WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Feb 23, 2022 – 12:28 pm GMT

PDB ID	:	7QIN
EMDB ID	:	EMD-13991
Title	:	In situ structure of actomyosin complex in skeletal sarcomere
Authors	:	Wang, Z.; Grange, M.; Pospich, S.; Wagner, T.; Kho, A.L.; Gautel, M.; Raunser, S.
Deposited on	:	2021-12-15
Resolution	:	6.60 Å(reported)
Based on initial models	:	3I5G, 5JLH

This is a wwPDB EM Validation Summary 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:
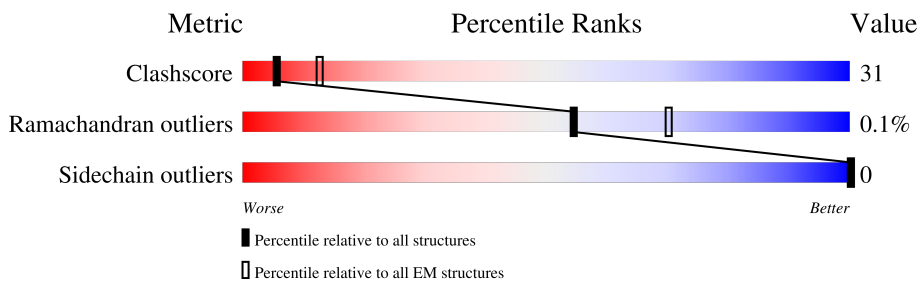
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 6.60 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	Percentile Ranks	Value
Clashscore		31
Ramachandran outliers		0.1%
Sidechain outliers		0

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	371	48% 51%
1	B	371	49% 50%
1	C	371	45% 54%
1	D	371	48% 51%
1	E	371	46% 53%
2	F	105	94% 6%
3	G	70	96%
4	H	117	7% 100%

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Mol	Chain	Length	Quality of chain
5	I	118	8% 100%
6	J	88	23% 100%
6	K	88	18% 100%
7	L	848	23% 35% 52% · 12%
7	M	848	18% 34% 53% · 12%

2   Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 29589 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, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	B	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	C	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	D	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	E	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		

- Molecule 2 is a protein called nebulin (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	105	Total	C	N	O	0	0
			546	333	105	108		

- Molecule 3 is a protein called nebulin (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	70	Total	C	N	O	0	0
			364	222	70	72		

- Molecule 4 is a protein called tropomyosin, alpha-1 (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	117	Total	C	N	O	0	0
			585	351	117	117		

- Molecule 5 is a protein called tropomyosin, alpha-1 (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	118	Total 590	C 354	N 118	O 118	0	0

- Molecule 6 is a protein called tropomyosin, alpha-1 (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	88	Total 440	C 264	N 88	O 88	0	0
6	K	88	Total 440	C 264	N 88	O 88	0	0

- Molecule 7 is a protein called Myosin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	749	Total 5992	C 3836	N 1002	O 1125	S 29	0	0
7	M	749	Total 5992	C 3836	N 1002	O 1125	S 29	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
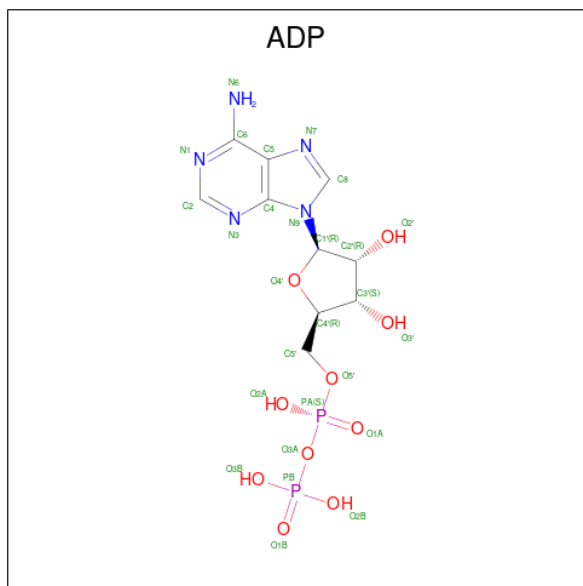
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 27	C 10	N 5	O 10	P 2	0
8	B	1	Total 27	C 10	N 5	O 10	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Mg	0
			1	1	
9	B	1	Total	Mg	0
			1	1	
9	C	1	Total	Mg	0
			1	1	
9	D	1	Total	Mg	0
			1	1	
9	E	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, alpha skeletal muscle
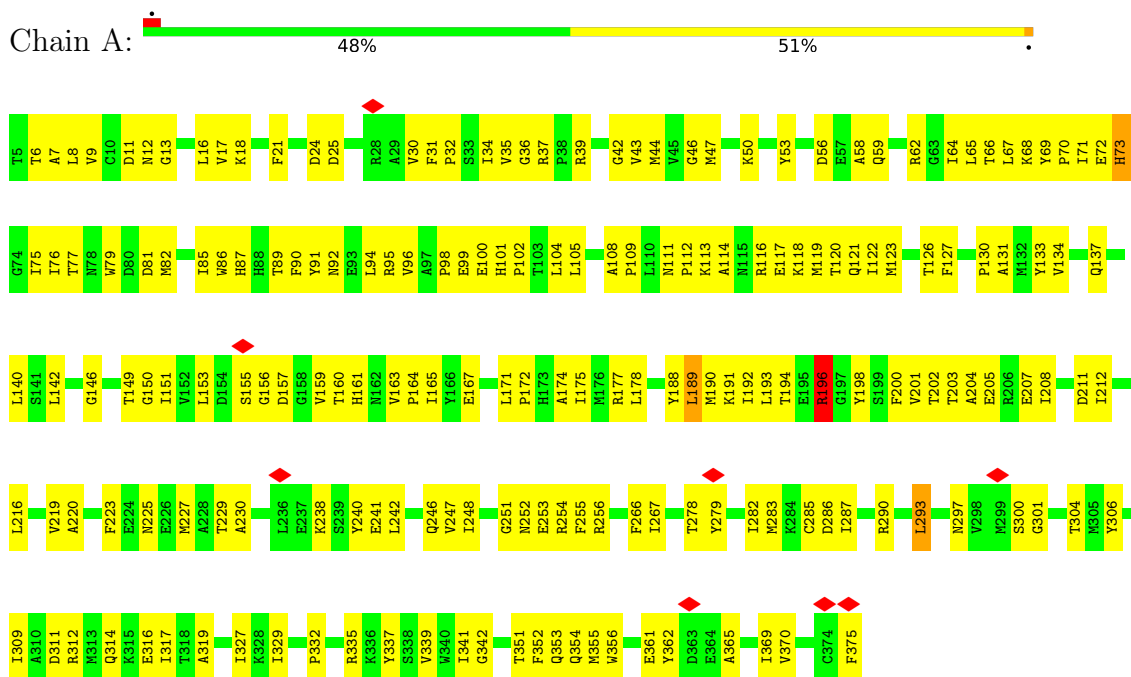
Chain A:

• Molecule 1: Actin, alpha skeletal muscle

Chain B:

• Molecule 1: Actin, alpha skeletal muscle

Chain C:

• Molecule 1: Actin, alpha skeletal muscle

Chain D:
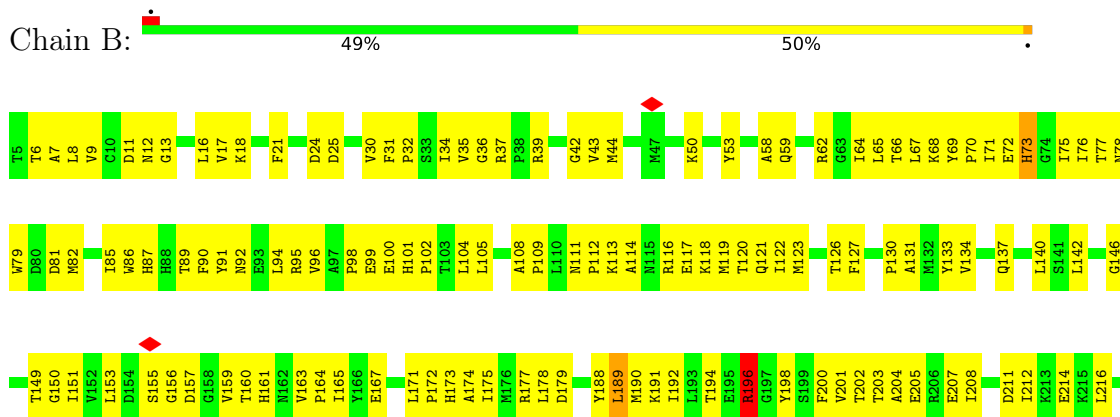
• Molecule 1: Actin, alpha skeletal muscle

Chain E:
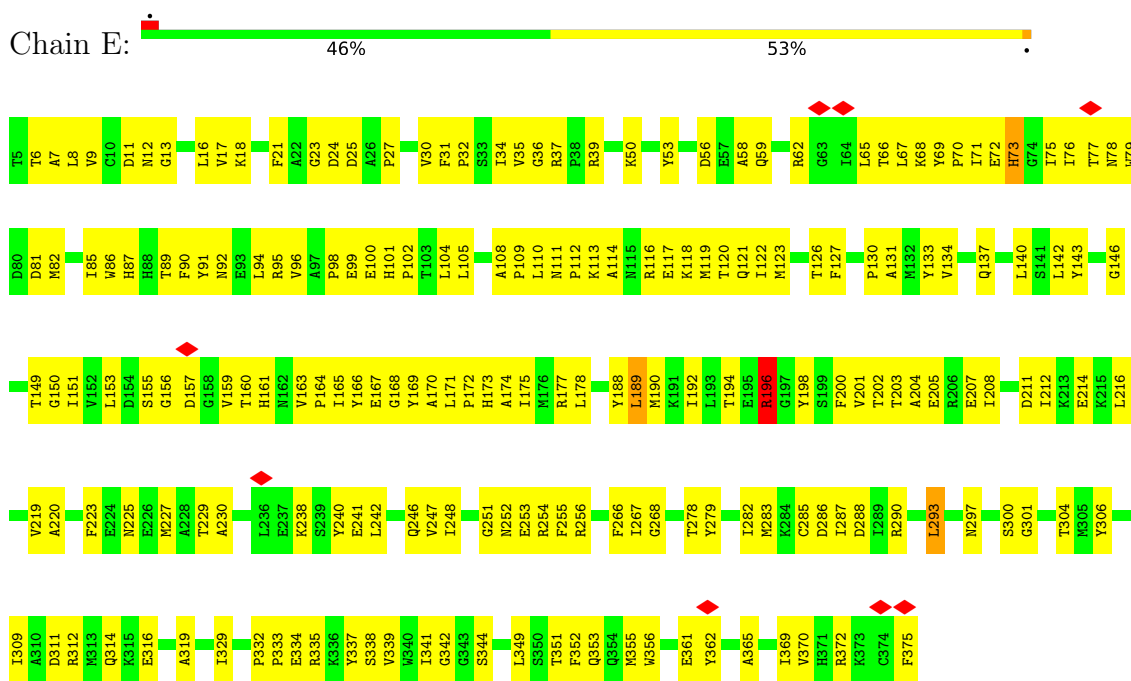
• Molecule 2: nebulin (mouse)

Chain F:
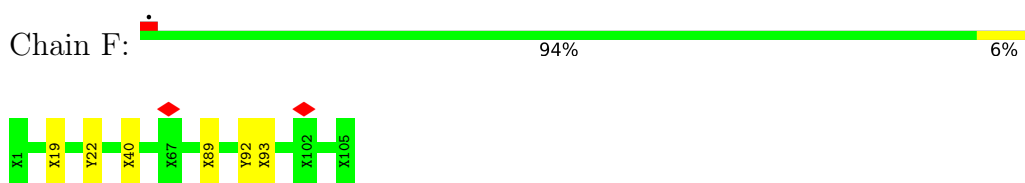
• Molecule 3: nebulin (mouse)

Chain G:
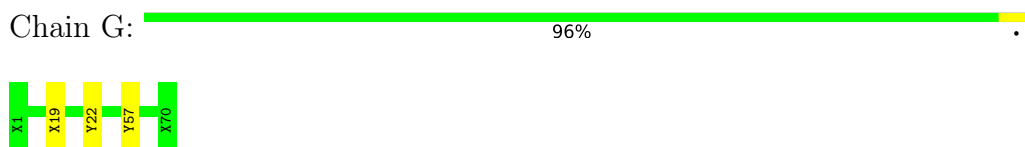
• Molecule 4: tropomyosin, alpha-1 (mouse)

Chain H:
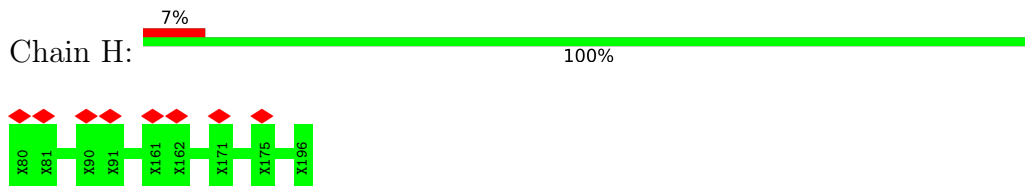
• Molecule 5: tropomyosin, alpha-1 (mouse)

Chain I:

X79 X119 X123 X129 X130 X131 X132 X133 X134 X135 X139 X196

• Molecule 6: tropomyosin, alpha-1 (mouse)

Chain J:

23%

100%

X78 X91 X98 X115 X118 X119 X122 X123 X126 X129 X132 X133 X139 X143 X146 X147 X160 X163 X164 X165

• Molecule 6: tropomyosin, alpha-1 (mouse)

Chain K:

18%

100%

X79 X80 X81 X84 X85 X91 X92 X93 X94 X95 X96 X97 X98 X101 X158 X159 X160 X161 X162 X163 X166

• Molecule 7: Myosin-4

Chain L:

23%

35%   52%   12%

• Molecule 7: Myosin-4

Chain M:

18%

34%

53%

12%

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	104302	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	3.4	Depositor
Minimum defocus (nm)	2400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	346.0, 346.0, 346.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.73, 1.73, 1.73	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.42	0/2950	0.66	3/3994 (0.1%)
1	B	0.42	0/2950	0.66	3/3994 (0.1%)
1	C	0.42	0/2950	0.66	3/3994 (0.1%)
1	D	0.42	0/2950	0.66	3/3994 (0.1%)
1	E	0.42	0/2950	0.66	3/3994 (0.1%)
2	F	0.51	0/36	0.54	0/45
3	G	0.48	0/24	0.56	0/30
7	L	0.39	0/6119	0.71	2/8251 (0.0%)
7	M	0.39	0/6119	0.71	2/8251 (0.0%)
All	All	0.41	0/27048	0.68	19/36547 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
7	L	0	11
7	M	0	11
All	All	0	37

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	196	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	196	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	196	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	E	196	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	D	196	ARG	NE-CZ-NH2	-6.73	116.93	120.30

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ARG	Sidechain
1	A	267	ILE	Peptide
1	A	301	GLY	Peptide
1	B	196	ARG	Sidechain
1	B	267	ILE	Peptide

5.2   Too-close contacts ⓘ

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	2900	0	2872	174	0
1	B	2900	0	2872	175	0
1	C	2900	0	2872	200	0
1	D	2900	0	2872	177	0
1	E	2900	0	2872	194	0
2	F	546	0	139	6	0
3	G	364	0	93	2	0
4	H	585	0	119	0	0
5	I	590	0	120	0	0
6	J	440	0	90	0	0
6	K	440	0	90	0	0
7	L	5992	0	5971	444	0
7	M	5992	0	5971	437	0
8	A	27	0	12	5	0
8	B	27	0	12	6	0
8	C	27	0	12	6	0
8	D	27	0	12	6	0
8	E	27	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
All	All	29589	0	27013	1739	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 31.

The worst 5 of 1739 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)
7:M:235:ASN:HD22	7:M:245:SER:HB3	1.29	0.96
1:E:333:PRO:HG3	7:L:416:LYS:H	1.28	0.96
7:M:196:PHE:HA	7:M:199:ILE:HD12	1.49	0.94
7:L:196:PHE:HA	7:L:199:ILE:HD12	1.50	0.94
7:M:359:VAL:HG13	7:M:431:ALA:HB1	1.50	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/371 (99%)	367 (100%)	1 (0%)	0	100	100
1	B	368/371 (99%)	367 (100%)	1 (0%)	0	100	100
1	C	368/371 (99%)	367 (100%)	1 (0%)	0	100	100
1	D	368/371 (99%)	367 (100%)	1 (0%)	0	100	100
1	E	368/371 (99%)	367 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	3/105 (3%)	3 (100%)	0	0	100	100
3	G	2/70 (3%)	2 (100%)	0	0	100	100
7	L	743/848 (88%)	740 (100%)	2 (0%)	1 (0%)	51	85
7	M	743/848 (88%)	740 (100%)	2 (0%)	1 (0%)	51	85
All	All	3331/3726 (89%)	3320 (100%)	9 (0%)	2 (0%)	54	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	L	181	SER
7	M	181	SER

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	313/313 (100%)	313 (100%)	0	100	100
1	B	313/313 (100%)	313 (100%)	0	100	100
1	C	313/313 (100%)	313 (100%)	0	100	100
1	D	313/313 (100%)	313 (100%)	0	100	100
1	E	313/313 (100%)	313 (100%)	0	100	100
2	F	3/3 (100%)	3 (100%)	0	100	100
3	G	2/2 (100%)	2 (100%)	0	100	100
7	L	648/727 (89%)	648 (100%)	0	100	100
7	M	648/727 (89%)	648 (100%)	0	100	100
All	All	2866/3024 (95%)	2866 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	137	GLN
1	E	137	GLN
7	M	690	HIS
1	D	162	ASN
1	E	12	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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
1	HIC	D	73	1	8,11,12	1.56	2 (25%)	6,14,16	1.65	1 (16%)
1	HIC	A	73	1	8,11,12	1.58	2 (25%)	6,14,16	1.66	1 (16%)
1	HIC	C	73	1	8,11,12	1.59	2 (25%)	6,14,16	1.67	1 (16%)
1	HIC	B	73	1	8,11,12	1.58	2 (25%)	6,14,16	1.66	1 (16%)
1	HIC	E	73	1	8,11,12	1.58	2 (25%)	6,14,16	1.65	1 (16%)

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
1	HIC	D	73	1	-	3/5/6/8	0/1/1/1
1	HIC	A	73	1	-	3/5/6/8	0/1/1/1
1	HIC	C	73	1	-	3/5/6/8	0/1/1/1
1	HIC	B	73	1	-	3/5/6/8	0/1/1/1
1	HIC	E	73	1	-	3/5/6/8	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	HIC	CD2-CG	3.29	1.41	1.36
1	A	73	HIC	CD2-CG	3.28	1.41	1.36
1	E	73	HIC	CD2-CG	3.23	1.41	1.36
1	D	73	HIC	CD2-CG	3.21	1.41	1.36
1	B	73	HIC	CD2-CG	3.21	1.41	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	73	HIC	CB-CA-C	-3.38	105.14	111.47
1	B	73	HIC	CB-CA-C	-3.36	105.16	111.47
1	E	73	HIC	CB-CA-C	-3.36	105.17	111.47
1	D	73	HIC	CB-CA-C	-3.35	105.19	111.47
1	A	73	HIC	CB-CA-C	-3.35	105.20	111.47

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	N-CA-CB-CG
1	A	73	HIC	CA-CB-CG-ND1
1	B	73	HIC	N-CA-CB-CG
1	B	73	HIC	CA-CB-CG-ND1
1	C	73	HIC	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	73	HIC	2	0
1	A	73	HIC	2	0
1	C	73	HIC	2	0
1	B	73	HIC	2	0
1	E	73	HIC	2	0

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#|Z| > 2$
8	ADP	D	401	9	24,29,29	0.91	1 (4%)	29,45,45	1.12	3 (10%)
8	ADP	A	401	9	24,29,29	0.92	1 (4%)	29,45,45	1.12	3 (10%)
8	ADP	C	401	9	24,29,29	0.92	1 (4%)	29,45,45	1.13	3 (10%)
8	ADP	B	401	9	24,29,29	0.92	1 (4%)	29,45,45	1.13	3 (10%)
8	ADP	E	401	9	24,29,29	0.92	1 (4%)	29,45,45	1.13	3 (10%)

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
8	ADP	D	401	9	-	5/12/32/32	0/3/3/3
8	ADP	A	401	9	-	5/12/32/32	0/3/3/3
8	ADP	C	401	9	-	5/12/32/32	0/3/3/3
8	ADP	B	401	9	-	5/12/32/32	0/3/3/3
8	ADP	E	401	9	-	5/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	401	ADP	C5-C4	2.28	1.47	1.40
8	C	401	ADP	C5-C4	2.28	1.47	1.40
8	A	401	ADP	C5-C4	2.27	1.46	1.40
8	E	401	ADP	C5-C4	2.26	1.46	1.40
8	B	401	ADP	C5-C4	2.25	1.46	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	401	ADP	N3-C2-N1	-2.89	124.16	128.68
8	C	401	ADP	N3-C2-N1	-2.88	124.18	128.68
8	E	401	ADP	N3-C2-N1	-2.86	124.21	128.68
8	D	401	ADP	N3-C2-N1	-2.86	124.22	128.68
8	A	401	ADP	N3-C2-N1	-2.84	124.24	128.68

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	401	ADP	C5'-O5'-PA-O2A
8	A	401	ADP	C5'-O5'-PA-O3A
8	B	401	ADP	C5'-O5'-PA-O2A
8	B	401	ADP	C5'-O5'-PA-O3A
8	C	401	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	401	ADP	6	0
8	A	401	ADP	5	0
8	C	401	ADP	6	0
8	B	401	ADP	6	0
8	E	401	ADP	6	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 401

Bond lengths

Bond angles

Torsions

Rings
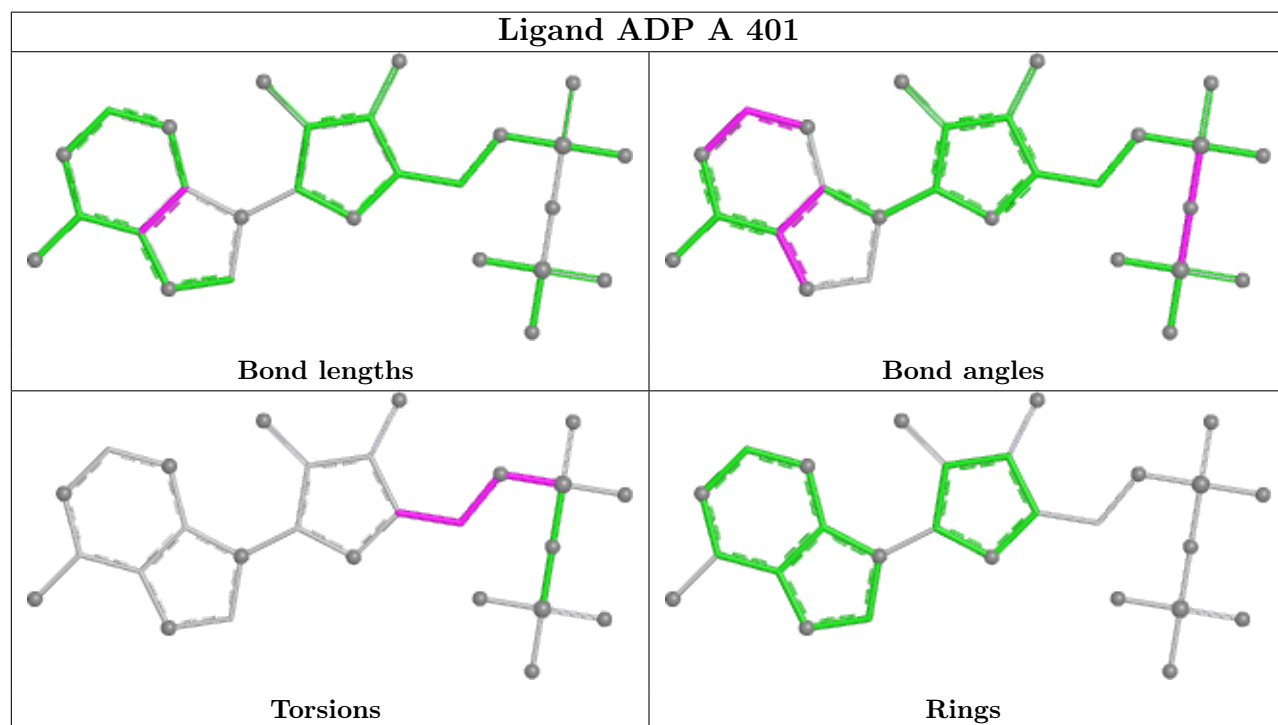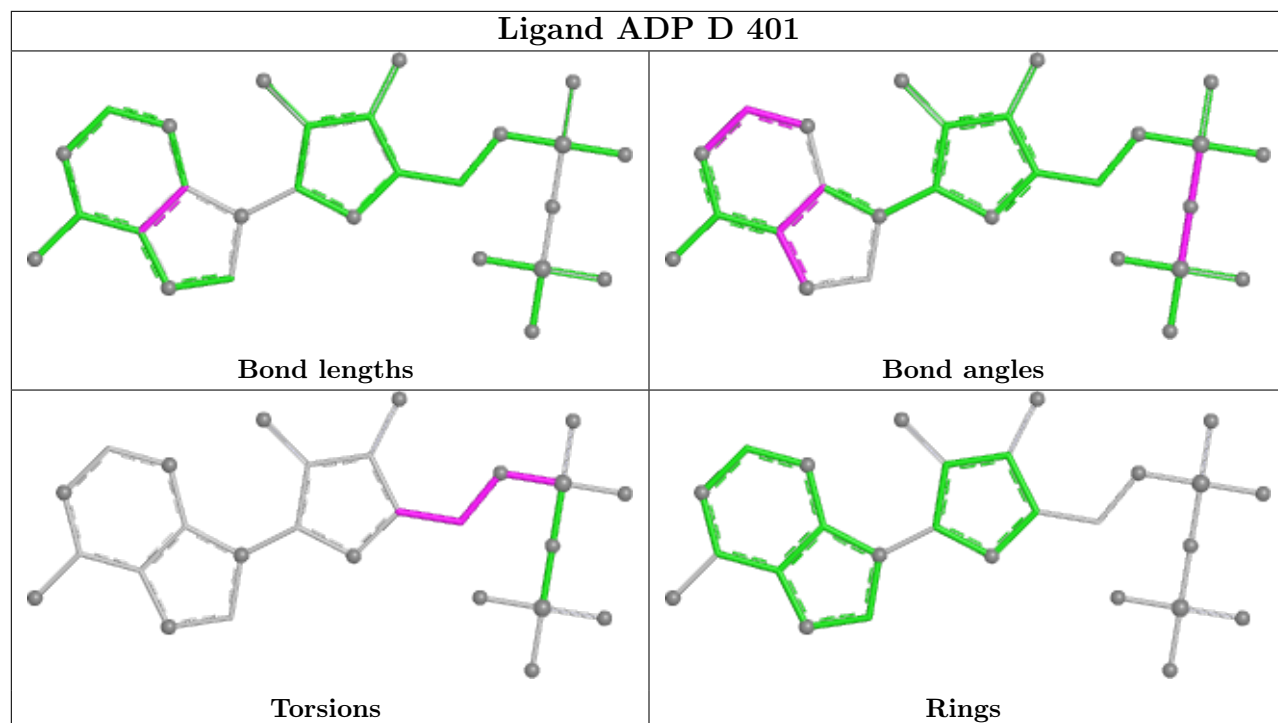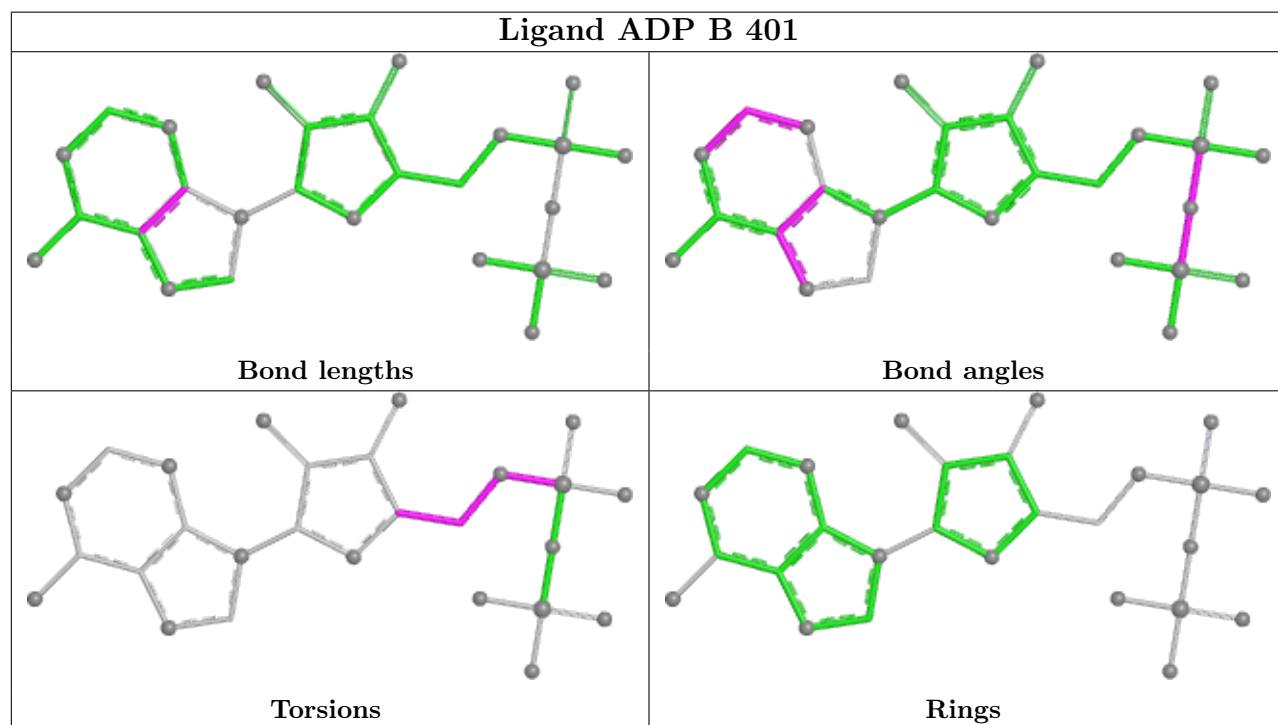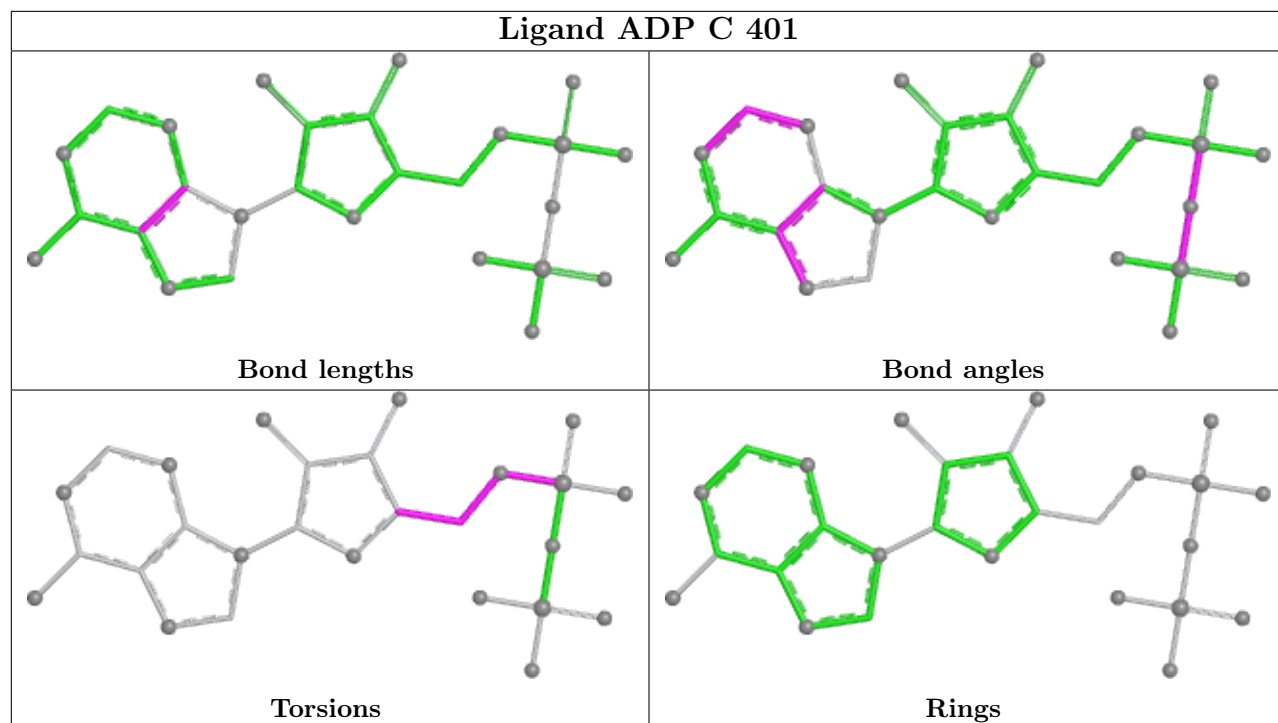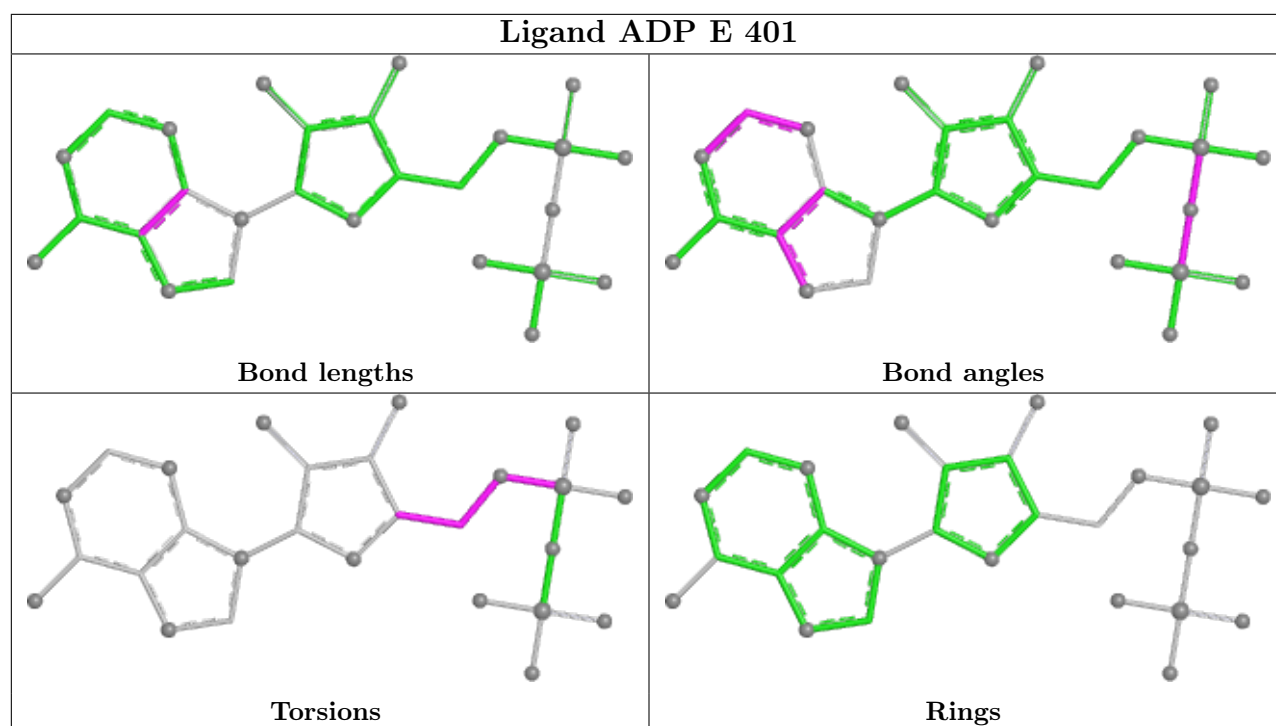
5.7 Other polymers ⓘ

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-13991. 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
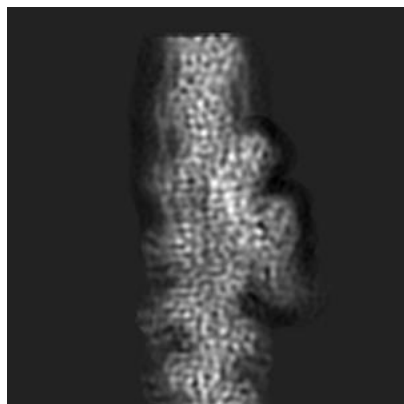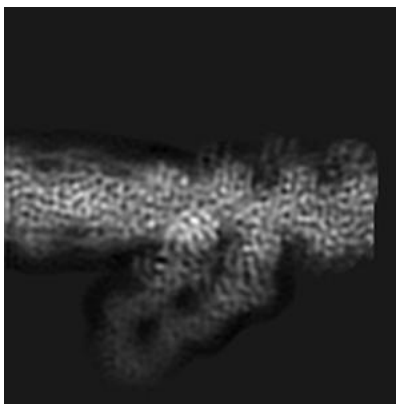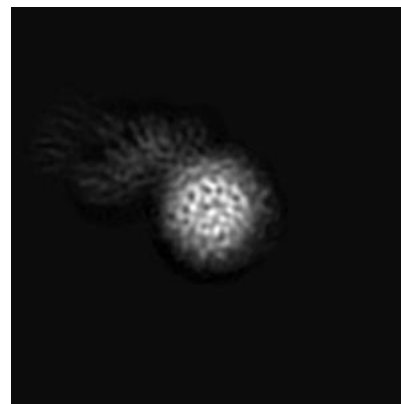
X   Y   Z

6.1.2 Raw map

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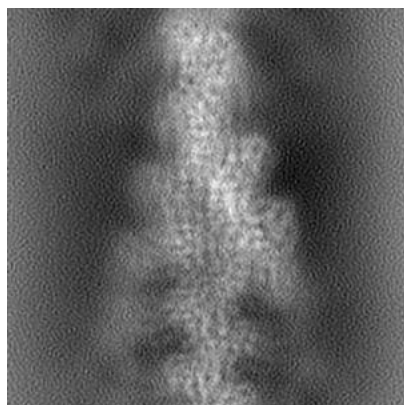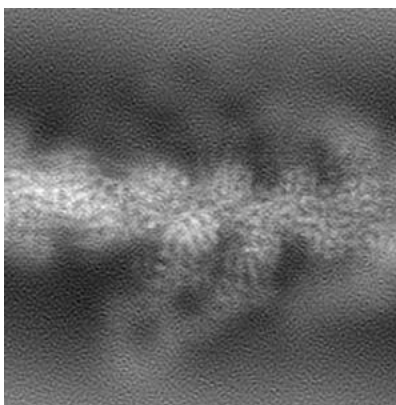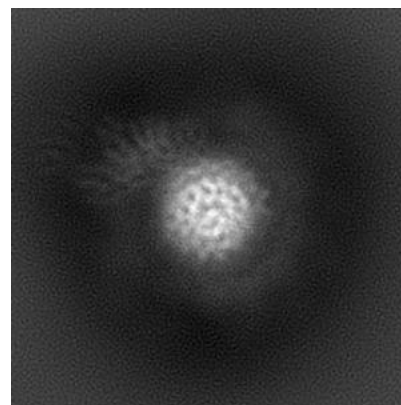
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
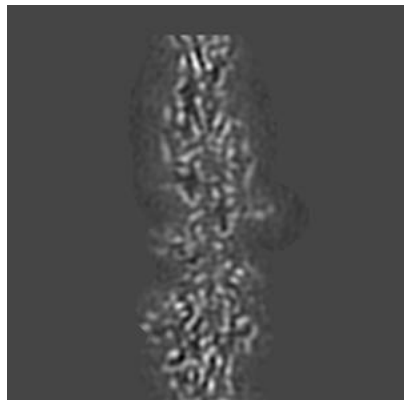
6.2.1 Primary map
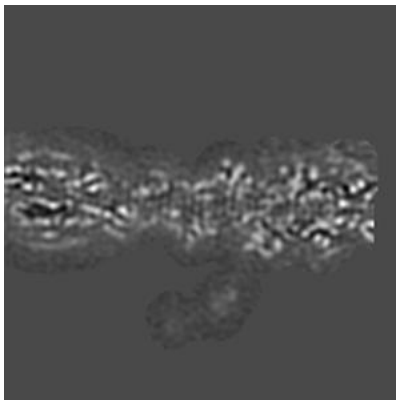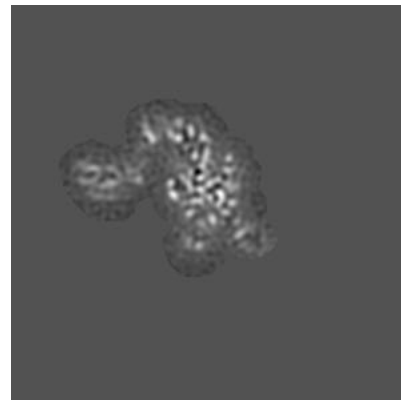
X Index: 100   Y Index: 100   Z Index: 100

6.2.2 Raw map
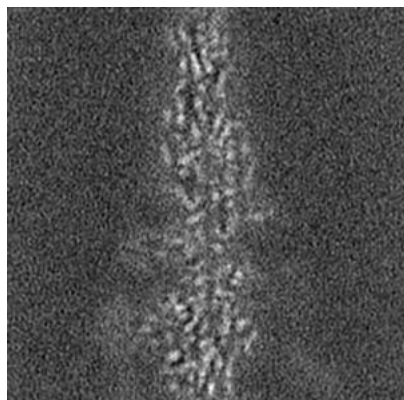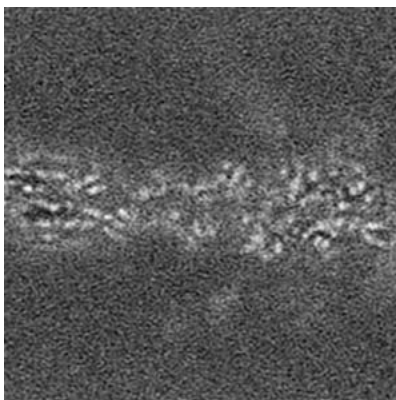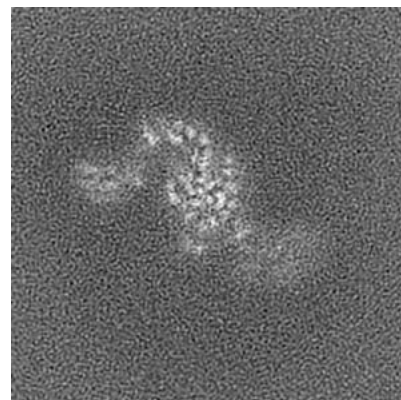
X Index: 100   Y Index: 100   Z Index: 100

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

6.3   Largest variance slices ⓘ
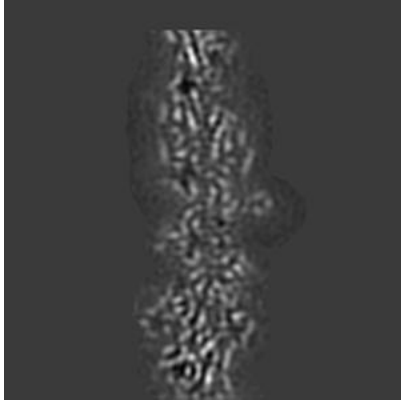
6.3.1   Primary map
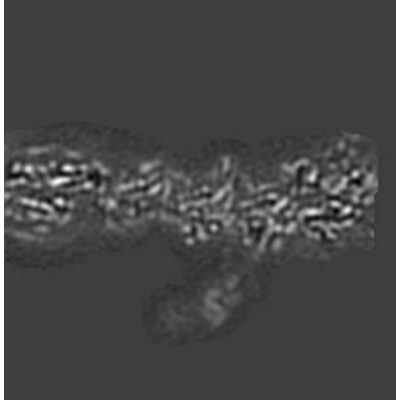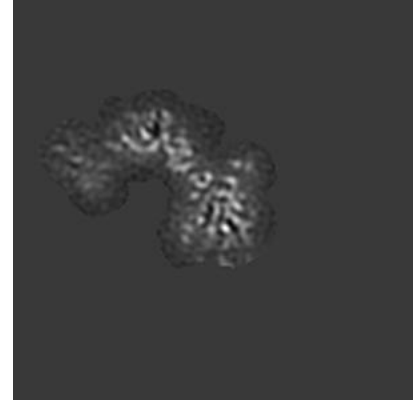
| X Index: 99 | Y Index: 103 | Z Index: 81 |

6.3.2   Raw map
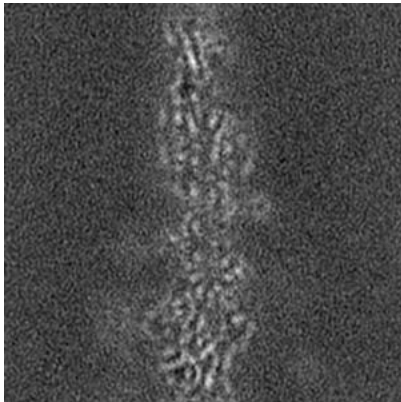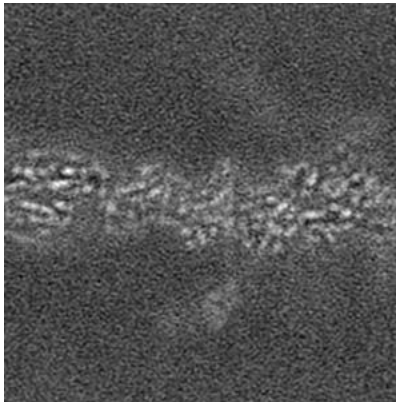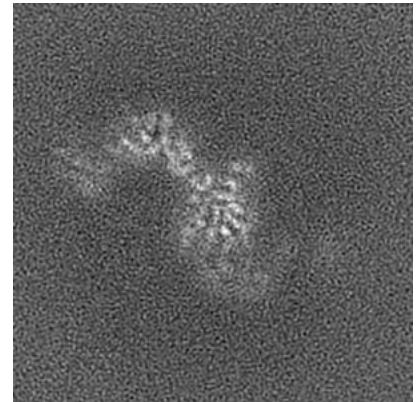
| X Index: 99 | Y Index: 103 | Z Index: 81 |

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

6.4   Orthogonal surface views ⓘ

6.4.1   Primary map

X   Y   Z
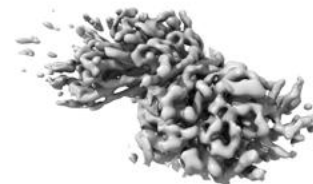
The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2   Raw map

X   Y   Z

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_13991_msk_1.map (i)

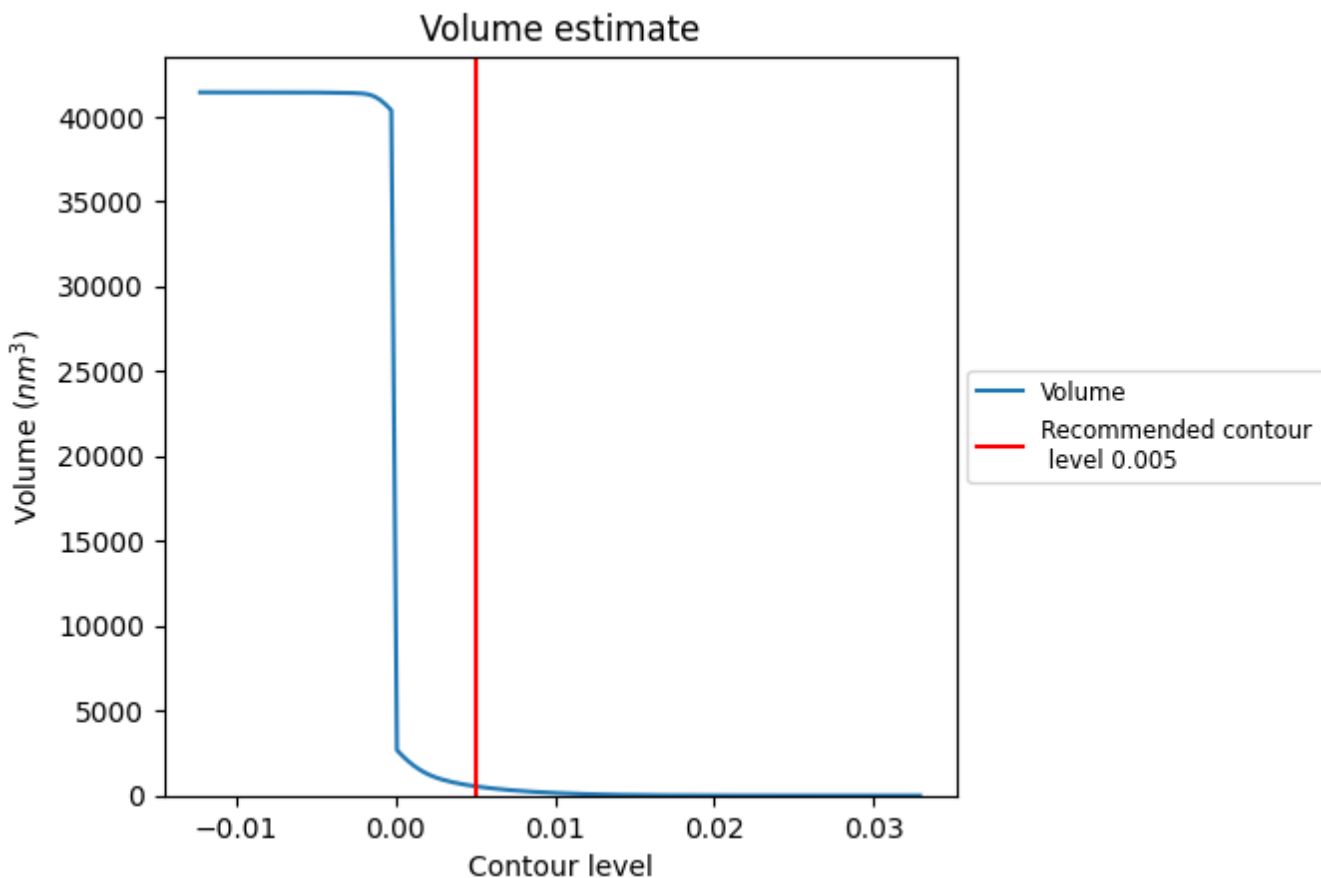X   Y   Z
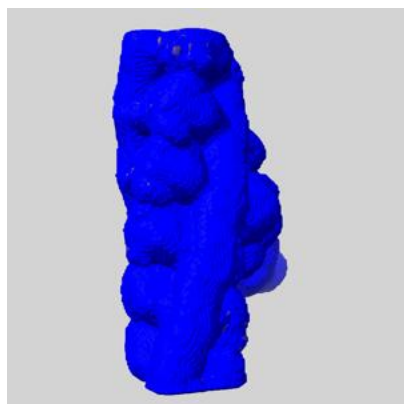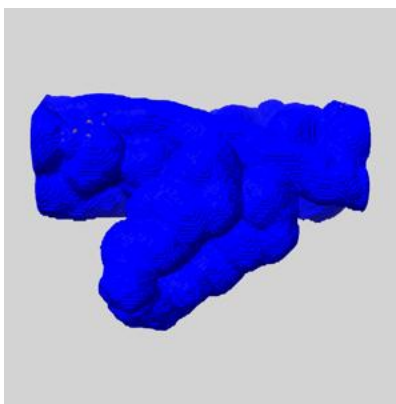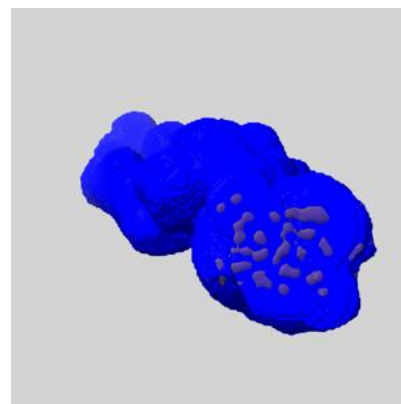
7　Map analysis ⓘ

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

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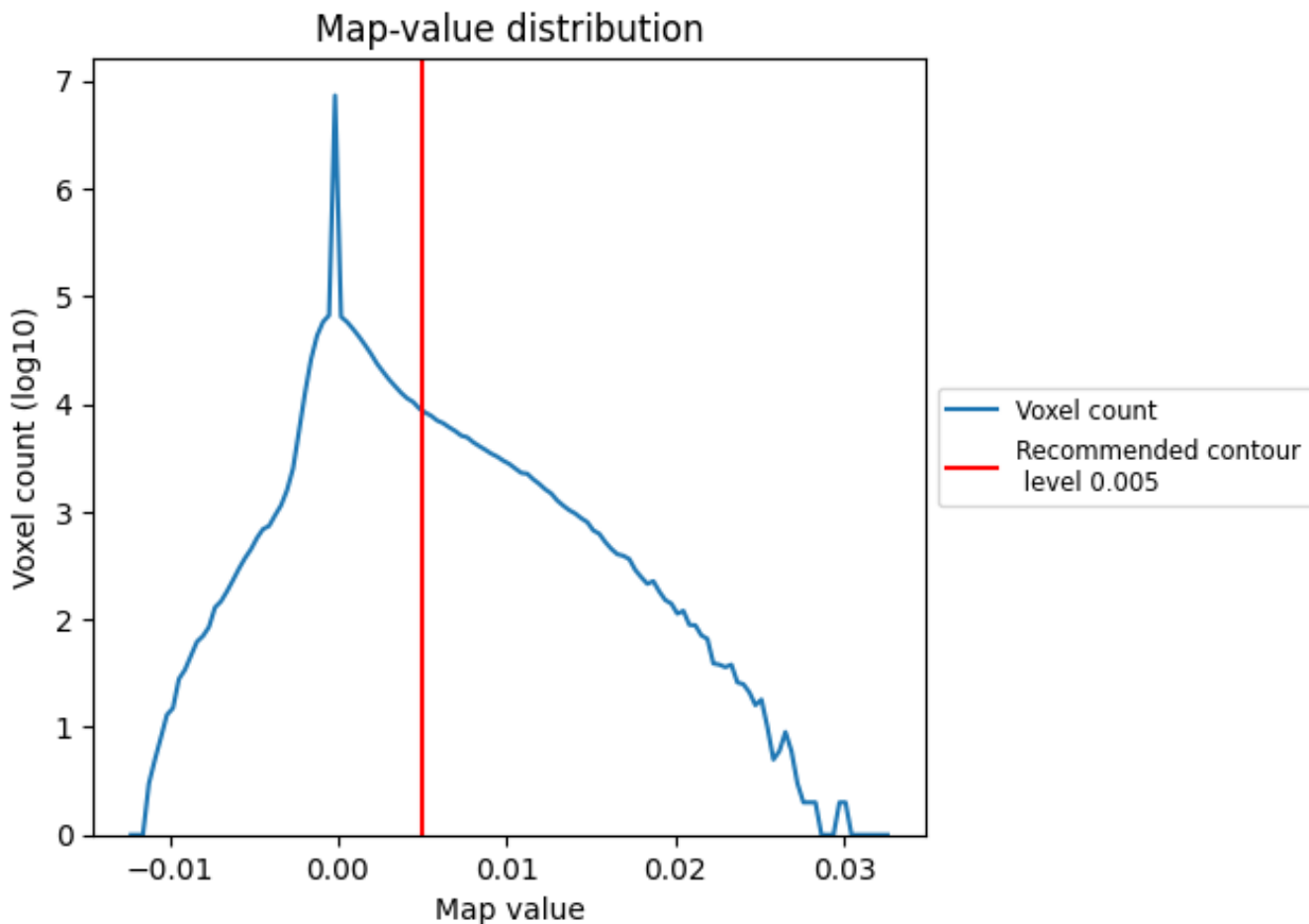
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ

The volume at the recommended contour level is 549 nm^3; this corresponds to an approximate mass of 496 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 ⓘ
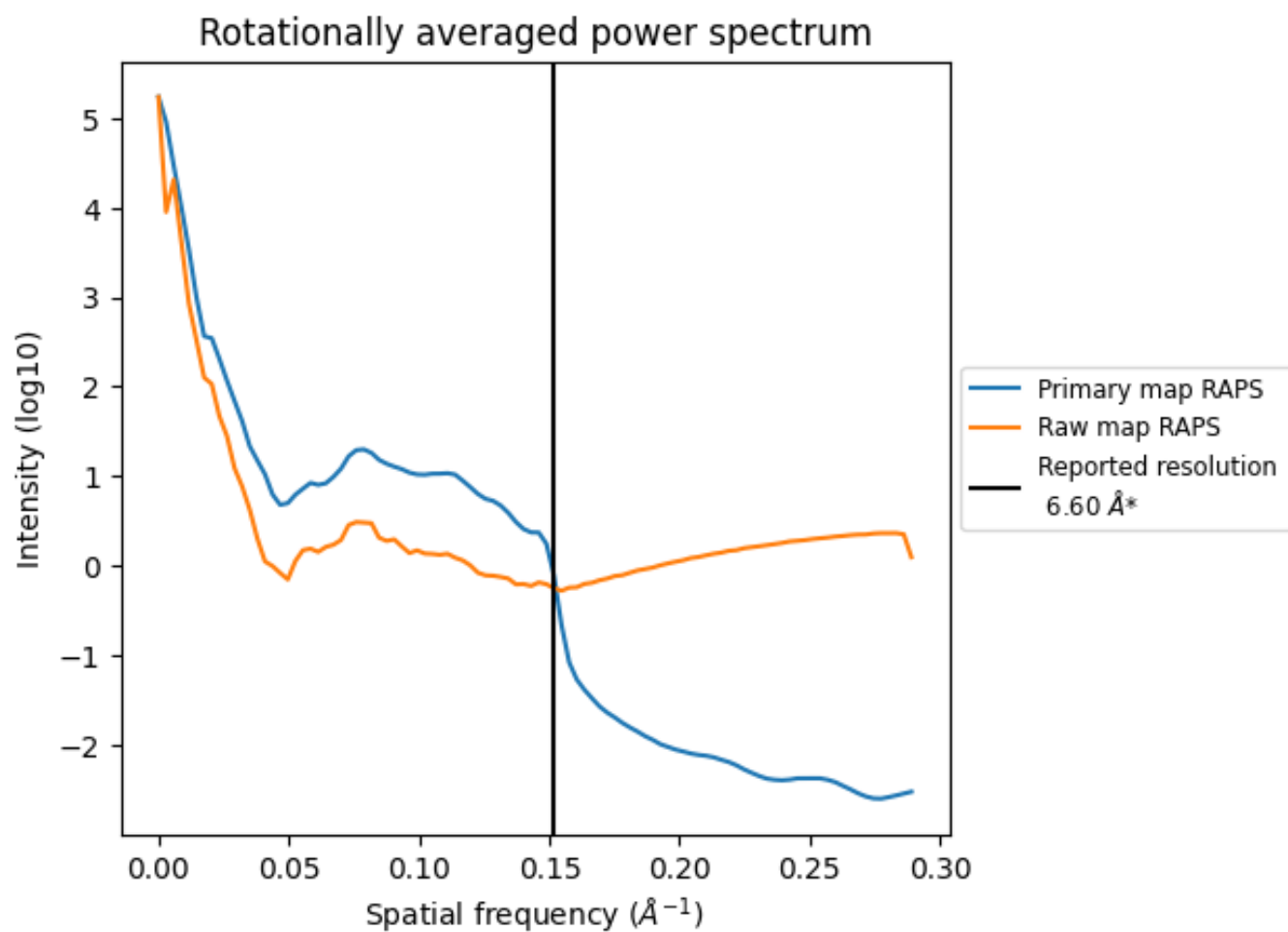
*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
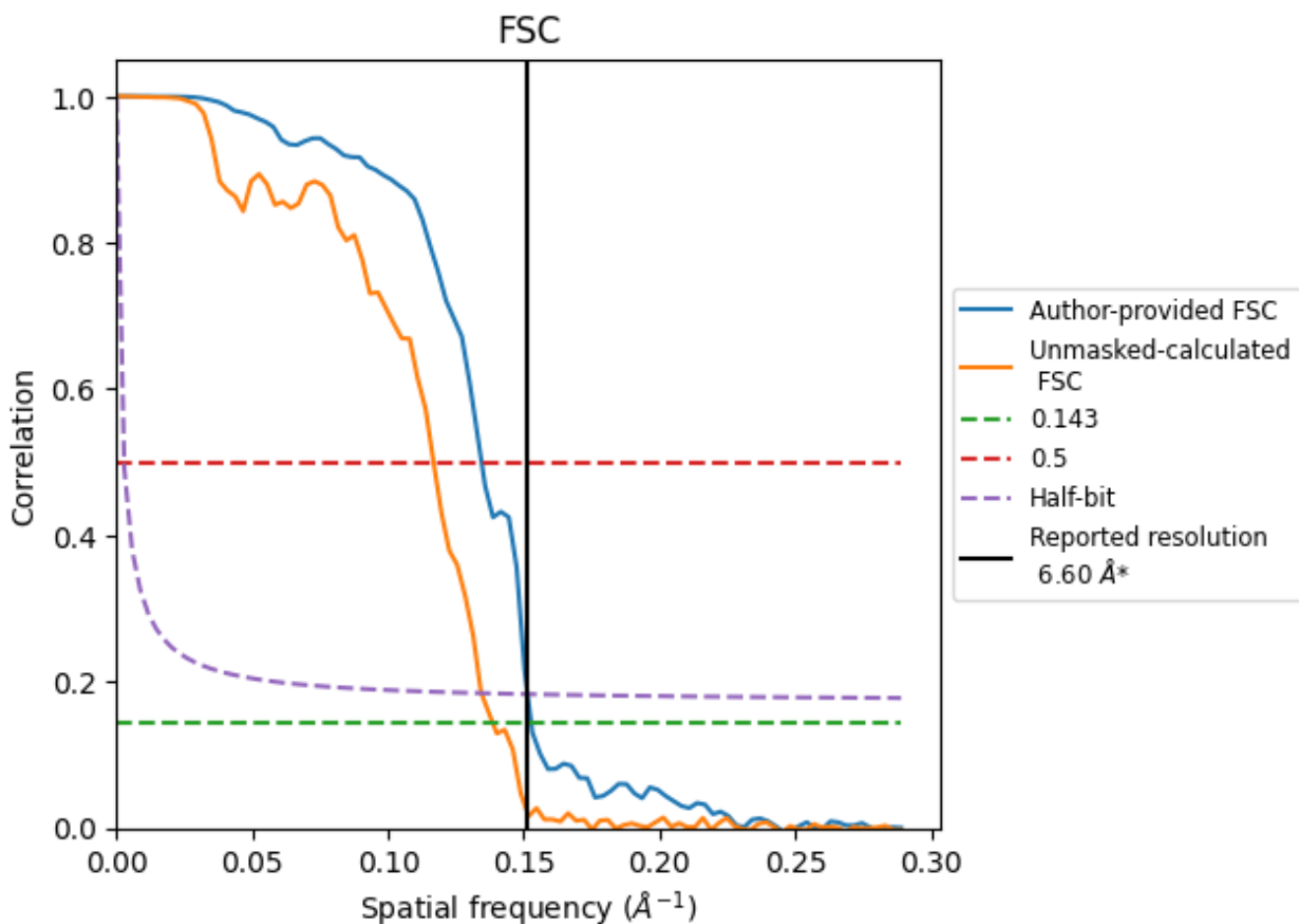
*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.55	7.43	6.61
Unmasked-calculated*	7.21	8.56	7.44

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-13991 and PDB model 7QIN. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ

X   Y   Z
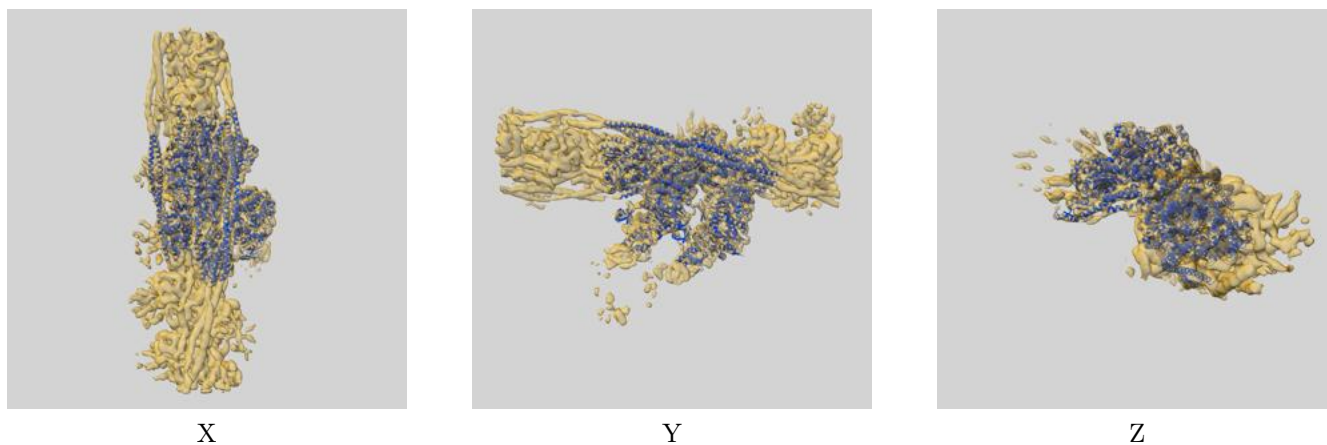
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion ⓘ
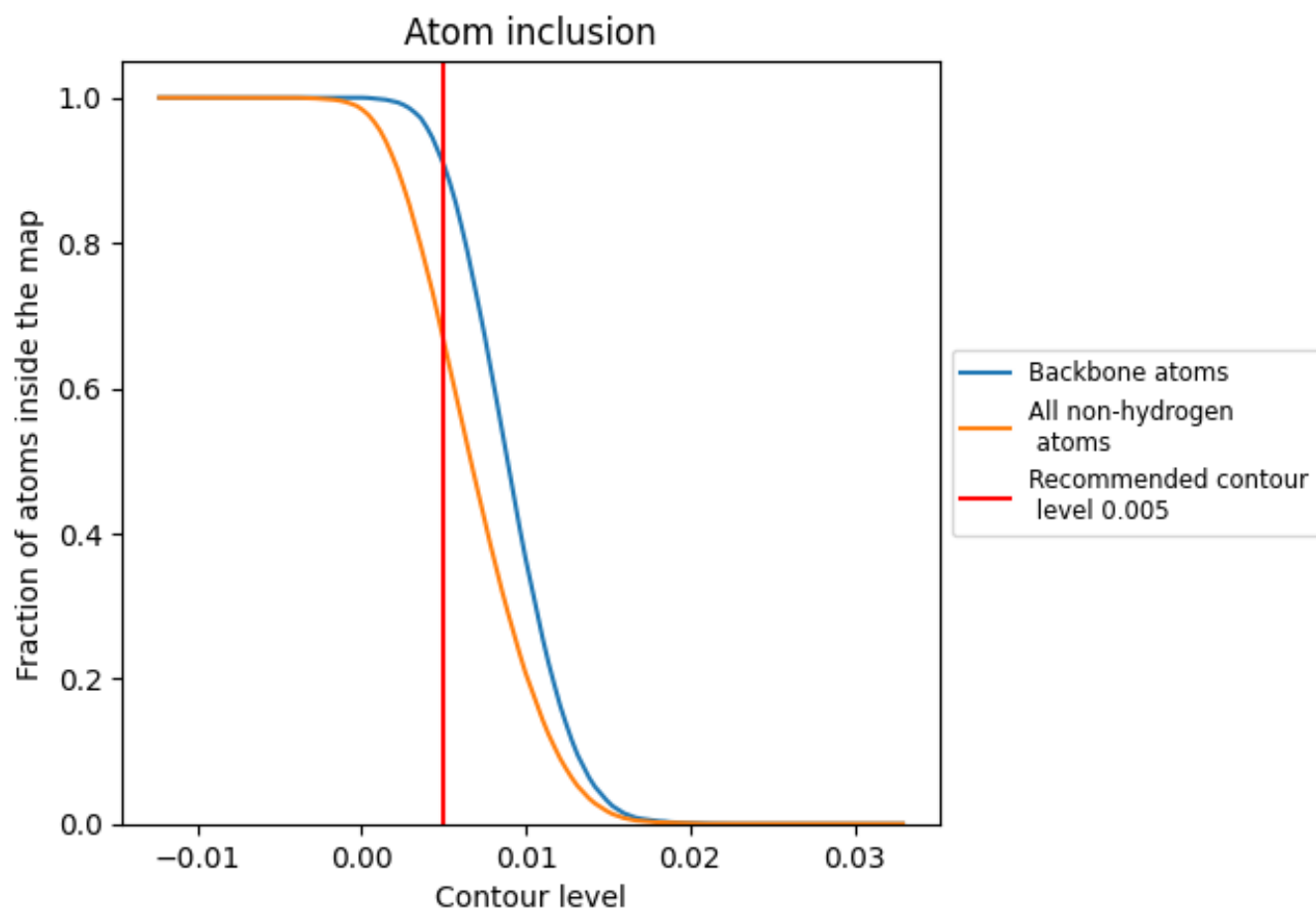
At the recommended contour level, 91% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.