



Full wwPDB EM Validation Report ⓘ

Sep 21, 2025 – 12:27 AM JST

PDB ID : 9M64 / pdb_00009m64
EMDB ID : EMD-63658
Title : Structure of SPIN90 dimer-Arp2/3 complexes-nucleated actin filaments (Doublet Complex)
Authors : Francis, J.; Pathri, A.K.; Chowdhury, S.
Deposited on : 2025-03-07
Resolution : 3.40 Å(reported)
Based on initial model : 7TPT

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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

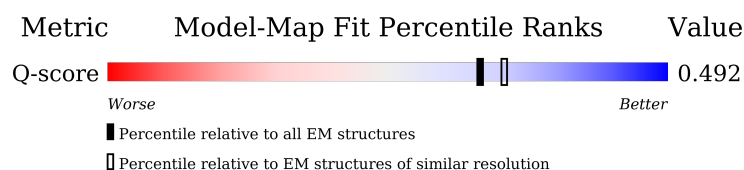
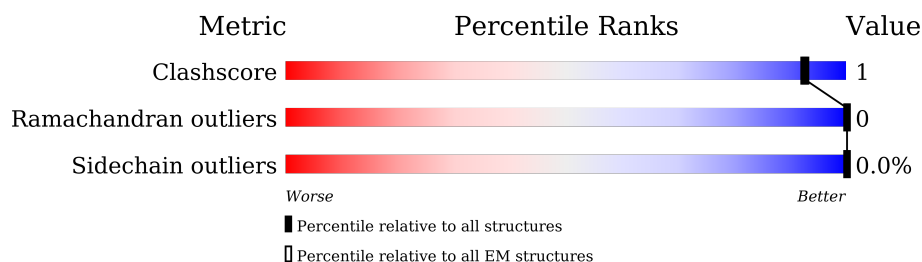
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.








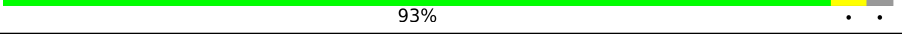
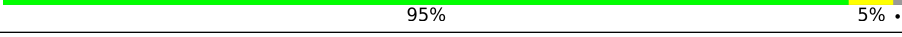

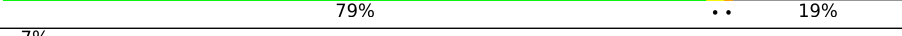

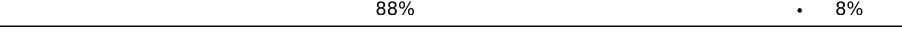
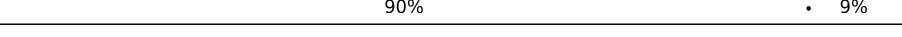
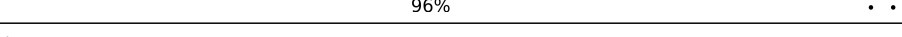
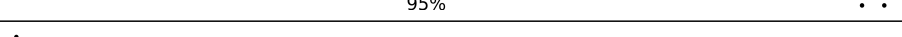
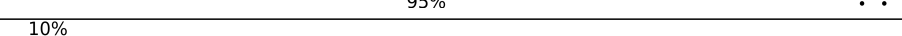
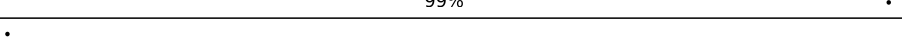
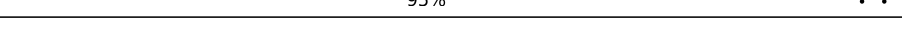
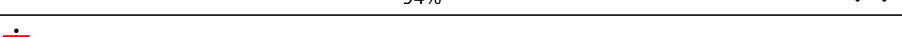
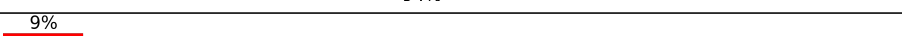

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	418	
1	a	418	
2	B	394	
2	b	394	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	372	
3	c	372	
4	D	300	
4	d	300	
5	E	178	
5	e	178	
6	F	168	
6	f	168	
7	G	151	
7	g	151	
8	H	454	
8	h	454	
9	I	377	
9	J	377	
9	K	377	
9	L	377	
9	i	377	
9	j	377	
9	k	377	
9	l	377	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 57141 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
1	A	411	Total	C	N	O	S	0	0
			3252	2084	552	601	15		
1	a	411	Total	C	N	O	S	0	0
			3257	2085	551	606	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	377	Total	C	N	O	S	0	0
			2963	1901	504	542	16		
2	b	380	Total	C	N	O	S	0	0
			3024	1936	511	560	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	314	Total	C	N	O	S	0	0
			2433	1546	426	441	20		
3	c	320	Total	C	N	O	S	0	0
			2445	1555	427	444	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	281	Total	C	N	O	S	0	0
			2260	1435	391	426	8		
4	d	281	Total	C	N	O	S	0	0
			2261	1438	393	422	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	178	Total	C	N	O	S	0	0
			1444	925	241	268	10		
5	e	173	Total	C	N	O	S	0	0
			1384	886	230	259	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	167	Total	C	N	O	S	0	0
			1371	875	239	248	9		
6	f	164	Total	C	N	O	S	0	0
			1344	859	235	241	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	123	Total	C	N	O	S	0	0
			903	565	160	175	3		
7	g	124	Total	C	N	O	S	0	0
			918	574	165	177	2		

- Molecule 8 is a protein called NCK-interacting protein with SH3 domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	416	Total	C	N	O	S	0	0
			3243	2059	563	594	27		
8	h	414	Total	C	N	O	S	0	0
			3251	2063	563	597	28		

- Molecule 9 is a protein called Actin, alpha skeletal muscle.

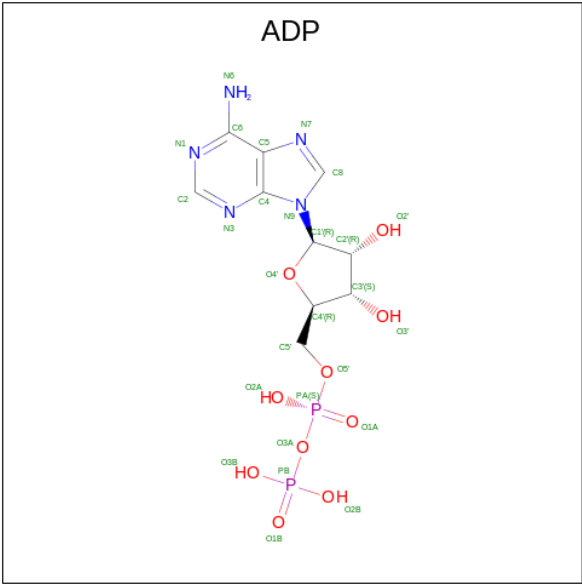
Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	371	Total	C	N	O	S	0	0
			2896	1835	489	551	21		
9	J	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
9	K	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
9	L	372	Total	C	N	O		0	0
			1878	1132	372	374			
9	i	371	Total	C	N	O	S	0	0
			2873	1819	485	549	20		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	369	Total	C	N	O	S	0	0
			2859	1812	485	542	20		
9	k	370	Total	C	N	O	S	0	0
			2877	1821	487	549	20		
9	l	372	Total	C	N	O		0	0
			1871	1126	372	373			

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	b	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	i	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	j	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	k	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	l	1	Total	C	N	O	P	0
			27	10	5	10	2	

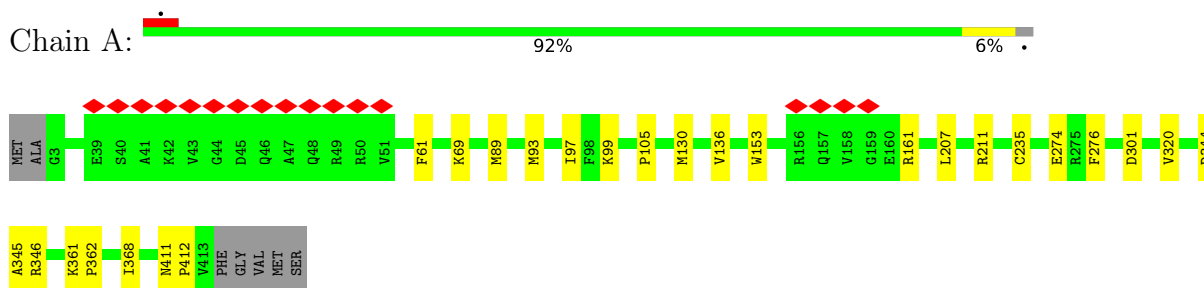
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	Mg	0
			1	1	
11	I	1	Total	Mg	0
			1	1	
11	J	1	Total	Mg	0
			1	1	
11	K	1	Total	Mg	0
			1	1	
11	a	1	Total	Mg	0
			1	1	
11	b	1	Total	Mg	0
			1	1	
11	i	1	Total	Mg	0
			1	1	
11	j	1	Total	Mg	0
			1	1	
11	k	1	Total	Mg	0
			1	1	
11	l	1	Total	Mg	0
			1	1	

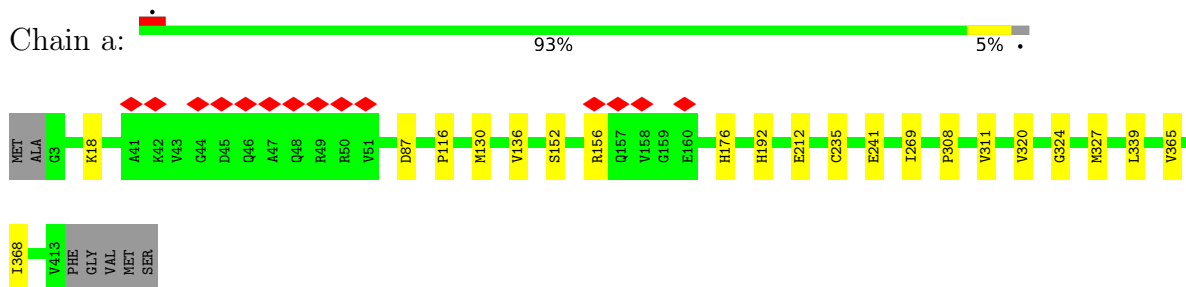
3 Residue-property plots

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.

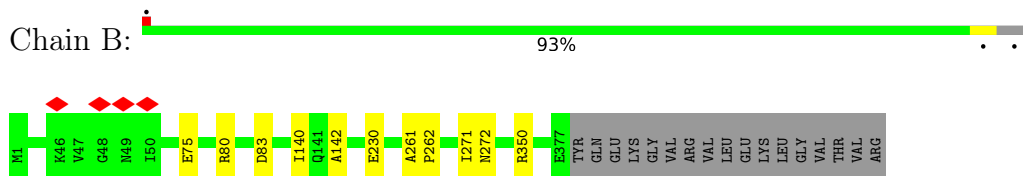
- Molecule 1: Actin-related protein 3



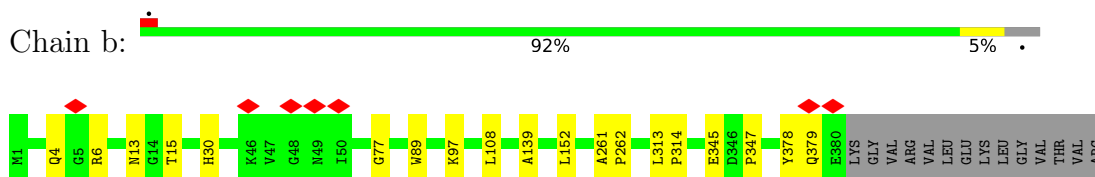
- Molecule 1: Actin-related protein 3




- Molecule 2: Actin-related protein 2

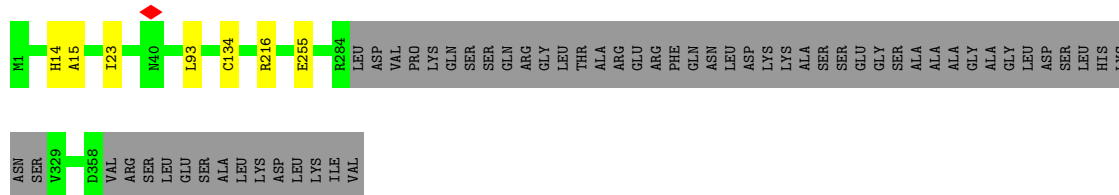


- Molecule 2: Actin-related protein 2




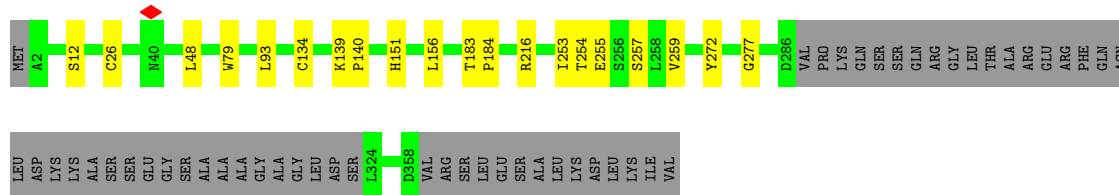
- Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain C:  83% 16%




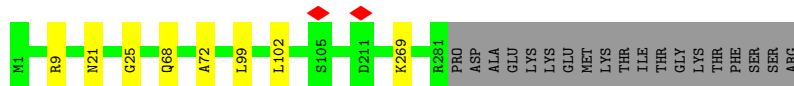
- Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain c:  81% 5% 14%




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

Chain D:  91% 6%



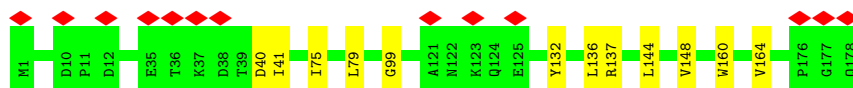
- Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain d:  90% 6%

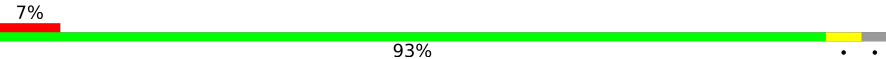


- Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:  93% 7% 7%



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

Chain e:  93% 7%

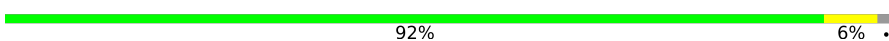


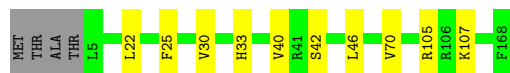
- Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:  95% 5% .




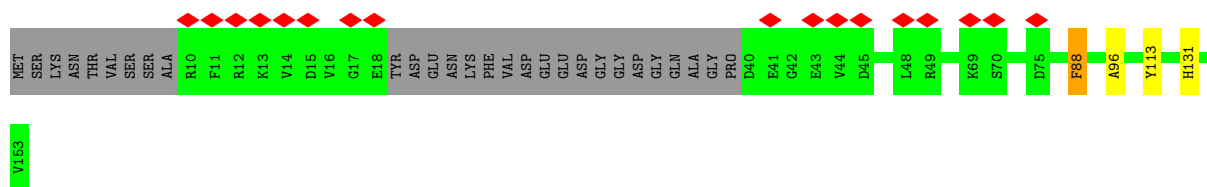
- Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain f:  92% 6% .




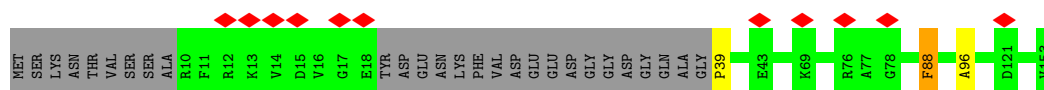
- Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:  11% 79% .. 19%




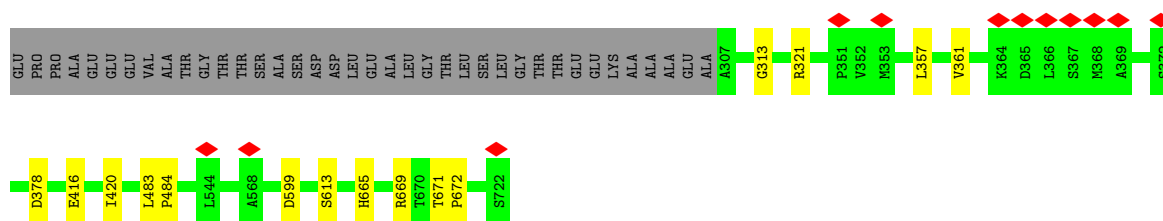
- Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain g:  7% 80% .. 18%




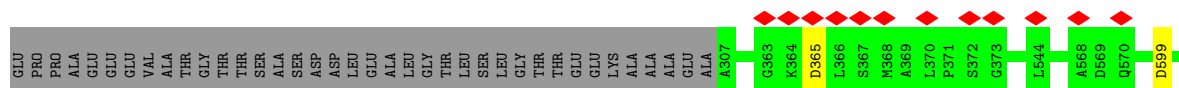
- Molecule 8: NCK-interacting protein with SH3 domain

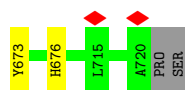
Chain H:  88% . 8%



- Molecule 8: NCK-interacting protein with SH3 domain

Chain h:  90% . 9%





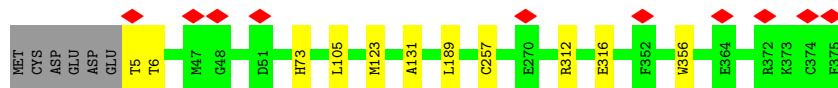
- Molecule 9: Actin, alpha skeletal muscle



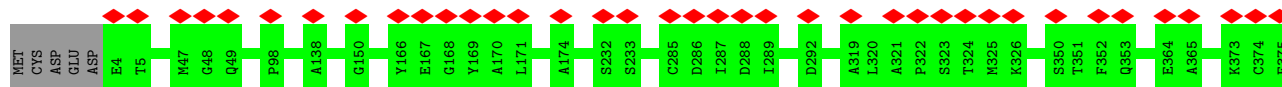
- Molecule 9: Actin, alpha skeletal muscle



- Molecule 9: Actin, alpha skeletal muscle



- Molecule 9: Actin, alpha skeletal muscle



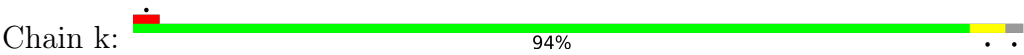
- Molecule 9: Actin, alpha skeletal muscle



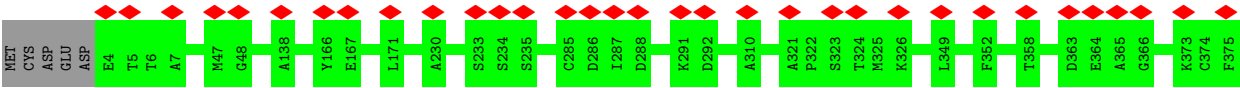
- Molecule 9: Actin, alpha skeletal muscle



- Molecule 9: Actin, alpha skeletal muscle



• Molecule 9: Actin, alpha skeletal muscle



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	27106	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.843	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.046	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.325	Depositor
Map size (Å)	480.00003, 480.00003, 480.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.19	0/3334	0.41	0/4526
1	a	0.20	0/3339	0.42	0/4534
2	B	0.18	0/3024	0.45	0/4094
2	b	0.19	0/3086	0.42	0/4174
3	C	0.19	0/2500	0.50	0/3398
3	c	0.20	0/2513	0.48	0/3423
4	D	0.20	0/2308	0.46	0/3119
4	d	0.17	0/2309	0.40	0/3118
5	E	0.17	0/1479	0.47	0/1994
5	e	0.18	0/1418	0.46	0/1920
6	F	0.20	0/1393	0.49	0/1868
6	f	0.21	0/1366	0.43	0/1832
7	G	0.15	0/911	0.39	0/1229
7	g	0.15	0/926	0.40	1/1246 (0.1%)
8	H	0.17	0/3304	0.42	0/4485
8	h	0.16	0/3311	0.40	0/4491
9	I	0.16	0/2946	0.40	0/3989
9	J	0.15	0/2950	0.42	0/3994
9	K	0.13	0/2950	0.38	0/3994
9	L	0.11	0/1891	0.39	0/2641
9	i	0.19	0/2923	0.40	0/3965
9	j	0.16	0/2908	0.41	0/3943
9	k	0.15	0/2926	0.42	0/3966
9	l	0.12	0/1883	0.39	0/2630
All	All	0.17	0/57898	0.42	1/78573 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	39	PRO	N-CA-CB	6.64	110.30	103.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	350	ARG	Sidechain

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	3252	0	3188	14	0
1	a	3257	0	3188	13	0
2	B	2963	0	2969	7	0
2	b	3024	0	3039	10	0
3	C	2433	0	2362	4	0
3	c	2445	0	2343	10	0
4	D	2260	0	2208	5	0
4	d	2261	0	2224	7	0
5	E	1444	0	1445	6	0
5	e	1384	0	1345	4	0
6	F	1371	0	1410	6	0
6	f	1344	0	1376	5	0
7	G	903	0	907	2	0
7	g	918	0	932	1	0
8	H	3243	0	3274	8	0
8	h	3251	0	3296	3	0
9	I	2896	0	2868	5	0
9	J	2900	0	2872	7	0
9	K	2900	0	2872	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	1878	0	959	0	0
9	i	2873	0	2813	6	0
9	j	2859	0	2822	8	0
9	k	2877	0	2841	8	0
9	l	1871	0	952	0	0
10	A	27	0	12	0	0
10	B	27	0	12	0	0
10	I	27	0	12	1	0
10	J	27	0	12	1	0
10	K	27	0	12	0	0
10	L	27	0	12	0	0
10	a	27	0	12	1	0
10	b	27	0	12	0	0
10	i	27	0	12	1	0
10	j	27	0	12	0	0
10	k	27	0	12	0	0
10	l	27	0	12	0	0
11	B	1	0	0	0	0
11	I	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	0	0
11	a	1	0	0	0	0
11	b	1	0	0	0	0
11	i	1	0	0	0	0
11	j	1	0	0	0	0
11	k	1	0	0	0	0
11	l	1	0	0	0	0
All	All	57141	0	54649	140	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 (140) 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)
9:J:149:THR:HG22	9:J:167:GLU:H	1.50	0.75
9:j:42:GLY:HA3	9:j:47:MET:HE1	1.84	0.60
3:c:253:ILE:HD11	3:c:259:VAL:HB	1.82	0.60
2:b:30:HIS:HB3	2:b:97:LYS:HD3	1.85	0.58
9:i:250:ILE:HG23	9:i:253:GLU:HB2	1.87	0.57
9:k:285:CYS:HB3	9:k:289:ILE:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ILE:HG21	1:A:105:PRO:HG3	1.87	0.56
9:I:285:CYS:HB3	9:I:289:ILE:HD11	1.88	0.55
9:k:131:ALA:HB1	9:k:356:TRP:HB3	1.86	0.55
9:J:103:THR:HG21	9:J:123:MET:HE2	1.88	0.54
8:H:313:GLY:H	8:H:361:VAL:HG11	1.73	0.54
1:A:320:VAL:HG22	1:A:368:ILE:HD11	1.90	0.54
9:i:14:SER:N	10:i:401:ADP:O3B	2.41	0.53
4:D:99:LEU:HA	4:D:102:LEU:HD23	1.91	0.53
9:I:39:ARG:HB3	9:I:66:THR:HG23	1.91	0.52
3:C:14:HIS:HB2	3:C:23:ILE:HD11	1.92	0.52
3:C:93:LEU:HA	3:C:134:CYS:SG	2.49	0.52
3:C:216:ARG:NH1	3:C:255:GLU:O	2.41	0.52
5:E:99:GLY:O	5:E:137:ARG:NH1	2.39	0.52
9:J:230:ALA:HB2	9:J:236:LEU:HD12	1.91	0.52
1:a:18:LYS:NZ	10:a:502:ADP:O2B	2.43	0.52
8:H:665:HIS:CD2	8:H:669:ARG:HH21	2.29	0.51
1:A:344:ASP:OD1	1:A:345:ALA:N	2.43	0.51
8:h:673:TYR:HA	8:h:676:HIS:CE1	2.46	0.51
9:j:139:VAL:HG22	9:j:165:ILE:HD11	1.92	0.51
9:k:155:SER:OG	9:k:304:THR:HG23	2.10	0.51
5:E:40:ASP:OD1	5:E:41:ILE:N	2.44	0.51
6:f:22:LEU:HD21	6:f:70:VAL:HG23	1.92	0.51
6:F:129:HIS:CE1	6:F:130:LYS:HE3	2.46	0.51
9:J:214:GLU:HG3	10:J:501:ADP:N3	2.26	0.51
1:a:320:VAL:HG22	1:a:368:ILE:HD11	1.92	0.51
1:a:212:GLU:HG2	1:a:269:ILE:HB	1.92	0.50
6:f:30:VAL:HG11	6:f:33:HIS:CE1	2.46	0.50
9:I:186:THR:HG22	9:I:213:LYS:HD3	1.94	0.50
9:j:358:THR:HG23	9:j:361:GLU:H	1.76	0.50
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.92	0.50
9:K:312:ARG:NH1	9:K:316:GLU:OE1	2.45	0.50
9:J:285:CYS:HB3	9:J:289:ILE:HD11	1.93	0.49
9:K:105:LEU:HD11	9:K:123:MET:HE3	1.92	0.49
3:c:12:SER:HB2	3:c:26:CYS:SG	2.52	0.49
1:A:61:PHE:CE1	1:A:69:LYS:HE2	2.48	0.48
9:I:214:GLU:HG2	10:I:402:ADP:C4	2.48	0.48
2:b:15:THR:HG21	2:b:77:GLY:H	1.79	0.48
1:A:411:ASN:HB2	1:A:412:PRO:HD2	1.95	0.48
2:b:4:GLN:OE1	2:b:6:ARG:NH1	2.44	0.48
9:j:287:ILE:H	9:j:287:ILE:HD12	1.79	0.47
2:B:271:ILE:HG22	2:B:272:ASN:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:254:THR:HG22	3:c:257:SER:HB3	1.96	0.47
7:G:88:PHE:CZ	7:G:96:ALA:HB2	2.50	0.47
2:b:261:ALA:HB3	2:b:262:PRO:HD3	1.95	0.47
5:e:82:LEU:HD22	5:e:149:PHE:CE2	2.49	0.47
9:k:274:ILE:O	9:k:278:THR:HG23	2.15	0.47
1:a:324:GLY:HA2	1:a:327:MET:HE3	1.97	0.47
5:E:75:ILE:HG23	5:E:144:LEU:HD11	1.97	0.46
5:e:38:ASP:OD1	5:e:39:THR:N	2.39	0.46
9:K:131:ALA:HB1	9:K:356:TRP:HB3	1.98	0.46
3:c:93:LEU:HA	3:c:134:CYS:SG	2.56	0.46
3:c:183:THR:HG23	3:c:184:PRO:HD2	1.97	0.46
9:K:189:LEU:HD13	9:K:257:CYS:SG	2.56	0.46
5:e:71:ILE:HD11	5:e:136:LEU:HD13	1.97	0.46
6:F:129:HIS:HE1	6:F:130:LYS:HE3	1.81	0.46
2:B:140:ILE:HG22	2:B:142:ALA:H	1.81	0.45
5:E:148:VAL:HG23	5:E:160:TRP:CB	2.47	0.45
7:g:88:PHE:CZ	7:g:96:ALA:HB2	2.50	0.45
1:a:130:MET:HE3	1:a:136:VAL:HG11	1.99	0.45
2:b:345:GLU:C	2:b:347:PRO:HD3	2.42	0.45
8:h:599:ASP:OD1	8:h:599:ASP:N	2.50	0.45
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.80	0.45
1:A:301:ASP:OD2	1:A:346:ARG:NH2	2.43	0.45
5:E:79:LEU:HB3	5:E:164:VAL:HG22	1.98	0.45
2:b:152:LEU:HA	9:j:44:MET:HE1	1.99	0.45
1:a:339:LEU:HB2	1:a:365:VAL:HG11	1.98	0.44
9:i:156:GLY:O	9:i:181:ALA:HB1	2.18	0.44
1:A:235:CYS:HB3	1:A:276:PHE:HB2	1.97	0.44
8:H:416:GLU:O	8:H:420:ILE:HG12	2.18	0.44
9:J:222:ASP:N	9:J:222:ASP:OD1	2.51	0.44
5:e:62:ASN:OD1	5:e:63:GLU:N	2.51	0.44
8:H:357:LEU:O	8:H:361:VAL:HG23	2.16	0.44
4:d:61:LEU:HD21	4:d:63:PHE:CE2	2.53	0.44
9:K:5:THR:HG23	9:K:6:THR:H	1.83	0.43
8:h:365:ASP:OD1	8:h:365:ASP:N	2.49	0.43
3:c:216:ARG:NH1	3:c:255:GLU:O	2.50	0.43
2:B:271:ILE:HG22	2:B:272:ASN:H	1.82	0.43
2:B:83:ASP:N	2:B:83:ASP:OD1	2.48	0.43
1:a:308:PRO:O	1:a:311:VAL:HG22	2.19	0.43
1:a:152:SER:O	1:a:156:ARG:HG2	2.19	0.43
2:B:75:GLU:OE1	2:B:80:ARG:NH1	2.51	0.43
4:d:148:ASP:N	4:d:148:ASP:OD1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:132:TYR:CE2	5:E:136:LEU:HD11	2.54	0.43
6:F:105:ARG:NH1	6:F:107:LYS:O	2.51	0.43
3:c:48:LEU:HD23	3:c:79:TRP:CD2	2.54	0.43
9:j:8:LEU:O	9:j:103:THR:HA	2.19	0.42
9:i:39:ARG:HG2	9:i:66:THR:HG23	2.01	0.42
9:K:5:THR:HG23	9:K:6:THR:N	2.34	0.42
9:i:51:ASP:OD1	9:i:52:SER:N	2.52	0.42
9:j:210:ARG:NH1	9:j:214:GLU:OE2	2.46	0.42
1:A:153:TRP:CE2	1:A:161:ARG:HB3	2.55	0.42
1:A:99:LYS:HE2	4:D:9:ARG:NH2	2.34	0.42
4:D:21:ASN:O	4:D:25:GLY:N	2.52	0.42
4:d:202:HIS:CD2	4:d:203:ARG:HG3	2.54	0.42
1:A:361:LYS:HD2	1:A:362:PRO:HD2	2.02	0.42
1:a:176:HIS:HD2	1:a:192:HIS:CD2	2.37	0.42
6:f:105:ARG:NH1	6:f:107:LYS:O	2.46	0.42
1:A:207:LEU:HD23	1:A:274:GLU:HB3	2.00	0.42
9:I:257:CYS:HB3	9:I:258:PRO:HD3	2.02	0.42
3:c:139:LYS:HB3	3:c:140:PRO:HD3	2.01	0.42
4:D:269:LYS:NZ	6:F:145:GLU:OE1	2.49	0.41
6:F:24:ASN:HA	6:F:120:ASN:ND2	2.35	0.41
9:i:104:LEU:HD13	9:i:133:TYR:HB3	2.01	0.41
3:C:15:ALA:O	3:C:23:ILE:HD12	2.20	0.41
4:D:68:GLN:HA	4:D:72:ALA:HB3	2.02	0.41
9:J:105:LEU:HD12	9:J:132:MET:HE3	2.02	0.41
9:k:317:ILE:HG23	9:k:327:ILE:HD13	2.02	0.41
4:d:51:ASP:OD1	4:d:51:ASP:N	2.48	0.41
2:b:313:LEU:HB3	2:b:314:PRO:HD3	2.01	0.41
9:k:102:PRO:HA	9:k:131:ALA:O	2.20	0.41
7:G:113:TYR:OH	7:G:131:HIS:HE1	2.04	0.41
3:c:151:HIS:HB2	3:c:156:LEU:HB2	2.02	0.41
4:d:41:VAL:HG21	4:d:117:LYS:HD2	2.03	0.41
1:A:89:MET:HE3	1:A:93:MET:HE3	2.03	0.41
1:a:116:PRO:HD2	1:a:176:HIS:CE1	2.56	0.41
2:B:230:GLU:OE2	6:F:35:LYS:NZ	2.54	0.41
1:a:87:ASP:OD1	4:d:267:ARG:NH1	2.53	0.41
6:f:25:PHE:CE2	6:f:46:LEU:HD21	2.56	0.41
8:H:483:LEU:HB3	8:H:484:PRO:HD3	2.01	0.41
2:b:13:ASN:ND2	2:b:89:TRP:HE1	2.18	0.41
2:b:378:TYR:CG	2:b:379:GLN:N	2.89	0.41
9:j:190:MET:HG2	9:j:209:VAL:HG11	2.02	0.41
1:a:235:CYS:HB2	1:a:241:GLU:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:272:TYR:CE1	3:c:277:GLY:HA2	2.56	0.41
9:k:302:GLY:O	9:k:305:MET:HG2	2.20	0.41
1:a:327:MET:HE2	1:a:327:MET:HB3	1.93	0.40
4:d:54:LYS:HB3	4:d:96:LEU:HD11	2.03	0.40
6:f:40:VAL:O	6:f:42:SER:N	2.54	0.40
2:b:108:LEU:HD11	2:b:139:ALA:HB2	2.03	0.40
8:H:321:ARG:HE	8:H:378:ASP:CG	2.28	0.40
8:H:599:ASP:OD1	8:H:613:SER:OG	2.36	0.40
1:A:130:MET:HE3	1:A:136:VAL:HG21	2.04	0.40
8:H:671:THR:HB	8:H:672:PRO:HD2	2.04	0.40
9:k:36:GLY:HA2	9:k:66:THR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/418 (98%)	386 (94%)	23 (6%)	0	100	100
1	a	409/418 (98%)	385 (94%)	24 (6%)	0	100	100
2	B	375/394 (95%)	356 (95%)	19 (5%)	0	100	100
2	b	378/394 (96%)	361 (96%)	17 (4%)	0	100	100
3	C	310/372 (83%)	289 (93%)	21 (7%)	0	100	100
3	c	316/372 (85%)	293 (93%)	23 (7%)	0	100	100
4	D	279/300 (93%)	268 (96%)	11 (4%)	0	100	100
4	d	279/300 (93%)	270 (97%)	9 (3%)	0	100	100
5	E	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
5	e	171/178 (96%)	159 (93%)	12 (7%)	0	100	100
6	F	165/168 (98%)	159 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	162/168 (96%)	156 (96%)	6 (4%)	0	100	100
7	G	119/151 (79%)	116 (98%)	3 (2%)	0	100	100
7	g	120/151 (80%)	119 (99%)	1 (1%)	0	100	100
8	H	414/454 (91%)	396 (96%)	18 (4%)	0	100	100
8	h	412/454 (91%)	396 (96%)	16 (4%)	0	100	100
9	I	368/377 (98%)	361 (98%)	7 (2%)	0	100	100
9	J	368/377 (98%)	356 (97%)	12 (3%)	0	100	100
9	K	368/377 (98%)	353 (96%)	15 (4%)	0	100	100
9	L	369/377 (98%)	340 (92%)	29 (8%)	0	100	100
9	i	368/377 (98%)	358 (97%)	10 (3%)	0	100	100
9	j	366/377 (97%)	359 (98%)	7 (2%)	0	100	100
9	k	367/377 (97%)	355 (97%)	12 (3%)	0	100	100
9	l	369/377 (98%)	348 (94%)	21 (6%)	0	100	100
All	All	7437/7886 (94%)	7108 (96%)	329 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	348/363 (96%)	348 (100%)	0	100	100
1	a	350/363 (96%)	350 (100%)	0	100	100
2	B	318/345 (92%)	318 (100%)	0	100	100
2	b	330/345 (96%)	330 (100%)	0	100	100
3	C	262/313 (84%)	262 (100%)	0	100	100
3	c	260/313 (83%)	260 (100%)	0	100	100
4	D	244/264 (92%)	244 (100%)	0	100	100
4	d	244/264 (92%)	244 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	159/159 (100%)	159 (100%)	0	100	100
5	e	149/159 (94%)	149 (100%)	0	100	100
6	F	154/155 (99%)	154 (100%)	0	100	100
6	f	150/155 (97%)	150 (100%)	0	100	100
7	G	93/123 (76%)	92 (99%)	1 (1%)	70	81
7	g	95/123 (77%)	94 (99%)	1 (1%)	70	81
8	H	356/391 (91%)	356 (100%)	0	100	100
8	h	360/391 (92%)	360 (100%)	0	100	100
9	I	312/319 (98%)	312 (100%)	0	100	100
9	J	313/319 (98%)	313 (100%)	0	100	100
9	K	313/319 (98%)	313 (100%)	0	100	100
9	L	20/319 (6%)	20 (100%)	0	100	100
9	i	306/319 (96%)	306 (100%)	0	100	100
9	j	305/319 (96%)	305 (100%)	0	100	100
9	k	309/319 (97%)	309 (100%)	0	100	100
9	l	19/319 (6%)	19 (100%)	0	100	100
All	All	5769/6778 (85%)	5767 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	88	PHE
7	g	88	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	366	GLN
1	A	411	ASN
2	B	81	ASN
2	B	87	HIS
2	B	141	GLN
2	B	165	HIS
4	D	239	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	129	HIS
6	F	137	HIS
7	G	131	HIS
8	H	343	GLN
8	H	595	ASN
8	H	665	HIS
8	H	678	HIS
9	I	280	ASN
9	K	40	HIS
9	K	49	GLN
9	K	137	GLN
1	a	95	GLN
1	a	108	HIS
1	a	176	HIS
1	a	192	HIS
2	b	13	ASN
3	c	46	HIS
4	d	21	ASN
4	d	26	ASN
4	d	92	ASN
4	d	112	GLN
4	d	119	ASN
4	d	145	HIS
4	d	202	HIS
4	d	219	ASN
5	e	86	ASN
6	f	28	GLN
6	f	33	HIS
7	g	71	GLN
7	g	129	GLN
8	h	343	GLN
8	h	355	GLN
8	h	498	HIS
8	h	562	ASN
8	h	633	HIS
9	i	161	HIS
9	i	162	ASN
9	j	225	ASN
9	k	12	ASN
9	k	275	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 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	HIC	l	73	9	3,4,12	0.61	0	2,4,16	0.85	0
9	HIC	L	73	9	3,4,12	0.70	0	2,4,16	0.86	0
9	HIC	I	73	9	8,11,12	1.06	1 (12%)	6,14,16	0.82	0
9	HIC	J	73	9	8,11,12	1.03	1 (12%)	6,14,16	0.72	0
9	HIC	i	73	9	8,11,12	1.08	1 (12%)	6,14,16	0.82	0
9	HIC	k	73	9	8,11,12	1.03	1 (12%)	6,14,16	0.71	0
9	HIC	K	73	9	8,11,12	1.08	1 (12%)	6,14,16	0.69	0
9	HIC	j	73	9	8,11,12	1.06	1 (12%)	6,14,16	0.80	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
9	HIC	l	73	9	-	0/0/2/8	-
9	HIC	L	73	9	-	0/0/2/8	-
9	HIC	I	73	9	-	0/5/6/8	0/1/1/1
9	HIC	J	73	9	-	0/5/6/8	0/1/1/1
9	HIC	i	73	9	-	1/5/6/8	0/1/1/1
9	HIC	k	73	9	-	0/5/6/8	0/1/1/1
9	HIC	K	73	9	-	0/5/6/8	0/1/1/1
9	HIC	j	73	9	-	1/5/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	73	HIC	CE1-ND1	-2.22	1.31	1.35
9	I	73	HIC	CE1-ND1	-2.20	1.31	1.35
9	j	73	HIC	CE1-ND1	-2.20	1.31	1.35
9	k	73	HIC	CE1-ND1	-2.14	1.31	1.35
9	K	73	HIC	CE1-ND1	-2.13	1.31	1.35
9	J	73	HIC	CE1-ND1	-2.12	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	i	73	HIC	CA-CB-CG-ND1
9	j	73	HIC	CA-CB-CG-ND1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	$\# Z > 2$
10	ADP	K	402	11	24,29,29	0.90	1 (4%)	29,45,45	1.31	5 (17%)
10	ADP	L	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.38	4 (13%)
10	ADP	B	402	11	24,29,29	0.92	1 (4%)	29,45,45	1.24	4 (13%)
10	ADP	b	402	11	24,29,29	0.93	1 (4%)	29,45,45	1.19	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ADP	j	402	11	24,29,29	0.94	1 (4%)	29,45,45	1.36	3 (10%)
10	ADP	a	502	11	24,29,29	0.89	1 (4%)	29,45,45	1.33	4 (13%)
10	ADP	k	401	11	24,29,29	0.95	1 (4%)	29,45,45	1.27	3 (10%)
10	ADP	l	501	11	24,29,29	0.89	1 (4%)	29,45,45	1.37	4 (13%)
10	ADP	A	501	-	24,29,29	0.91	1 (4%)	29,45,45	1.50	4 (13%)
10	ADP	I	402	11	24,29,29	1.01	2 (8%)	29,45,45	1.29	3 (10%)
10	ADP	J	501	11	24,29,29	1.03	2 (8%)	29,45,45	1.40	5 (17%)
10	ADP	i	401	11	24,29,29	0.93	1 (4%)	29,45,45	1.51	4 (13%)

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
10	ADP	K	402	11	-	0/12/32/32	0/3/3/3
10	ADP	L	501	-	-	4/12/32/32	0/3/3/3
10	ADP	B	402	11	-	7/12/32/32	0/3/3/3
10	ADP	b	402	11	-	7/12/32/32	0/3/3/3
10	ADP	j	402	11	-	0/12/32/32	0/3/3/3
10	ADP	a	502	11	-	0/12/32/32	0/3/3/3
10	ADP	k	401	11	-	0/12/32/32	0/3/3/3
10	ADP	l	501	11	-	2/12/32/32	0/3/3/3
10	ADP	A	501	-	-	2/12/32/32	0/3/3/3
10	ADP	I	402	11	-	2/12/32/32	0/3/3/3
10	ADP	J	501	11	-	2/12/32/32	0/3/3/3
10	ADP	i	401	11	-	2/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	501	ADP	O4'-C1'	2.53	1.44	1.41
10	I	402	ADP	O4'-C1'	2.50	1.44	1.41
10	L	501	ADP	C5-C4	2.42	1.47	1.40
10	K	402	ADP	C5-C4	2.37	1.47	1.40
10	l	501	ADP	C5-C4	2.29	1.47	1.40
10	k	401	ADP	C5-C4	2.28	1.47	1.40
10	i	401	ADP	C5-C4	2.27	1.46	1.40
10	J	501	ADP	C5-C4	2.25	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	402	ADP	C5-C4	2.23	1.46	1.40
10	A	501	ADP	C5-C4	2.23	1.46	1.40
10	j	402	ADP	C5-C4	2.22	1.46	1.40
10	b	402	ADP	C5-C4	2.21	1.46	1.40
10	I	402	ADP	C5-C4	2.20	1.46	1.40
10	a	502	ADP	C5-C4	2.13	1.46	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	i	401	ADP	PA-O3A-PB	-4.15	118.57	132.83
10	j	402	ADP	PA-O3A-PB	-4.01	119.07	132.83
10	L	501	ADP	PA-O3A-PB	-3.99	119.15	132.83
10	A	501	ADP	O4'-C1'-C2'	-3.62	101.63	106.93
10	J	501	ADP	N3-C2-N1	-3.31	123.50	128.68
10	A	501	ADP	N3-C2-N1	-3.29	123.54	128.68
10	a	502	ADP	N3-C2-N1	-3.29	123.54	128.68
10	I	402	ADP	N3-C2-N1	-3.28	123.55	128.68
10	l	501	ADP	PA-O3A-PB	-3.26	121.66	132.83
10	A	501	ADP	PA-O3A-PB	-3.24	121.70	132.83
10	j	402	ADP	N3-C2-N1	-3.23	123.64	128.68
10	l	501	ADP	N3-C2-N1	-3.18	123.71	128.68
10	i	401	ADP	N3-C2-N1	-3.09	123.85	128.68
10	K	402	ADP	N3-C2-N1	-3.06	123.89	128.68
10	L	501	ADP	N3-C2-N1	-3.06	123.89	128.68
10	k	401	ADP	N3-C2-N1	-3.04	123.92	128.68
10	b	402	ADP	N3-C2-N1	-3.04	123.92	128.68
10	a	502	ADP	PA-O3A-PB	-3.01	122.51	132.83
10	B	402	ADP	N3-C2-N1	-2.99	124.00	128.68
10	J	501	ADP	PA-O3A-PB	-2.88	122.94	132.83
10	B	402	ADP	PA-O3A-PB	-2.84	123.09	132.83
10	I	402	ADP	PA-O3A-PB	-2.80	123.20	132.83
10	I	402	ADP	C4-C5-N7	-2.79	106.50	109.40
10	J	501	ADP	C4-C5-N7	-2.70	106.58	109.40
10	A	501	ADP	C4-C5-N7	-2.70	106.59	109.40
10	i	401	ADP	C3'-C2'-C1'	2.69	105.03	100.98
10	l	501	ADP	O4'-C1'-C2'	-2.68	103.00	106.93
10	L	501	ADP	C4-C5-N7	-2.68	106.61	109.40
10	j	402	ADP	C4-C5-N7	-2.62	106.67	109.40
10	k	401	ADP	C4-C5-N7	-2.59	106.70	109.40
10	b	402	ADP	PA-O3A-PB	-2.58	123.96	132.83
10	K	402	ADP	PA-O3A-PB	-2.56	124.06	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	402	ADP	O4'-C1'-C2'	-2.52	103.24	106.93
10	l	501	ADP	C4-C5-N7	-2.51	106.78	109.40
10	a	502	ADP	C4-C5-N7	-2.48	106.81	109.40
10	J	501	ADP	C3'-C2'-C1'	-2.42	97.34	100.98
10	K	402	ADP	C3'-C2'-C1'	2.41	104.61	100.98
10	i	401	ADP	C4-C5-N7	-2.39	106.91	109.40
10	b	402	ADP	C4-C5-N7	-2.38	106.91	109.40
10	a	502	ADP	O4'-C4'-C3'	-2.36	100.44	105.11
10	K	402	ADP	C4-C5-N7	-2.32	106.98	109.40
10	B	402	ADP	C4-C5-N7	-2.28	107.02	109.40
10	k	401	ADP	PA-O3A-PB	-2.25	125.10	132.83
10	L	501	ADP	O4'-C1'-C2'	-2.13	103.81	106.93
10	B	402	ADP	O4'-C1'-C2'	-2.08	103.88	106.93
10	J	501	ADP	O4'-C1'-C2'	-2.04	103.94	106.93

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	501	ADP	PA-O3A-PB-O2B
10	B	402	ADP	C5'-O5'-PA-O3A
10	B	402	ADP	O4'-C4'-C5'-O5'
10	B	402	ADP	C3'-C4'-C5'-O5'
10	J	501	ADP	O4'-C4'-C5'-O5'
10	L	501	ADP	C5'-O5'-PA-O2A
10	b	402	ADP	C5'-O5'-PA-O1A
10	b	402	ADP	C5'-O5'-PA-O2A
10	l	501	ADP	PA-O3A-PB-O2B
10	b	402	ADP	O4'-C4'-C5'-O5'
10	b	402	ADP	C3'-C4'-C5'-O5'
10	b	402	ADP	C4'-C5'-O5'-PA
10	i	401	ADP	PB-O3A-PA-O1A
10	B	402	ADP	C4'-C5'-O5'-PA
10	A	501	ADP	PA-O3A-PB-O1B
10	L	501	ADP	C5'-O5'-PA-O3A
10	I	402	ADP	PB-O3A-PA-O2A
10	b	402	ADP	PB-O3A-PA-O2A
10	B	402	ADP	C5'-O5'-PA-O2A
10	L	501	ADP	C5'-O5'-PA-O1A
10	B	402	ADP	PB-O3A-PA-O1A
10	i	401	ADP	PB-O3A-PA-O2A
10	J	501	ADP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

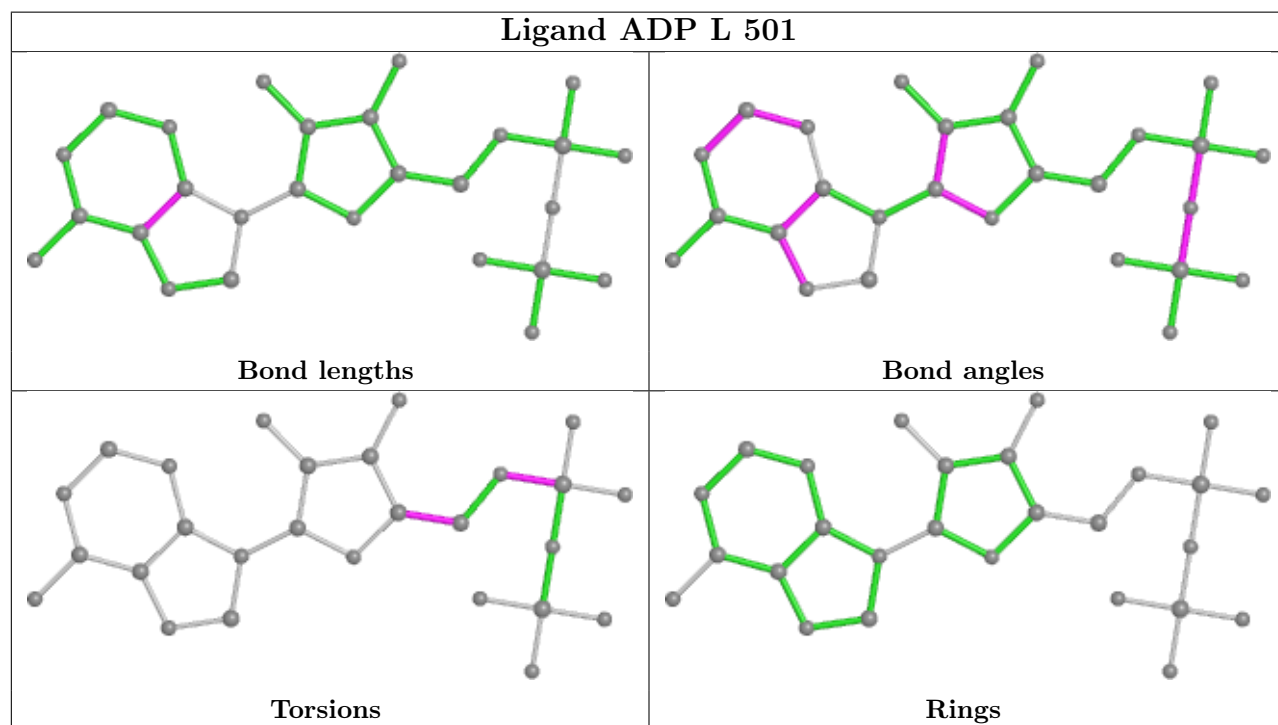
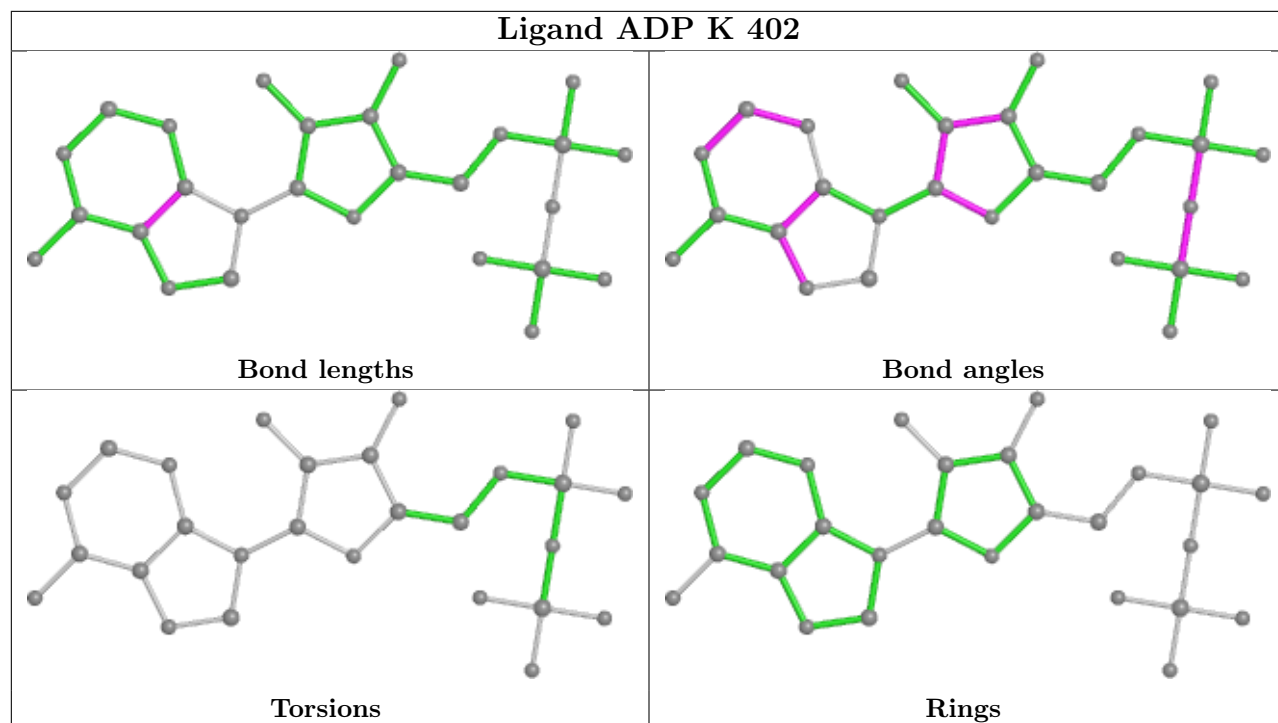
Mol	Chain	Res	Type	Atoms
10	l	501	ADP	PA-O3A-PB-O1B
10	B	402	ADP	PB-O3A-PA-O2A
10	b	402	ADP	C5'-O5'-PA-O3A
10	L	501	ADP	O4'-C4'-C5'-O5'
10	I	402	ADP	O4'-C4'-C5'-O5'

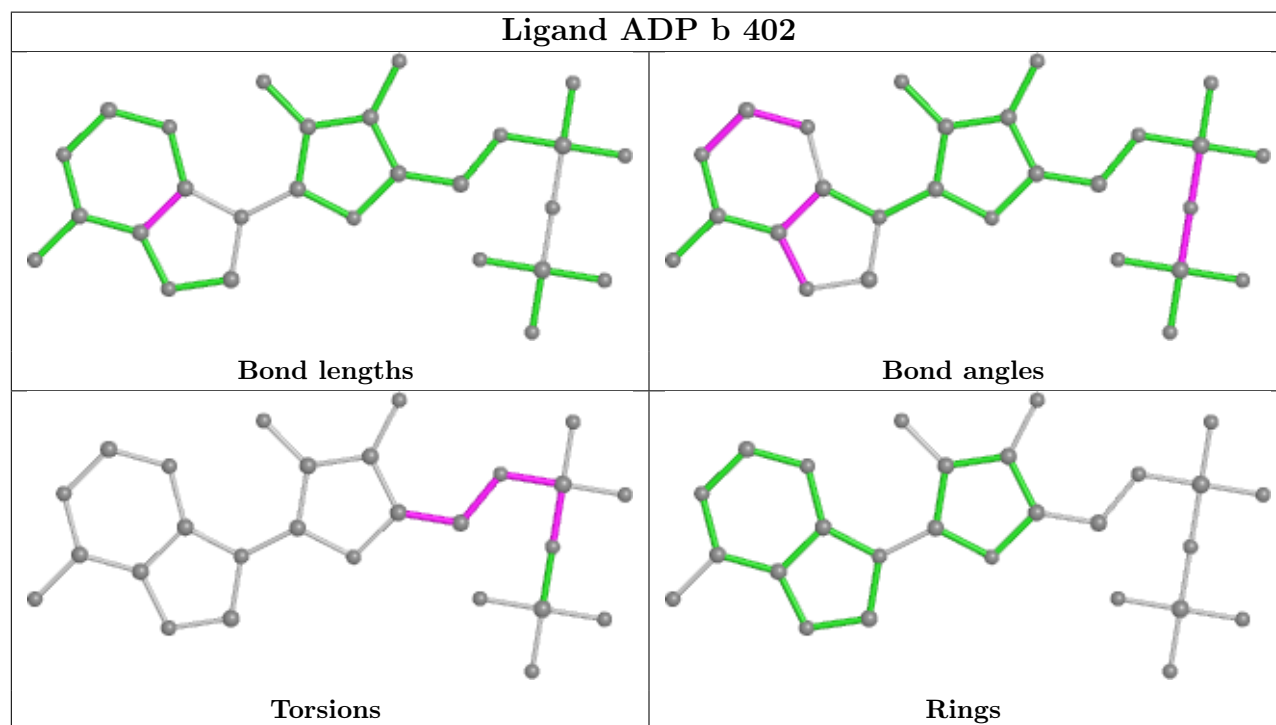
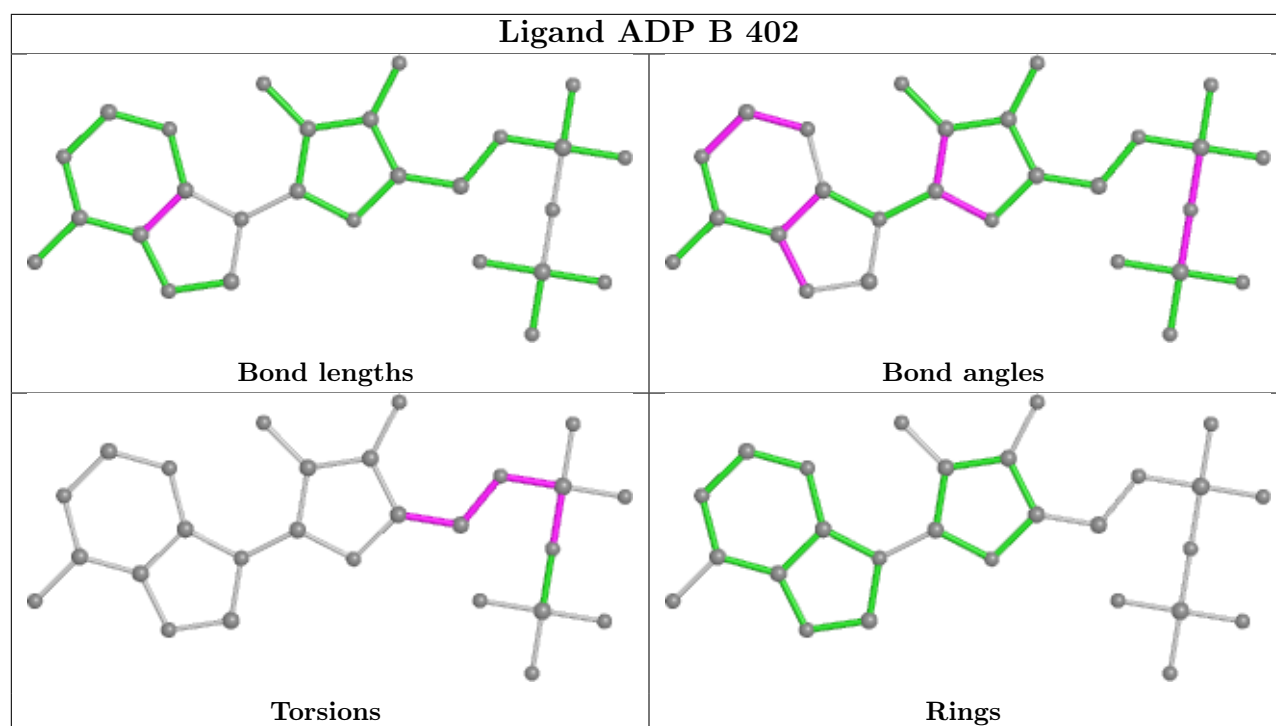
There are no ring outliers.

4 monomers are involved in 4 short contacts:

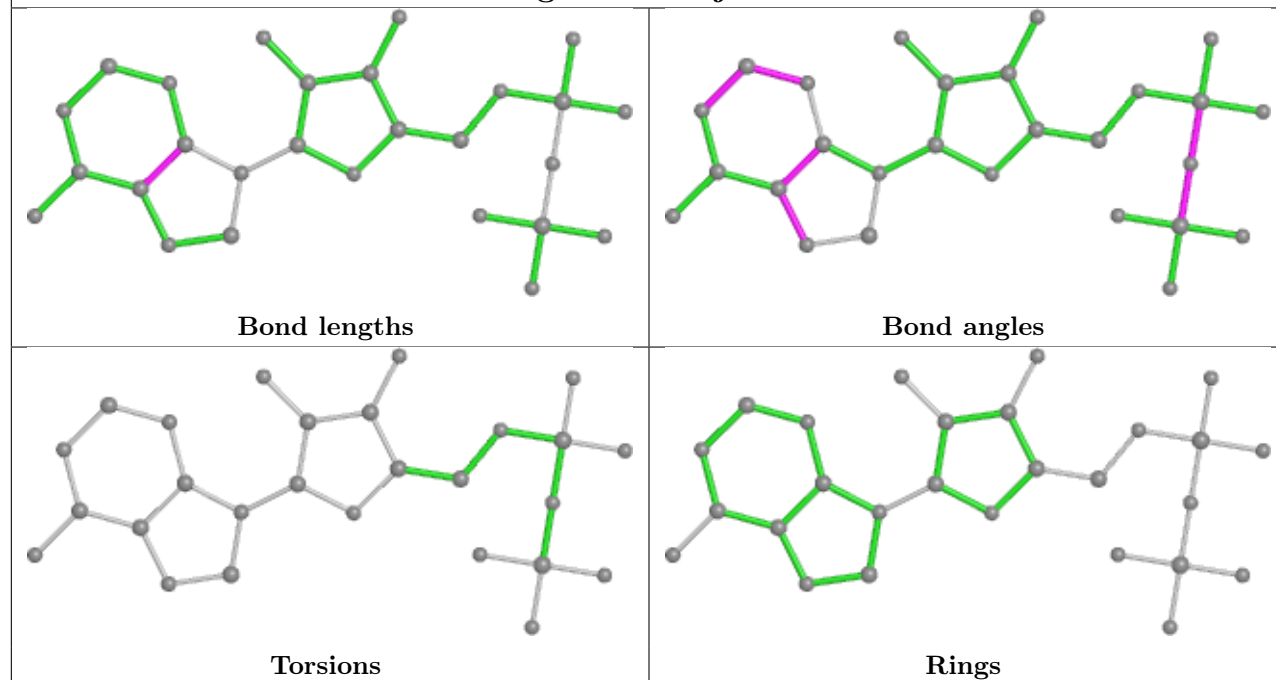
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	a	502	ADP	1	0
10	I	402	ADP	1	0
10	J	501	ADP	1	0
10	i	401	ADP	1	0

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.

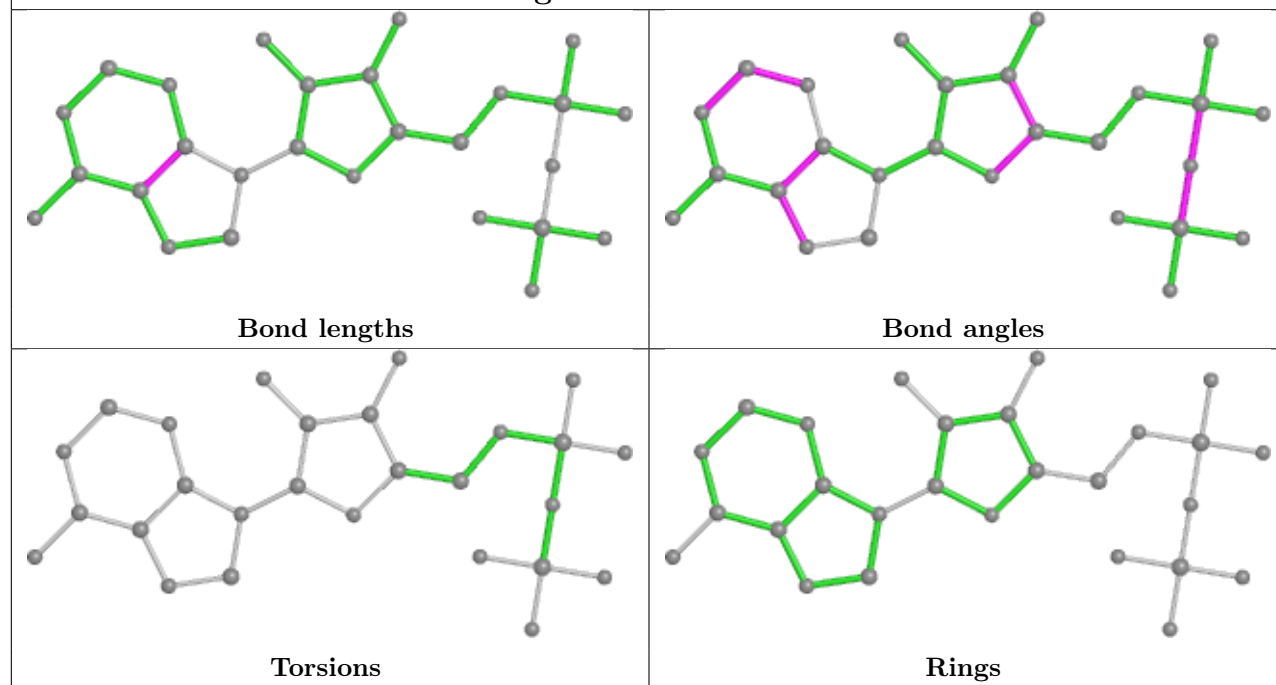


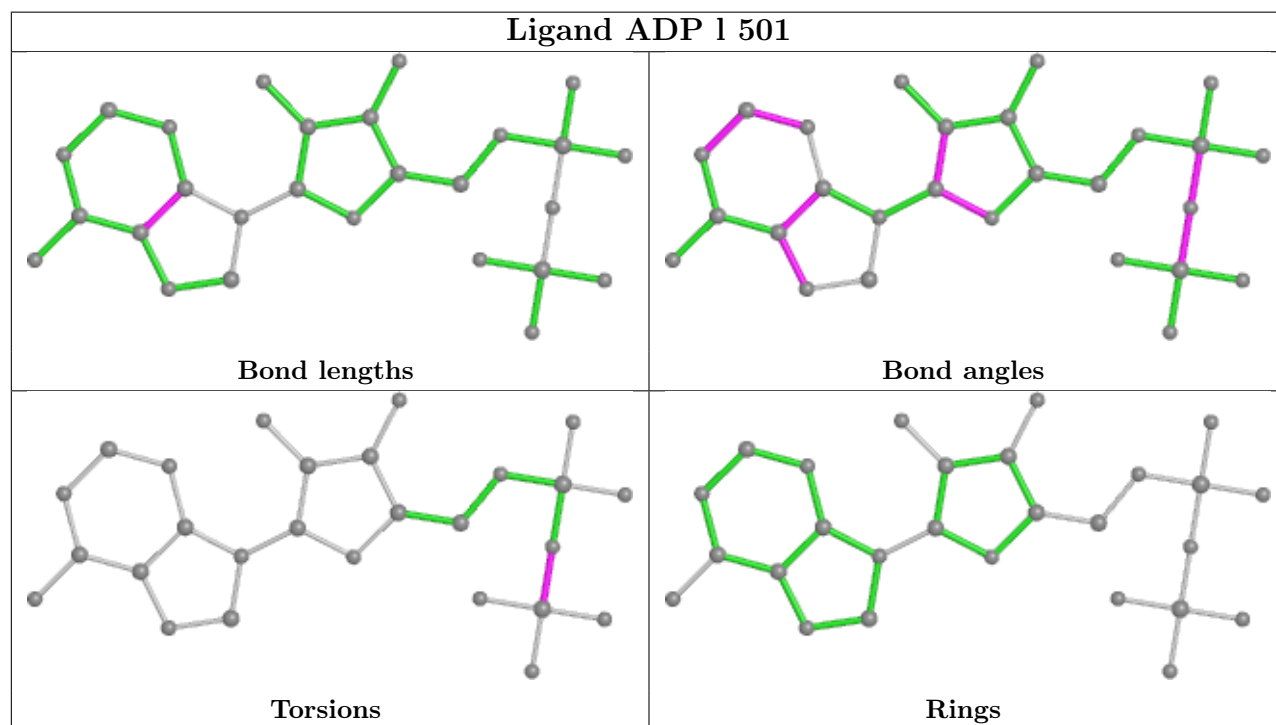
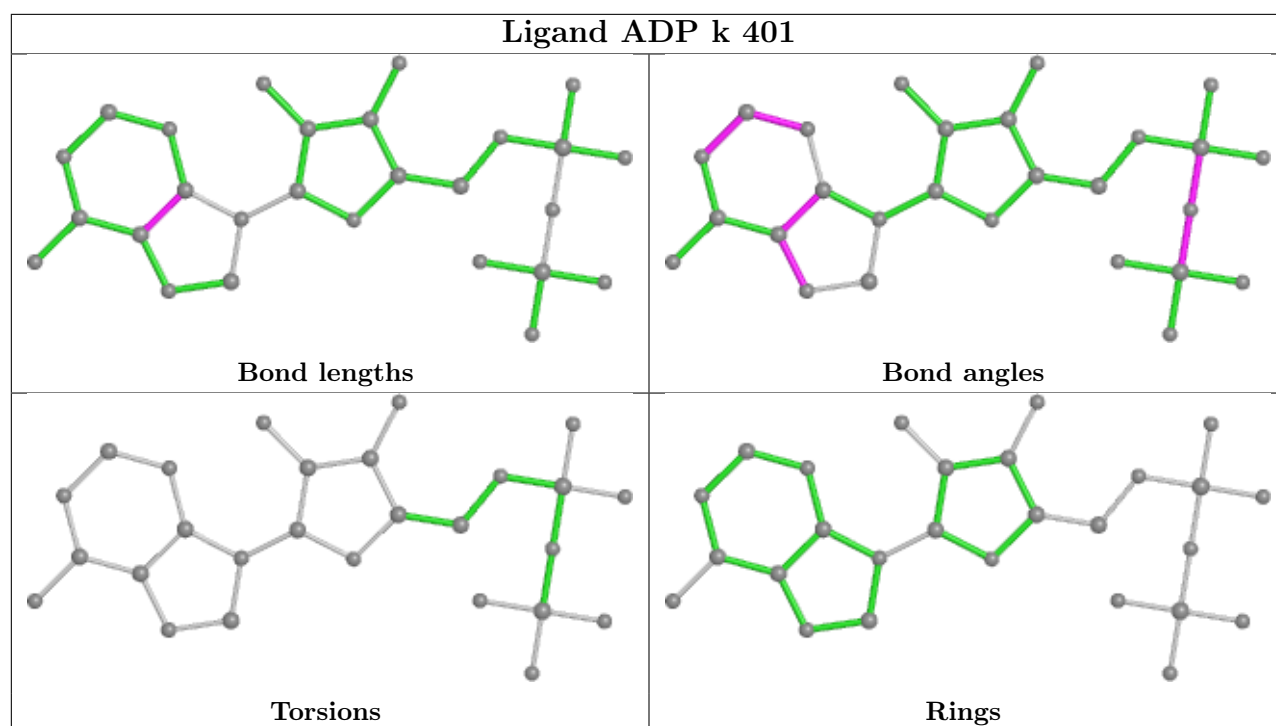


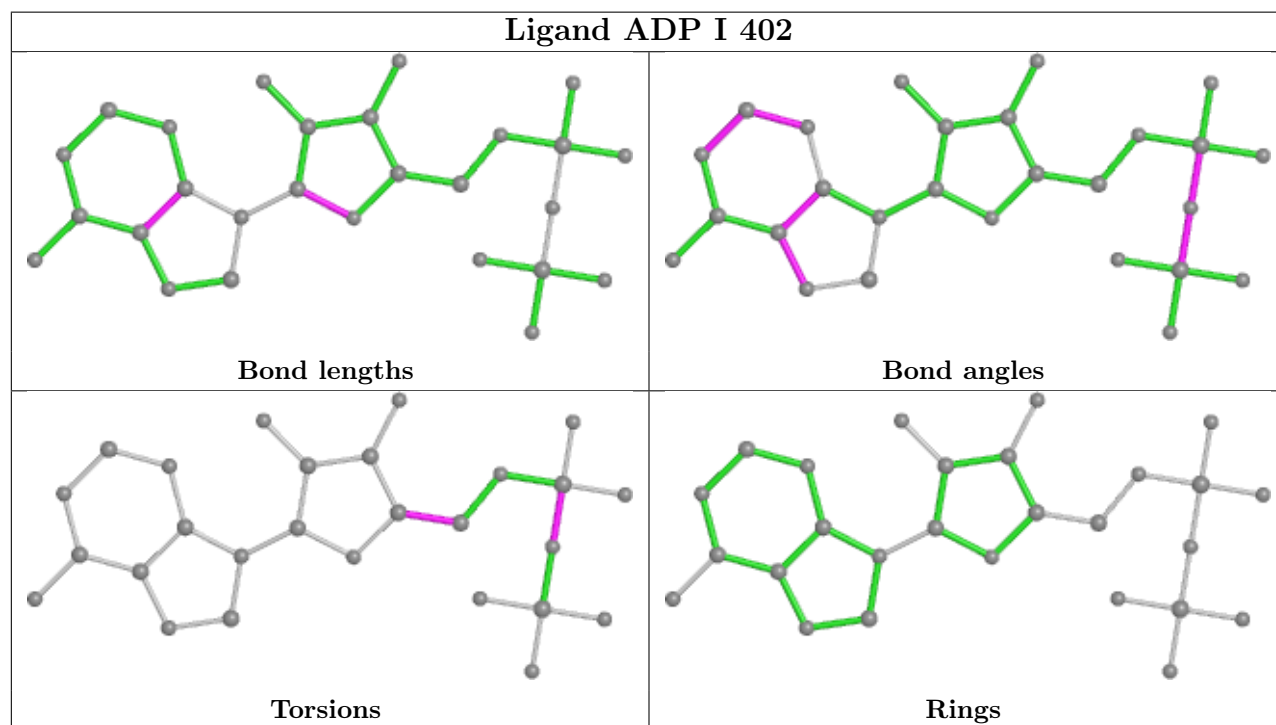
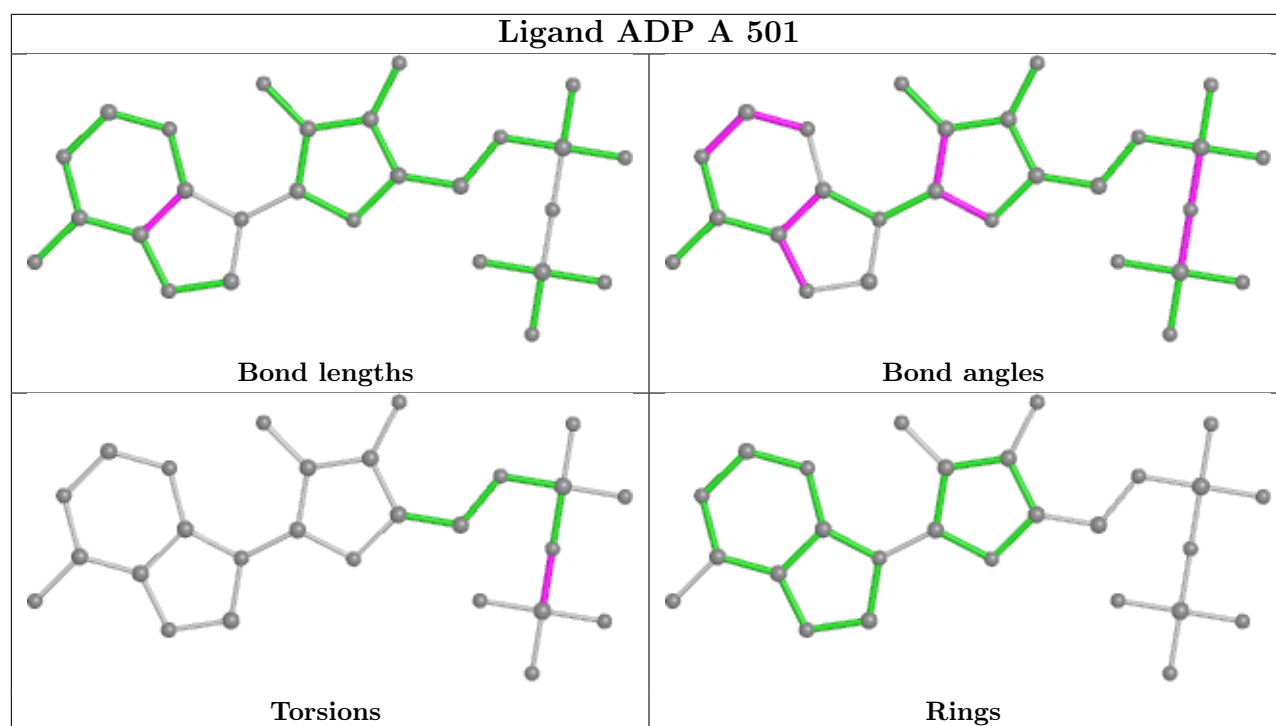
Ligand ADP j 402

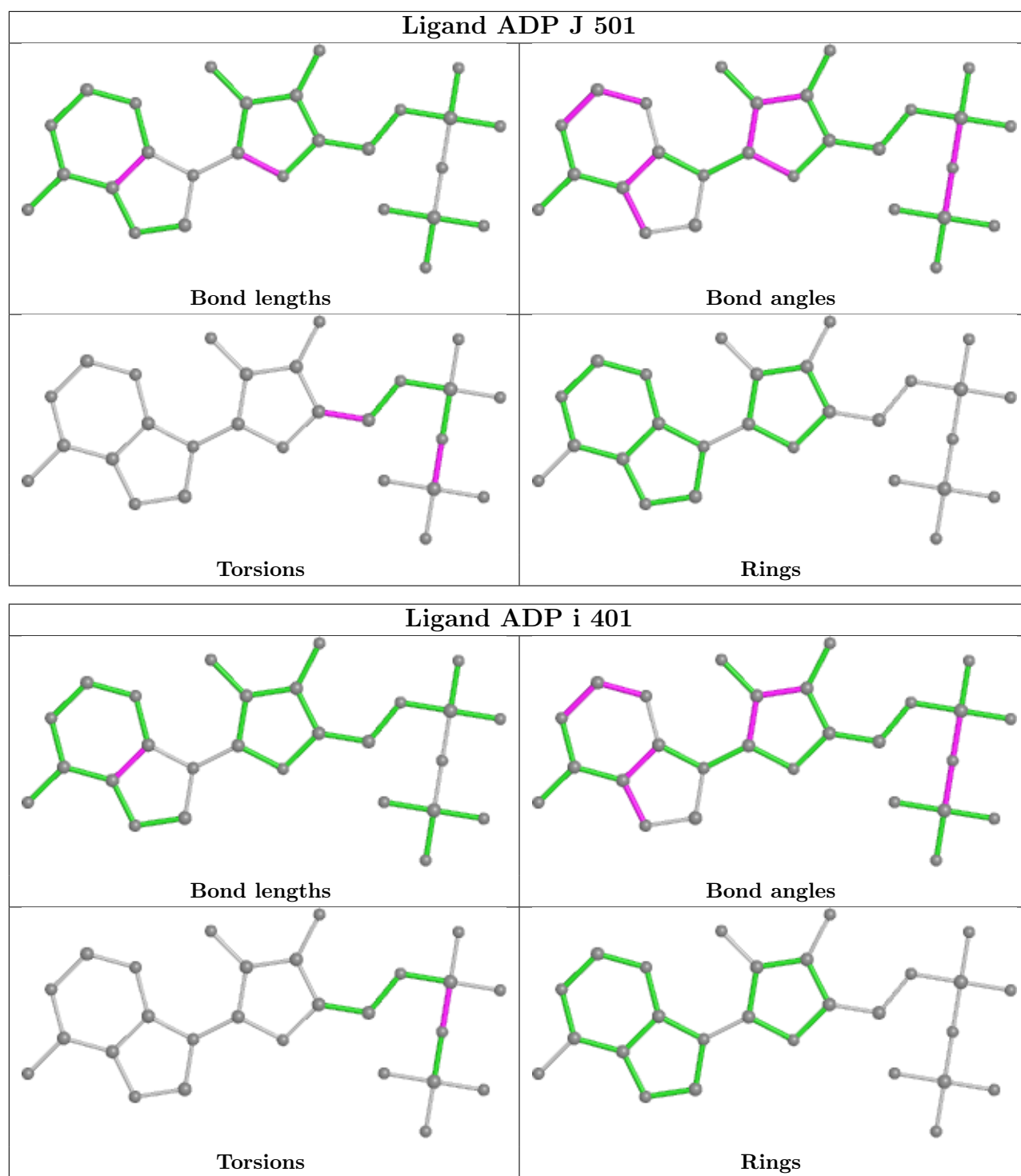


Ligand ADP a 502









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

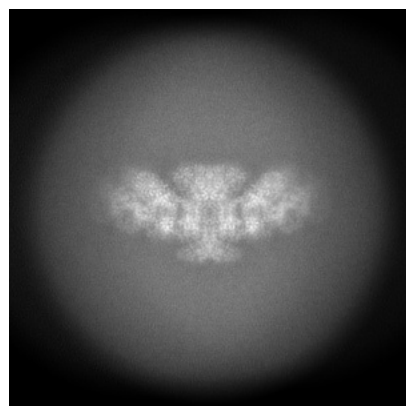
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63658. These allow visual inspection of the internal detail of the map and identification of artifacts.

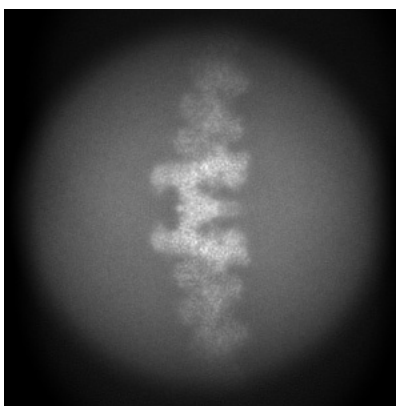
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

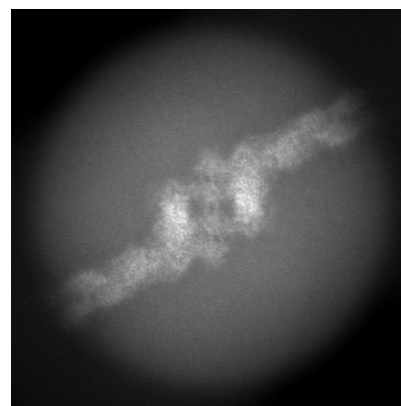
6.1.1 Primary map



X

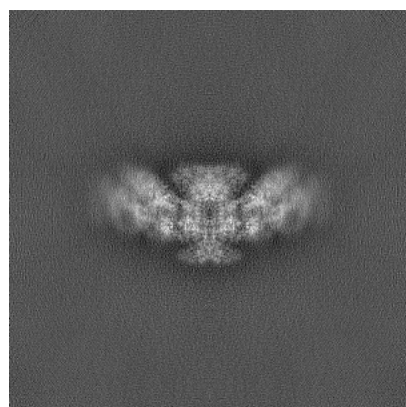


Y

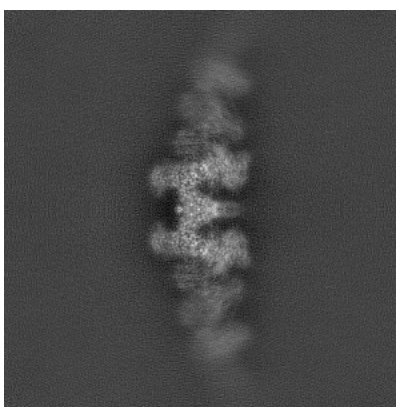


Z

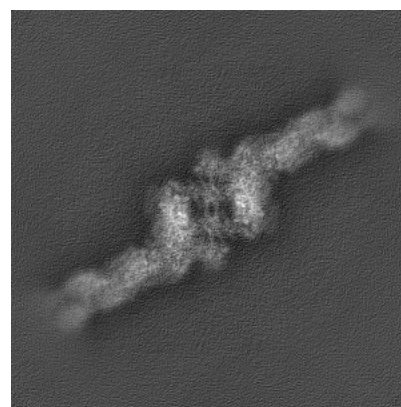
6.1.2 Raw map



X



Y

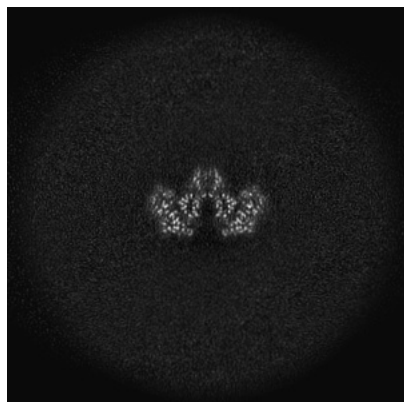


Z

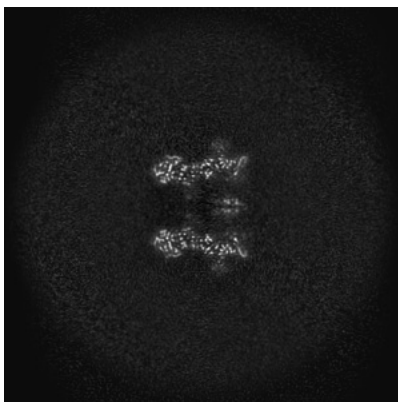
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

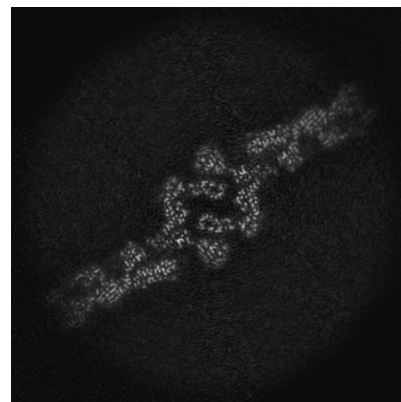
6.2.1 Primary map



X Index: 200

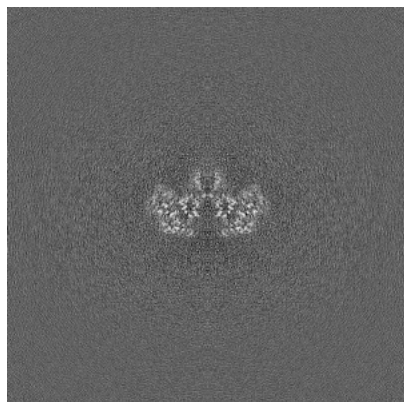


Y Index: 200

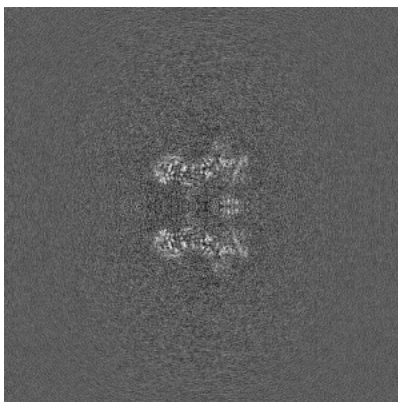


Z Index: 200

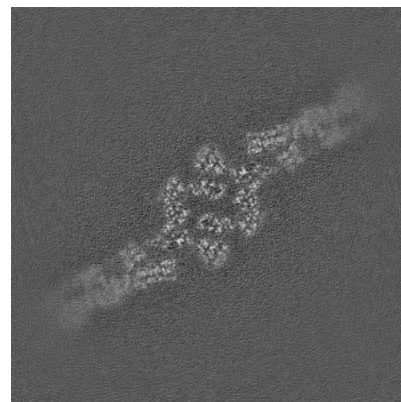
6.2.2 Raw map



X Index: 200



Y Index: 200

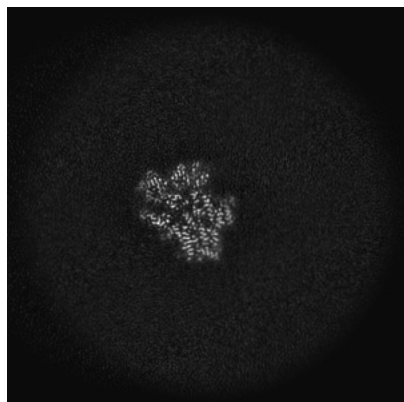


Z Index: 200

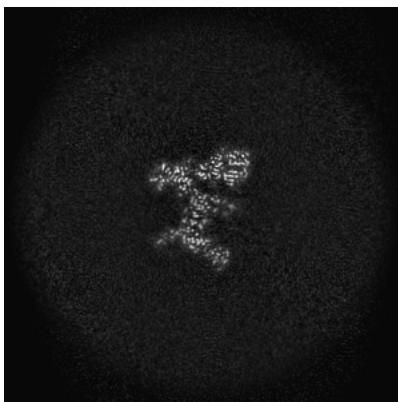
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

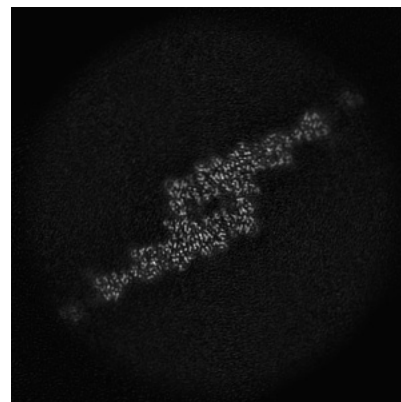
6.3.1 Primary map



X Index: 167

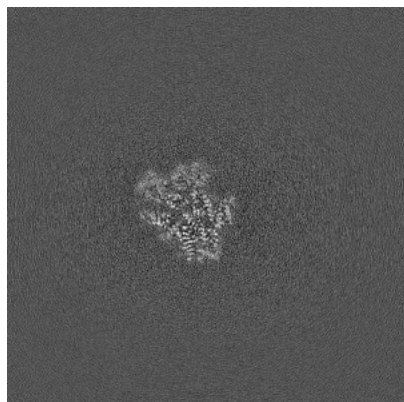


Y Index: 213

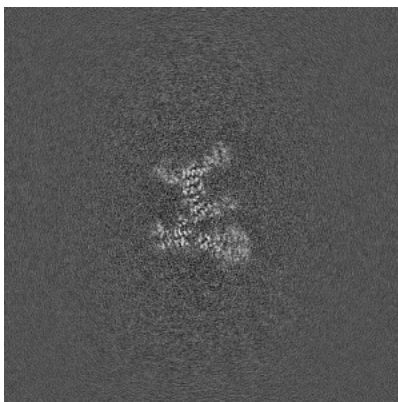


Z Index: 187

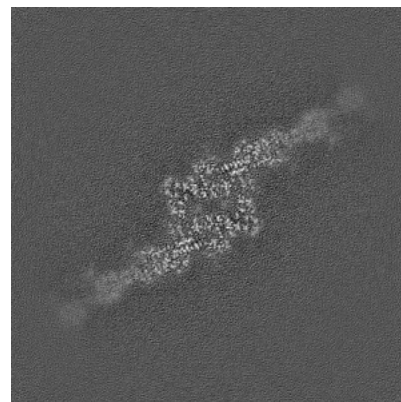
6.3.2 Raw map



X Index: 167



Y Index: 188

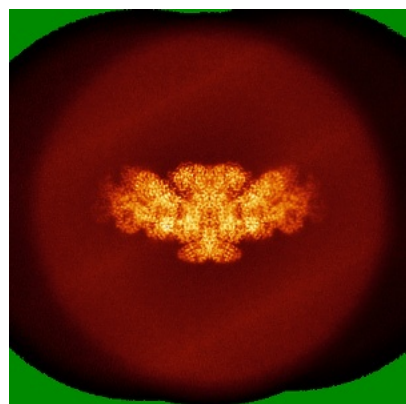


Z Index: 190

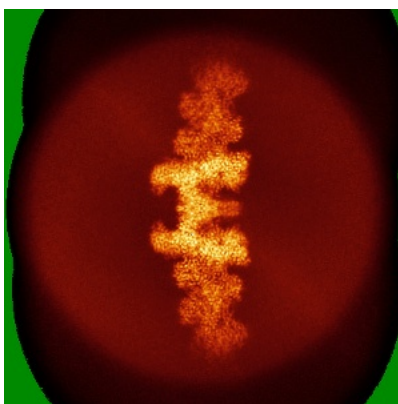
The images above show the largest variance slices of the map in three orthogonal directions.

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

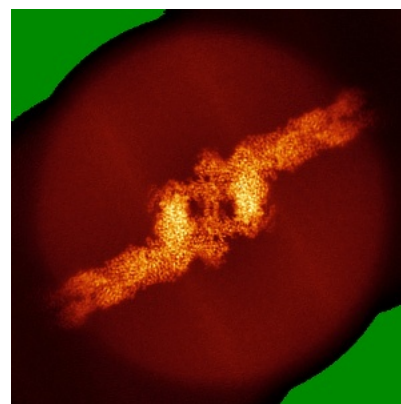
6.4.1 Primary map



X

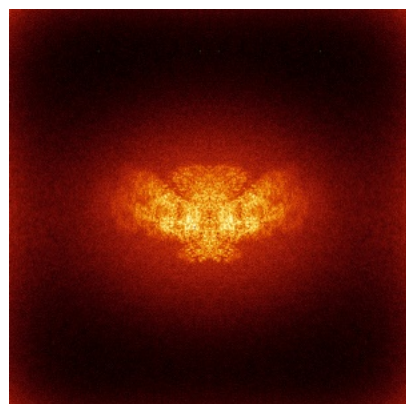


Y

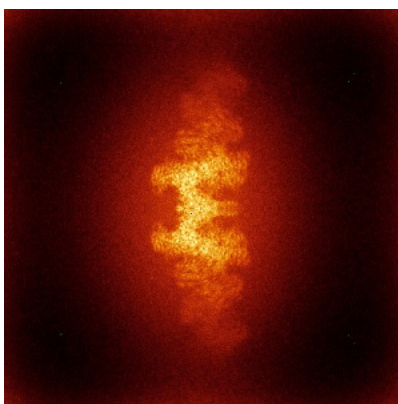


Z

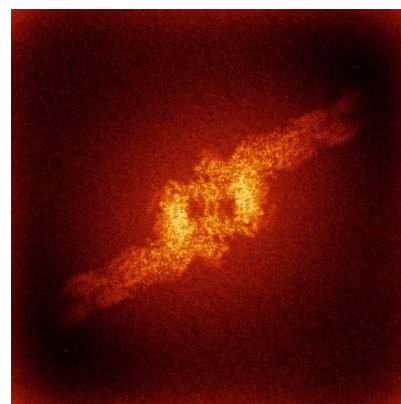
6.4.2 Raw map



X



Y

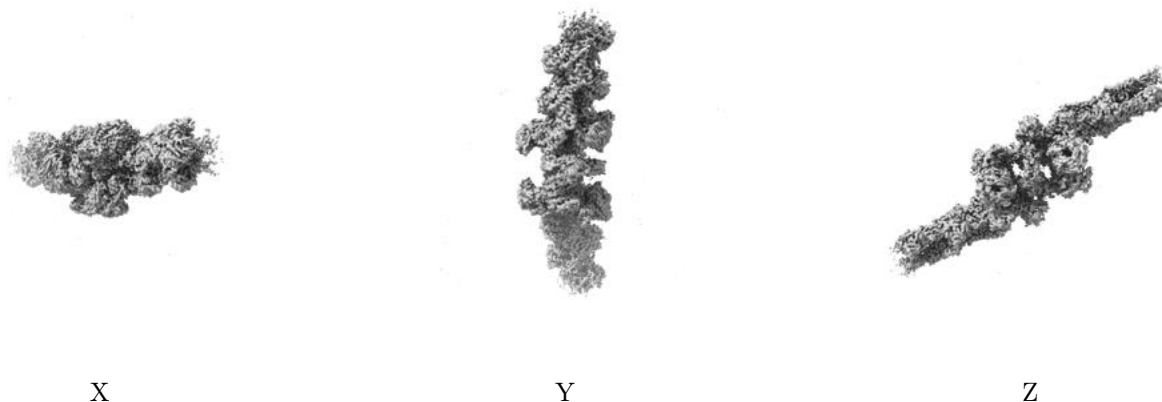


Z

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.

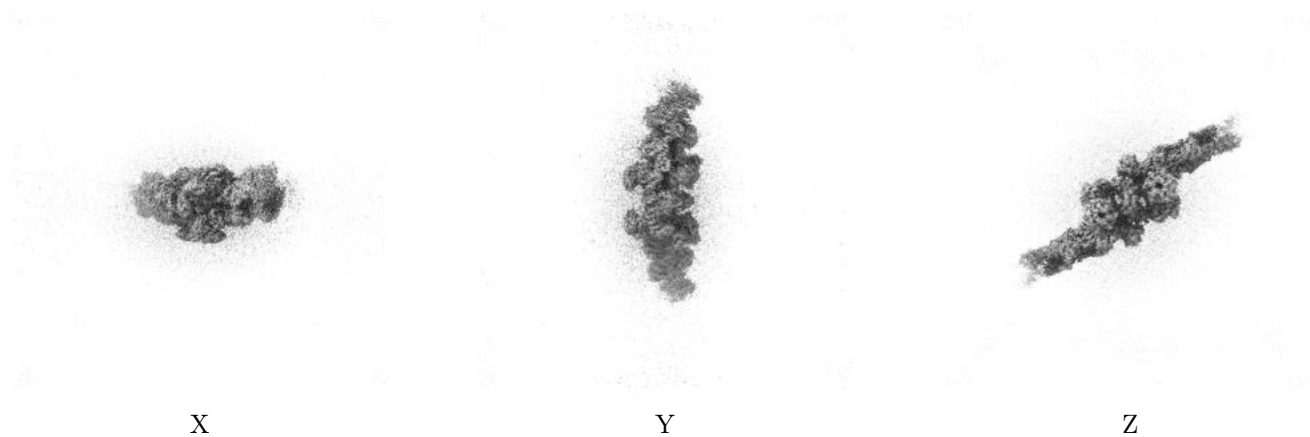
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

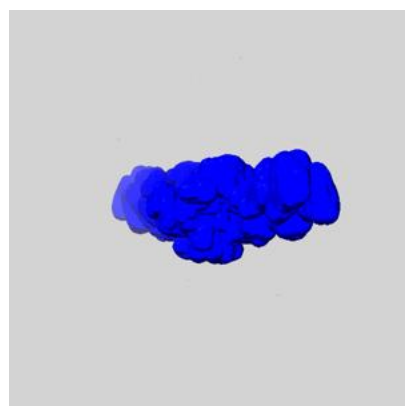
6.6 Mask visualisation [i](#)

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

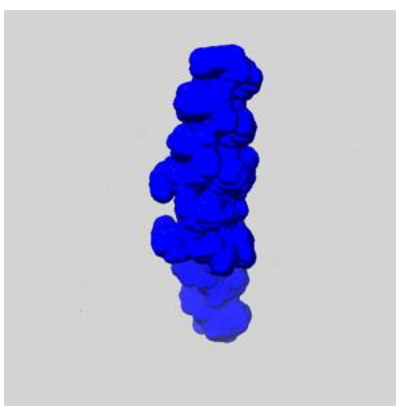
A mask typically either:

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

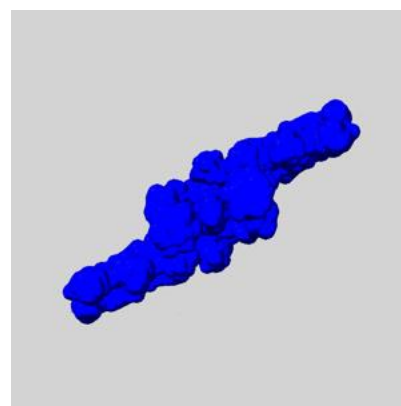
6.6.1 emd_63658_msk_1.map [i](#)



X



Y

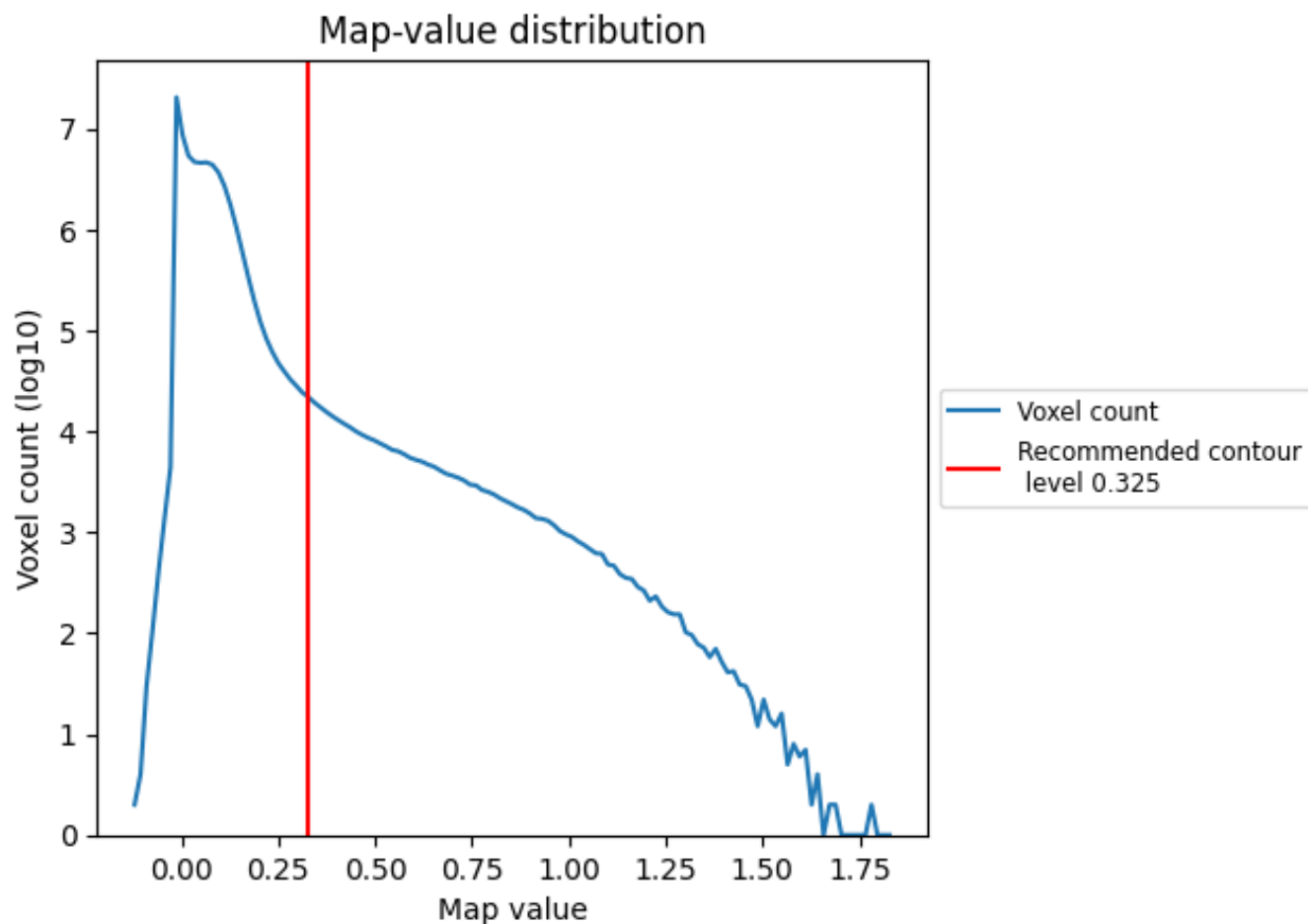


Z

7 Map analysis [i](#)

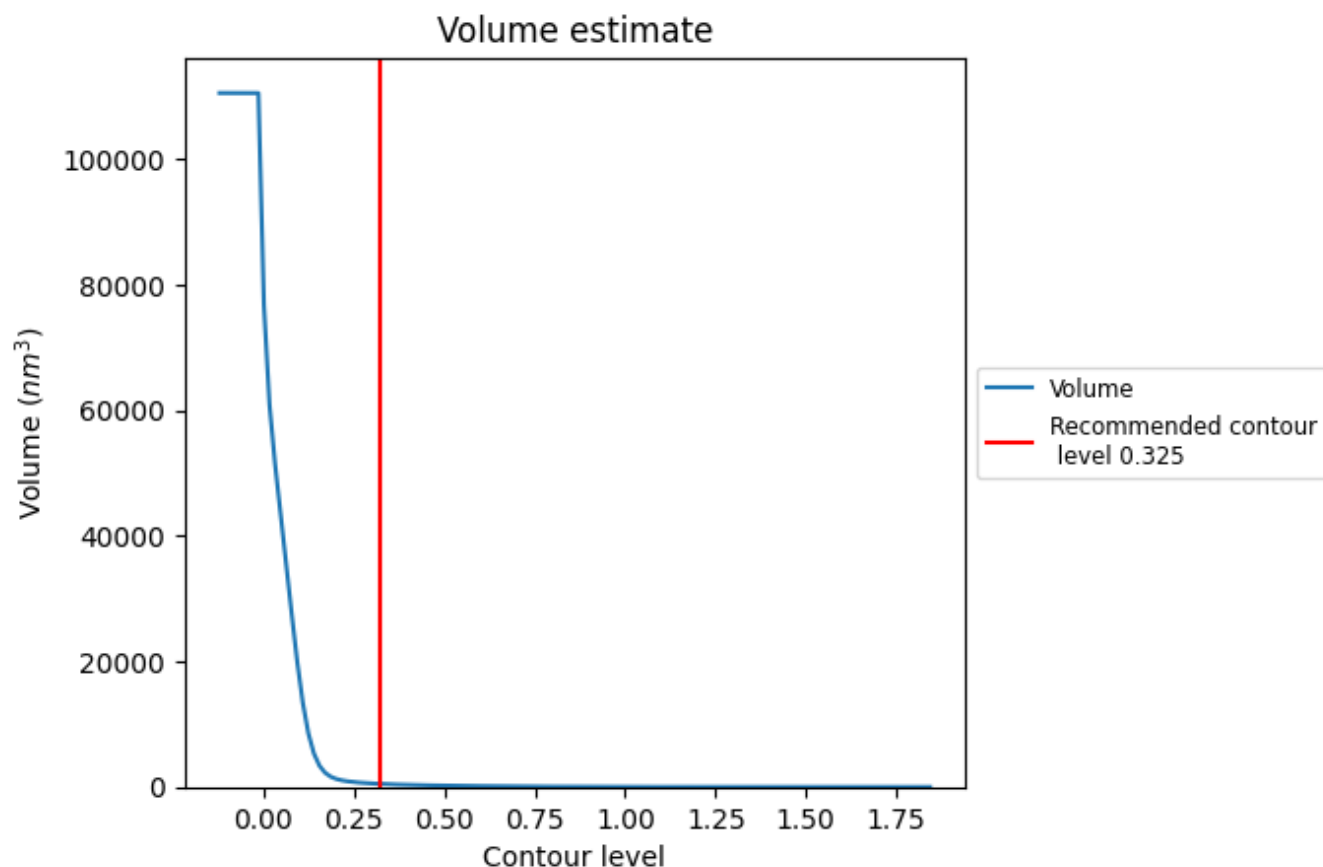
This section contains the results of statistical analysis of the map.

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.

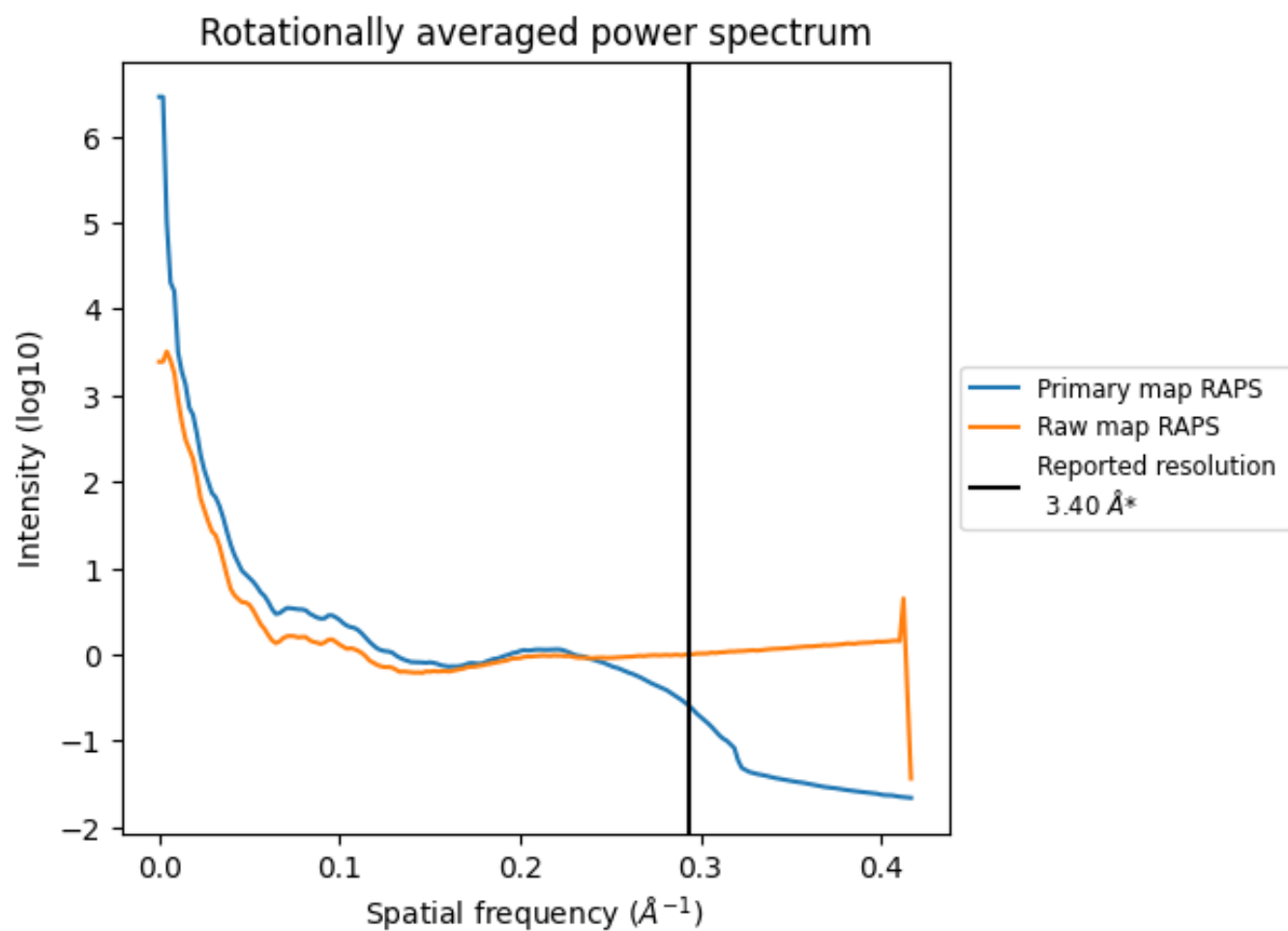
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 486 nm^3 ; this corresponds to an approximate mass of 439 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 ⓘ

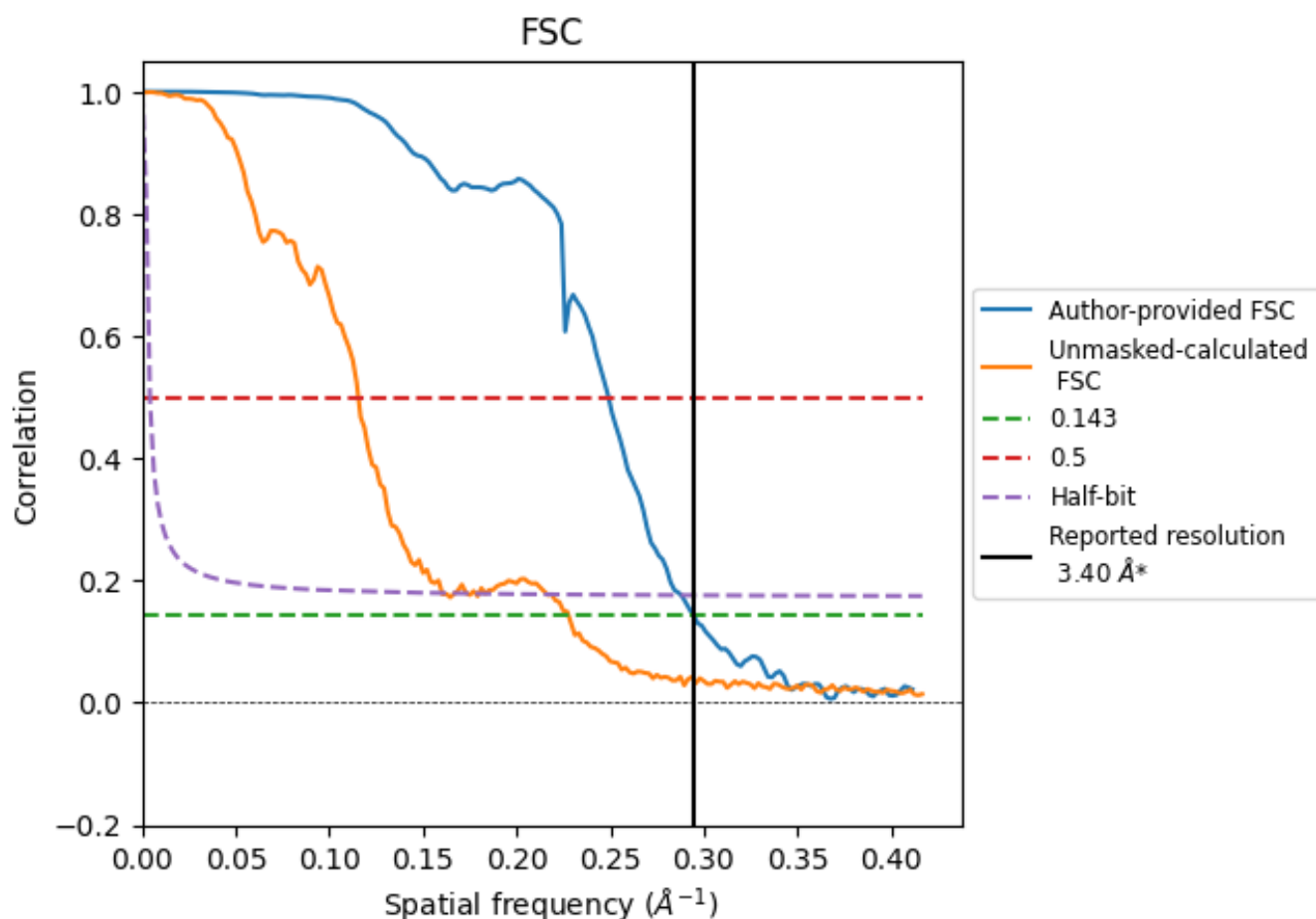


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

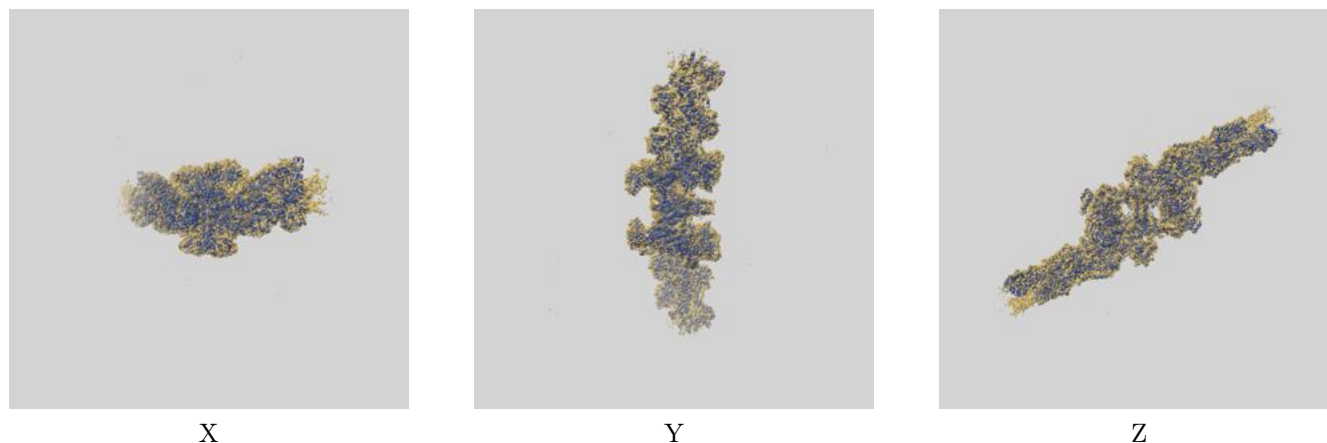
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	4.01	3.47
Unmasked-calculated*	4.39	8.67	6.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

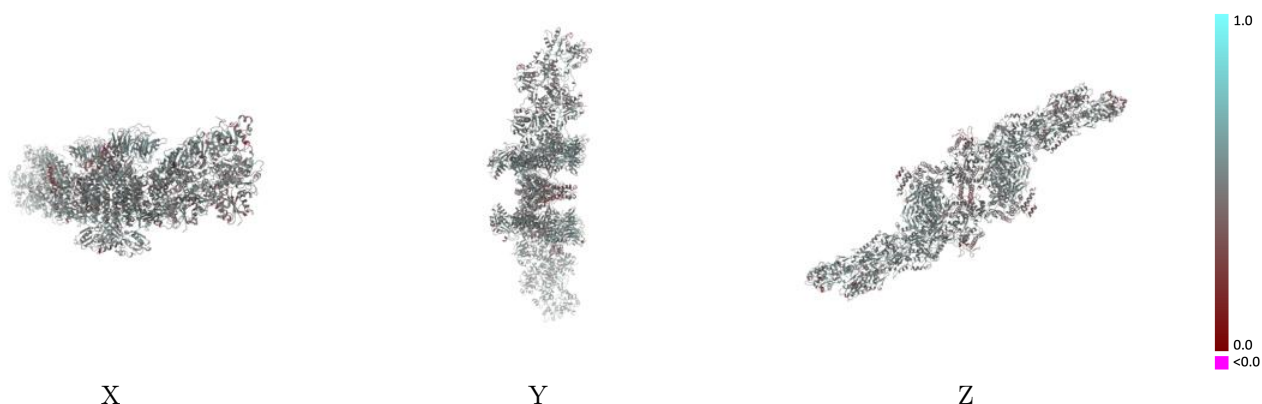
This section contains information regarding the fit between EMDB map EMD-63658 and PDB model 9M64. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



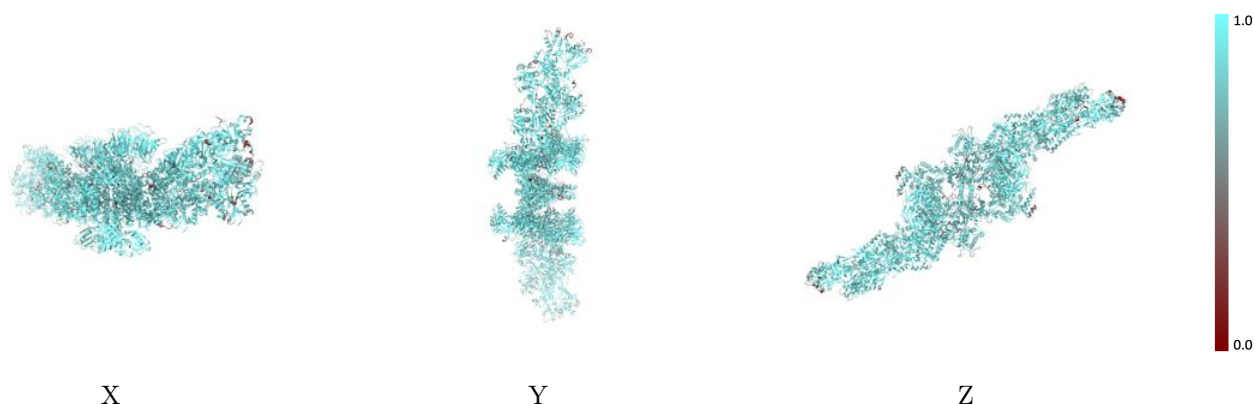
The images above show the 3D surface view of the map at the recommended contour level 0.325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



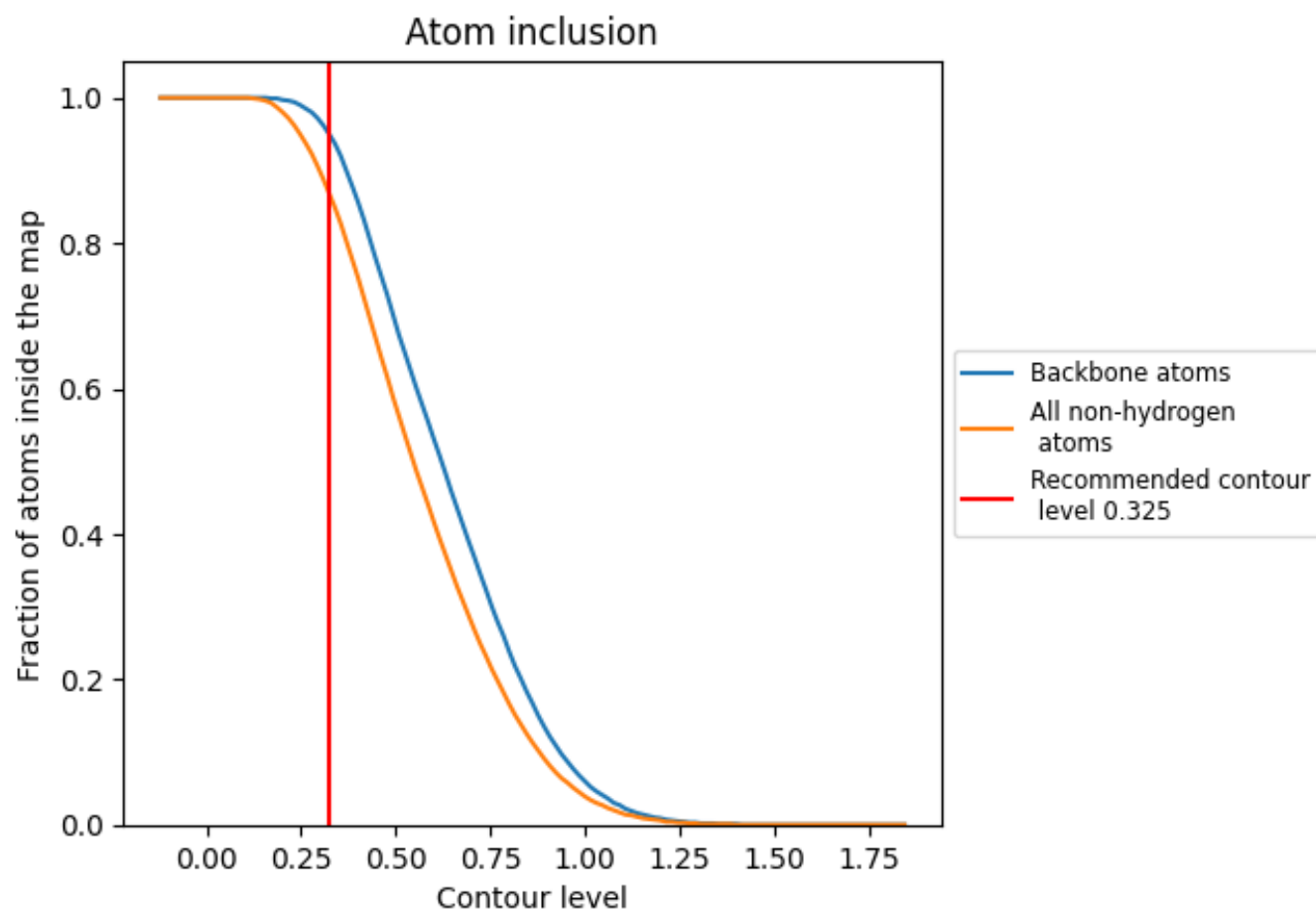
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.325).



















































9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8670	 0.4920
A	 0.8770	 0.5020
B	 0.8810	 0.5130
C	 0.9230	 0.5130
D	 0.9000	 0.4890
E	 0.7770	 0.4210
F	 0.9260	 0.5220
G	 0.7430	 0.4500
H	 0.8640	 0.4680
I	 0.8850	 0.4930
J	 0.8640	 0.4880
K	 0.8080	 0.4610
L	 0.8100	 0.4800
a	 0.8780	 0.5100
b	 0.8760	 0.5130
c	 0.9300	 0.5160
d	 0.8990	 0.4910
e	 0.8010	 0.4350
f	 0.9180	 0.5220
g	 0.7500	 0.4600
h	 0.8550	 0.4620
i	 0.9070	 0.5180
j	 0.8940	 0.5130
k	 0.8320	 0.4880
l	 0.8170	 0.5040

