



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 12:36 AM EST

PDB ID : 7TR9
EMDB ID : EMD-26083
Title : Cascade complex from type I-A CRISPR-Cas system
Authors : Hu, C.; Ni, D.; Nam, K.H.; Majumdar, S.; McLean, J.; Stahlberg, H.; Terns, M.; Ke, A.
Deposited on : 2022-01-28
Resolution : 3.90 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:

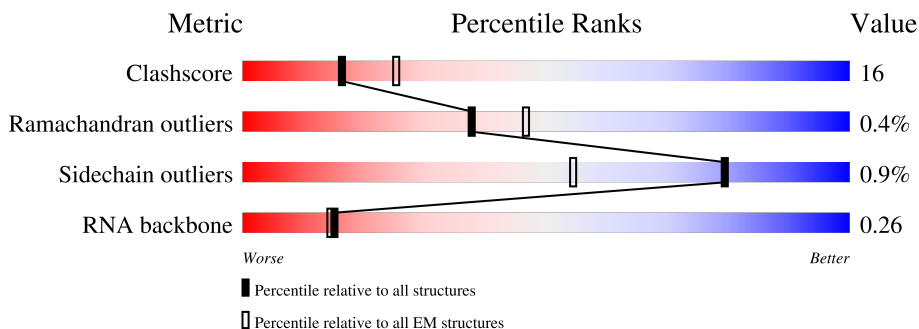
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	C	341	
2	D	108	
2	E	108	
2	F	108	
2	G	108	
2	H	108	
3	I	336	

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Mol	Chain	Length	Quality of chain
3	J	336	<p>5% 68% 32%</p>
3	K	336	<p>7% 55% 44%</p>
3	L	336	<p>10% 65% 35%</p>
3	M	336	<p>12% 61% 39%</p>
3	N	336	<p>10% 59% 36%</p>
3	O	336	<p>12% 57% 25% 18%</p>
4	P	256	<p>10% 55% 38% 6%</p>
5	R	45	<p>27% 51% 22%</p>
6	A	572	<p>21% 67% 32%</p>
7	Q	237	<p>30% 66% 34%</p>
8	S	22	<p>32% 64% 5%</p>
9	T	8	<p>12% 25% 75%</p>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 34208 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 Cas8a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	333	2662	1730	439	484	9	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	24	VAL	GLU	conflict	UNP Q8U338
C	64	SER	GLU	conflict	UNP Q8U338
C	110	LEU	VAL	conflict	UNP Q8U338
C	?	-	SER	deletion	UNP Q8U338
C	?	-	LEU	deletion	UNP Q8U338
C	?	-	GLY	deletion	UNP Q8U338

- Molecule 2 is a protein called Cas11a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	107	856	550	144	160	2	0	0
2	E	108	860	552	145	161	2	0	0
2	F	107	856	550	144	160	2	0	0
2	G	107	856	550	144	160	2	0	0
2	H	107	856	550	144	160	2	0	0

- Molecule 3 is a protein called Cas7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	335	2597	1655	450	487	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	336	Total	C	N	O	S	0	0
			2603	1659	451	488	5		
3	K	336	Total	C	N	O	S	0	0
			2596	1656	448	487	5		
3	L	336	Total	C	N	O	S	0	0
			2597	1656	448	488	5		
3	M	336	Total	C	N	O	S	0	0
			2597	1656	448	488	5		
3	N	321	Total	C	N	O	S	0	0
			2494	1595	431	463	5		
3	O	274	Total	C	N	O	S	0	0
			2134	1370	364	396	4		

- Molecule 4 is a protein called Cas5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	240	Total	C	N	O	S	0	0
			1936	1266	315	349	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	?	-	THR	deletion	UNP A0A5C0XNV9

- Molecule 5 is a RNA chain called crRNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	45	Total	C	N	O	P	0	0
			949	427	166	312	44		

- Molecule 6 is a protein called CRISPR-associated helicase Cas3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	572	Total	C	N	O	S	0	0
			4307	2752	745	802	8		

- Molecule 7 is a protein called CRISPR-associated endonuclease Cas3-HD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	237	Total	C	N	O	S	0	0
			1823	1167	314	329	13		

- Molecule 8 is a DNA chain called Target strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	S	22	464	217	92	133	22	0	0

- Molecule 9 is a DNA chain called Non-Target strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	T	8	163	77	31	47	8	0	0

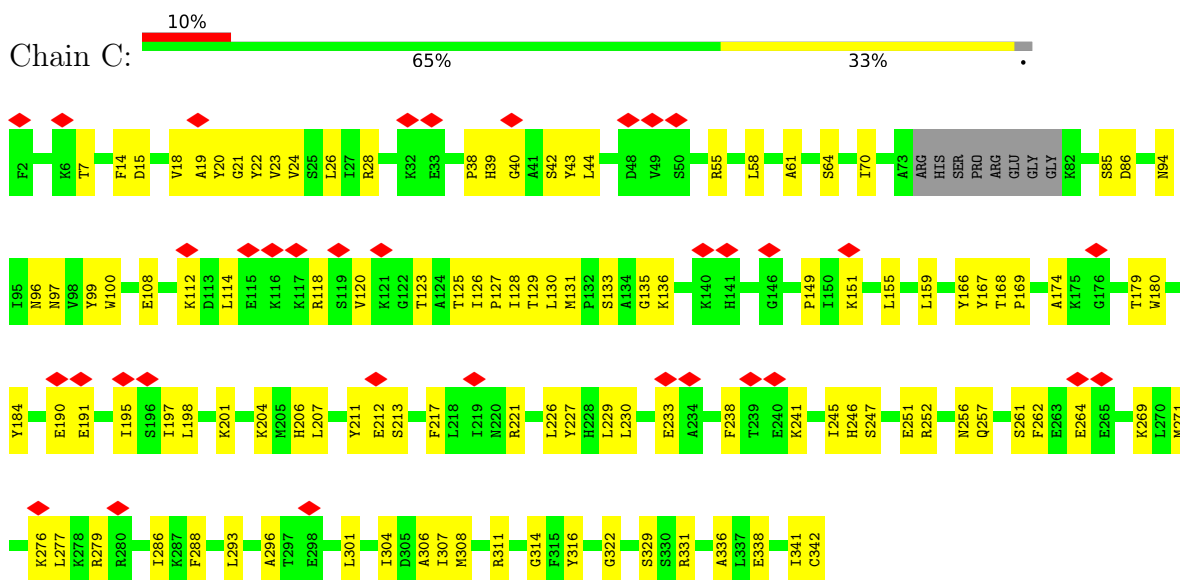
- Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	Q	2	Total	Ni	0
			2	2	

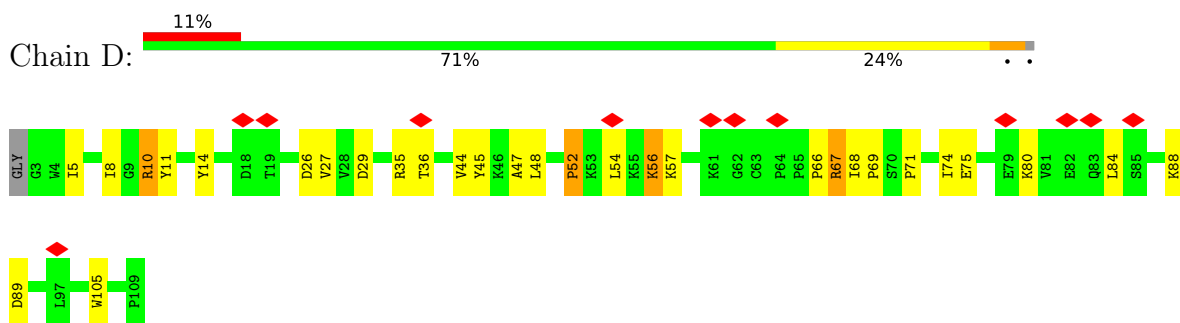
3 Residue-property plots

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.

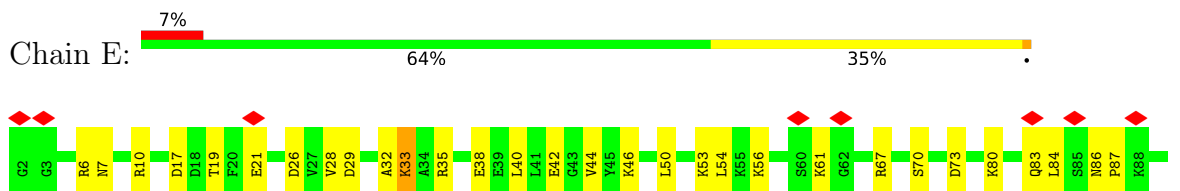
- Molecule 1: Cas8a

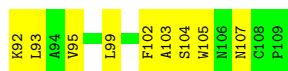


- Molecule 2: Cas11a

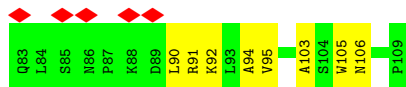


- Molecule 2: Cas11a

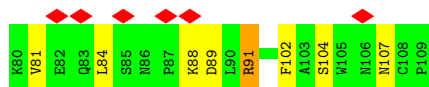
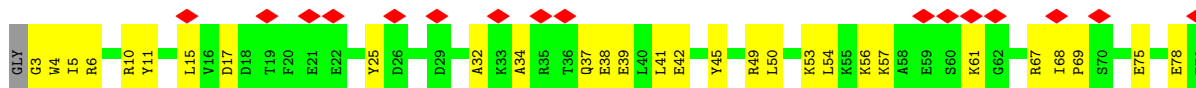




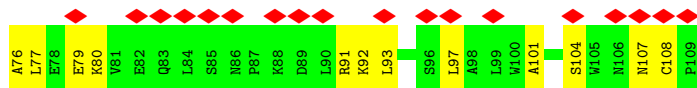
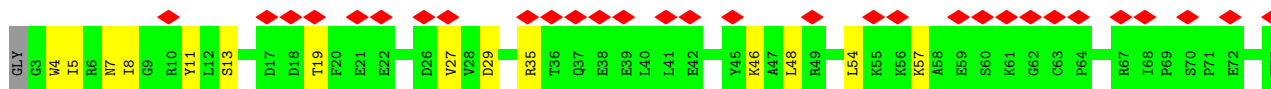
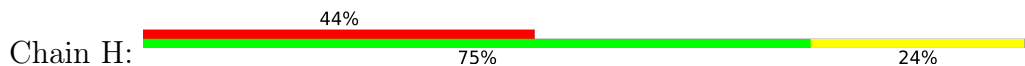
• Molecule 2: Cas11a



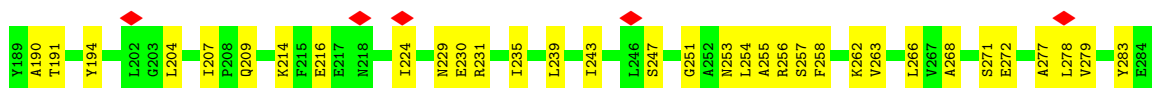
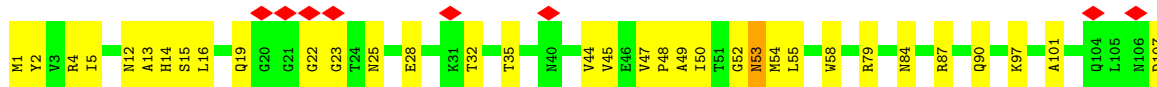
• Molecule 2: Cas11a

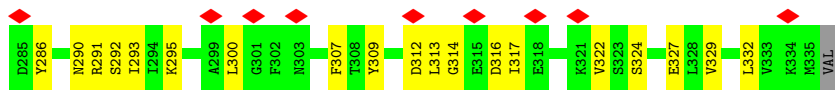


• Molecule 2: Cas11a

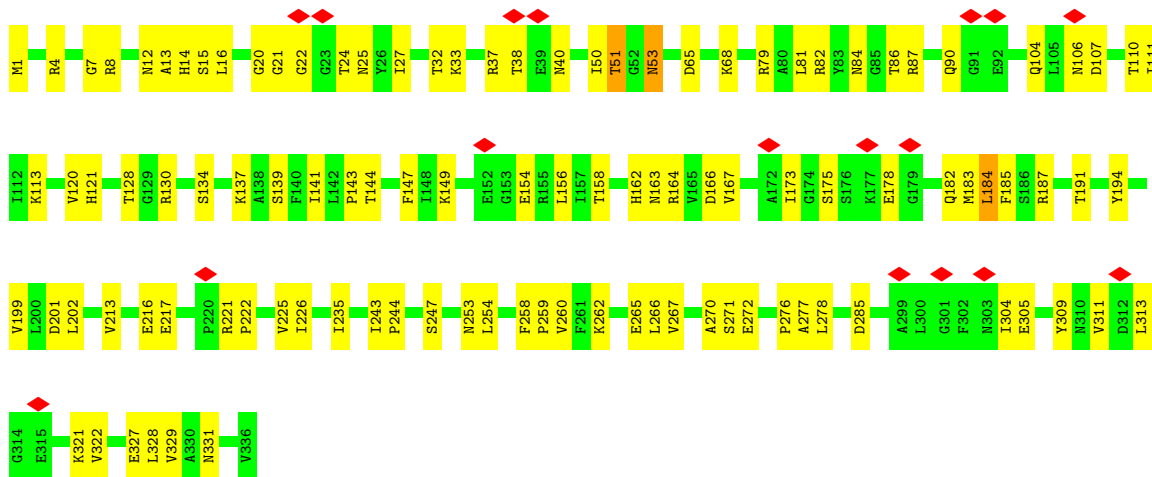


• Molecule 3: Cas7a

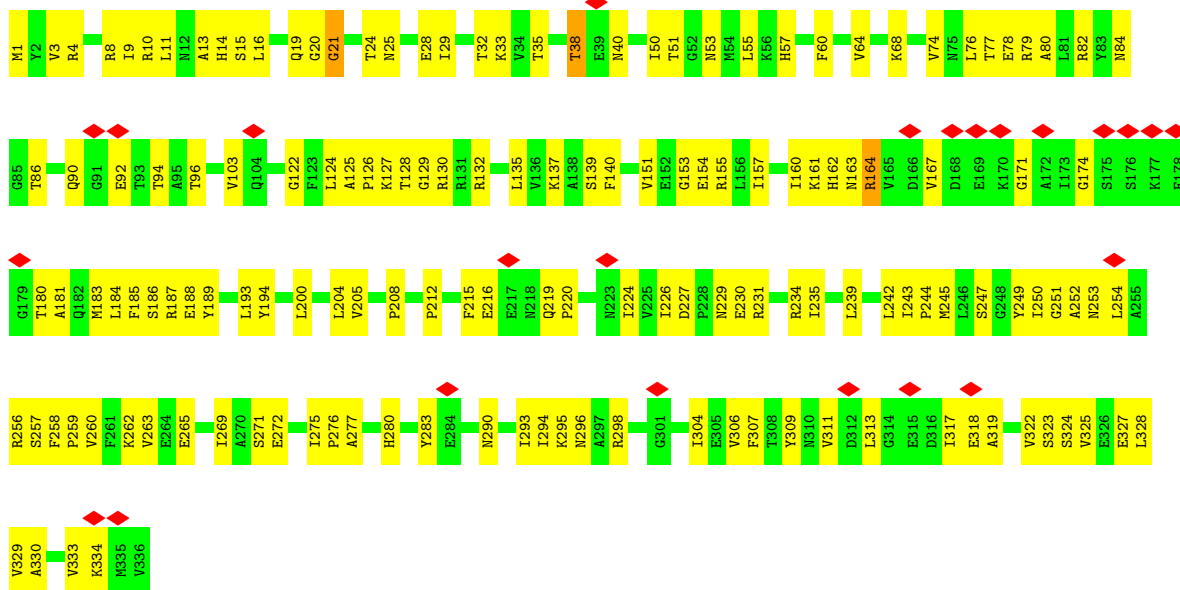




• Molecule 3: Cas7a



• Molecule 3: Cas7a

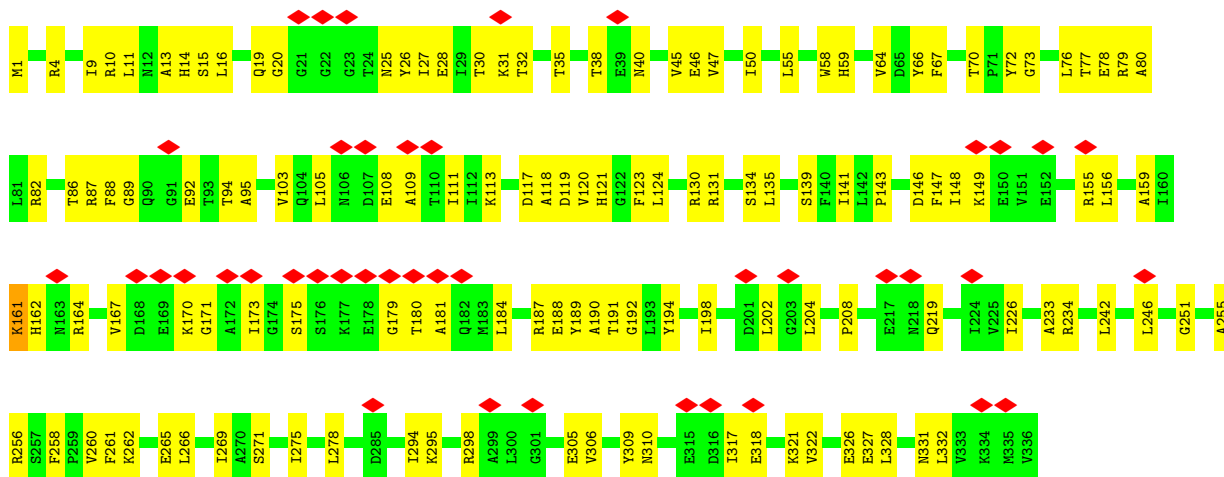


• Molecule 3: Cas7a

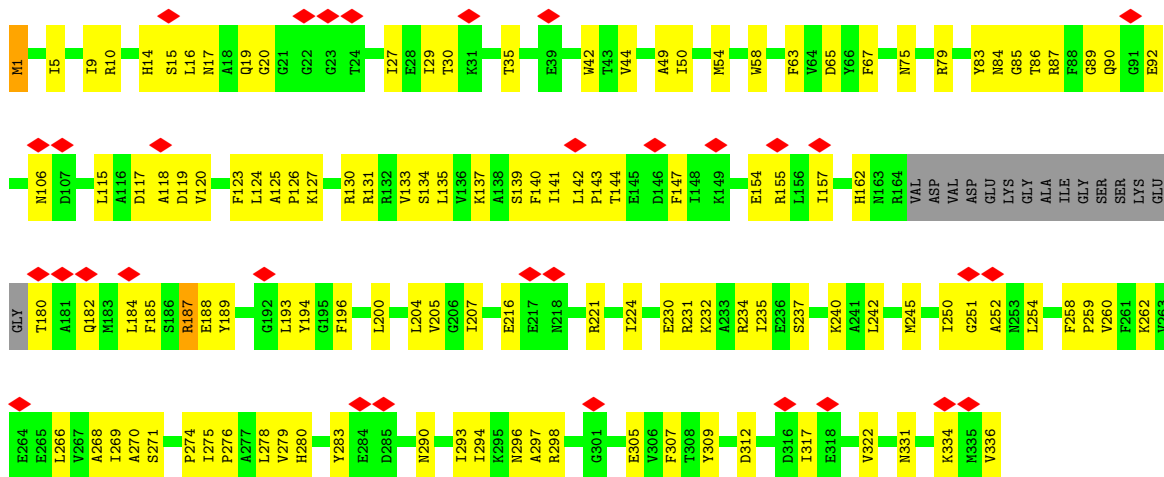




• Molecule 3: Cas7a

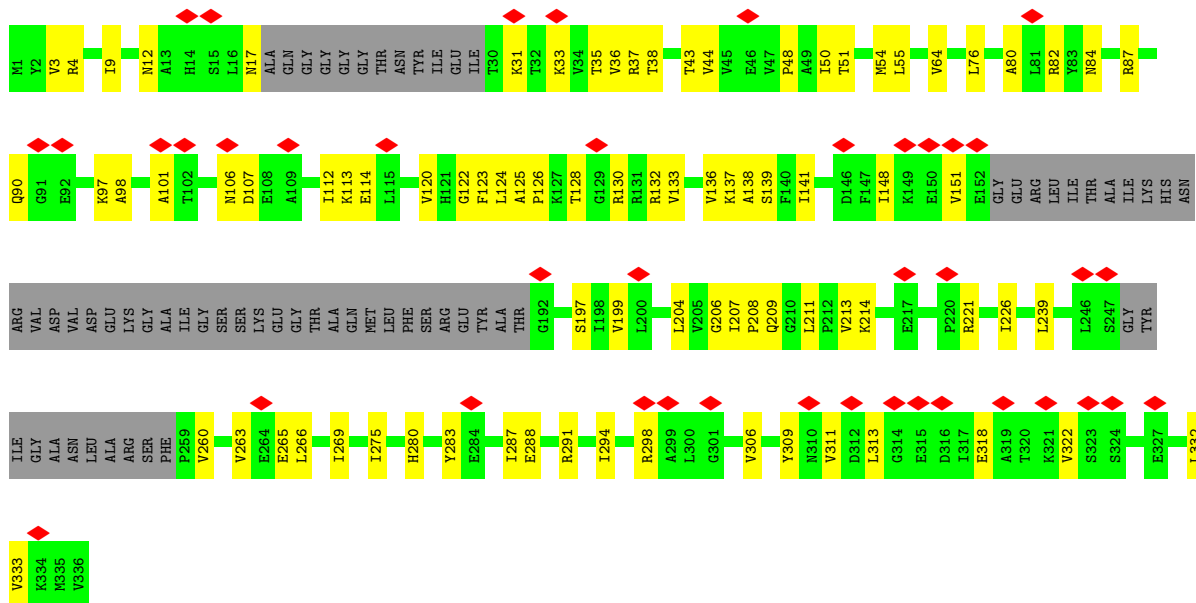


• Molecule 3: Cas7a

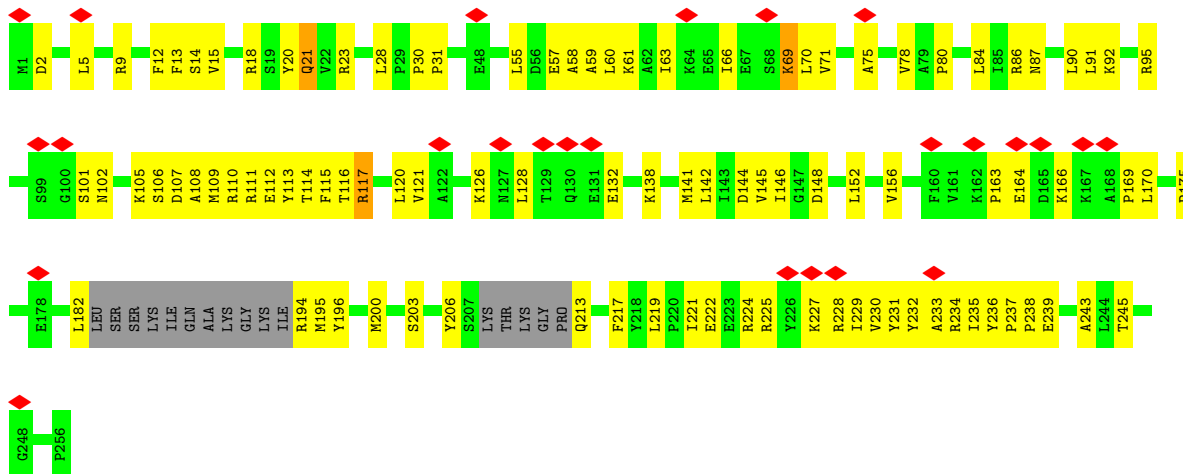


• Molecule 3: Cas7a





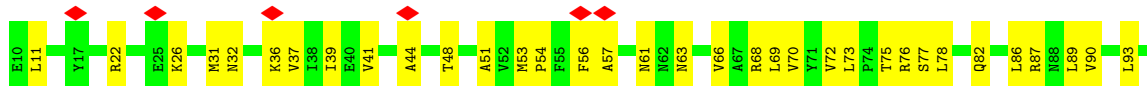
• Molecule 4: Cas5a

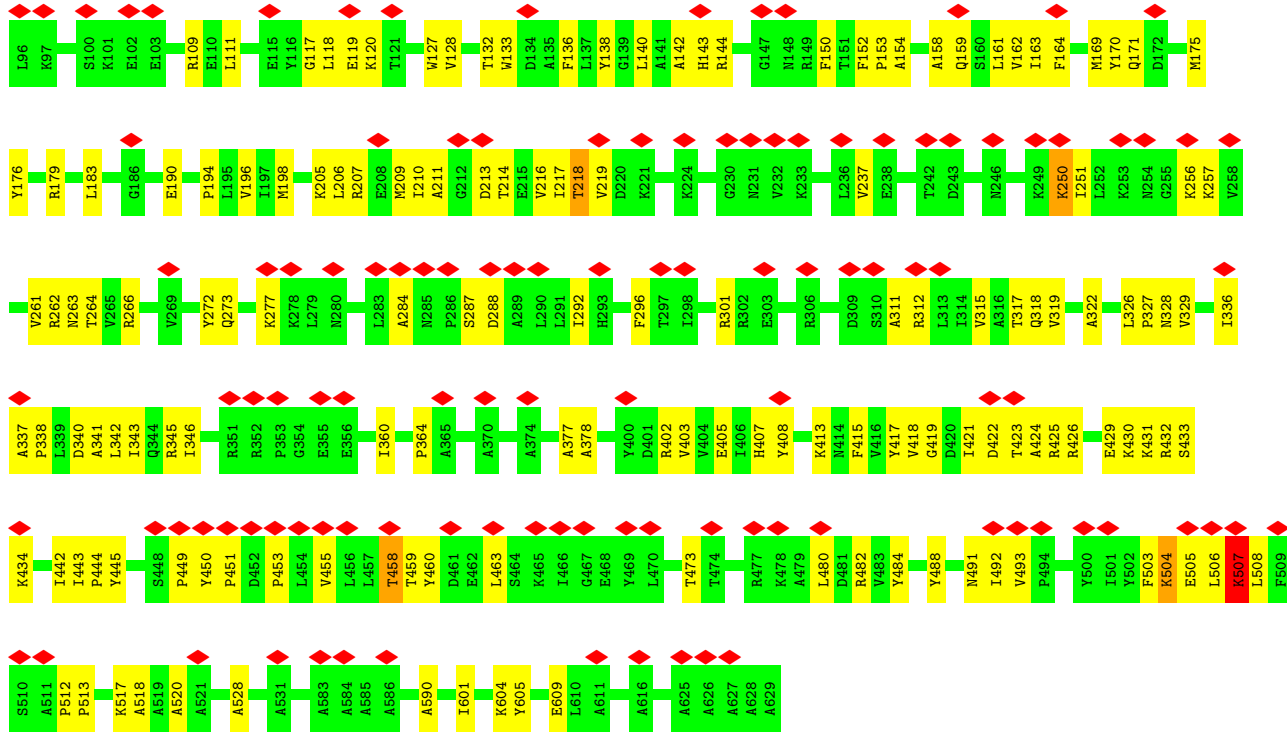


• Molecule 5: crRNA (45-MER)

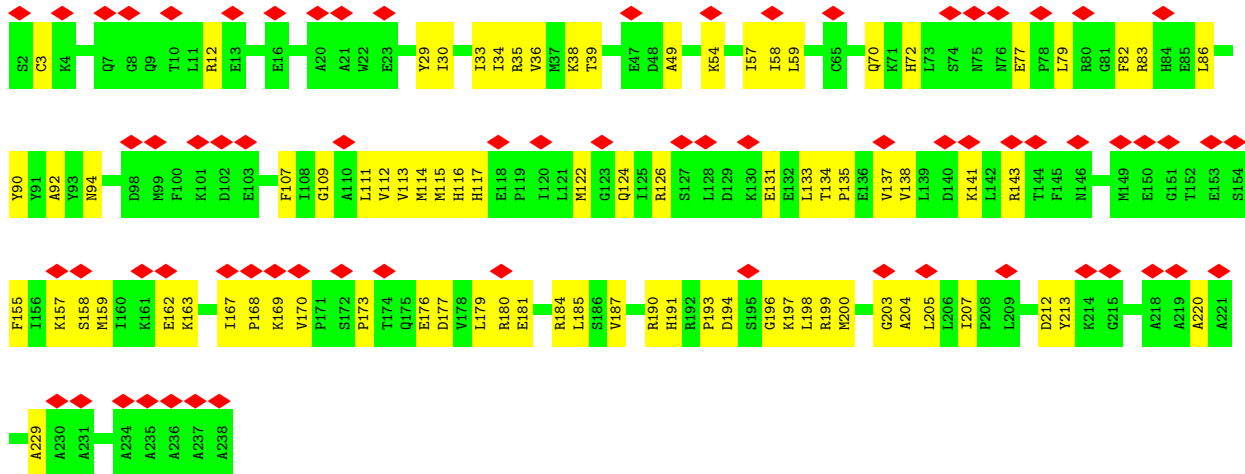


• Molecule 6: CRISPR-associated helicase Cas3





• Molecule 7: CRISPR-associated endonuclease Cas3-HD



• Molecule 8: Target strand DNA



• Molecule 9: Non-Target strand DNA



G17	A18	C19	C20	C21	A22	G23	T24
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13781	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.826	Depositor
Minimum map value	-0.281	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.155	Depositor
Map size (\AA)	372.0, 372.0, 372.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.24, 1.24, 1.24	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:
NI

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	C	0.25	0/2723	0.49	0/3684
2	D	0.26	0/876	0.53	0/1188
2	E	0.26	0/880	0.52	0/1193
2	F	0.25	0/876	0.54	0/1188
2	G	0.25	0/876	0.51	0/1188
2	H	0.25	0/876	0.52	0/1188
3	I	0.27	0/2645	0.54	0/3583
3	J	0.29	0/2651	0.56	1/3592 (0.0%)
3	K	0.27	0/2644	0.55	0/3584
3	L	0.27	0/2645	0.53	0/3585
3	M	0.24	0/2645	0.51	0/3585
3	N	0.25	0/2541	0.51	0/3445
3	O	0.25	0/2173	0.49	0/2946
4	P	0.25	0/1977	0.52	0/2673
5	R	0.37	0/1060	0.77	1/1649 (0.1%)
6	A	0.25	0/4379	0.53	0/5951
7	Q	0.26	0/1854	0.51	0/2502
8	S	0.60	1/522 (0.2%)	0.82	0/807
9	T	0.34	0/182	0.81	0/278
All	All	0.27	1/35025 (0.0%)	0.54	2/47809 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	46	DT	O3'-P	6.04	1.68	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	18	C	P-O3'-C3'	5.36	126.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	51	THR	CB-CA-C	-5.02	98.04	111.60

There are no chirality outliers.

There are no planarity outliers.

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	C	2662	0	2667	111	0
2	D	856	0	860	28	0
2	E	860	0	863	28	0
2	F	856	0	860	29	0
2	G	856	0	860	29	0
2	H	856	0	860	24	0
3	I	2597	0	2628	99	0
3	J	2603	0	2635	105	0
3	K	2596	0	2621	127	0
3	L	2597	0	2624	95	0
3	M	2597	0	2624	98	0
3	N	2494	0	2524	95	0
3	O	2134	0	2168	58	0
4	P	1936	0	2018	82	0
5	R	949	0	481	37	0
6	A	4307	0	4415	132	0
7	Q	1823	0	1891	66	0
8	S	464	0	247	53	0
9	T	163	0	90	7	0
10	Q	2	0	0	0	0
All	All	34208	0	33936	1075	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 1075 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)
1:C:136:LYS:NZ	8:S:61:DG:N7	1.63	1.42
1:C:128:ILE:HD11	8:S:61:DG:OP1	1.44	1.16
3:J:134:SER:HB2	5:R:12:G:OP1	1.55	1.06
1:C:97:ASN:ND2	9:T:21:DC:H1'	1.71	1.03
3:K:20:GLY:HA3	5:R:21:A:H8	1.22	1.01

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	C	329/341 (96%)	306 (93%)	23 (7%)	0	100	100
2	D	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	E	106/108 (98%)	100 (94%)	5 (5%)	1 (1%)	17	54
2	F	105/108 (97%)	90 (86%)	15 (14%)	0	100	100
2	G	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
3	I	333/336 (99%)	310 (93%)	22 (7%)	1 (0%)	41	75
3	J	334/336 (99%)	303 (91%)	31 (9%)	0	100	100
3	K	334/336 (99%)	305 (91%)	27 (8%)	2 (1%)	25	63
3	L	334/336 (99%)	302 (90%)	32 (10%)	0	100	100
3	M	334/336 (99%)	307 (92%)	27 (8%)	0	100	100
3	N	317/336 (94%)	300 (95%)	17 (5%)	0	100	100
3	O	266/336 (79%)	251 (94%)	15 (6%)	0	100	100
4	P	234/256 (91%)	214 (92%)	18 (8%)	2 (1%)	17	54
6	A	568/572 (99%)	476 (84%)	82 (14%)	10 (2%)	8	42
7	Q	235/237 (99%)	213 (91%)	22 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4144/4298 (96%)	3766 (91%)	362 (9%)	16 (0%)	38 71

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	102	ASN
6	A	455	VAL
2	E	19	THR
6	A	507	LYS
3	K	21	GLY

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	C	282/292 (97%)	282 (100%)	0	100 100
2	D	91/91 (100%)	87 (96%)	4 (4%)	28 56
2	E	91/91 (100%)	88 (97%)	3 (3%)	38 63
2	F	91/91 (100%)	90 (99%)	1 (1%)	73 84
2	G	91/91 (100%)	89 (98%)	2 (2%)	52 71
2	H	91/91 (100%)	91 (100%)	0	100 100
3	I	275/277 (99%)	273 (99%)	2 (1%)	84 90
3	J	276/277 (100%)	273 (99%)	3 (1%)	73 84
3	K	274/277 (99%)	270 (98%)	4 (2%)	65 80
3	L	275/277 (99%)	275 (100%)	0	100 100
3	M	275/277 (99%)	274 (100%)	1 (0%)	91 94
3	N	264/277 (95%)	262 (99%)	2 (1%)	81 89
3	O	230/277 (83%)	230 (100%)	0	100 100
4	P	211/224 (94%)	209 (99%)	2 (1%)	78 87
6	A	422/427 (99%)	417 (99%)	5 (1%)	71 83
7	Q	191/191 (100%)	190 (100%)	1 (0%)	88 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3430/3528 (97%)	3400 (99%)	30 (1%)	79 87

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	184	LEU
6	A	432	ARG
3	K	256	ARG
7	Q	180	ARG
6	A	205	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	104	GLN
3	J	106	ASN
3	M	59	HIS
3	L	17	ASN
3	M	17	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	R	45/45 (100%)	17 (37%)	7 (15%)

5 of 17 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	R	2	U
5	R	9	A
5	R	11	U
5	R	14	U
5	R	15	U

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	R	15	U
5	R	18	C
5	R	21	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	19	C
5	R	14	U

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	531:ALA	C	580:ALA	N	37.08

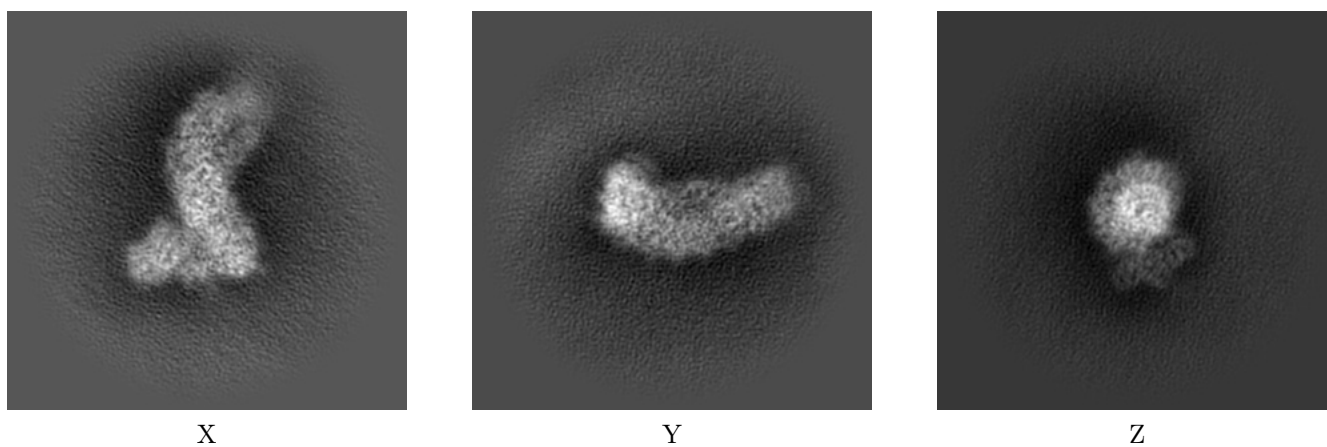
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26083. 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](#)

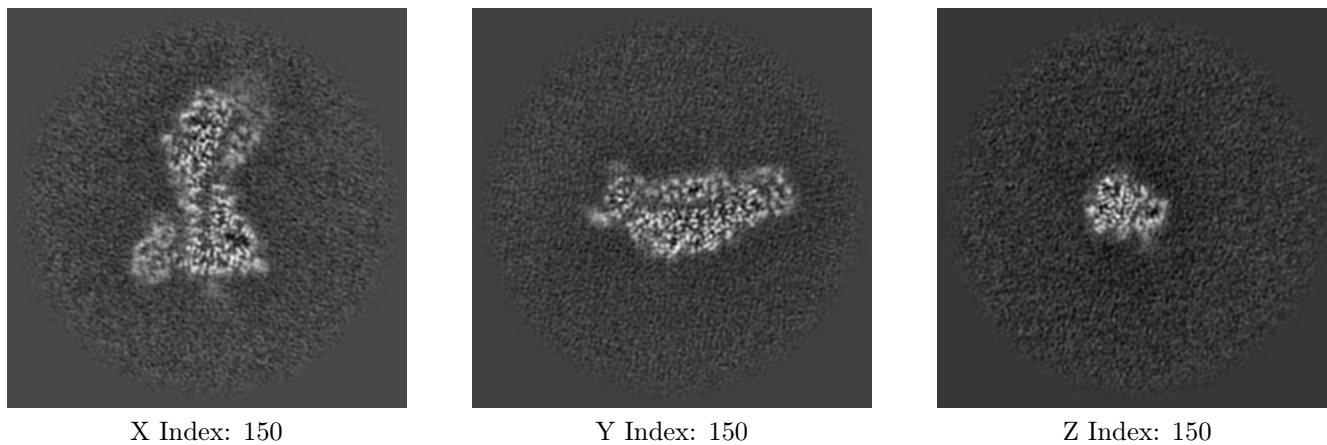
6.1.1 Primary map



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

6.2 Central slices [i](#)

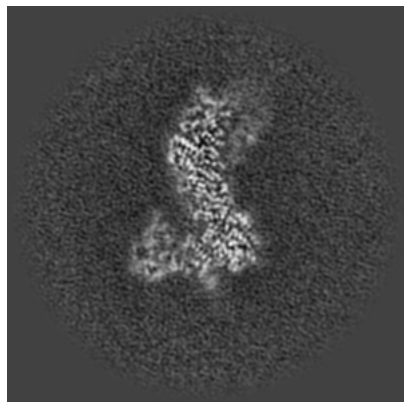
6.2.1 Primary map



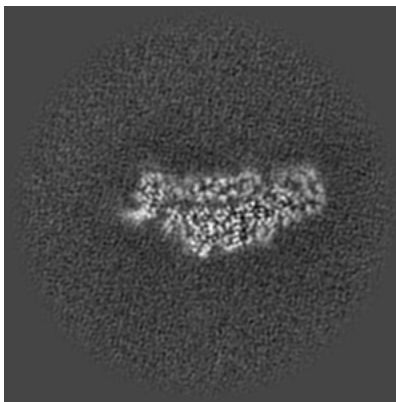
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

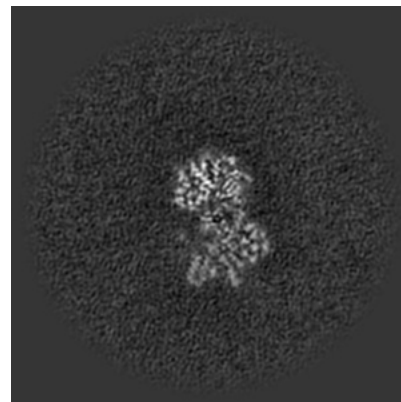
6.3.1 Primary map



X Index: 146



Y Index: 148



Z Index: 121

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.155. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

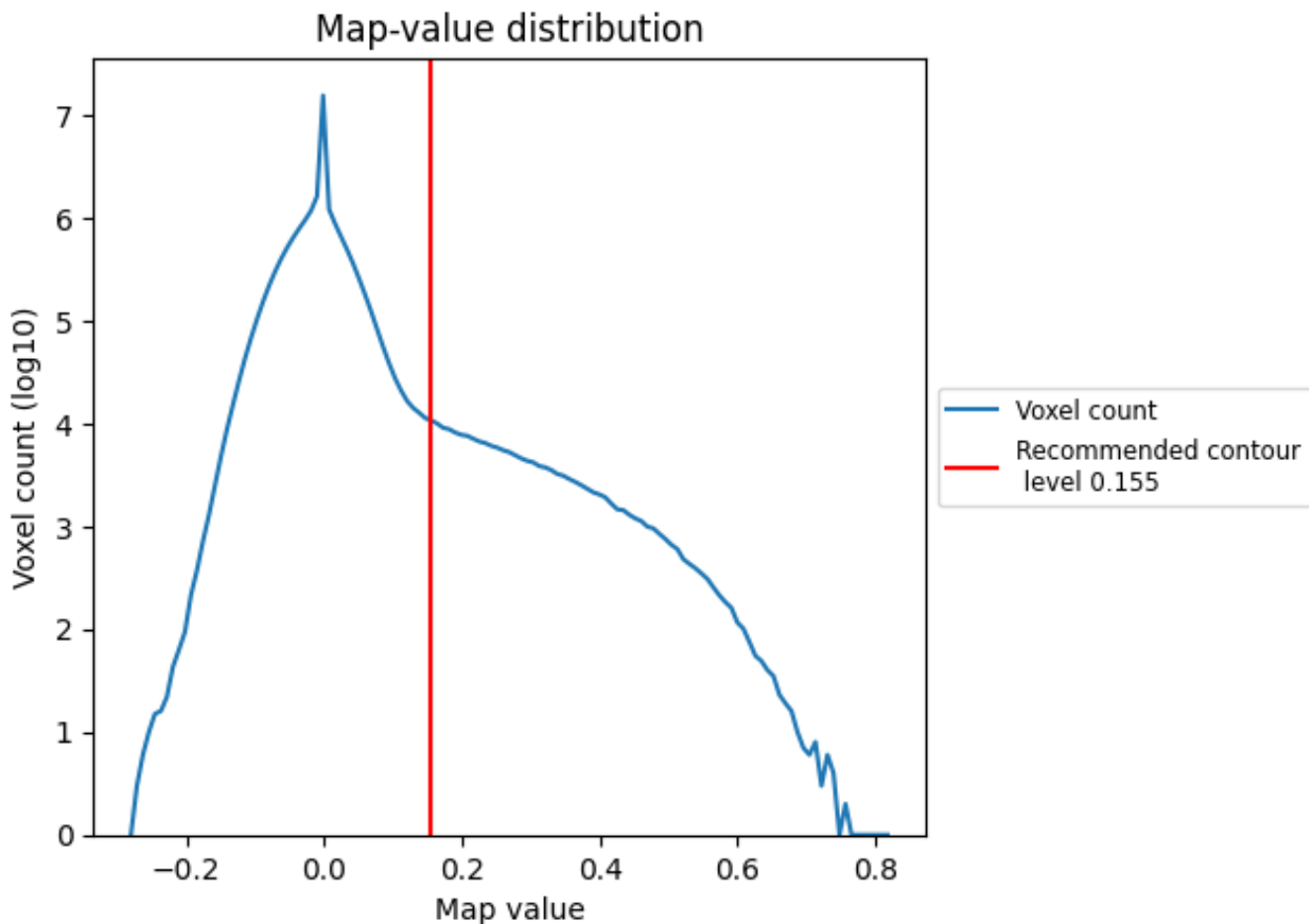
6.5 Mask visualisation

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

7 Map analysis [i](#)

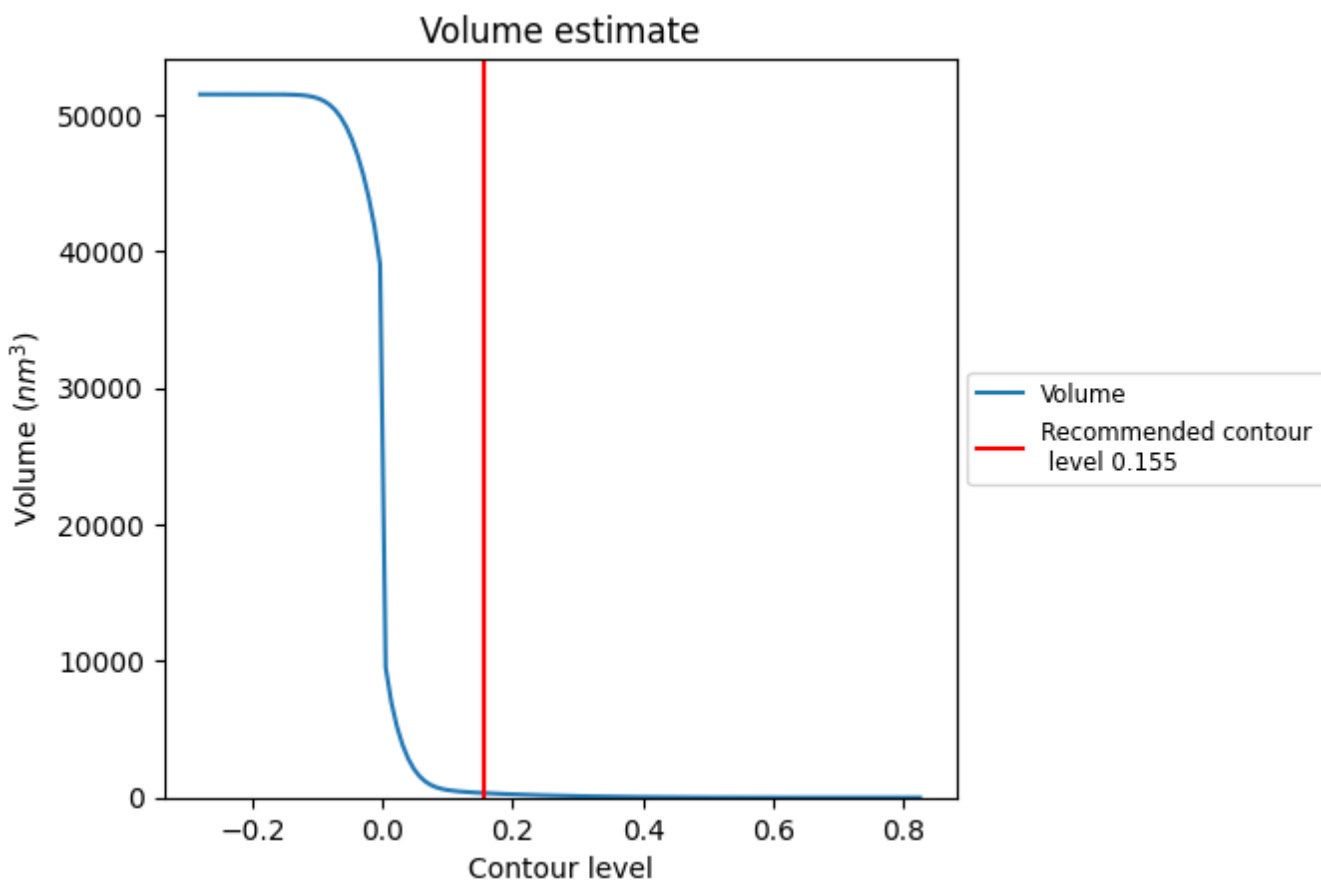
This section contains the results of statistical analysis of the map.

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.

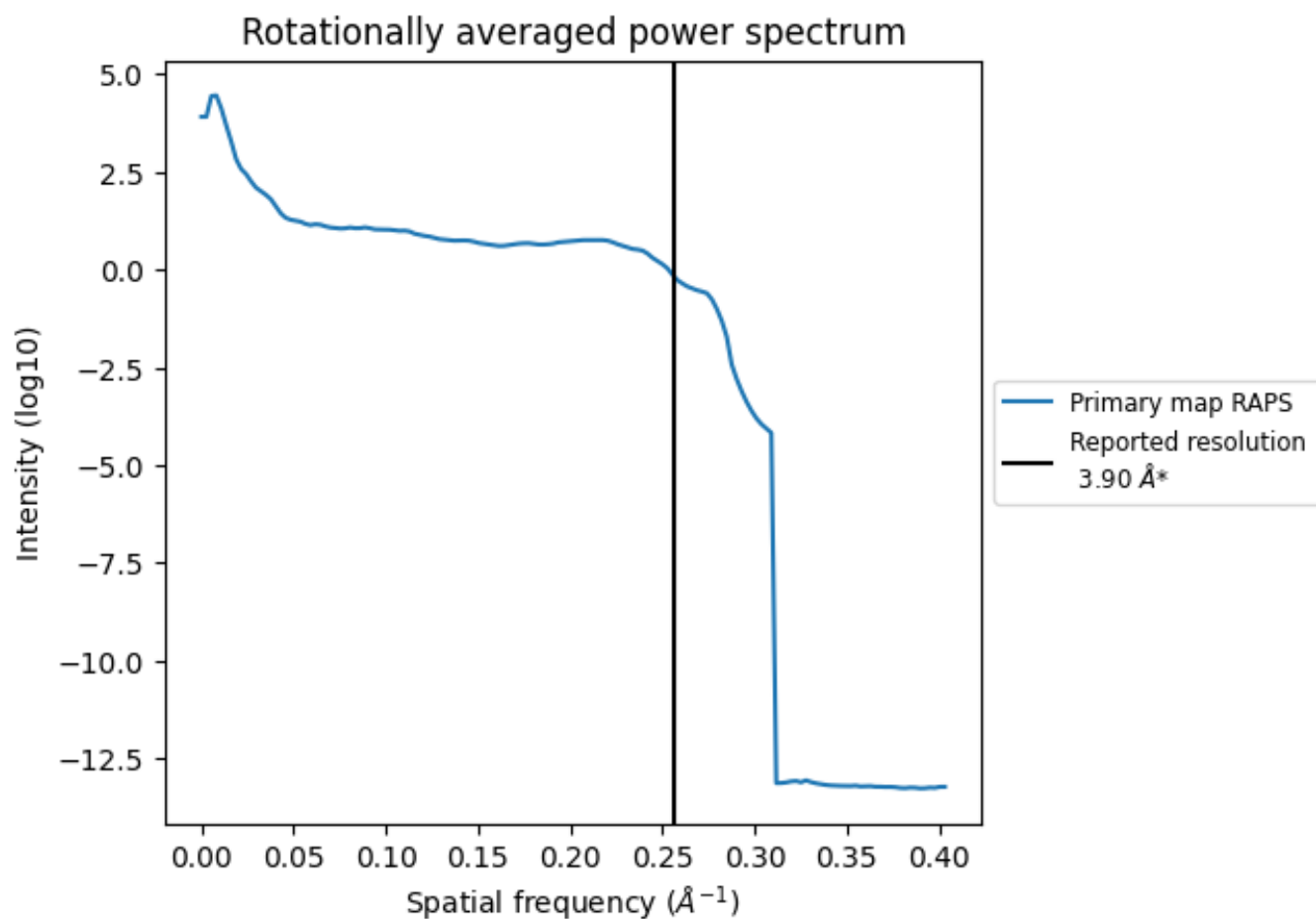
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 330 nm³; this corresponds to an approximate mass of 298 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

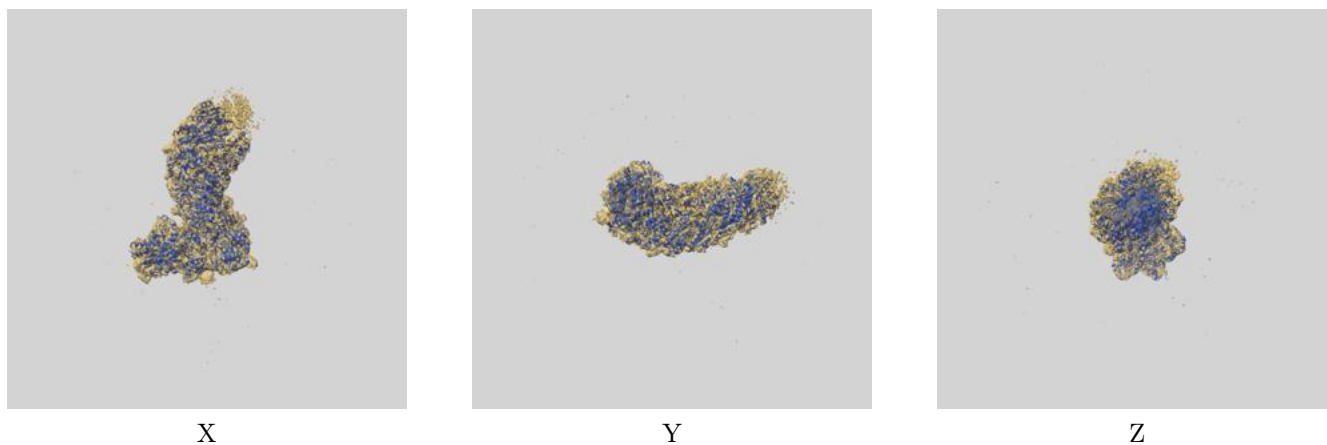
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

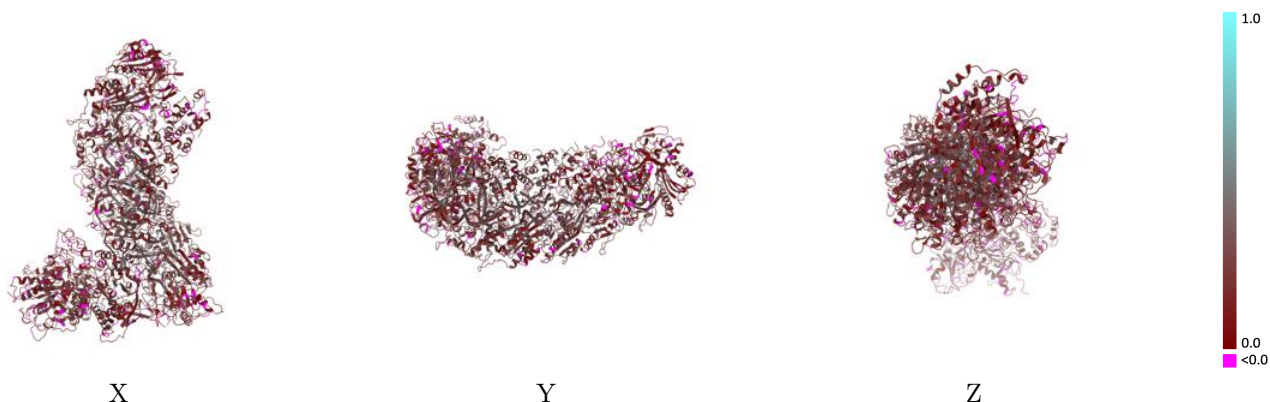
This section contains information regarding the fit between EMDB map EMD-26083 and PDB model 7TR9. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



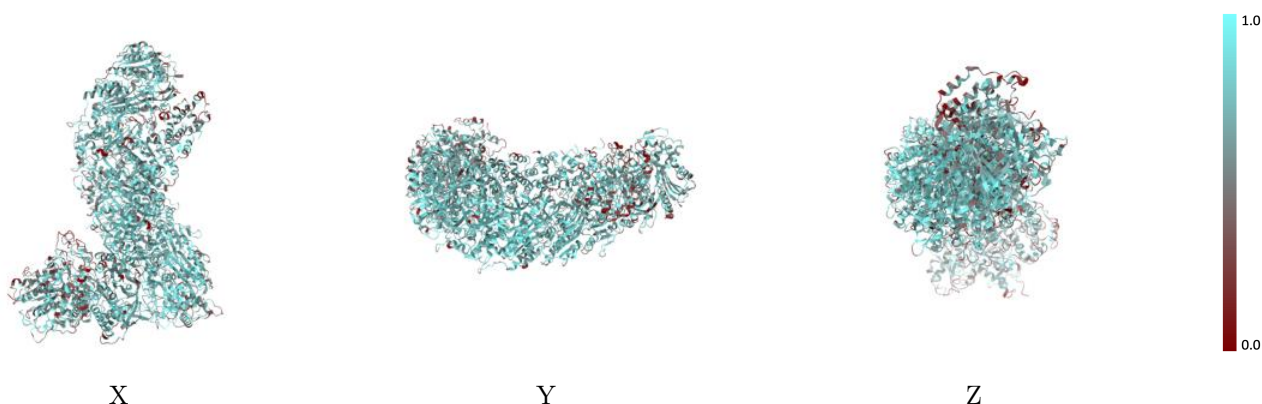
The images above show the 3D surface view of the map at the recommended contour level 0.155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



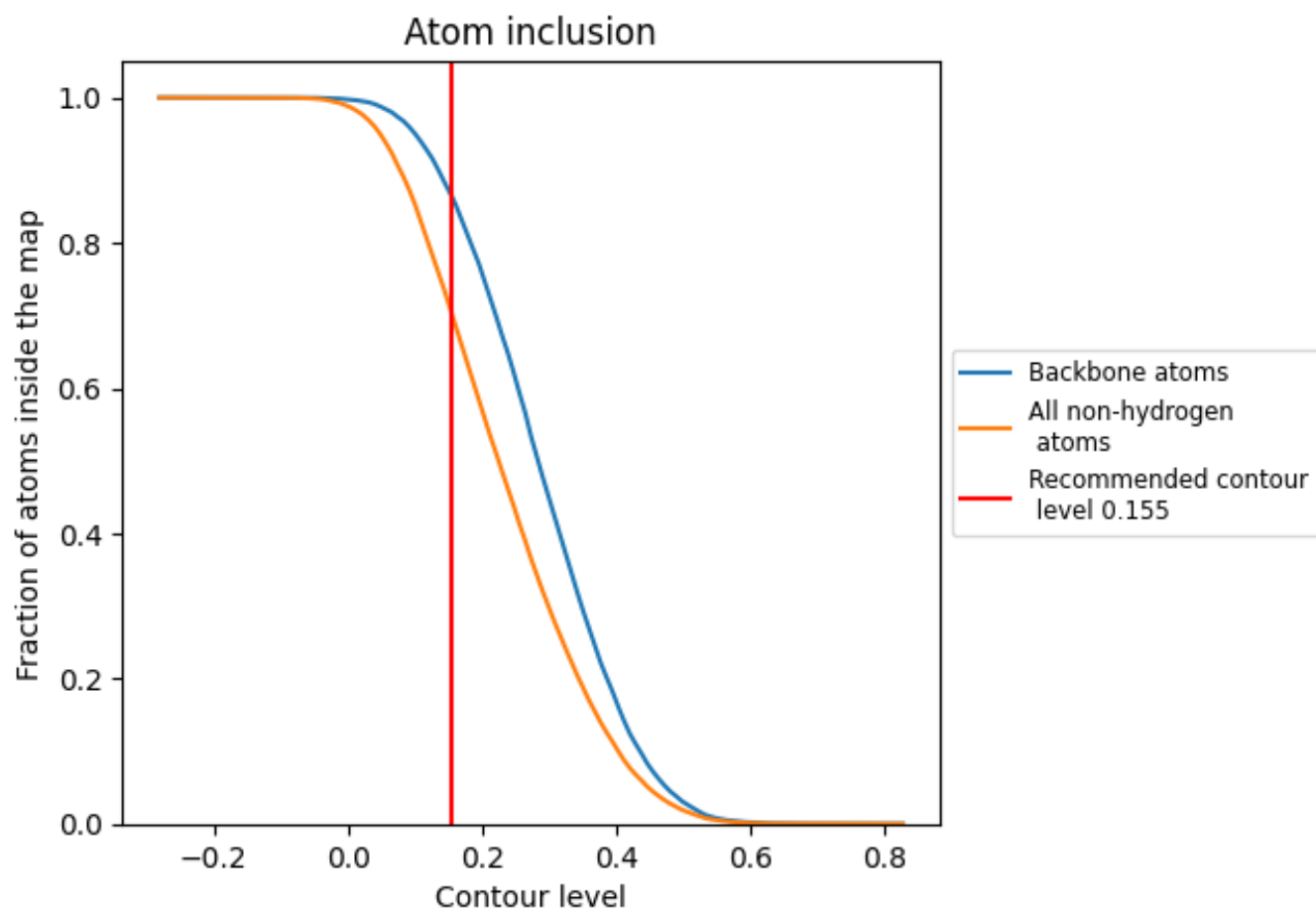
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.155).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 70% 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 (0.155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7011	 0.2250
A	 0.6115	 0.1930
C	 0.7076	 0.2490
D	 0.7392	 0.2220
E	 0.7583	 0.2600
F	 0.6878	 0.2090
G	 0.6124	 0.1840
H	 0.4486	 0.1520
I	 0.7478	 0.2400
J	 0.7951	 0.2730
K	 0.7821	 0.2490
L	 0.7476	 0.2460
M	 0.7045	 0.2320
N	 0.6986	 0.2320
O	 0.6546	 0.1940
P	 0.7079	 0.1950
Q	 0.5791	 0.1890
R	 0.8714	 0.2850
S	 0.7500	 0.2030
T	 0.7669	 0.2260

