wwPDB EM Validation Summary Report

Apr 24, 2023 – 02:26 PM JST

PDB ID	:	8I03
EMDB ID	:	EMD-35093
Title	:	Cryo-EM structure of the SIN3L complex from S. pombe
Authors	:	Wang, C.; Guo, Z.; Zhan, X.
Deposited on	:	2023-01-10
Resolution	:	3.20 Å(reported)

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 ⓘ 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:

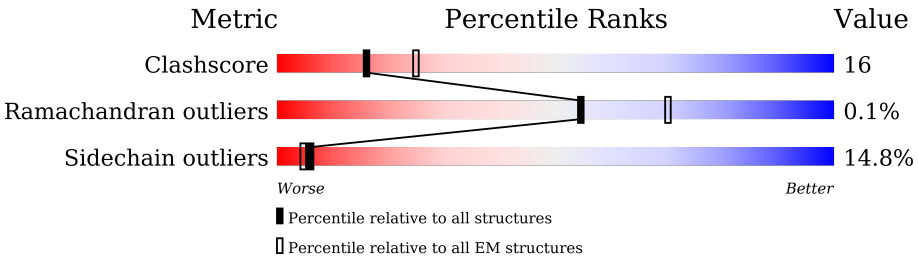
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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)
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	1522	26% 13% 60%
2	B	1154	36% 18% 45%
3	C	405	75% 15% 9%
3	D	405	70% 17% 10%
4	E	491	26% 8% 66%
5	F	240	69% 21% 5% 5%
6	G	267	9% 46% 14% 38%
7	H	305	28% 11% 59%

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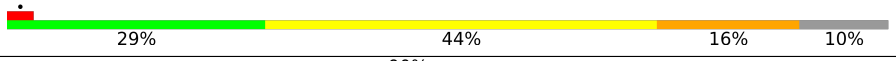
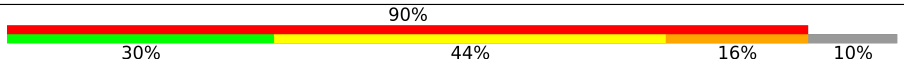
Mol	Chain	Length	Quality of chain
8	I	351	
9	J	431	
9	K	431	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 29430 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 Paired amphipathic helix protein pst1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	616	5072	3237	869	941	25	0	0

- Molecule 2 is a protein called Paired amphipathic helix protein pst3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	639	5305	3399	909	975	22	0	0

- Molecule 3 is a protein called Histone deacetylase clr6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	370	2962	1881	505	557	19	0	0
3	D	363	2911	1847	496	549	19	0	0

- Molecule 4 is a protein called Transcriptional regulatory protein dep1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	169	1328	829	242	249	8	0	0

- Molecule 5 is a protein called Transcriptional regulatory protein rxt2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	F	228	1831	1137	314	368	4	8	0	0

- Molecule 6 is a protein called Transcriptional regulatory protein sds3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	166	Total	C	N	O	S	0	0
			1306	805	235	261	5		

- Molecule 7 is a protein called Chromatin modification-related protein png2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	126	Total	C	N	O	S	0	0
			994	621	167	200	6		

- Molecule 8 is a protein called Transcriptional regulatory protein rxt3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	185	Total	C	N	O	S	0	0
			1505	972	256	273	4		

- Molecule 9 is a protein called RbAp48-related WD40 repeat-containing protein prw1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	388	Total	C	N	O	S	0	0
			3105	1957	533	599	16		
9	K	388	Total	C	N	O	S	0	0
			3105	1957	533	599	16		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	Zn	0
			1	1	
10	D	1	Total	Zn	0
			1	1	

- Molecule 11 is POTASSIUM ION (three-letter code: K) (formula: K).

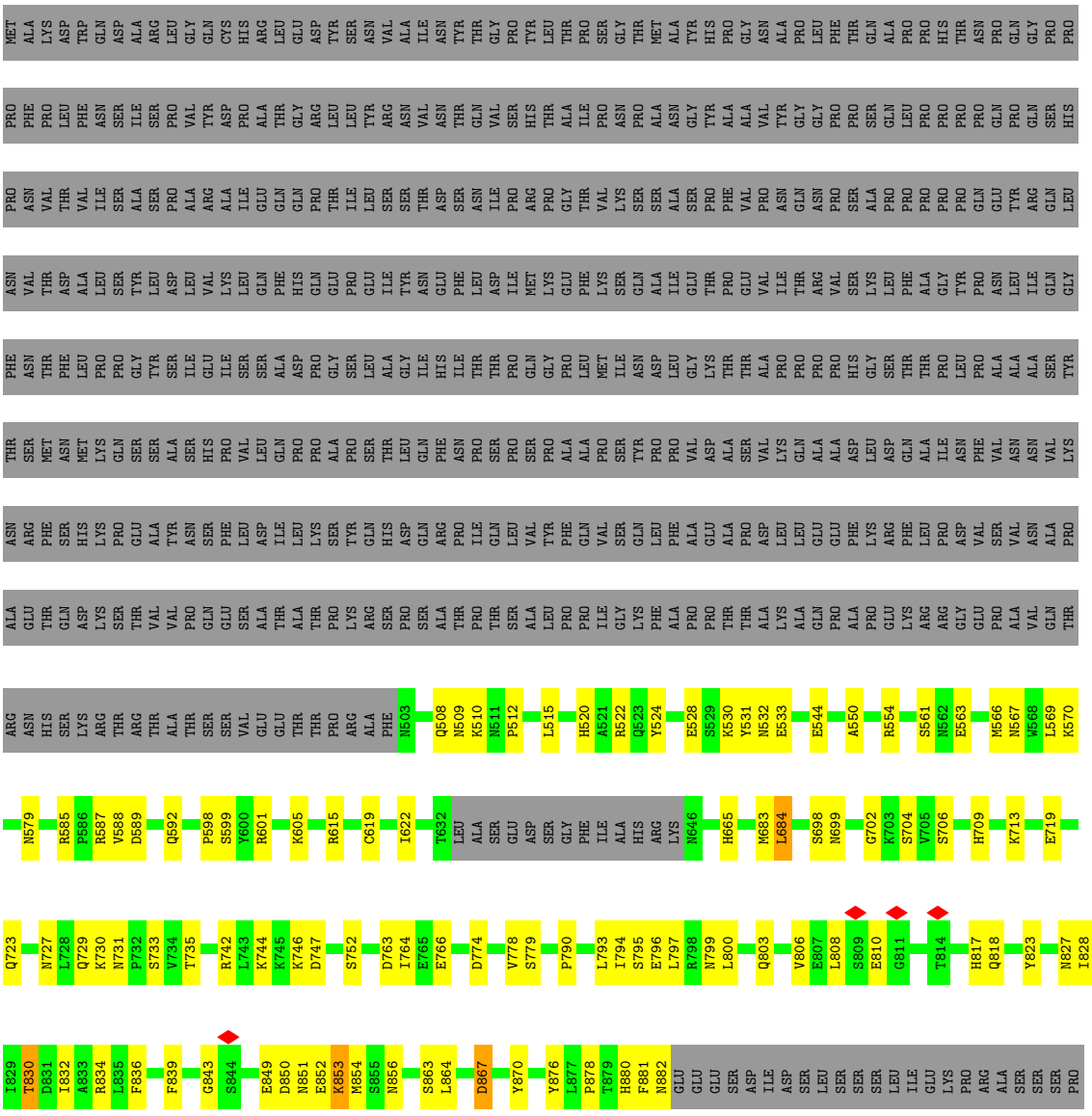
Mol	Chain	Residues	Atoms		AltConf
11	C	2	Total	K	0
			2	2	
11	D	2	Total	K	0
			2	2	

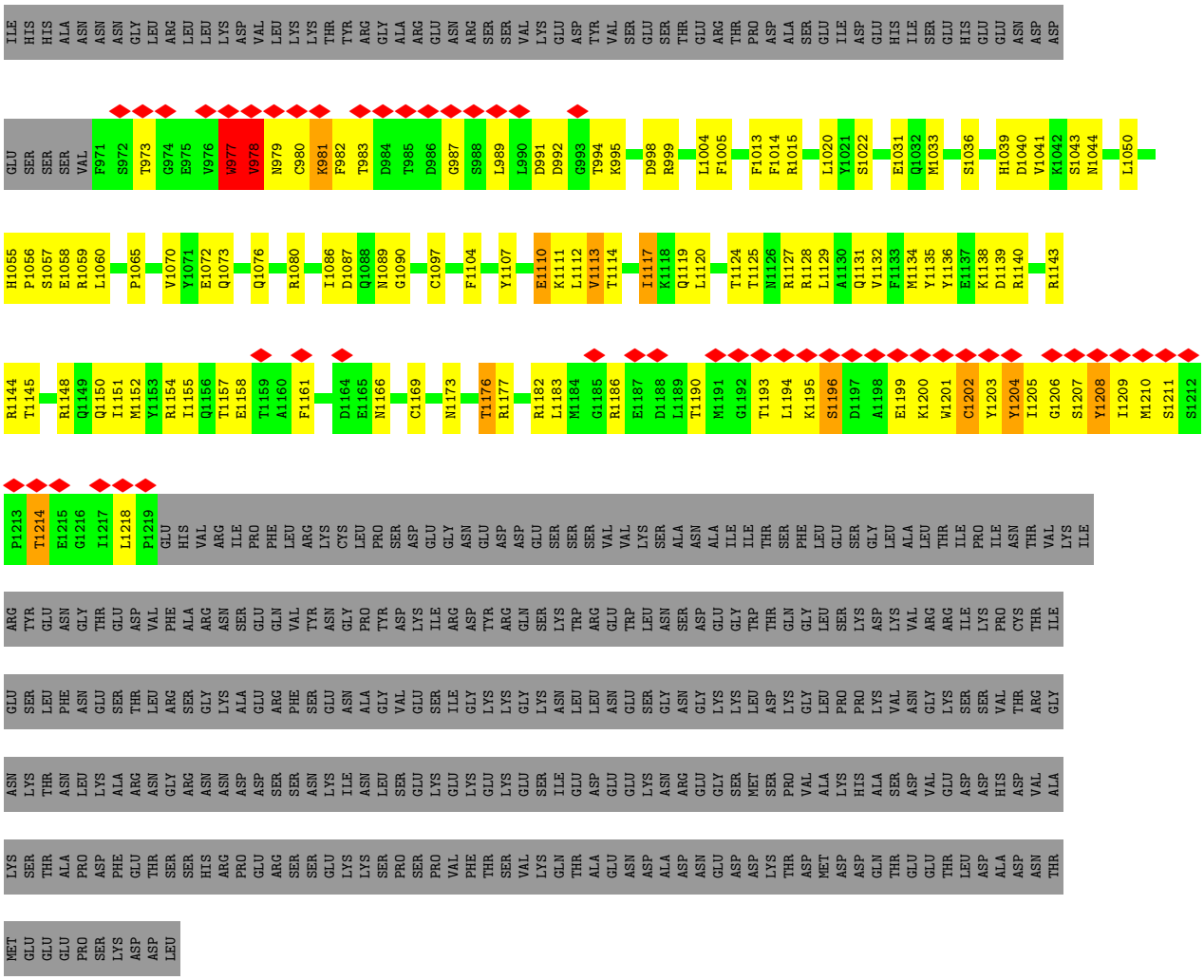
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Paired amphipathic helix protein pst1

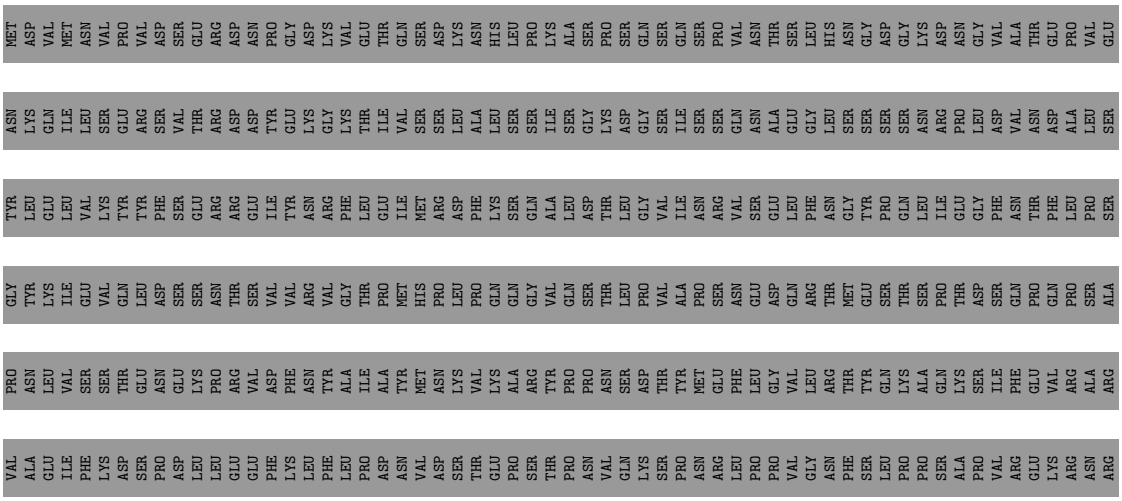
Chain A:

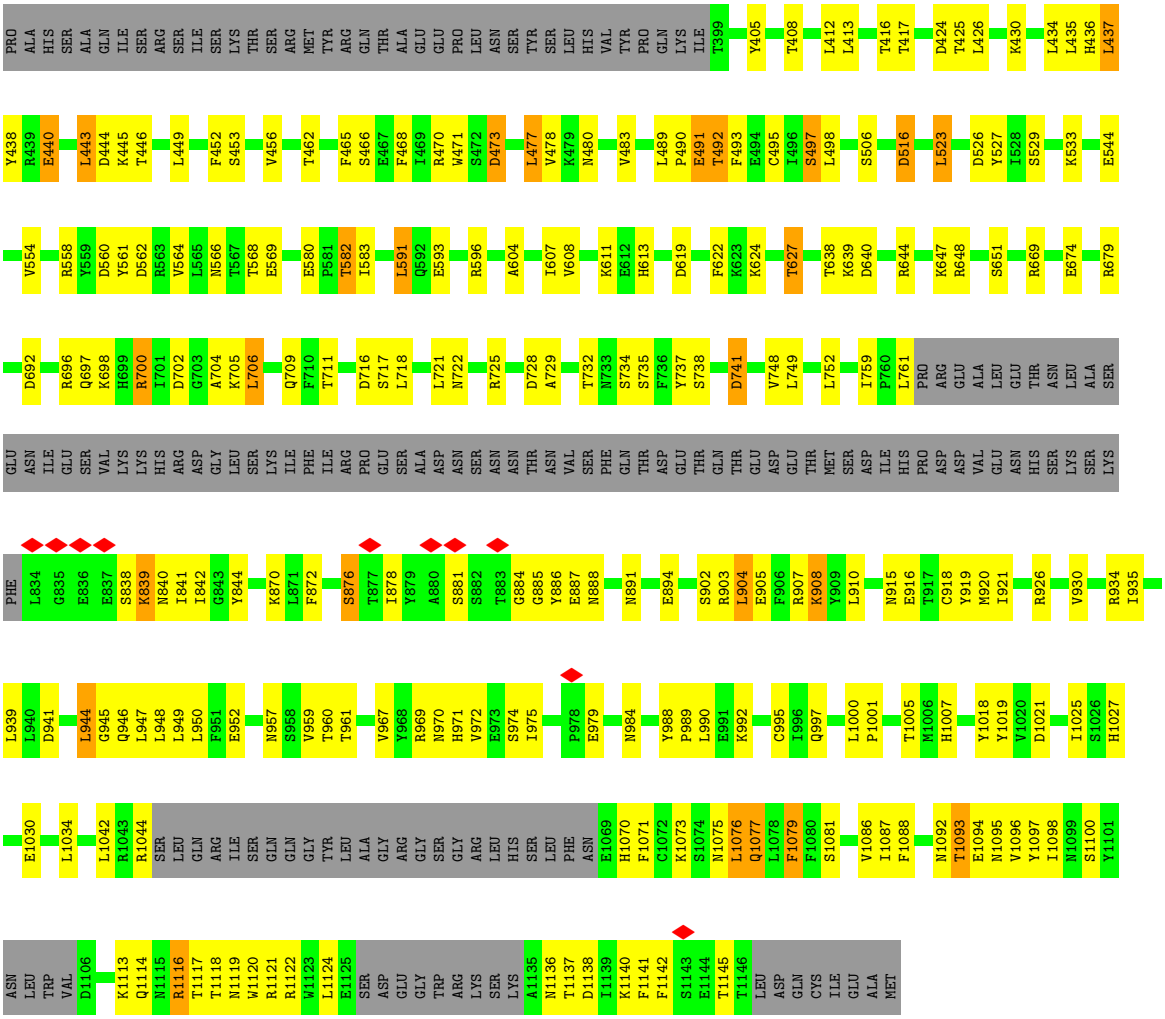




• Molecule 2: Paired amphipathic helix protein pst3

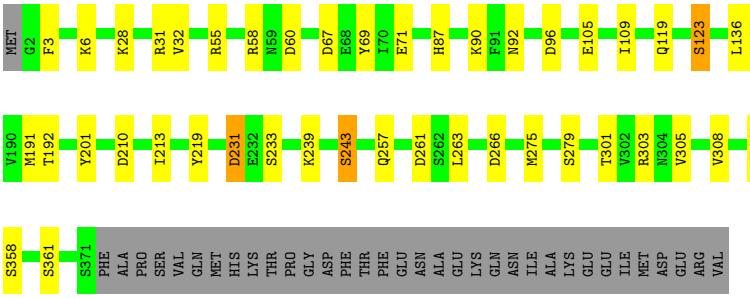
Chain B:





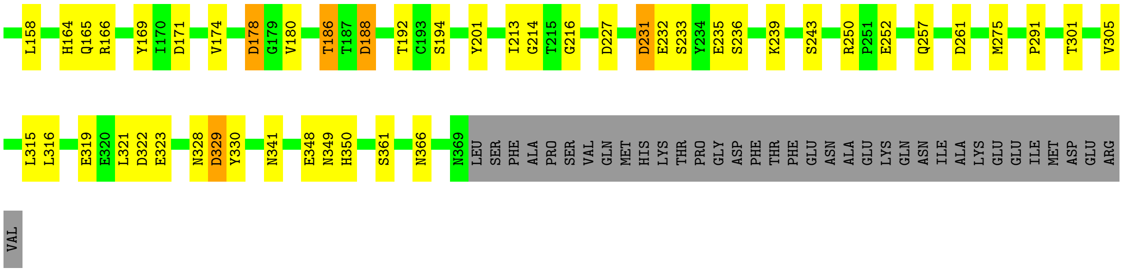
• Molecule 3: Histone deacetylase clr6

Chain C:



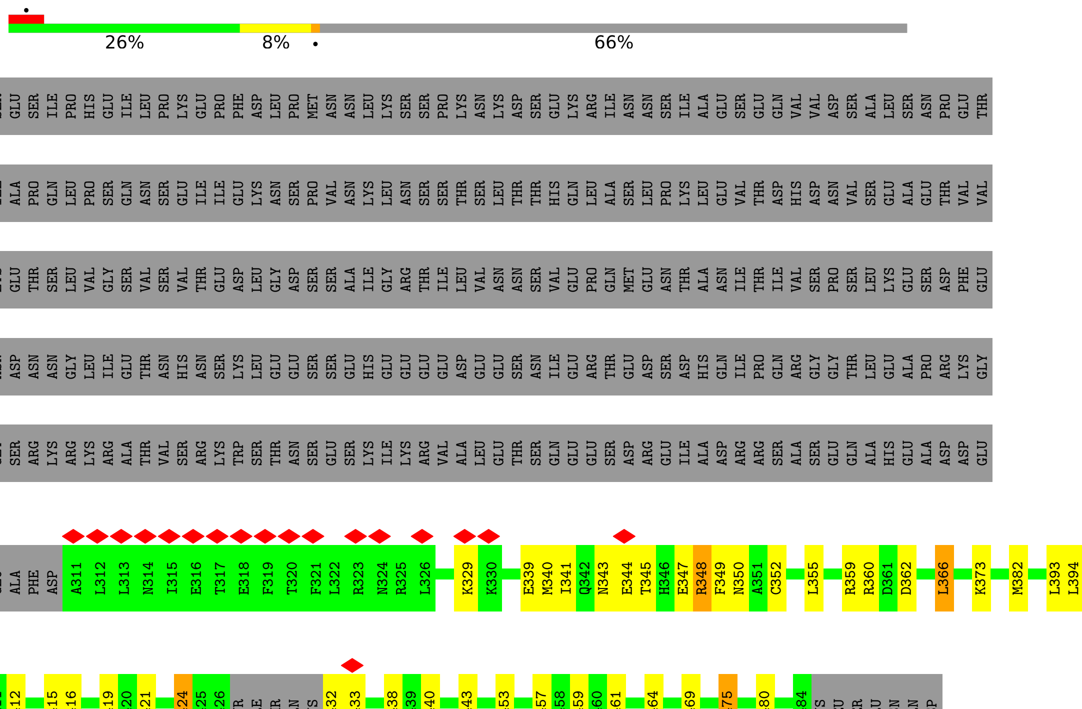
• Molecule 3: Histone deacetylase clr6

Chain D:



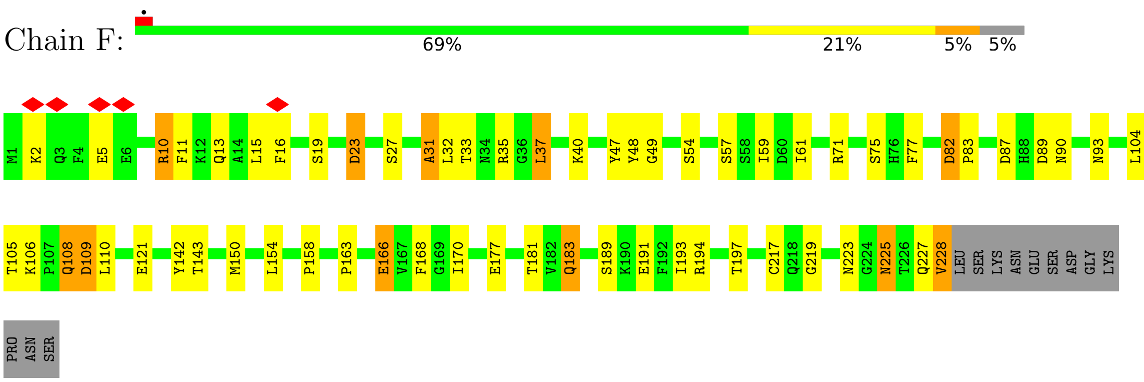
• Molecule 4: Transcriptional regulatory protein dep1

Chain E:



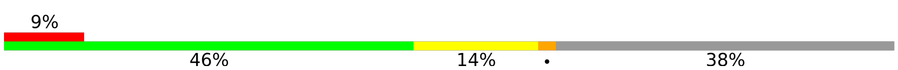
• Molecule 5: Transcriptional regulatory protein rxt2

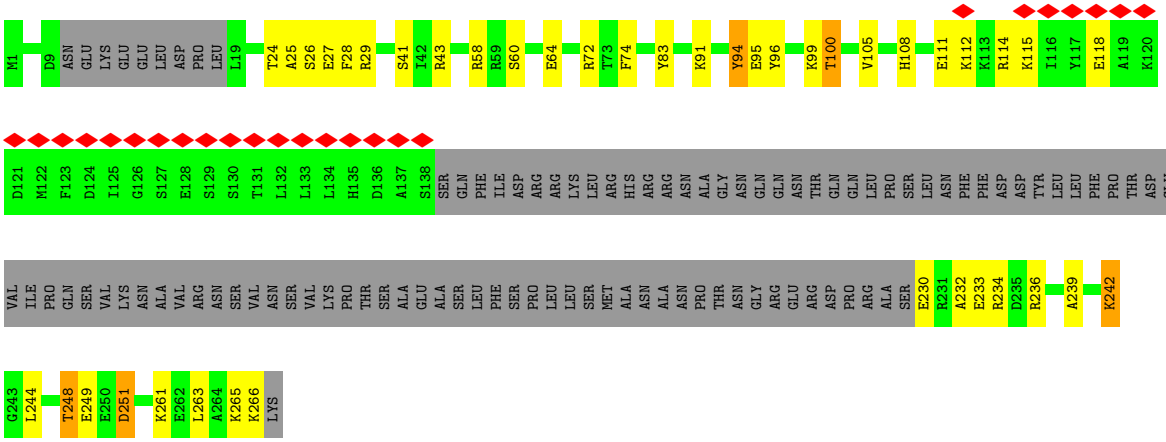
Chain F:



• Molecule 6: Transcriptional regulatory protein sds3

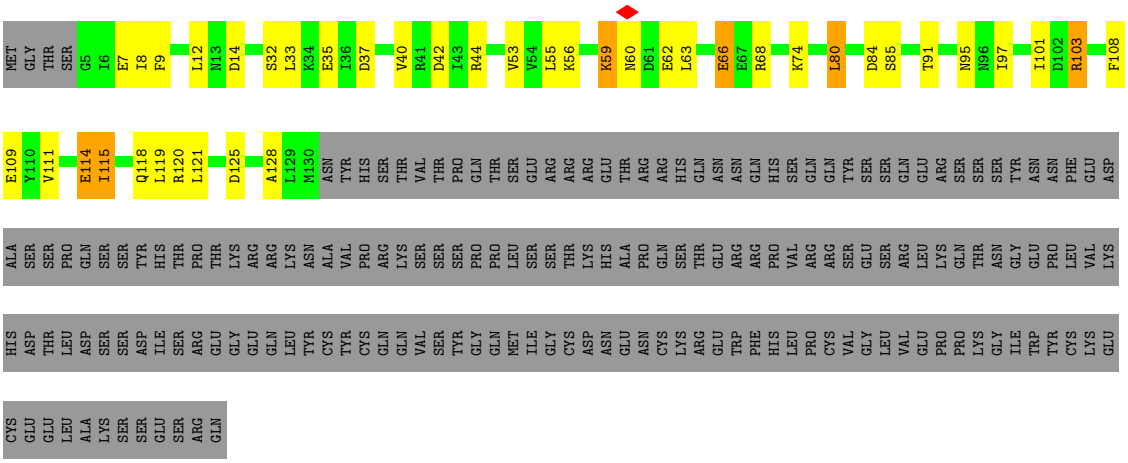
Chain G:





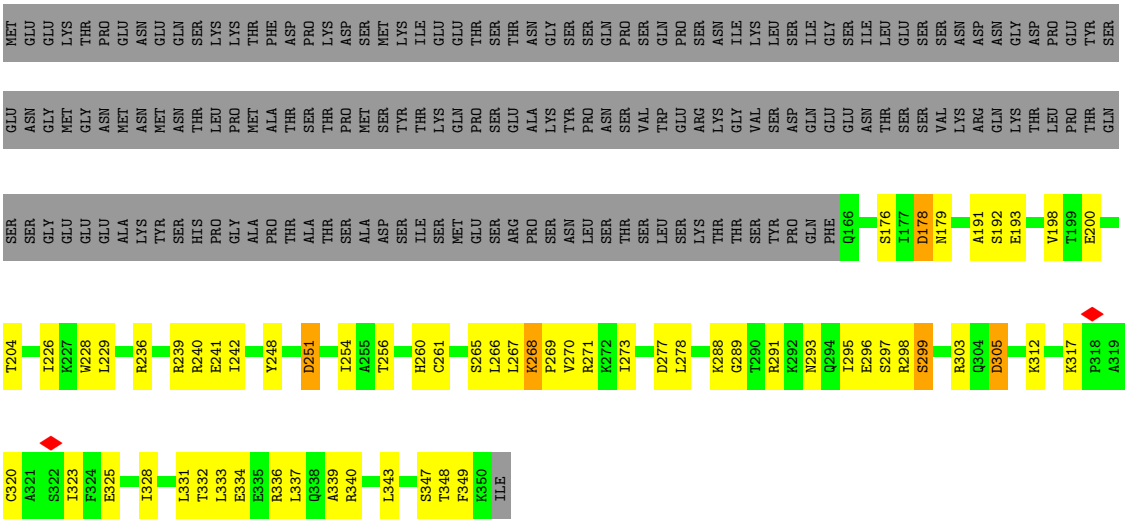
• Molecule 7: Chromatin modification-related protein png2

Chain H:



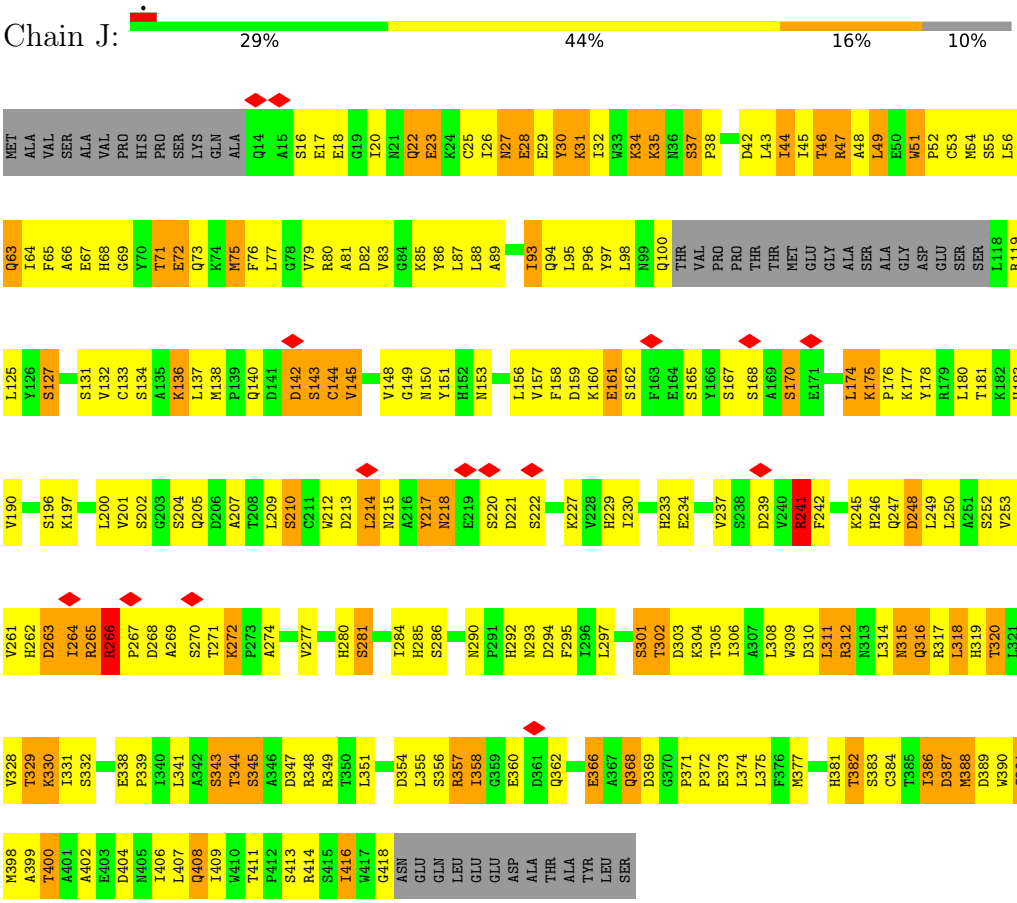
• Molecule 8: Transcriptional regulatory protein rxt3

Chain I:



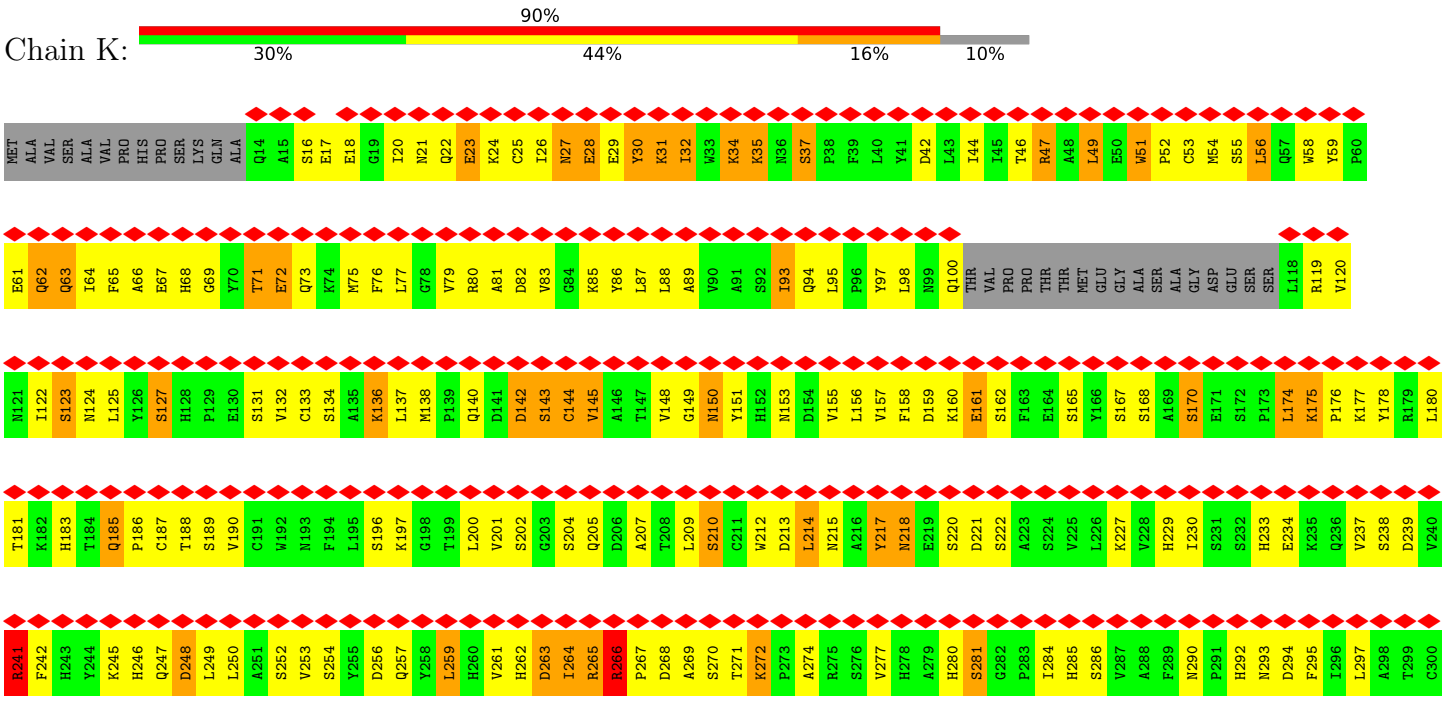
• Molecule 9: RbAp48-related WD40 repeat-containing protein prw1

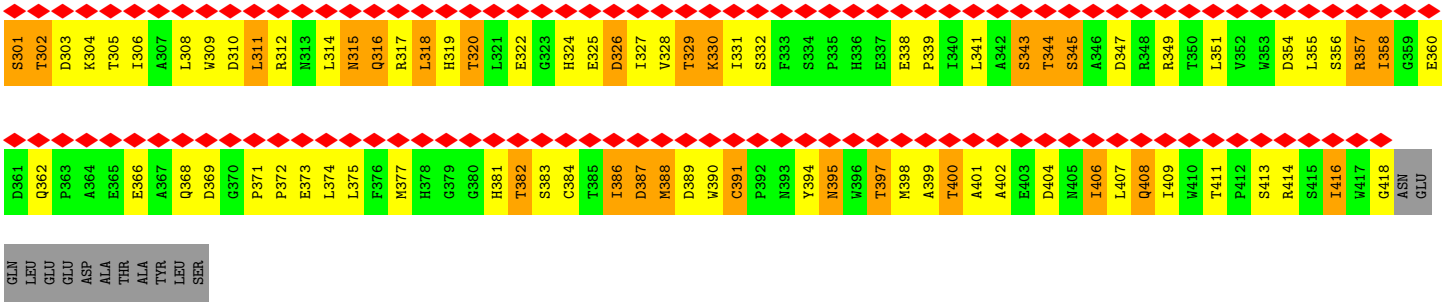
Chain J:



• Molecule 9: RbAp48-related WD40 repeat-containing protein prw1

Chain K:




S301 T302 D303 K304 T305 I306 A307 L308 W309 D310 L311 R312 N313 L314 N315 Q316 R317 L318 H319 T320 L321 E322 G323 H324 E325 D326 I327 V328 T329 K330 I331 S332 F333 S334 P335 H336 E337 E338 P339 I340 L341 A342 S343 T344 S345 A346 D347 R348 R349 T350 L351 V352 W353 D354 L355 S356 R357 I358 G359 E360

D361 Q362 P363 A364 E365 E366 A367 Q368 D369 G370 P371 P372 E373 L374 L375 F376 M377 H378 G379 G380 H381 T382 S383 C384 T385 I386 D387 M388 D389 W390 C391 P392 N393 Y394 N395 W396 T397 M398 A399 T400 A401 A402 E403 D404 M405 I406 L407 Q408 I409 W410 T411 P412 S413 R414 S415 I416 W417 G418 ASN GLU

GLN LEU GLU GLU ASP ALA THR ALA TYR LEU SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	389222	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.00	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: SEP, ZN, K

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	0.47	0/5194	0.52	1/7023 (0.0%)
2	B	0.46	0/5421	0.49	0/7321
3	C	0.72	0/3040	0.54	0/4121
3	D	0.70	0/2988	0.54	0/4054
4	E	0.47	0/1342	0.49	0/1804
5	F	0.59	0/1823	0.55	0/2458
6	G	0.43	0/1314	0.45	0/1755
7	H	0.50	0/1004	0.58	0/1353
8	I	0.54	0/1543	0.49	0/2099
9	J	0.32	0/3190	0.63	4/4345 (0.1%)
9	K	0.32	0/3190	0.63	4/4345 (0.1%)
All	All	0.51	0/30049	0.54	9/40678 (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
1	A	0	3
5	F	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	684	LEU	CA-CB-CG	6.20	129.56	115.30
9	K	266	ARG	NE-CZ-NH1	5.93	123.27	120.30
9	J	266	ARG	NE-CZ-NH1	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	241	ARG	NE-CZ-NH1	5.53	123.07	120.30
9	J	241	ARG	NE-CZ-NH1	5.53	123.06	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1204	TYR	Peptide
1	A	977	TRP	Peptide
1	A	978	VAL	Peptide
5	F	49	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5072	0	4988	182	0
2	B	5305	0	5285	216	0
3	C	2962	0	2818	35	0
3	D	2911	0	2761	39	0
4	E	1328	0	1304	32	0
5	F	1831	0	1768	68	0
6	G	1306	0	1267	28	0
7	H	994	0	997	26	0
8	I	1505	0	1524	52	0
9	J	3105	0	2960	197	0
9	K	3105	0	2960	206	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	C	2	0	0	0	0
11	D	2	0	0	0	0
All	All	29430	0	28632	930	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 16.

The worst 5 of 930 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)
2:B:435:LEU:HD11	5:F:11:PHE:CD1	1.64	1.30
2:B:1076:LEU:HD13	2:B:1095:ASN:ND2	1.55	1.21
2:B:1093:THR:OG1	9:J:48:ALA:HB3	1.44	1.16
2:B:1076:LEU:HD22	2:B:1095:ASN:OD1	1.46	1.15
2:B:1093:THR:HG1	9:J:48:ALA:HB3	1.08	1.09

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	610/1522 (40%)	555 (91%)	55 (9%)	0	100	100
2	B	629/1154 (54%)	585 (93%)	44 (7%)	0	100	100
3	C	368/405 (91%)	341 (93%)	27 (7%)	0	100	100
3	D	361/405 (89%)	330 (91%)	31 (9%)	0	100	100
4	E	165/491 (34%)	158 (96%)	7 (4%)	0	100	100
5	F	222/240 (92%)	190 (86%)	30 (14%)	2 (1%)	17	56
6	G	160/267 (60%)	155 (97%)	5 (3%)	0	100	100
7	H	124/305 (41%)	113 (91%)	11 (9%)	0	100	100
8	I	183/351 (52%)	167 (91%)	16 (9%)	0	100	100
9	J	384/431 (89%)	368 (96%)	16 (4%)	0	100	100
9	K	384/431 (89%)	368 (96%)	16 (4%)	0	100	100
All	All	3590/6002 (60%)	3330 (93%)	258 (7%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	32	LEU
5	F	31	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	567/1364 (42%)	521 (92%)	46 (8%)	11 42
2	B	590/1060 (56%)	537 (91%)	53 (9%)	9 34
3	C	320/351 (91%)	300 (94%)	20 (6%)	18 52
3	D	315/351 (90%)	284 (90%)	31 (10%)	8 31
4	E	137/448 (31%)	125 (91%)	12 (9%)	10 36
5	F	198/209 (95%)	182 (92%)	16 (8%)	11 42
6	G	130/238 (55%)	120 (92%)	10 (8%)	13 44
7	H	112/280 (40%)	95 (85%)	17 (15%)	3 13
8	I	170/322 (53%)	158 (93%)	12 (7%)	14 47
9	J	348/382 (91%)	217 (62%)	131 (38%)	0 0
9	K	348/382 (91%)	217 (62%)	131 (38%)	0 0
All	All	3235/5387 (60%)	2756 (85%)	479 (15%)	6 14

5 of 479 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	49	LEU
9	K	315	ASN
9	J	241	ARG
9	K	304	LYS
9	K	400	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
9	J	285	HIS
9	J	319	HIS
9	K	260	HIS
2	B	1114	GLN
2	B	1095	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\|>2$
5	SEP	F	24	5	8,9,10	0.64	0	8,12,14	0.62	0
5	SEP	F	27	5	8,9,10	0.64	0	8,12,14	0.61	0
5	SEP	F	19	5	8,9,10	0.63	0	8,12,14	0.71	0
5	SEP	F	22	5	8,9,10	0.64	0	8,12,14	0.61	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
5	SEP	F	24	5	-	1/5/8/10	-
5	SEP	F	27	5	-	0/5/8/10	-
5	SEP	F	19	5	-	1/5/8/10	-
5	SEP	F	22	5	-	3/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	19	SEP	N-CA-CB-OG
5	F	22	SEP	CB-OG-P-O1P
5	F	22	SEP	CB-OG-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	F	24	SEP	N-CA-CB-OG
5	F	22	SEP	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	27	SEP	1	0
5	F	19	SEP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

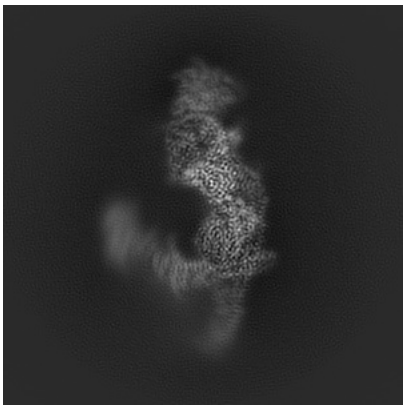
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35093. These allow visual inspection of the internal detail of the map and identification of artifacts.

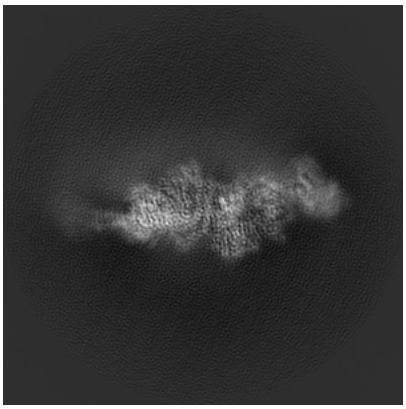
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

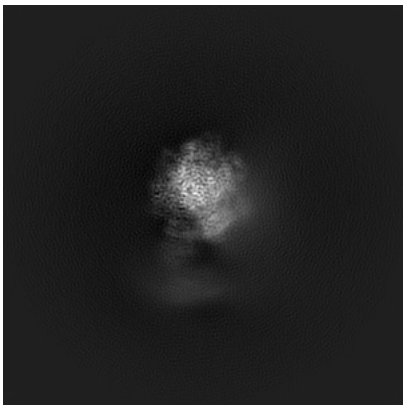
6.1.1 Primary map



X

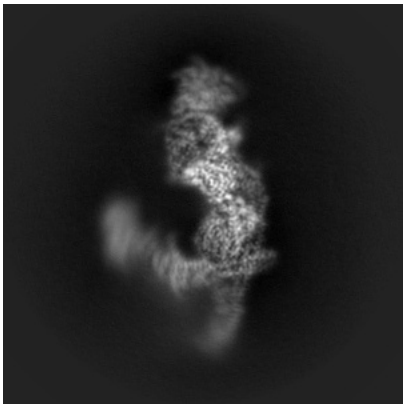


Y

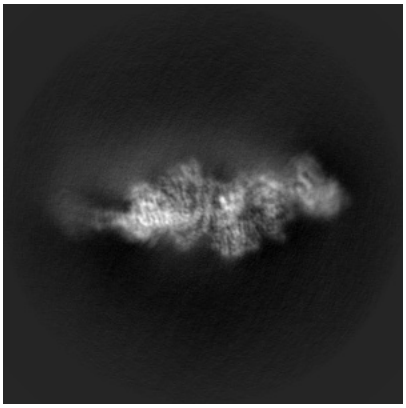


Z

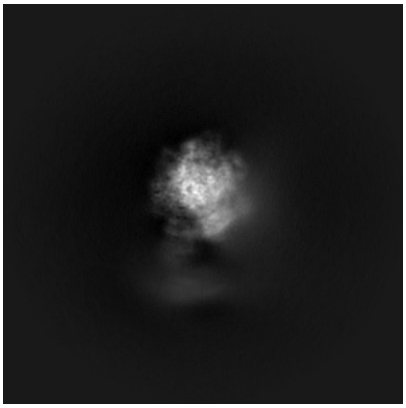
6.1.2 Raw map



X



Y

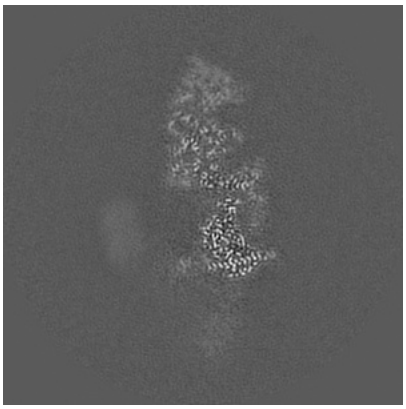


Z

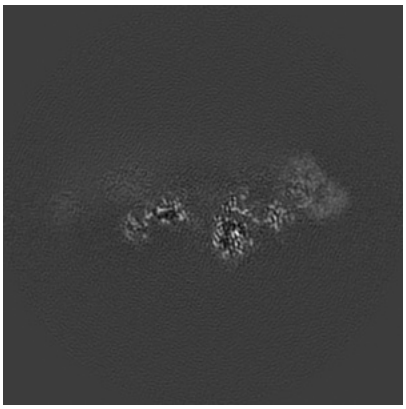
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

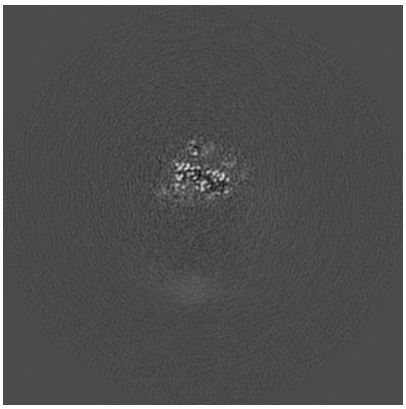
6.2.1 Primary map



X Index: 180

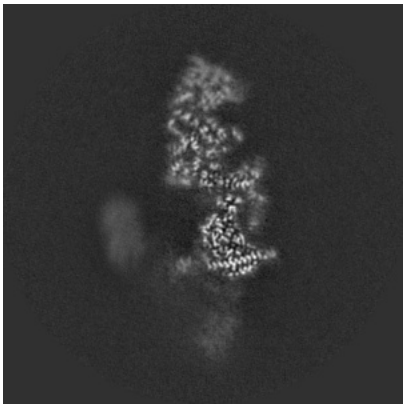


Y Index: 180

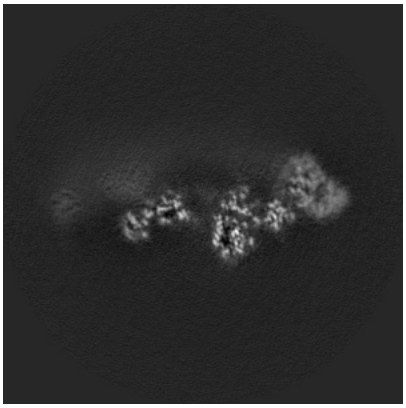


Z Index: 180

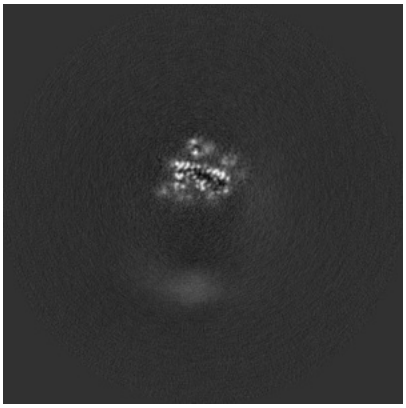
6.2.2 Raw map



X Index: 180



Y Index: 180

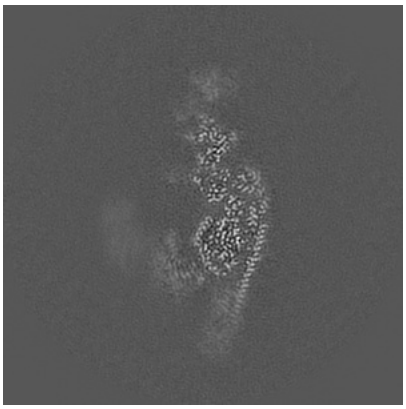


Z Index: 180

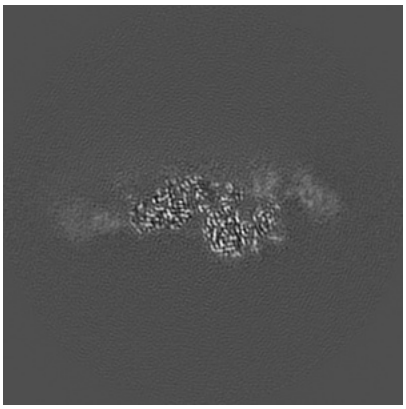
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

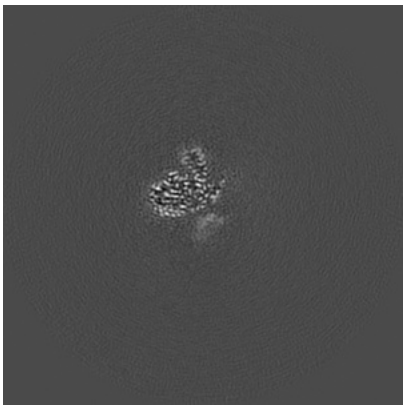
6.3.1 Primary map



X Index: 170

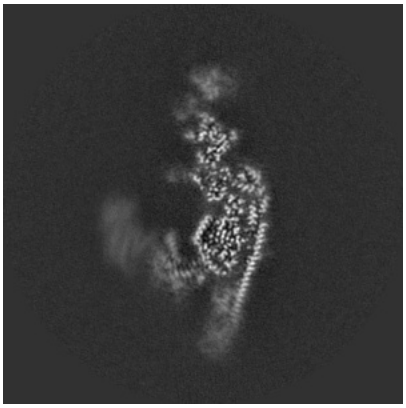


Y Index: 197

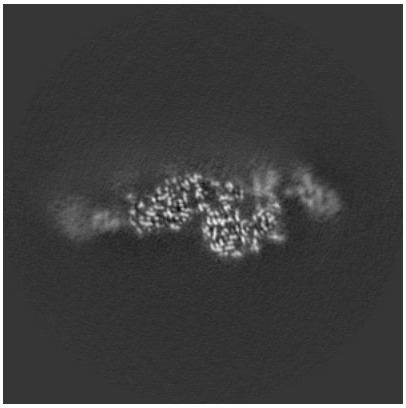


Z Index: 200

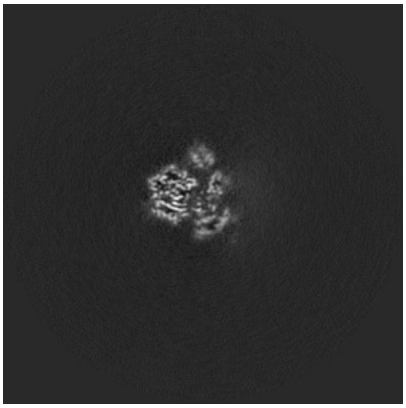
6.3.2 Raw map



X Index: 170



Y Index: 197

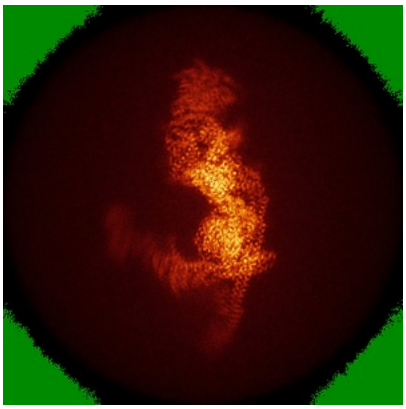


Z Index: 210

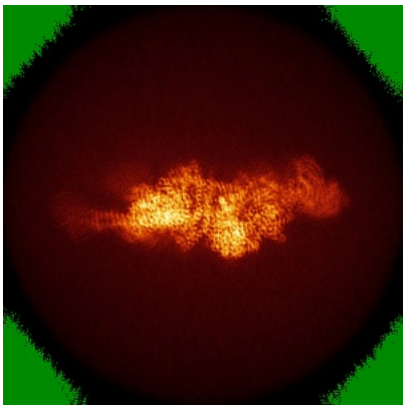
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

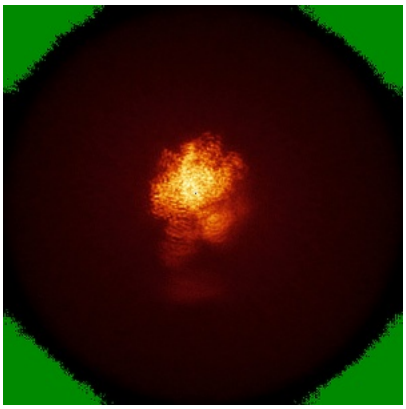
6.4.1 Primary map



X

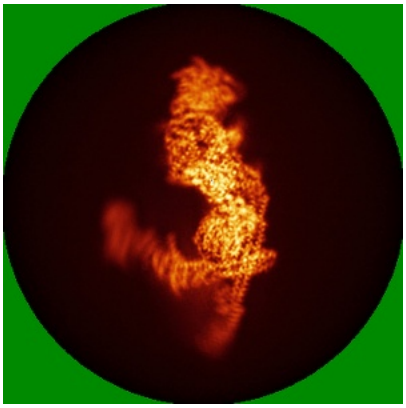


Y



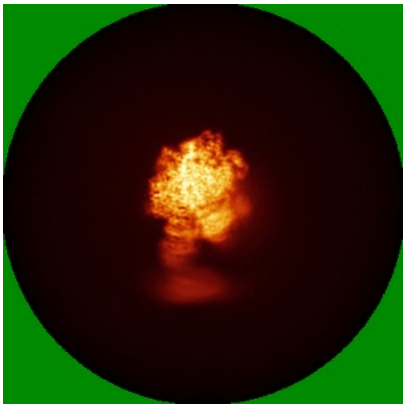
Z

6.4.2 Raw map



X

Y

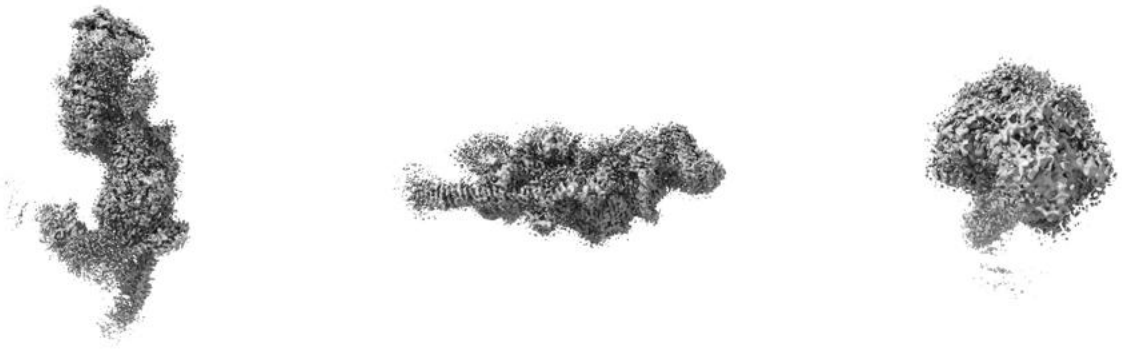


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. 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

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.

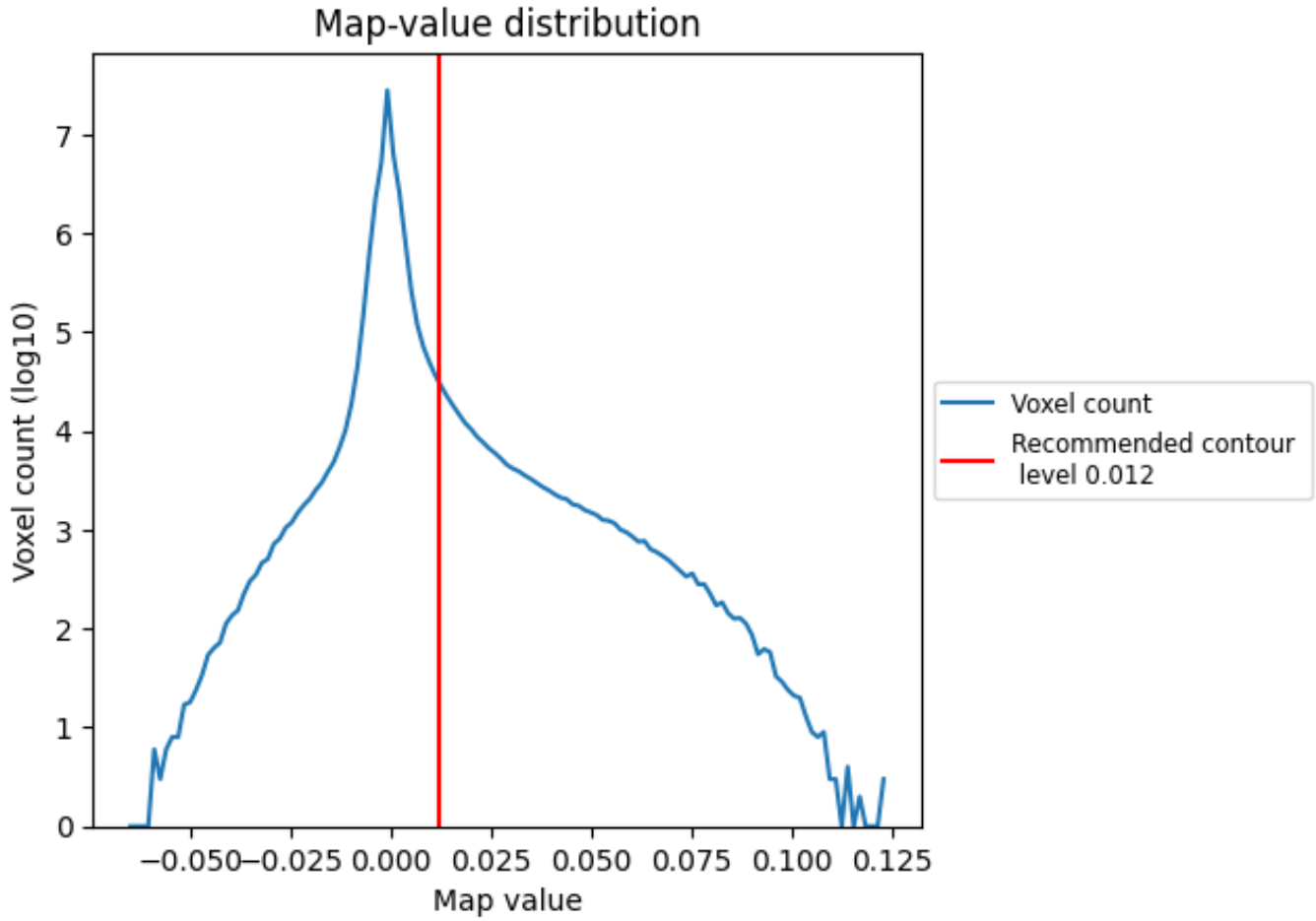
6.6 Mask visualisation (i)

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

7 Map analysis

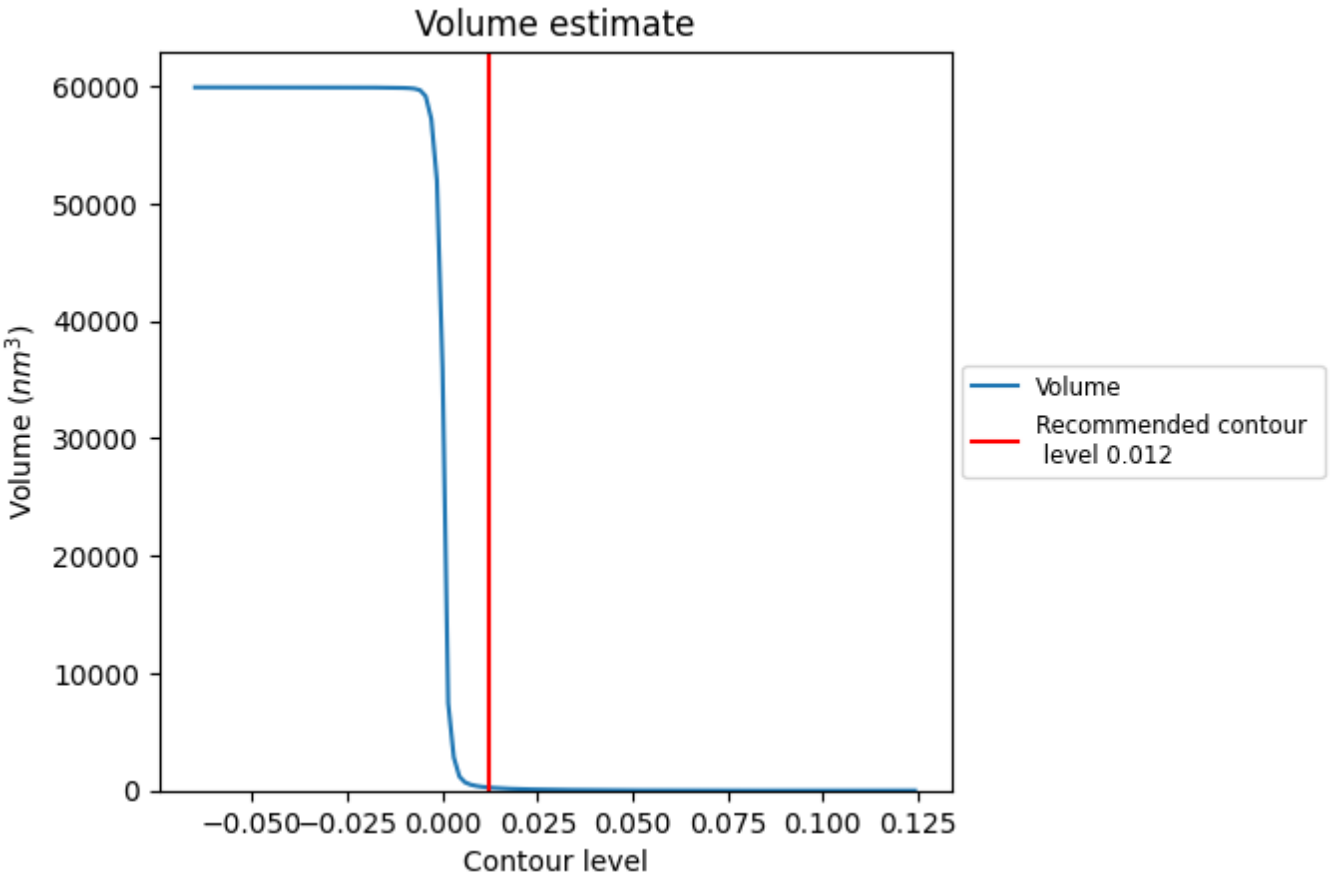
This section contains the results of statistical analysis of the map.

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.

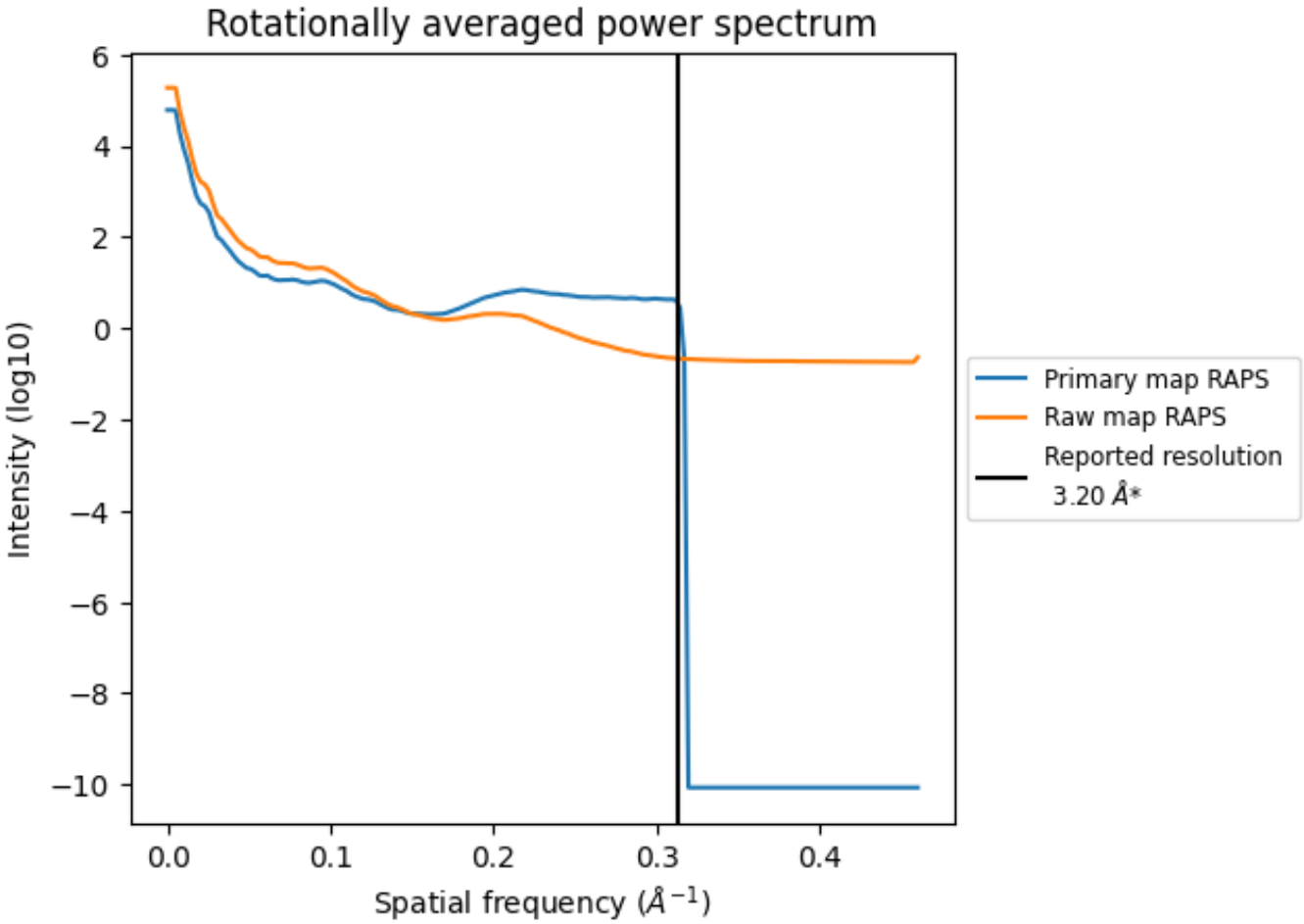
7.2 Volume estimate (i)



The volume at the recommended contour level is 265 nm^3; this corresponds to an approximate mass of 240 kDa.

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

7.3 Rotationally averaged power spectrum (i)

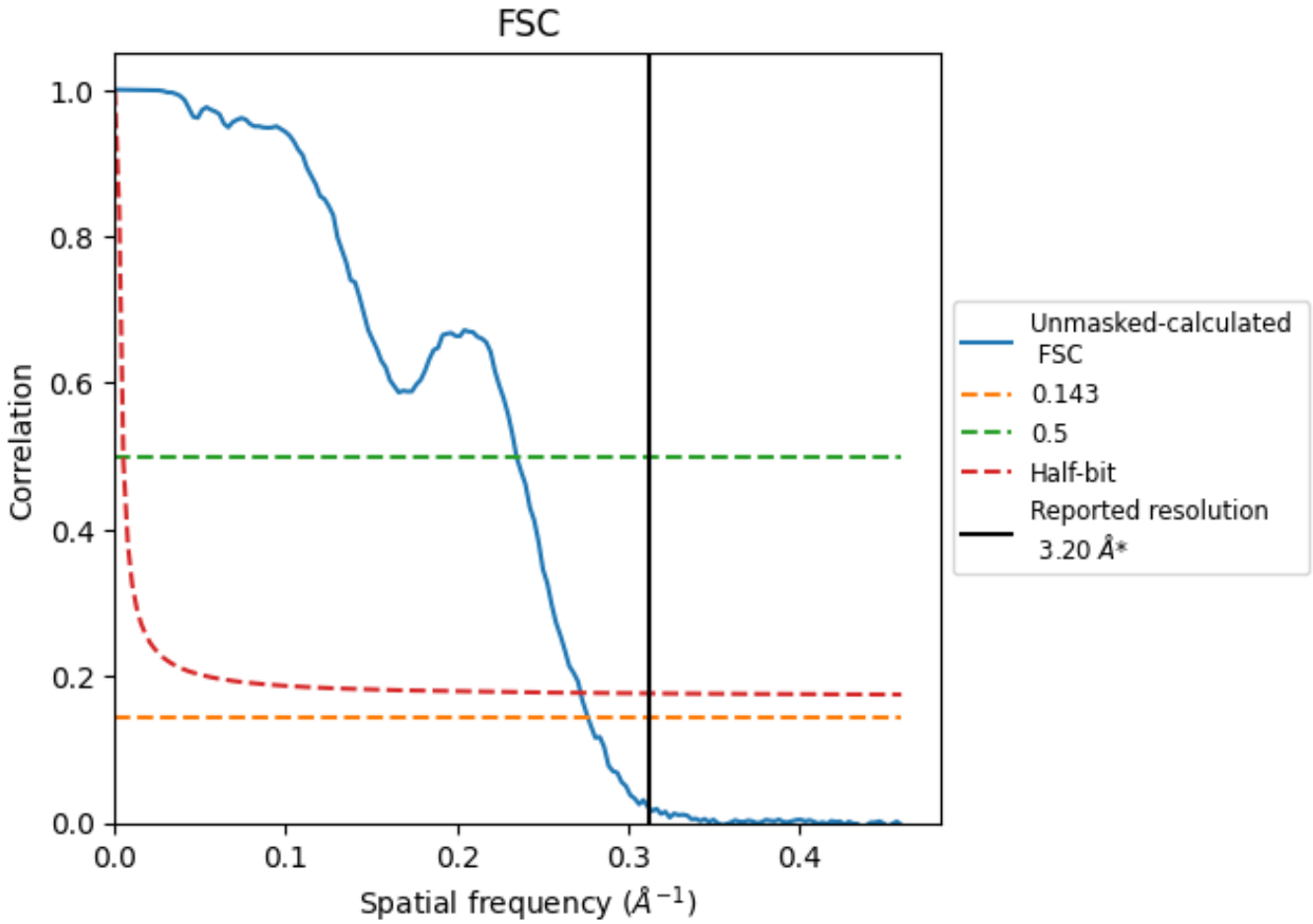


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

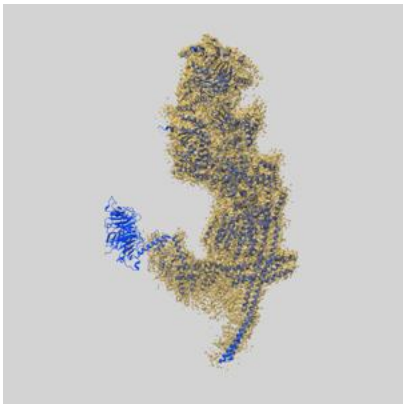
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.26	3.67

*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 3.61 differs from the reported value 3.2 by more than 10 %

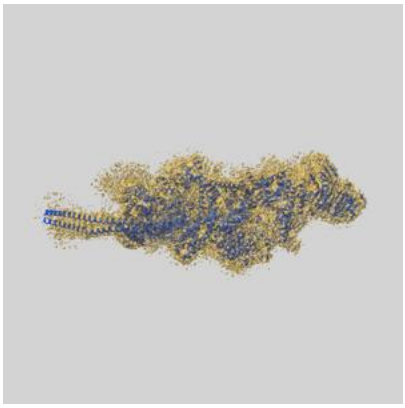
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35093 and PDB model 8I03. Per-residue inclusion information can be found in section 3 on page 6.

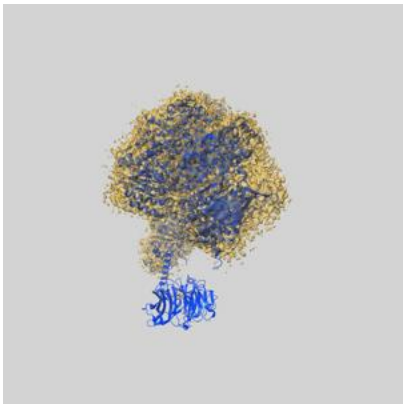
9.1 Map-model overlay



X



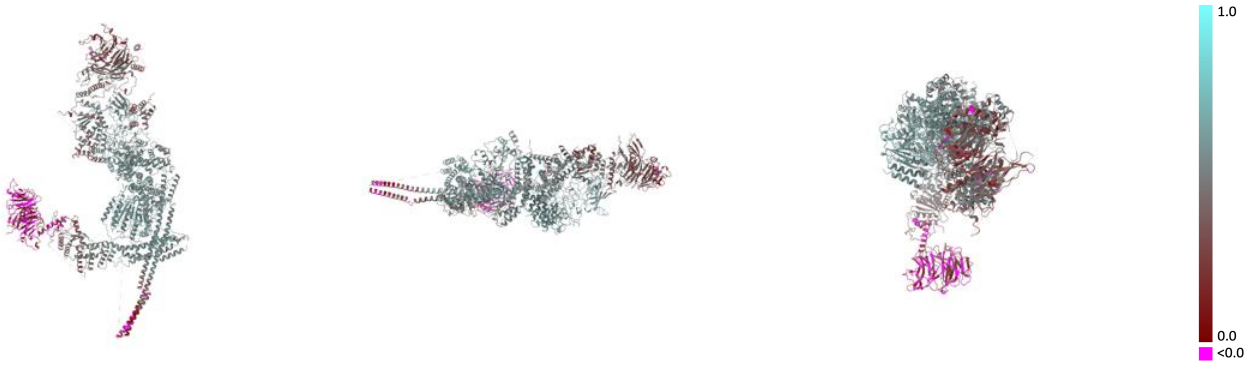
Y



Z

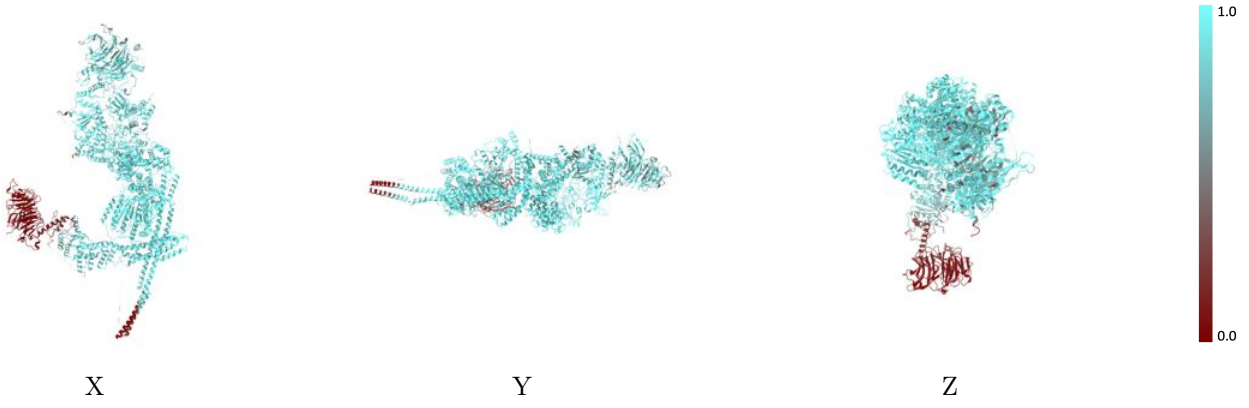
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



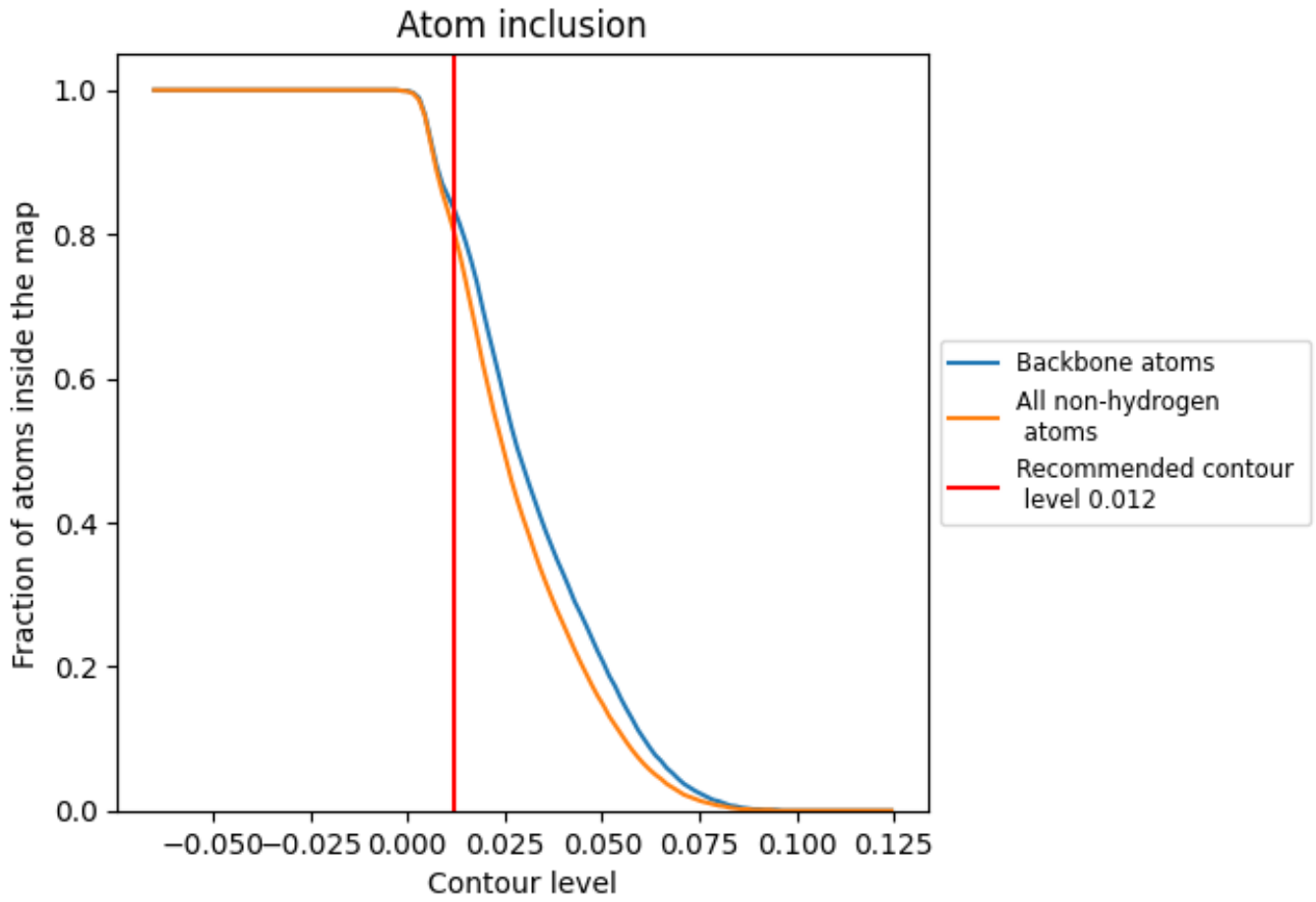
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 80% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.4440
A	0.8470	0.4620
B	0.9070	0.4810
C	0.9780	0.5940
D	0.9780	0.5890
E	0.8730	0.4760
F	0.9310	0.5430
G	0.8140	0.4590
H	0.9380	0.5430
I	0.9300	0.5300
J	0.8000	0.3300
K	0.0070	0.0360