wwPDB EM Validation Summary Report (i)

Mar 4, 2024 – 05:51 PM EST

PDB ID	:	6D6Q
EMDB ID	:	EMD-7808
Title	:	Human nuclear exosome-MTR4 RNA complex - overall reconstruction
Authors	:	Weick, E.-M.; Lima, C.D.
Deposited on	:	2018-04-22
Resolution	:	3.45 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 (i) 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 (1)) were used in the production of this report:

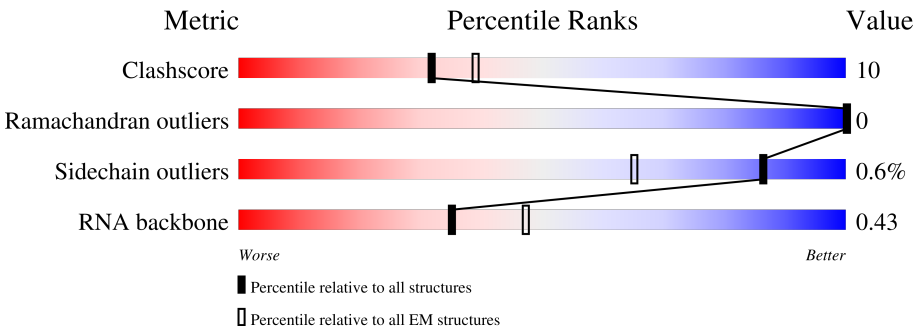
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.45 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 <=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	473	• 43% 18% 39%
2	B	249	6% 75% 21% • •
3	C	278	7% 76% 19% 5%
4	D	237	• 65% 23% 12%
5	E	293	7% 82% 15% • •
6	F	272	8% 76% 15% • 7%
7	G	277	13% 66% 19% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	296	8% 78% 20%
9	I	197	30% 75% 18% 7%
10	J	761	99%
11	K	960	38% 66% 22% 11%
12	L	162	18% 37% 5% 58%
13	M	1045	19% 52% 16% 32%
14	N	16	81% 81% 19%
15	O	62	37% 37% 23% 18% 23%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 31639 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 Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	287	2264	1423	404	419	18	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP Q06265
A	-15	GLY	-	expression tag	UNP Q06265
A	-14	SER	-	expression tag	UNP Q06265
A	-13	SER	-	expression tag	UNP Q06265
A	-12	HIS	-	expression tag	UNP Q06265
A	-11	HIS	-	expression tag	UNP Q06265
A	-10	HIS	-	expression tag	UNP Q06265
A	-9	HIS	-	expression tag	UNP Q06265
A	-8	HIS	-	expression tag	UNP Q06265
A	-7	HIS	-	expression tag	UNP Q06265
A	-6	SER	-	expression tag	UNP Q06265
A	-5	GLN	-	expression tag	UNP Q06265
A	-4	ASP	-	expression tag	UNP Q06265
A	-3	PRO	-	expression tag	UNP Q06265
A	-2	ASN	-	expression tag	UNP Q06265
A	-1	SER	-	expression tag	UNP Q06265
A	0	HIS	-	expression tag	UNP Q06265

- Molecule 2 is a protein called Exosome complex component RRP41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	241	1824	1126	345	344	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	expression tag	UNP Q9NPD3
B	-3	ALA	-	expression tag	UNP Q9NPD3
B	-2	ASP	-	expression tag	UNP Q9NPD3
B	-1	PRO	-	expression tag	UNP Q9NPD3

- Molecule 3 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	265	2020	1272	337	397	14	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ASP	-	expression tag	UNP Q96B26
C	0	PRO	-	expression tag	UNP Q96B26

- Molecule 4 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	208	1566	979	278	297	12	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	expression tag	UNP Q9NQT4
D	0	LEU	-	expression tag	UNP Q9NQT4

- Molecule 5 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	286	2194	1373	374	432	15	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASP	-	expression tag	UNP Q15024
E	0	PRO	-	expression tag	UNP Q15024

- Molecule 6 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	252	1859	1154	353	345	7	0	0

- Molecule 7 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	237	1806	1136	329	329	12	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	ASP	-	expression tag	UNP Q9NQT5
G	0	PRO	-	expression tag	UNP Q9NQT5
G	225	HIS	TYR	variant	UNP Q9NQT5

- Molecule 8 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	289	2263	1424	405	419	15	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	ASP	-	expression tag	UNP Q13868
H	-1	PRO	-	expression tag	UNP Q13868
H	0	HIS	-	expression tag	UNP Q13868

- Molecule 9 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	183	1407	884	247	266	10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	ASP	-	expression tag	UNP Q9Y3B2
I	0	PRO	-	expression tag	UNP Q9Y3B2

- Molecule 10 is a protein called Exosome component 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	11	86	56	14	16	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	SER	-	expression tag	UNP Q01780
J	313	ASN	ASP	engineered mutation	UNP Q01780
J	649	SER	-	linker	UNP Q01780
J	650	ARG	-	linker	UNP Q01780
J	651	GLY	-	linker	UNP Q01780
J	652	SER	-	linker	UNP Q01780
J	653	GLY	-	linker	UNP Q01780
J	654	SER	-	linker	UNP Q01780
J	655	GLY	-	linker	UNP Q01780
J	656	SER	-	linker	UNP Q01780
J	657	GLY	-	linker	UNP Q01780
J	658	SER	-	linker	UNP Q01780
J	659	GLY	-	linker	UNP Q01780
J	660	SER	-	linker	UNP Q01780

- Molecule 11 is a protein called Exosome complex exonuclease RRP44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	853	6856	4329	1233	1260	34	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLY	-	expression tag	UNP Q9Y2L1
K	0	SER	-	expression tag	UNP Q9Y2L1
K	146	ASN	ASP	engineered mutation	UNP Q9Y2L1
K	269	SER	ASN	variant	UNP Q9Y2L1
K	487	ASN	ASP	engineered mutation	UNP Q9Y2L1
K	843	ASN	LYS	variant	UNP Q9Y2L1

- Molecule 12 is a protein called M-phase phosphoprotein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	68	573	371	95	101	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	ASP	-	expression tag	UNP Q99547
L	0	PRO	-	expression tag	UNP Q99547

- Molecule 13 is a protein called Exosome RNA helicase MTR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	709	5648	3589	963	1052	44	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP P42285
M	-1	GLY	-	expression tag	UNP P42285
M	0	ASP	-	expression tag	UNP P42285

- Molecule 14 is a RNA chain called RNA (5'-R(*AP*GP*CP*AP*CP*CP*GP*UP*AP*AP *AP*GP*AP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	13	278	126	56	84	12	0	0

- Molecule 15 is DNA/RNA hybrid called DNA/RNA (62-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	O	48	966	443	172	304	47	0	0

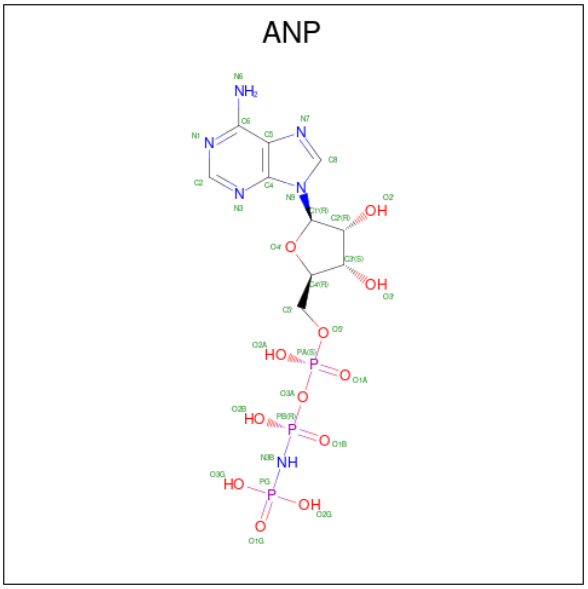
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
16	K	1	1	1	0

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
17	K	1	1	1	0

- Molecule 18 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



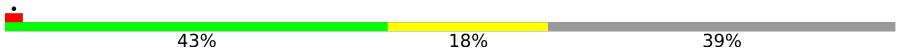
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	M	1	27	10	6	9	2	0

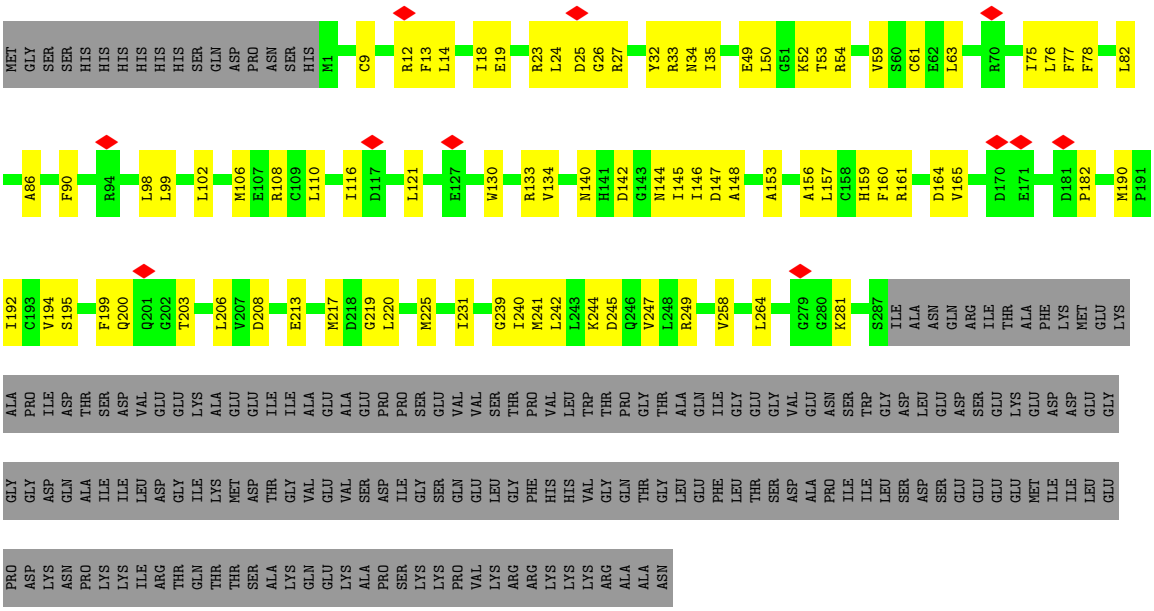
3 Residue-property plots (i)

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: Exosome complex component RRP45

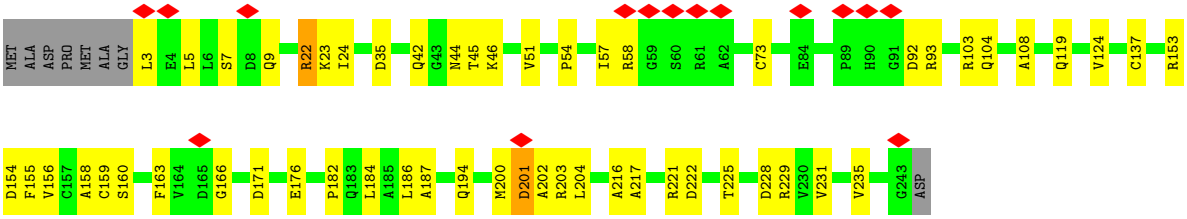
Chain A:





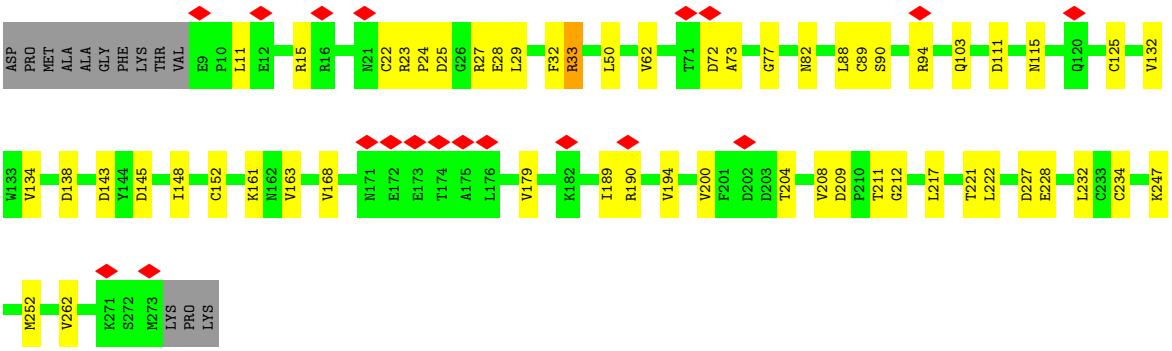
• Molecule 2: Exosome complex component RRP41

Chain B:



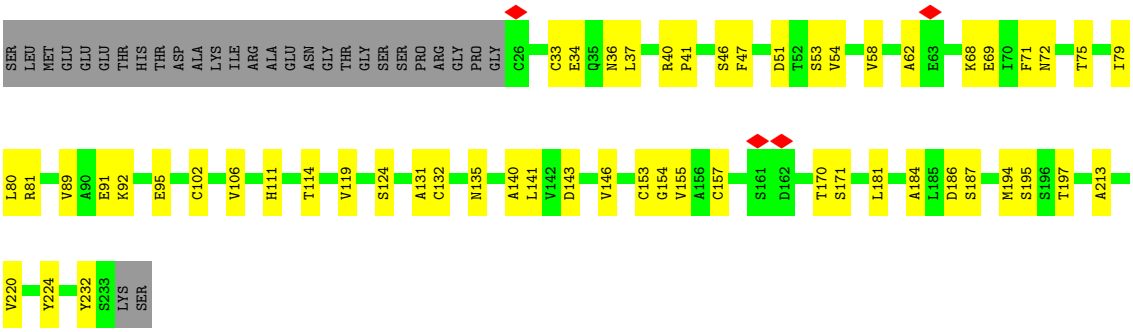
• Molecule 3: Exosome complex component RRP43

Chain C:



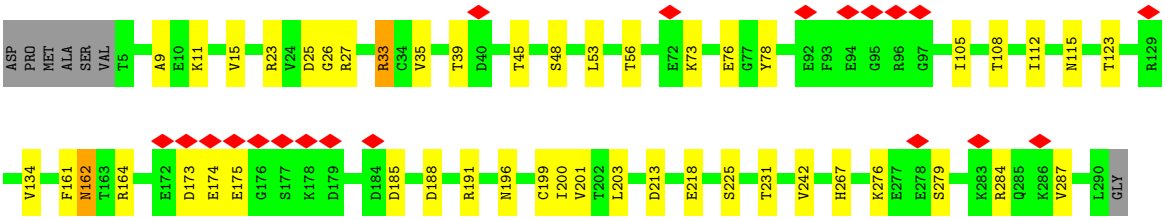
• Molecule 4: Exosome complex component RRP46

Chain D:



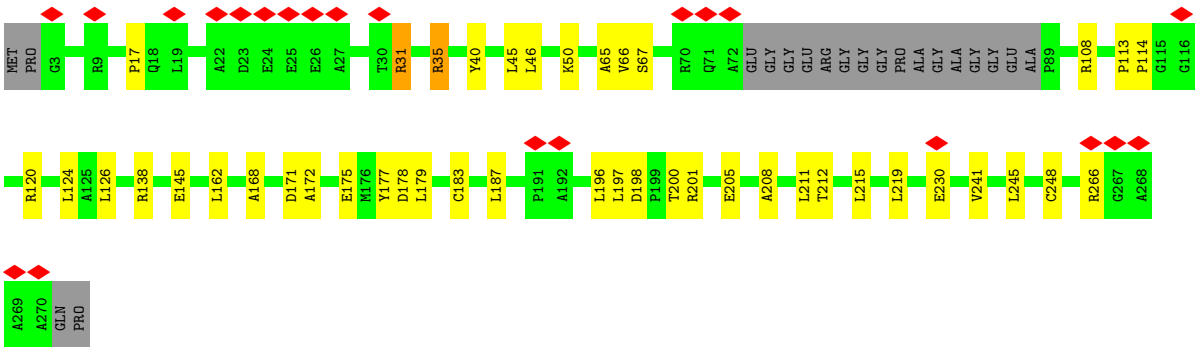
• Molecule 5: Exosome complex component RRP42

Chain E:



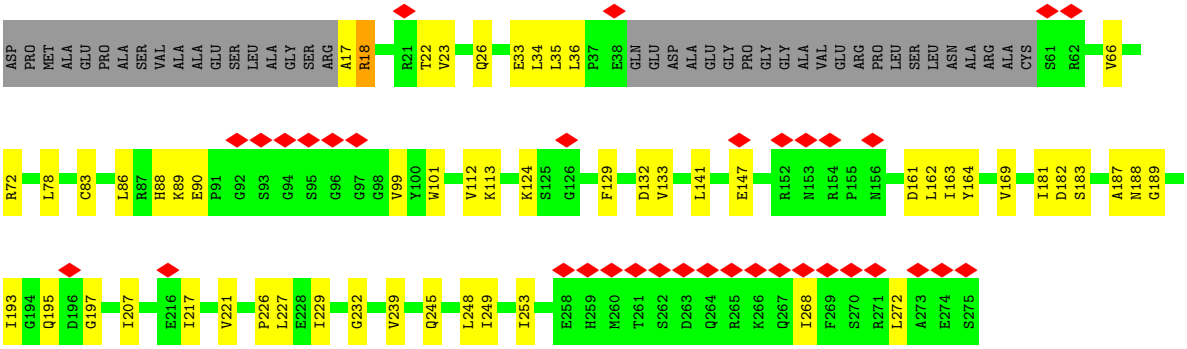
• Molecule 6: Exosome complex component MTR3

Chain F:



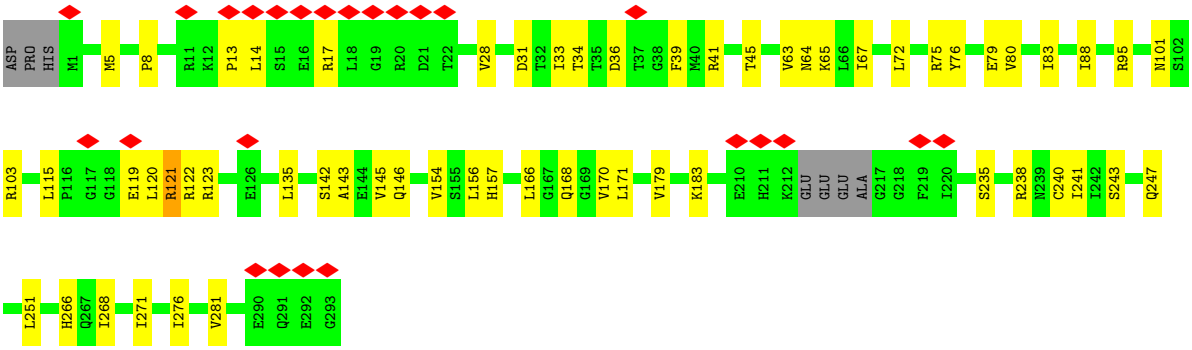
- Molecule 7: Exosome complex component RRP40

Chain G:



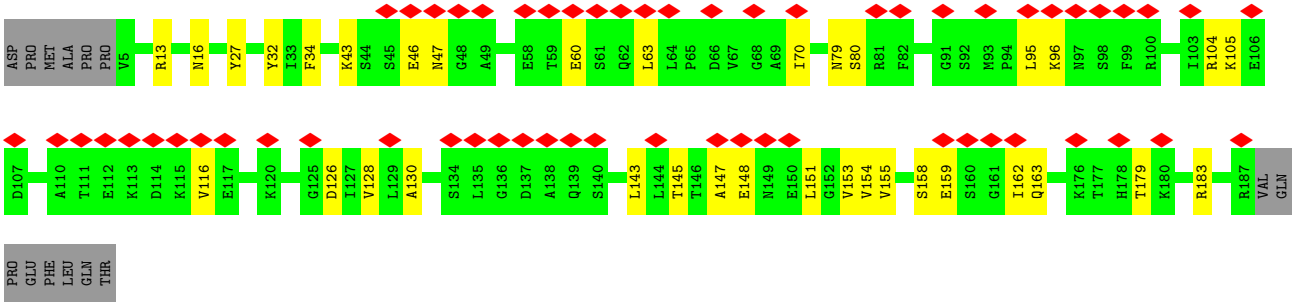
- Molecule 8: Exosome complex component RRP4

Chain H:



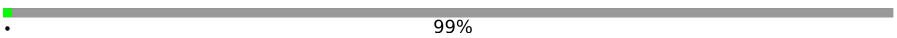
- Molecule 9: Exosome complex component CSL4

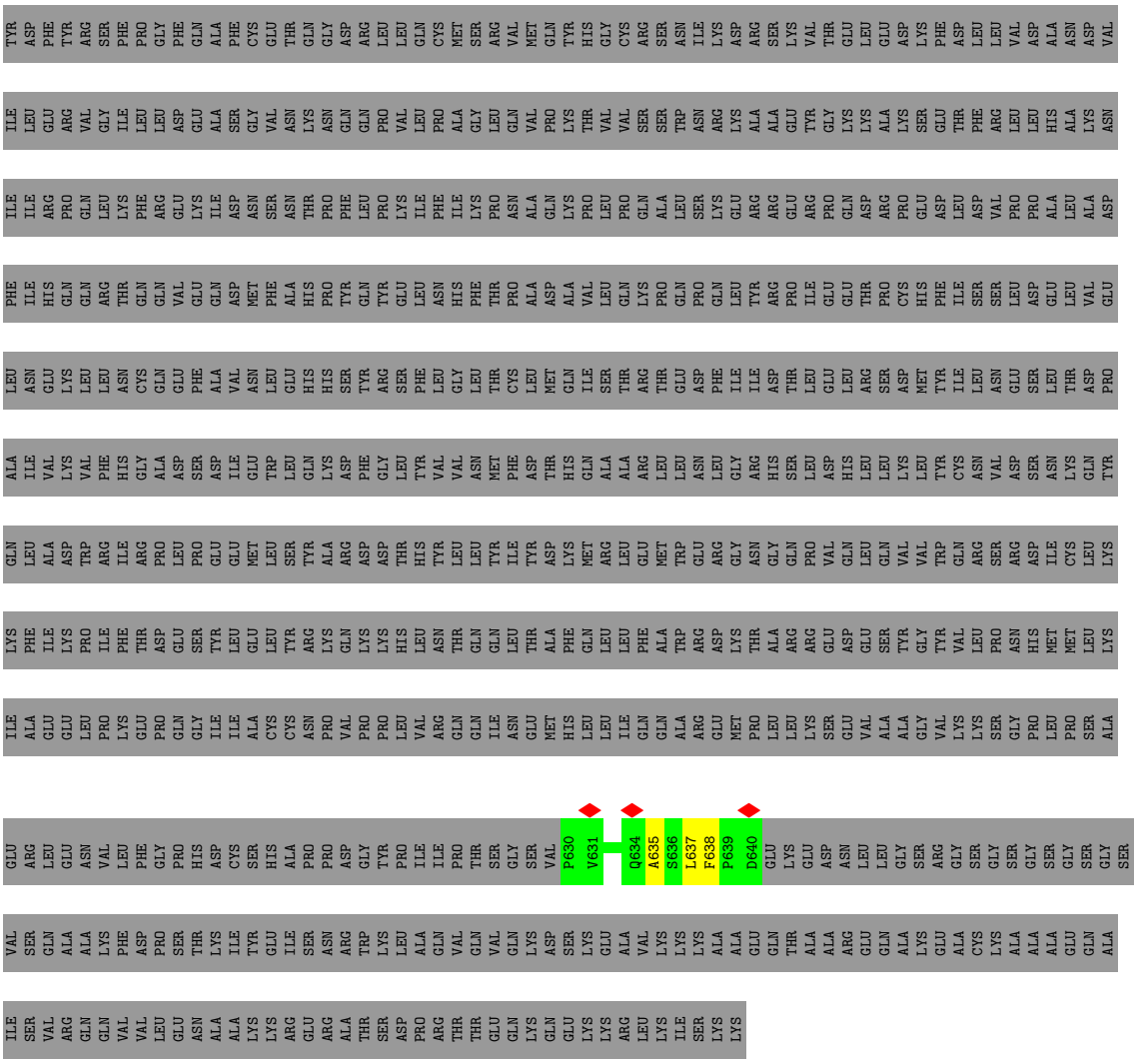
Chain I:



- Molecule 10: Exosome component 10

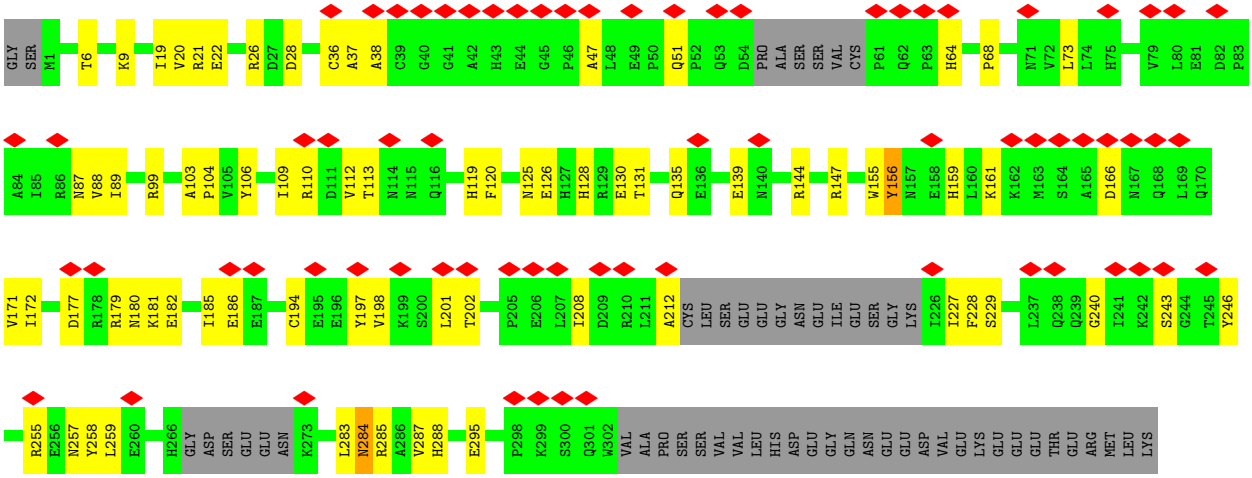
Chain J:





• Molecule 11: Exosome complex exonuclease RRP44

Chain K:



THR ALA VAL SER GLU LYS MET LEU K340 R344 V345 V346 C357 L360 S363 D364 I365 K366 E367 S368 R369 R370 H371 L372 R379 I380 P381 R382 I383 R384 I385 E386 T387 R388 R397 I398 I399 W405 P406 R407 R410 Y411 V417 R418 N419 L420 E425 T428 E429

T430 E431 V432 L433 Q442 L449 L452 P453 K454 M455 P456 W457 S458 I459 T460 E461 K462 D463 M464 K465 N466 R467 E468 D469 L470 R471 H472 L473 C474 I475 C476 S477 V478 D479 P480 P481 G482 C483 T484 D485 I486 N487 D488 A489 L490 H491 C492 R493 E494 L495 E496 N497 G498 N499 L500 E501

H505 I506 A507 D508 V509 S510 H511 F512 I513 G516 N517 A518 L519 D520 Q521 E522 R525 R526 T529 V530 Y531 L532 C533 R536 I537 D538 E542 L543 L544 S545 S546 N547 K552 C553 D554 V555 D556 S561 C562 I563 W564 E565 M566 N567 H568 N569 A570 E571 I572 L573 K574 T575 K576

S584 K585 A586 S587 L588 T589 E592 A593 Q594 L595 R596 I597 D598 S599 A600 N601 M602 N603 D604 D605 I606 T607 T608 S609 L610 R611 G612 L613 N614 K615 L616 A617 K618 I619 L620 K621 K622 R623 R624 I625 E626 K627 G628 A629 L630 T631 L632 S633 S634 P635 E636 V637 R638 F639 H640 MET ASP SER

GLU THR HIS ASP P648 I649 D650 L651 Q652 T653 K654 E655 L656 R657 E658 T659 N660 S661 M662 V663 E664 E665 F666 M667 L668 A675 I678 H679 E680 E681 E684 H685 A686 L687 L688 R689 A693 P694 P695 P696 S697 N698 Y699 E700 I701 L702 V703 K704 A705 A706 R707 S708 R709 N710 L711 E712

I713 K714 T715 D716 T717 A718 K719 S720 L721 A722 E723 S724 L725 D726 Q727 A728 E729 S730 P731 T732 F733 P734 Y735 L736 N737 T738 L739 L740 R741 I742 R746 C747 M748 M749 Q750 Y753 F754 C755 S756 G757 M758 D759 N760 D761 F762 H763 H764 L767 A768 S769 P770 I771 Y772 T773 H774 R780

D784 H788 R789 L790 L791 A792 V793 A794 I795 G796 A797 D798 C799 T800 Y801 P802 E803 L804 T805 D806 K807 H808 K809 L810 A811 D812 R829 Q837 S842 N843 G844 I845 V846 S847 E848 E849 A850 Y851 I852 L853 F854 V855 R856 K857 M858 A859 I860 V861 V862 L863 I864 P865 K866 Y867 G868

L869 E870 G871 T872 V873 F874 F875 E876 GLU LYS ASP LYS PRO ASN PRO Q884 L885 I886 Y887 D888 D889 E890 I891 P892 S893 L894 K895 I896 E897 D898 T899 V900 F901 H902 V903 F904 D905 K906 V907 K908 V909 K910 I911 M912 L913 D914 S915 S916 Q919 H920 Q921 K922 I923 R924 M925 S926 L927 V928 E929

PRO GLN ILE PRO GLY ILE SER ILE PRO THR ASP THR SER ASN MET ASP LEU ASN GLY PRO LYS LYS LYS LYS MET LYS LEU GLY LYS

- Molecule 12: M-phase phosphoprotein 6

Chain L: 18% 37% 5% 58%

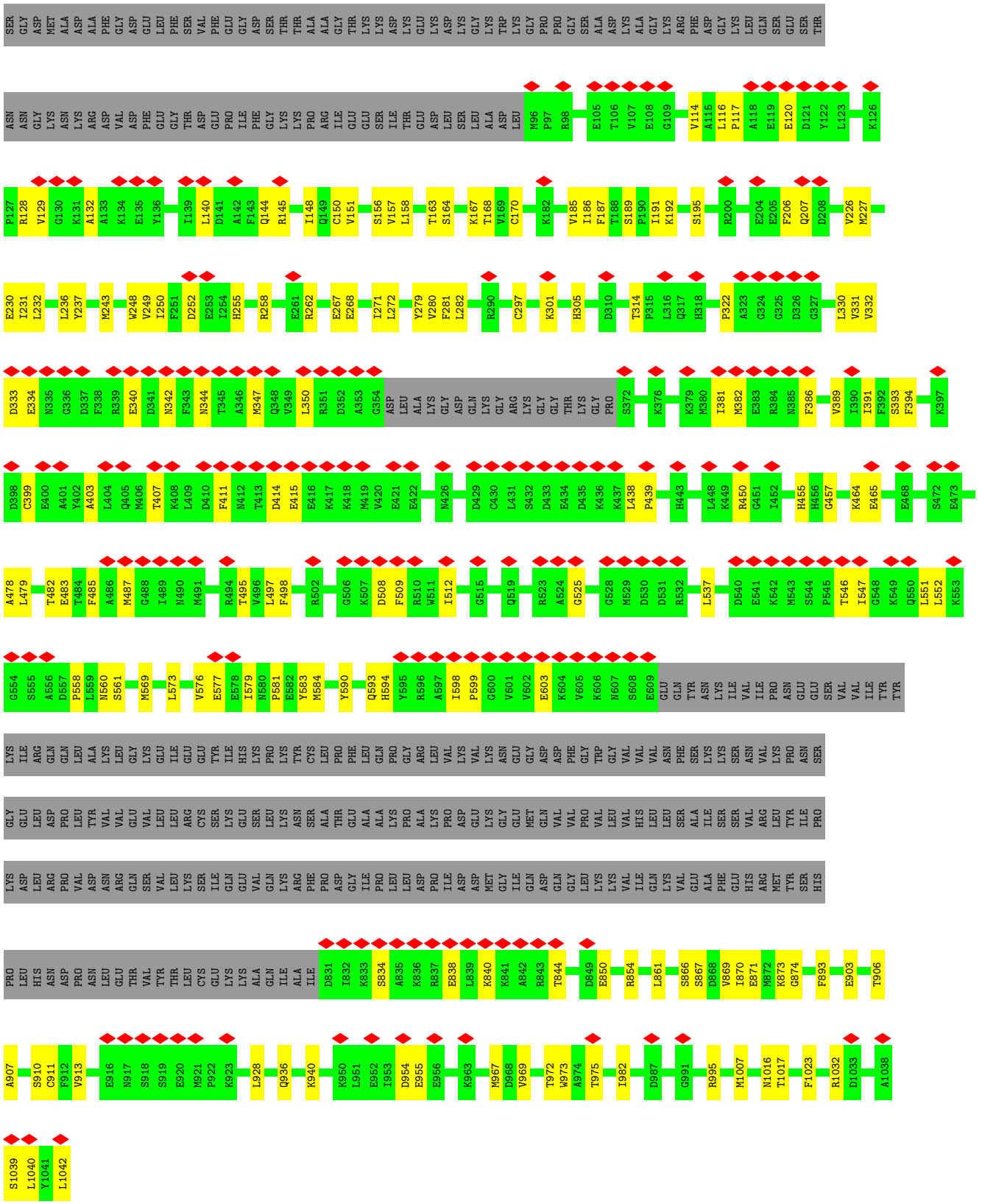
ASP PRO MET ALA ALA GLU R5 K6 T7 R8 L9 S10 K11 N12 L13 L14 R15 M16 K17 F18 M19 Q20 R21 GLY LEU ASP SER GLU THR LYS LYS GLN LEU GLU GLU GLU GLU LYS LYS ILE ILE SER GLU GLU H43 D47 L48 P49 E50 L51 K52 E53 K54 E55 S56 E60 D69

Y72 G73 R74 R78 E83 K86 A93 LYS HIS LYS ALA GLU GLU VAL GLU ASP GLU THR VAL GLU LEU ASP VAL SER ASP GLU GLU MET ALA ARG ARG TYR GLU THR LEU VAL GLY THR ILE GLY LYS LYS PHE ALA ARG LYS ARG ASP HIS ALA ASN TYR GLU GLU ASP

GLU ASN GLY ASP ILE THR PRO ILE LYS ALA LYS LYS MET PHE LEU LYS PRO GLN ASP

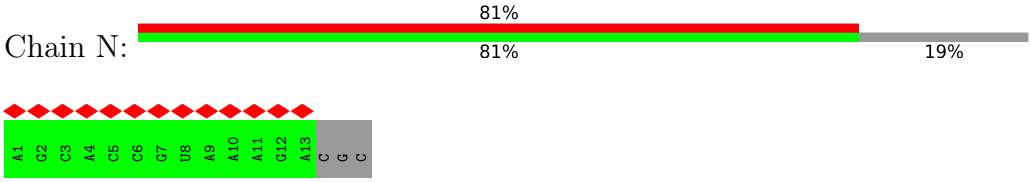
- Molecule 13: Exosome RNA helicase MTR4

Chain M: 19% 52% 16% 32%



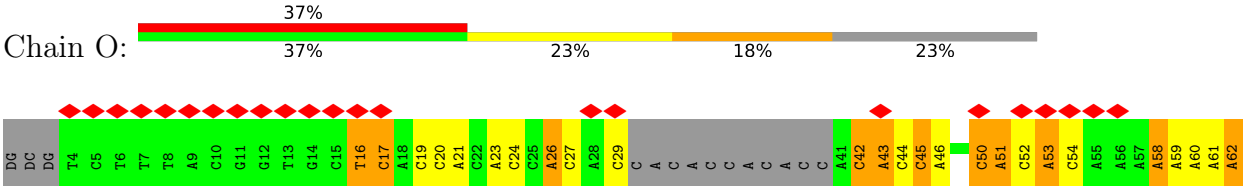
• Molecule 14: RNA (5'-R(*AP*GP*CP*AP*CP*CP*GP*UP*AP*AP*AP*GP*AP*CP*GP*C)-3')

Chain N:



• Molecule 15: DNA/RNA (62-MER)

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122703	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	85.23	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: ZN, MG, ANP

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	0.39	0/2297	0.52	0/3094
2	B	0.41	0/1849	0.54	0/2500
3	C	0.38	0/2053	0.51	0/2786
4	D	0.39	0/1586	0.53	0/2145
5	E	0.40	0/2225	0.51	0/3007
6	F	0.37	0/1889	0.54	0/2562
7	G	0.34	0/1832	0.49	0/2467
8	H	0.40	0/2296	0.51	0/3092
9	I	0.30	0/1431	0.50	0/1932
10	J	0.26	0/88	0.47	0/118
11	K	0.30	0/6991	0.49	1/9444 (0.0%)
12	L	0.28	0/583	0.49	0/776
13	M	0.31	0/5751	0.47	0/7752
14	N	0.22	0/312	0.76	0/485
15	O	0.60	3/1077 (0.3%)	0.98	5/1668 (0.3%)
All	All	0.36	3/32260 (0.0%)	0.53	6/43828 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
11	K	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	17	C	P-OP2	11.40	1.68	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	16	DT	O3'-P	8.20	1.71	1.61
15	O	17	C	P-OP1	6.26	1.59	1.49

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	16	DT	O3'-P-O5'	10.97	124.84	104.00
11	K	648	PRO	CA-N-CD	-8.84	99.13	111.50
15	O	16	DT	P-O3'-C3'	-6.69	111.67	119.70
15	O	16	DT	OP2-P-O3'	-6.29	91.36	105.20
15	O	17	C	OP1-P-OP2	-5.92	110.72	119.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	201	ASP	Peptide
11	K	455	MET	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	2264	0	2315	70	0
2	B	1824	0	1823	43	0
3	C	2020	0	2035	41	0
4	D	1566	0	1605	35	0
5	E	2194	0	2205	38	0
6	F	1859	0	1889	26	0
7	G	1806	0	1865	43	0
8	H	2263	0	2337	44	0
9	I	1407	0	1432	22	0
10	J	86	0	86	3	0
11	K	6856	0	6907	150	0
12	L	573	0	575	6	0
13	M	5648	0	5681	107	0
14	N	278	0	144	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	966	0	518	28	0
16	K	1	0	0	0	0
17	K	1	0	0	0	0
18	M	27	0	12	2	0
All	All	31639	0	31429	601	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 10.

The worst 5 of 601 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)
13:M:237:TYR:OH	13:M:268:GLU:OE2	1.78	0.99
11:K:780:ARG:NH2	15:O:61:A:OP2	1.97	0.97
3:C:111:ASP:OD1	3:C:115:ASN:ND2	1.97	0.96
15:O:42:C:O2'	15:O:43:A:O5'	1.82	0.95
11:K:565:GLU:OE1	11:K:574:LYS:NZ	2.05	0.88

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	285/473 (60%)	263 (92%)	22 (8%)	0	100	100
2	B	239/249 (96%)	215 (90%)	24 (10%)	0	100	100
3	C	263/278 (95%)	237 (90%)	26 (10%)	0	100	100
4	D	206/237 (87%)	197 (96%)	9 (4%)	0	100	100
5	E	284/293 (97%)	249 (88%)	35 (12%)	0	100	100
6	F	248/272 (91%)	230 (93%)	18 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	233/277 (84%)	211 (91%)	22 (9%)	0	100	100
8	H	285/296 (96%)	240 (84%)	45 (16%)	0	100	100
9	I	181/197 (92%)	159 (88%)	22 (12%)	0	100	100
10	J	9/761 (1%)	5 (56%)	4 (44%)	0	100	100
11	K	839/960 (87%)	752 (90%)	87 (10%)	0	100	100
12	L	64/162 (40%)	54 (84%)	10 (16%)	0	100	100
13	M	703/1045 (67%)	647 (92%)	56 (8%)	0	100	100
All	All	3839/5500 (70%)	3459 (90%)	380 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	252/411 (61%)	251 (100%)	1 (0%)	91	97
2	B	184/189 (97%)	182 (99%)	2 (1%)	73	88
3	C	227/237 (96%)	225 (99%)	2 (1%)	78	91
4	D	172/195 (88%)	172 (100%)	0	100	100
5	E	249/254 (98%)	247 (99%)	2 (1%)	81	92
6	F	179/188 (95%)	177 (99%)	2 (1%)	73	88
7	G	196/223 (88%)	195 (100%)	1 (0%)	88	95
8	H	251/257 (98%)	247 (98%)	4 (2%)	62	83
9	I	159/172 (92%)	159 (100%)	0	100	100
10	J	10/672 (2%)	10 (100%)	0	100	100
11	K	758/854 (89%)	753 (99%)	5 (1%)	84	93
12	L	63/148 (43%)	63 (100%)	0	100	100
13	M	618/911 (68%)	616 (100%)	2 (0%)	92	98
All	All	3318/4711 (70%)	3297 (99%)	21 (1%)	86	95

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	144	ARG
11	K	569	ASN
13	M	347	MET
11	K	689	ARG
11	K	284	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	837	GLN
13	M	291	GLN
13	M	300	HIS
11	K	170	GLN
11	K	266	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	N	12/16 (75%)	0	0
15	O	33/62 (53%)	14 (42%)	2 (6%)
All	All	45/78 (57%)	14 (31%)	2 (4%)

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	O	24	C
15	O	26	A
15	O	29	C
15	O	42	C
15	O	43	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	O	42	C
15	O	53	A

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	ANP	M	2001	-	24,29,33	1.57	3 (12%)	25,45,52	1.16	2 (8%)

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
18	ANP	M	2001	-	-	5/9/32/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	M	2001	ANP	PB-O1B	6.30	1.56	1.46
18	M	2001	ANP	PB-O2B	-2.58	1.49	1.56
18	M	2001	ANP	PB-O3A	-2.26	1.56	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	M	2001	ANP	PB-O3A-PA	-4.29	118.94	132.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	M	2001	ANP	C5-C6-N6	2.35	123.92	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	M	2001	ANP	C5'-O5'-PA-O1A
18	M	2001	ANP	C5'-O5'-PA-O2A
18	M	2001	ANP	O4'-C4'-C5'-O5'
18	M	2001	ANP	C3'-C4'-C5'-O5'
18	M	2001	ANP	C5'-O5'-PA-O3A

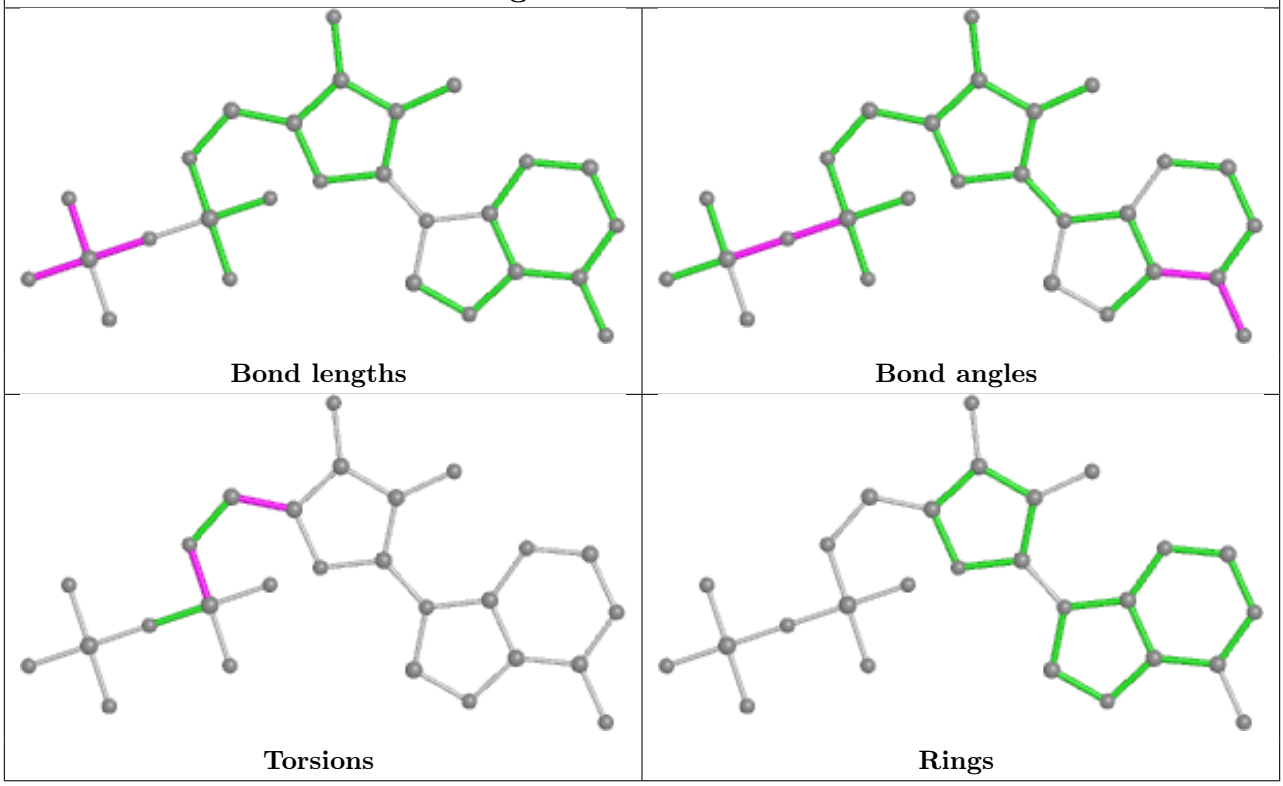
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	M	2001	ANP	2	0

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

Ligand ANP M 2001



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.

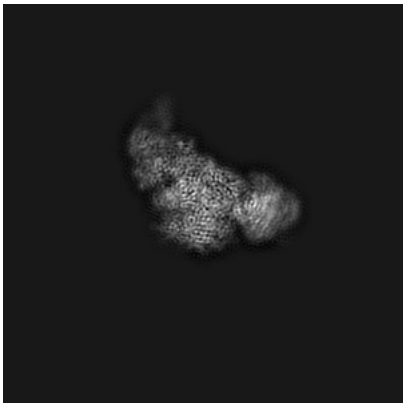
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7808. These allow visual inspection of the internal detail of the map and identification of artifacts.

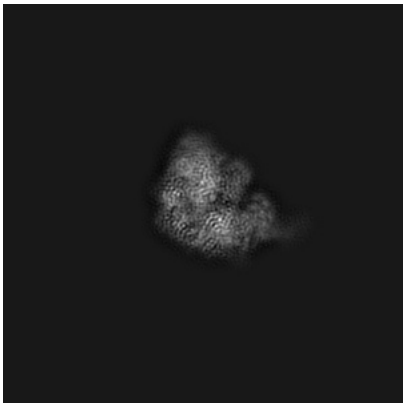
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

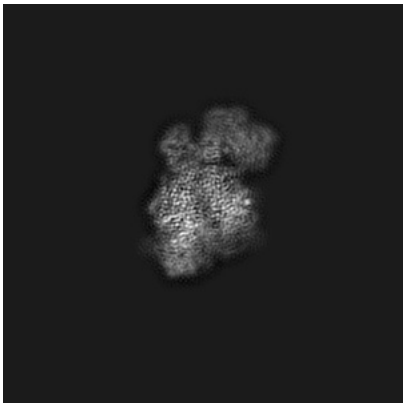
6.1.1 Primary map



X



Y

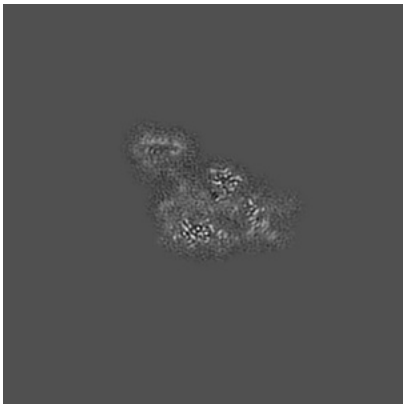


Z

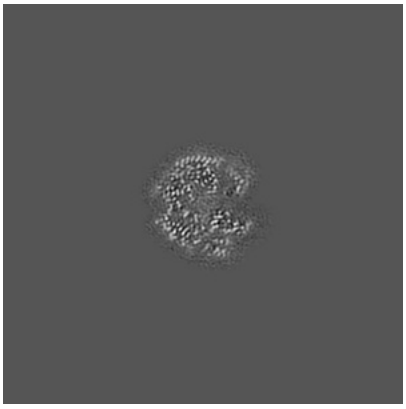
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

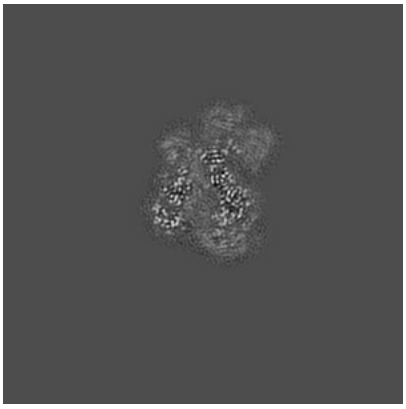
6.2.1 Primary map



X Index: 192



Y Index: 192

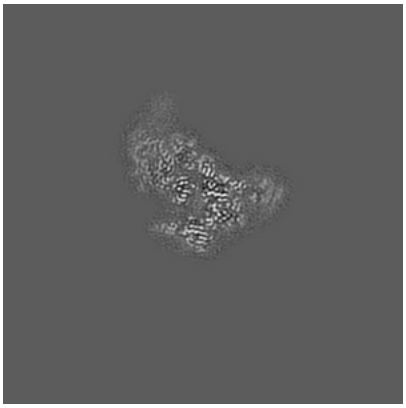


Z Index: 192

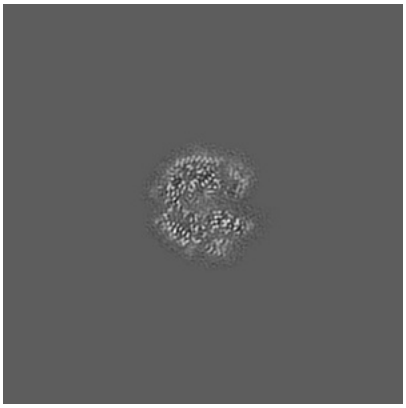
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

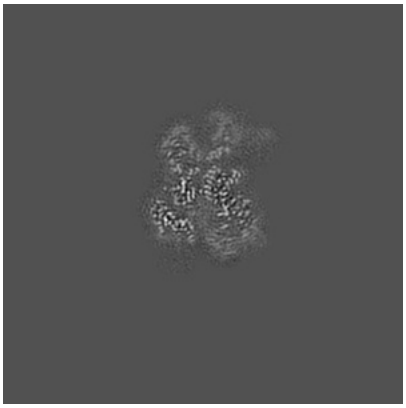
6.3.1 Primary map



X Index: 173



Y Index: 193

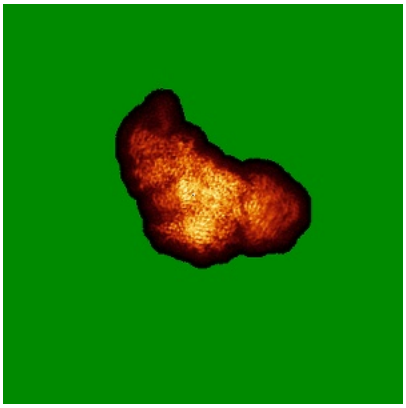


Z Index: 200

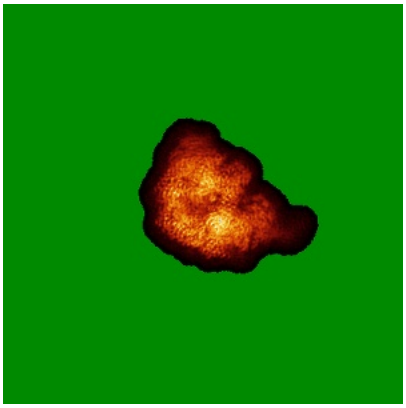
The images above show the largest variance slices of the map in three orthogonal directions.

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

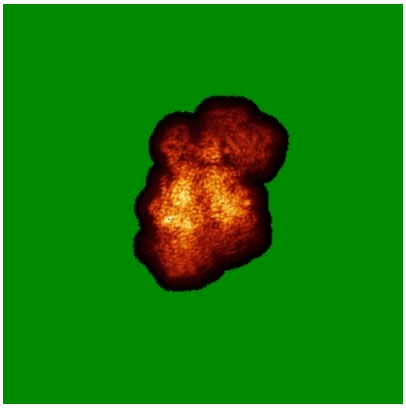
6.4.1 Primary map



X



Y

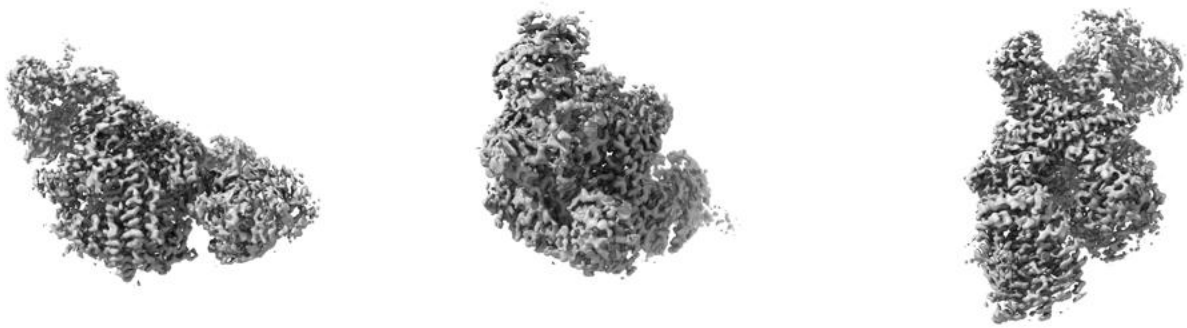


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

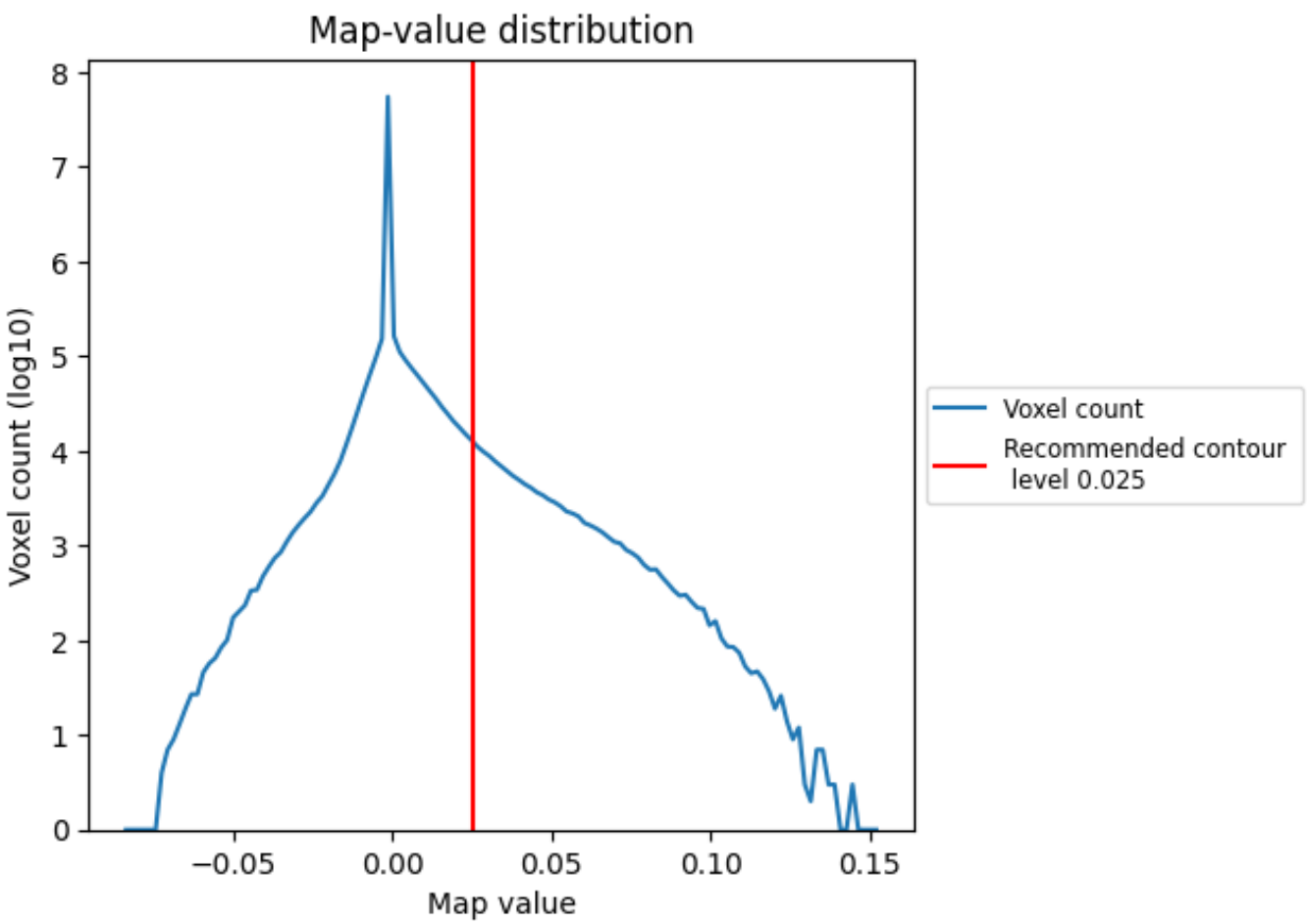
6.6 Mask visualisation (i)

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

7 Map analysis (i)

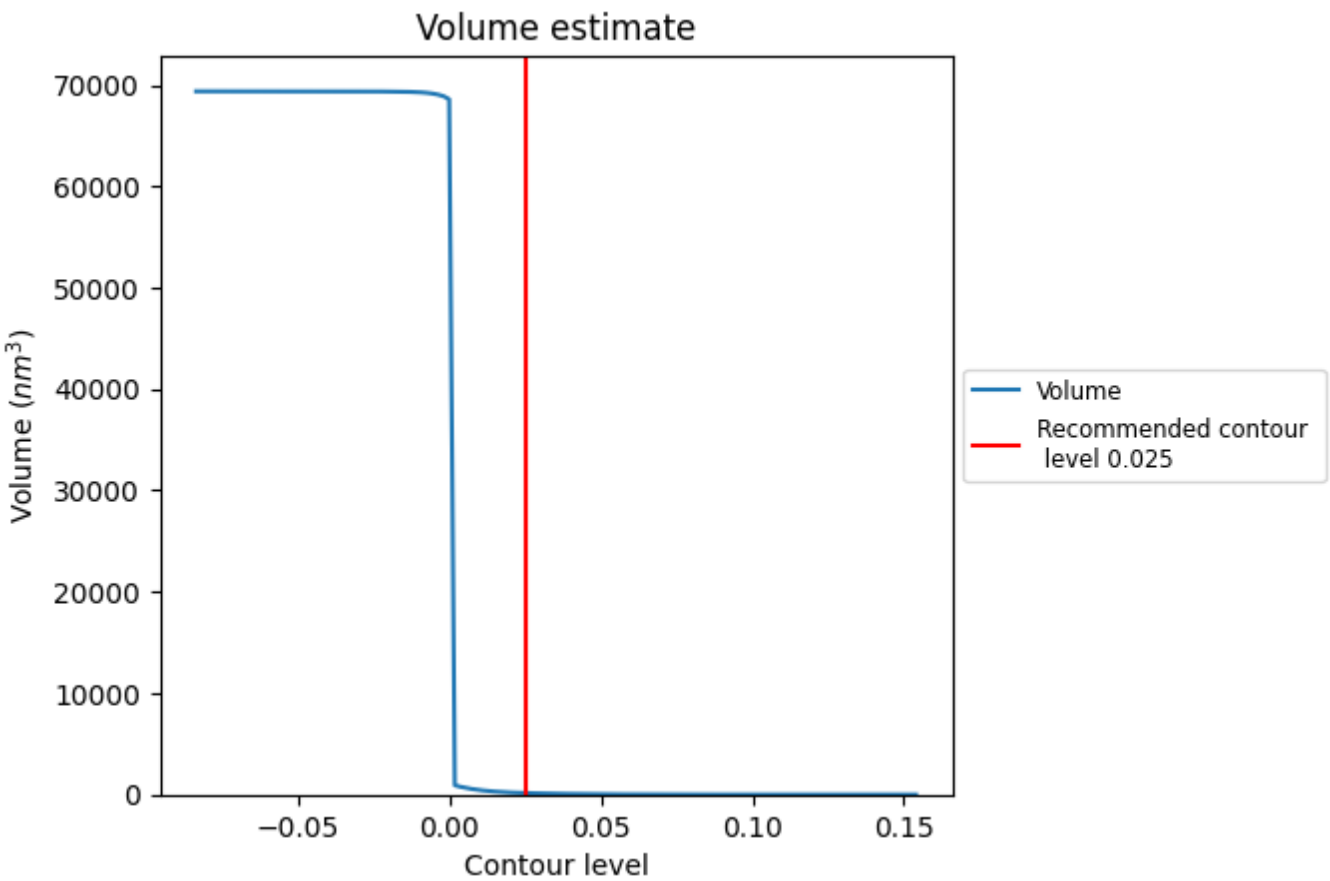
This section contains the results of statistical analysis of the map.

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.

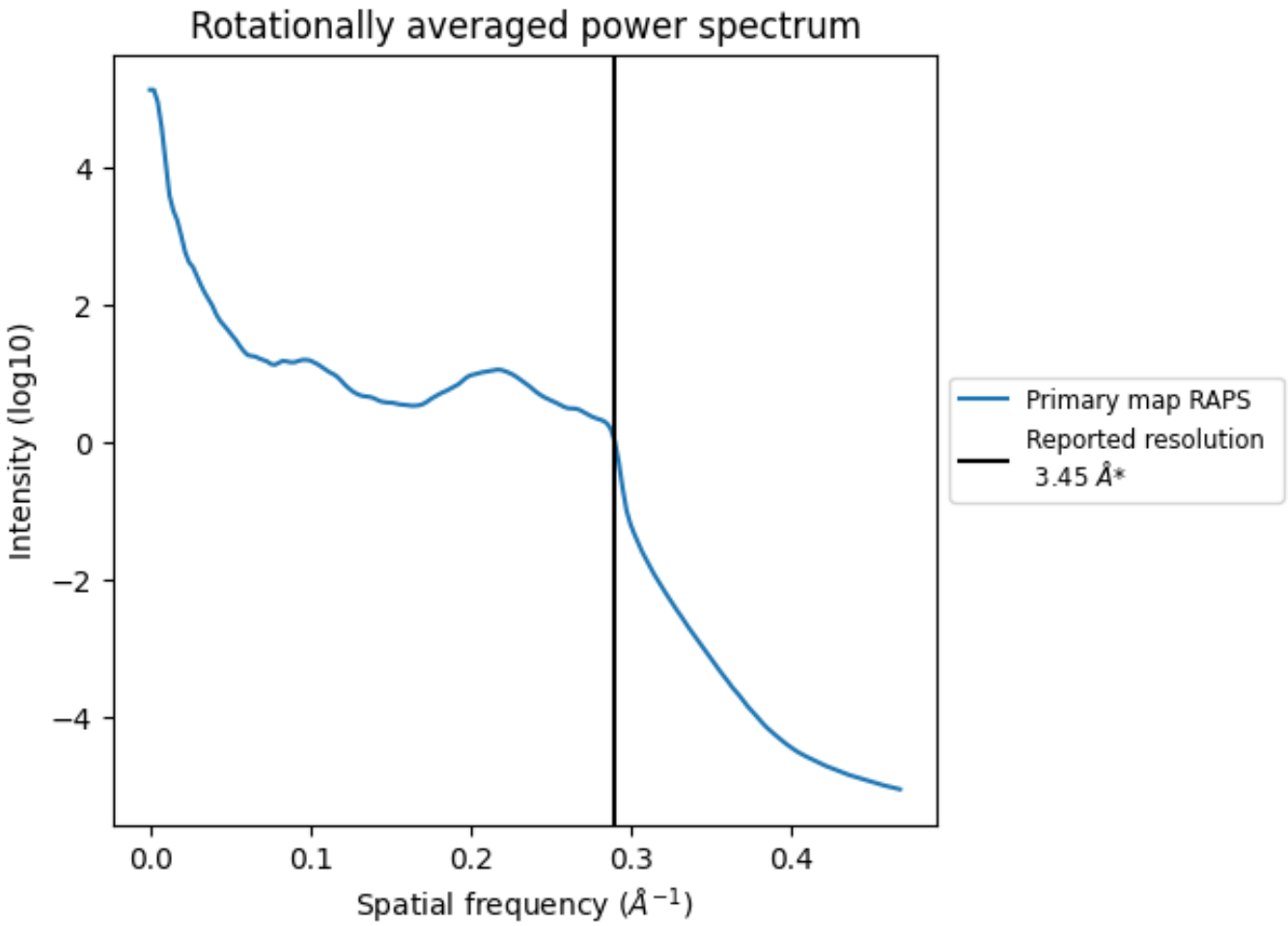
7.2 Volume estimate (i)



The volume at the recommended contour level is 149 nm^3; this corresponds to an approximate mass of 134 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)

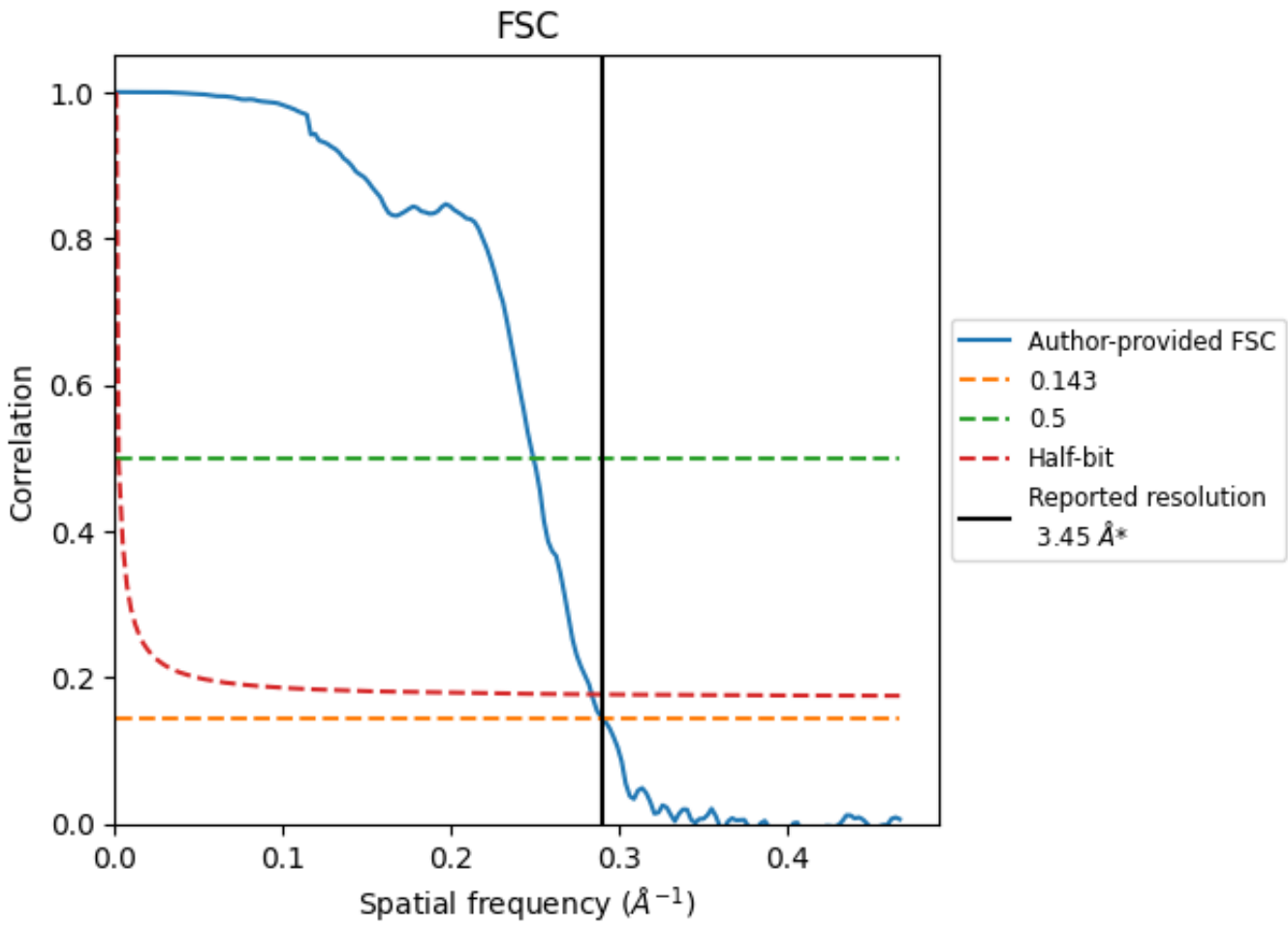


*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

8.2 Resolution estimates (i)

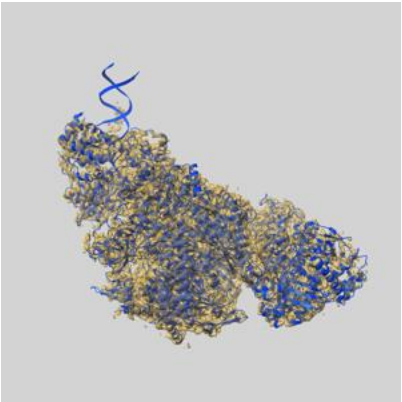
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.44	4.01	3.52
Unmasked-calculated*	-	-	-

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

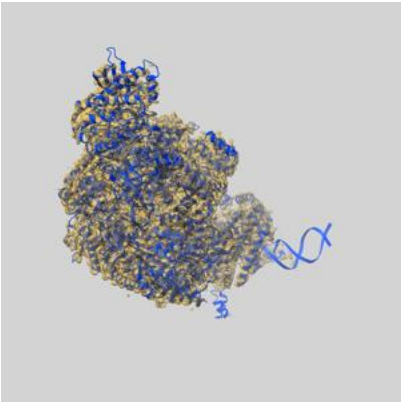
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7808 and PDB model 6D6Q. Per-residue inclusion information can be found in section 3 on page 10.

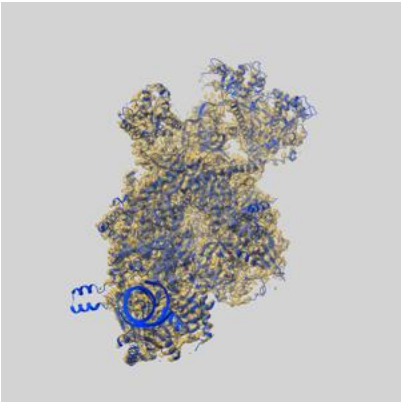
9.1 Map-model overlay (i)



X



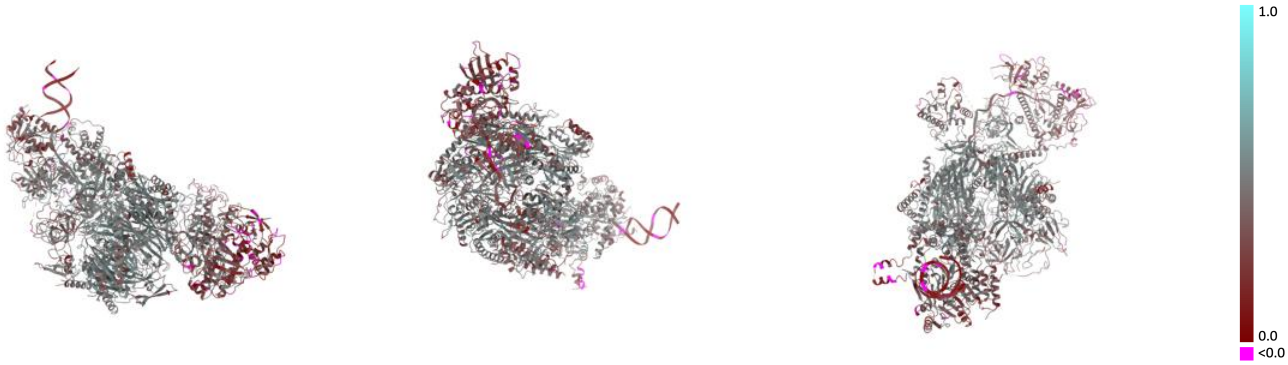
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

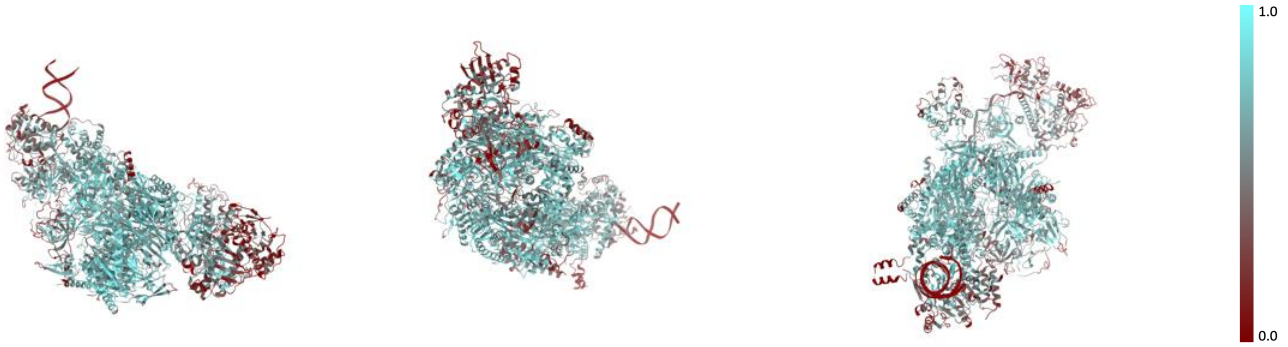
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

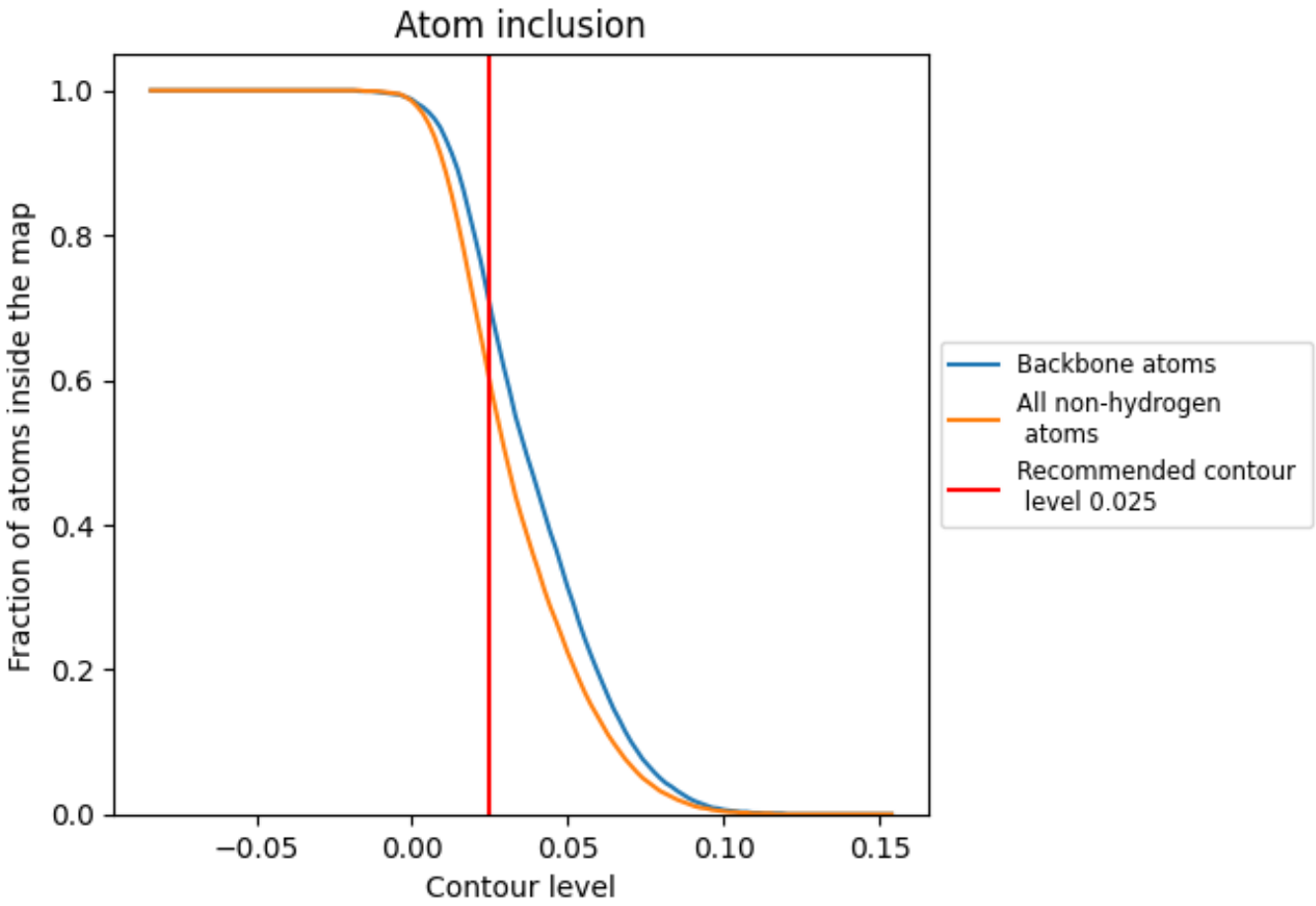
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.4130
A	0.7300	0.4860
B	0.7460	0.4890
C	0.7270	0.4740
D	0.7620	0.4930
E	0.7160	0.4750
F	0.7060	0.4750
G	0.6380	0.4350
H	0.7090	0.4770
I	0.5060	0.4070
J	0.5120	0.4210
K	0.4530	0.3270
L	0.4730	0.3880
M	0.5370	0.3850
N	0.0250	0.0810
O	0.4270	0.2940