



# Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:33 AM EST

PDB ID : 7TPT  
EMDB ID : EMD-26063  
Title : Single-particle Cryo-EM structure of Arp2/3 complex at branched-actin junction.  
Authors : Ding, B.; Narvaez-Ortiz, H.Y.; Nolen, B.J.; Chowdhury, S.  
Deposited on : 2022-01-26  
Resolution : 3.90 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](mailto: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>.

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

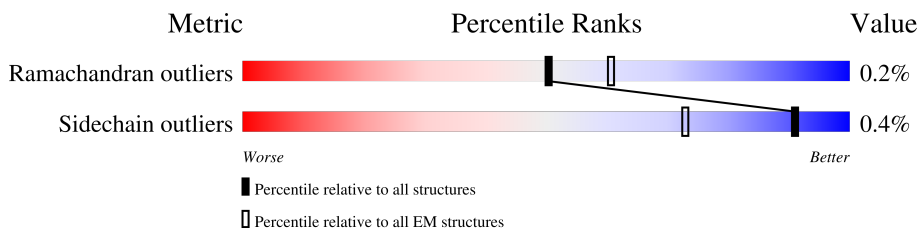
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	418	99%
2	B	394	98%
3	C	372	98%
4	D	300	5% 94% 6%
5	E	178	97%
6	F	168	100%
7	G	151	6% 88% 11%
8	H	377	98%
8	I	377	5% 98%

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Mol	Chain	Length	Quality of chain		
8	J	377	31%	99%	.
8	K	377	52%	99%	.
8	L	377	31%	99%	.
8	M	377	9%	99%	.
8	N	377	6%	98%	.
8	O	377	.	98%	.
8	P	377	.	98%	.
8	Q	377	.	98%	.
8	R	377	.	98%	.
8	S	377	.	98%	.
8	T	377	16%	99%	.
8	U	377	39%	99%	.
9	a	7	57%	29%	14%
9	b	7	57%	29%	14%
9	c	7	14%	57%	29%
9	d	7	57%	29%	14%
9	e	7	71%	57%	29%
9	f	7	14%	57%	29%
9	g	7	57%	29%	14%
9	h	7	14%	57%	29%
9	i	7	57%	29%	14%
9	j	7	57%	29%	14%
9	k	7	57%	29%	14%
9	l	7	57%	29%	14%
9	m	7	57%	29%	14%

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Mol	Chain	Length	Quality of chain
9	n	7	
9	o	7	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 50755 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	414	3310	2119	561	615	15	0	0

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	385	3081	1972	527	566	16	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	363	2744	1729	492	504	19	0	0

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	283	2287	1453	396	430	8	0	0

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	173	1411	906	235	261	9	0	0

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	168	1379	880	240	249	10	0	0

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	134	1002	628	177	194	3	0	0

- Molecule 8 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	371	2900	1837	489	553	21	0	0
8	I	372	2909	1842	490	556	21	0	0
8	J	372	1833	1088	372	373		0	0
8	K	372	1833	1088	372	373		0	0
8	L	372	1833	1088	372	373		0	0
8	M	372	1840	1094	372	374		0	0
8	N	372	2909	1842	490	556	21	0	0
8	O	372	2909	1842	490	556	21	0	0
8	P	372	2909	1842	490	556	21	0	0
8	Q	372	2909	1842	490	556	21	0	0
8	R	372	2909	1842	490	556	21	0	0
8	S	372	2909	1842	490	556	21	0	0
8	T	372	1833	1088	372	373		0	0
8	U	372	1833	1088	372	373		0	0

- Molecule 9 is a protein called Phalloidin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	a	7	55	35	8	11	1	0	0
9	b	7	55	35	8	11	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	c	7	55	35	8	11	1	0	0
9	d	7	55	35	8	11	1	0	0
9	e	7	55	35	8	11	1	0	0
9	f	7	55	35	8	11	1	0	0
9	g	7	55	35	8	11	1	0	0
9	h	7	55	35	8	11	1	0	0
9	i	7	55	35	8	11	1	0	0
9	j	7	55	35	8	11	1	0	0
9	k	7	55	35	8	11	1	0	0
9	l	7	55	35	8	11	1	0	0
9	m	7	55	35	8	11	1	0	0
9	n	7	55	35	8	11	1	0	0
9	o	7	55	35	8	11	1	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

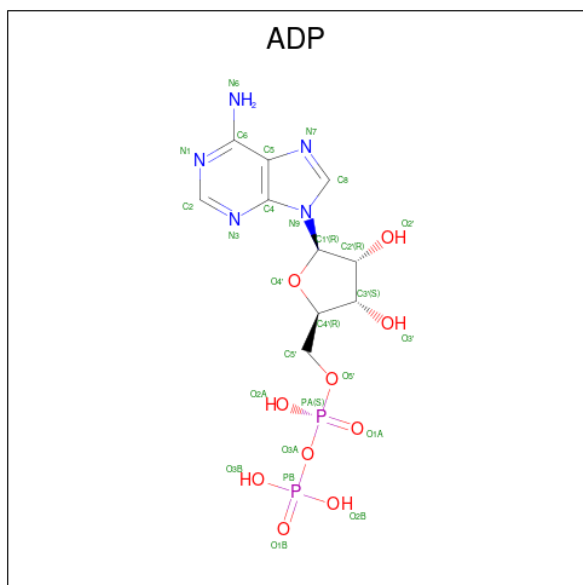
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total 1	Mg 1	0
10	B	1	Total 1	Mg 1	0
10	H	1	Total 1	Mg 1	0
10	I	1	Total 1	Mg 1	0
10	J	1	Total 1	Mg 1	0
10	K	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
10	L	1	Total	Mg	0
			1	1	
10	M	1	Total	Mg	0
			1	1	
10	N	1	Total	Mg	0
			1	1	
10	O	1	Total	Mg	0
			1	1	
10	P	1	Total	Mg	0
			1	1	
10	Q	1	Total	Mg	0
			1	1	
10	R	1	Total	Mg	0
			1	1	
10	S	1	Total	Mg	0
			1	1	
10	T	1	Total	Mg	0
			1	1	
10	U	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf	
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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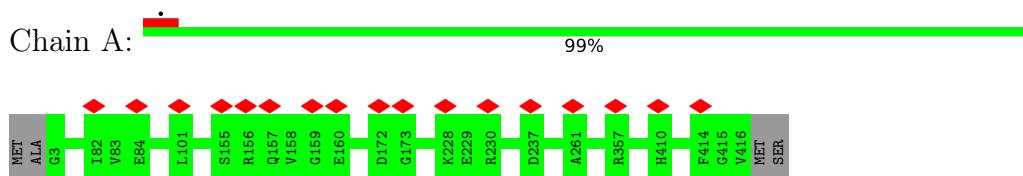
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	B	1	Total 27	C 10	N 5	O 10	P 2	0
11	H	1	Total 27	C 10	N 5	O 10	P 2	0
11	I	1	Total 27	C 10	N 5	O 10	P 2	0
11	J	1	Total 27	C 10	N 5	O 10	P 2	0
11	K	1	Total 27	C 10	N 5	O 10	P 2	0
11	L	1	Total 27	C 10	N 5	O 10	P 2	0
11	M	1	Total 27	C 10	N 5	O 10	P 2	0
11	N	1	Total 27	C 10	N 5	O 10	P 2	0
11	O	1	Total 27	C 10	N 5	O 10	P 2	0
11	P	1	Total 27	C 10	N 5	O 10	P 2	0
11	Q	1	Total 27	C 10	N 5	O 10	P 2	0
11	R	1	Total 27	C 10	N 5	O 10	P 2	0
11	S	1	Total 27	C 10	N 5	O 10	P 2	0
11	T	1	Total 27	C 10	N 5	O 10	P 2	0
11	U	1	Total 27	C 10	N 5	O 10	P 2	0

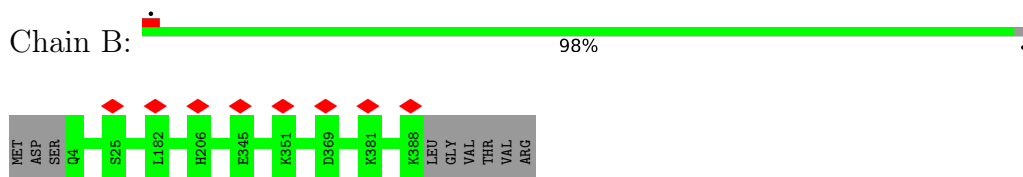
### 3 Residue-property plots [i](#)

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.

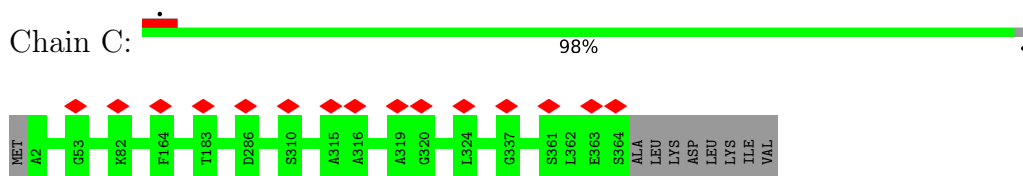
- Molecule 1: Actin-related protein 3



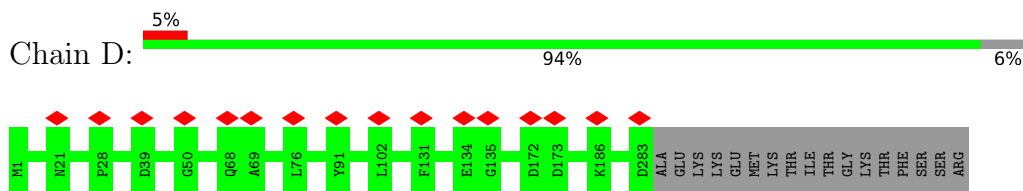
- Molecule 2: Actin-related protein 2



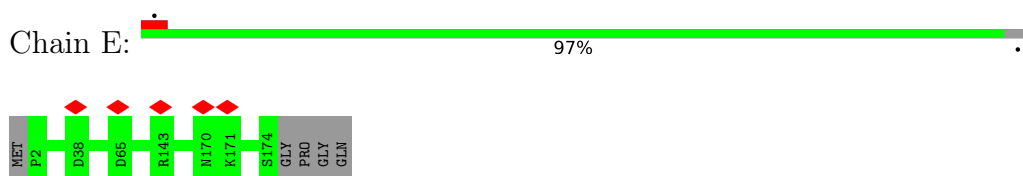
- Molecule 3: Actin-related protein 2/3 complex subunit 1B



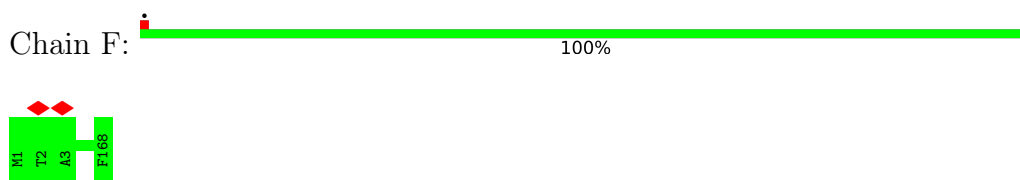
- Molecule 4: Actin-related protein 2/3 complex subunit 2



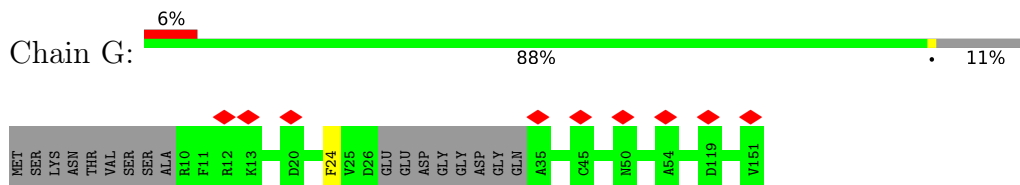
- Molecule 5: Actin-related protein 2/3 complex subunit 3



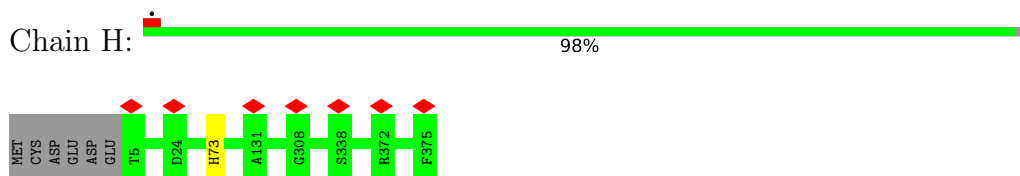
- Molecule 6: Actin-related protein 2/3 complex subunit 4



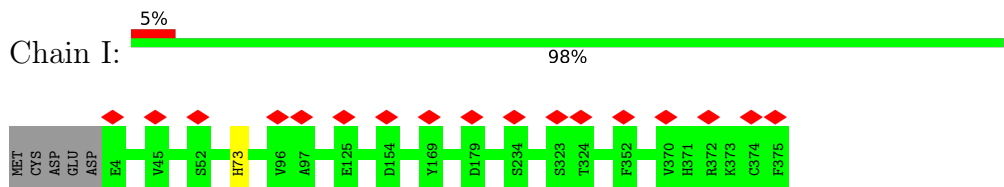
- Molecule 7: Actin-related protein 2/3 complex subunit 5



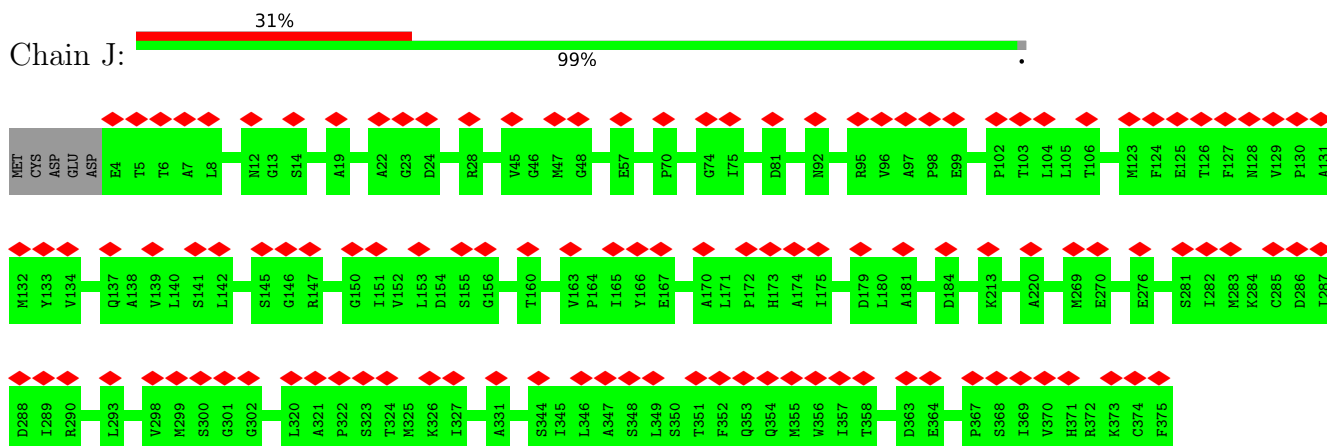
- Molecule 8: Actin, alpha skeletal muscle



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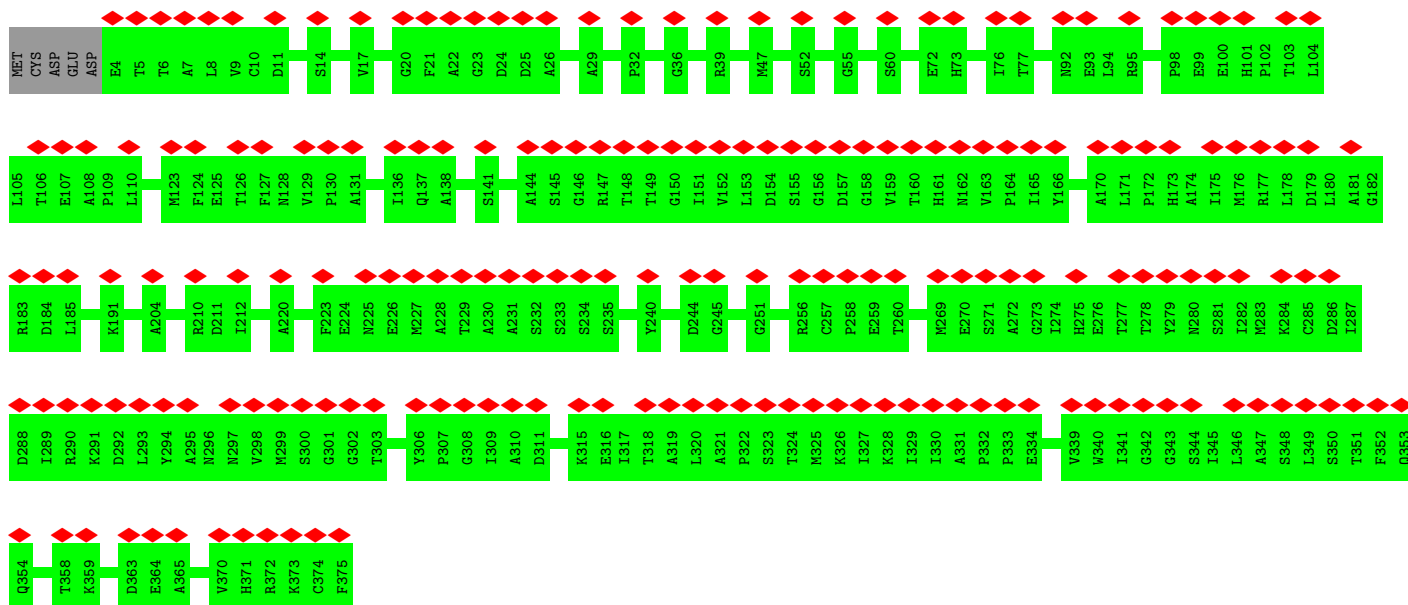


- Molecule 8: Actin, alpha skeletal muscle

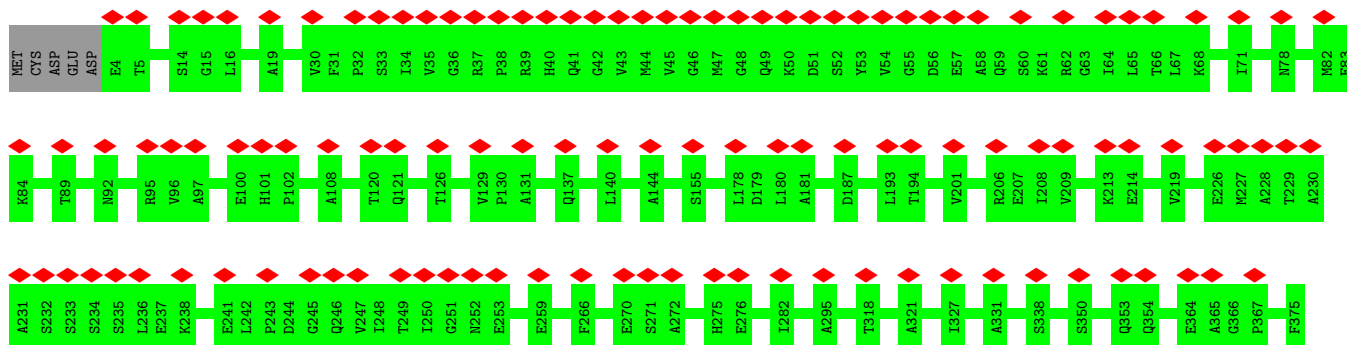


- Molecule 8: Actin, alpha skeletal muscle

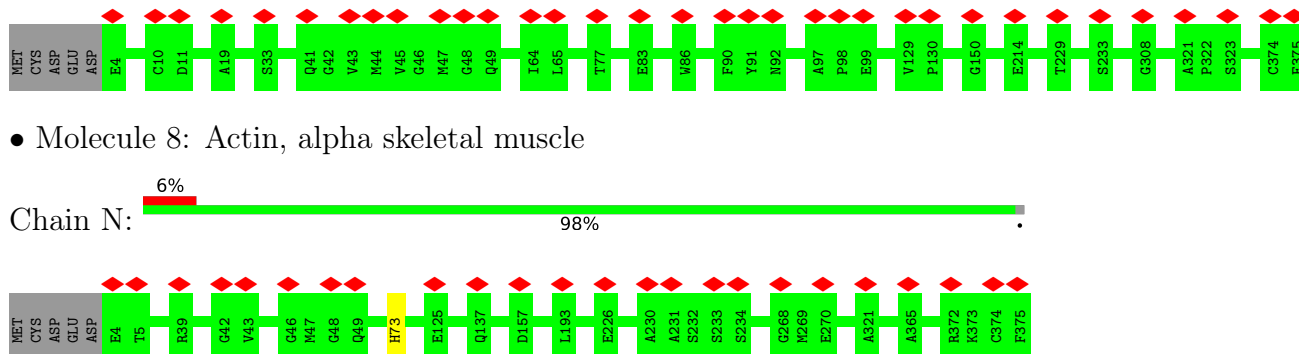




• Molecule 8: Actin, alpha skeletal muscle

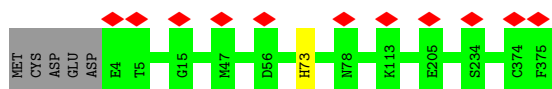


• Molecule 8: Actin, alpha skeletal muscle



• Molecule 8: Actin, alpha skeletal muscle

Chain O:  98%



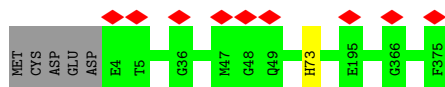
• Molecule 8: Actin, alpha skeletal muscle

Chain P:  98%



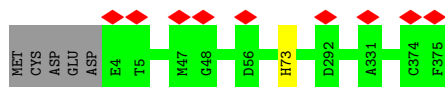
• Molecule 8: Actin, alpha skeletal muscle

Chain Q:  98%



• Molecule 8: Actin, alpha skeletal muscle

Chain R:  98%



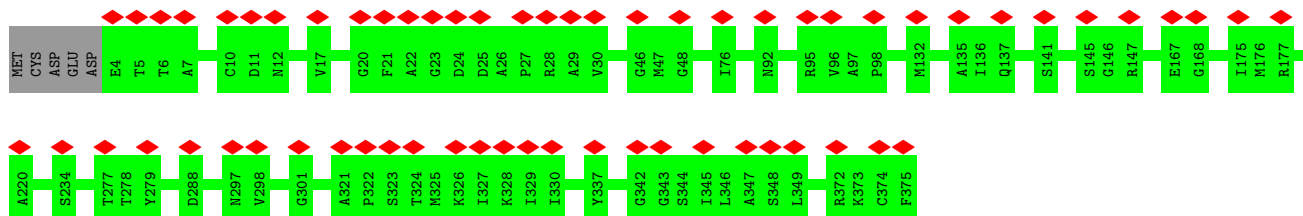
• Molecule 8: Actin, alpha skeletal muscle

Chain S:  98%

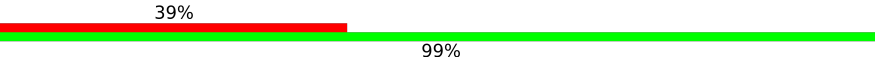


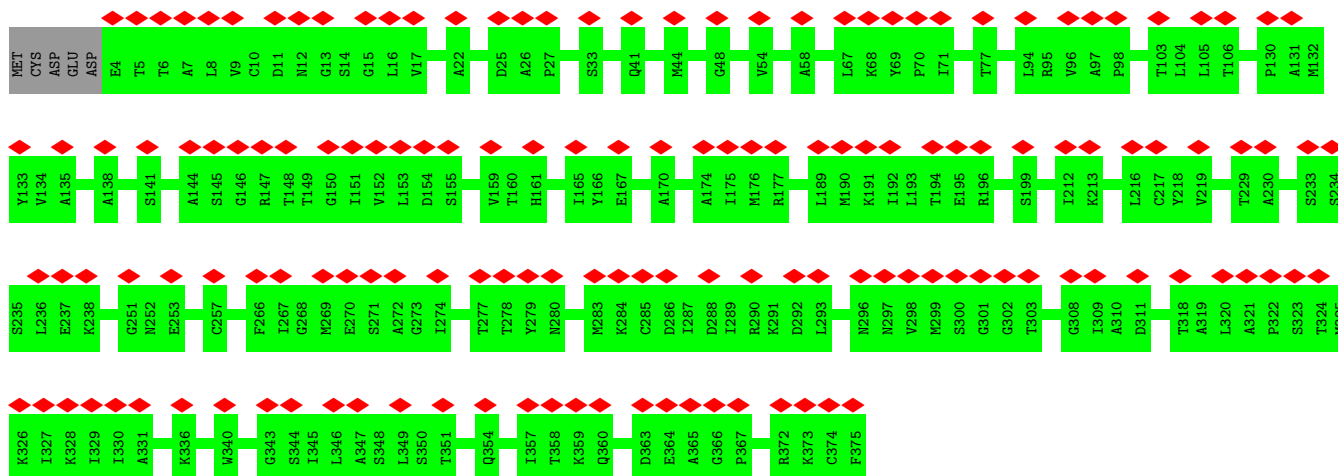
• Molecule 8: Actin, alpha skeletal muscle

Chain T:  16% 99%



• Molecule 8: Actin, alpha skeletal muscle

Chain U:  39% 99%



• Molecule 9: Phalloidin



• Molecule 9: Phalloidin



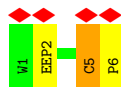
• Molecule 9: Phalloidin



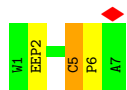
• Molecule 9: Phalloidin



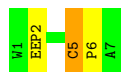
• Molecule 9: Phalloidin



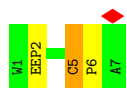
● Molecule 9: Phalloidin



● Molecule 9: Phalloidin



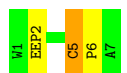
● Molecule 9: Phalloidin



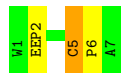
● Molecule 9: Phalloidin



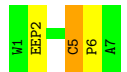
● Molecule 9: Phalloidin



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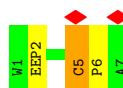
● Molecule 9: Phalloidin



● Molecule 9: Phalloidin



- Molecule 9: Phalloidin



- Molecule 9: Phalloidin





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	127093	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Particles were CTF-corrected during projection matching and back projection	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	41.97	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.307	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	412.16, 412.16, 412.16	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.12, 1.12, 1.12	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, EEP, DTH, HIC, ADP, HYP

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	0.32	0/3393	0.53	0/4602
2	B	0.31	0/3143	0.53	0/4247
3	C	0.24	0/2814	0.50	0/3824
4	D	0.26	0/2336	0.51	0/3154
5	E	0.25	0/1445	0.46	0/1949
6	F	0.25	0/1401	0.49	0/1878
7	G	0.35	0/1013	0.48	0/1363
8	H	0.34	0/2950	0.55	0/3994
8	I	0.27	0/2959	0.49	0/4006
8	J	0.24	0/1826	0.43	0/2535
8	K	0.24	0/1826	0.43	0/2535
8	L	0.24	0/1826	0.43	0/2535
8	M	0.26	0/1834	0.45	0/2546
8	N	0.25	0/2959	0.49	0/4006
8	O	0.36	0/2959	0.58	0/4006
8	P	0.36	0/2959	0.52	0/4006
8	Q	0.27	0/2959	0.49	0/4006
8	R	0.26	0/2959	0.50	0/4006
8	S	0.27	0/2959	0.49	0/4006
8	T	0.24	0/1826	0.43	0/2535
8	U	0.24	0/1826	0.43	0/2535
9	a	1.03	0/28	1.40	0/33
9	b	1.02	0/28	1.42	0/33
9	c	1.03	0/28	1.40	0/33
9	d	1.04	0/28	1.41	0/33
9	e	1.03	0/28	1.41	0/33
9	f	1.02	0/28	1.41	0/33
9	g	1.04	0/28	1.42	0/33
9	h	1.02	0/28	1.41	0/33
9	i	1.03	0/28	1.42	0/33
9	j	1.02	0/28	1.40	0/33
9	k	1.03	0/28	1.42	0/33

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	l	1.02	0/28	1.42	0/33
9	m	1.02	0/28	1.42	0/33
9	n	1.04	0/28	1.40	0/33
9	o	1.02	0/28	1.42	0/33
All	All	0.30	0/50592	0.51	0/68769

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/418 (99%)	383 (93%)	29 (7%)	0	100	100
2	B	383/394 (97%)	361 (94%)	22 (6%)	0	100	100
3	C	361/372 (97%)	338 (94%)	23 (6%)	0	100	100
4	D	281/300 (94%)	260 (92%)	21 (8%)	0	100	100
5	E	171/178 (96%)	159 (93%)	12 (7%)	0	100	100
6	F	166/168 (99%)	157 (95%)	9 (5%)	0	100	100
7	G	130/151 (86%)	112 (86%)	18 (14%)	0	100	100
8	H	368/377 (98%)	360 (98%)	8 (2%)	0	100	100
8	I	369/377 (98%)	358 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	369/377 (98%)	359 (97%)	10 (3%)	0	100	100
8	K	369/377 (98%)	359 (97%)	10 (3%)	0	100	100
8	L	369/377 (98%)	359 (97%)	10 (3%)	0	100	100
8	M	369/377 (98%)	359 (97%)	10 (3%)	0	100	100
8	N	369/377 (98%)	358 (97%)	11 (3%)	0	100	100
8	O	369/377 (98%)	357 (97%)	12 (3%)	0	100	100
8	P	369/377 (98%)	354 (96%)	15 (4%)	0	100	100
8	Q	369/377 (98%)	359 (97%)	10 (3%)	0	100	100
8	R	369/377 (98%)	359 (97%)	10 (3%)	0	100	100
8	S	369/377 (98%)	358 (97%)	11 (3%)	0	100	100
8	T	369/377 (98%)	359 (97%)	10 (3%)	0	100	100
8	U	369/377 (98%)	359 (97%)	10 (3%)	0	100	100
9	a	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	b	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	c	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	d	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	e	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	f	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	g	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	h	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	i	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	j	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	k	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	l	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	m	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	n	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
9	o	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
All	All	7099/7364 (96%)	6802 (96%)	282 (4%)	15 (0%)	50	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	a	5	CYS

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Mol	Chain	Res	Type
9	b	5	CYS
9	c	5	CYS
9	d	5	CYS
9	e	5	CYS
9	f	5	CYS
9	g	5	CYS
9	h	5	CYS
9	i	5	CYS
9	j	5	CYS
9	k	5	CYS
9	l	5	CYS
9	m	5	CYS
9	n	5	CYS
9	o	5	CYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/363 (99%)	360 (100%)	0	100	100
2	B	337/345 (98%)	337 (100%)	0	100	100
3	C	282/313 (90%)	282 (100%)	0	100	100
4	D	249/264 (94%)	249 (100%)	0	100	100
5	E	156/159 (98%)	156 (100%)	0	100	100
6	F	155/155 (100%)	155 (100%)	0	100	100
7	G	105/123 (85%)	104 (99%)	1 (1%)	76	86
8	H	313/319 (98%)	313 (100%)	0	100	100
8	I	314/319 (98%)	314 (100%)	0	100	100
8	M	1/319 (0%)	1 (100%)	0	100	100
8	N	314/319 (98%)	314 (100%)	0	100	100
8	O	314/319 (98%)	314 (100%)	0	100	100
8	P	314/319 (98%)	314 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Q	314/319 (98%)	314 (100%)	0	100	100
8	R	314/319 (98%)	314 (100%)	0	100	100
8	S	314/319 (98%)	314 (100%)	0	100	100
9	a	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	b	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	c	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	d	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	e	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	f	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	g	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	h	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	i	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	j	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	k	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	l	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	m	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	n	2/2 (100%)	1 (50%)	1 (50%)	0	0
9	o	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	4186/4623 (90%)	4170 (100%)	16 (0%)	91	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	24	PHE
9	a	5	CYS
9	b	5	CYS
9	c	5	CYS
9	d	5	CYS
9	e	5	CYS
9	f	5	CYS
9	g	5	CYS
9	h	5	CYS
9	i	5	CYS
9	j	5	CYS
9	k	5	CYS
9	l	5	CYS

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Mol	Chain	Res	Type
9	m	5	CYS
9	n	5	CYS
9	o	5	CYS

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

59 non-standard protein/DNA/RNA residues are modelled in this entry.

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
9	HYP	i	6	9	6,8,9	0.50	0	5,10,12	1.25	1 (20%)
8	HIC	I	73	8	8,11,12	1.68	2 (25%)	6,14,16	1.10	1 (16%)
8	HIC	M	73	8	3,4,12	0.89	0	2,4,16	0.87	0
8	HIC	U	73	8	3,4,12	0.92	0	2,4,16	0.89	0
8	HIC	N	73	8	8,11,12	1.67	2 (25%)	6,14,16	1.19	1 (16%)
9	HYP	d	6	9	6,8,9	0.51	0	5,10,12	1.24	1 (20%)
9	EEP	l	2	9	8,9,10	1.39	2 (25%)	5,12,14	0.99	0
9	EEP	b	2	9	8,9,10	1.39	2 (25%)	5,12,14	1.01	0
9	EEP	n	2	9	8,9,10	1.40	2 (25%)	5,12,14	1.00	0
9	HYP	h	6	9	6,8,9	0.50	0	5,10,12	1.25	1 (20%)
9	EEP	c	2	9	8,9,10	1.39	2 (25%)	5,12,14	1.00	0
9	EEP	e	2	9	8,9,10	1.37	2 (25%)	5,12,14	1.01	0
9	EEP	g	2	9	8,9,10	1.43	2 (25%)	5,12,14	0.99	0
9	EEP	a	2	9	8,9,10	1.39	2 (25%)	5,12,14	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	HYP	o	6	9	6,8,9	0.50	0	5,10,12	1.24	1 (20%)
9	HYP	c	6	9	6,8,9	0.52	0	5,10,12	1.24	1 (20%)
9	HYP	k	6	9	6,8,9	0.51	0	5,10,12	1.24	1 (20%)
8	HIC	J	73	8	3,4,12	0.90	0	2,4,16	0.88	0
8	HIC	T	73	8	3,4,12	0.91	0	2,4,16	0.89	0
8	HIC	O	73	8	8,11,12	1.68	2 (25%)	6,14,16	1.12	1 (16%)
9	EEP	j	2	9	8,9,10	1.38	2 (25%)	5,12,14	1.02	0
9	HYP	j	6	9	6,8,9	0.52	0	5,10,12	1.25	1 (20%)
8	HIC	R	73	8	8,11,12	1.66	2 (25%)	6,14,16	1.15	1 (16%)
9	EEP	m	2	9	8,9,10	1.39	2 (25%)	5,12,14	1.01	0
8	HIC	H	73	8	8,11,12	1.66	2 (25%)	6,14,16	1.13	1 (16%)
8	HIC	S	73	8	8,11,12	1.66	2 (25%)	6,14,16	1.18	1 (16%)
9	HYP	e	6	9	6,8,9	0.50	0	5,10,12	1.26	1 (20%)
9	HYP	m	6	9	6,8,9	0.50	0	5,10,12	1.26	1 (20%)
9	HYP	n	6	9	6,8,9	0.50	0	5,10,12	1.25	1 (20%)
9	EEP	h	2	9	8,9,10	1.40	2 (25%)	5,12,14	1.00	0
8	HIC	K	73	8	3,4,12	0.89	0	2,4,16	0.88	0
9	HYP	l	6	9	6,8,9	0.51	0	5,10,12	1.25	1 (20%)
9	HYP	b	6	9	6,8,9	0.49	0	5,10,12	1.26	1 (20%)
9	EEP	k	2	9	8,9,10	1.40	2 (25%)	5,12,14	1.00	0
8	HIC	Q	73	8	8,11,12	1.70	2 (25%)	6,14,16	1.11	1 (16%)
9	EEP	o	2	9	8,9,10	1.38	2 (25%)	5,12,14	1.00	0
8	HIC	L	73	8	3,4,12	0.90	0	2,4,16	0.88	0
9	HYP	a	6	9	6,8,9	0.51	0	5,10,12	1.27	1 (20%)
8	HIC	P	73	8	8,11,12	1.71	2 (25%)	6,14,16	1.09	1 (16%)
9	EEP	f	2	9	8,9,10	1.39	2 (25%)	5,12,14	1.00	0
9	EEP	i	2	9	8,9,10	1.36	2 (25%)	5,12,14	1.01	0
9	HYP	f	6	9	6,8,9	0.51	0	5,10,12	1.24	1 (20%)
9	EEP	d	2	9	8,9,10	1.41	2 (25%)	5,12,14	0.99	0
9	HYP	g	6	9	6,8,9	0.52	0	5,10,12	1.26	1 (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
9	HYP	i	6	9	-	0/0/11/13	0/1/1/1
8	HIC	I	73	8	-	2/5/6/8	0/1/1/1
8	HIC	M	73	8	-	0/0/2/8	-
8	HIC	U	73	8	-	0/0/2/8	-
8	HIC	N	73	8	-	0/5/6/8	0/1/1/1
9	HYP	d	6	9	-	0/0/11/13	0/1/1/1
9	EEP	l	2	9	-	3/9/10/12	-
9	EEP	b	2	9	-	3/9/10/12	-
9	EEP	n	2	9	-	3/9/10/12	-
9	HYP	h	6	9	-	0/0/11/13	0/1/1/1
9	EEP	c	2	9	-	3/9/10/12	-
9	EEP	e	2	9	-	3/9/10/12	-
9	EEP	g	2	9	-	3/9/10/12	-
9	EEP	a	2	9	-	3/9/10/12	-
9	HYP	o	6	9	-	0/0/11/13	0/1/1/1
9	HYP	c	6	9	-	0/0/11/13	0/1/1/1
9	HYP	k	6	9	-	0/0/11/13	0/1/1/1
8	HIC	J	73	8	-	0/0/2/8	-
8	HIC	T	73	8	-	0/0/2/8	-
8	HIC	O	73	8	-	2/5/6/8	0/1/1/1
9	EEP	j	2	9	-	3/9/10/12	-
9	HYP	j	6	9	-	0/0/11/13	0/1/1/1
8	HIC	R	73	8	-	2/5/6/8	0/1/1/1
9	EEP	m	2	9	-	3/9/10/12	-
8	HIC	H	73	8	-	2/5/6/8	0/1/1/1
8	HIC	S	73	8	-	0/5/6/8	0/1/1/1
9	HYP	e	6	9	-	0/0/11/13	0/1/1/1
9	HYP	m	6	9	-	0/0/11/13	0/1/1/1
9	HYP	n	6	9	-	0/0/11/13	0/1/1/1
9	EEP	h	2	9	-	3/9/10/12	-
8	HIC	K	73	8	-	0/0/2/8	-
9	HYP	l	6	9	-	0/0/11/13	0/1/1/1
9	HYP	b	6	9	-	0/0/11/13	0/1/1/1
9	EEP	k	2	9	-	3/9/10/12	-
8	HIC	Q	73	8	-	2/5/6/8	0/1/1/1
9	EEP	o	2	9	-	3/9/10/12	-
8	HIC	L	73	8	-	0/0/2/8	-
9	HYP	a	6	9	-	0/0/11/13	0/1/1/1
8	HIC	P	73	8	-	2/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EEP	f	2	9	-	3/9/10/12	-
9	EEP	i	2	9	-	3/9/10/12	-
9	HYP	f	6	9	-	0/0/11/13	0/1/1/1
9	EEP	d	2	9	-	3/9/10/12	-
9	HYP	g	6	9	-	0/0/11/13	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	73	HIC	CD2-CG	3.73	1.41	1.36
8	Q	73	HIC	CD2-CG	3.69	1.41	1.36
8	O	73	HIC	CD2-CG	3.67	1.41	1.36
8	N	73	HIC	CD2-CG	3.66	1.41	1.36
8	I	73	HIC	CD2-CG	3.64	1.41	1.36
8	R	73	HIC	CD2-CG	3.63	1.41	1.36
8	S	73	HIC	CD2-CG	3.63	1.41	1.36
8	H	73	HIC	CD2-CG	3.62	1.41	1.36
9	d	2	EEP	CB-CA	-2.86	1.50	1.54
9	n	2	EEP	CB-CA	-2.83	1.50	1.54
9	m	2	EEP	CB-CA	-2.82	1.50	1.54
9	k	2	EEP	CB-CA	-2.81	1.50	1.54
9	j	2	EEP	CB-CA	-2.81	1.50	1.54
9	g	2	EEP	CB-CA	-2.80	1.50	1.54
9	e	2	EEP	CB-CA	-2.80	1.50	1.54
9	o	2	EEP	CB-CA	-2.78	1.50	1.54
9	f	2	EEP	CB-CA	-2.77	1.50	1.54
9	b	2	EEP	CB-CA	-2.76	1.50	1.54
9	c	2	EEP	CB-CA	-2.76	1.50	1.54
9	i	2	EEP	CB-CA	-2.75	1.50	1.54
9	l	2	EEP	CB-CA	-2.73	1.50	1.54
9	h	2	EEP	CB-CA	-2.73	1.50	1.54
9	a	2	EEP	CB-CA	-2.70	1.50	1.54
9	g	2	EEP	CB-CG	-2.37	1.50	1.53
9	h	2	EEP	CB-CG	-2.35	1.50	1.53
9	c	2	EEP	CB-CG	-2.31	1.50	1.53
9	a	2	EEP	CB-CG	-2.31	1.50	1.53
9	d	2	EEP	CB-CG	-2.31	1.50	1.53
9	l	2	EEP	CB-CG	-2.28	1.50	1.53
9	f	2	EEP	CB-CG	-2.27	1.50	1.53
9	k	2	EEP	CB-CG	-2.26	1.50	1.53
9	m	2	EEP	CB-CG	-2.25	1.50	1.53
9	n	2	EEP	CB-CG	-2.24	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	2	EEP	CB-CG	-2.24	1.50	1.53
9	o	2	EEP	CB-CG	-2.24	1.50	1.53
9	i	2	EEP	CB-CG	-2.22	1.51	1.53
9	e	2	EEP	CB-CG	-2.18	1.51	1.53
9	j	2	EEP	CB-CG	-2.18	1.51	1.53
8	I	73	HIC	CZ-NE2	-2.06	1.42	1.48
8	S	73	HIC	CZ-NE2	-2.05	1.42	1.48
8	P	73	HIC	CZ-NE2	-2.04	1.42	1.48
8	Q	73	HIC	CZ-NE2	-2.04	1.42	1.48
8	N	73	HIC	CZ-NE2	-2.03	1.42	1.48
8	H	73	HIC	CZ-NE2	-2.03	1.42	1.48
8	R	73	HIC	CZ-NE2	-2.02	1.42	1.48
8	O	73	HIC	CZ-NE2	-2.01	1.42	1.48

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	j	6	HYP	O-C-CA	-2.30	118.74	124.78
9	a	6	HYP	O-C-CA	-2.30	118.75	124.78
9	b	6	HYP	O-C-CA	-2.30	118.75	124.78
9	d	6	HYP	O-C-CA	-2.30	118.76	124.78
9	g	6	HYP	O-C-CA	-2.29	118.77	124.78
9	e	6	HYP	O-C-CA	-2.29	118.77	124.78
9	h	6	HYP	O-C-CA	-2.29	118.78	124.78
9	n	6	HYP	O-C-CA	-2.28	118.80	124.78
9	m	6	HYP	O-C-CA	-2.28	118.80	124.78
9	i	6	HYP	O-C-CA	-2.27	118.83	124.78
9	l	6	HYP	O-C-CA	-2.27	118.83	124.78
9	k	6	HYP	O-C-CA	-2.27	118.83	124.78
9	o	6	HYP	O-C-CA	-2.27	118.84	124.78
9	f	6	HYP	O-C-CA	-2.26	118.85	124.78
9	c	6	HYP	O-C-CA	-2.25	118.87	124.78
8	N	73	HIC	CB-CA-C	-2.09	107.55	111.47
8	I	73	HIC	CB-CA-C	-2.09	107.56	111.47
8	Q	73	HIC	CB-CA-C	-2.08	107.56	111.47
8	R	73	HIC	CB-CA-C	-2.08	107.58	111.47
8	P	73	HIC	CB-CA-C	-2.07	107.58	111.47
8	O	73	HIC	CB-CA-C	-2.07	107.58	111.47
8	S	73	HIC	CB-CA-C	-2.07	107.59	111.47
8	H	73	HIC	CB-CA-C	-2.06	107.60	111.47

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	73	HIC	CA-CB-CG-ND1
8	H	73	HIC	CA-CB-CG-CD2
8	I	73	HIC	CA-CB-CG-ND1
8	O	73	HIC	CA-CB-CG-ND1
8	O	73	HIC	CA-CB-CG-CD2
8	P	73	HIC	CA-CB-CG-ND1
8	Q	73	HIC	CA-CB-CG-ND1
8	Q	73	HIC	CA-CB-CG-CD2
8	R	73	HIC	CA-CB-CG-ND1
9	a	2	EEP	O2-CD1-CG-CB
9	a	2	EEP	O2-CD1-CG-O1
9	a	2	EEP	O2-CD1-CG-CD2
9	b	2	EEP	O2-CD1-CG-CB
9	b	2	EEP	O2-CD1-CG-O1
9	b	2	EEP	O2-CD1-CG-CD2
9	c	2	EEP	O2-CD1-CG-CB
9	c	2	EEP	O2-CD1-CG-O1
9	c	2	EEP	O2-CD1-CG-CD2
9	d	2	EEP	O2-CD1-CG-CB
9	d	2	EEP	O2-CD1-CG-O1
9	d	2	EEP	O2-CD1-CG-CD2
9	e	2	EEP	O2-CD1-CG-CB
9	e	2	EEP	O2-CD1-CG-O1
9	e	2	EEP	O2-CD1-CG-CD2
9	f	2	EEP	O2-CD1-CG-CB
9	f	2	EEP	O2-CD1-CG-O1
9	f	2	EEP	O2-CD1-CG-CD2
9	g	2	EEP	O2-CD1-CG-CB
9	g	2	EEP	O2-CD1-CG-O1
9	g	2	EEP	O2-CD1-CG-CD2
9	h	2	EEP	O2-CD1-CG-CB
9	h	2	EEP	O2-CD1-CG-O1
9	h	2	EEP	O2-CD1-CG-CD2
9	i	2	EEP	O2-CD1-CG-CB
9	i	2	EEP	O2-CD1-CG-O1
9	i	2	EEP	O2-CD1-CG-CD2
9	j	2	EEP	O2-CD1-CG-CB
9	j	2	EEP	O2-CD1-CG-O1
9	j	2	EEP	O2-CD1-CG-CD2
9	k	2	EEP	O2-CD1-CG-CB
9	k	2	EEP	O2-CD1-CG-O1
9	k	2	EEP	O2-CD1-CG-CD2

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Mol	Chain	Res	Type	Atoms
9	l	2	EEP	O2-CD1-CG-CB
9	l	2	EEP	O2-CD1-CG-O1
9	l	2	EEP	O2-CD1-CG-CD2
9	m	2	EEP	O2-CD1-CG-CB
9	m	2	EEP	O2-CD1-CG-O1
9	m	2	EEP	O2-CD1-CG-CD2
9	n	2	EEP	O2-CD1-CG-CB
9	n	2	EEP	O2-CD1-CG-O1
9	n	2	EEP	O2-CD1-CG-CD2
9	o	2	EEP	O2-CD1-CG-CB
9	o	2	EEP	O2-CD1-CG-O1
9	o	2	EEP	O2-CD1-CG-CD2
8	R	73	HIC	CA-CB-CG-CD2
8	I	73	HIC	CA-CB-CG-CD2
8	P	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	$\# Z  > 2$
11	ADP	A	502	10	24,29,29	2.74	12 (50%)	29,45,45	2.34	6 (20%)
11	ADP	L	501	10	24,29,29	2.73	12 (50%)	29,45,45	2.35	6 (20%)
11	ADP	M	501	10	24,29,29	2.73	12 (50%)	29,45,45	2.36	7 (24%)
11	ADP	R	501	10	24,29,29	2.50	11 (45%)	29,45,45	2.34	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	ADP	J	501	10	24,29,29	2.74	12 (50%)	29,45,45	2.34	6 (20%)
11	ADP	K	501	10	24,29,29	2.73	12 (50%)	29,45,45	2.33	6 (20%)
11	ADP	P	501	10	24,29,29	2.62	12 (50%)	29,45,45	2.29	6 (20%)
11	ADP	I	501	10	24,29,29	2.73	12 (50%)	29,45,45	2.35	6 (20%)
11	ADP	S	501	10	24,29,29	2.73	12 (50%)	29,45,45	2.33	6 (20%)
11	ADP	T	501	10	24,29,29	2.50	11 (45%)	29,45,45	2.31	6 (20%)
11	ADP	N	501	10	24,29,29	2.60	12 (50%)	29,45,45	2.33	6 (20%)
11	ADP	O	501	10	24,29,29	2.73	12 (50%)	29,45,45	2.27	6 (20%)
11	ADP	U	501	10	24,29,29	2.73	12 (50%)	29,45,45	2.33	6 (20%)
11	ADP	H	401	10	24,29,29	2.72	12 (50%)	29,45,45	2.33	6 (20%)
11	ADP	Q	501	10	24,29,29	2.72	12 (50%)	29,45,45	2.34	6 (20%)
11	ADP	B	502	10	24,29,29	2.73	12 (50%)	29,45,45	2.28	6 (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
11	ADP	A	502	10	-	2/12/32/32	0/3/3/3
11	ADP	L	501	10	-	4/12/32/32	0/3/3/3
11	ADP	M	501	10	-	4/12/32/32	0/3/3/3
11	ADP	R	501	10	-	4/12/32/32	0/3/3/3
11	ADP	J	501	10	-	5/12/32/32	0/3/3/3
11	ADP	K	501	10	-	5/12/32/32	0/3/3/3
11	ADP	P	501	10	-	2/12/32/32	0/3/3/3
11	ADP	I	501	10	-	3/12/32/32	0/3/3/3
11	ADP	S	501	10	-	3/12/32/32	0/3/3/3
11	ADP	T	501	10	-	6/12/32/32	0/3/3/3
11	ADP	N	501	10	-	2/12/32/32	0/3/3/3
11	ADP	O	501	10	-	4/12/32/32	0/3/3/3
11	ADP	U	501	10	-	5/12/32/32	0/3/3/3
11	ADP	H	401	10	-	5/12/32/32	0/3/3/3
11	ADP	Q	501	10	-	3/12/32/32	0/3/3/3
11	ADP	B	502	10	-	5/12/32/32	0/3/3/3

All (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	501	ADP	O4'-C1'	7.40	1.51	1.41
11	A	502	ADP	O4'-C1'	7.36	1.51	1.41
11	K	501	ADP	O4'-C1'	7.35	1.51	1.41
11	J	501	ADP	O4'-C1'	7.34	1.51	1.41
11	T	501	ADP	O4'-C1'	7.34	1.51	1.41
11	U	501	ADP	O4'-C1'	7.32	1.51	1.41
11	M	501	ADP	O4'-C1'	7.31	1.51	1.41
11	B	502	ADP	O4'-C1'	7.31	1.51	1.41
11	L	501	ADP	O4'-C1'	7.31	1.51	1.41
11	P	501	ADP	O4'-C1'	7.28	1.51	1.41
11	S	501	ADP	O4'-C1'	7.28	1.51	1.41
11	O	501	ADP	O4'-C1'	7.28	1.51	1.41
11	Q	501	ADP	O4'-C1'	7.25	1.51	1.41
11	I	501	ADP	O4'-C1'	7.25	1.51	1.41
11	H	401	ADP	O4'-C1'	7.24	1.51	1.41
11	N	501	ADP	O4'-C1'	7.15	1.51	1.41
11	U	501	ADP	PB-O1B	4.58	1.65	1.50
11	I	501	ADP	PB-O1B	4.58	1.65	1.50
11	J	501	ADP	PB-O1B	4.57	1.65	1.50
11	M	501	ADP	PB-O1B	4.56	1.65	1.50
11	H	401	ADP	PB-O1B	4.55	1.65	1.50
11	Q	501	ADP	PB-O1B	4.55	1.65	1.50
11	A	502	ADP	PB-O1B	4.54	1.65	1.50
11	S	501	ADP	PB-O1B	4.54	1.65	1.50
11	B	502	ADP	PB-O1B	4.54	1.65	1.50
11	P	501	ADP	PB-O1B	4.53	1.65	1.50
11	K	501	ADP	PB-O1B	4.53	1.65	1.50
11	O	501	ADP	PB-O1B	4.53	1.65	1.50
11	L	501	ADP	PB-O1B	4.52	1.65	1.50
11	N	501	ADP	PB-O1B	4.50	1.65	1.50
11	M	501	ADP	PA-O1A	4.06	1.65	1.50
11	S	501	ADP	PA-O1A	4.05	1.65	1.50
11	K	501	ADP	PA-O1A	4.05	1.65	1.50
11	J	501	ADP	PA-O1A	4.05	1.65	1.50
11	L	501	ADP	PA-O1A	4.04	1.65	1.50
11	U	501	ADP	PA-O1A	4.04	1.65	1.50
11	B	502	ADP	PA-O1A	4.04	1.65	1.50
11	I	501	ADP	PA-O1A	4.03	1.65	1.50
11	O	501	ADP	PA-O1A	4.03	1.65	1.50
11	Q	501	ADP	PA-O1A	4.03	1.65	1.50
11	A	502	ADP	PA-O1A	4.03	1.65	1.50
11	H	401	ADP	PA-O1A	4.02	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	501	ADP	C2'-C1'	-3.48	1.48	1.53
11	Q	501	ADP	C2'-C1'	-3.43	1.48	1.53
11	N	501	ADP	C2'-C1'	-3.43	1.48	1.53
11	T	501	ADP	C2'-C1'	-3.40	1.48	1.53
11	M	501	ADP	C2'-C1'	-3.40	1.48	1.53
11	S	501	ADP	C2'-C1'	-3.39	1.48	1.53
11	B	502	ADP	C2'-C1'	-3.38	1.48	1.53
11	A	502	ADP	C2'-C1'	-3.37	1.48	1.53
11	P	501	ADP	C2'-C1'	-3.36	1.48	1.53
11	J	501	ADP	C2'-C1'	-3.36	1.48	1.53
11	H	401	ADP	C2'-C1'	-3.36	1.48	1.53
11	I	501	ADP	C2'-C1'	-3.34	1.48	1.53
11	K	501	ADP	C2'-C1'	-3.34	1.48	1.53
11	L	501	ADP	C2'-C1'	-3.33	1.48	1.53
11	R	501	ADP	C2'-C1'	-3.31	1.48	1.53
11	U	501	ADP	C2'-C1'	-3.30	1.48	1.53
11	K	501	ADP	C6-N6	3.25	1.45	1.34
11	L	501	ADP	C6-N6	3.25	1.45	1.34
11	T	501	ADP	C6-N6	3.24	1.45	1.34
11	R	501	ADP	C6-N6	3.24	1.45	1.34
11	U	501	ADP	C6-N6	3.24	1.45	1.34
11	Q	501	ADP	C6-N6	3.24	1.45	1.34
11	N	501	ADP	C6-N6	3.23	1.45	1.34
11	S	501	ADP	C6-N6	3.23	1.45	1.34
11	J	501	ADP	C6-N6	3.23	1.45	1.34
11	P	501	ADP	C6-N6	3.22	1.45	1.34
11	A	502	ADP	C6-N6	3.22	1.45	1.34
11	M	501	ADP	C6-N6	3.22	1.45	1.34
11	I	501	ADP	C6-N6	3.21	1.45	1.34
11	O	501	ADP	C6-N6	3.21	1.45	1.34
11	H	401	ADP	C6-N6	3.20	1.45	1.34
11	B	502	ADP	C6-N6	3.20	1.45	1.34
11	T	501	ADP	C2'-C3'	-2.85	1.45	1.53
11	A	502	ADP	C2'-C3'	-2.84	1.45	1.53
11	B	502	ADP	C2'-C3'	-2.84	1.45	1.53
11	P	501	ADP	C2'-C3'	-2.83	1.45	1.53
11	O	501	ADP	C2'-C3'	-2.83	1.45	1.53
11	H	401	ADP	C2'-C3'	-2.83	1.45	1.53
11	N	501	ADP	C2'-C3'	-2.83	1.45	1.53
11	R	501	ADP	C2'-C3'	-2.82	1.45	1.53
11	S	501	ADP	C2'-C3'	-2.81	1.45	1.53
11	I	501	ADP	C2'-C3'	-2.81	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	501	ADP	C2'-C3'	-2.80	1.45	1.53
11	Q	501	ADP	C2'-C3'	-2.80	1.45	1.53
11	J	501	ADP	C2'-C3'	-2.79	1.45	1.53
11	L	501	ADP	O4'-C4'	2.78	1.51	1.45
11	L	501	ADP	C2'-C3'	-2.77	1.45	1.53
11	K	501	ADP	C2'-C3'	-2.77	1.45	1.53
11	J	501	ADP	O4'-C4'	2.76	1.51	1.45
11	U	501	ADP	C2'-C3'	-2.75	1.45	1.53
11	U	501	ADP	O4'-C4'	2.74	1.51	1.45
11	O	501	ADP	O4'-C4'	2.72	1.51	1.45
11	K	501	ADP	O4'-C4'	2.72	1.51	1.45
11	T	501	ADP	O4'-C4'	2.71	1.51	1.45
11	A	502	ADP	PB-O3B	2.71	1.65	1.54
11	H	401	ADP	PB-O3B	2.70	1.65	1.54
11	R	501	ADP	PB-O3B	2.70	1.65	1.54
11	I	501	ADP	PB-O2B	2.70	1.65	1.54
11	B	502	ADP	PB-O2B	2.70	1.65	1.54
11	T	501	ADP	PB-O2B	2.69	1.65	1.54
11	P	501	ADP	PB-O3B	2.69	1.65	1.54
11	A	502	ADP	O4'-C4'	2.69	1.51	1.45
11	P	501	ADP	O4'-C4'	2.69	1.51	1.45
11	N	501	ADP	PB-O3B	2.69	1.65	1.54
11	U	501	ADP	PB-O3B	2.69	1.65	1.54
11	T	501	ADP	PB-O3B	2.69	1.65	1.54
11	K	501	ADP	PB-O2B	2.69	1.65	1.54
11	R	501	ADP	PB-O2B	2.68	1.65	1.54
11	J	501	ADP	PB-O3B	2.68	1.65	1.54
11	I	501	ADP	O4'-C4'	2.68	1.51	1.45
11	B	502	ADP	O4'-C4'	2.68	1.51	1.45
11	R	501	ADP	O4'-C4'	2.68	1.51	1.45
11	S	501	ADP	O4'-C4'	2.67	1.51	1.45
11	L	501	ADP	PB-O3B	2.67	1.65	1.54
11	Q	501	ADP	PB-O2B	2.67	1.65	1.54
11	M	501	ADP	O4'-C4'	2.67	1.51	1.45
11	M	501	ADP	PB-O2B	2.67	1.65	1.54
11	H	401	ADP	O4'-C4'	2.67	1.51	1.45
11	O	501	ADP	PB-O2B	2.67	1.65	1.54
11	S	501	ADP	PB-O2B	2.66	1.65	1.54
11	Q	501	ADP	O4'-C4'	2.62	1.50	1.45
11	A	502	ADP	C4-N3	-2.60	1.32	1.35
11	N	501	ADP	O4'-C4'	2.55	1.50	1.45
11	S	501	ADP	C4-N3	-2.53	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	S	501	ADP	C2-N3	2.53	1.36	1.32
11	I	501	ADP	C4-N3	-2.52	1.32	1.35
11	Q	501	ADP	C4-N3	-2.52	1.32	1.35
11	N	501	ADP	C4-N3	-2.52	1.32	1.35
11	U	501	ADP	C2-N3	2.51	1.36	1.32
11	K	501	ADP	C2-N3	2.51	1.36	1.32
11	O	501	ADP	C2-N3	2.51	1.36	1.32
11	L	501	ADP	C2-N3	2.50	1.36	1.32
11	P	501	ADP	C2-N3	2.50	1.36	1.32
11	T	501	ADP	C4-N3	-2.49	1.32	1.35
11	O	501	ADP	C4-N3	-2.49	1.32	1.35
11	P	501	ADP	C4-N3	-2.49	1.32	1.35
11	R	501	ADP	C2-N3	2.49	1.36	1.32
11	R	501	ADP	C4-N3	-2.48	1.32	1.35
11	K	501	ADP	C4-N3	-2.48	1.32	1.35
11	B	502	ADP	C2-N3	2.48	1.36	1.32
11	I	501	ADP	C2-N3	2.47	1.36	1.32
11	H	401	ADP	C4-N3	-2.47	1.32	1.35
11	J	501	ADP	C2-N3	2.46	1.36	1.32
11	M	501	ADP	C2-N3	2.43	1.36	1.32
11	H	401	ADP	C2-N3	2.43	1.36	1.32
11	Q	501	ADP	C2-N3	2.43	1.36	1.32
11	B	502	ADP	C4-N3	-2.43	1.32	1.35
11	N	501	ADP	C2-N3	2.42	1.36	1.32
11	J	501	ADP	C4-N3	-2.42	1.32	1.35
11	L	501	ADP	C4-N3	-2.42	1.32	1.35
11	T	501	ADP	C2-N3	2.42	1.36	1.32
11	M	501	ADP	C4-N3	-2.40	1.32	1.35
11	A	502	ADP	C2-N3	2.39	1.35	1.32
11	U	501	ADP	C4-N3	-2.38	1.32	1.35
11	H	401	ADP	PB-O2B	-2.17	1.46	1.54
11	J	501	ADP	PB-O2B	-2.16	1.46	1.54
11	M	501	ADP	PB-O3B	-2.16	1.46	1.54
11	A	502	ADP	PB-O2B	-2.16	1.46	1.54
11	I	501	ADP	PB-O3B	-2.16	1.46	1.54
11	S	501	ADP	PB-O3B	-2.16	1.46	1.54
11	O	501	ADP	PB-O3B	-2.15	1.46	1.54
11	N	501	ADP	PB-O2B	-2.15	1.46	1.54
11	U	501	ADP	PB-O2B	-2.15	1.46	1.54
11	K	501	ADP	PB-O3B	-2.14	1.46	1.54
11	L	501	ADP	PB-O2B	-2.14	1.46	1.54
11	P	501	ADP	PB-O2B	-2.14	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	501	ADP	PA-O2A	2.14	1.65	1.55
11	Q	501	ADP	PB-O3B	-2.14	1.46	1.54
11	B	502	ADP	PB-O3B	-2.14	1.46	1.54
11	R	501	ADP	PA-O2A	2.13	1.65	1.55
11	P	501	ADP	PA-O2A	2.12	1.65	1.55
11	N	501	ADP	PA-O2A	2.12	1.65	1.55
11	O	501	ADP	C6-C5	-2.11	1.35	1.43
11	S	501	ADP	C6-C5	-2.08	1.35	1.43
11	M	501	ADP	C6-C5	-2.08	1.35	1.43
11	B	502	ADP	C6-C5	-2.07	1.35	1.43
11	N	501	ADP	C6-C5	-2.07	1.35	1.43
11	R	501	ADP	C6-C5	-2.07	1.35	1.43
11	U	501	ADP	C6-C5	-2.07	1.35	1.43
11	I	501	ADP	C6-C5	-2.07	1.35	1.43
11	Q	501	ADP	C6-C5	-2.07	1.35	1.43
11	P	501	ADP	C6-C5	-2.06	1.35	1.43
11	K	501	ADP	C6-C5	-2.06	1.35	1.43
11	L	501	ADP	C6-C5	-2.06	1.35	1.43
11	H	401	ADP	C6-C5	-2.05	1.35	1.43
11	J	501	ADP	C6-C5	-2.04	1.35	1.43
11	T	501	ADP	C6-C5	-2.04	1.35	1.43
11	A	502	ADP	C6-C5	-2.04	1.35	1.43

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	501	ADP	PA-O3A-PB	-7.22	108.05	132.83
11	O	501	ADP	PA-O3A-PB	-7.13	108.37	132.83
11	Q	501	ADP	PA-O3A-PB	-7.10	108.46	132.83
11	P	501	ADP	PA-O3A-PB	-7.03	108.70	132.83
11	B	502	ADP	PA-O3A-PB	-6.98	108.89	132.83
11	S	501	ADP	PA-O3A-PB	-6.90	109.16	132.83
11	L	501	ADP	PA-O3A-PB	-6.88	109.21	132.83
11	K	501	ADP	PA-O3A-PB	-6.86	109.29	132.83
11	T	501	ADP	PA-O3A-PB	-6.83	109.38	132.83
11	R	501	ADP	PA-O3A-PB	-6.82	109.44	132.83
11	N	501	ADP	PA-O3A-PB	-6.78	109.55	132.83
11	J	501	ADP	PA-O3A-PB	-6.77	109.60	132.83
11	M	501	ADP	PA-O3A-PB	-6.74	109.69	132.83
11	A	502	ADP	PA-O3A-PB	-6.72	109.77	132.83
11	U	501	ADP	PA-O3A-PB	-6.67	109.94	132.83
11	H	401	ADP	PA-O3A-PB	-6.51	110.50	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	501	ADP	N3-C2-N1	-5.28	120.43	128.68
11	H	401	ADP	N3-C2-N1	-5.27	120.44	128.68
11	Q	501	ADP	N3-C2-N1	-5.25	120.47	128.68
11	J	501	ADP	N3-C2-N1	-5.24	120.49	128.68
11	T	501	ADP	N3-C2-N1	-5.24	120.49	128.68
11	R	501	ADP	N3-C2-N1	-5.23	120.50	128.68
11	M	501	ADP	N3-C2-N1	-5.23	120.51	128.68
11	P	501	ADP	N3-C2-N1	-5.22	120.52	128.68
11	U	501	ADP	N3-C2-N1	-5.22	120.53	128.68
11	B	502	ADP	N3-C2-N1	-5.22	120.53	128.68
11	L	501	ADP	N3-C2-N1	-5.22	120.53	128.68
11	S	501	ADP	N3-C2-N1	-5.20	120.55	128.68
11	K	501	ADP	N3-C2-N1	-5.20	120.55	128.68
11	I	501	ADP	N3-C2-N1	-5.19	120.57	128.68
11	A	502	ADP	N3-C2-N1	-5.19	120.57	128.68
11	O	501	ADP	N3-C2-N1	-5.12	120.68	128.68
11	U	501	ADP	C3'-C2'-C1'	5.00	108.51	100.98
11	K	501	ADP	C3'-C2'-C1'	4.99	108.50	100.98
11	L	501	ADP	C3'-C2'-C1'	4.95	108.43	100.98
11	M	501	ADP	C3'-C2'-C1'	4.93	108.39	100.98
11	J	501	ADP	C3'-C2'-C1'	4.92	108.39	100.98
11	H	401	ADP	C3'-C2'-C1'	4.89	108.34	100.98
11	A	502	ADP	C3'-C2'-C1'	4.83	108.25	100.98
11	R	501	ADP	C3'-C2'-C1'	4.81	108.22	100.98
11	N	501	ADP	C3'-C2'-C1'	4.76	108.15	100.98
11	S	501	ADP	C3'-C2'-C1'	4.73	108.10	100.98
11	T	501	ADP	C3'-C2'-C1'	4.72	108.08	100.98
11	I	501	ADP	C3'-C2'-C1'	4.66	108.00	100.98
11	B	502	ADP	C3'-C2'-C1'	4.60	107.90	100.98
11	Q	501	ADP	C3'-C2'-C1'	4.59	107.89	100.98
11	M	501	ADP	C1'-N9-C4	-4.46	118.81	126.64
11	P	501	ADP	C3'-C2'-C1'	4.43	107.66	100.98
11	A	502	ADP	C1'-N9-C4	-4.40	118.91	126.64
11	H	401	ADP	C1'-N9-C4	-4.38	118.94	126.64
11	O	501	ADP	C3'-C2'-C1'	4.36	107.54	100.98
11	N	501	ADP	C1'-N9-C4	-4.34	119.01	126.64
11	R	501	ADP	C1'-N9-C4	-4.29	119.10	126.64
11	T	501	ADP	C1'-N9-C4	-4.28	119.12	126.64
11	Q	501	ADP	C1'-N9-C4	-4.25	119.18	126.64
11	B	502	ADP	C1'-N9-C4	-4.25	119.18	126.64
11	I	501	ADP	C1'-N9-C4	-4.24	119.20	126.64
11	P	501	ADP	C1'-N9-C4	-4.19	119.28	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	501	ADP	C1'-N9-C4	-4.19	119.29	126.64
11	J	501	ADP	C1'-N9-C4	-4.18	119.30	126.64
11	L	501	ADP	C1'-N9-C4	-4.15	119.34	126.64
11	U	501	ADP	C1'-N9-C4	-4.14	119.37	126.64
11	O	501	ADP	C1'-N9-C4	-4.09	119.46	126.64
11	K	501	ADP	C1'-N9-C4	-4.04	119.55	126.64
11	J	501	ADP	C4-C5-N7	-3.85	105.38	109.40
11	H	401	ADP	C4-C5-N7	-3.83	105.41	109.40
11	R	501	ADP	C4-C5-N7	-3.82	105.42	109.40
11	U	501	ADP	C4-C5-N7	-3.82	105.42	109.40
11	A	502	ADP	C4-C5-N7	-3.81	105.42	109.40
11	I	501	ADP	C4-C5-N7	-3.80	105.44	109.40
11	L	501	ADP	C4-C5-N7	-3.80	105.44	109.40
11	K	501	ADP	C4-C5-N7	-3.78	105.45	109.40
11	B	502	ADP	C4-C5-N7	-3.78	105.46	109.40
11	M	501	ADP	C4-C5-N7	-3.77	105.47	109.40
11	Q	501	ADP	C4-C5-N7	-3.77	105.47	109.40
11	T	501	ADP	C4-C5-N7	-3.76	105.48	109.40
11	S	501	ADP	C4-C5-N7	-3.74	105.50	109.40
11	N	501	ADP	C4-C5-N7	-3.74	105.50	109.40
11	P	501	ADP	C4-C5-N7	-3.73	105.51	109.40
11	O	501	ADP	C4-C5-N7	-3.64	105.60	109.40
11	H	401	ADP	C2'-C3'-C4'	3.13	108.72	102.64
11	U	501	ADP	C2'-C3'-C4'	3.05	108.56	102.64
11	M	501	ADP	C2'-C3'-C4'	3.01	108.48	102.64
11	J	501	ADP	C2'-C3'-C4'	3.00	108.48	102.64
11	L	501	ADP	C2'-C3'-C4'	2.99	108.45	102.64
11	A	502	ADP	C2'-C3'-C4'	2.99	108.44	102.64
11	K	501	ADP	C2'-C3'-C4'	2.97	108.41	102.64
11	R	501	ADP	C2'-C3'-C4'	2.96	108.40	102.64
11	S	501	ADP	C2'-C3'-C4'	2.90	108.28	102.64
11	N	501	ADP	C2'-C3'-C4'	2.84	108.16	102.64
11	I	501	ADP	C2'-C3'-C4'	2.75	107.99	102.64
11	Q	501	ADP	C2'-C3'-C4'	2.75	107.98	102.64
11	T	501	ADP	C2'-C3'-C4'	2.72	107.93	102.64
11	P	501	ADP	C2'-C3'-C4'	2.53	107.56	102.64
11	O	501	ADP	C2'-C3'-C4'	2.49	107.49	102.64
11	B	502	ADP	C2'-C3'-C4'	2.31	107.13	102.64
11	M	501	ADP	PA-O5'-C5'	-2.05	109.65	121.68

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	502	ADP	C5'-O5'-PA-O1A
11	B	502	ADP	C5'-O5'-PA-O1A
11	B	502	ADP	C5'-O5'-PA-O3A
11	B	502	ADP	O4'-C4'-C5'-O5'
11	B	502	ADP	C3'-C4'-C5'-O5'
11	H	401	ADP	C5'-O5'-PA-O1A
11	J	501	ADP	C5'-O5'-PA-O1A
11	K	501	ADP	C5'-O5'-PA-O1A
11	K	501	ADP	C5'-O5'-PA-O3A
11	L	501	ADP	C5'-O5'-PA-O1A
11	M	501	ADP	C5'-O5'-PA-O1A
11	O	501	ADP	C5'-O5'-PA-O1A
11	R	501	ADP	PA-O3A-PB-O2B
11	R	501	ADP	PA-O3A-PB-O3B
11	T	501	ADP	C5'-O5'-PA-O3A
11	U	501	ADP	C5'-O5'-PA-O1A
11	U	501	ADP	C5'-O5'-PA-O3A
11	H	401	ADP	O4'-C4'-C5'-O5'
11	H	401	ADP	C3'-C4'-C5'-O5'
11	K	501	ADP	O4'-C4'-C5'-O5'
11	K	501	ADP	C3'-C4'-C5'-O5'
11	J	501	ADP	O4'-C4'-C5'-O5'
11	T	501	ADP	O4'-C4'-C5'-O5'
11	J	501	ADP	C3'-C4'-C5'-O5'
11	T	501	ADP	C3'-C4'-C5'-O5'
11	Q	501	ADP	C3'-C4'-C5'-O5'
11	R	501	ADP	C3'-C4'-C5'-O5'
11	Q	501	ADP	O4'-C4'-C5'-O5'
11	R	501	ADP	O4'-C4'-C5'-O5'
11	H	401	ADP	C4'-C5'-O5'-PA
11	J	501	ADP	C5'-O5'-PA-O3A
11	M	501	ADP	C5'-O5'-PA-O3A
11	O	501	ADP	C5'-O5'-PA-O3A
11	O	501	ADP	C3'-C4'-C5'-O5'
11	U	501	ADP	O4'-C4'-C5'-O5'
11	U	501	ADP	C3'-C4'-C5'-O5'
11	B	502	ADP	C5'-O5'-PA-O2A
11	T	501	ADP	C5'-O5'-PA-O2A
11	I	501	ADP	C3'-C4'-C5'-O5'
11	L	501	ADP	C3'-C4'-C5'-O5'
11	P	501	ADP	C3'-C4'-C5'-O5'
11	L	501	ADP	O4'-C4'-C5'-O5'
11	O	501	ADP	O4'-C4'-C5'-O5'

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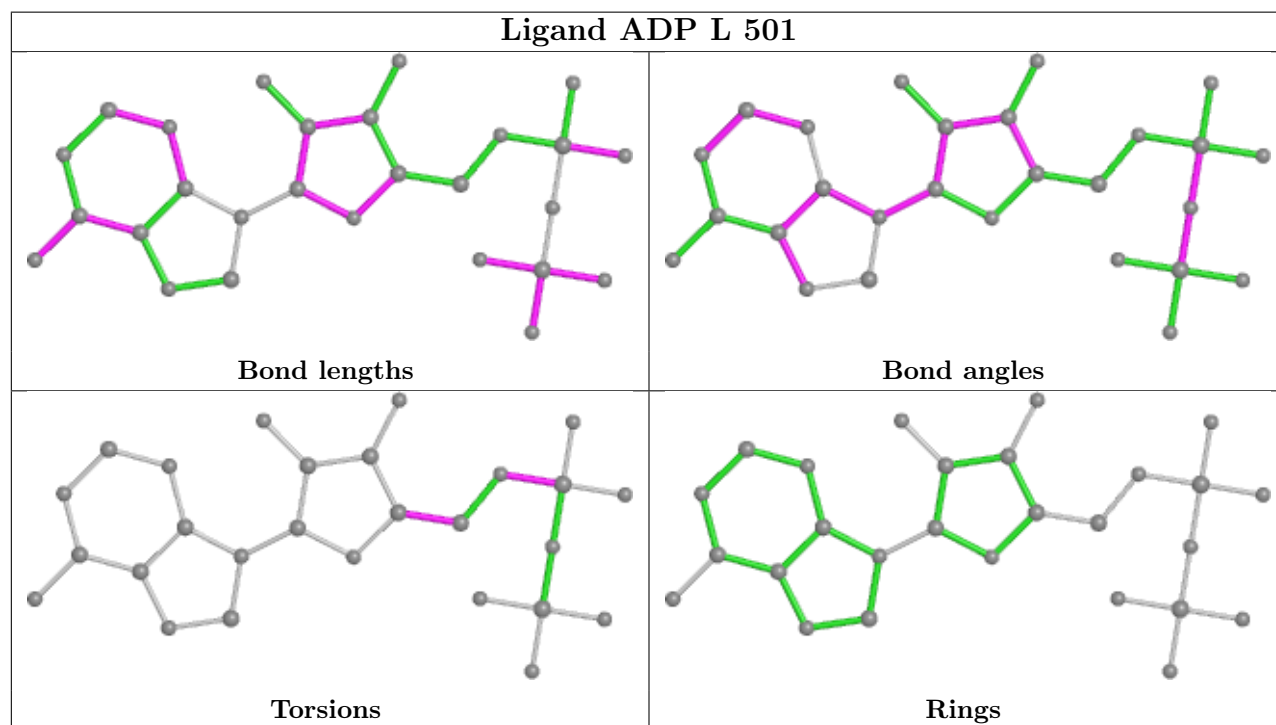
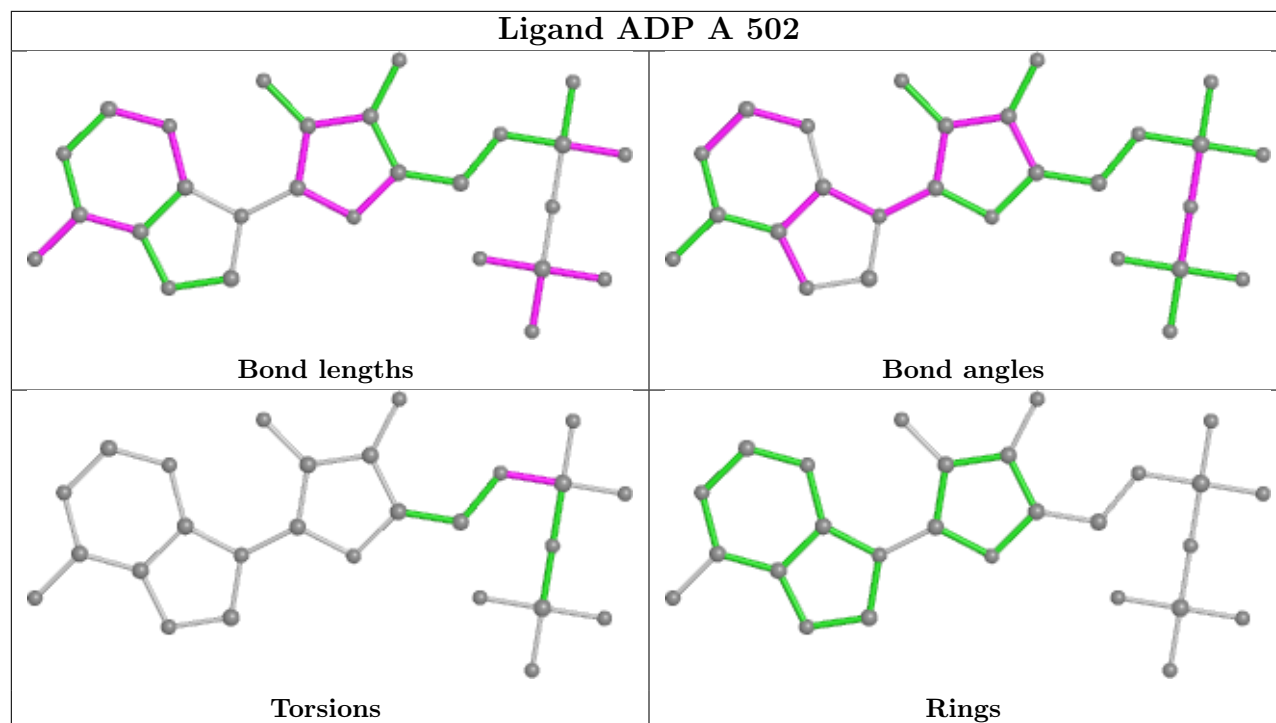
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
11	P	501	ADP	O4'-C4'-C5'-O5'
11	T	501	ADP	C4'-C5'-O5'-PA
11	K	501	ADP	C4'-C5'-O5'-PA
11	M	501	ADP	C4'-C5'-O5'-PA
11	U	501	ADP	C4'-C5'-O5'-PA
11	I	501	ADP	O4'-C4'-C5'-O5'
11	N	501	ADP	C3'-C4'-C5'-O5'
11	J	501	ADP	C4'-C5'-O5'-PA
11	S	501	ADP	C3'-C4'-C5'-O5'
11	M	501	ADP	PA-O3A-PB-O2B
11	A	502	ADP	C5'-O5'-PA-O3A
11	H	401	ADP	C5'-O5'-PA-O3A
11	L	501	ADP	C5'-O5'-PA-O3A
11	N	501	ADP	O4'-C4'-C5'-O5'
11	S	501	ADP	O4'-C4'-C5'-O5'
11	I	501	ADP	C5'-O5'-PA-O1A
11	Q	501	ADP	C5'-O5'-PA-O1A
11	S	501	ADP	C5'-O5'-PA-O1A
11	T	501	ADP	C5'-O5'-PA-O1A

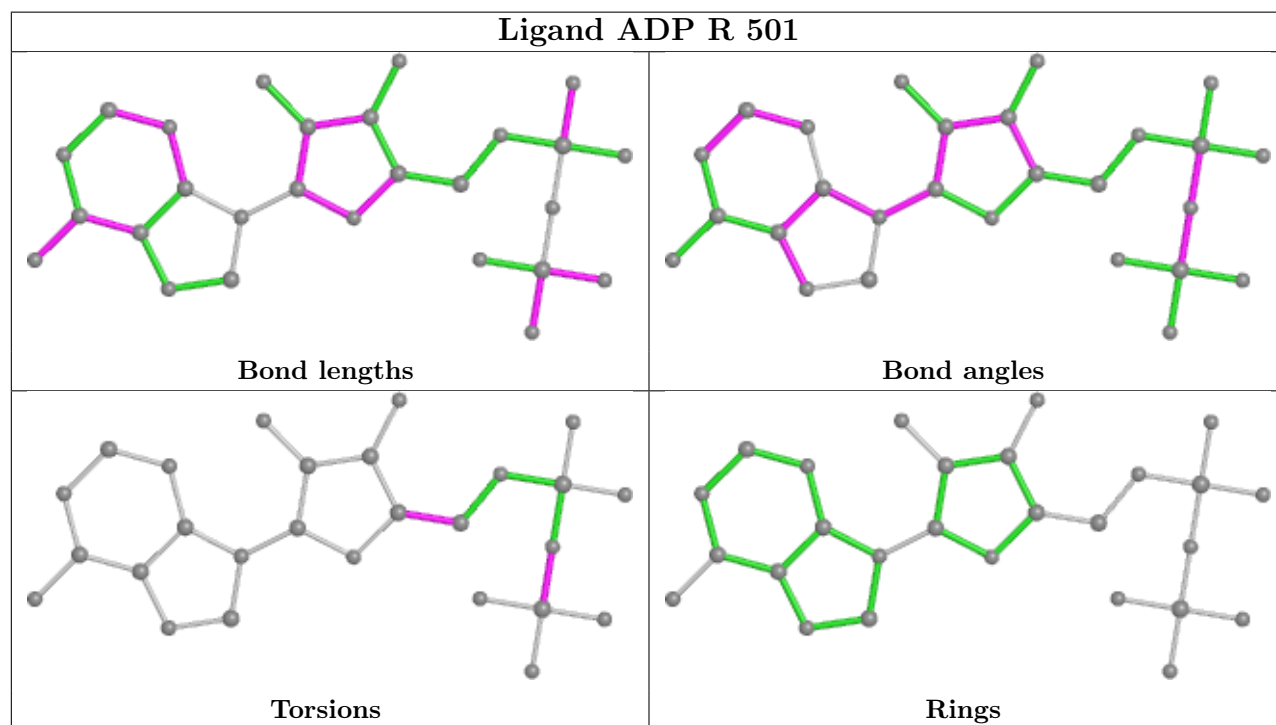
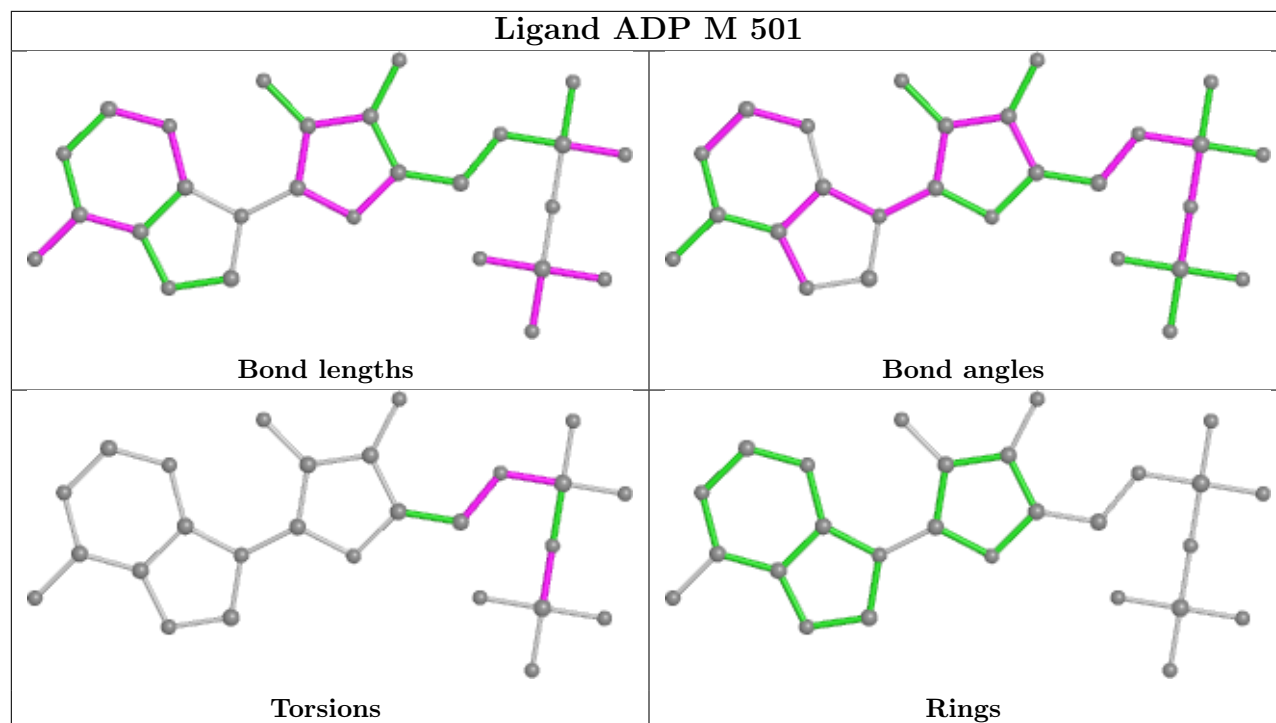
There are no ring outliers.

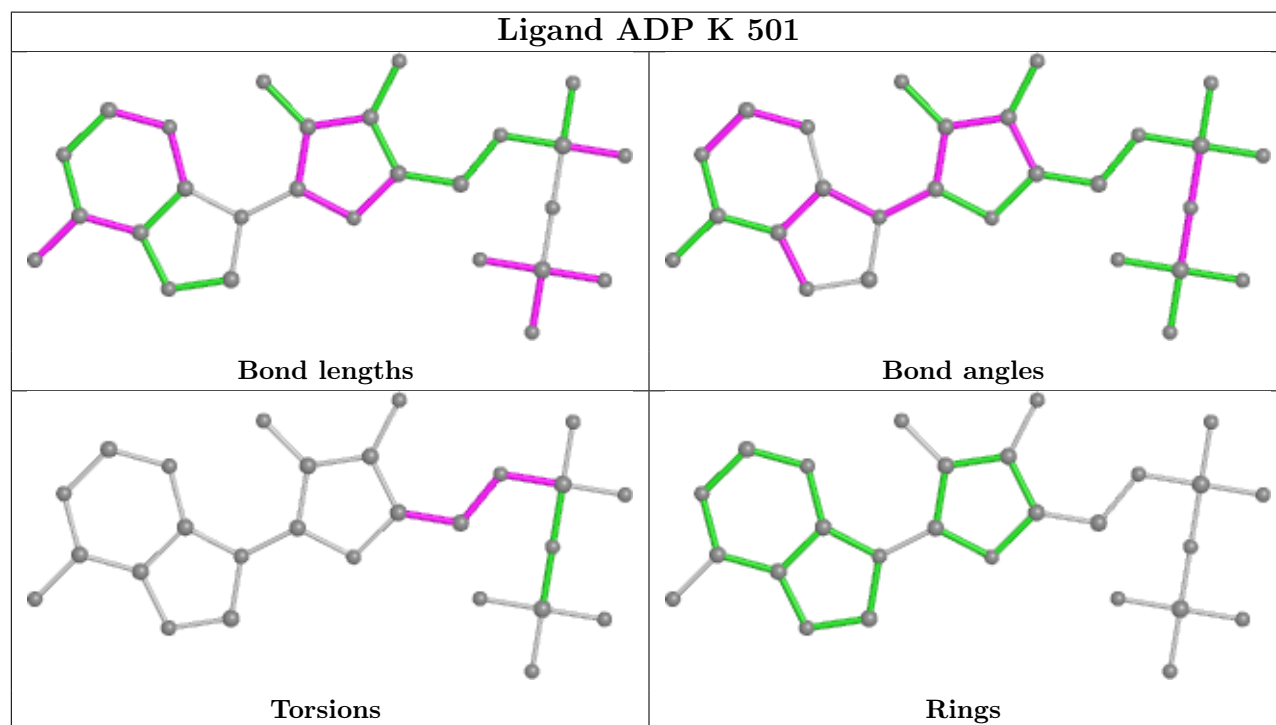
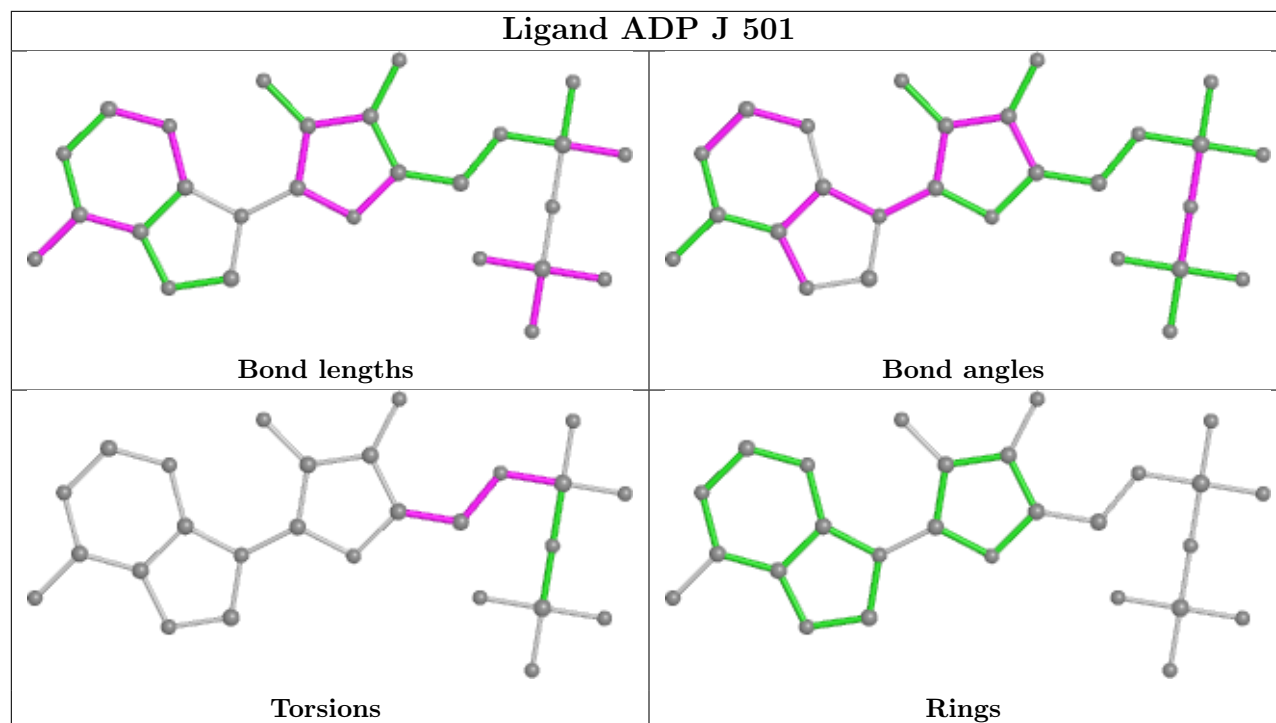
No monomer is involved in short contacts.

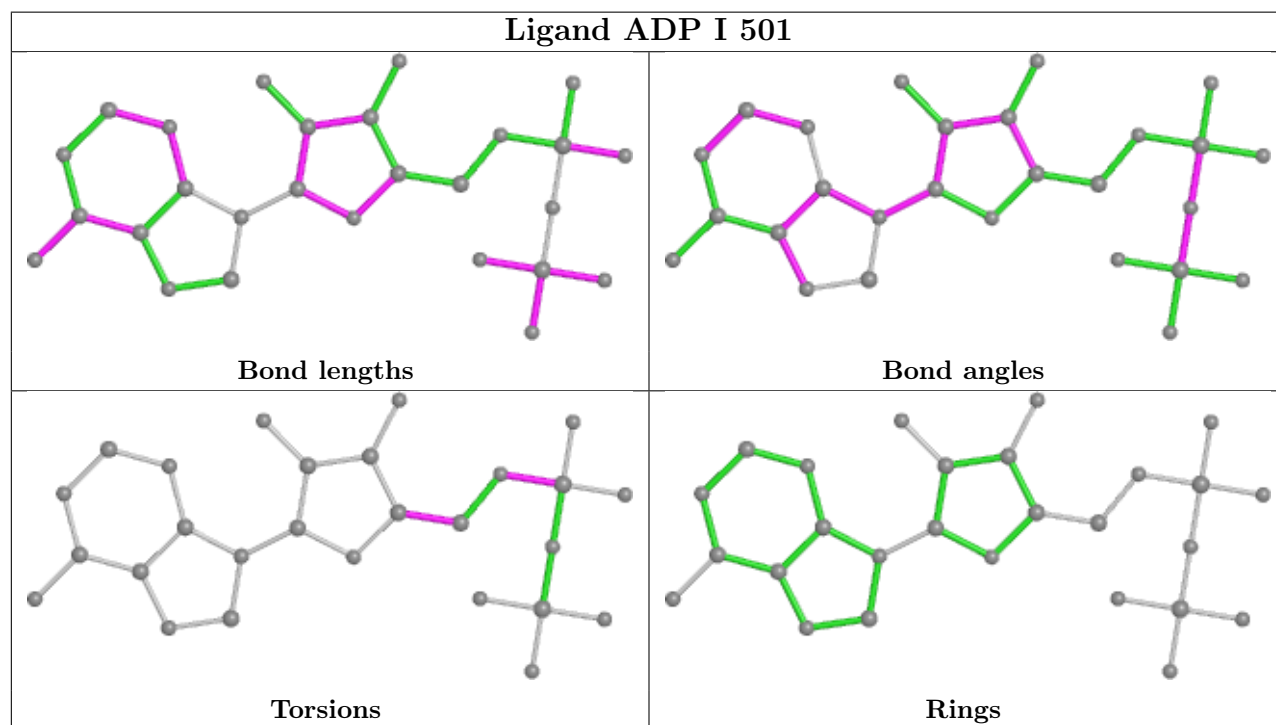
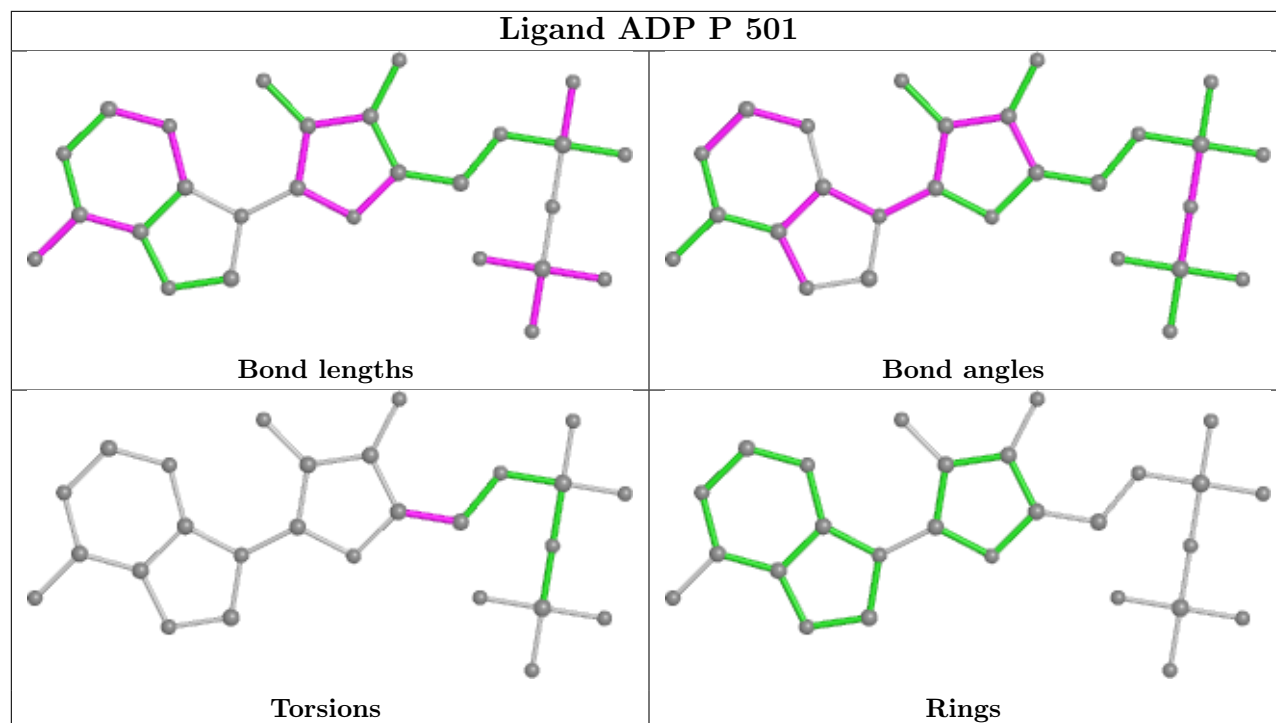
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

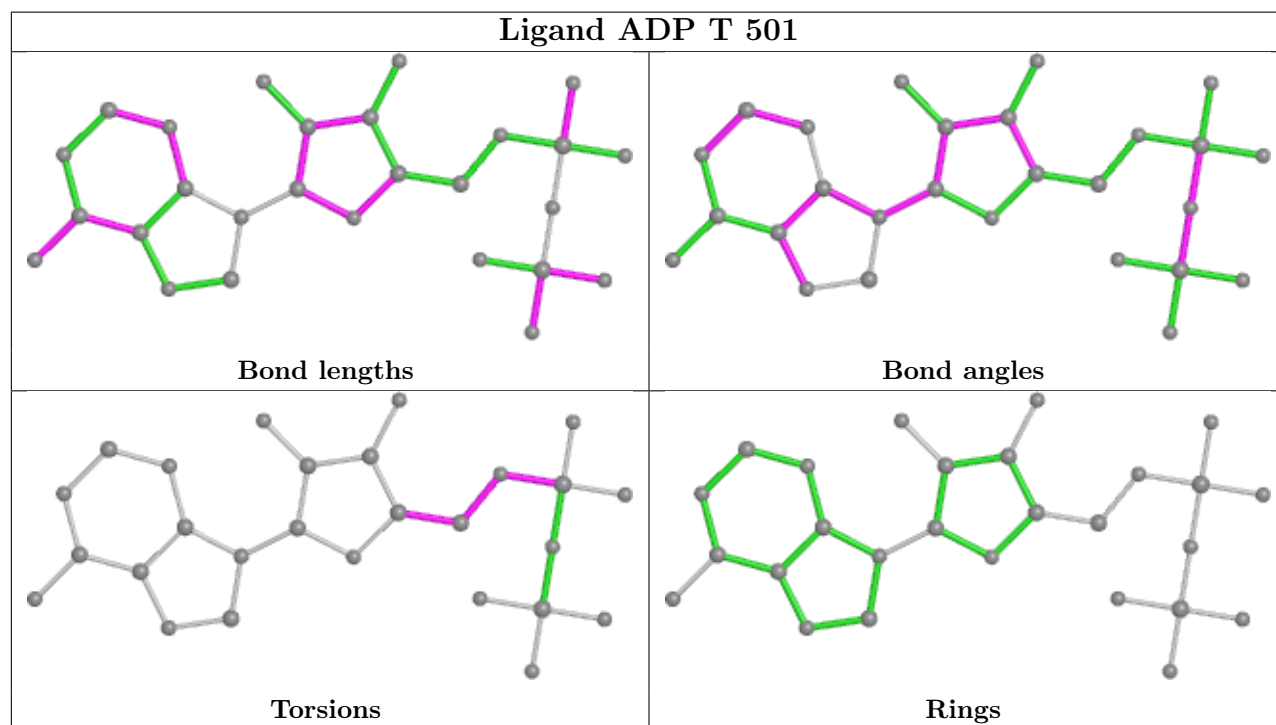
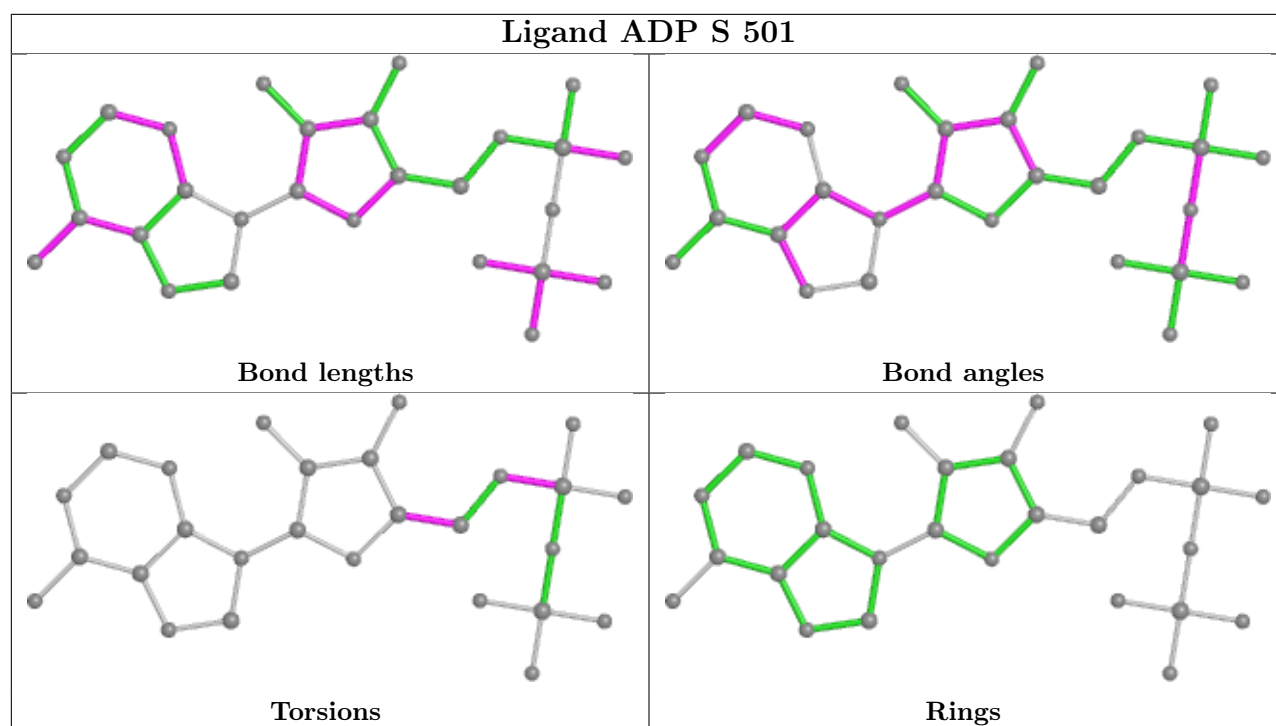


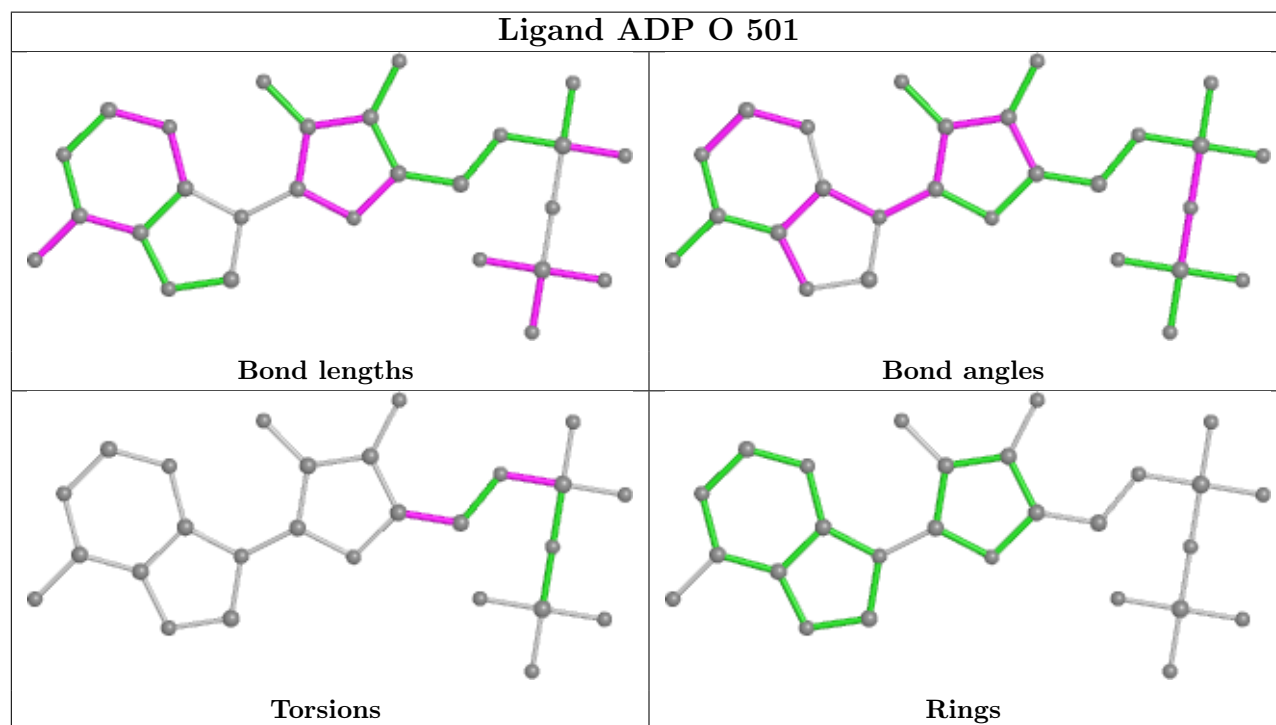
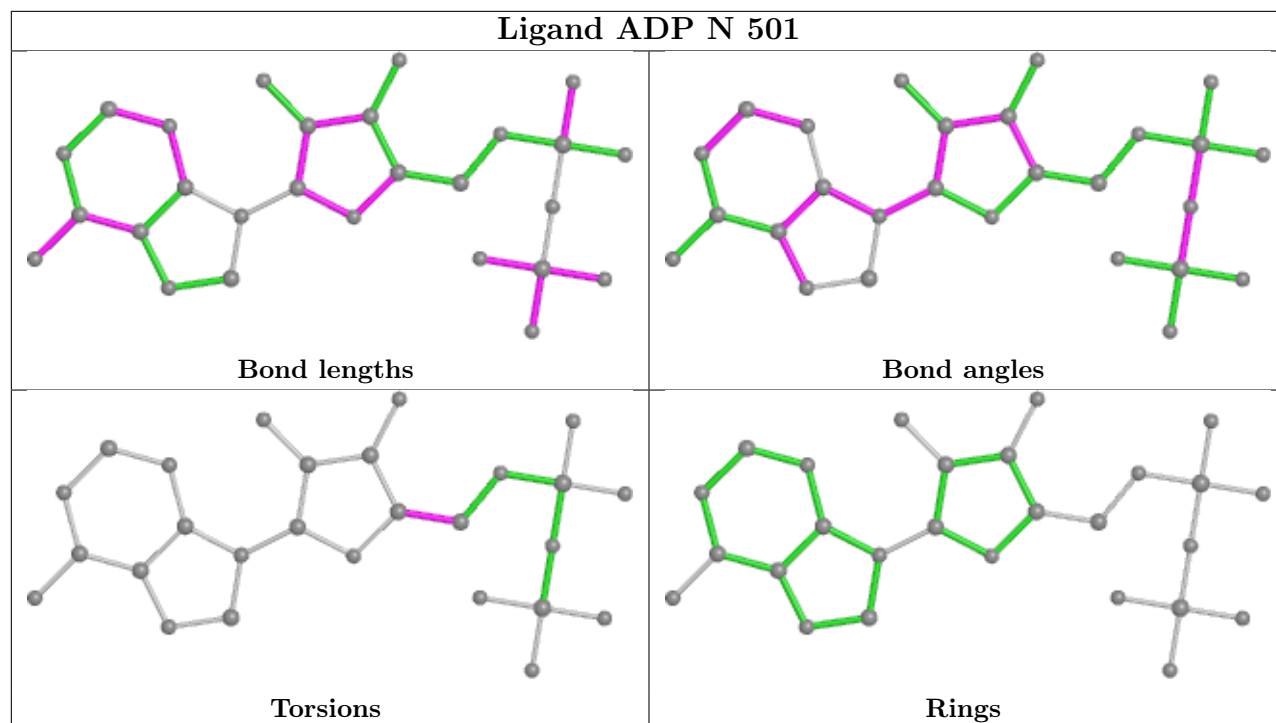


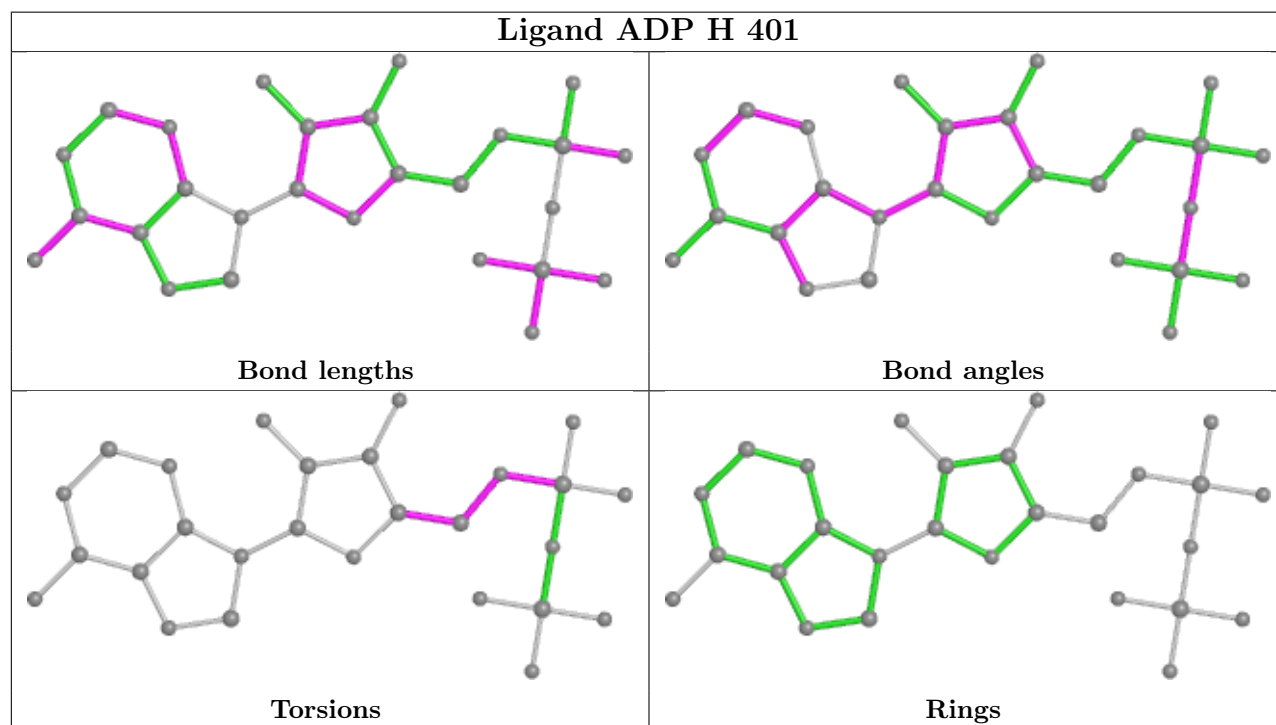
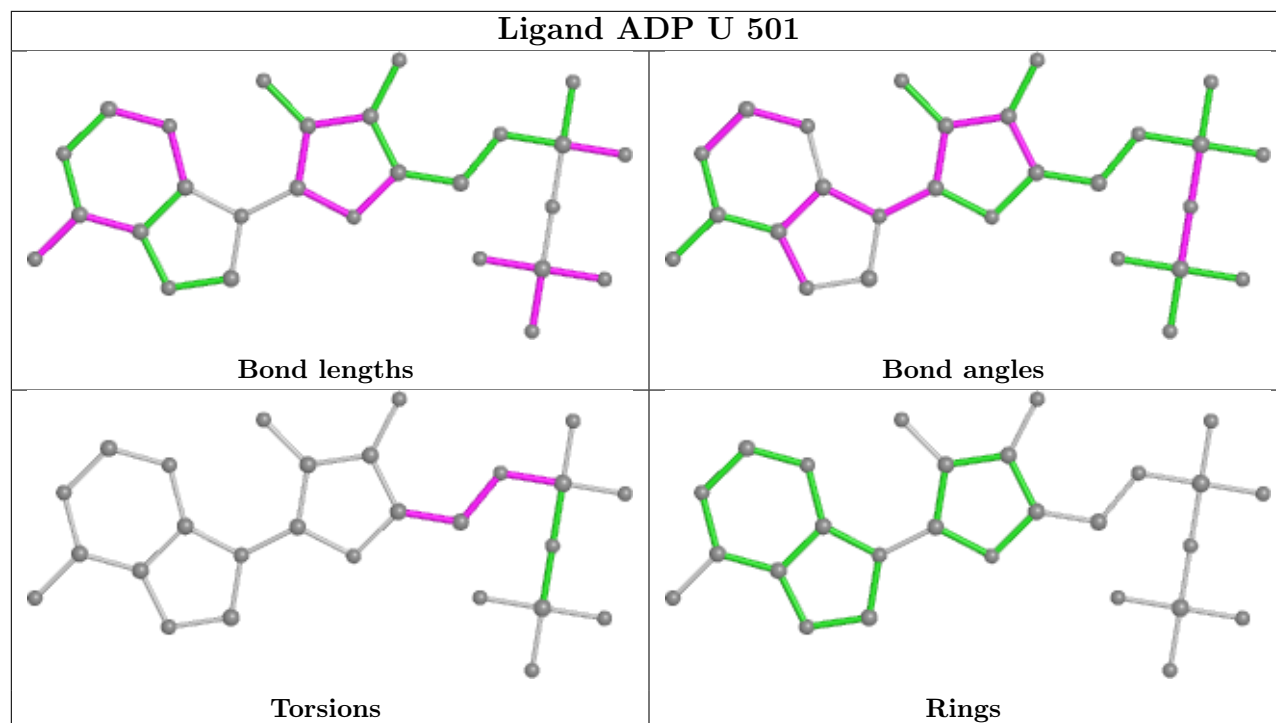


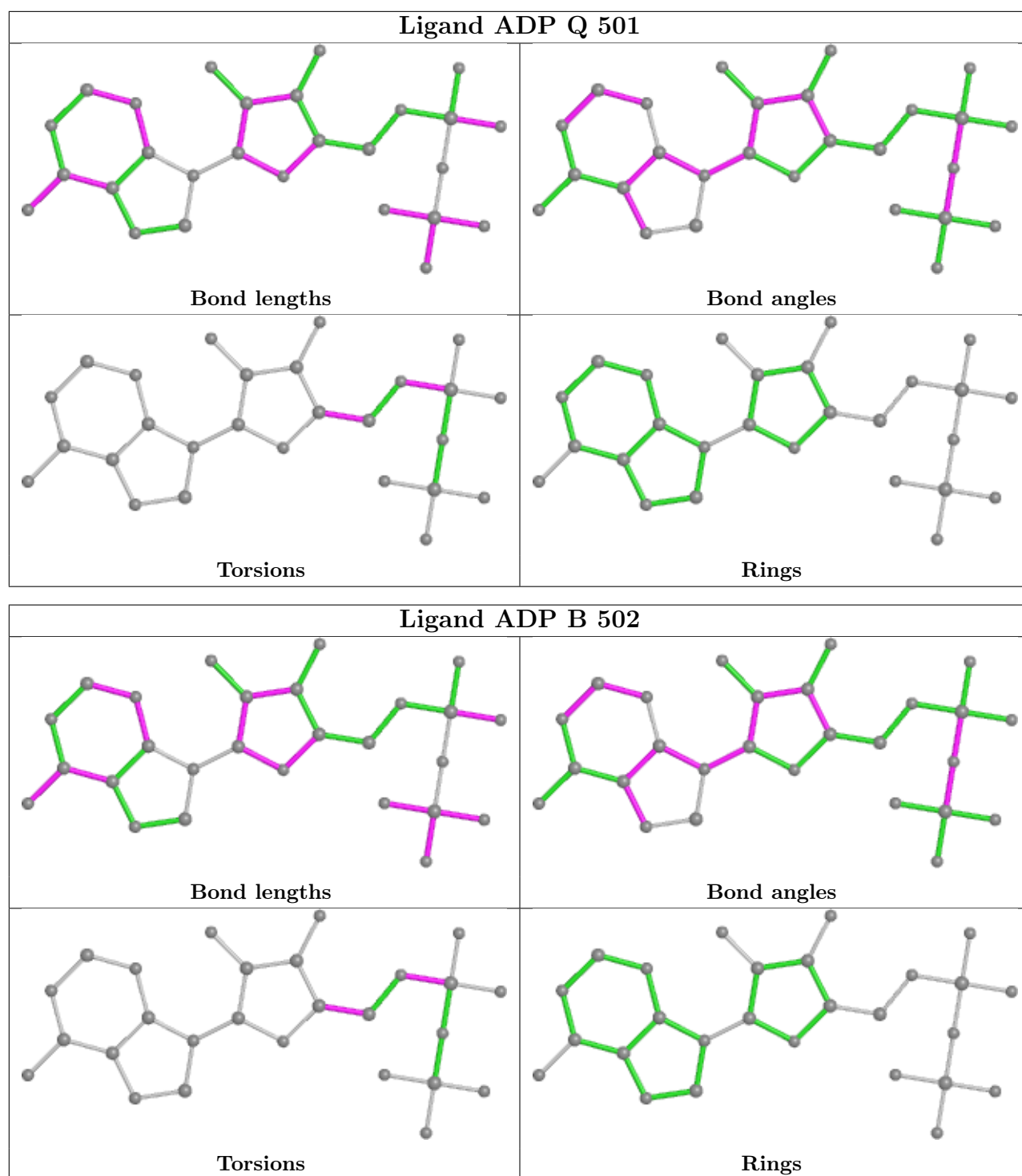












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



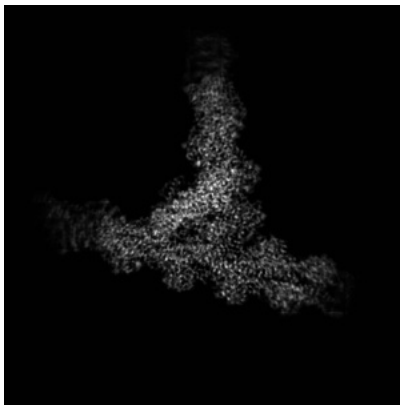
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26063. These allow visual inspection of the internal detail of the map and identification of artifacts.

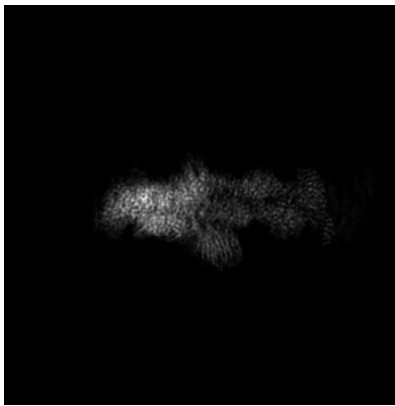
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

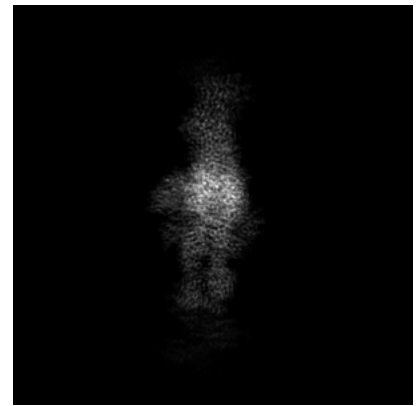
#### 6.1.1 Primary map



X

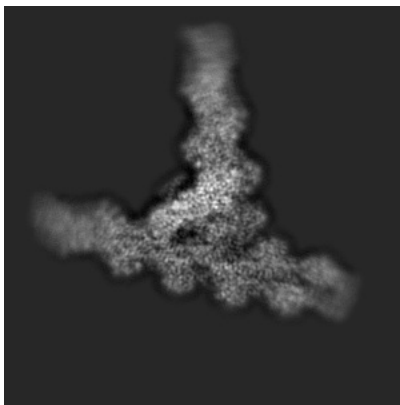


Y

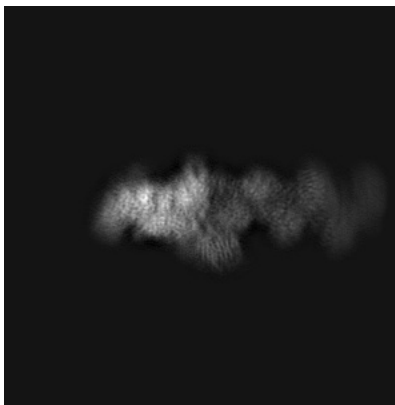


Z

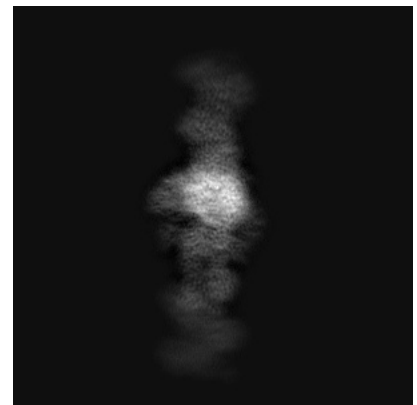
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

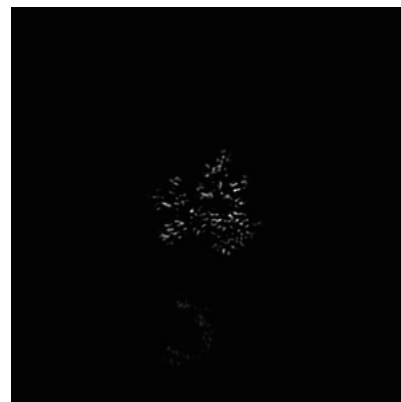
### 6.2.1 Primary map



X Index: 184

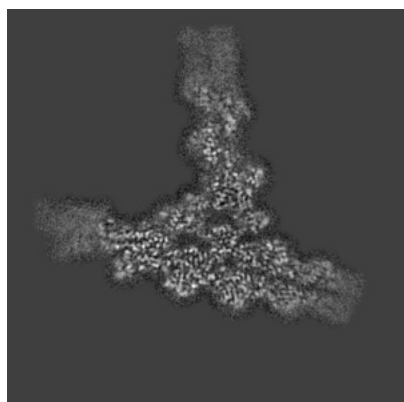


Y Index: 184

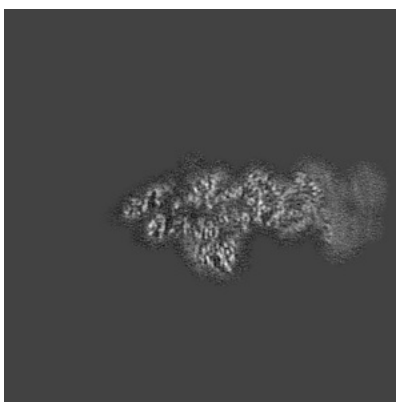


Z Index: 184

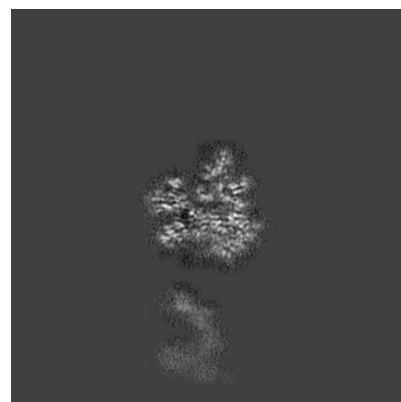
### 6.2.2 Raw map



X Index: 184



Y Index: 184



Z Index: 184

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: 189

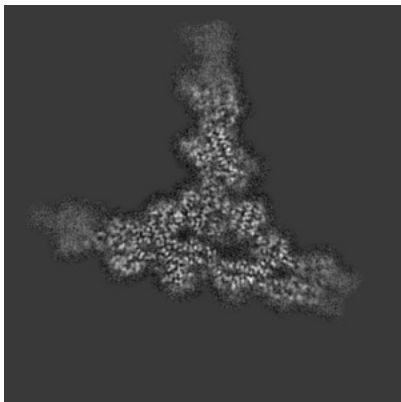


Y Index: 196

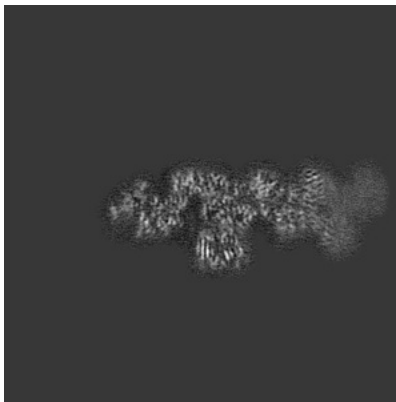


Z Index: 130

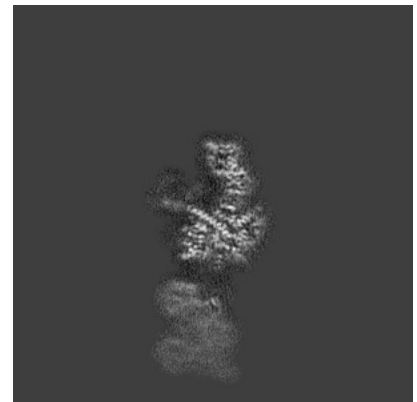
### 6.3.2 Raw map



X Index: 193



Y Index: 195

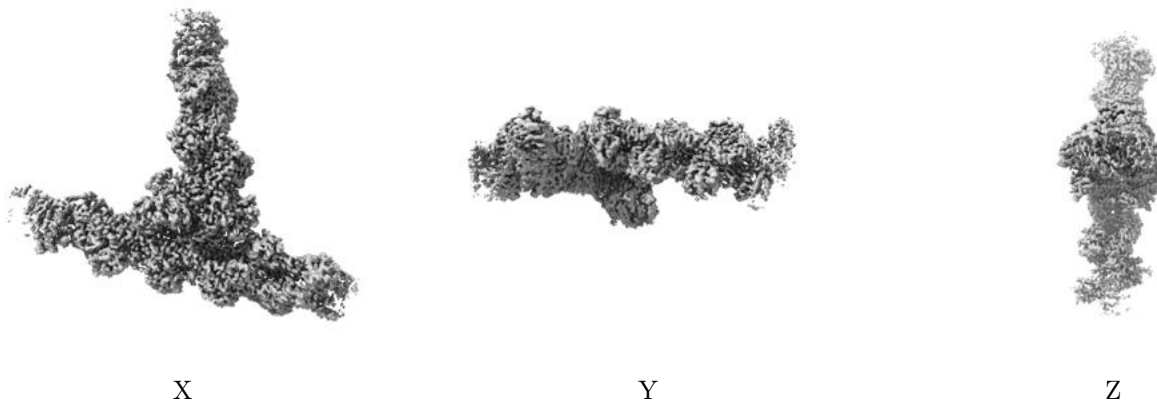


Z Index: 173

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

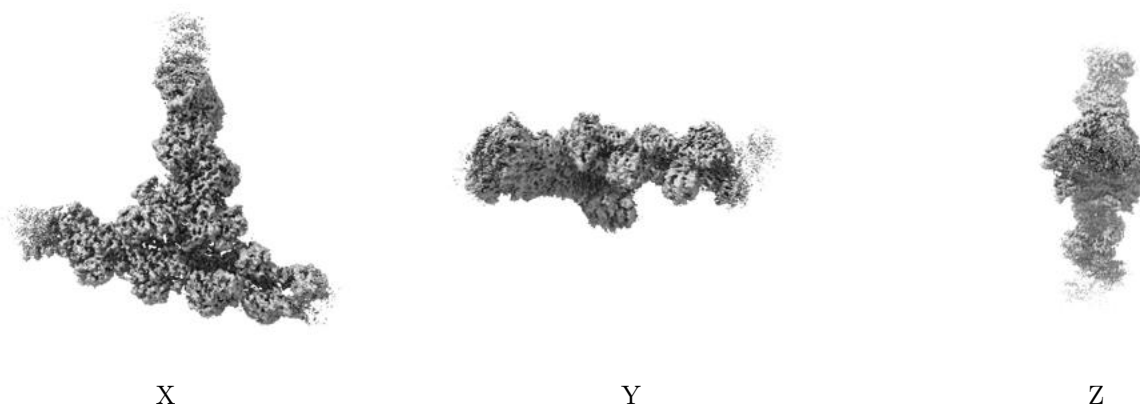
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

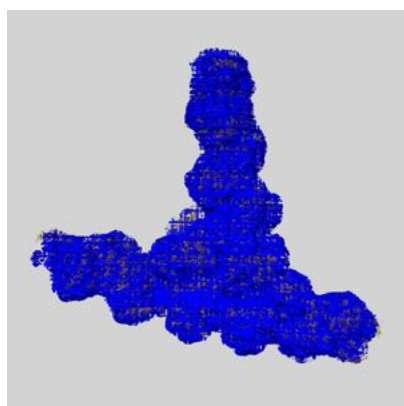
## 6.5 Mask visualisation [i](#)

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

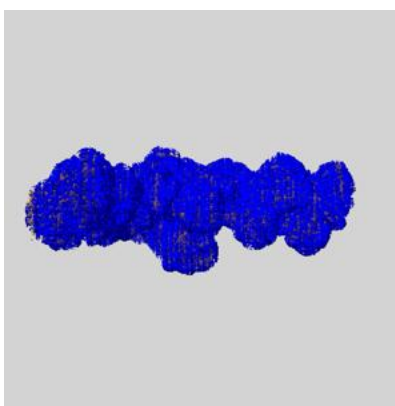
A mask typically either:

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

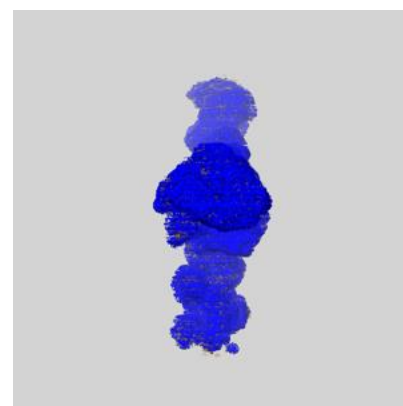
### 6.5.1 emd\_26063\_msk\_1.map [i](#)



X



Y

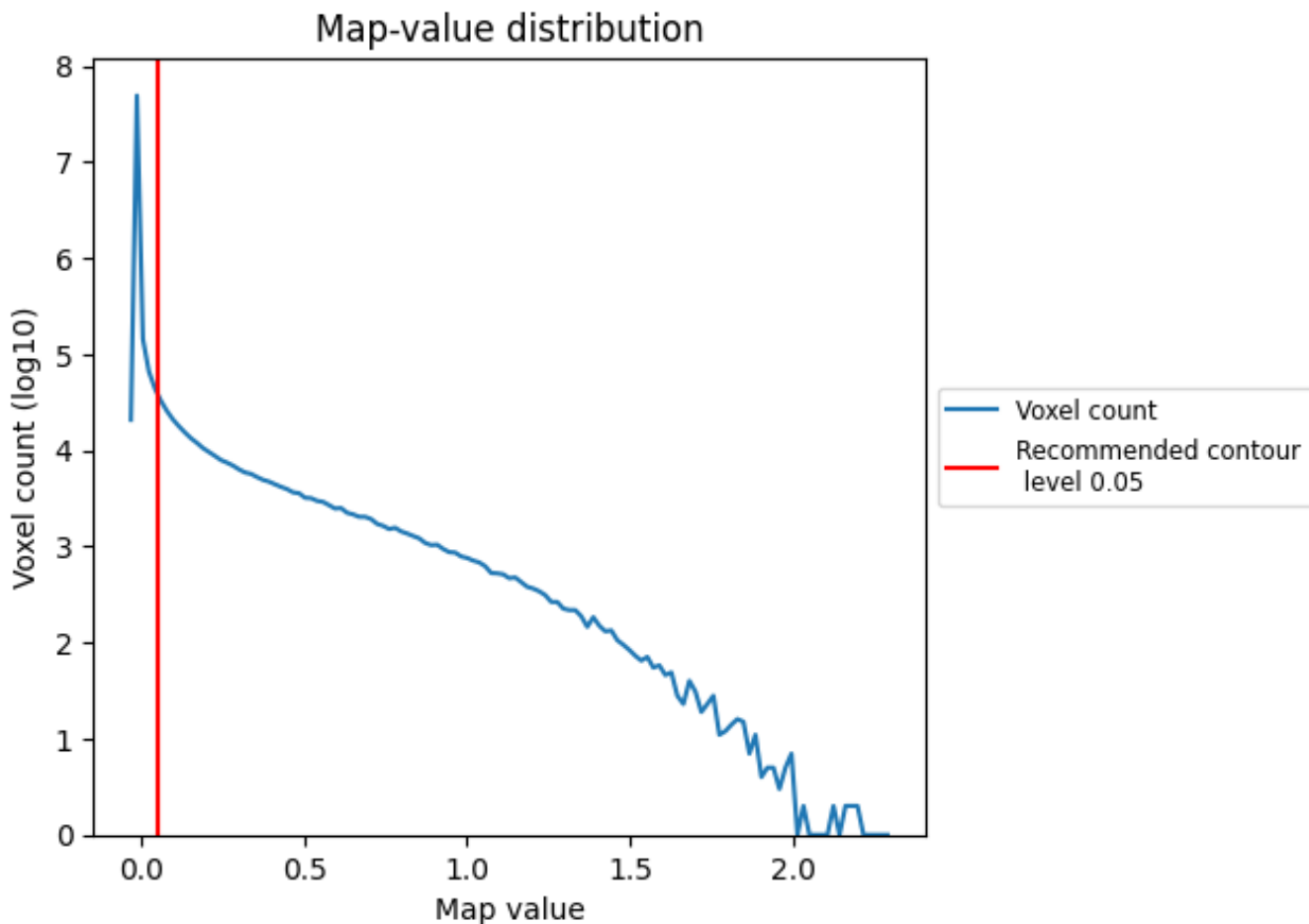


Z

## 7 Map analysis [i](#)

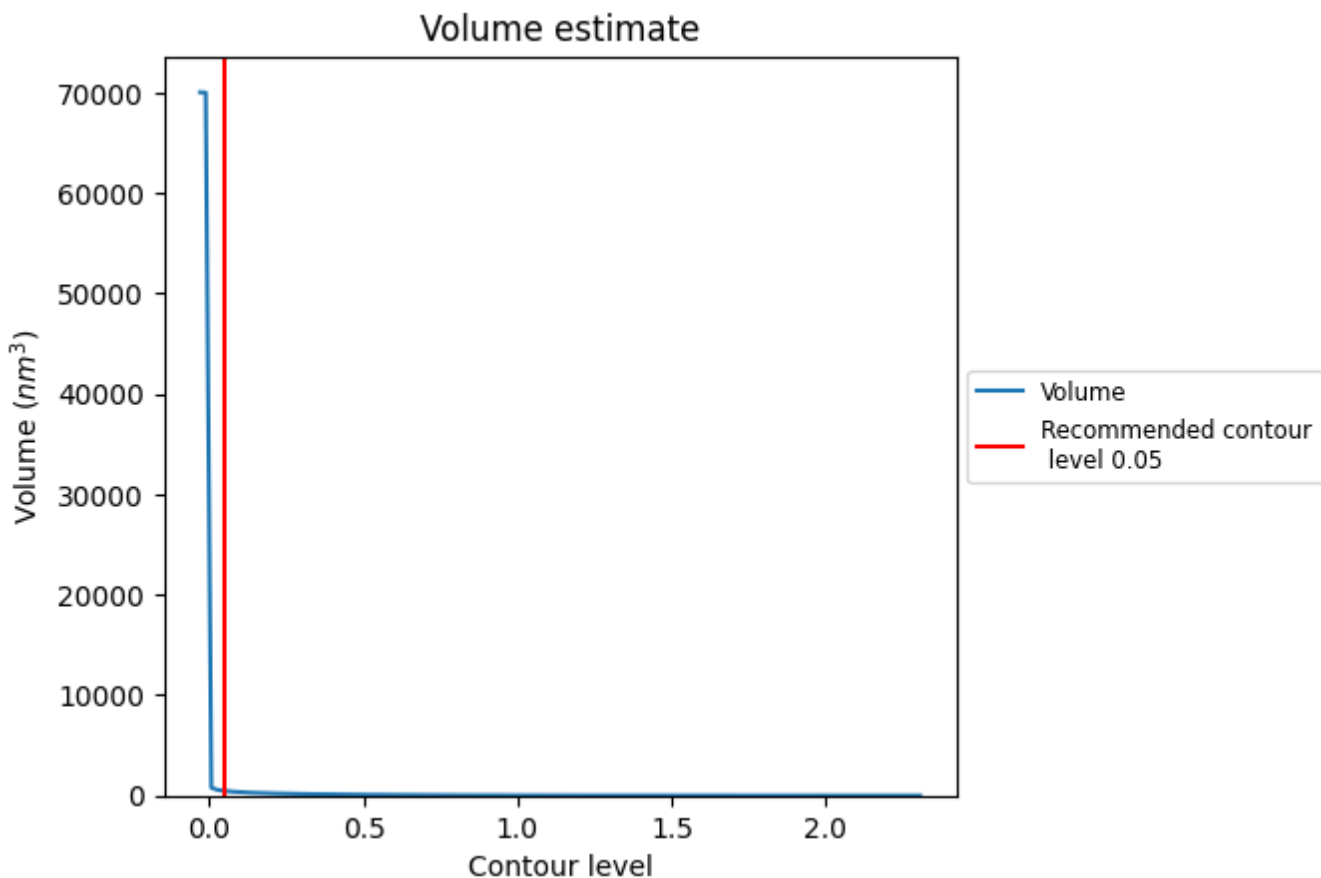
This section contains the results of statistical analysis of the map.

### 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.

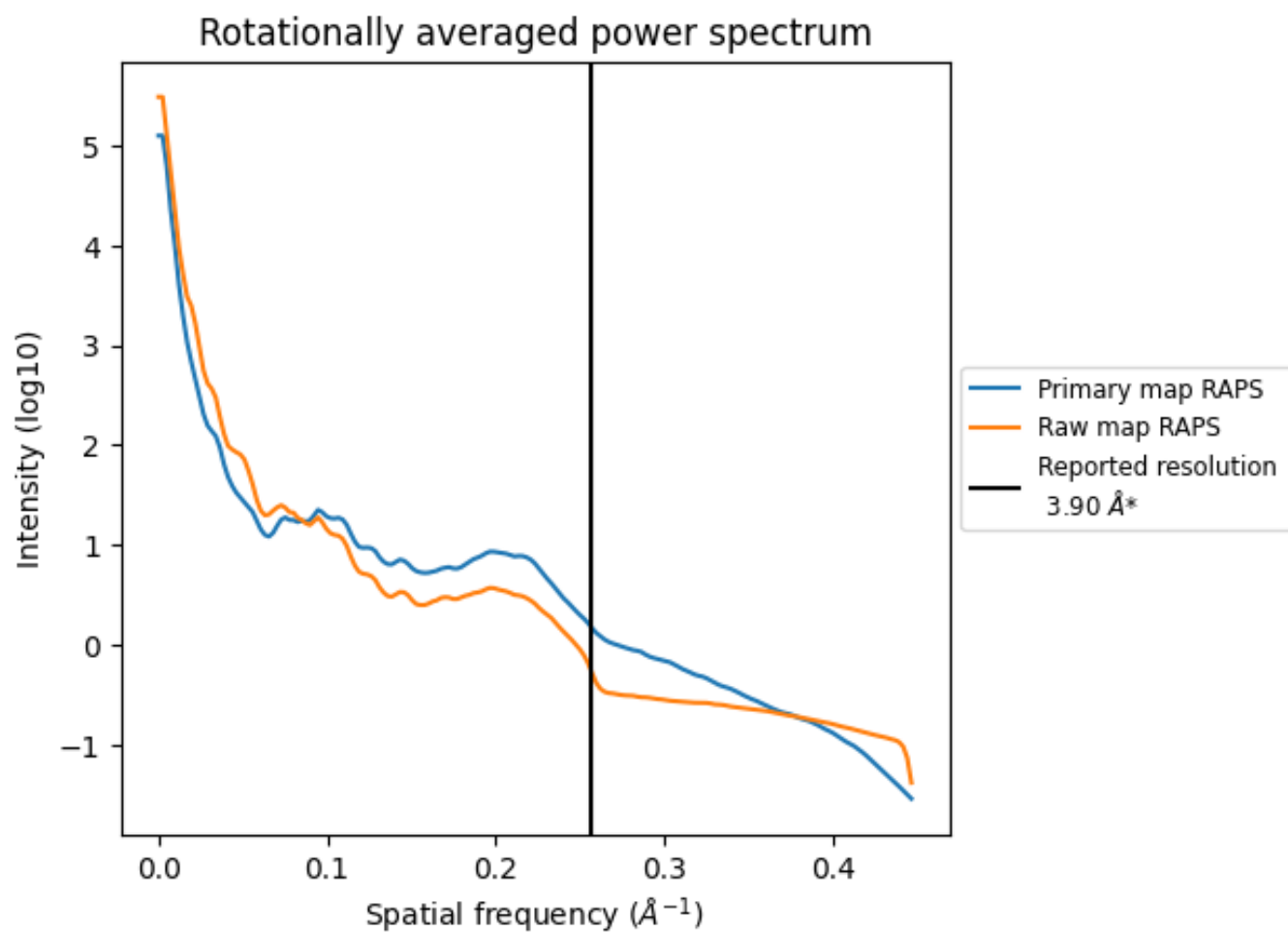
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 462 nm<sup>3</sup>; this corresponds to an approximate mass of 418 kDa.

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

### 7.3 Rotationally averaged power spectrum i



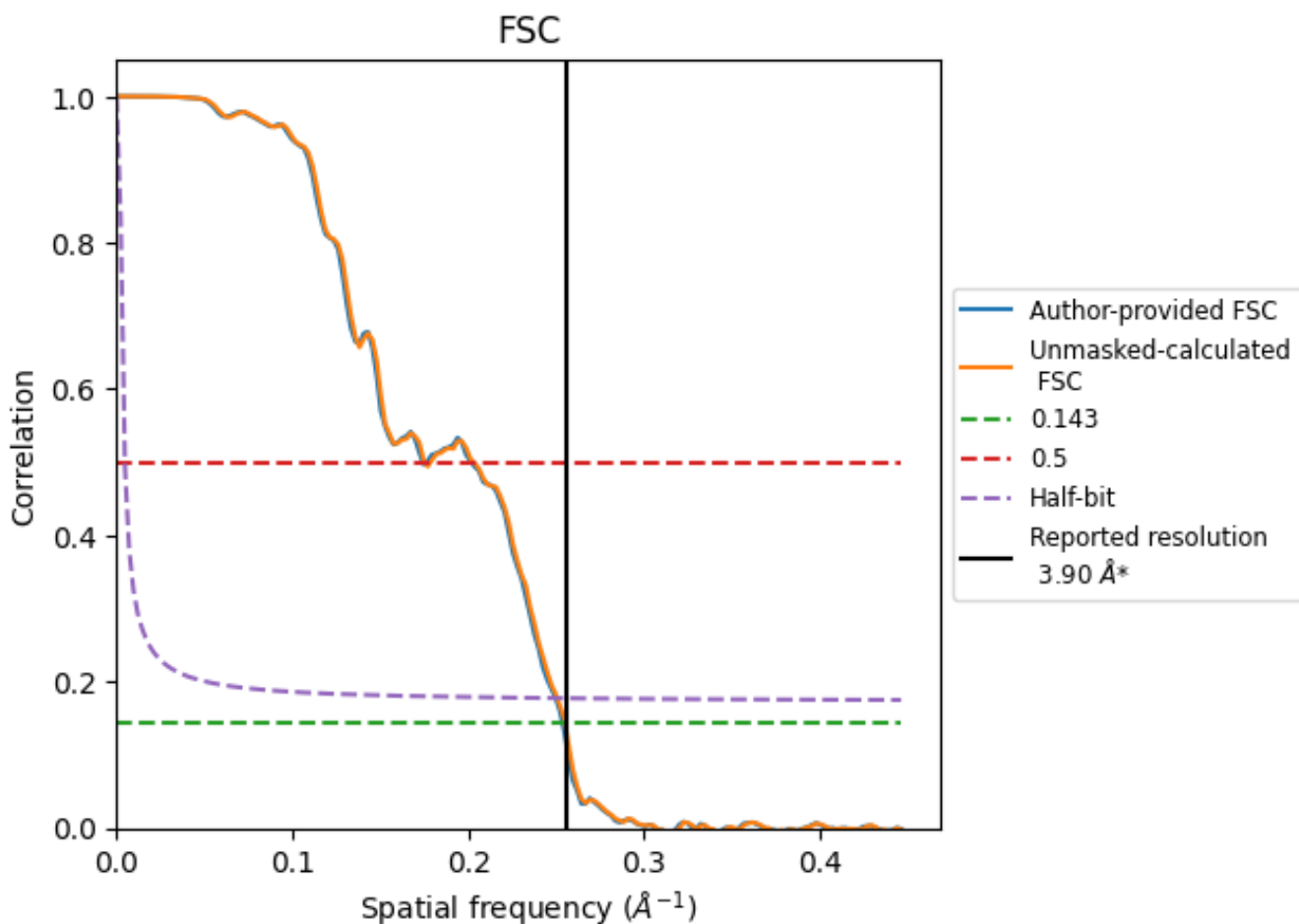
\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

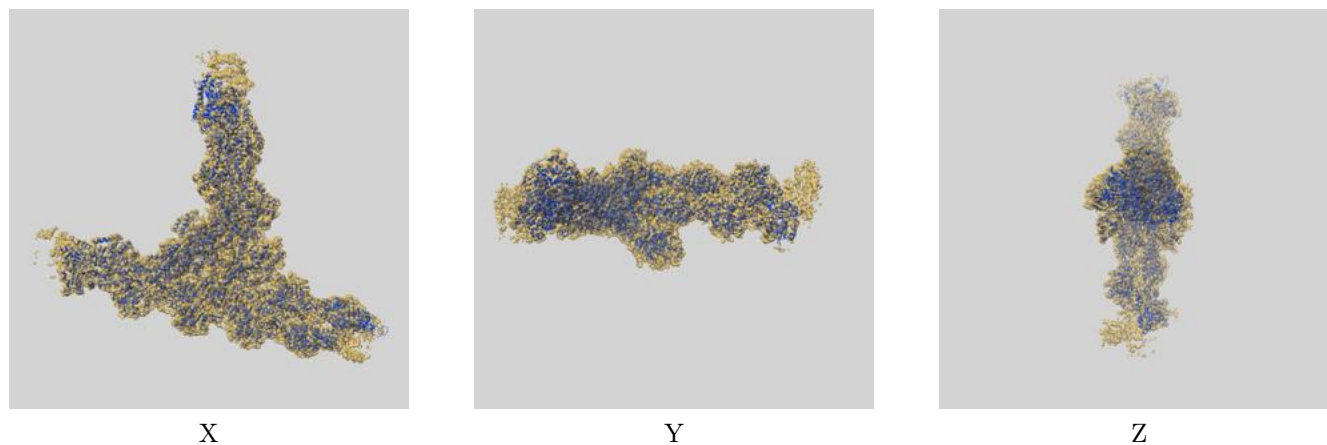
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.94	5.74	4.00
Unmasked-calculated*	3.92	5.69	3.99

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

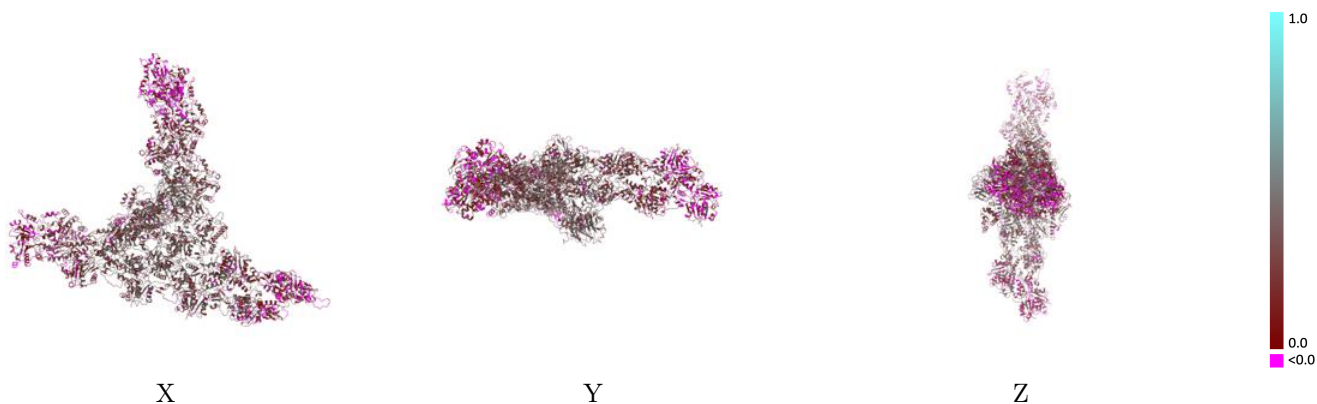
This section contains information regarding the fit between EMDB map EMD-26063 and PDB model 7TPT. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



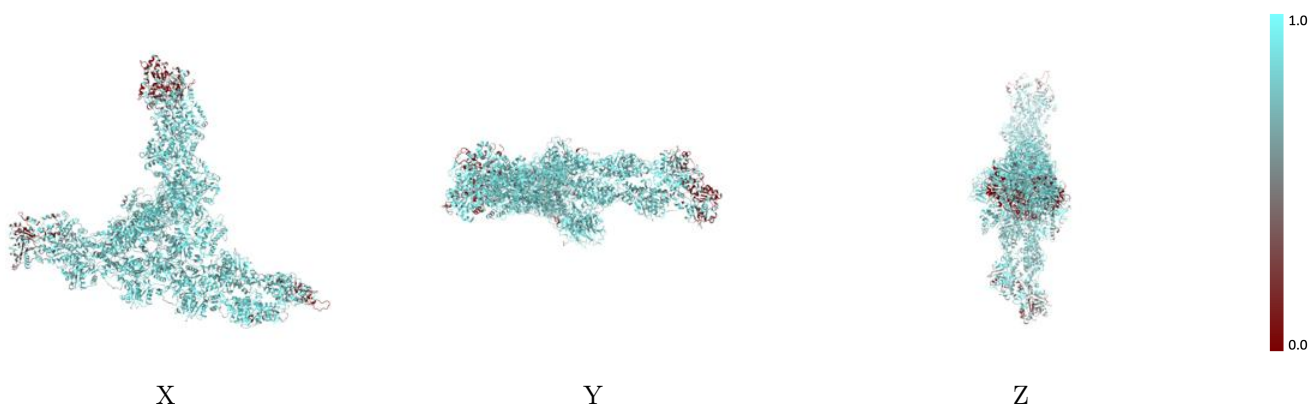
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



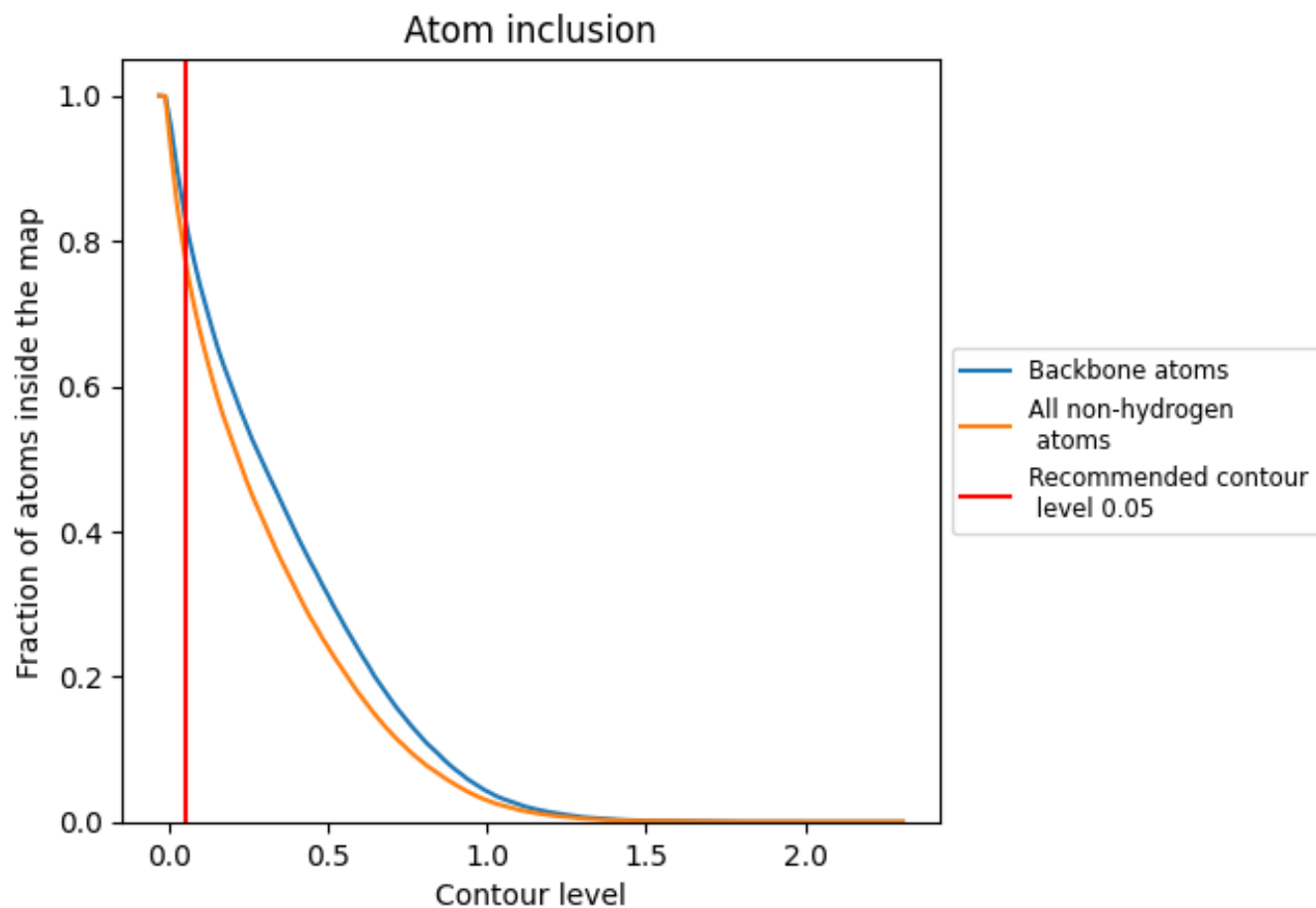
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7764	 0.2660
A	 0.8214	 0.3320
B	 0.8185	 0.3320
C	 0.8361	 0.3530
D	 0.7966	 0.3100
E	 0.8304	 0.3250
F	 0.8373	 0.3430
G	 0.7692	 0.2940
H	 0.8081	 0.2720
I	 0.7772	 0.2200
J	 0.6362	 0.1270
K	 0.4514	 0.0690
L	 0.6292	 0.1340
M	 0.8174	 0.2030
N	 0.7980	 0.2500
O	 0.8212	 0.2900
P	 0.8403	 0.3260
Q	 0.8476	 0.3270
R	 0.8199	 0.3130
S	 0.7990	 0.2520
T	 0.7442	 0.2080
U	 0.5615	 0.1170
a	 0.8889	 0.3540
b	 0.9444	 0.4360
c	 0.9074	 0.3110
d	 0.8519	 0.3010
e	 0.3148	 0.0300
f	 0.7407	 0.2280
g	 0.8519	 0.3460
h	 0.8704	 0.3540
i	 0.9259	 0.4350
j	 0.9074	 0.4310
k	 0.8704	 0.4000
l	 0.8889	 0.4040
m	 0.8889	 0.3710



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Chain	Atom inclusion	Q-score
n	 0.5926	 -0.0130
o	 0.6852	 0.1670