408	0	31269	133	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 (133) 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)
13:e:918:GLY:HA2	13:e:950:GLY:HA2	1.45	0.97
13:n:918:GLY:HA2	13:n:950:GLY:HA2	1.48	0.96
13:m:918:GLY:HA2	13:m:950:GLY:HA2	1.49	0.91
13:e:918:GLY:HA2	13:e:950:GLY:CA	2.10	0.82
13:n:918:GLY:HA2	13:n:950:GLY:CA	2.13	0.79
13:m:918:GLY:HA2	13:m:950:GLY:CA	2.13	0.78
15:r:85:GLY:O	15:r:110:ASP:N	2.21	0.74
13:e:918:GLY:CA	13:e:950:GLY:HA2	2.17	0.73
5:L:125:ASP:CA	15:q:426:GLU:N	2.52	0.72
13:m:1057:TYR:C	13:m:1059:CYS:H	1.97	0.70
5:L:163:ARG:O	5:L:203:VAL:N	2.25	0.70
13:m:918:GLY:CA	13:m:950:GLY:HA2	2.20	0.70
13:n:918:GLY:CA	13:n:950:GLY:HA2	2.20	0.70
13:n:4288:VAL:N	13:n:4292:LYS:O	2.26	0.69
15:i:262:CYS:O	15:i:266:GLY:N	2.26	0.69
13:m:4288:VAL:N	13:m:4292:LYS:O	2.26	0.69
13:e:4288:VAL:N	13:e:4292:LYS:O	2.26	0.68
15:r:262:CYS:O	15:r:266:GLY:N	2.26	0.68
13:e:3767:ILE:O	13:e:3771:GLU:N	2.29	0.66
13:m:3767:ILE:O	13:m:3771:GLU:N	2.29	0.66
13:n:3767:ILE:O	13:n:3771:GLU:N	2.29	0.65
13:f:4288:VAL:N	13:f:4292:LYS:O	2.31	0.64
15:r:37:SER:C	15:r:39:ILE:N	2.55	0.64
21:n:4705:ANP:O1G	21:n:4705:ANP:O2B	2.18	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:e:4705:ANP:O1G	21:e:4705:ANP:O2B	2.18	0.62
13:f:3767:ILE:O	13:f:3771:GLU:N	2.32	0.61
15:i:56:ASN:O	15:i:132:LEU:N	2.27	0.61
15:r:56:ASN:O	15:r:132:LEU:N	2.27	0.61
21:m:4705:ANP:O2B	21:m:4705:ANP:O1G	2.18	0.60
7:R:36:GLY:O	7:R:40:VAL:N	2.35	0.59
13:m:1057:TYR:C	13:m:1059:CYS:N	2.60	0.59
15:r:273:SER:O	15:r:277:GLU:N	2.36	0.59
15:i:273:SER:O	15:i:277:GLU:N	2.36	0.59
13:f:1911:GLY:N	17:f:4701:ADP:O2B	2.31	0.58
6:P:298:ALA:O	6:P:300:HIS:N	2.38	0.57
13:n:1909:GLY:N	17:n:4701:ADP:O1B	2.27	0.56
14:o:280:ARG:O	14:o:592:GLY:N	2.40	0.55
14:p:280:ARG:O	14:p:592:GLY:N	2.40	0.54
14:g:280:ARG:O	14:g:592:GLY:N	2.40	0.54
13:e:3891:LYS:O	13:e:3895:THR:N	2.41	0.53
13:e:1407:ALA:CA	13:e:3658:GLY:HA3	2.39	0.53
16:k:69:LEU:N	16:k:80:VAL:O	2.41	0.53
13:n:3891:LYS:O	13:n:3895:THR:N	2.42	0.53
13:e:4087:ALA:O	13:e:4091:GLY:N	2.43	0.52
13:n:2373:MET:O	19:n:4702:ATP:H2	1.93	0.52
6:M:144:LEU:O	6:M:148:LYS:N	2.41	0.52
13:m:3891:LYS:O	13:m:3895:THR:N	2.42	0.52
15:q:55:LYS:O	15:q:105:ASN:N	2.42	0.51
11:W:279:ASN:O	11:W:280:ASP:C	2.48	0.51
13:m:975:ILE:C	13:m:977:GLU:N	2.68	0.51
13:m:4087:ALA:O	13:m:4091:GLY:N	2.43	0.51
11:w:279:ASN:O	11:w:283:GLN:N	2.39	0.50
13:f:676:HIS:O	13:f:680:GLN:N	2.42	0.50
13:m:1029:GLY:C	13:m:1031:VAL:H	2.20	0.50
8:S:1124:MET:O	8:S:1128:LEU:N	2.44	0.50
13:n:4087:ALA:O	13:n:4091:GLY:N	2.43	0.49
13:f:1347:LYS:O	13:f:1349:GLN:N	2.41	0.49
13:n:2228:SER:N	19:n:4702:ATP:O2B	2.43	0.49
13:n:1054:TRP:C	13:n:1056:GLN:H	2.19	0.49
3:J:378:TYR:O	3:J:382:GLY:N	2.46	0.49
13:f:3891:LYS:O	13:f:3895:THR:N	2.46	0.49
21:f:4703:ANP:O1G	21:f:4703:ANP:O2B	2.30	0.48
13:n:315:SER:O	13:n:319:ASP:N	2.43	0.48
13:e:2232:MET:N	19:e:4702:ATP:O1A	2.43	0.48
13:f:3498:ASN:O	13:f:3501:SER:N	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:4087:ALA:O	13:f:4091:GLY:N	2.46	0.48
13:f:315:SER:O	13:f:319:ASP:N	2.47	0.47
1:E:45:VAL:O	1:G:175:ALA:N	2.37	0.47
13:e:2694:ARG:O	13:e:2698:GLN:N	2.48	0.47
14:h:280:ARG:O	14:h:592:GLY:N	2.48	0.47
12:Y:387:ALA:O	12:Y:391:ASP:N	2.47	0.47
16:l:57:VAL:O	16:l:61:ASP:N	2.36	0.47
13:m:2694:ARG:O	13:m:2698:GLN:N	2.48	0.47
13:n:2694:ARG:O	13:n:2698:GLN:N	2.48	0.47
13:f:3498:ASN:O	13:f:3500:MET:N	2.48	0.47
13:m:176:ASP:C	13:m:178:MET:H	2.23	0.47
13:m:3407:LYS:O	13:m:3408:ARG:C	2.58	0.46
14:p:392:THR:N	14:p:395:ALA:O	2.49	0.46
13:f:176:ASP:C	13:f:178:MET:H	2.22	0.46
16:k:83:ASP:N	16:k:86:TYR:O	2.48	0.46
14:o:392:THR:N	14:o:395:ALA:O	2.49	0.46
13:n:1054:TRP:C	13:n:1056:GLN:N	2.73	0.46
13:n:1057:TYR:C	13:n:1059:CYS:H	2.22	0.45
14:g:392:THR:N	14:g:395:ALA:O	2.49	0.45
1:E:298:ILE:O	1:E:331:SER:N	2.46	0.45
9:U:126:GLY:N	9:U:143:ILE:O	2.48	0.45
1:B:330:ILE:N	6:Q:88:TYR:O	2.48	0.45
13:n:3407:LYS:O	13:n:3408:ARG:C	2.59	0.45
13:f:1001:SER:C	13:f:1003:ARG:H	2.24	0.45
4:K:99:ASP:O	4:K:103:LYS:N	2.50	0.44
10:V:27:VAL:N	10:V:46:CYS:O	2.47	0.44
13:m:975:ILE:O	13:m:978:CYS:N	2.50	0.44
1:B:332:ALA:H	6:Q:86:GLY:HA3	1.82	0.44
1:B:318:VAL:O	1:B:322:ALA:N	2.48	0.44
13:e:1057:TYR:C	13:e:1059:CYS:N	2.74	0.44
1:F:200:LYS:O	1:G:117:PRO:CA	2.66	0.44
12:Y:395:ASP:O	12:Y:399:VAL:N	2.48	0.44
6:P:274:ALA:O	6:P:275:LEU:C	2.59	0.43
13:e:1911:GLY:CA	17:e:4701:ADP:C8	3.00	0.43
13:n:176:ASP:C	13:n:178:MET:H	2.25	0.43
1:B:332:ALA:O	6:Q:86:GLY:N	2.52	0.43
13:f:2694:ARG:O	13:f:2698:GLN:N	2.51	0.43
14:g:551:LEU:O	14:g:562:THR:N	2.52	0.43
13:f:3407:LYS:O	13:f:3408:ARG:C	2.59	0.43
16:k:18:GLN:N	16:k:91:ILE:O	2.52	0.43
14:p:551:LEU:O	14:p:562:THR:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o:551:LEU:O	14:o:562:THR:N	2.52	0.43
13:e:3407:LYS:O	13:e:3408:ARG:C	2.59	0.43
6:M:147:LEU:O	6:M:151:LEU:N	2.47	0.42
13:e:1057:TYR:C	13:e:1059:CYS:H	2.27	0.42
7:R:85:GLN:O	7:R:89:ALA:N	2.49	0.42
13:e:456:HIS:O	13:e:460:GLN:N	2.44	0.41
13:e:2943:LYS:O	21:e:4705:ANP:O1B	2.37	0.41
13:n:3378:ASN:C	13:n:3380:GLU:H	2.27	0.41
1:I:298:ILE:O	1:I:331:SER:N	2.53	0.41
1:E:332:ALA:O	6:P:18:ASP:O	2.39	0.41
1:F:290:LEU:O	1:F:291:ARG:C	2.62	0.41
6:P:298:ALA:C	6:P:300:HIS:N	2.79	0.41
13:e:2943:LYS:O	21:e:4705:ANP:O2A	2.38	0.41
13:n:3469:GLU:O	13:n:3470:ALA:C	2.63	0.41
15:i:85:GLY:O	15:i:110:ASP:N	2.48	0.41
13:n:1057:TYR:C	13:n:1059:CYS:N	2.79	0.41
13:e:3410:GLU:O	13:e:3411:PRO:C	2.63	0.41
13:f:1064:GLN:C	13:f:1066:GLU:N	2.78	0.41
13:e:582:PHE:O	13:e:586:SER:N	2.49	0.41
13:m:2943:LYS:O	21:m:4705:ANP:O2A	2.39	0.41
7:R:173:CYS:O	7:R:177:ALA:N	2.46	0.40
15:i:47:ALA:C	15:i:48:ARG:O	2.63	0.40
15:j:46:ARG:O	15:j:47:ALA:C	2.65	0.40
8:S:1118:VAL:O	8:S:1122:ALA:N	2.55	0.40
13:n:2943:LYS:O	21:n:4705:ANP:O2A	2.39	0.40
13:f:1909:GLY:N	17:f:4701:ADP:O1B	2.51	0.40
15:q:46:ARG:O	15:q:47:ALA:C	2.63	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	A	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	B	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	C	373/376 (99%)	362 (97%)	11 (3%)	0	100	100
1	D	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	E	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	F	368/376 (98%)	358 (97%)	10 (3%)	0	100	100
1	G	367/376 (98%)	356 (97%)	11 (3%)	0	100	100
1	I	368/376 (98%)	354 (96%)	14 (4%)	0	100	100
2	H	370/375 (99%)	364 (98%)	6 (2%)	0	100	100
3	J	377/417 (90%)	361 (96%)	16 (4%)	0	100	100
4	K	276/286 (96%)	264 (96%)	12 (4%)	0	100	100
5	L	267/272 (98%)	260 (97%)	7 (3%)	0	100	100
6	M	330/405 (82%)	298 (90%)	30 (9%)	2 (1%)	21	59
6	N	270/405 (67%)	258 (96%)	10 (4%)	2 (1%)	18	56
6	P	335/405 (83%)	305 (91%)	28 (8%)	2 (1%)	21	59
6	Q	319/405 (79%)	302 (95%)	17 (5%)	0	100	100
7	O	168/186 (90%)	154 (92%)	13 (8%)	1 (1%)	21	59
7	R	177/186 (95%)	159 (90%)	15 (8%)	3 (2%)	7	36
8	S	147/1281 (12%)	139 (95%)	7 (5%)	1 (1%)	18	56
8	T	190/1281 (15%)	176 (93%)	13 (7%)	1 (0%)	24	63
9	U	176/190 (93%)	161 (92%)	15 (8%)	0	100	100
10	V	180/182 (99%)	175 (97%)	3 (2%)	2 (1%)	11	46
11	W	205/577 (36%)	205 (100%)	0	0	100	100
11	X	267/577 (46%)	265 (99%)	2 (1%)	0	100	100
11	w	205/577 (36%)	204 (100%)	1 (0%)	0	100	100
11	x	238/577 (41%)	238 (100%)	0	0	100	100
12	Y	373/467 (80%)	352 (94%)	21 (6%)	0	100	100
13	e	4571/4646 (98%)	4476 (98%)	94 (2%)	1 (0%)	100	100
13	f	4571/4646 (98%)	4500 (98%)	65 (1%)	6 (0%)	48	83
13	m	4552/4646 (98%)	4458 (98%)	92 (2%)	2 (0%)	100	100
13	n	4556/4646 (98%)	4464 (98%)	91 (2%)	1 (0%)	100	100
14	g	390/638 (61%)	384 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	h	392/638 (61%)	383 (98%)	9 (2%)	0	100	100
14	o	390/638 (61%)	382 (98%)	8 (2%)	0	100	100
14	p	397/638 (62%)	391 (98%)	6 (2%)	0	100	100
15	i	295/492 (60%)	281 (95%)	13 (4%)	1 (0%)	36	72
15	j	324/492 (66%)	318 (98%)	6 (2%)	0	100	100
15	q	319/492 (65%)	310 (97%)	9 (3%)	0	100	100
15	r	295/492 (60%)	281 (95%)	14 (5%)	0	100	100
16	k	91/96 (95%)	79 (87%)	12 (13%)	0	100	100
16	l	91/96 (95%)	81 (89%)	9 (10%)	1 (1%)	11	46
16	s	91/96 (95%)	84 (92%)	7 (8%)	0	100	100
16	t	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
All	All	29234/35547 (82%)	28458 (97%)	750 (3%)	26 (0%)	49	83

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	217	PRO
6	P	204	PRO
7	R	24	PRO
8	S	1142	PRO
10	V	80	VAL
13	f	203	PRO
13	f	1309	THR
13	f	1348	GLU
13	f	3499	GLN
15	i	48	ARG
13	m	1309	THR
13	e	1309	THR
13	f	1314	GLY
13	n	1309	THR
6	P	299	LYS
13	m	976	GLU
6	N	158	LYS
6	N	163	ASP
7	R	61	ILE
7	R	69	ASP
16	l	82	PRO
7	O	69	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	f	3498	ASN
6	M	166	ILE
8	T	1147	PRO
10	V	79	GLY

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 43 ligands modelled in this entry, 17 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	ADP	m	4701	-	28,29,29	1.37	4 (14%)	43,45,45	1.95	10 (23%)
17	ADP	F	802	18	28,29,29	0.51	0	43,45,45	0.55	0
21	ANP	f	4703	-	33,33,33	0.83	2 (6%)	45,52,52	0.74	2 (4%)
17	ADP	n	4701	-	28,29,29	1.37	4 (14%)	43,45,45	1.95	10 (23%)
19	ATP	f	4702	18	32,33,33	0.68	0	48,52,52	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	ANP	m	4704	-	33,33,33	0.92	4 (12%)	45,52,52	0.64	0
21	ANP	m	4705	-	33,33,33	0.92	4 (12%)	45,52,52	0.63	0
21	ANP	n	4704	-	33,33,33	0.92	4 (12%)	45,52,52	0.64	0
21	ANP	n	4705	-	33,33,33	0.92	4 (12%)	45,52,52	0.63	0
17	ADP	I	800	18	28,29,29	0.47	0	43,45,45	0.57	0
17	ADP	f	4701	-	28,29,29	1.37	4 (14%)	43,45,45	1.95	10 (23%)
17	ADP	D	800	18	28,29,29	1.35	4 (14%)	43,45,45	1.88	11 (25%)
19	ATP	m	4702	18	32,33,33	0.65	2 (6%)	48,52,52	0.72	0
19	ATP	J	800	18	32,33,33	0.54	0	48,52,52	0.59	0
17	ADP	C	800	18	28,29,29	1.36	5 (17%)	43,45,45	1.85	11 (25%)
17	ADP	E	800	18	28,29,29	1.36	4 (14%)	43,45,45	1.85	11 (25%)
17	ADP	B	800	18	28,29,29	1.35	4 (14%)	43,45,45	1.87	11 (25%)
19	ATP	n	4702	18	32,33,33	0.66	2 (6%)	48,52,52	0.72	0
19	ATP	e	4702	18	32,33,33	0.65	1 (3%)	48,52,52	0.72	0
21	ANP	e	4705	-	33,33,33	0.92	4 (12%)	45,52,52	0.63	0
21	ANP	e	4704	-	33,33,33	0.92	4 (12%)	45,52,52	0.64	0
17	ADP	e	4701	-	28,29,29	1.37	4 (14%)	43,45,45	1.95	10 (23%)
17	ADP	H	800	18	28,29,29	0.47	0	43,45,45	0.55	0
17	ADP	A	800	18	28,29,29	1.38	5 (17%)	43,45,45	1.86	10 (23%)
21	ANP	f	4705	-	33,33,33	0.91	4 (12%)	45,52,52	0.64	0
17	ADP	G	800	18	28,29,29	0.52	0	43,45,45	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	m	4701	-	-	5/16/32/32	0/3/3/3
17	ADP	F	802	18	-	0/16/32/32	0/3/3/3
21	ANP	f	4703	-	-	5/18/38/38	0/3/3/3
17	ADP	n	4701	-	-	5/16/32/32	0/3/3/3
19	ATP	f	4702	18	-	2/22/38/38	0/3/3/3
21	ANP	m	4704	-	-	7/18/38/38	0/3/3/3
21	ANP	m	4705	-	-	5/18/38/38	0/3/3/3
21	ANP	n	4704	-	-	7/18/38/38	0/3/3/3
21	ANP	n	4705	-	-	5/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	I	800	18	-	0/16/32/32	0/3/3/3
17	ADP	f	4701	-	-	5/16/32/32	0/3/3/3
17	ADP	D	800	18	-	3/16/32/32	0/3/3/3
19	ATP	m	4702	18	-	2/22/38/38	0/3/3/3
19	ATP	J	800	18	-	2/22/38/38	0/3/3/3
17	ADP	C	800	18	-	3/16/32/32	0/3/3/3
17	ADP	E	800	18	-	3/16/32/32	0/3/3/3
17	ADP	B	800	18	-	0/16/32/32	0/3/3/3
19	ATP	n	4702	18	-	2/22/38/38	0/3/3/3
19	ATP	e	4702	18	-	2/22/38/38	0/3/3/3
21	ANP	e	4705	-	-	5/18/38/38	0/3/3/3
21	ANP	e	4704	-	-	7/18/38/38	0/3/3/3
17	ADP	e	4701	-	-	5/16/32/32	0/3/3/3
17	ADP	H	800	18	-	0/16/32/32	0/3/3/3
17	ADP	A	800	18	-	0/16/32/32	0/3/3/3
21	ANP	f	4705	-	-	7/18/38/38	0/3/3/3
17	ADP	G	800	18	-	0/16/32/32	0/3/3/3

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	800	ADP	C5-C4	4.45	1.47	1.39
17	E	800	ADP	C5-C4	4.43	1.47	1.39
17	C	800	ADP	C5-C4	4.42	1.47	1.39
17	n	4701	ADP	C5-C4	4.42	1.47	1.39
17	B	800	ADP	C5-C4	4.42	1.47	1.39
17	m	4701	ADP	C5-C4	4.41	1.47	1.39
17	f	4701	ADP	C5-C4	4.41	1.47	1.39
17	D	800	ADP	C5-C4	4.40	1.46	1.39
17	e	4701	ADP	C5-C4	4.38	1.46	1.39
21	f	4703	ANP	PG-O1G	2.70	1.50	1.46
17	A	800	ADP	C5-C6	2.66	1.48	1.41
21	n	4704	ANP	PB-O3A	-2.61	1.55	1.59
21	m	4704	ANP	PB-O3A	-2.61	1.55	1.59
21	e	4704	ANP	PB-O3A	-2.60	1.55	1.59
21	f	4705	ANP	PB-O3A	-2.57	1.55	1.59
17	D	800	ADP	C5-C6	2.56	1.48	1.41
17	C	800	ADP	C5-C6	2.55	1.48	1.41
17	B	800	ADP	C5-C6	2.54	1.48	1.41
19	n	4702	ATP	PB-O3B	-2.54	1.56	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	800	ADP	C5-C6	2.53	1.48	1.41
21	f	4705	ANP	PG-O1G	2.53	1.50	1.46
19	m	4702	ATP	PB-O3B	-2.51	1.56	1.59
19	e	4702	ATP	PB-O3B	-2.50	1.56	1.59
21	e	4705	ANP	PG-O1G	2.50	1.50	1.46
17	C	800	ADP	C5-N7	-2.50	1.34	1.39
21	n	4704	ANP	PG-O1G	2.49	1.50	1.46
21	m	4704	ANP	PG-O1G	2.49	1.50	1.46
21	m	4705	ANP	PG-O1G	2.49	1.50	1.46
17	n	4701	ADP	C5-N7	-2.48	1.34	1.39
21	n	4705	ANP	PG-O1G	2.47	1.49	1.46
17	e	4701	ADP	C5-N7	-2.47	1.34	1.39
21	e	4704	ANP	PG-O1G	2.47	1.49	1.46
17	f	4701	ADP	C5-C6	2.47	1.47	1.41
21	e	4705	ANP	PB-O3A	-2.46	1.56	1.59
17	e	4701	ADP	C5-C6	2.46	1.47	1.41
21	m	4705	ANP	PB-O3A	-2.46	1.56	1.59
17	m	4701	ADP	C5-C6	2.46	1.47	1.41
17	E	800	ADP	C5-N7	-2.46	1.34	1.39
17	f	4701	ADP	C5-N7	-2.45	1.34	1.39
17	n	4701	ADP	C5-C6	2.45	1.47	1.41
21	n	4705	ANP	PB-O3A	-2.44	1.56	1.59
17	m	4701	ADP	C5-N7	-2.44	1.34	1.39
17	A	800	ADP	C5-N7	-2.38	1.34	1.39
21	f	4703	ANP	PB-O2B	-2.37	1.50	1.56
17	B	800	ADP	C5-N7	-2.36	1.34	1.39
21	e	4704	ANP	PG-N3B	2.36	1.69	1.63
17	D	800	ADP	C5-N7	-2.35	1.34	1.39
21	n	4704	ANP	PG-N3B	2.33	1.69	1.63
21	m	4704	ANP	PG-N3B	2.33	1.69	1.63
21	f	4705	ANP	PG-N3B	2.32	1.69	1.63
17	A	800	ADP	C8-N7	2.32	1.36	1.31
21	m	4705	ANP	PB-O1B	2.32	1.49	1.46
21	e	4705	ANP	PB-O1B	2.31	1.49	1.46
21	n	4705	ANP	PB-O1B	2.30	1.49	1.46
21	n	4705	ANP	PG-N3B	2.29	1.69	1.63
21	e	4705	ANP	PG-N3B	2.29	1.69	1.63
17	C	800	ADP	C8-N7	2.28	1.36	1.31
17	B	800	ADP	C8-N7	2.28	1.36	1.31
21	m	4705	ANP	PG-N3B	2.27	1.69	1.63
17	D	800	ADP	C8-N7	2.26	1.36	1.31
17	E	800	ADP	C8-N7	2.25	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	n	4701	ADP	C8-N7	2.17	1.35	1.31
17	m	4701	ADP	C8-N7	2.17	1.35	1.31
17	f	4701	ADP	C8-N7	2.16	1.35	1.31
17	e	4701	ADP	C8-N7	2.14	1.35	1.31
21	e	4704	ANP	PB-O1B	2.14	1.49	1.46
17	A	800	ADP	C4-N9	-2.11	1.33	1.37
21	m	4704	ANP	PB-O1B	2.10	1.49	1.46
21	n	4704	ANP	PB-O1B	2.09	1.49	1.46
17	C	800	ADP	C4-N9	-2.09	1.33	1.37
21	f	4705	ANP	PB-O1B	2.07	1.49	1.46
19	n	4702	ATP	PA-O3A	-2.05	1.57	1.59
19	m	4702	ATP	PA-O3A	-2.01	1.57	1.59

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	m	4701	ADP	C5-C4-N3	-6.00	118.46	126.72
17	f	4701	ADP	C5-C4-N3	-5.98	118.48	126.72
17	e	4701	ADP	C5-C4-N3	-5.98	118.48	126.72
17	n	4701	ADP	C5-C4-N3	-5.97	118.50	126.72
17	D	800	ADP	C5-C4-N3	-5.74	118.81	126.72
17	E	800	ADP	C5-C4-N3	-5.72	118.84	126.72
17	B	800	ADP	C5-C4-N3	-5.71	118.85	126.72
17	A	800	ADP	C5-C4-N3	-5.68	118.89	126.72
17	C	800	ADP	C5-C4-N3	-5.66	118.93	126.72
17	f	4701	ADP	N3-C4-N9	4.99	135.66	127.17
17	m	4701	ADP	N3-C4-N9	4.99	135.65	127.17
17	n	4701	ADP	N3-C4-N9	4.98	135.64	127.17
17	e	4701	ADP	N3-C4-N9	4.97	135.62	127.17
17	E	800	ADP	N3-C4-N9	4.62	135.02	127.17
17	B	800	ADP	N3-C4-N9	4.54	134.88	127.17
17	D	800	ADP	N3-C4-N9	4.53	134.88	127.17
17	C	800	ADP	N3-C4-N9	4.49	134.79	127.17
17	A	800	ADP	N3-C4-N9	4.39	134.63	127.17
17	n	4701	ADP	C2-N3-C4	3.86	121.25	111.83
17	m	4701	ADP	C2-N3-C4	3.85	121.24	111.83
17	e	4701	ADP	C2-N3-C4	3.85	121.24	111.83
17	f	4701	ADP	C2-N3-C4	3.85	121.22	111.83
17	D	800	ADP	C2-N3-C4	3.82	121.17	111.83
17	B	800	ADP	C2-N3-C4	3.79	121.09	111.83
17	A	800	ADP	C2-N3-C4	3.77	121.04	111.83
17	E	800	ADP	C2-N3-C4	3.75	120.98	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	n	4701	ADP	N3-C2-N1	-3.72	122.95	128.58
17	C	800	ADP	C2-N3-C4	3.71	120.89	111.83
17	e	4701	ADP	N3-C2-N1	-3.70	122.98	128.58
17	f	4701	ADP	N3-C2-N1	-3.69	123.00	128.58
17	m	4701	ADP	N3-C2-N1	-3.69	123.00	128.58
17	D	800	ADP	N3-C2-N1	-3.66	123.04	128.58
17	A	800	ADP	C4-C5-N7	-3.60	106.47	110.58
17	B	800	ADP	N3-C2-N1	-3.58	123.16	128.58
17	E	800	ADP	N3-C2-N1	-3.52	123.25	128.58
17	D	800	ADP	C4-C5-N7	-3.50	106.58	110.58
17	A	800	ADP	N3-C2-N1	-3.49	123.31	128.58
17	C	800	ADP	N3-C2-N1	-3.48	123.31	128.58
17	B	800	ADP	C4-C5-N7	-3.45	106.64	110.58
17	C	800	ADP	C4-C5-N7	-3.40	106.69	110.58
17	E	800	ADP	C4-C5-N7	-3.39	106.70	110.58
17	n	4701	ADP	C4-C5-N7	-3.25	106.86	110.58
17	e	4701	ADP	C4-C5-N7	-3.25	106.86	110.58
17	m	4701	ADP	C4-C5-N7	-3.25	106.86	110.58
17	f	4701	ADP	C4-C5-N7	-3.23	106.89	110.58
17	n	4701	ADP	C4-N9-C8	3.04	108.93	105.74
17	m	4701	ADP	C4-N9-C8	3.03	108.92	105.74
17	f	4701	ADP	C4-N9-C8	3.01	108.90	105.74
17	e	4701	ADP	C4-N9-C8	3.00	108.89	105.74
17	E	800	ADP	C4-N9-C8	2.94	108.83	105.74
17	B	800	ADP	C4-N9-C8	2.87	108.75	105.74
17	D	800	ADP	C4-N9-C8	2.87	108.75	105.74
17	C	800	ADP	C4-N9-C8	2.86	108.74	105.74
17	A	800	ADP	C4-N9-C8	2.84	108.72	105.74
17	A	800	ADP	C5-N7-C8	2.73	107.74	103.45
17	D	800	ADP	C5-N7-C8	2.69	107.68	103.45
17	e	4701	ADP	C5-N7-C8	2.68	107.66	103.45
17	n	4701	ADP	C5-N7-C8	2.68	107.66	103.45
17	E	800	ADP	C5-N7-C8	2.67	107.65	103.45
17	m	4701	ADP	C5-N7-C8	2.67	107.64	103.45
17	B	800	ADP	C5-N7-C8	2.67	107.64	103.45
17	f	4701	ADP	C5-N7-C8	2.65	107.61	103.45
17	C	800	ADP	C5-N7-C8	2.64	107.59	103.45
21	f	4703	ANP	O2G-PG-O1G	-2.63	106.86	113.45
17	B	800	ADP	C3'-C2'-C1'	2.39	105.98	101.46
17	e	4701	ADP	C3'-C2'-C1'	2.38	105.96	101.46
17	m	4701	ADP	C3'-C2'-C1'	2.37	105.95	101.46
17	n	4701	ADP	C3'-C2'-C1'	2.37	105.94	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	800	ADP	N9-C8-N7	-2.36	110.59	113.94
21	f	4703	ANP	O3G-PG-O1G	-2.36	107.54	113.45
17	f	4701	ADP	C3'-C2'-C1'	2.36	105.92	101.46
17	C	800	ADP	C3'-C2'-C1'	2.31	105.84	101.46
17	E	800	ADP	N9-C8-N7	-2.30	110.67	113.94
17	D	800	ADP	N9-C8-N7	-2.29	110.68	113.94
17	m	4701	ADP	N9-C8-N7	-2.29	110.69	113.94
17	e	4701	ADP	N9-C8-N7	-2.29	110.69	113.94
17	n	4701	ADP	N9-C8-N7	-2.29	110.69	113.94
17	C	800	ADP	N9-C8-N7	-2.29	110.69	113.94
17	D	800	ADP	C3'-C2'-C1'	2.28	105.78	101.46
17	B	800	ADP	N9-C8-N7	-2.28	110.70	113.94
17	f	4701	ADP	N9-C8-N7	-2.26	110.73	113.94
17	E	800	ADP	C3'-C2'-C1'	2.26	105.73	101.46
17	A	800	ADP	C6-C5-N7	2.25	136.43	132.09
17	B	800	ADP	C6-C5-N7	2.17	136.27	132.09
17	D	800	ADP	C6-C5-N7	2.16	136.26	132.09
17	C	800	ADP	C6-C5-N7	2.10	136.14	132.09
17	A	800	ADP	C3'-C2'-C1'	2.09	105.42	101.46
17	C	800	ADP	C2-N1-C6	2.06	122.12	118.73
17	E	800	ADP	C6-C5-N7	2.05	136.04	132.09
17	f	4701	ADP	C2'-C3'-C4'	2.04	106.55	102.61
17	m	4701	ADP	C2'-C3'-C4'	2.03	106.54	102.61
17	D	800	ADP	C2-N1-C6	2.03	122.06	118.73
17	B	800	ADP	C2-N1-C6	2.03	122.06	118.73
17	E	800	ADP	C2-N1-C6	2.02	122.05	118.73
17	e	4701	ADP	C2'-C3'-C4'	2.02	106.51	102.61
17	n	4701	ADP	C2'-C3'-C4'	2.02	106.51	102.61

There are no chirality outliers.

All (87) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	e	4701	ADP	C5'-O5'-PA-O3A
17	f	4701	ADP	PA-O3A-PB-O2B
17	f	4701	ADP	C5'-O5'-PA-O2A
17	f	4701	ADP	C5'-O5'-PA-O3A
17	m	4701	ADP	PA-O3A-PB-O2B
17	m	4701	ADP	C5'-O5'-PA-O2A
17	m	4701	ADP	C5'-O5'-PA-O3A
17	n	4701	ADP	PA-O3A-PB-O2B
17	n	4701	ADP	C5'-O5'-PA-O2A
17	n	4701	ADP	C5'-O5'-PA-O3A
19	e	4702	ATP	PB-O3B-PG-O2G
19	f	4702	ATP	PB-O3B-PG-O2G
19	f	4702	ATP	PB-O3B-PG-O3G
19	m	4702	ATP	PB-O3B-PG-O2G
19	n	4702	ATP	PB-O3B-PG-O2G
21	e	4704	ANP	PG-N3B-PB-O1B
21	e	4704	ANP	PG-N3B-PB-O3A
21	e	4705	ANP	PB-N3B-PG-O1G
21	e	4705	ANP	PG-N3B-PB-O1B
21	e	4705	ANP	C5'-O5'-PA-O1A
21	e	4705	ANP	C5'-O5'-PA-O3A
21	f	4703	ANP	PB-N3B-PG-O1G
21	f	4703	ANP	PG-N3B-PB-O1B
21	f	4703	ANP	C5'-O5'-PA-O1A
21	f	4703	ANP	C5'-O5'-PA-O3A
21	f	4705	ANP	PG-N3B-PB-O1B
21	f	4705	ANP	PG-N3B-PB-O3A
21	m	4704	ANP	PG-N3B-PB-O1B
21	m	4704	ANP	PG-N3B-PB-O3A
21	m	4705	ANP	PB-N3B-PG-O1G
21	m	4705	ANP	PG-N3B-PB-O1B
21	m	4705	ANP	C5'-O5'-PA-O1A
21	m	4705	ANP	C5'-O5'-PA-O3A
21	n	4704	ANP	PG-N3B-PB-O1B
21	n	4704	ANP	PG-N3B-PB-O3A
21	n	4705	ANP	PB-N3B-PG-O1G
21	n	4705	ANP	PG-N3B-PB-O1B
21	n	4705	ANP	C5'-O5'-PA-O1A
21	n	4705	ANP	C5'-O5'-PA-O3A
21	e	4704	ANP	O4'-C4'-C5'-O5'
21	f	4705	ANP	O4'-C4'-C5'-O5'
21	m	4704	ANP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	n	4704	ANP	O4'-C4'-C5'-O5'
19	J	800	ATP	PB-O3B-PG-O1G
19	J	800	ATP	PB-O3B-PG-O2G
19	e	4702	ATP	PB-O3B-PG-O3G
19	m	4702	ATP	PB-O3B-PG-O3G
19	n	4702	ATP	PB-O3B-PG-O3G
21	e	4704	ANP	C3'-C4'-C5'-O5'
21	f	4705	ANP	C3'-C4'-C5'-O5'
21	m	4704	ANP	C3'-C4'-C5'-O5'
21	n	4704	ANP	C3'-C4'-C5'-O5'
17	C	800	ADP	C5'-O5'-PA-O2A
17	D	800	ADP	C5'-O5'-PA-O2A
17	e	4701	ADP	C5'-O5'-PA-O1A
17	f	4701	ADP	C5'-O5'-PA-O1A
17	m	4701	ADP	C5'-O5'-PA-O1A
17	n	4701	ADP	C5'-O5'-PA-O1A
21	e	4704	ANP	C5'-O5'-PA-O1A
21	e	4704	ANP	C5'-O5'-PA-O2A
21	e	4704	ANP	C5'-O5'-PA-O3A
21	e	4705	ANP	C5'-O5'-PA-O2A
21	f	4703	ANP	C5'-O5'-PA-O2A
21	f	4705	ANP	C5'-O5'-PA-O1A
21	f	4705	ANP	C5'-O5'-PA-O2A
21	f	4705	ANP	C5'-O5'-PA-O3A
21	m	4704	ANP	C5'-O5'-PA-O1A
21	m	4704	ANP	C5'-O5'-PA-O2A
21	m	4704	ANP	C5'-O5'-PA-O3A
21	m	4705	ANP	C5'-O5'-PA-O2A
21	n	4704	ANP	C5'-O5'-PA-O1A
21	n	4704	ANP	C5'-O5'-PA-O2A
21	n	4704	ANP	C5'-O5'-PA-O3A
21	n	4705	ANP	C5'-O5'-PA-O2A
17	e	4701	ADP	PA-O3A-PB-O1B
17	f	4701	ADP	PA-O3A-PB-O1B
17	m	4701	ADP	PA-O3A-PB-O1B
17	n	4701	ADP	PA-O3A-PB-O1B

There are no ring outliers.

9 monomers are involved in 15 short contacts:

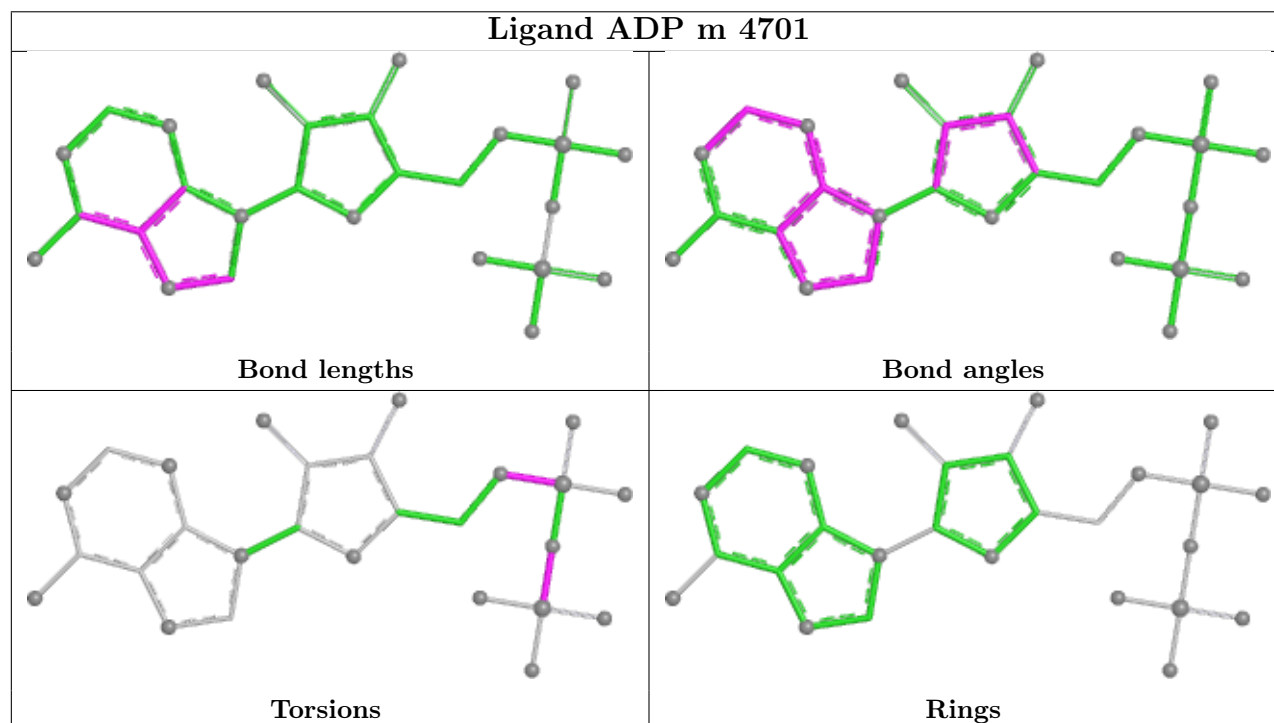
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	f	4703	ANP	1	0

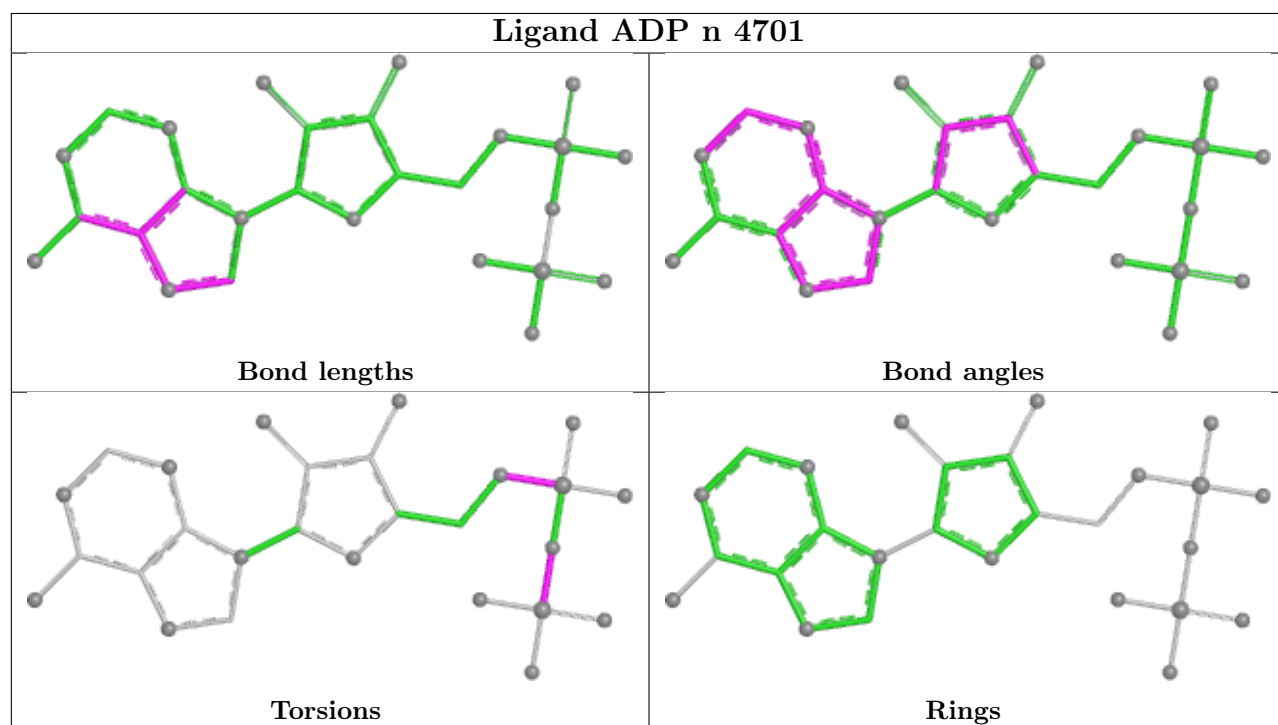
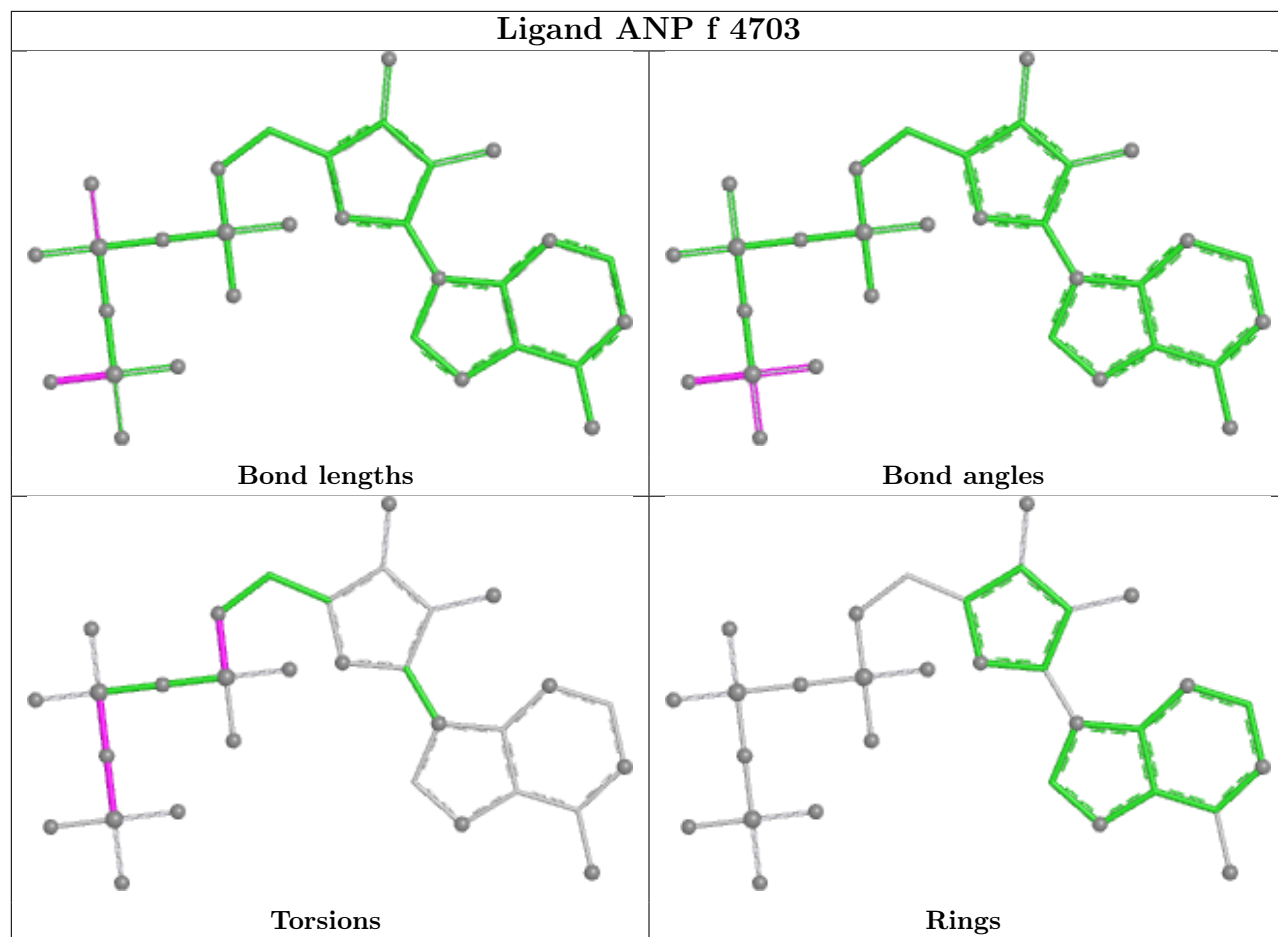
Continued on next page...

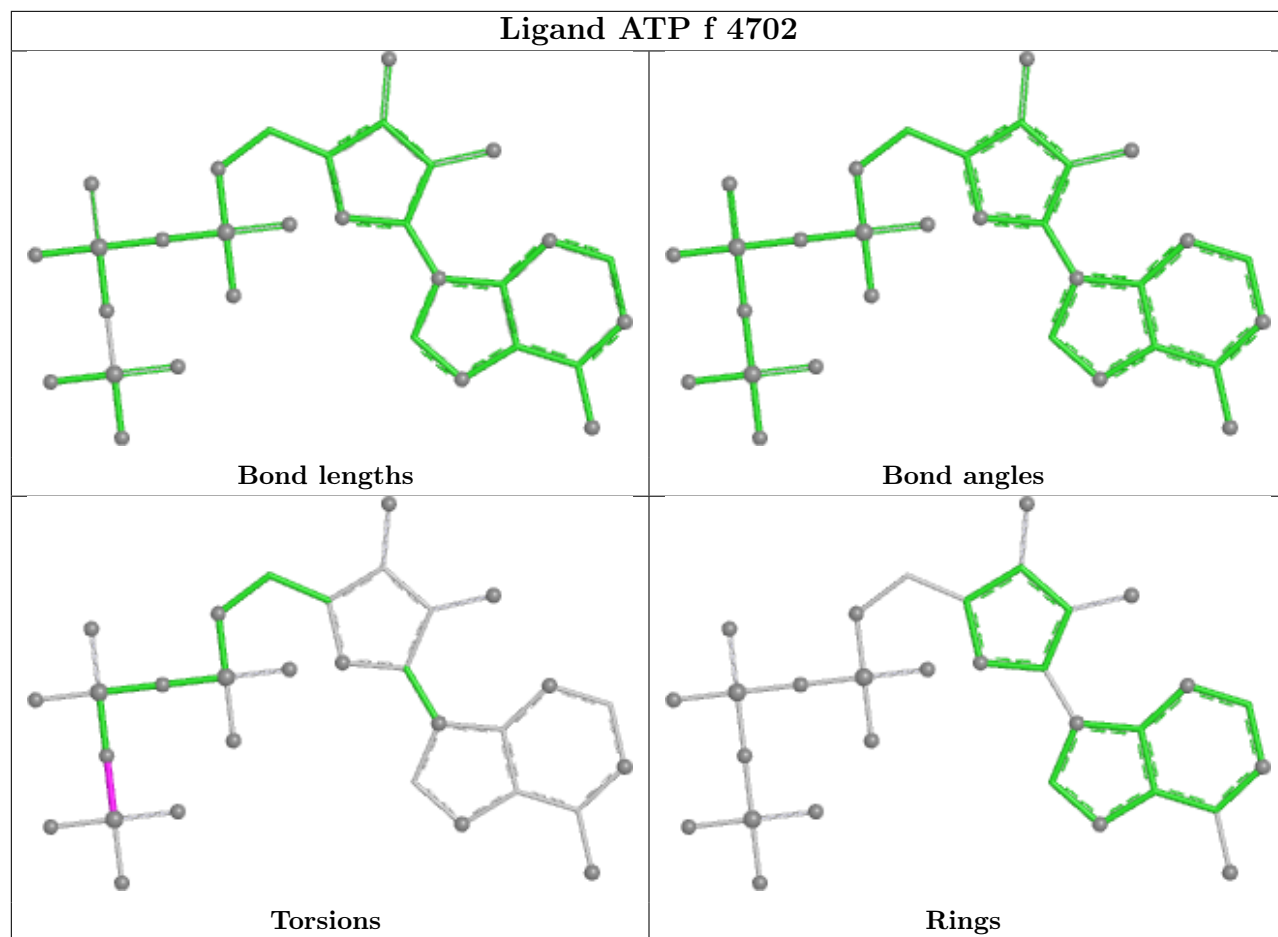
Continued from previous page...

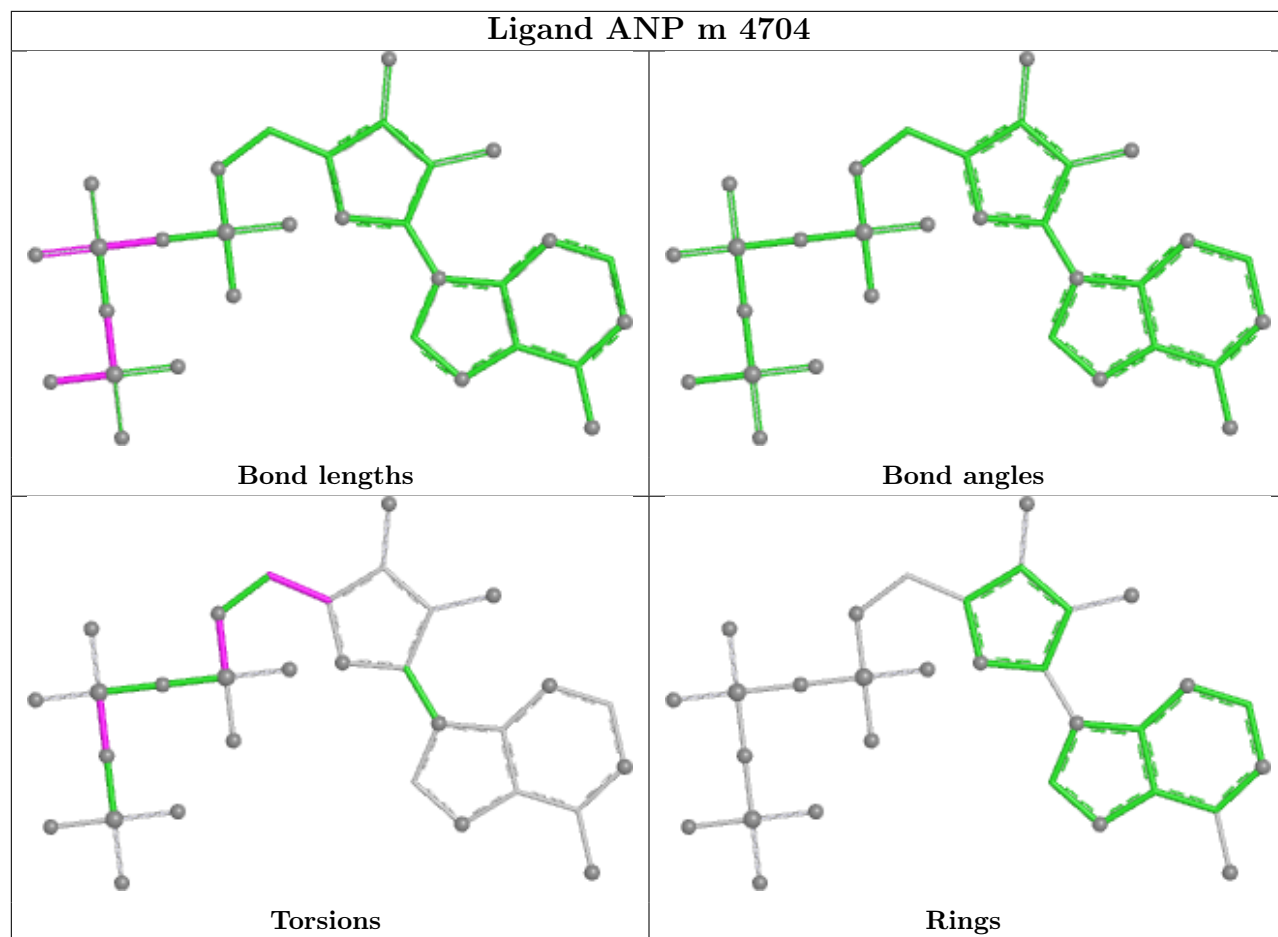
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	n	4701	ADP	1	0
21	m	4705	ANP	2	0
21	n	4705	ANP	2	0
17	f	4701	ADP	2	0
19	n	4702	ATP	2	0
19	e	4702	ATP	1	0
21	e	4705	ANP	3	0
17	e	4701	ADP	1	0

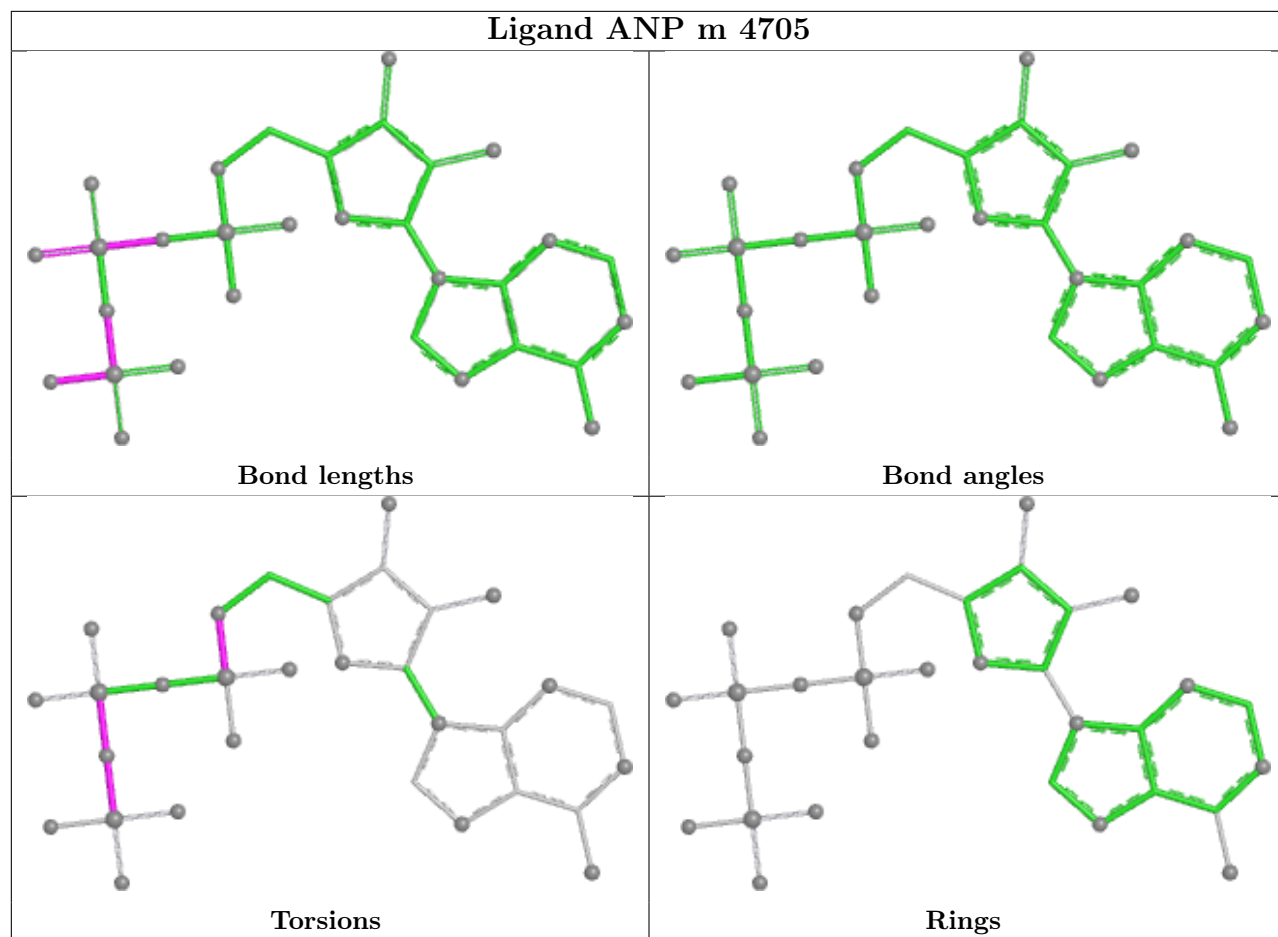
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

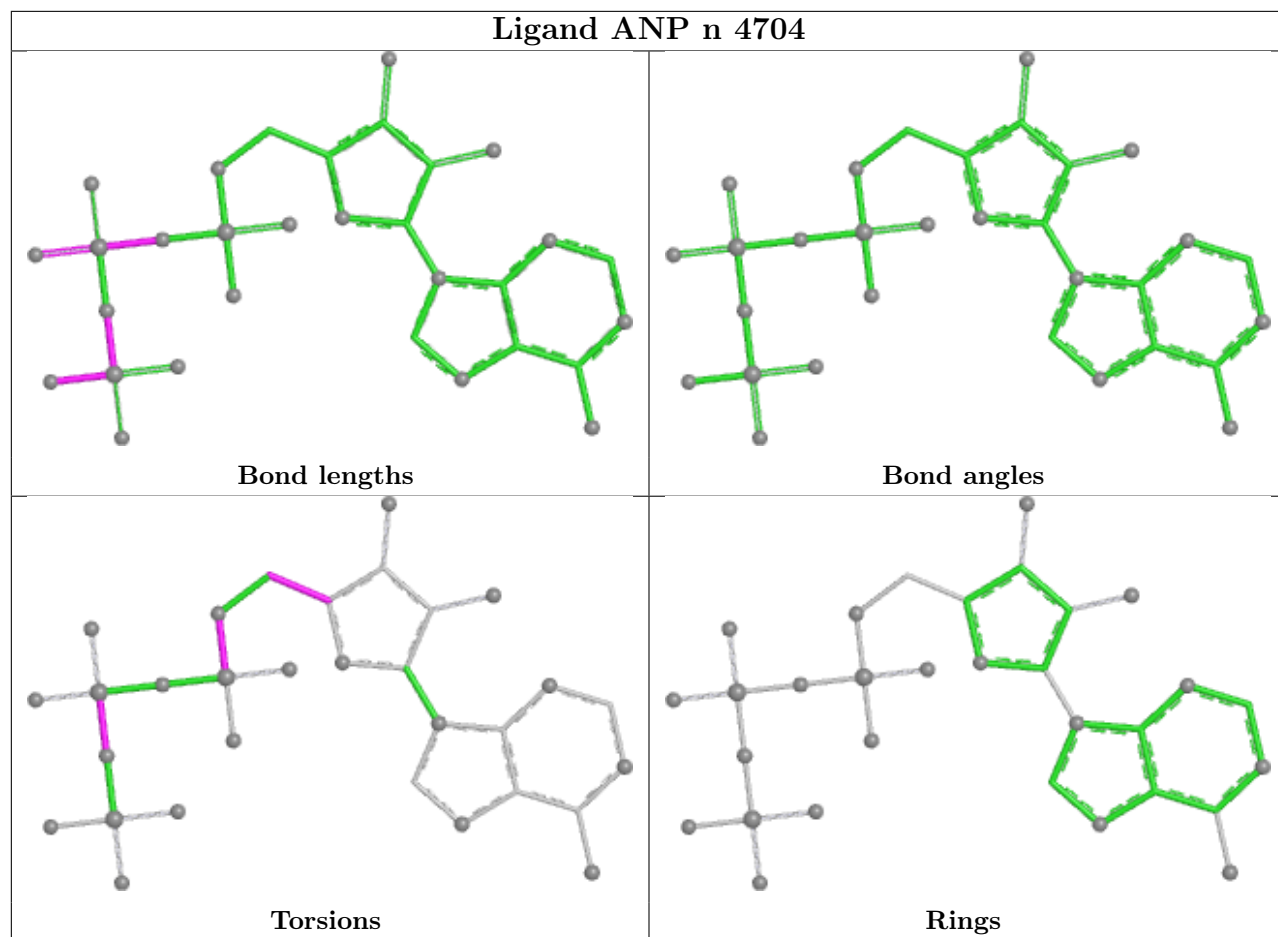


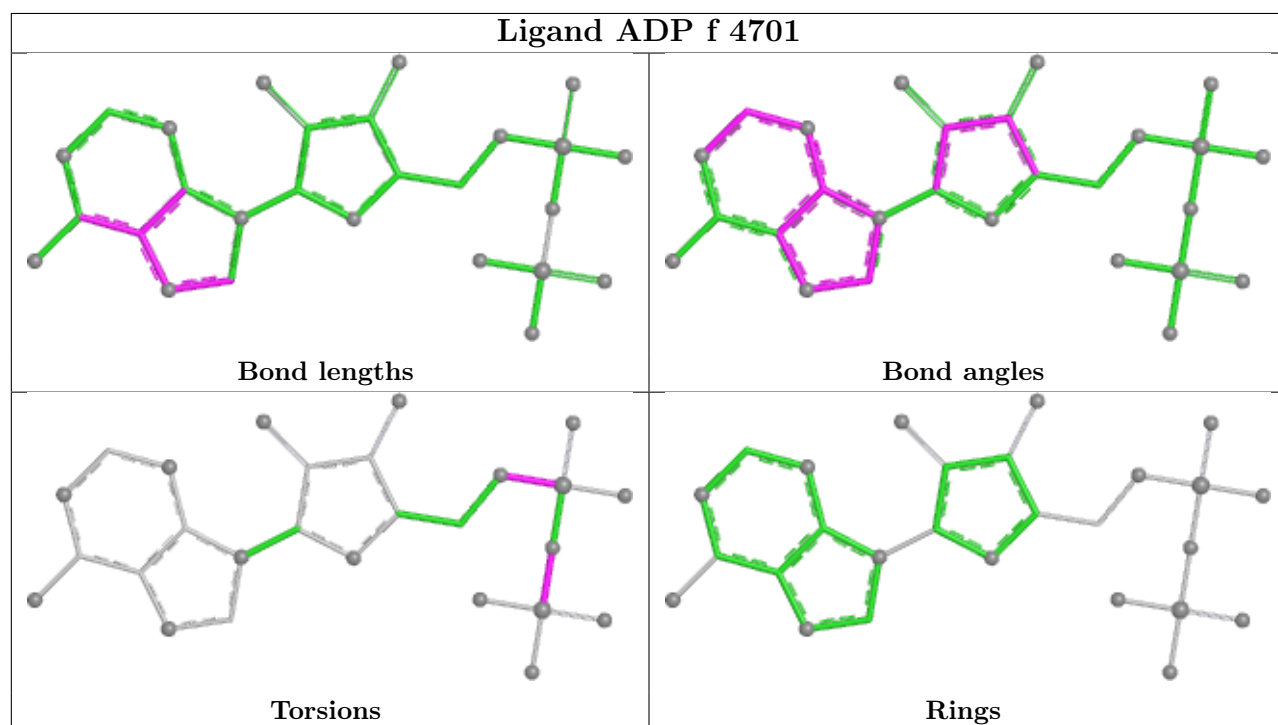
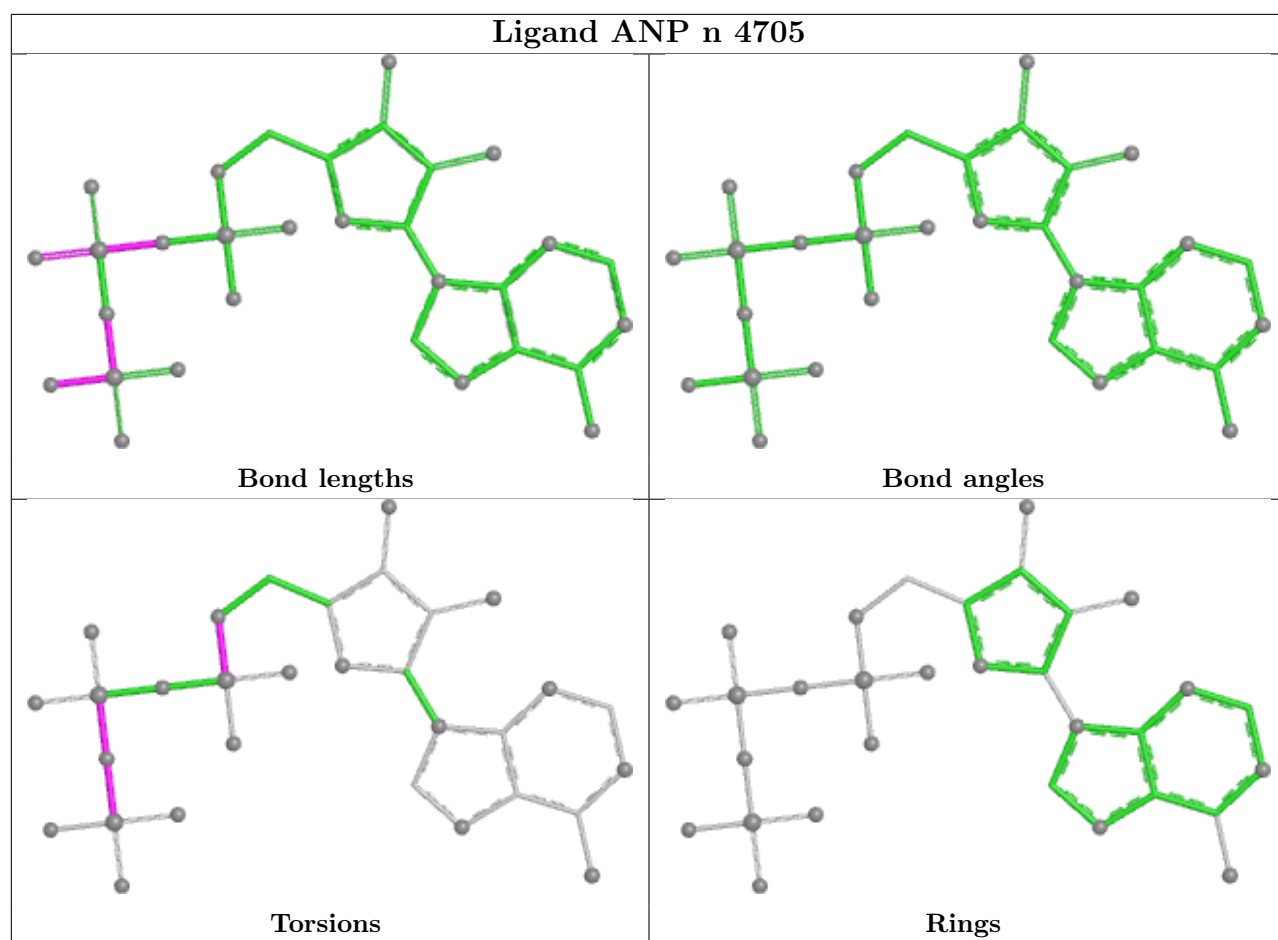


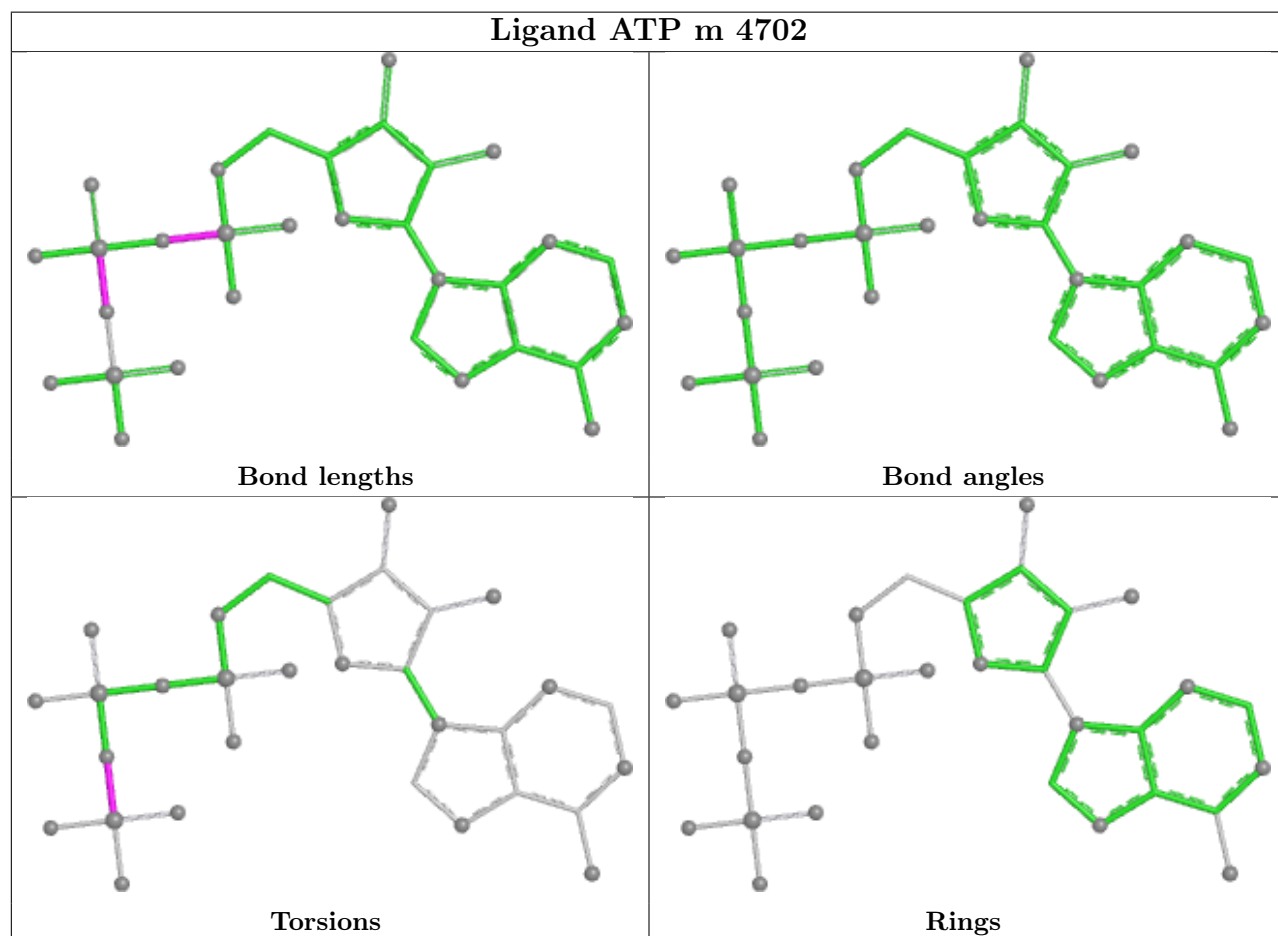
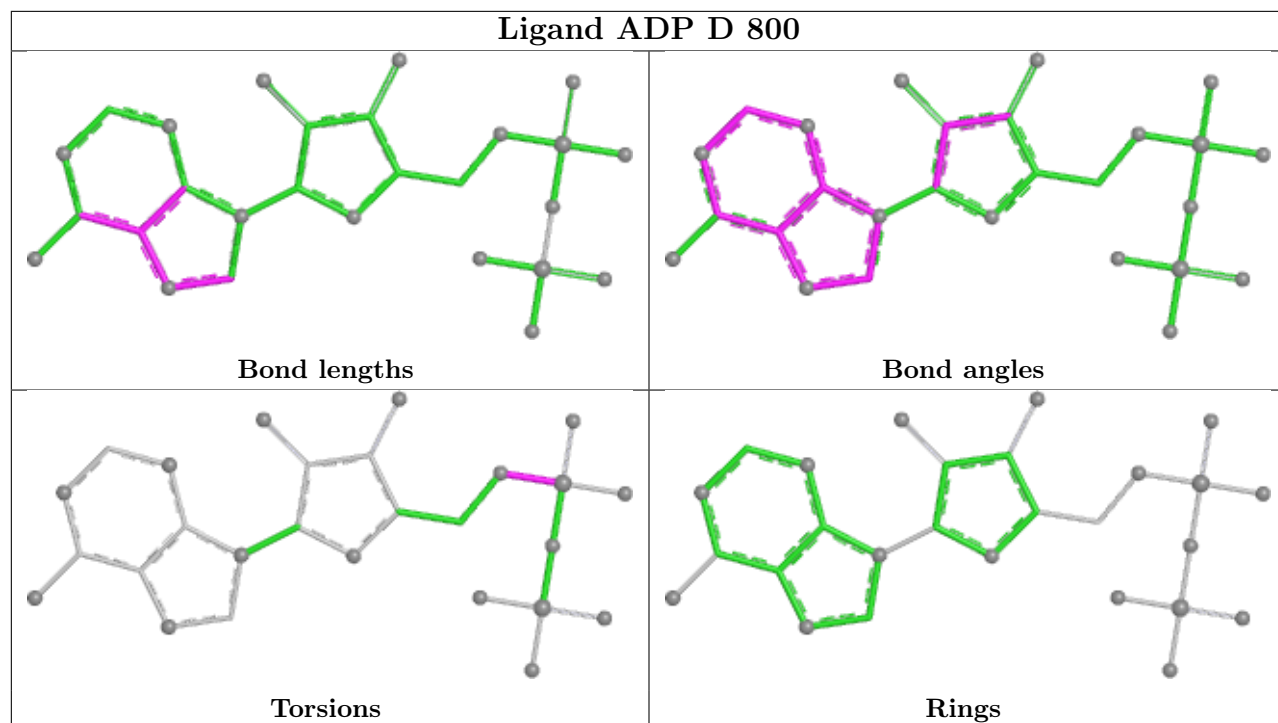




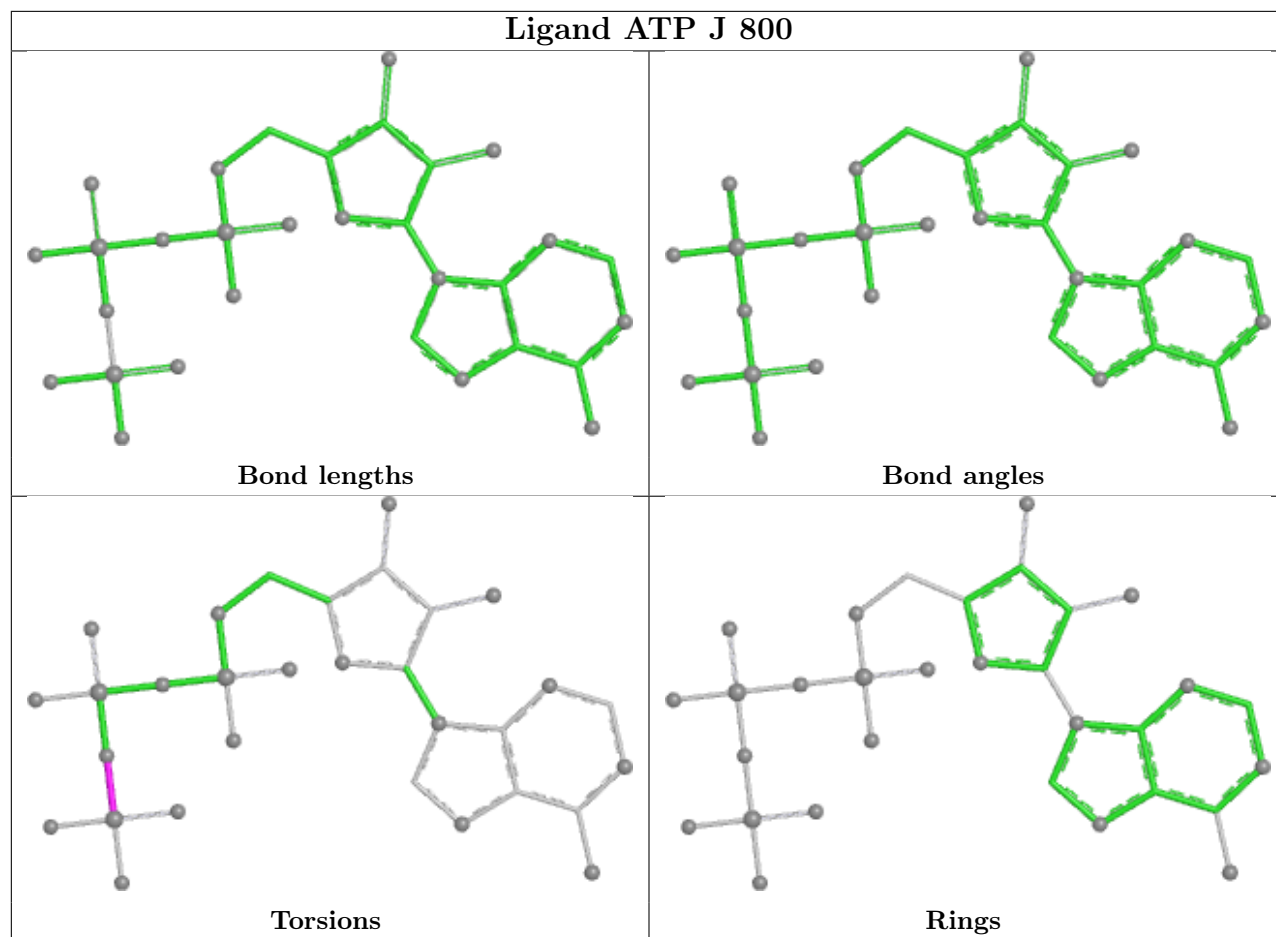




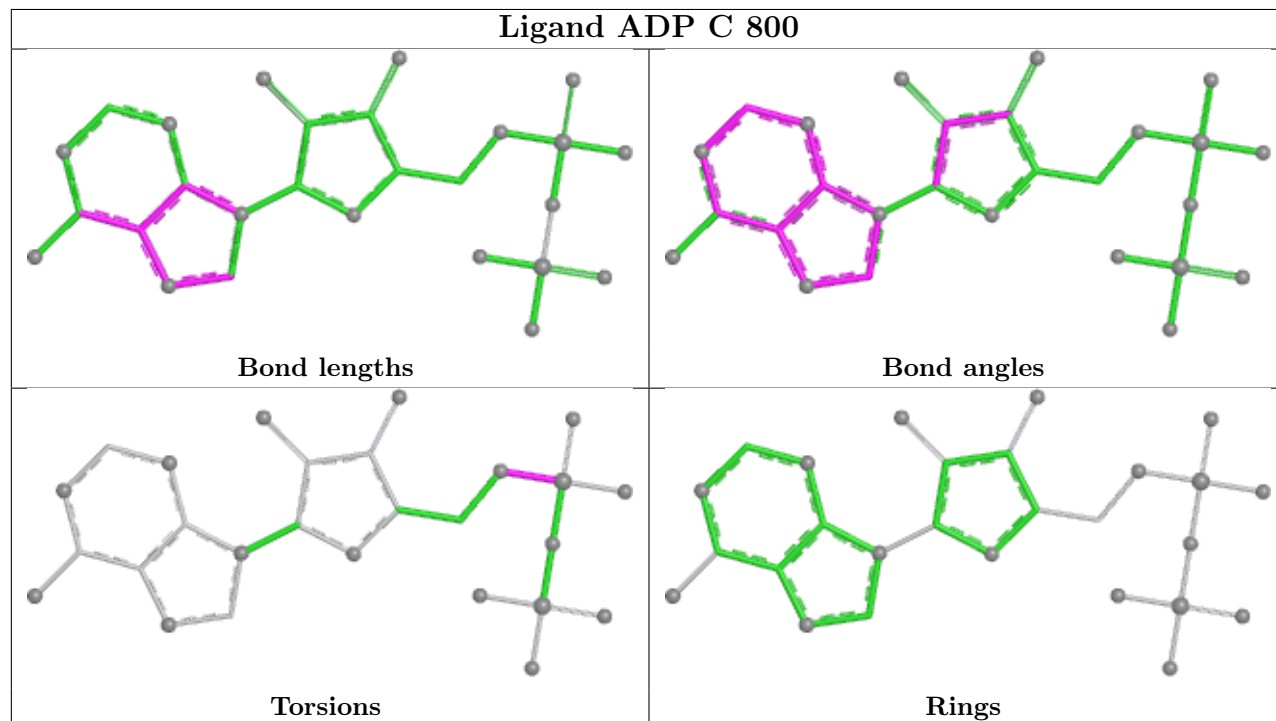


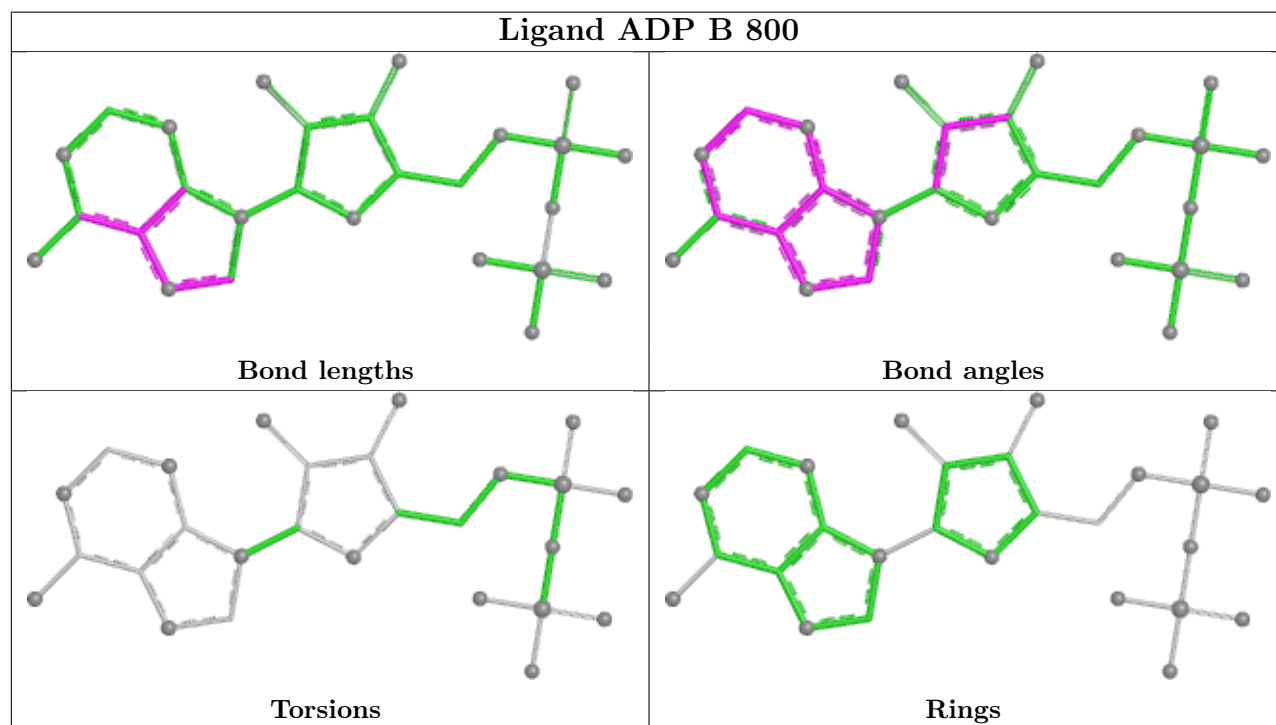
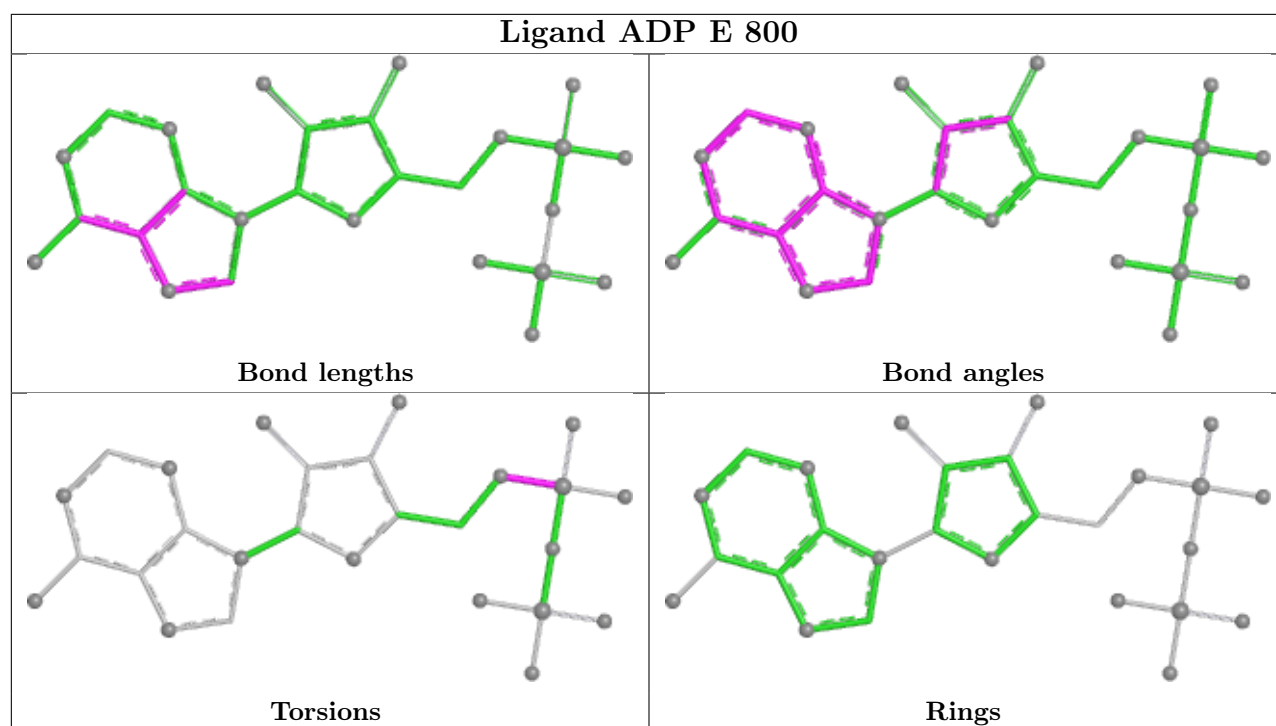


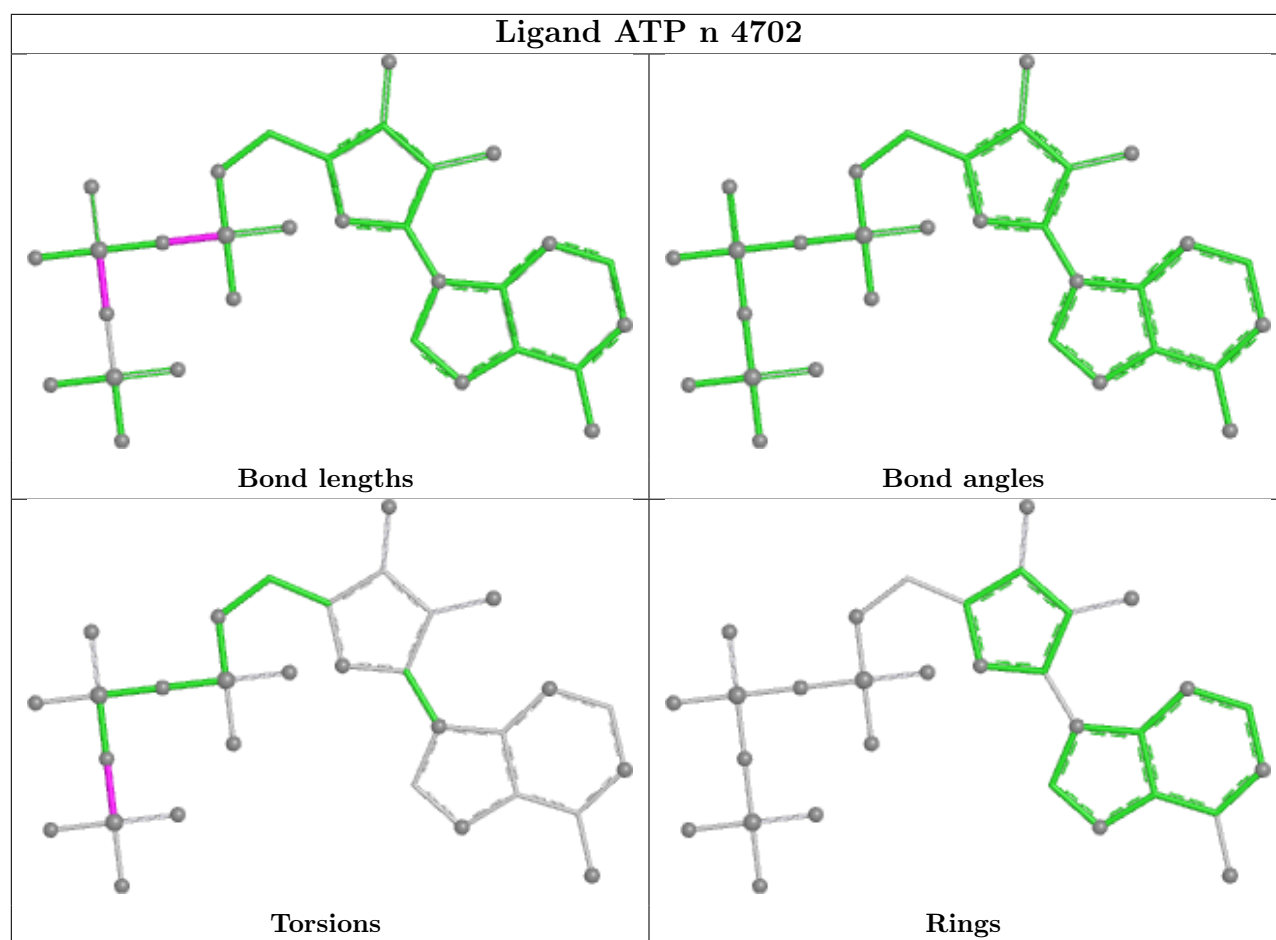
Ligand ATP J 800

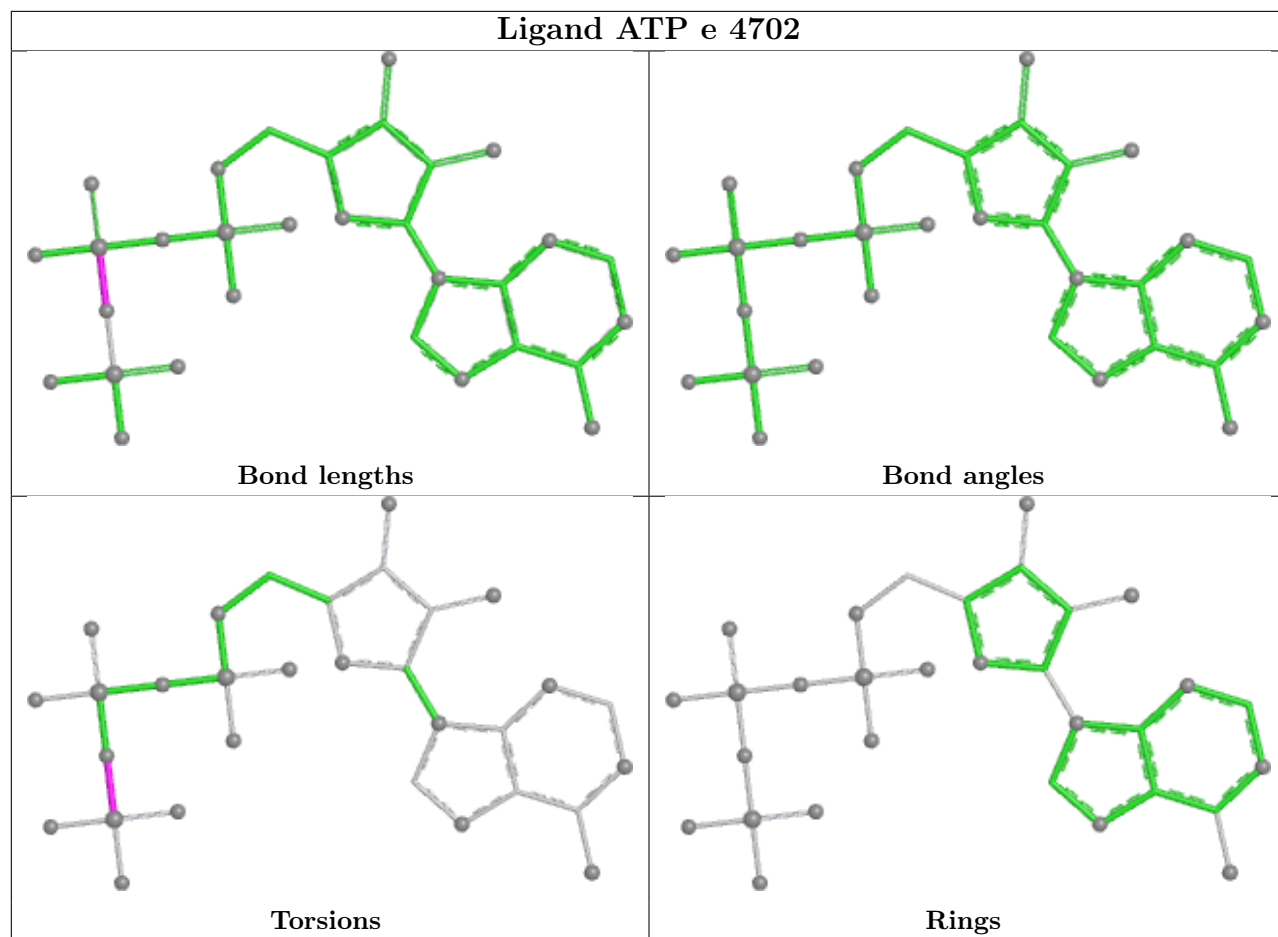


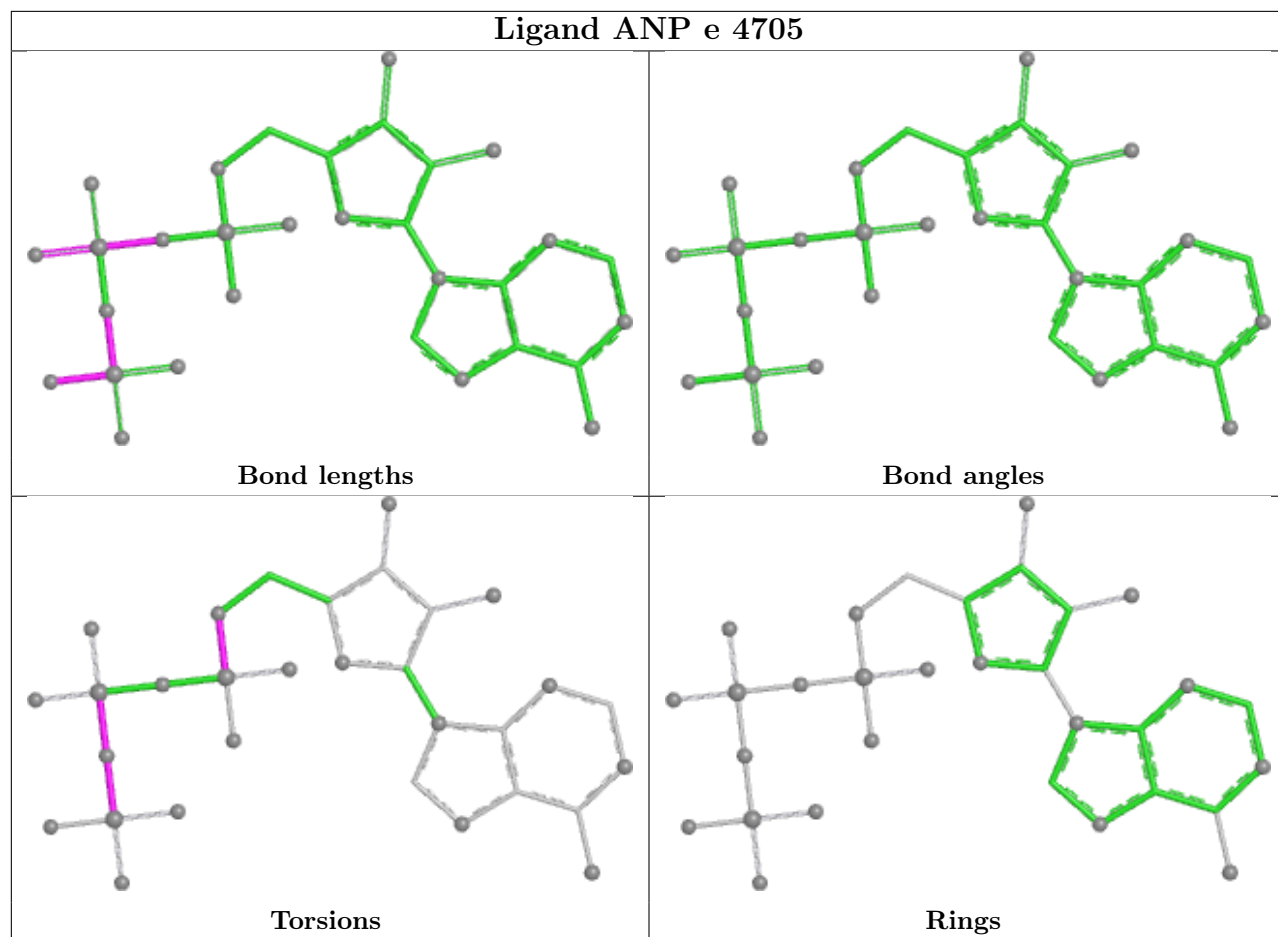
Ligand ADP C 800

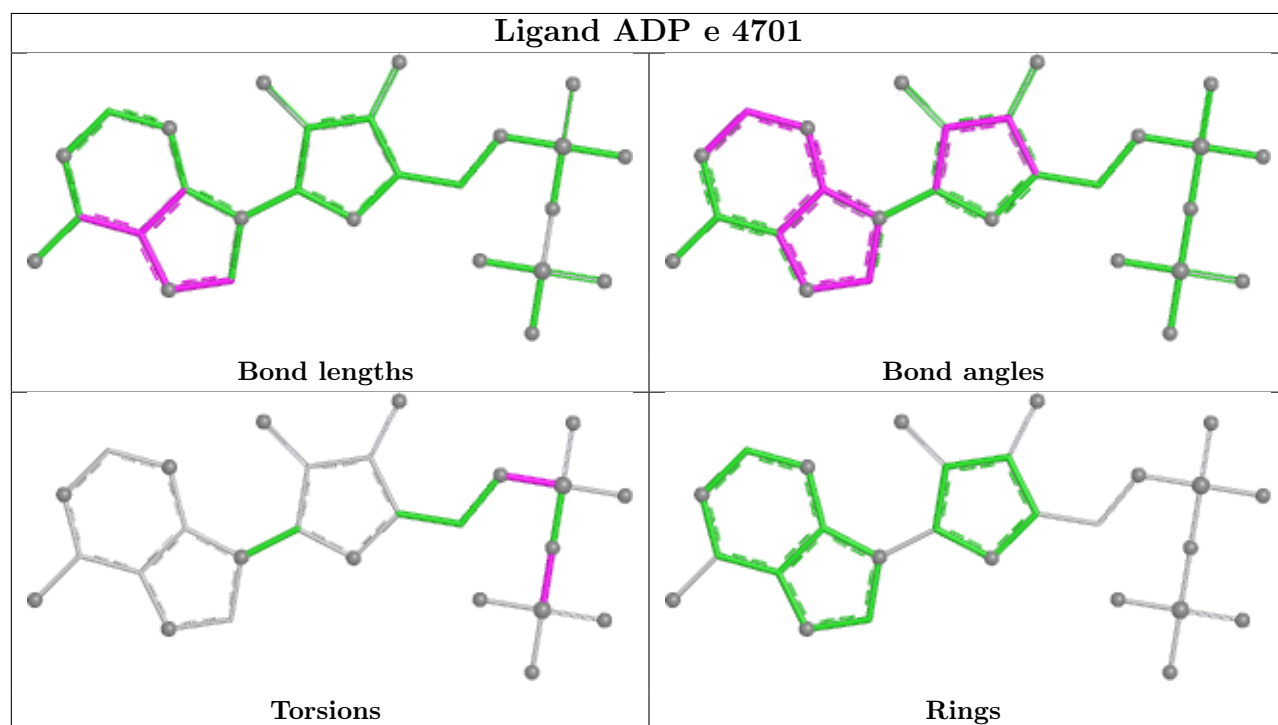
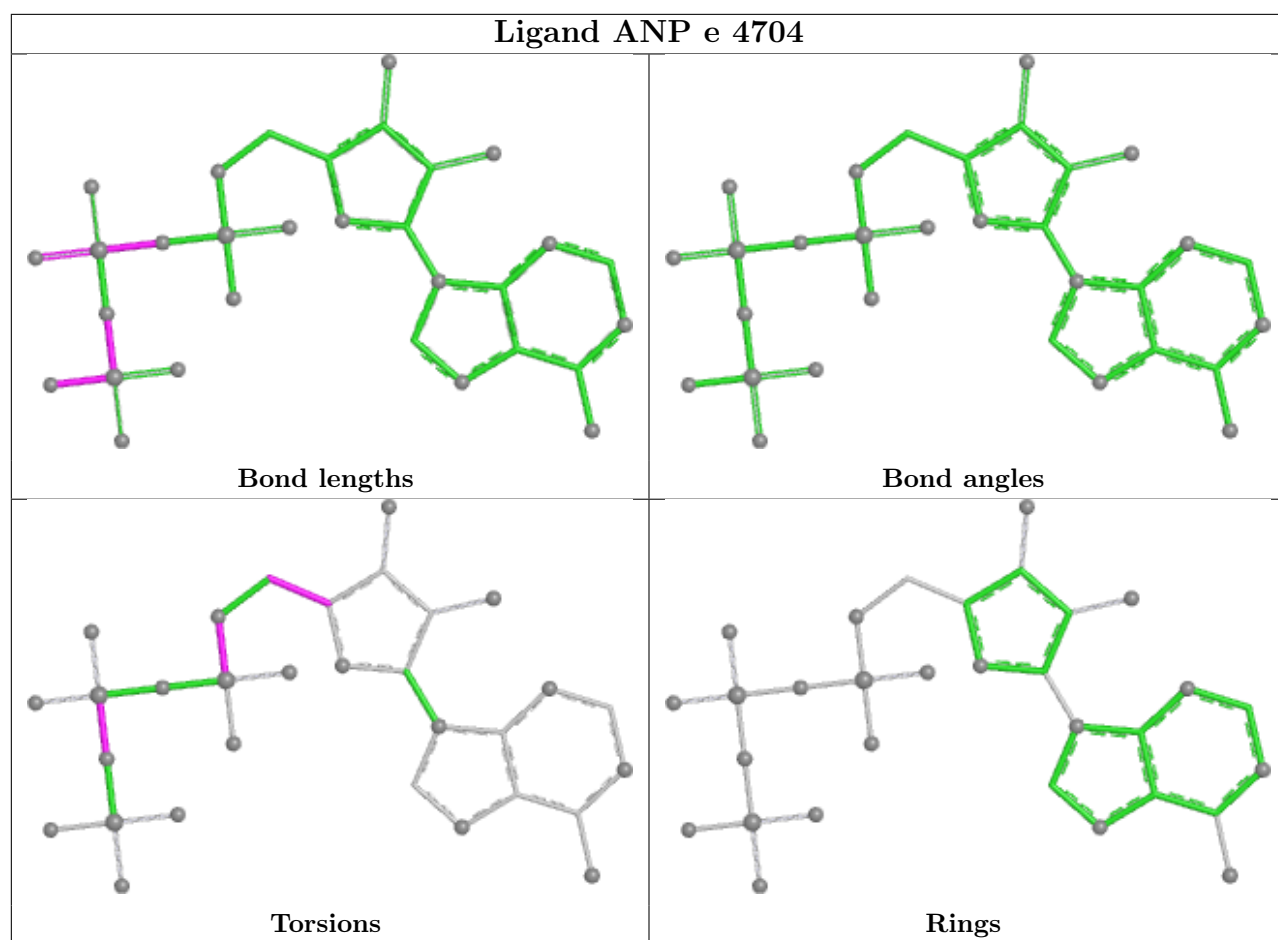


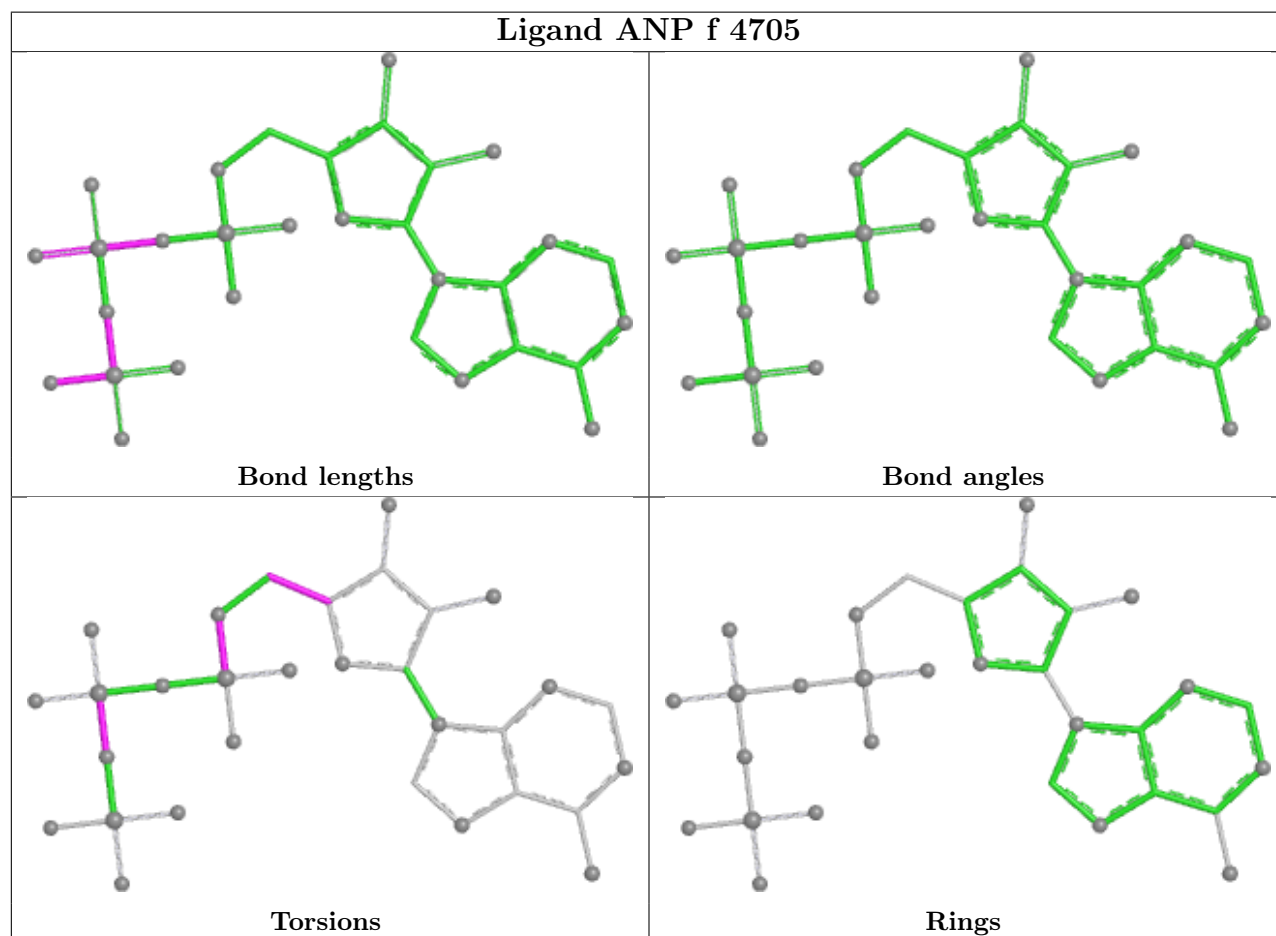
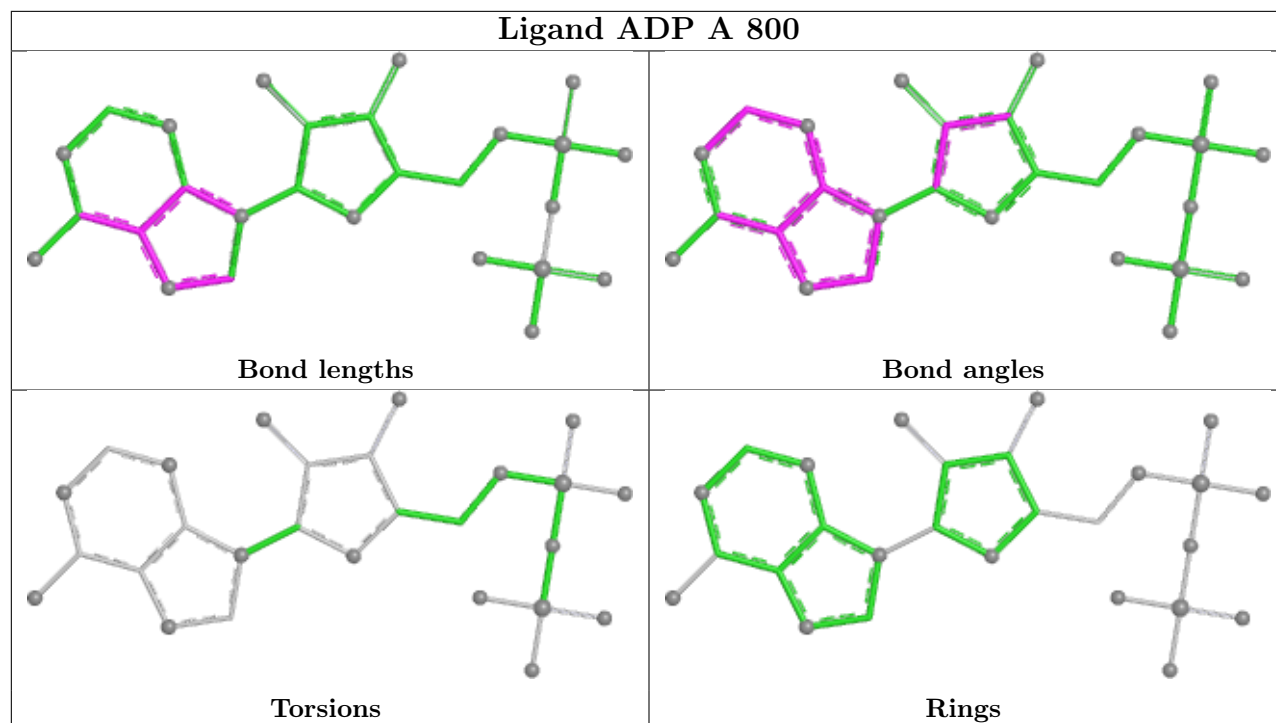












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	S	1

All chain breaks are listed below:

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

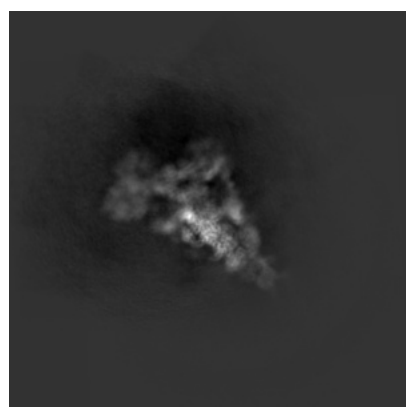
6 Map visualisation [i](#)

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

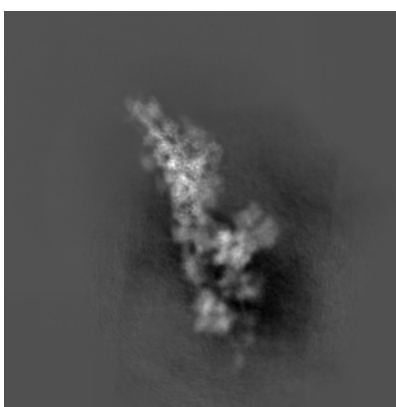
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

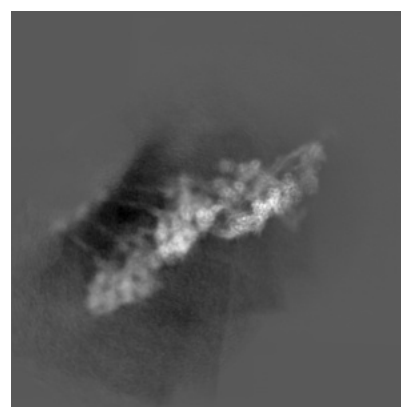
6.1.1 Primary map



X



Y

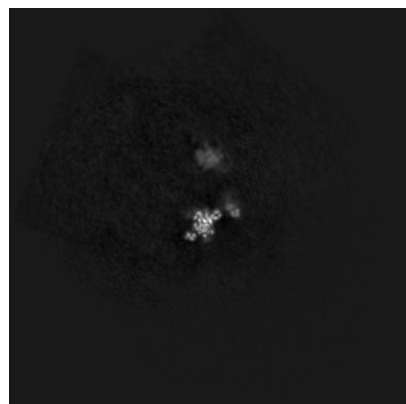


Z

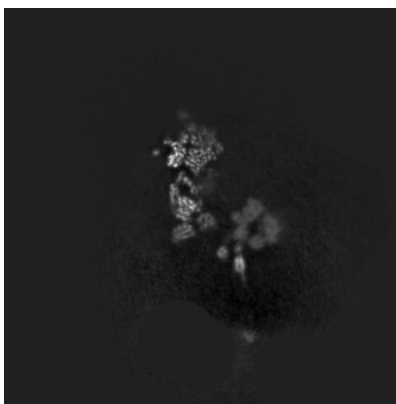
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

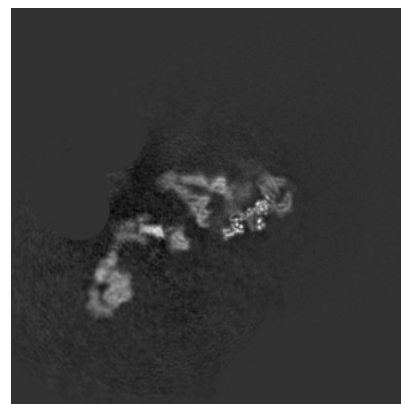
6.2.1 Primary map



X Index: 192



Y Index: 192

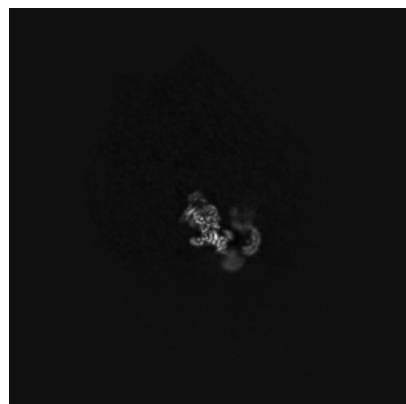


Z Index: 192

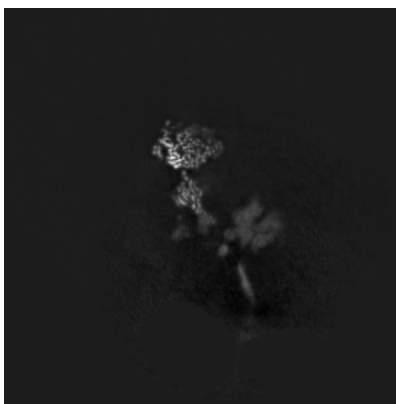
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

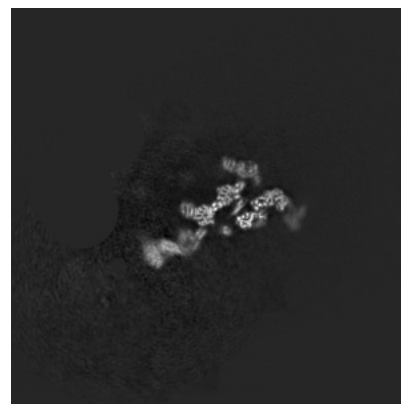
6.3.1 Primary map



X Index: 236



Y Index: 197

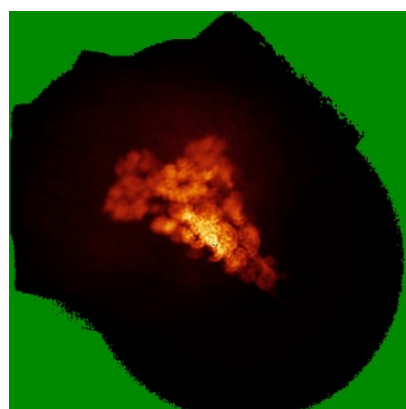


Z Index: 175

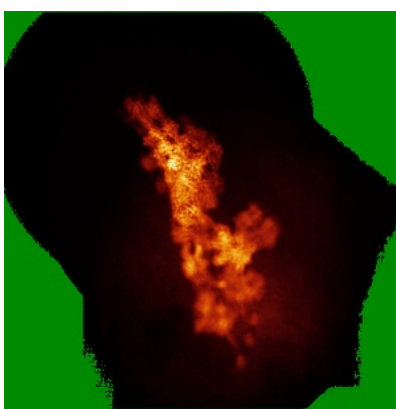
The images above show the largest variance slices of the map in three orthogonal directions.

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

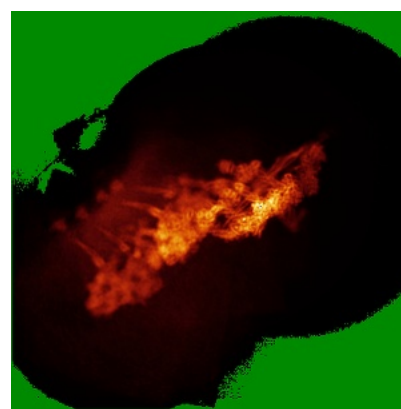
6.4.1 Primary map



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 0.0851. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

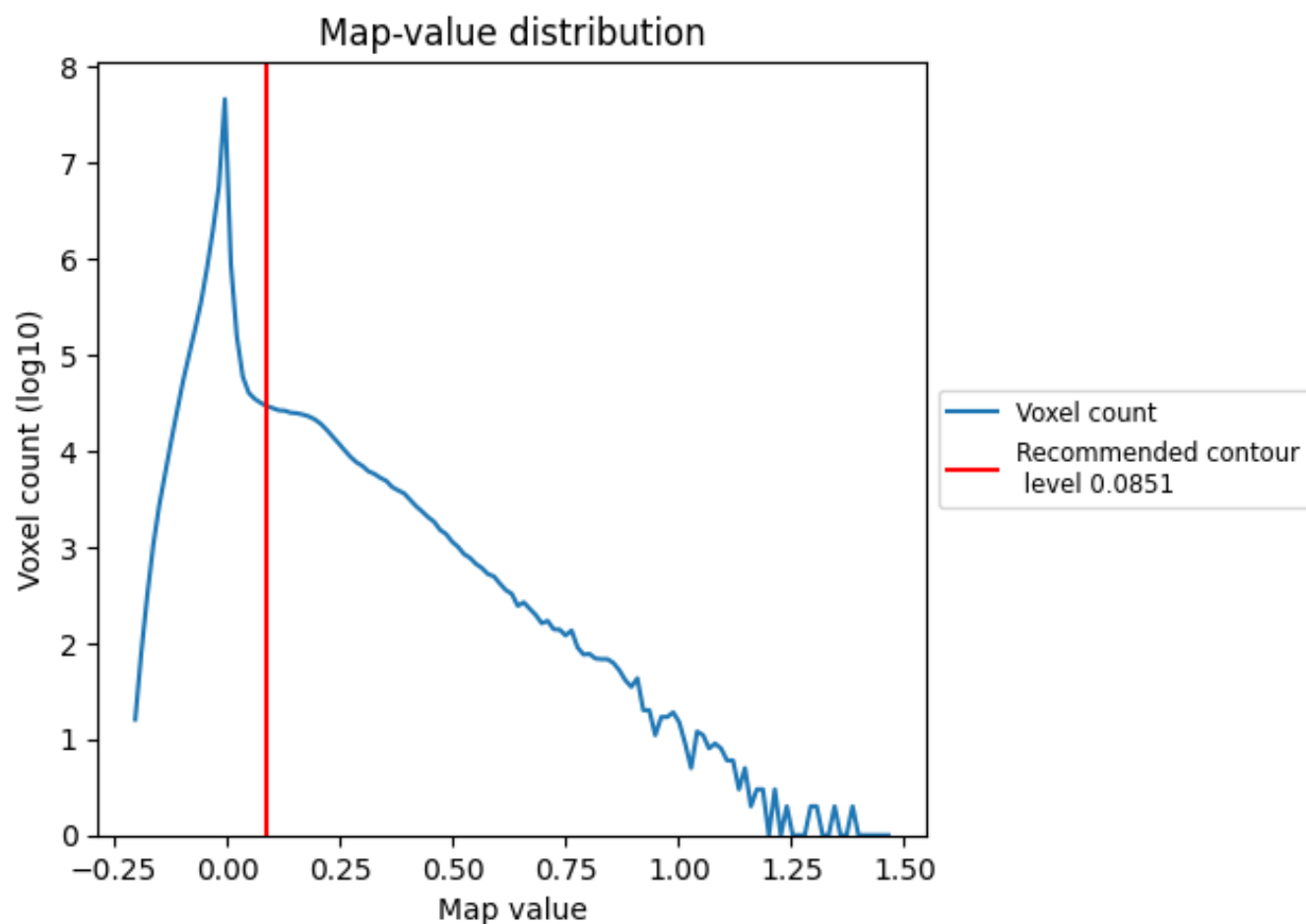
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

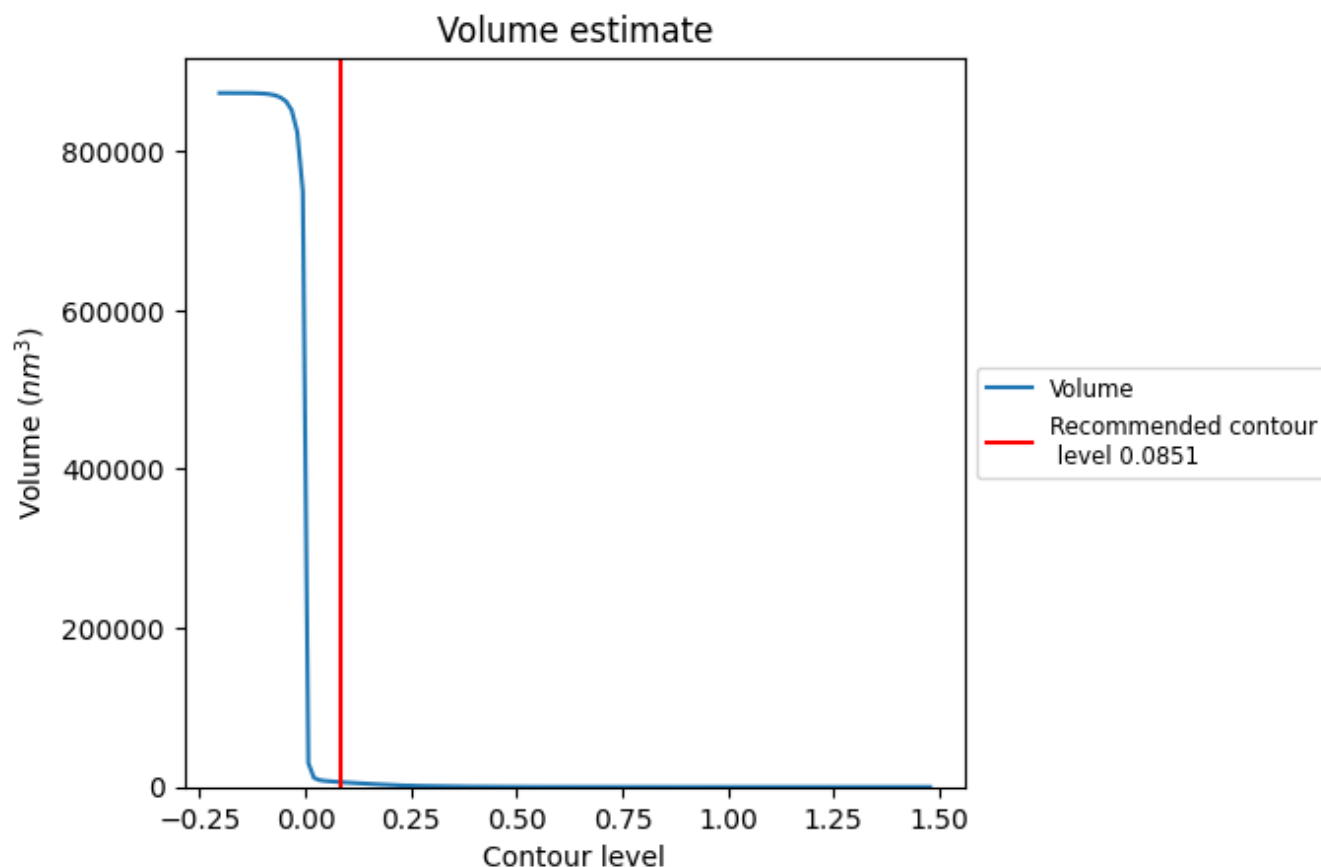
This section contains the results of statistical analysis of the map.

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.

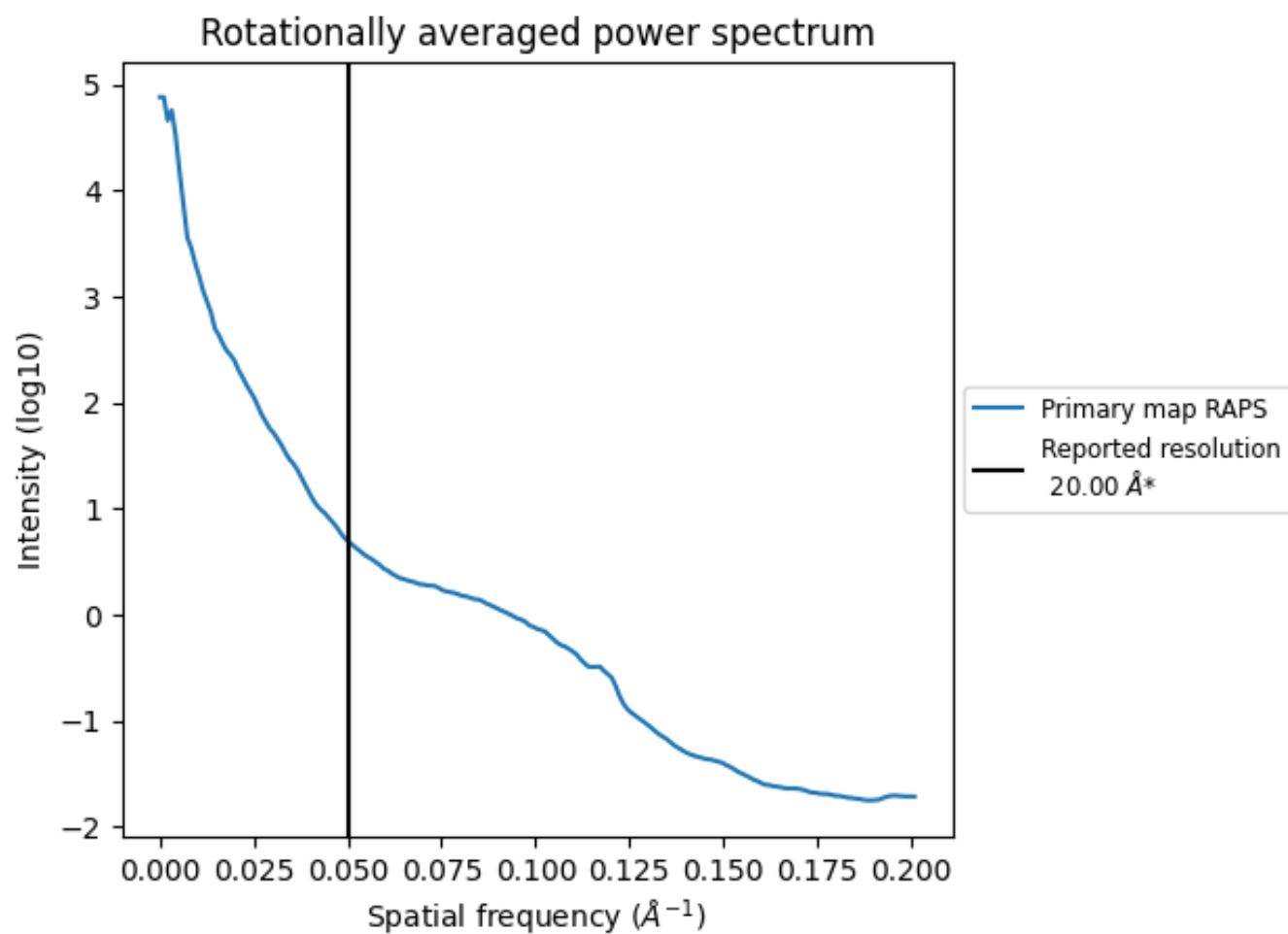
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.050 Å⁻¹

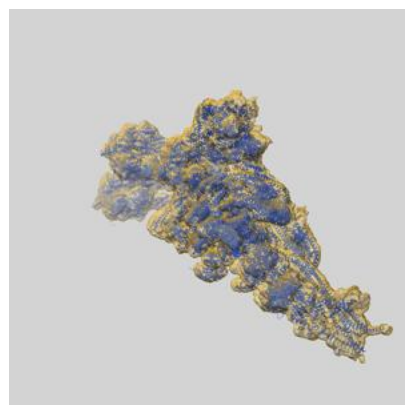
8 Fourier-Shell correlation ⓘ

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

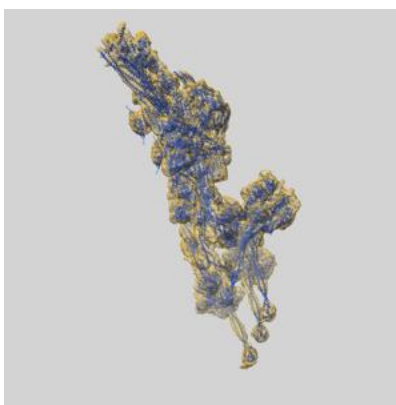
9 Map-model fit [i](#)

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

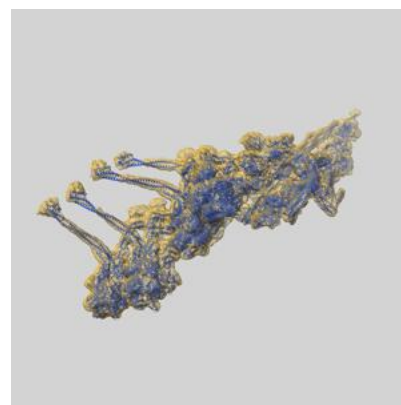
9.1 Map-model overlay [i](#)



X



Y



Z

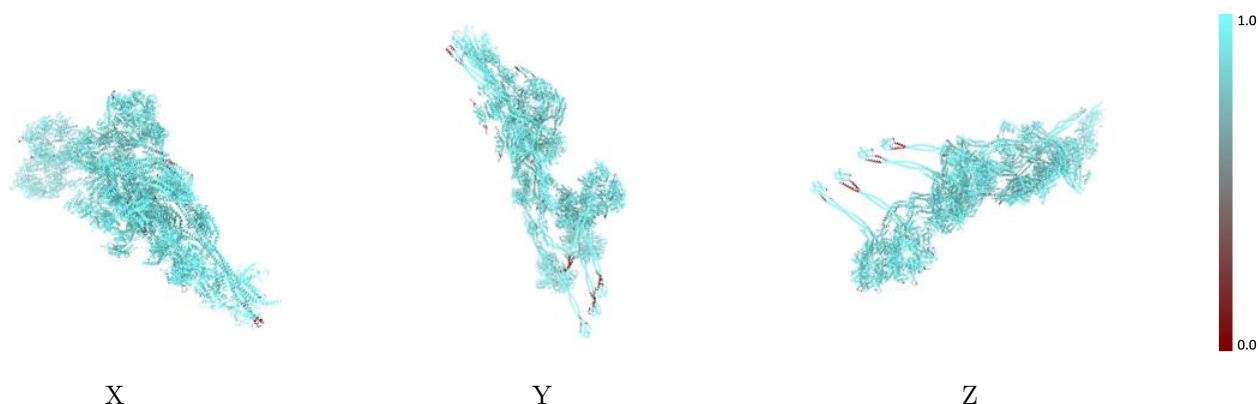
The images above show the 3D surface view of the map at the recommended contour level 0.0851 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



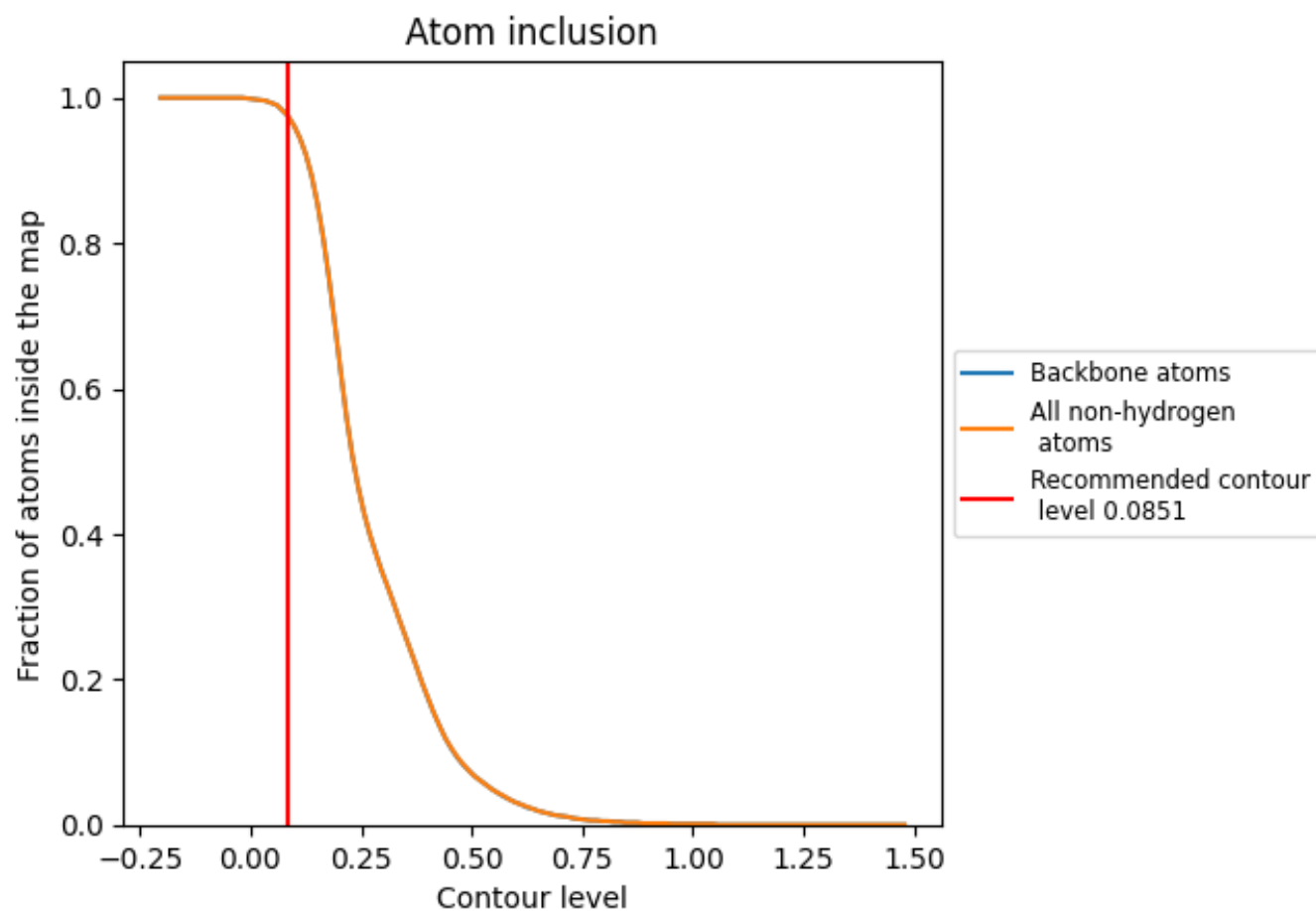
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0851).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0851) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.2150
A	 0.9970	 0.3320
B	 1.0000	 0.3610
C	 1.0000	 0.3660
D	 1.0000	 0.3570
E	 1.0000	 0.3460
F	 0.9990	 0.3370
G	 0.9990	 0.3310
H	 1.0000	 0.3300
I	 0.9820	 0.3350
J	 0.9960	 0.3520
K	 0.9990	 0.3250
L	 1.0000	 0.3360
M	 0.9740	 0.2620
N	 0.9290	 0.2250
O	 0.9910	 0.2500
P	 0.9800	 0.2830
Q	 0.9950	 0.2850
R	 1.0000	 0.2690
S	 0.9760	 0.2410
T	 0.9950	 0.3050
U	 0.9640	 0.3190
V	 0.9890	 0.3350
W	 0.9120	 0.2270
X	 0.9800	 0.2620
Y	 0.9960	 0.3200
e	 0.9630	 0.1650
f	 0.9770	 0.2590
g	 1.0000	 0.2600
h	 1.0000	 0.2840
i	 1.0000	 0.2370
j	 0.9800	 0.2030
k	 1.0000	 0.1580
l	 1.0000	 0.1940
m	 0.9570	 0.1370



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n	 0.9690	 0.1260
o	 1.0000	 0.3580
p	 0.9790	 0.1810
q	 0.9910	 0.1620
r	 0.9980	 0.0950
s	 0.9950	 0.2170
t	 1.0000	 0.2590
w	 0.9370	 0.2010
x	 0.9730	 0.2600