



Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 08:49 AM EDT

PDB ID : 7U05
EMDB ID : EMD-26254
Title : Structure of the yeast TRAPPII-Rab11/Ypt32 complex in the closed/closed state (composite structure)
Authors : Bagde, S.R.; Fromme, J.C.
Deposited on : 2022-02-17
Resolution : 3.70 Å (reported)
Based on initial models : 3CUE, 3RWO, 3PR6

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:

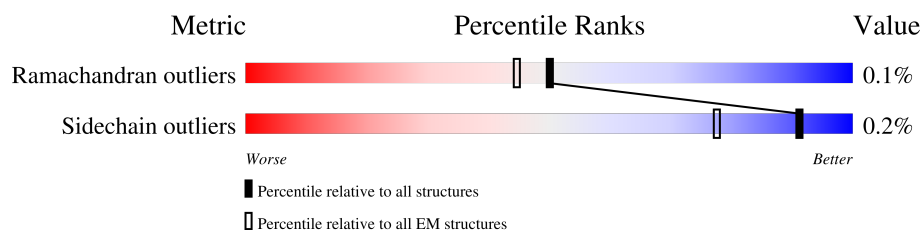
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.70 Å.

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



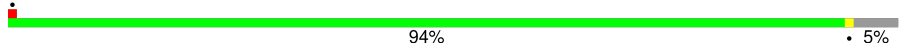
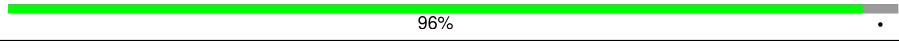
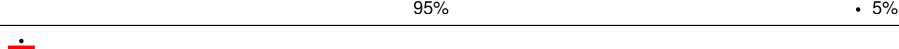
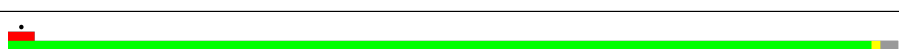



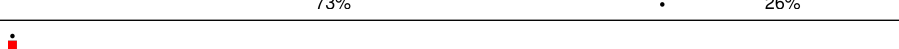
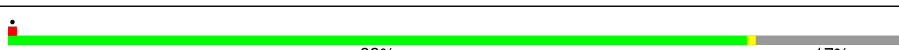


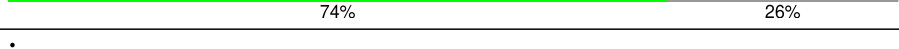

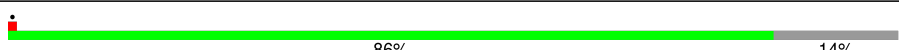





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	M	242	
1	m	242	
2	C	560	
2	c	560	
3	D	152	
3	d	152	
4	E	268	
4	e	268	
5	F	193	

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Mol	Chain	Length	Quality of chain
5	I	193	
5	f	193	
5	i	193	
6	G	159	
6	g	159	
7	H	219	
7	h	219	
8	J	283	
8	j	283	
9	K	175	
9	k	175	
10	L	227	
10	l	227	
11	B	1104	
11	b	1104	
12	A	1289	
12	a	1289	
13	N	210	
13	n	210	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 130986 atoms, of which 65392 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 Trafficking protein particle complex II-specific subunit 130.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	227	Total	C	H	N	O	0	0
			2040	681	905	227	227		
1	m	227	Total	C	H	N	O	0	0
			2040	681	905	227	227		

- Molecule 2 is a protein called Trafficking protein particle complex II-specific subunit 65.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	286	Total	C	H	N	O	0	0
			4652	1488	2353	372	434		
2	c	286	Total	C	H	N	O	0	0
			4652	1488	2353	372	434		

- Molecule 3 is a protein called TRAPP-associated protein TCA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	140	Total	C	H	N	O	0	0
			2262	729	1145	175	209		
3	d	140	Total	C	H	N	O	0	0
			2262	729	1145	175	209		

- Molecule 4 is a protein called Trafficking protein particle complex subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	207	Total	C	H	N	O	0	0
			3430	1092	1736	286	308		
4	e	207	Total	C	H	N	O	0	0
			3430	1092	1736	286	308		

- Molecule 5 is a protein called Trafficking protein particle complex subunit BET3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	186	Total	C	H	N	O	S	0	0
			2997	955	1500	246	285	11		
5	I	184	Total	C	H	N	O	S	0	0
			2971	947	1489	244	280	11		
5	f	186	Total	C	H	N	O	S	0	0
			2997	955	1500	246	285	11		
5	i	184	Total	C	H	N	O	S	0	0
			2971	947	1489	244	280	11		

- Molecule 6 is a protein called Trafficking protein particle complex subunit BET5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	156	Total	C	H	N	O	S	0	0
			2518	813	1245	216	238	6		
6	g	156	Total	C	H	N	O	S	0	0
			2518	813	1245	216	238	6		

- Molecule 7 is a protein called Trafficking protein particle complex subunit 23.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	179	Total	C	H	N	O	S	0	0
			2863	921	1432	230	272	8		
7	h	179	Total	C	H	N	O	S	0	0
			2863	921	1432	230	272	8		

- Molecule 8 is a protein called Trafficking protein particle complex subunit 31.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	210	Total	C	H	N	O	S	0	0
			3343	1077	1652	288	317	9		
8	j	210	Total	C	H	N	O	S	0	0
			3343	1077	1652	288	317	9		

- Molecule 9 is a protein called Trafficking protein particle complex subunit 20.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	146	Total	C	H	N	O	S	0	0
			2342	766	1152	197	222	5		
9	k	146	Total	C	H	N	O	S	0	0
			2342	766	1152	197	222	5		

- Molecule 10 is a protein called GTP-binding protein YPT32/YPT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	193	Total	C	H	N	O	S	0	0
			2982	949	1477	254	298	4		
10	l	193	Total	C	H	N	O	S	0	0
			2982	949	1477	254	298	4		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	221	HIS	-	expression tag	UNP P51996
L	222	HIS	-	expression tag	UNP P51996
L	223	HIS	-	expression tag	UNP P51996
L	224	HIS	-	expression tag	UNP P51996
L	225	HIS	-	expression tag	UNP P51996
L	226	HIS	-	expression tag	UNP P51996
L	227	HIS	-	expression tag	UNP P51996
l	221	HIS	-	expression tag	UNP P51996
l	222	HIS	-	expression tag	UNP P51996
l	223	HIS	-	expression tag	UNP P51996
l	224	HIS	-	expression tag	UNP P51996
l	225	HIS	-	expression tag	UNP P51996
l	226	HIS	-	expression tag	UNP P51996
l	227	HIS	-	expression tag	UNP P51996

- Molecule 11 is a protein called Trafficking protein particle complex II-specific subunit 130.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	B	815	Total	C	H	N	O	S	0	0
			13433	4334	6748	1081	1242	28		
11	b	815	Total	C	H	N	O	S	0	0
			13433	4334	6748	1081	1242	28		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1103	ALA	-	expression tag	UNP Q03660
B	1104	ALA	-	expression tag	UNP Q03660
b	1103	ALA	-	expression tag	UNP Q03660
b	1104	ALA	-	expression tag	UNP Q03660

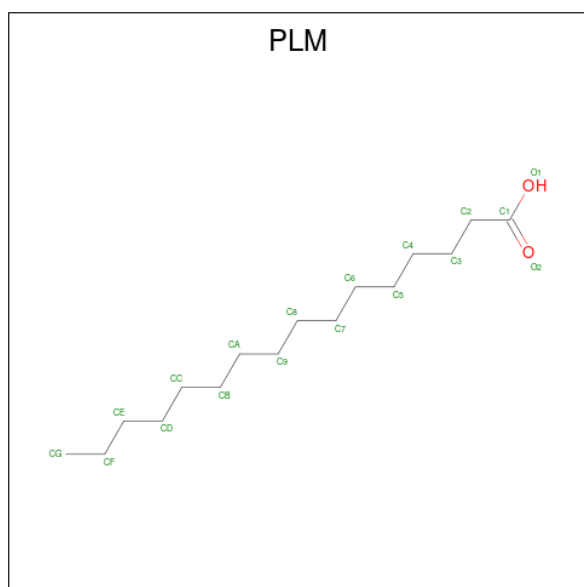
- Molecule 12 is a protein called Trafficking protein particle complex II-specific subunit 120.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	A	1114	Total	C	H	N	O	S	0	0
			18376	5905	9272	1477	1680	42		
12	a	1114	Total	C	H	N	O	S	0	0
			18376	5905	9272	1477	1680	42		

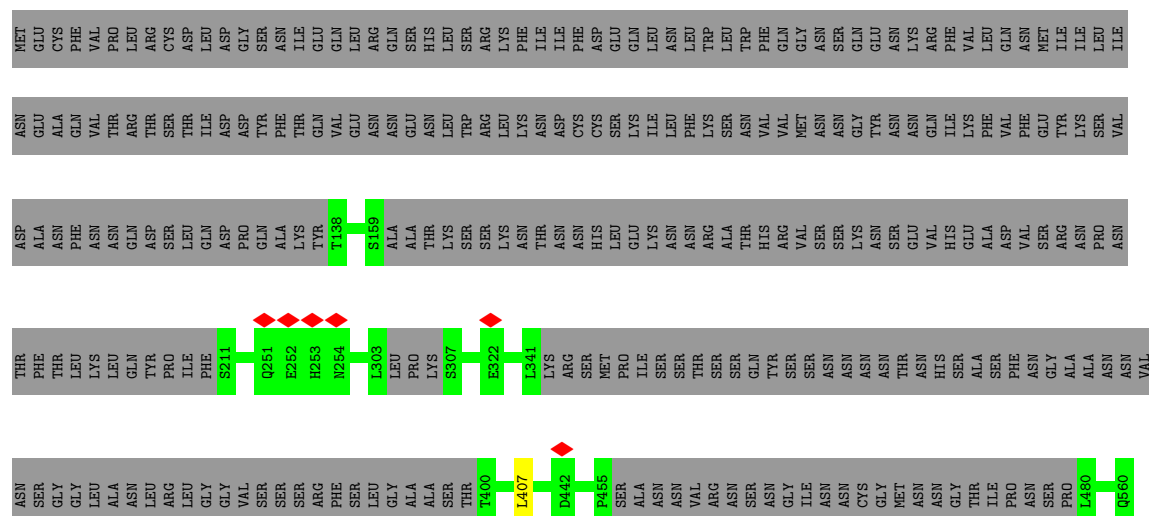
- Molecule 13 is a protein called Trafficking protein particle complex II-specific subunit 65.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	132	Total	C	H	N	O	0	0
			1188	396	528	132	132		
13	n	132	Total	C	H	N	O	0	0
			1188	396	528	132	132		

- Molecule 14 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	F	1	Total	C	H	O	0
			48	16	31	1	
14	I	1	Total	C	H	O	0
			48	16	31	1	
14	f	1	Total	C	H	O	0
			48	16	31	1	
14	i	1	Total	C	H	O	0
			48	16	31	1	



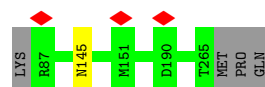
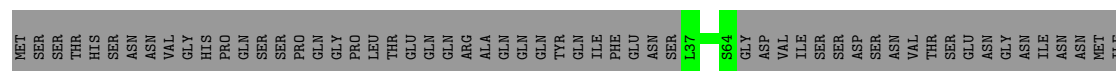
- Molecule 3: TRAPP-associated protein TCA17



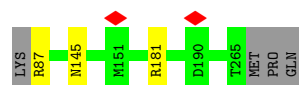
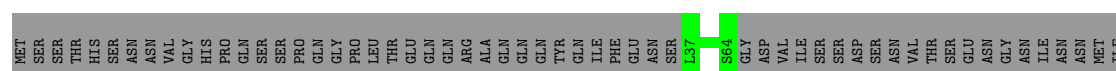
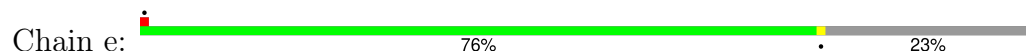
- Molecule 3: TRAPP-associated protein TCA17



- Molecule 4: Trafficking protein particle complex subunit 33

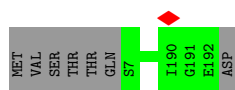


- Molecule 4: Trafficking protein particle complex subunit 33



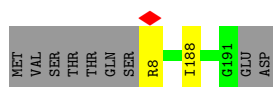
- Molecule 5: Trafficking protein particle complex subunit BET3

Chain F:  96% .



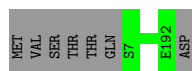
- Molecule 5: Trafficking protein particle complex subunit BET3

Chain I:  94% . 5%



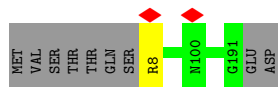
- Molecule 5: Trafficking protein particle complex subunit BET3

Chain f:  96% .



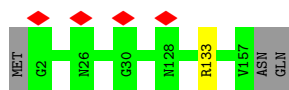
- Molecule 5: Trafficking protein particle complex subunit BET3

Chain i:  95% . 5%



- Molecule 6: Trafficking protein particle complex subunit BET5

Chain G:  97% ..




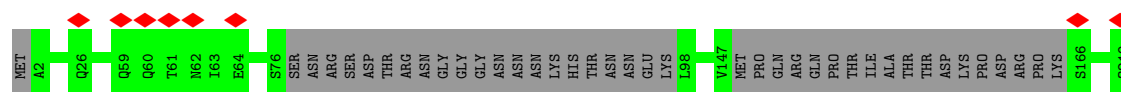
- Molecule 6: Trafficking protein particle complex subunit BET5

Chain g:  97% ..

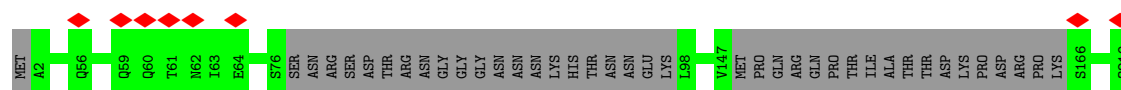
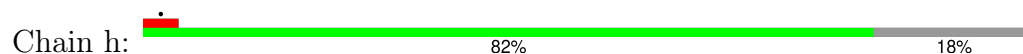


- Molecule 7: Trafficking protein particle complex subunit 23

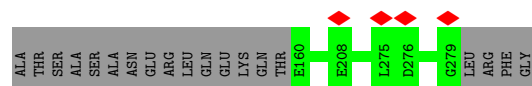
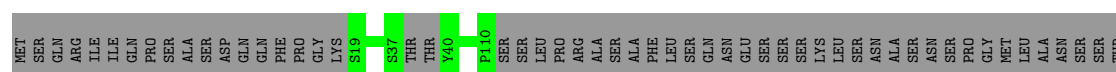
Chain H:  82% 18%



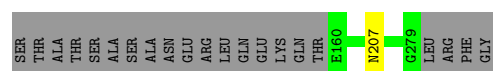
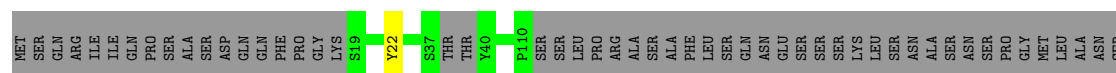
- Molecule 7: Trafficking protein particle complex subunit 23



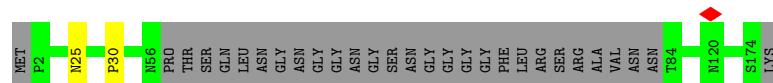
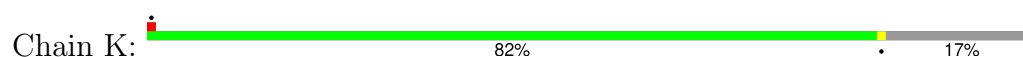
- Molecule 8: Trafficking protein particle complex subunit 31



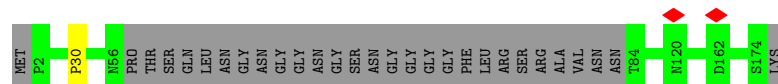
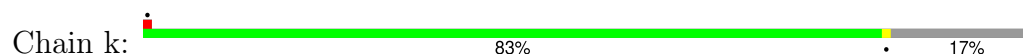
- Molecule 8: Trafficking protein particle complex subunit 31



- Molecule 9: Trafficking protein particle complex subunit 20



- Molecule 9: Trafficking protein particle complex subunit 20



- Molecule 10: GTP-binding protein YPT32/YPT11

Responsibility	Percentage
Current government	85%
Previous government	15%



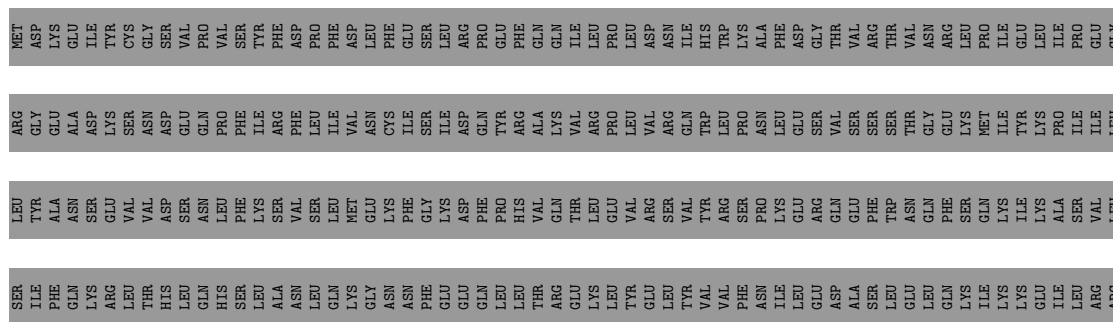
Response	Percentage
Agree	85%
Disagree	15%

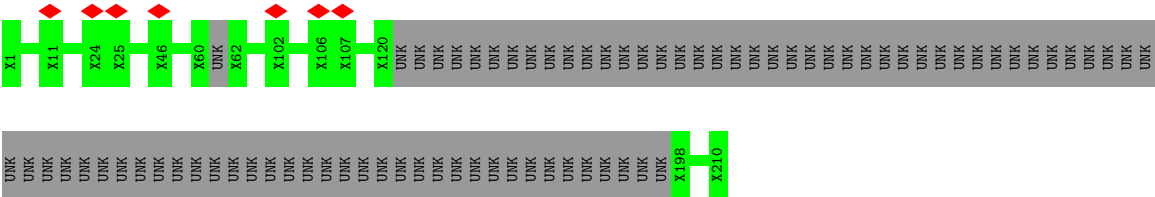


Response	Percentage
U.S. is a democracy	74%
U.S. is not a democracy	26%

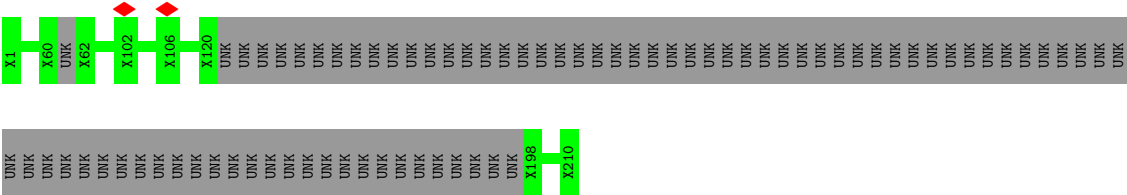


Response	Percentage
U.S. is a democracy	74%
U.S. is not a democracy	26%





• Molecule 13: Trafficking protein particle complex II-specific subunit 65



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	369488	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	63000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	39.609	Depositor
Minimum map value	-22.623	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.657	Depositor
Recommended contour level	2.5	Depositor
Map size (\AA)	572.8, 572.8, 572.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.4319999, 1.4319999, 1.4319999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLM

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
2	C	0.27	0/2344	0.57	0/3176
2	c	0.29	0/2344	0.58	1/3176 (0.0%)
3	D	0.29	0/1135	0.56	0/1530
3	d	0.30	0/1135	0.60	0/1530
4	E	0.30	0/1726	0.60	0/2323
4	e	0.30	0/1726	0.61	0/2323
5	F	0.29	0/1524	0.57	0/2060
5	I	0.30	0/1509	0.59	0/2040
5	f	0.29	0/1524	0.55	0/2060
5	i	0.28	0/1509	0.56	0/2040
6	G	0.28	0/1302	0.59	0/1758
6	g	0.29	0/1302	0.60	0/1758
7	H	0.30	0/1457	0.53	0/1968
7	h	0.29	0/1457	0.55	0/1968
8	J	0.30	0/1727	0.63	0/2328
8	j	0.30	0/1727	0.61	0/2328
9	K	0.31	0/1221	0.59	0/1655
9	k	0.30	0/1221	0.60	0/1655
10	L	0.28	0/1530	0.58	0/2070
10	l	0.28	0/1530	0.58	0/2070
11	B	0.28	0/6814	0.56	0/9188
11	b	0.29	0/6814	0.57	0/9188
12	A	0.28	0/9303	0.57	0/12602
12	a	0.29	0/9303	0.57	0/12602
All	All	0.29	0/63184	0.58	1/85396 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	407	LEU	CA-CB-CG	5.23	127.32	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	276/560 (49%)	254 (92%)	22 (8%)	0	100	100
2	c	276/560 (49%)	252 (91%)	24 (9%)	0	100	100
3	D	136/152 (90%)	125 (92%)	11 (8%)	0	100	100
3	d	136/152 (90%)	124 (91%)	12 (9%)	0	100	100
4	E	203/268 (76%)	178 (88%)	25 (12%)	0	100	100
4	e	203/268 (76%)	177 (87%)	26 (13%)	0	100	100
5	F	184/193 (95%)	172 (94%)	12 (6%)	0	100	100
5	I	182/193 (94%)	165 (91%)	16 (9%)	1 (0%)	25	57
5	f	184/193 (95%)	173 (94%)	11 (6%)	0	100	100
5	i	182/193 (94%)	163 (90%)	19 (10%)	0	100	100
6	G	154/159 (97%)	132 (86%)	22 (14%)	0	100	100
6	g	154/159 (97%)	129 (84%)	24 (16%)	1 (1%)	22	54
7	H	173/219 (79%)	155 (90%)	18 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	173/219 (79%)	157 (91%)	16 (9%)	0	100	100
8	J	204/283 (72%)	183 (90%)	21 (10%)	0	100	100
8	j	204/283 (72%)	185 (91%)	18 (9%)	1 (0%)	25	57
9	K	142/175 (81%)	128 (90%)	13 (9%)	1 (1%)	19	51
9	k	142/175 (81%)	130 (92%)	11 (8%)	1 (1%)	19	51
10	L	189/227 (83%)	169 (89%)	20 (11%)	0	100	100
10	l	189/227 (83%)	170 (90%)	19 (10%)	0	100	100
11	B	805/1104 (73%)	732 (91%)	73 (9%)	0	100	100
11	b	805/1104 (73%)	731 (91%)	73 (9%)	1 (0%)	48	78
12	A	1100/1289 (85%)	987 (90%)	112 (10%)	1 (0%)	48	78
12	a	1100/1289 (85%)	991 (90%)	109 (10%)	0	100	100
All	All	7496/9644 (78%)	6762 (90%)	727 (10%)	7 (0%)	50	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	188	ILE
8	j	22	TYR
6	g	95	LYS
11	b	294	GLN
12	A	1273	GLN
9	K	30	PRO
9	k	30	PRO

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	
2	C	270/518 (52%)	269 (100%)	1 (0%)	89	93
2	c	270/518 (52%)	270 (100%)	0	100	100
3	D	127/142 (89%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	d	127/142 (89%)	127 (100%)	0	100	100
4	E	192/248 (77%)	191 (100%)	1 (0%)	86	92
4	e	192/248 (77%)	189 (98%)	3 (2%)	58	74
5	F	171/178 (96%)	171 (100%)	0	100	100
5	I	169/178 (95%)	168 (99%)	1 (1%)	84	90
5	f	171/178 (96%)	171 (100%)	0	100	100
5	i	169/178 (95%)	168 (99%)	1 (1%)	84	90
6	G	142/145 (98%)	141 (99%)	1 (1%)	81	88
6	g	142/145 (98%)	142 (100%)	0	100	100
7	H	162/199 (81%)	162 (100%)	0	100	100
7	h	162/199 (81%)	162 (100%)	0	100	100
8	J	187/249 (75%)	187 (100%)	0	100	100
8	j	187/249 (75%)	186 (100%)	1 (0%)	86	92
9	K	132/152 (87%)	131 (99%)	1 (1%)	79	85
9	k	132/152 (87%)	132 (100%)	0	100	100
10	L	162/194 (84%)	162 (100%)	0	100	100
10	l	162/194 (84%)	162 (100%)	0	100	100
11	B	753/1023 (74%)	753 (100%)	0	100	100
11	b	753/1023 (74%)	753 (100%)	0	100	100
12	A	1054/1213 (87%)	1053 (100%)	1 (0%)	92	96
12	a	1054/1213 (87%)	1053 (100%)	1 (0%)	92	96
All	All	7042/8878 (79%)	7030 (100%)	12 (0%)	91	96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	219	ASN
4	E	145	ASN
6	G	133	ARG
5	I	8	ARG
9	K	25	ASN
12	A	728	LYS
4	e	87	ARG
4	e	145	ASN
4	e	181	ARG

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Mol	Chain	Res	Type
5	i	8	ARG
8	j	207	ASN
12	a	173	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	219	ASN
11	B	405	ASN
11	B	535	HIS
11	B	837	ASN
12	A	467	ASN
4	e	106	HIS
8	j	207	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
14	PLM	f	201	5	15,16,17	0.50	0	14,15,17	0.39	0
14	PLM	F	201	5	15,16,17	0.52	0	14,15,17	0.39	0
14	PLM	i	201	5	15,16,17	0.46	0	14,15,17	0.39	0
14	PLM	I	201	5	15,16,17	0.50	0	14,15,17	0.41	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
14	PLM	f	201	5	-	7/14/14/15	-
14	PLM	F	201	5	-	7/14/14/15	-
14	PLM	i	201	5	-	4/14/14/15	-
14	PLM	I	201	5	-	4/14/14/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	I	201	PLM	O2-C1-C2-C3
14	i	201	PLM	O2-C1-C2-C3
14	f	201	PLM	C4-C5-C6-C7
14	F	201	PLM	C4-C5-C6-C7
14	f	201	PLM	C2-C3-C4-C5
14	F	201	PLM	C2-C3-C4-C5
14	F	201	PLM	C3-C4-C5-C6
14	f	201	PLM	C3-C4-C5-C6
14	I	201	PLM	CB-CC-CD-CE
14	f	201	PLM	CD-CE-CF-CG
14	F	201	PLM	CD-CE-CF-CG
14	i	201	PLM	CB-CC-CD-CE
14	I	201	PLM	C8-C9-CA-CB
14	f	201	PLM	CB-CC-CD-CE
14	I	201	PLM	C7-C8-C9-CA
14	i	201	PLM	C9-CA-CB-CC
14	f	201	PLM	C6-C7-C8-C9
14	F	201	PLM	C6-C7-C8-C9

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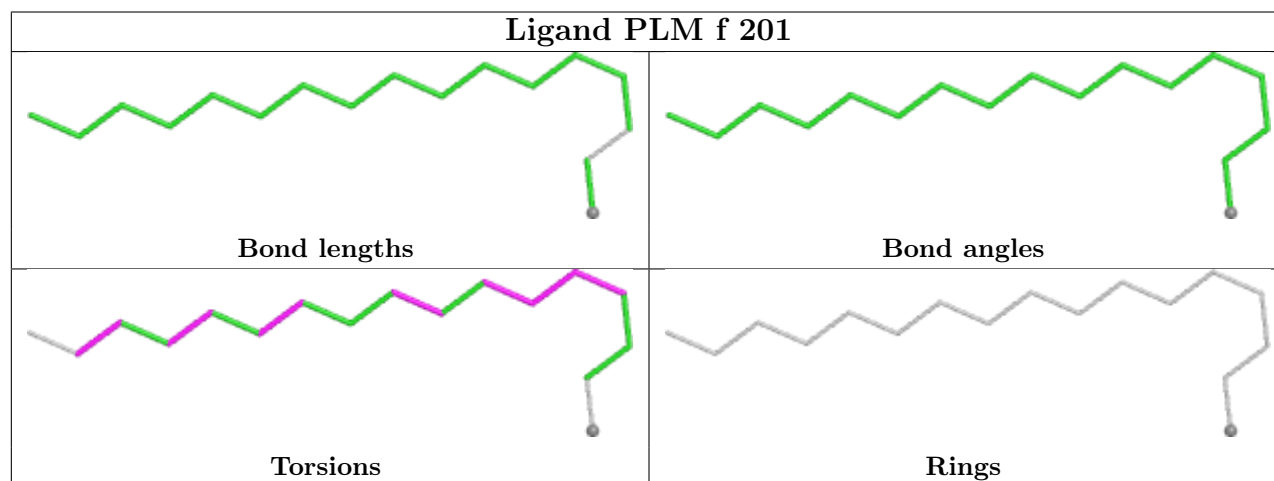
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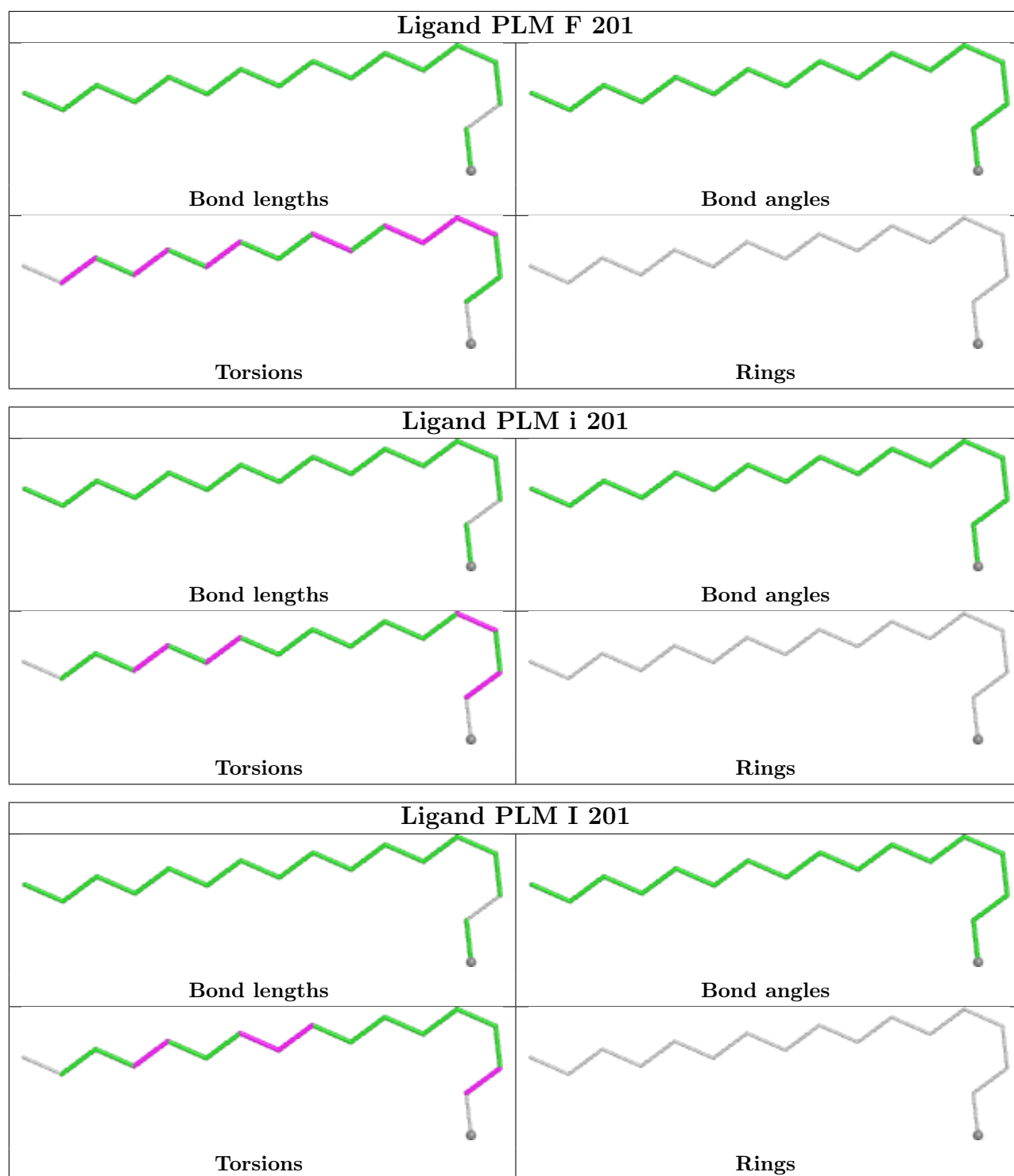
Mol	Chain	Res	Type	Atoms
14	F	201	PLM	CB-CC-CD-CE
14	F	201	PLM	C9-CA-CB-CC
14	i	201	PLM	C2-C3-C4-C5
14	f	201	PLM	C9-CA-CB-CC

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

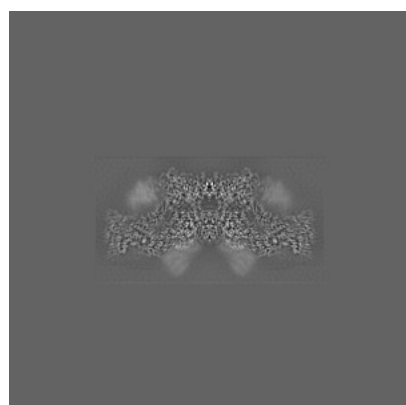
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26254. These allow visual inspection of the internal detail of the map and identification of artifacts.

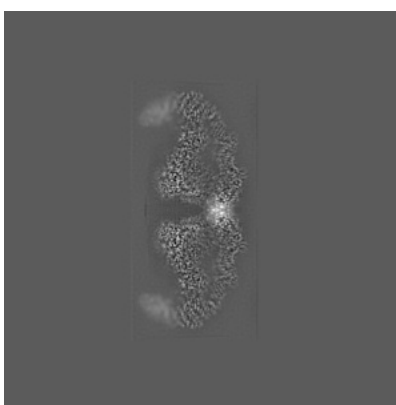
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

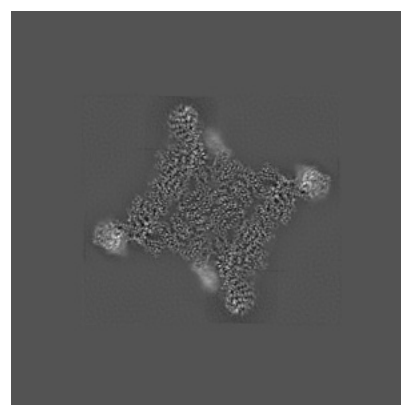
6.1.1 Primary map



X



Y

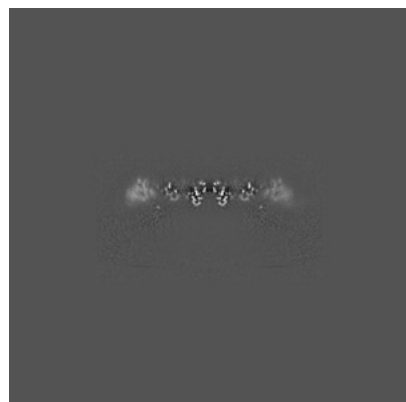


Z

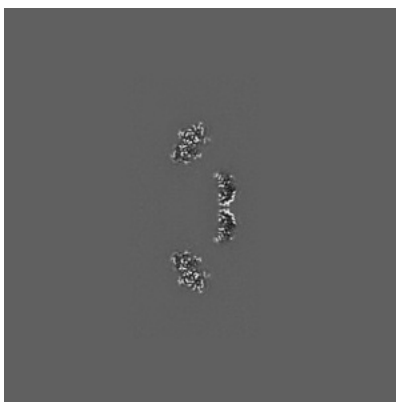
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

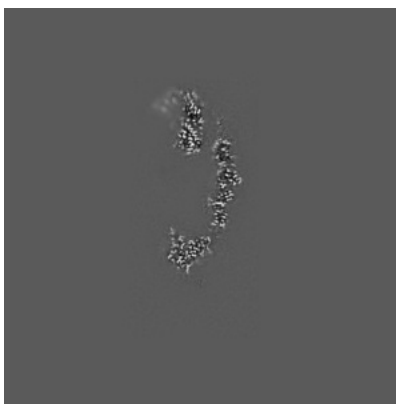
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

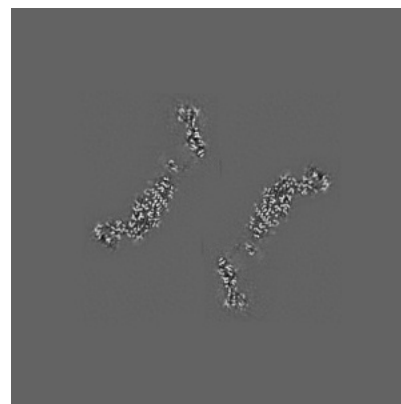
6.3.1 Primary map



X Index: 181



Y Index: 218

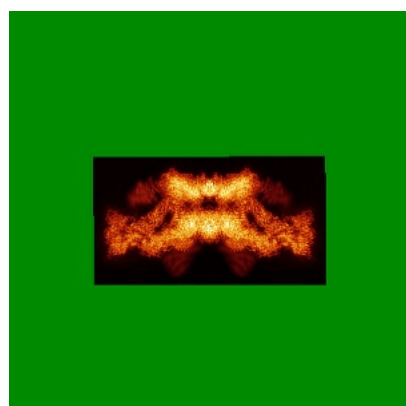


Z Index: 184

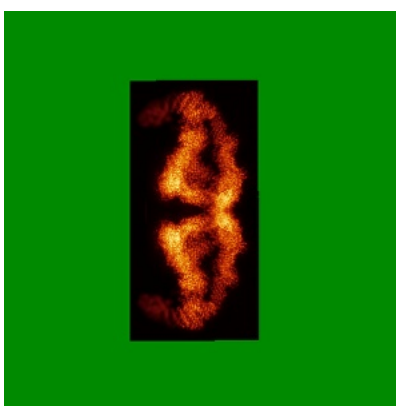
The images above show the largest variance slices of the map in three orthogonal directions.

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

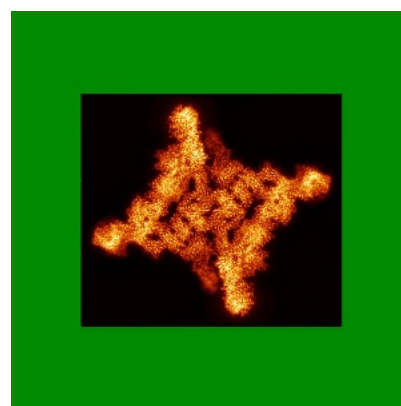
6.4.1 Primary map



X



Y

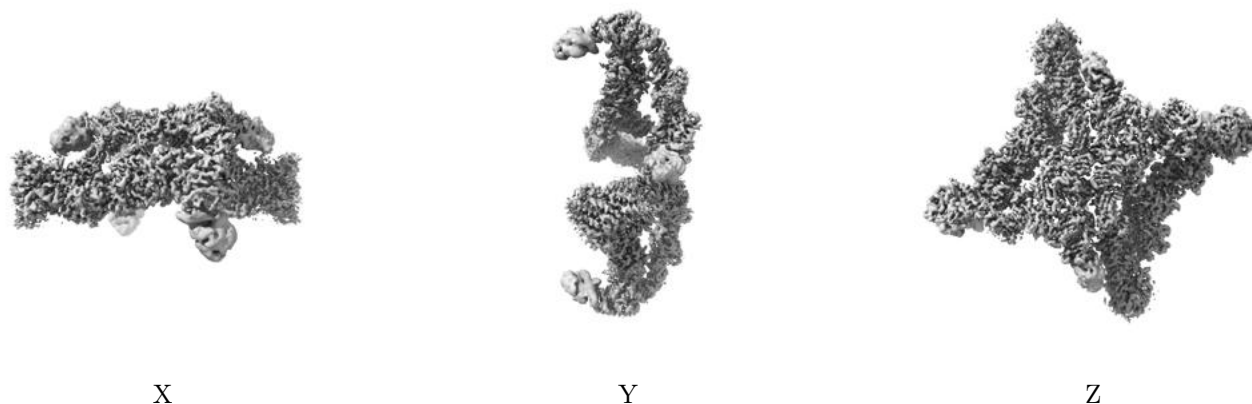


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

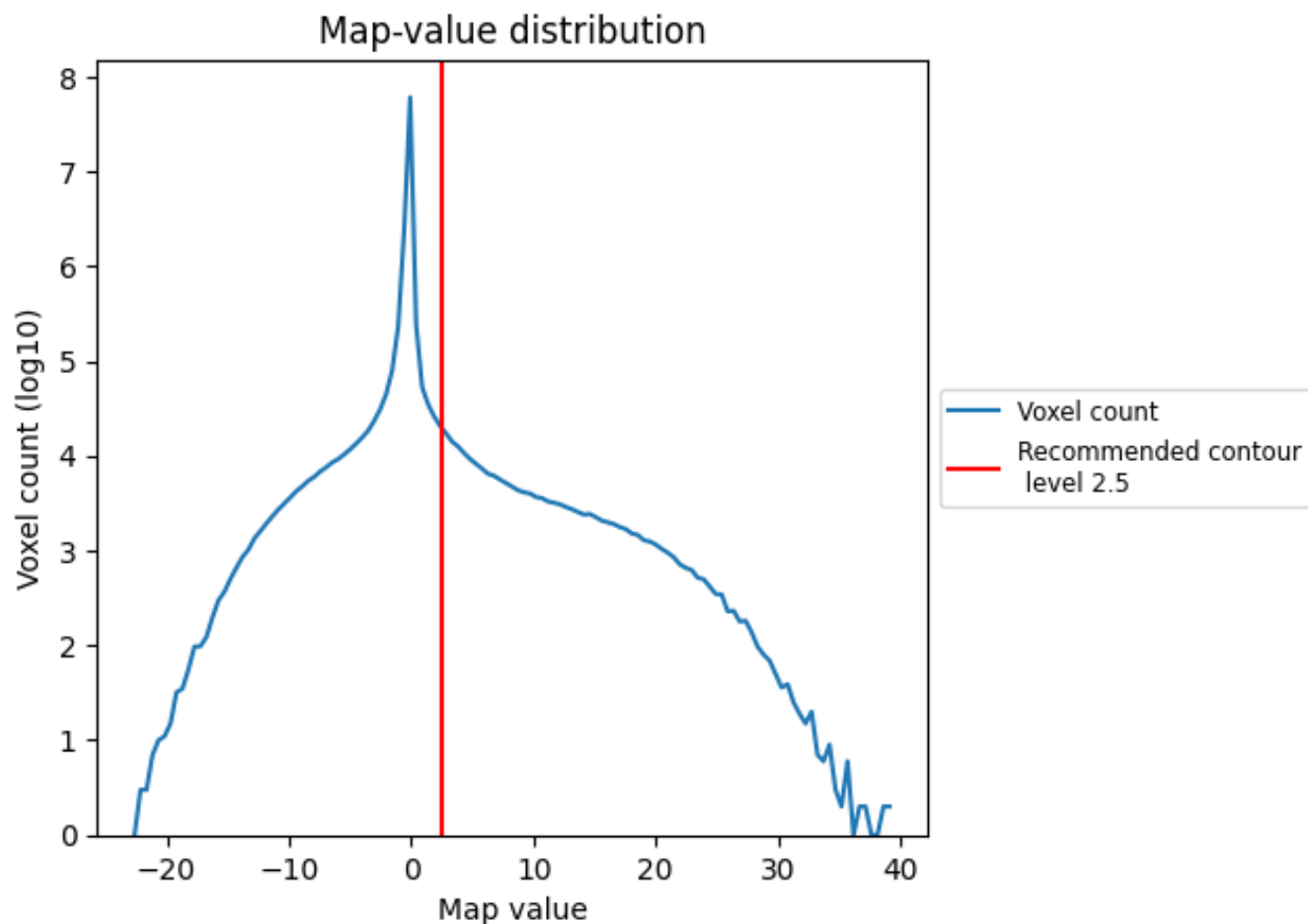
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

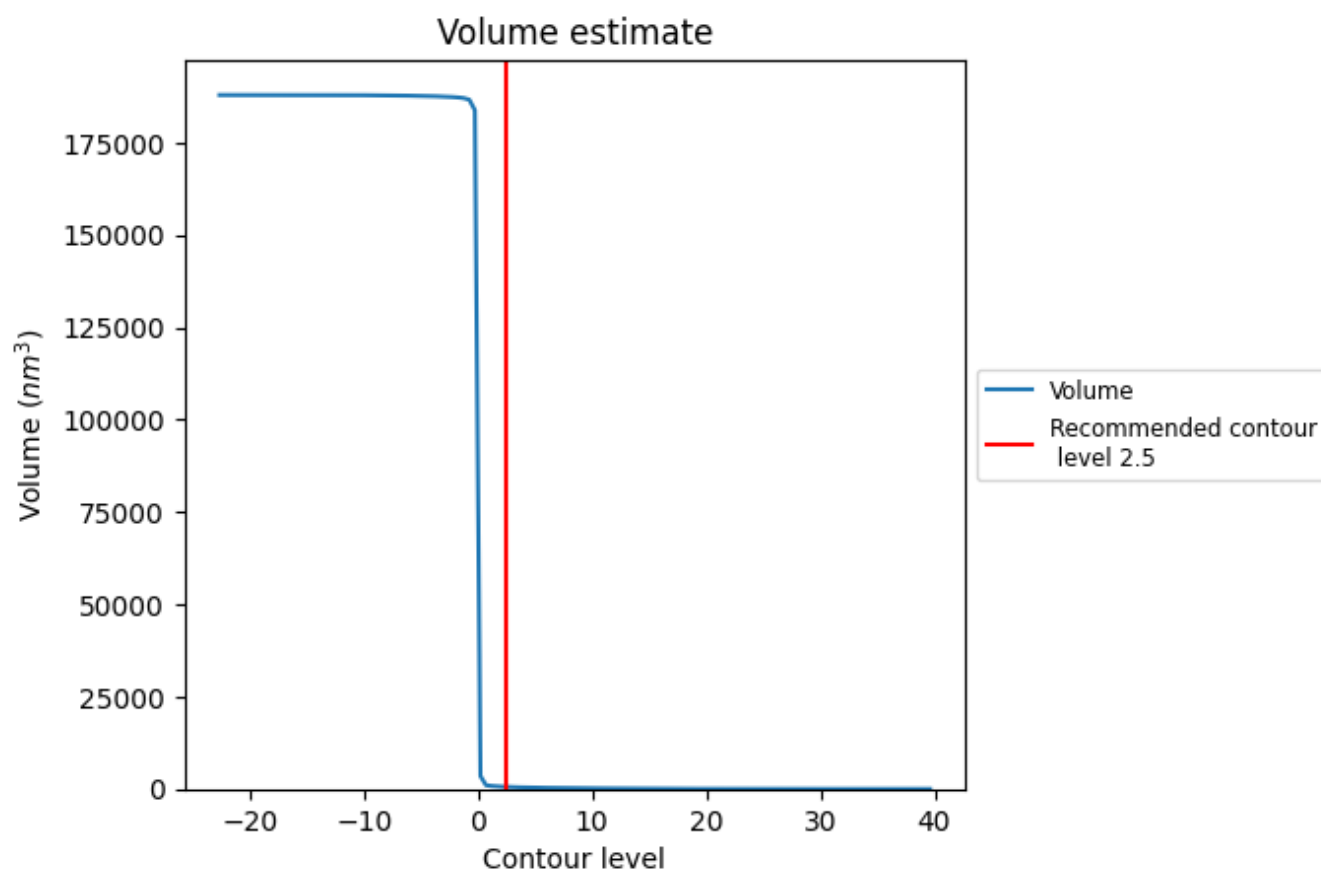
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

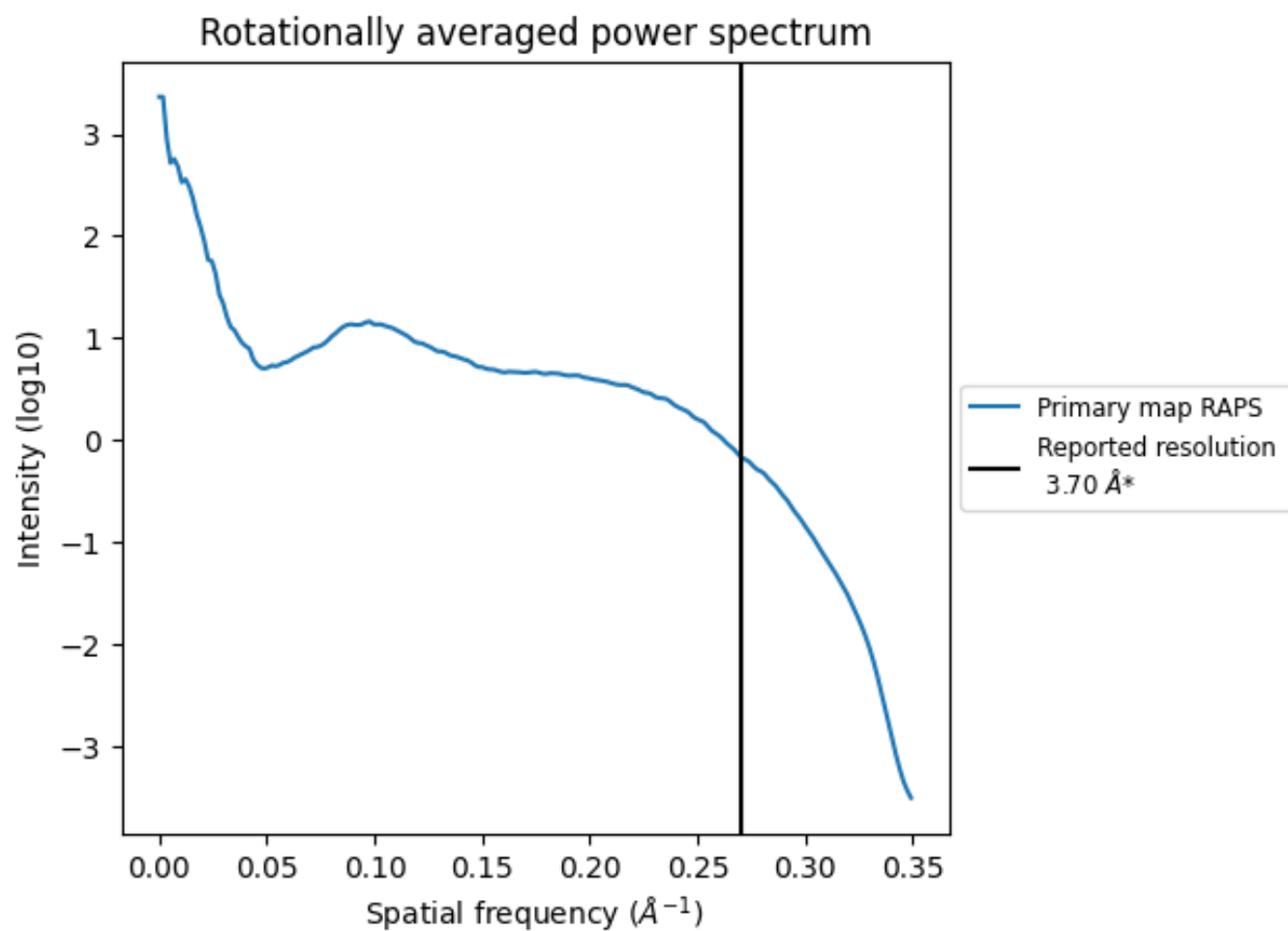
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 563 nm^3 ; this corresponds to an approximate mass of 509 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 0.270 Å⁻¹

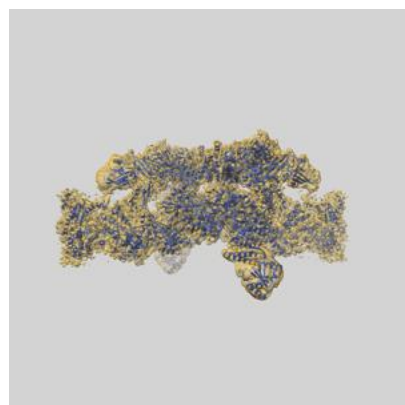
8 Fourier-Shell correlation

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

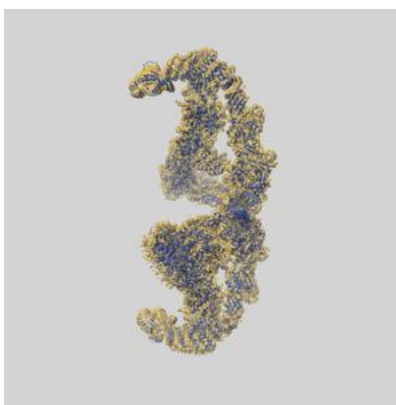
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26254 and PDB model 7U05. Per-residue inclusion information can be found in section [3](#) on page [8](#).

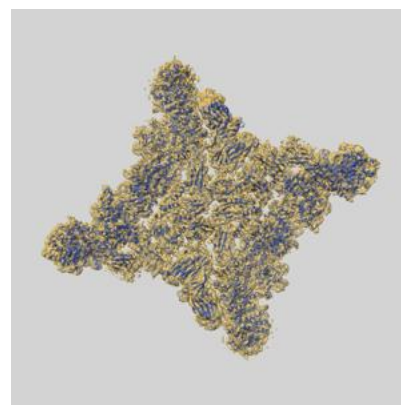
9.1 Map-model overlay [i](#)



X



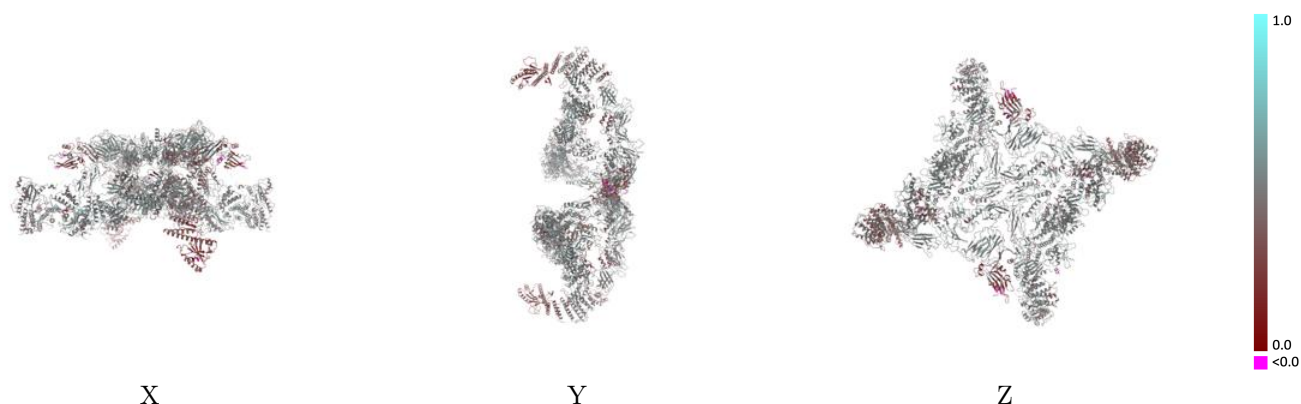
Y



Z

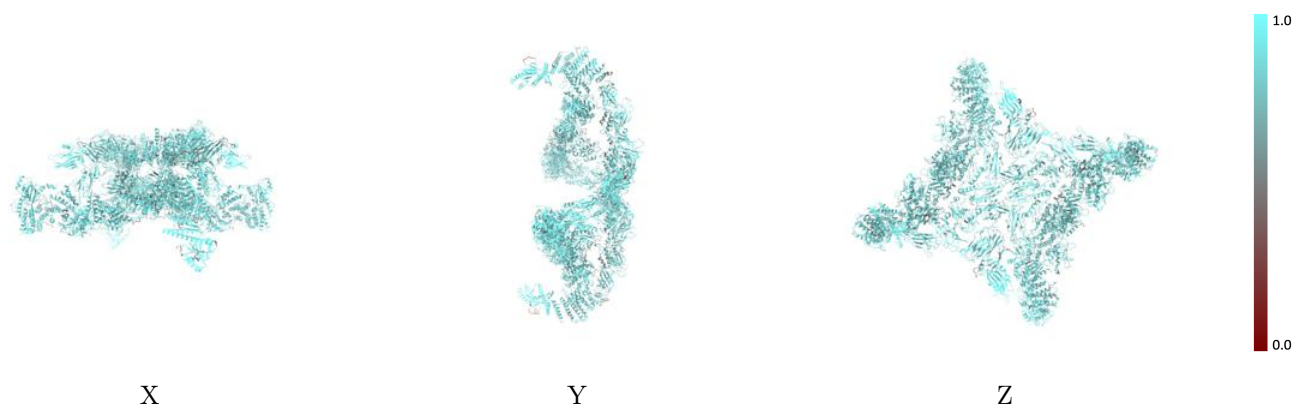
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



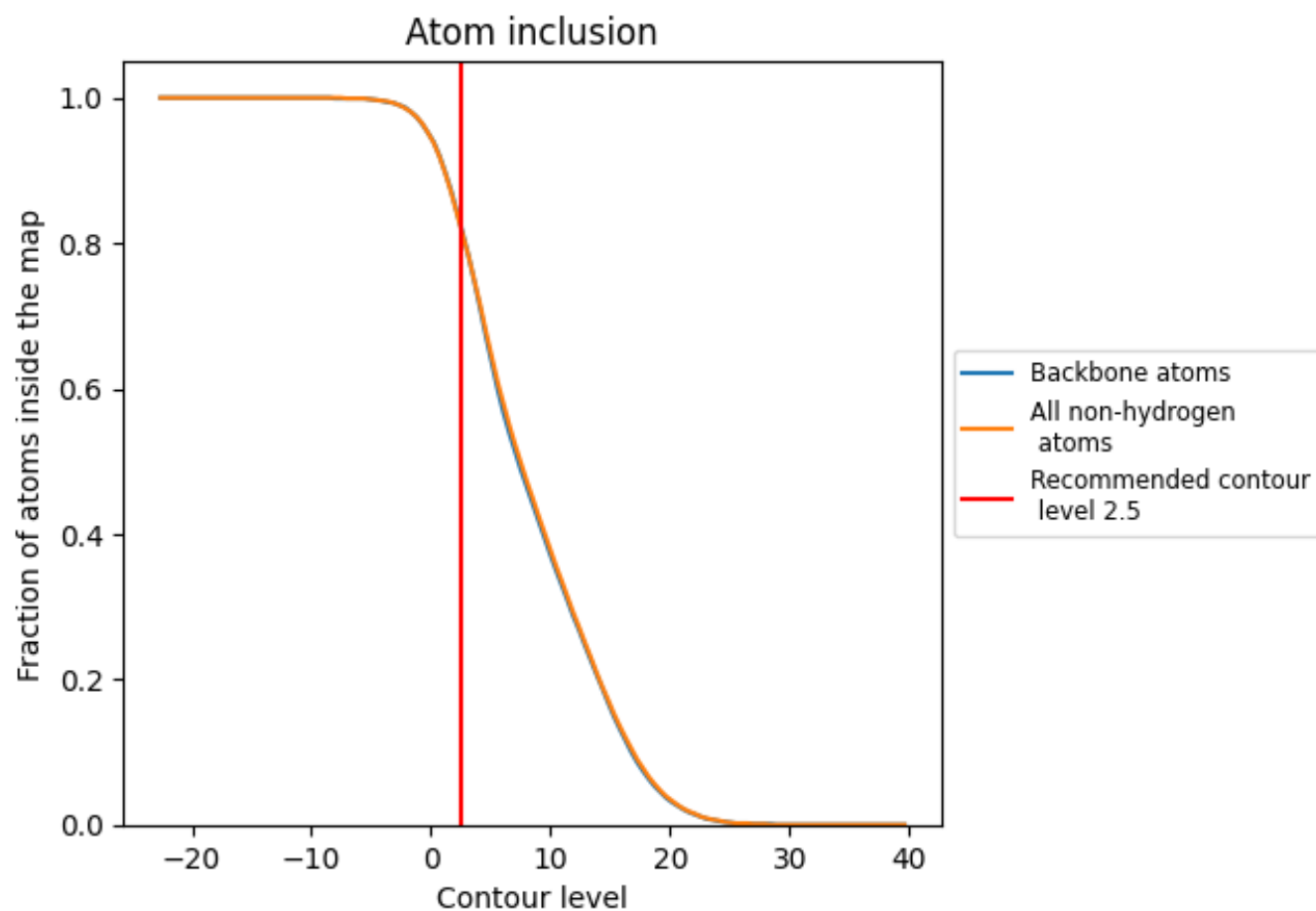
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.4520
A	 0.8400	 0.4710
B	 0.7980	 0.4410
C	 0.7890	 0.4540
D	 0.8120	 0.4440
E	 0.8220	 0.4620
F	 0.8450	 0.4840
G	 0.8410	 0.4870
H	 0.7890	 0.4740
I	 0.8350	 0.4950
J	 0.8530	 0.4830
K	 0.8530	 0.4940
L	 0.7670	 0.4540
M	 0.9100	 0.2470
N	 0.9180	 0.2490
a	 0.8430	 0.4710
b	 0.7950	 0.4400
c	 0.7940	 0.4470
d	 0.8090	 0.4440
e	 0.8190	 0.4510
f	 0.8300	 0.4820
g	 0.8480	 0.4860
h	 0.8020	 0.4750
i	 0.8280	 0.4850
j	 0.8580	 0.4830
k	 0.8620	 0.4900
l	 0.7710	 0.4560
m	 0.9180	 0.2450
n	 0.9740	 0.2530

