wwPDB EM Validation Summary Report

Mar 8, 2026 – 10:41 AM UTC

PDB ID	:	6S8B / pdb_00006s8b
EMDB ID	:	EMD-10117
Title	:	Cryo-EM structure of the Type III-B Cmr-beta bound to cognate target RNA and AMPPnP, state 1
Authors	:	Sofos, N.; Montoya, G.; Stella, S.
Deposited on	:	2019-07-09
Resolution	:	2.41 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:

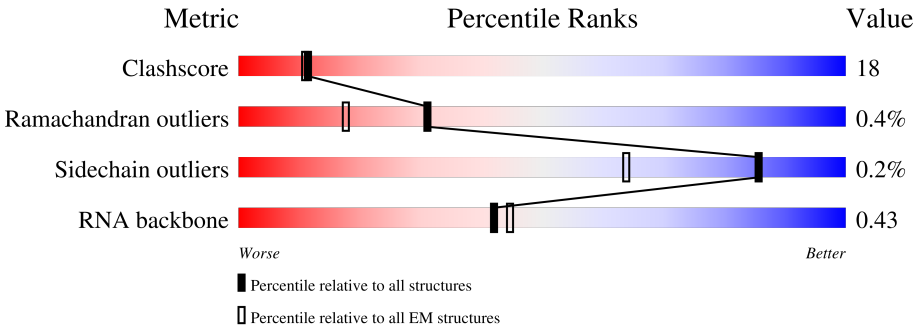
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

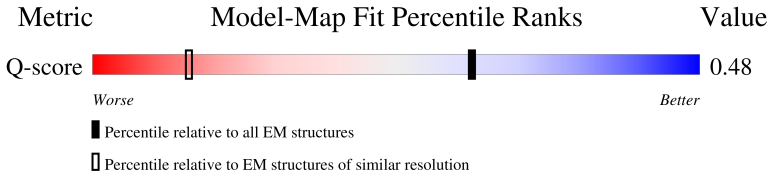
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.41 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5662 (1.92 - 2.91)

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	155	65% 34%
1	B	155	66% 32%
1	C	155	77% 21%

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Mol	Chain	Length	Quality of chain
2	D	286	78% 21%
2	E	286	70% 29%
2	F	286	74% 26%
2	G	286	73% 26%
3	H	313	60% 37%
4	I	296	72% 24%
5	J	476	66% 33%
6	U	46	9% 43% 35% 17%
7	V	51	33% 49% 14%
8	L	174	6% 62% 37%
8	M	174	6% 52% 47%
8	N	174	18% 51% 47%
8	O	174	14% 53% 46%
8	P	174	30% 51% 48%
8	Q	174	13% 51% 48%
8	R	174	17% 52% 47%
8	S	174	73% 46% 53%
8	T	174	29% 55% 44%
8	W	174	49% 55% 43%
8	X	174	76% 46% 53%
8	l	174	6% 64% 36%
8	m	174	55% 45%
8	n	174	20% 44% 55%
8	o	174	18% 52% 47%
8	p	174	31% 62% 37%

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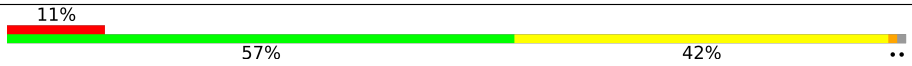
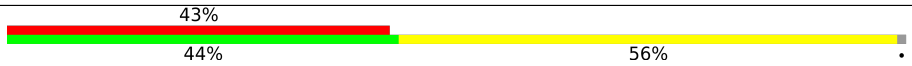
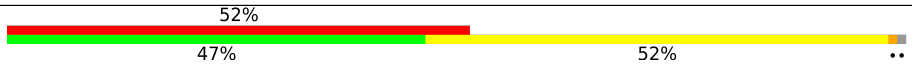
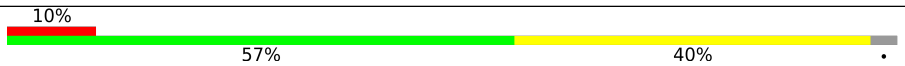
Mol	Chain	Length	Quality of chain
8	q	174	
8	r	174	
8	s	174	
8	t	174	
8	w	174	
8	x	174	
9	K	1037	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 62151 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 CRISPR-associated protein, Cmr5 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	153	Total	C	N	O	S	0	0
			1253	817	205	230	1		
1	B	154	Total	C	N	O	S	0	0
			1261	823	206	231	1		
1	C	154	Total	C	N	O	S	0	0
			1261	823	206	231	1		

- Molecule 2 is a protein called CRISPR-associated RAMP protein, Cmr4 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	285	Total	C	N	O	S	0	0
			2274	1478	369	425	2		
2	E	285	Total	C	N	O	S	0	0
			2274	1478	369	425	2		
2	F	285	Total	C	N	O	S	0	0
			2274	1478	369	425	2		
2	G	285	Total	C	N	O	S	0	0
			2273	1478	369	424	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	31	ALA	ASP	conflict	UNP F0NDX6
E	31	ALA	ASP	conflict	UNP F0NDX6
F	31	ALA	ASP	conflict	UNP F0NDX6
G	31	ALA	ASP	conflict	UNP F0NDX6

- Molecule 3 is a protein called CRISPR-associated protein, Cmr3 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	304	Total	C	N	O	S	0	0
			2468	1593	408	460	7		

- Molecule 4 is a protein called CRISPR-associated RAMP protein, Cmr6 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	284	Total	C	N	O	S	0	0
			2282	1470	381	427	4		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	284	ALA	-	expression tag	UNP F0NDX3
I	285	ALA	-	expression tag	UNP F0NDX3
I	286	ALA	-	expression tag	UNP F0NDX3
I	287	HIS	-	expression tag	UNP F0NDX3
I	288	HIS	-	expression tag	UNP F0NDX3
I	289	HIS	-	expression tag	UNP F0NDX3
I	290	HIS	-	expression tag	UNP F0NDX3
I	291	HIS	-	expression tag	UNP F0NDX3
I	292	HIS	-	expression tag	UNP F0NDX3
I	293	HIS	-	expression tag	UNP F0NDX3
I	294	HIS	-	expression tag	UNP F0NDX3
I	295	HIS	-	expression tag	UNP F0NDX3
I	296	HIS	-	expression tag	UNP F0NDX3

- Molecule 5 is a protein called Cmr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	475	Total	C	N	O	S	0	0
			3889	2517	632	727	13		

- Molecule 6 is a RNA chain called Cognate target RNA (46-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	44	Total	C	N	O	P	0	0
			933	418	162	309	44		

- Molecule 7 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	49	Total	C	N	O	P	0	0
			1045	470	195	332	48		

- Molecule 8 is a protein called CRISPR-associated protein Cmrx.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	M	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	N	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	O	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	P	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	Q	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	R	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	S	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	T	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	W	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	X	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	l	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	m	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	n	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	o	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	p	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	q	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	r	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	s	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	t	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	w	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	x	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		

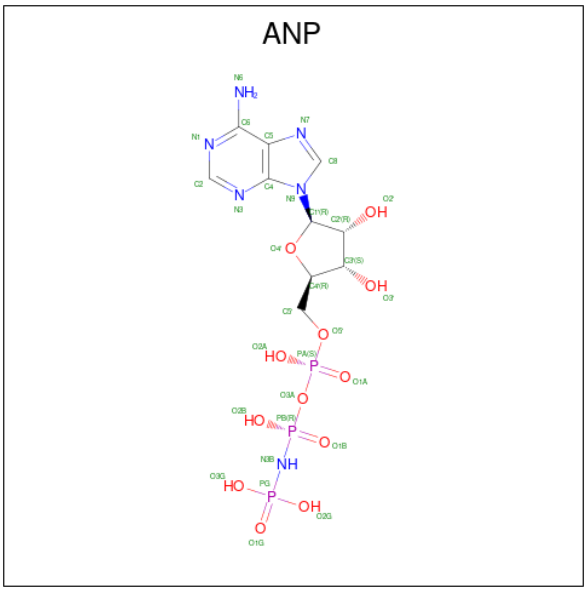
- Molecule 9 is a protein called CRISPR-associated protein, Cmr2 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	1009	8282	5360	1366	1532	24	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 11 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	K	1	31	10	6	12	3	0
11	K	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
12	K	3	3	3	0

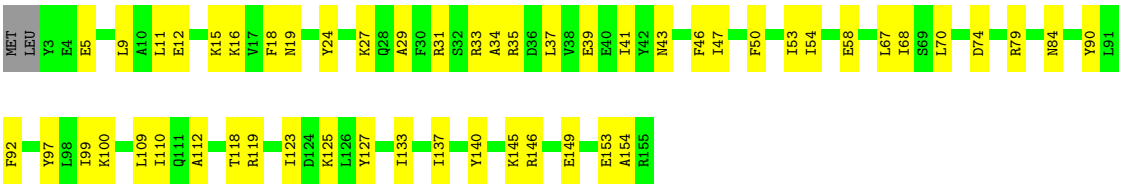
3 Residue-property plots (i)

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: CRISPR-associated protein, Cmr5 family

Chain A:

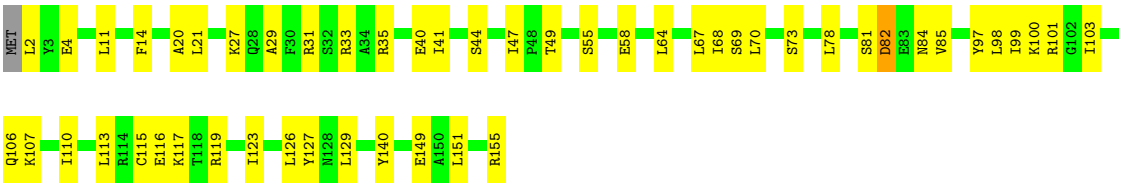




• Molecule 1: CRISPR-associated protein, Cmr5 family

Chain B:

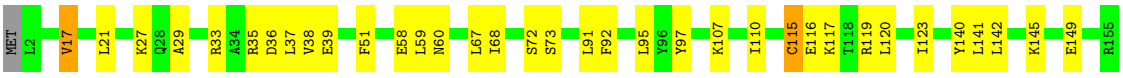




• Molecule 1: CRISPR-associated protein, Cmr5 family

Chain C:

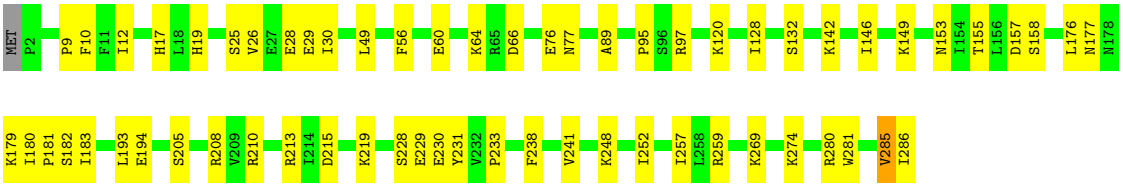




• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

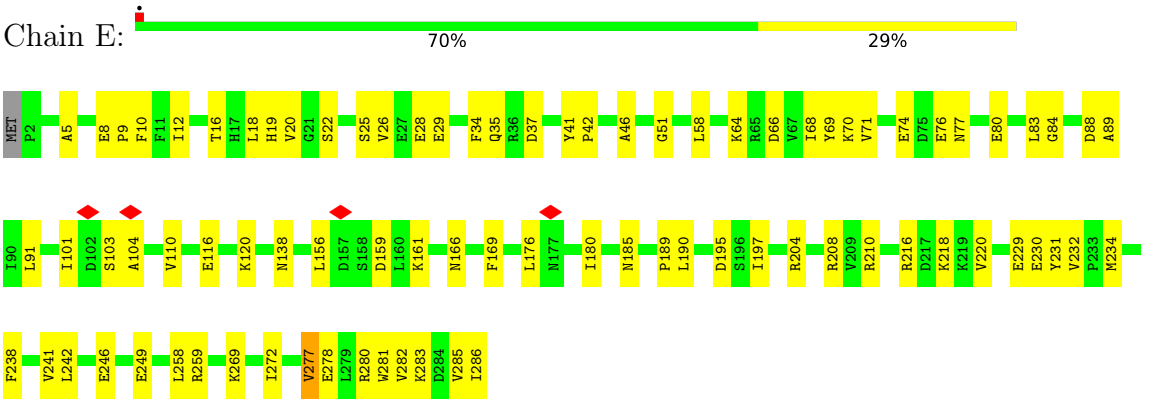
Chain D:





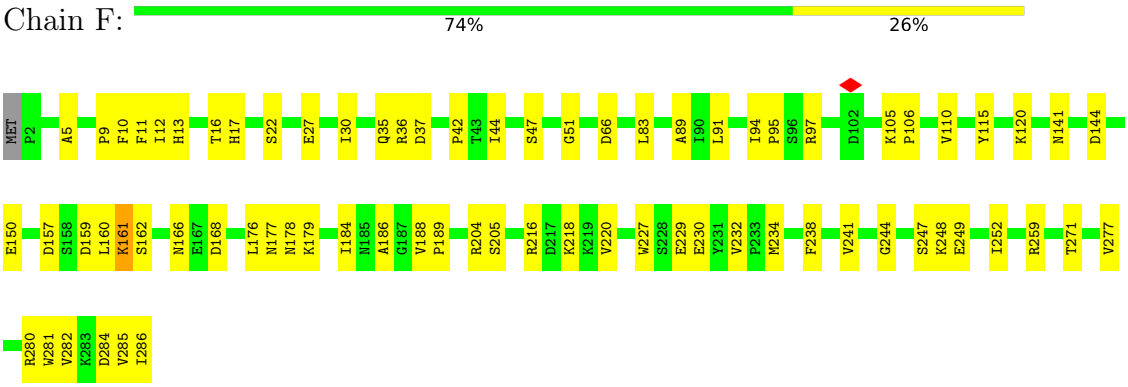
• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

Chain E:



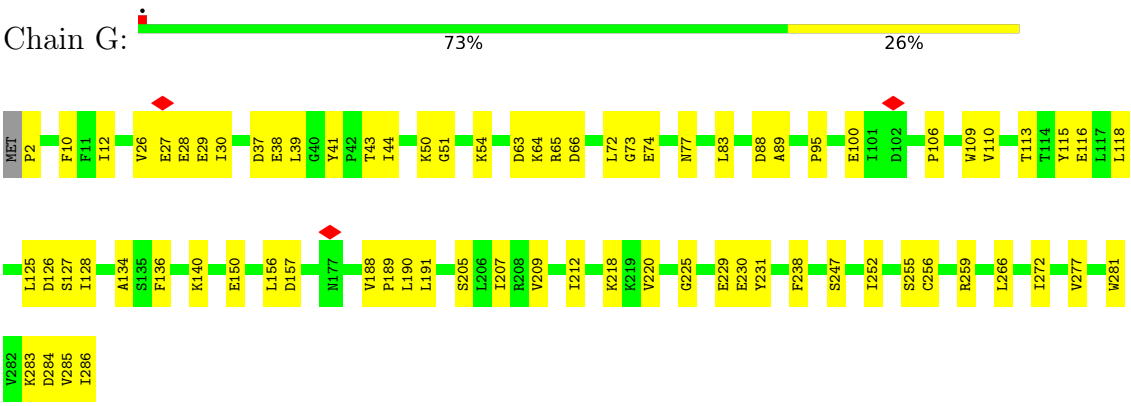
• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

Chain F:



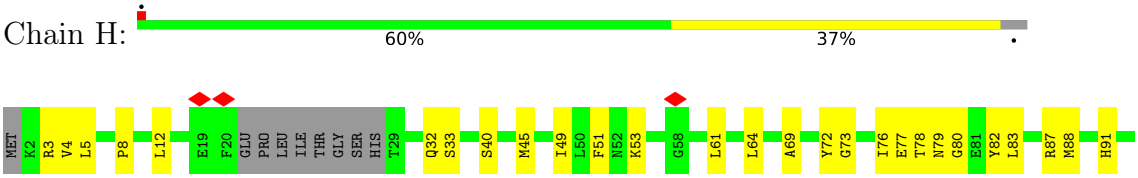
• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

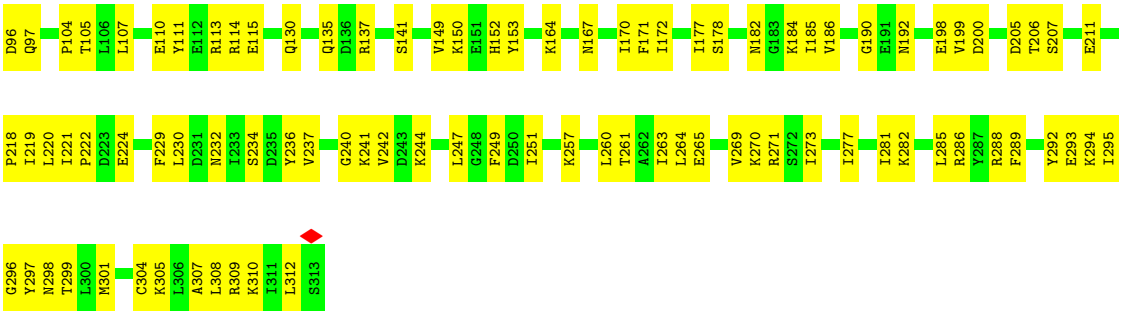
Chain G:



• Molecule 3: CRISPR-associated protein, Cmr3 family

Chain H:

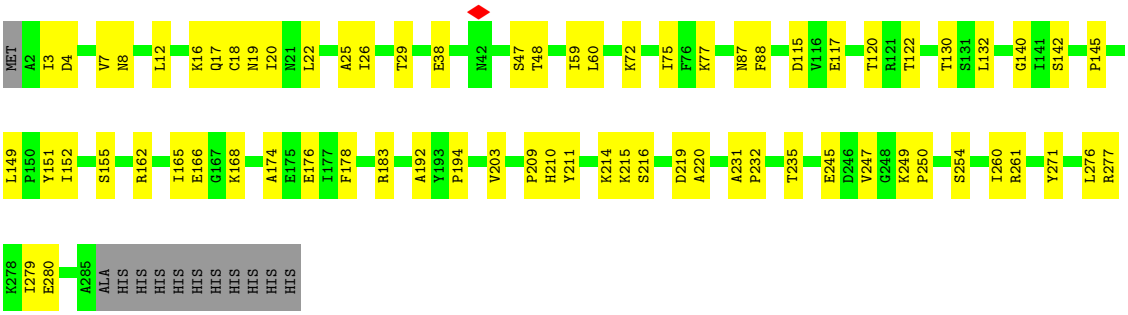




• Molecule 4: CRISPR-associated RAMP protein, Cmr6 family

Chain I:

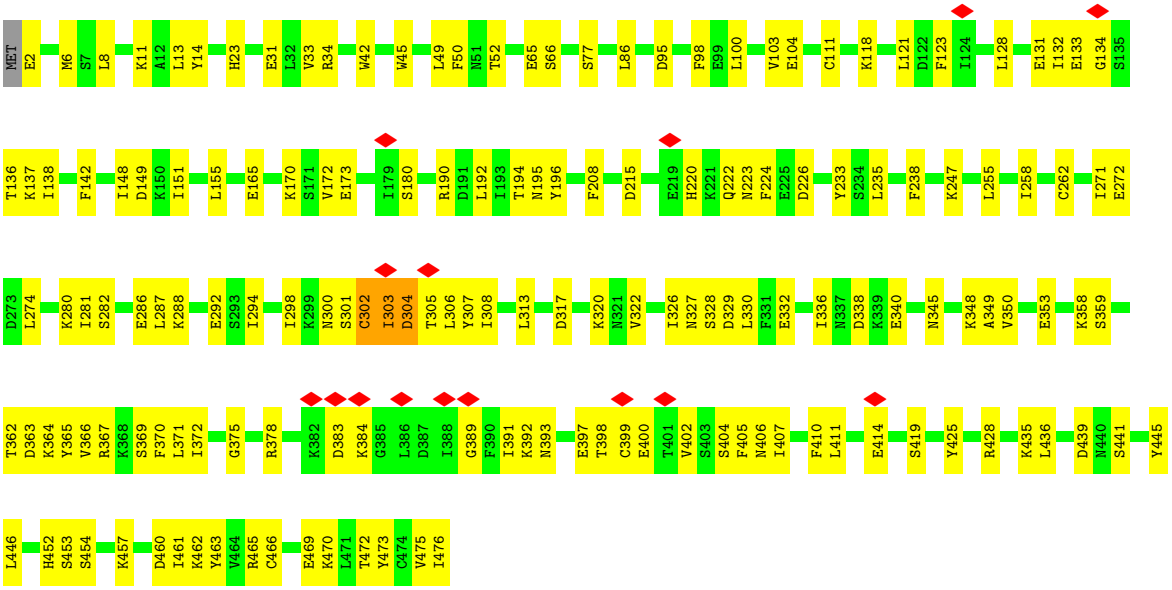




• Molecule 5: Cmr1

Chain J:

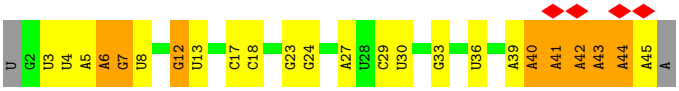




• Molecule 6: Cognate target RNA (46-mer)

Chain U:

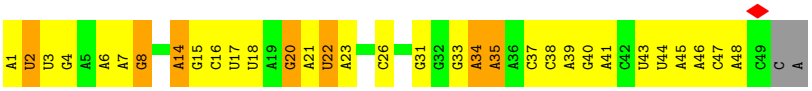




• Molecule 7: crRNA

Chain V:

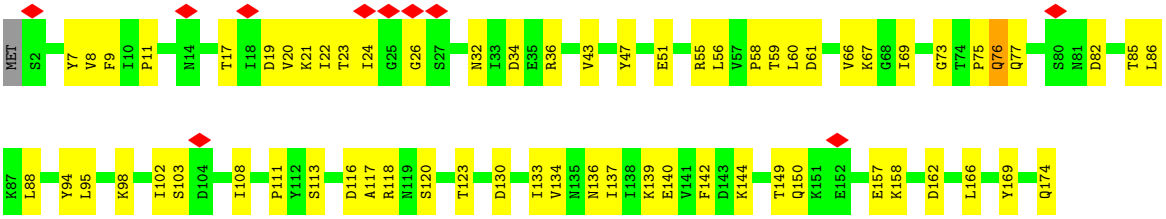




• Molecule 8: CRISPR-associated protein Cmrx

Chain L:

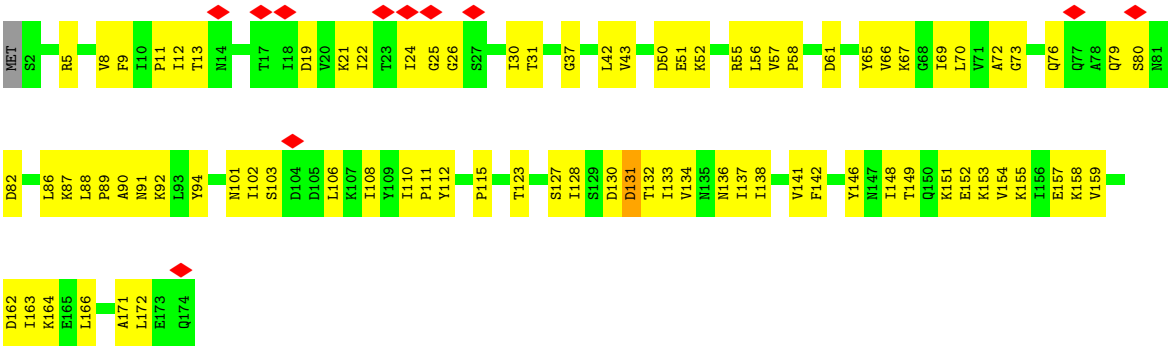




• Molecule 8: CRISPR-associated protein Cmrx

Chain M:

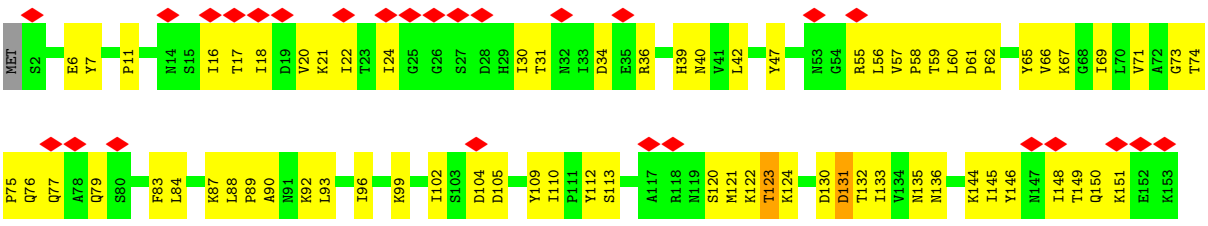


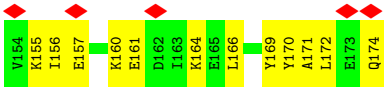


• Molecule 8: CRISPR-associated protein Cmrx

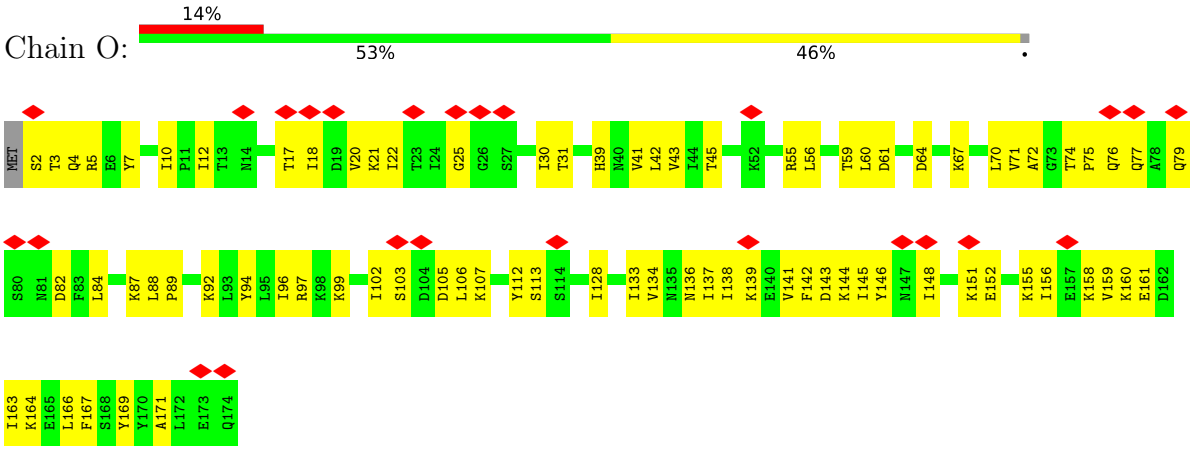
Chain N:



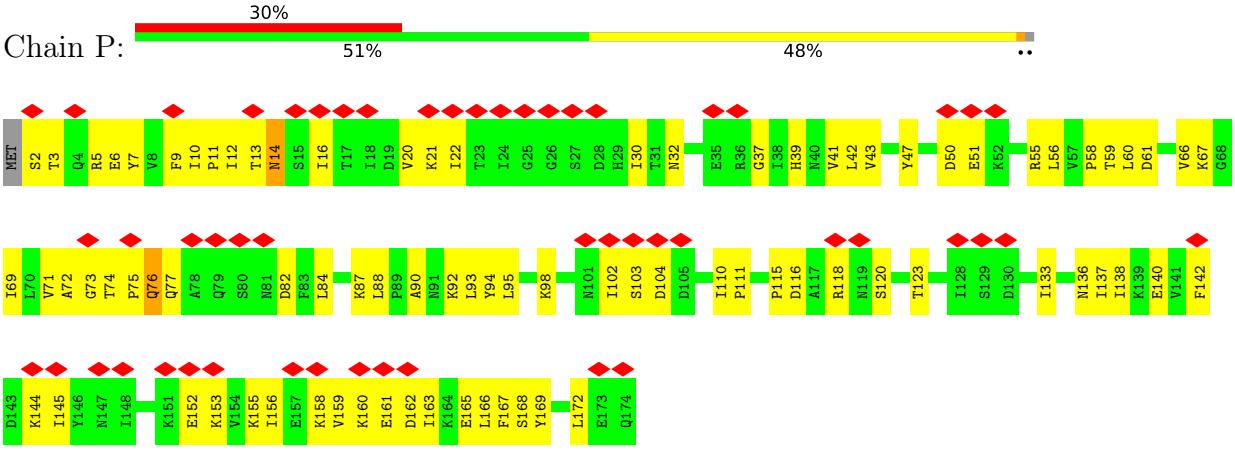




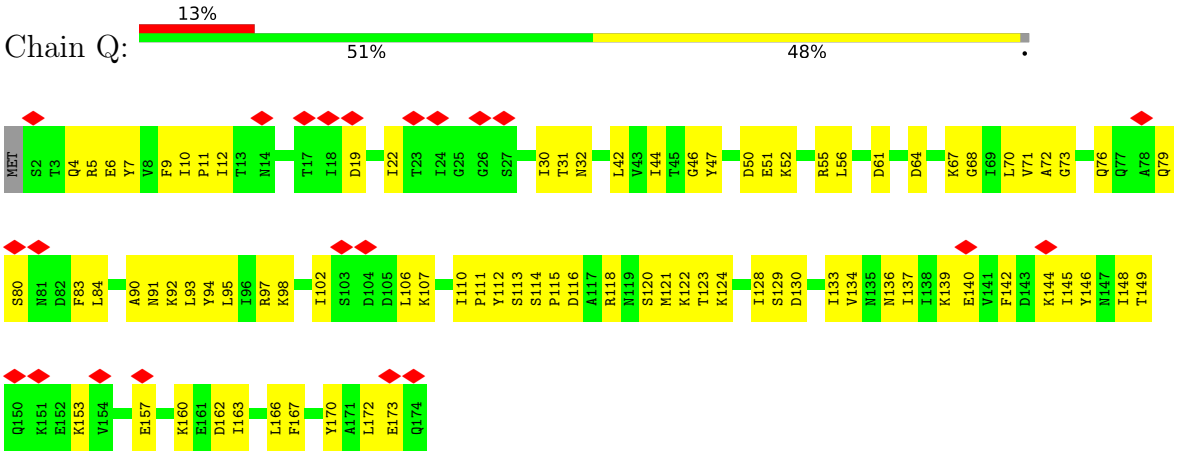
• Molecule 8: CRISPR-associated protein Cmrx



• Molecule 8: CRISPR-associated protein Cmrx

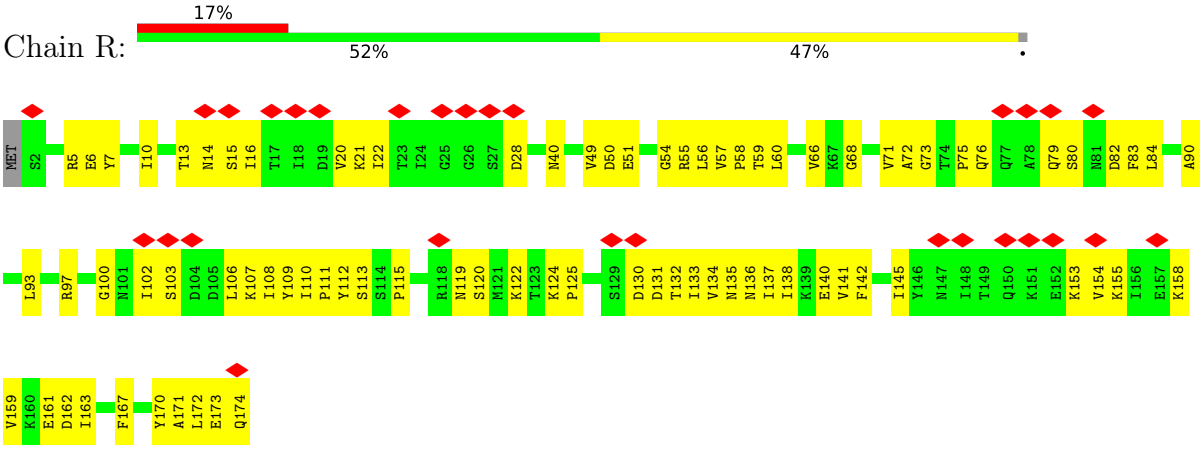


• Molecule 8: CRISPR-associated protein Cmrx



• Molecule 8: CRISPR-associated protein Cmrx

Chain R:



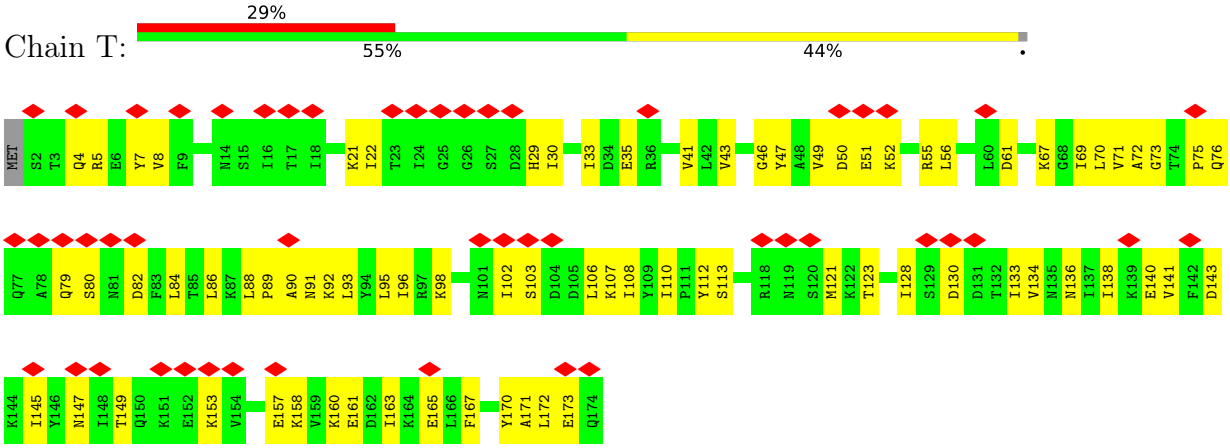
• Molecule 8: CRISPR-associated protein Cmrx

Chain S:



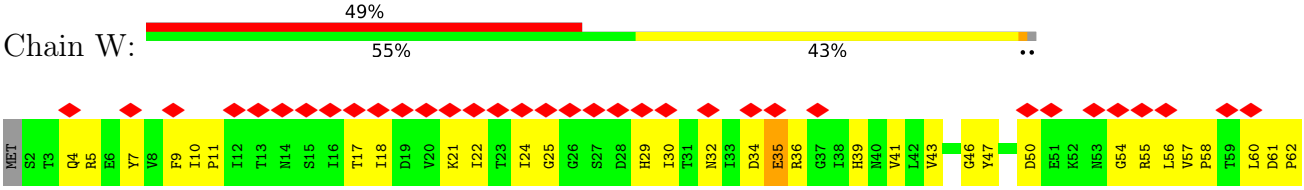
• Molecule 8: CRISPR-associated protein Cmrx

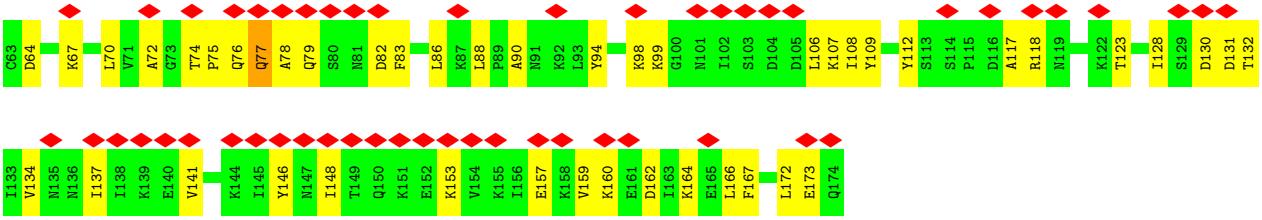
Chain T:



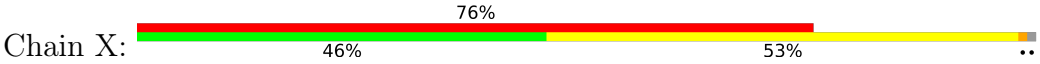
• Molecule 8: CRISPR-associated protein Cmrx

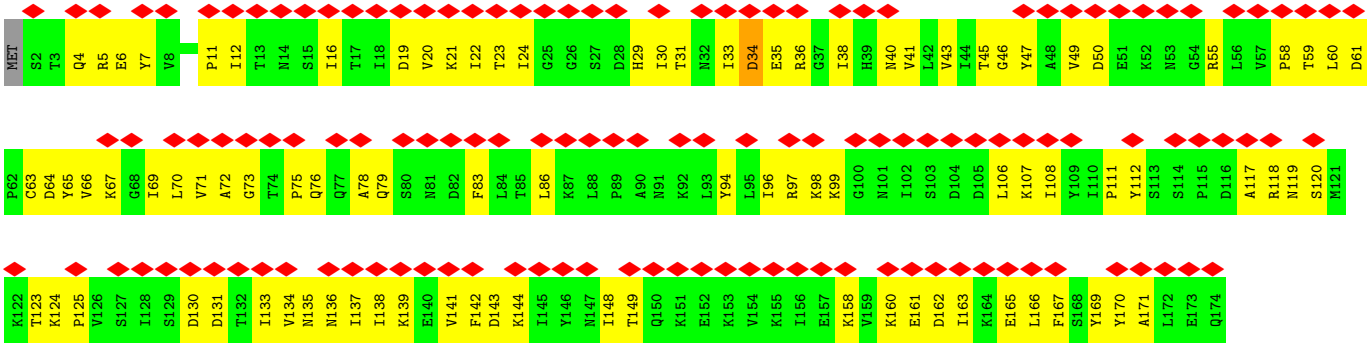
Chain W:





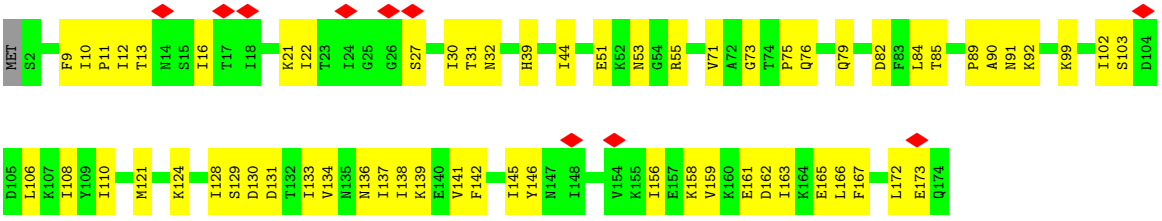
• Molecule 8: CRISPR-associated protein Cmrx





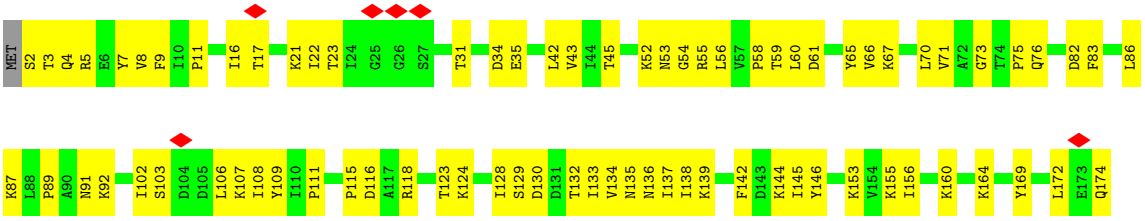
• Molecule 8: CRISPR-associated protein Cmrx





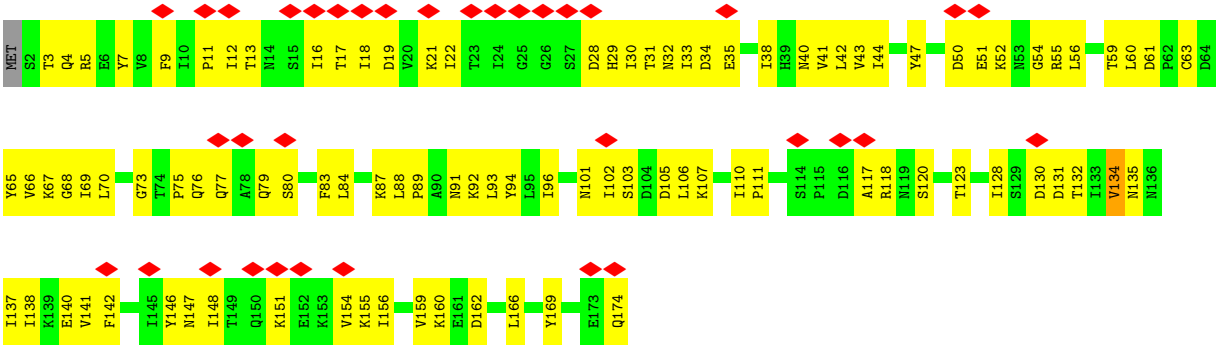
• Molecule 8: CRISPR-associated protein Cmrx





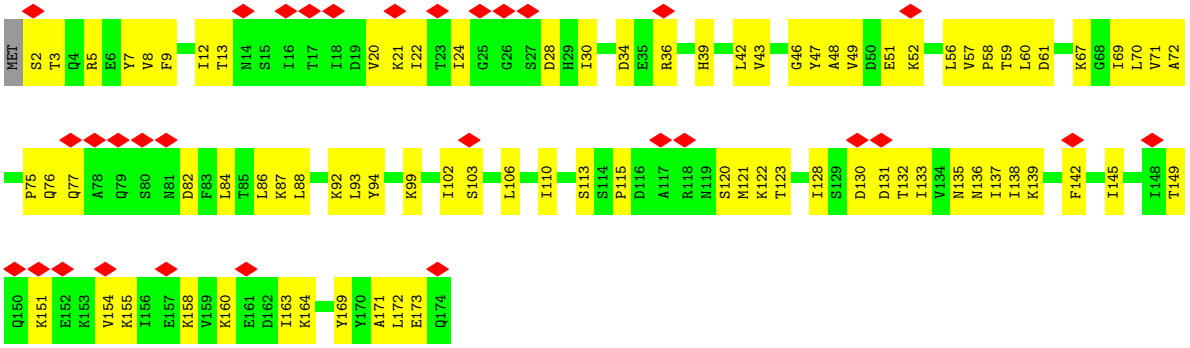
• Molecule 8: CRISPR-associated protein Cmrx





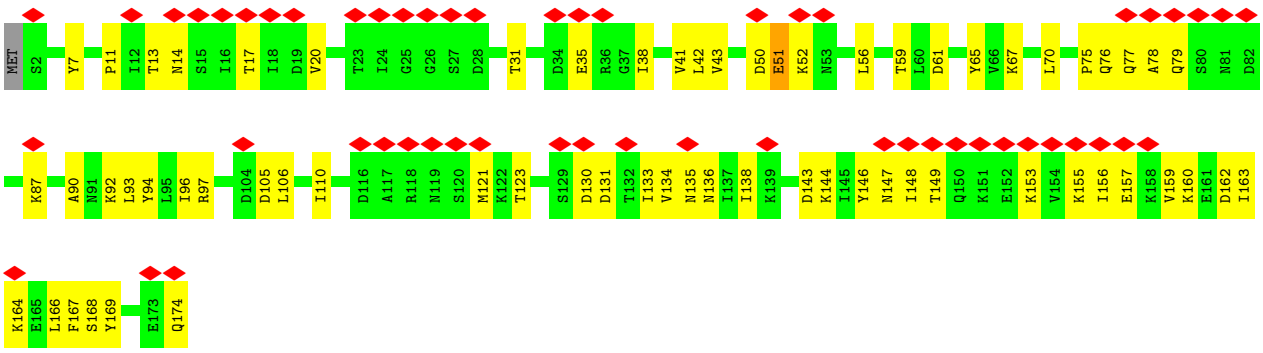
• Molecule 8: CRISPR-associated protein Cmrx





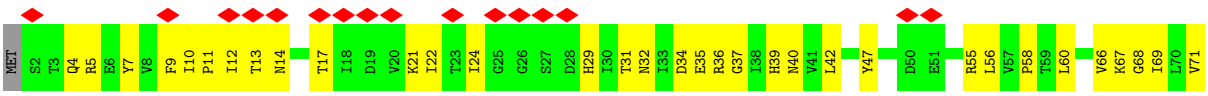
• Molecule 8: CRISPR-associated protein Cmrx

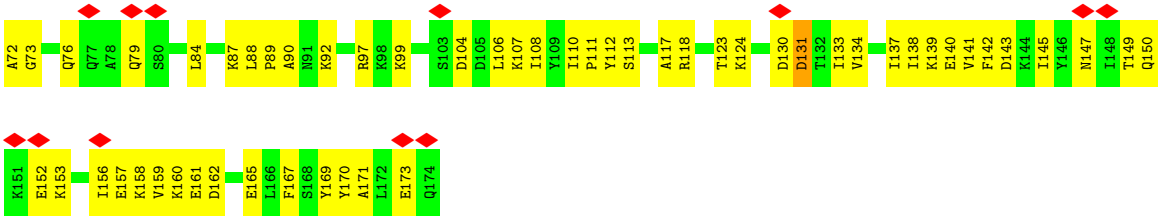




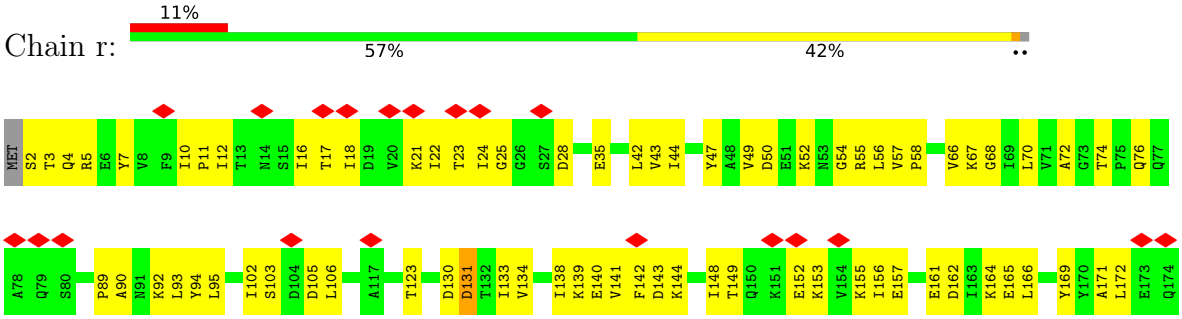
• Molecule 8: CRISPR-associated protein Cmrx



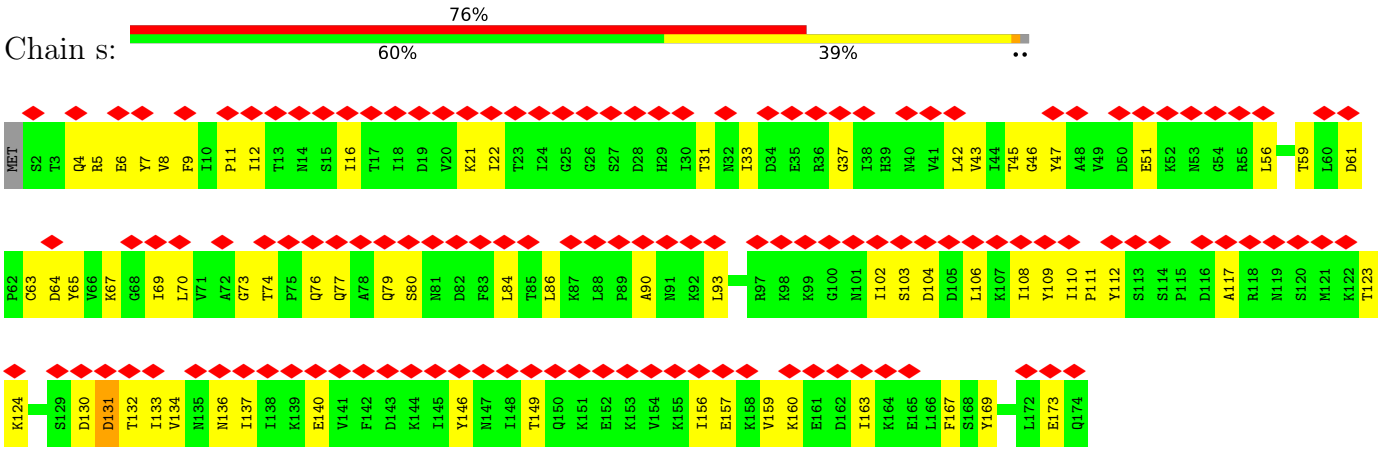




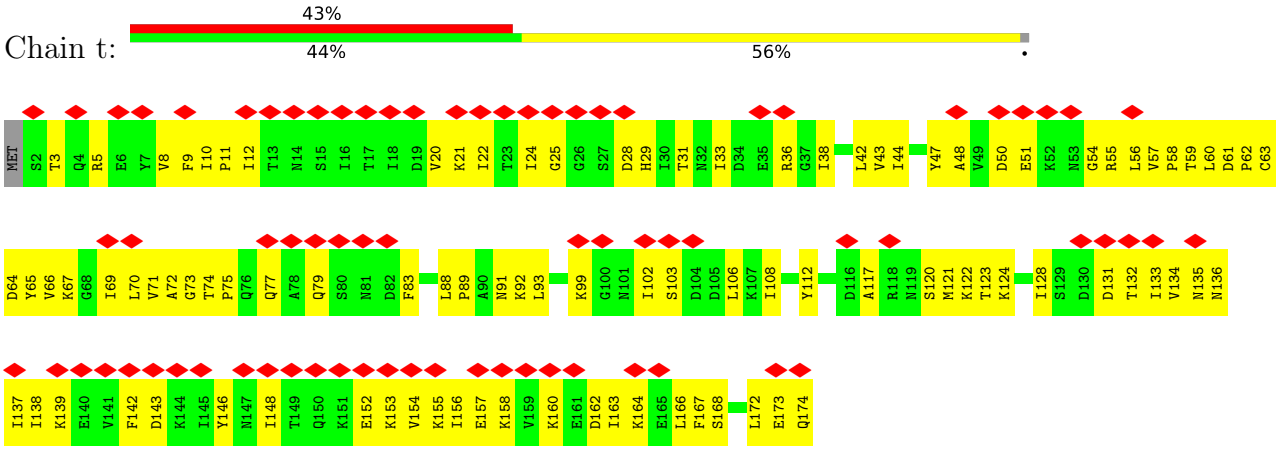
• Molecule 8: CRISPR-associated protein Cmrx



• Molecule 8: CRISPR-associated protein Cmrx

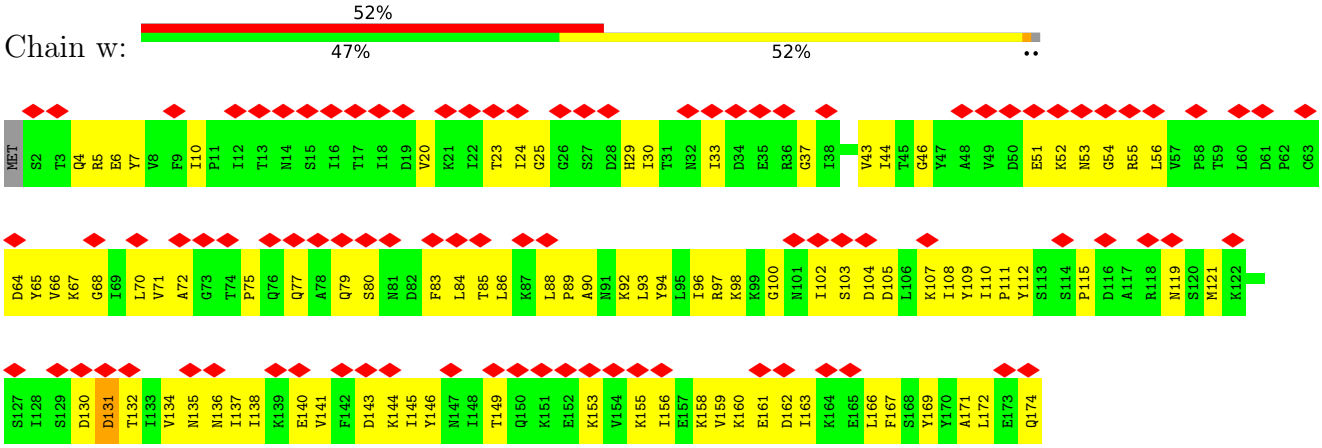


• Molecule 8: CRISPR-associated protein Cmrx



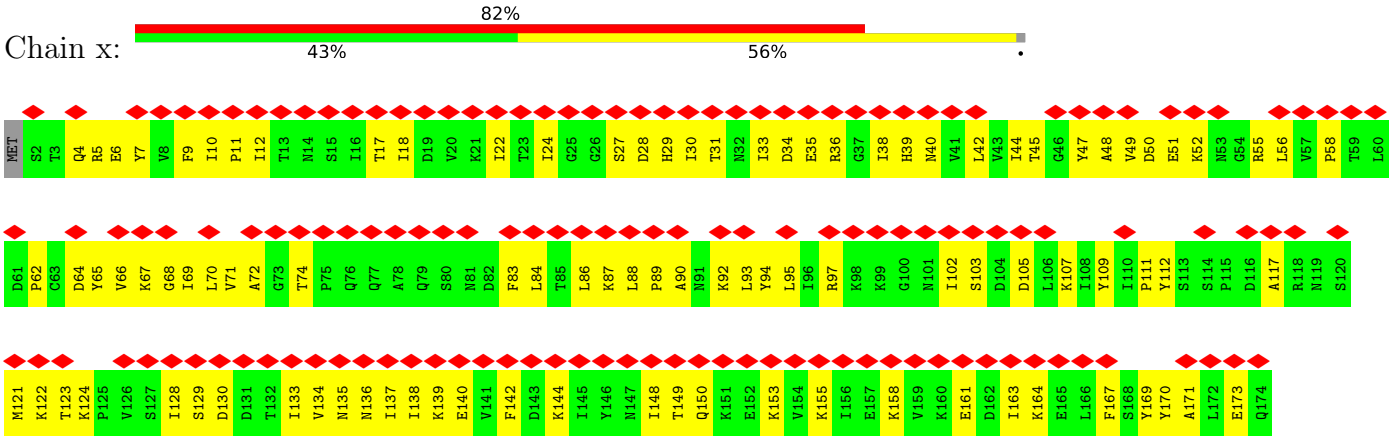
• Molecule 8: CRISPR-associated protein Cmrx

Chain w:



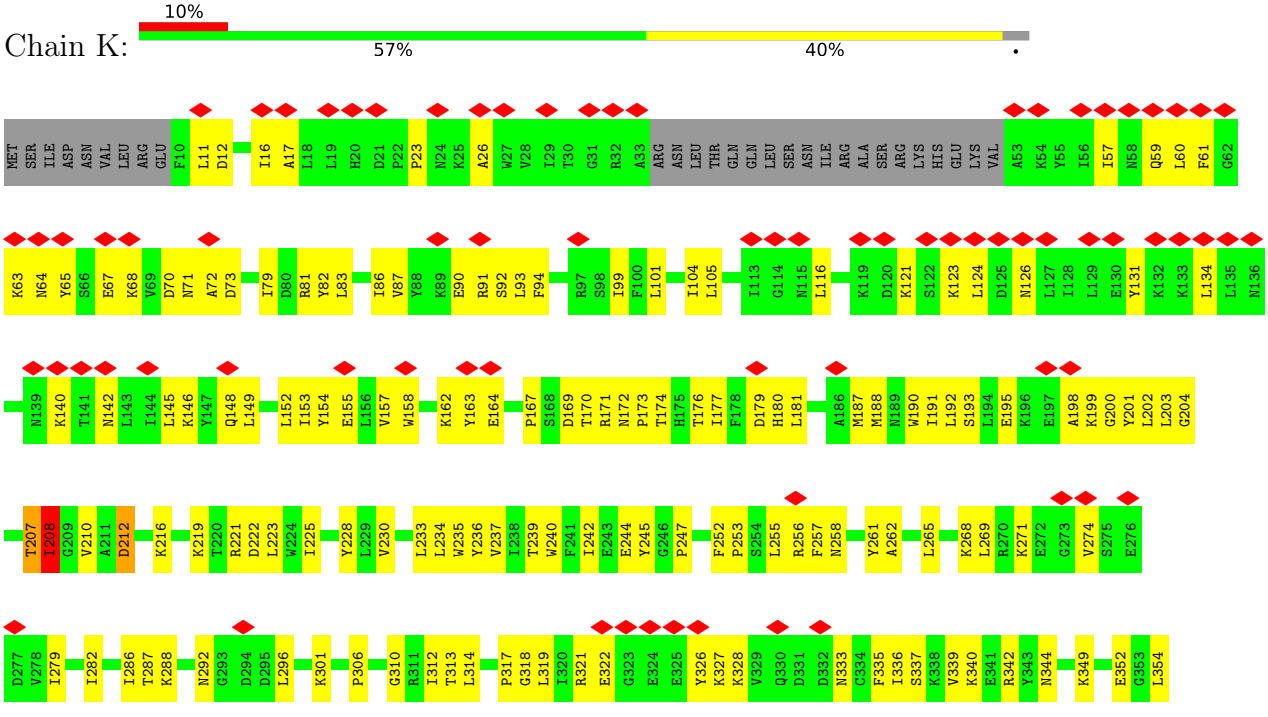
• Molecule 8: CRISPR-associated protein Cmrx

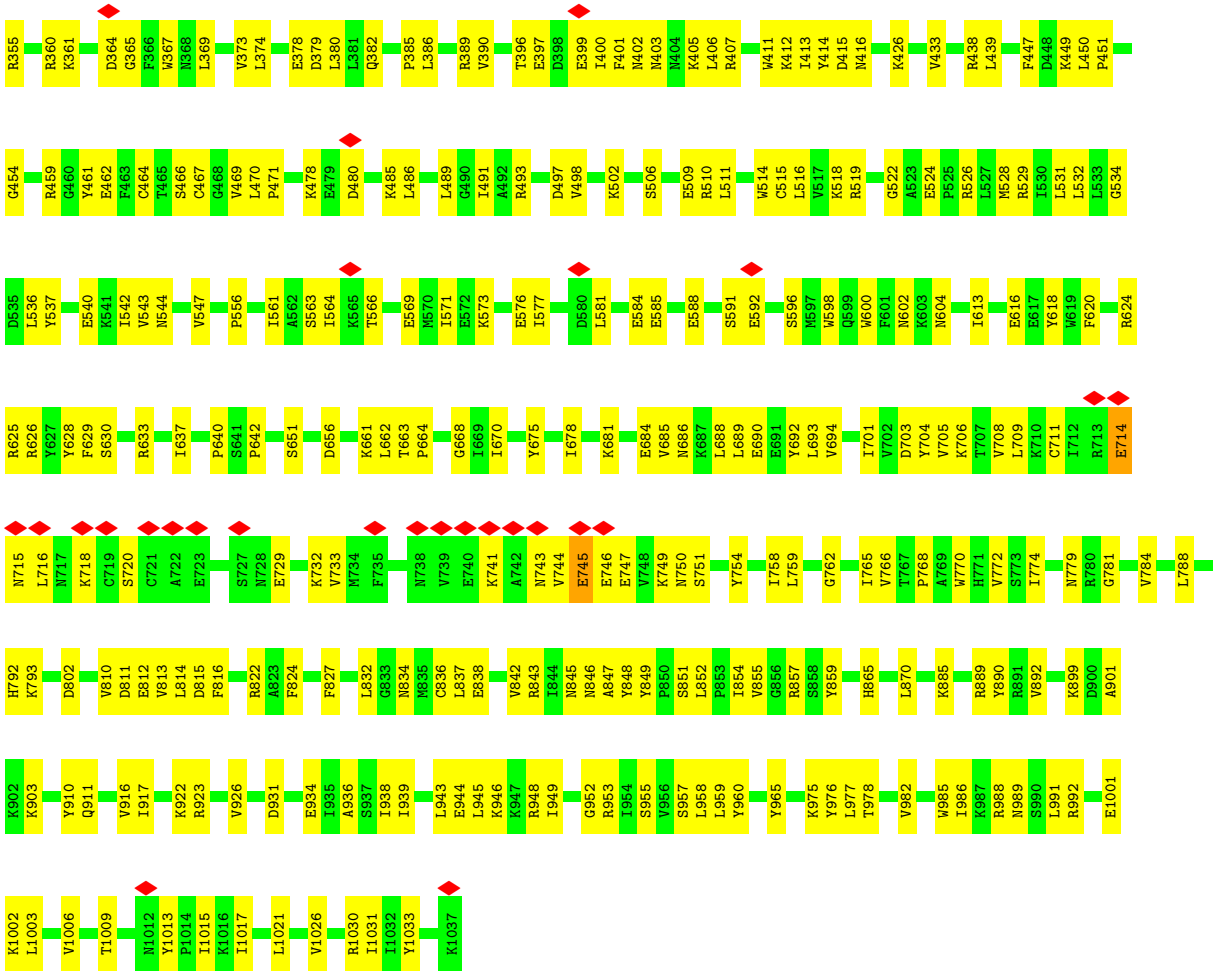
Chain x:



• Molecule 9: CRISPR-associated protein, Cmr2 family

Chain K:




R355 R360 K361 D364 G365 F366 W367 N368 L369 V373 L374 E378 D379 L380 L381 Q382 P385 L386 R389 V390 T396 E397 D398 E399 I400 F401 N402 N403 N404 K405 L406 R407 W411 K412 I413 Y414 D415 N416 K426 V433 R438 L439 F447 D448 K449 L450 P451
G454 R459 G460 Y461 E462 F463 C464 T465 S466 C467 G468 V469 L470 P471 K478 E479 D480 K485 L486 L489 G490 I491 A492 R493 D497 V498 K502 S506 E509 R510 L511 W514 C515 L516 W517 K518 R519 G522 A523 E524 P525 R526 L527 M528 R529 I530 L531 L532 L533 G534
D535 L536 Y537 E540 K541 I542 V543 N544 V547 P556 I561 A562 S563 I564 K565 T566 E569 K570 I571 E572 K573 E576 I577 D580 L581 E584 E585 E588 S591 E592 S596 M597 W598 Q599 W600 F601 N602 K603 N604 I613 E616 E617 Y618 W619 F620 R624
R625 R626 Y627 Y628 F629 S630 R633 I637 P640 S641 P642 S651 D656 K661 L662 T663 P664 G668 I669 I670 Y675 I678 K681 E684 V685 N686 K687 L688 L689 E690 E691 Y692 L693 V694 I701 V702 D703 Y704 V705 K706 T707 V708 L709 K710 C711 I712 R713 E714
N715 L716 N717 K718 C719 S720 C721 A722 E723 S727 N728 E729 K732 V733 M734 F735 N738 V739 E740 K741 A742 N743 V744 E745 E746 E747 V748 K749 N750 S751 Y754 I758 L759 G762 I765 V766 T767 P768 A769 W770 H771 V772 S773 I774 N779 R780 G781 V784 L788
H792 K793 D802 V810 D811 E812 V813 L814 D815 F816 R822 A823 F824 F827 L832 G833 N834 M835 C836 L837 E838 V842 R843 I844 N845 N846 A847 Y848 Y849 P850 S851 L852 P853 I854 V855 G856 R857 S858 Y859 H865 L870 K885 R889 Y890 R891 V892 K899 D900 A901
K902 K903 Y910 Q911 V916 I917 K922 R923 V926 D931 E934 I935 A936 S937 I938 I939 L943 E944 L945 K946 K947 R948 I949 G952 R953 I954 S955 V956 S957 L958 L959 Y960 Y965 K975 Y976 L977 T978 V982 W985 I986 K987 R988 N989 S990 L991 R992 E1001
K1002 L1003 V1006 T1009 N1012 Y1013 P1014 I1015 K1016 I1017 L1021 V1026 R1030 I1031 I1032 Y1033 K1037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82571	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	34.130	Depositor
Minimum map value	-15.312	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.723	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, 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	0.33	0/1275	0.41	0/1716
1	B	0.34	0/1283	0.46	0/1727
1	C	0.33	0/1283	0.40	0/1727
2	D	0.38	0/2318	0.46	1/3134 (0.0%)
2	E	0.38	0/2318	0.42	0/3134
2	F	0.39	0/2318	0.46	0/3134
2	G	0.36	0/2317	0.45	0/3133
3	H	0.29	0/2511	0.42	0/3382
4	I	0.34	0/2325	0.43	0/3138
5	J	0.28	0/3956	0.45	1/5319 (0.0%)
6	U	0.37	0/1042	0.34	0/1620
7	V	0.49	0/1171	0.47	0/1823
8	L	0.24	0/1400	0.48	0/1895
8	M	0.23	0/1400	0.49	1/1895 (0.1%)
8	N	0.18	0/1400	0.48	1/1895 (0.1%)
8	O	0.20	0/1400	0.47	0/1895
8	P	0.19	0/1400	0.52	0/1895
8	Q	0.19	0/1400	0.44	0/1895
8	R	0.17	0/1400	0.44	0/1895
8	S	0.18	0/1400	0.50	0/1895
8	T	0.18	0/1400	0.47	0/1895
8	W	0.17	0/1400	0.54	0/1895
8	X	0.19	0/1400	0.50	0/1895
8	l	0.25	0/1400	0.49	0/1895
8	m	0.25	0/1400	0.49	0/1895
8	n	0.19	0/1400	0.50	1/1895 (0.1%)
8	o	0.21	0/1400	0.50	0/1895
8	p	0.18	0/1400	0.46	0/1895
8	q	0.20	0/1400	0.46	0/1895
8	r	0.19	0/1400	0.48	0/1895
8	s	0.17	0/1400	0.47	0/1895
8	t	0.18	0/1400	0.52	0/1895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
8	w	0.17	0/1400	0.46	0/1895
8	x	0.18	0/1400	0.49	0/1895
9	K	0.24	0/8452	0.45	1/11416 (0.0%)
All	All	0.27	0/63369	0.46	6/86093 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
5	J	0	2
8	P	0	1
8	S	0	1
8	X	0	1
9	K	0	1
All	All	0	7

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	154	VAL	N-CA-C	-7.51	104.17	112.80
2	D	285	VAL	N-CA-C	-6.16	107.86	113.71
5	J	271	ILE	N-CA-C	-5.99	107.05	111.90
9	K	208	ILE	N-CA-C	5.48	116.97	111.00
8	N	24	ILE	N-CA-C	-5.25	107.47	111.62

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	115	CYS	Peptide
5	J	302	CYS	Peptide
5	J	398	THR	Peptide
8	P	14	ASN	Peptide
8	S	153	LYS	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	1253	0	1287	39	0
1	B	1261	0	1298	38	0
1	C	1261	0	1298	27	0
2	D	2274	0	2342	44	0
2	E	2274	0	2342	59	0
2	F	2274	0	2342	58	0
2	G	2273	0	2339	55	0
3	H	2468	0	2523	91	0
4	I	2282	0	2331	47	0
5	J	3889	0	3975	118	0
6	U	933	0	471	25	0
7	V	1045	0	531	39	0
8	L	1378	0	1418	50	0
8	M	1378	0	1418	66	0
8	N	1378	0	1417	67	0
8	O	1378	0	1417	62	0
8	P	1378	0	1418	70	0
8	Q	1378	0	1417	63	0
8	R	1378	0	1417	57	0
8	S	1378	0	1417	70	0
8	T	1378	0	1418	60	0
8	W	1378	0	1418	65	0
8	X	1378	0	1417	80	0
8	l	1378	0	1417	45	0
8	m	1378	0	1417	58	0
8	n	1378	0	1418	85	0
8	o	1378	0	1418	60	0
8	p	1378	0	1417	53	0
8	q	1378	0	1418	74	0
8	r	1378	0	1418	51	0
8	s	1378	0	1418	54	0
8	t	1378	0	1418	85	0
8	w	1378	0	1417	72	0
8	x	1378	0	1418	89	0
9	K	8282	0	8427	318	0
10	K	1	0	0	0	0
11	K	62	0	26	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	K	3	0	0	0	0
All	All	62151	0	62718	2233	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 18.

The worst 5 of 2233 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)
9:K:208:ILE:CD1	9:K:389:ARG:HG3	1.86	1.04
8:x:123:THR:HA	8:x:171:ALA:O	1.64	0.96
9:K:208:ILE:HD11	9:K:389:ARG:HG3	1.48	0.94
8:w:85:THR:HA	8:w:108:ILE:O	1.69	0.92
8:M:37:GLY:H	8:M:158:LYS:HZ3	1.20	0.86

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	151/155 (97%)	143 (95%)	8 (5%)	0	100	100
1	B	152/155 (98%)	146 (96%)	5 (3%)	1 (1%)	18	27
1	C	152/155 (98%)	147 (97%)	5 (3%)	0	100	100
2	D	283/286 (99%)	259 (92%)	24 (8%)	0	100	100
2	E	283/286 (99%)	264 (93%)	19 (7%)	0	100	100
2	F	283/286 (99%)	252 (89%)	30 (11%)	1 (0%)	30	42
2	G	283/286 (99%)	242 (86%)	41 (14%)	0	100	100
3	H	300/313 (96%)	270 (90%)	30 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	282/296 (95%)	263 (93%)	19 (7%)	0	100	100
5	J	473/476 (99%)	424 (90%)	47 (10%)	2 (0%)	30	42
8	L	171/174 (98%)	136 (80%)	33 (19%)	2 (1%)	10	15
8	M	171/174 (98%)	134 (78%)	35 (20%)	2 (1%)	10	15
8	N	171/174 (98%)	138 (81%)	32 (19%)	1 (1%)	21	30
8	O	171/174 (98%)	138 (81%)	33 (19%)	0	100	100
8	P	171/174 (98%)	130 (76%)	40 (23%)	1 (1%)	21	30
8	Q	171/174 (98%)	125 (73%)	45 (26%)	1 (1%)	21	30
8	R	171/174 (98%)	137 (80%)	34 (20%)	0	100	100
8	S	171/174 (98%)	134 (78%)	35 (20%)	2 (1%)	10	15
8	T	171/174 (98%)	130 (76%)	39 (23%)	2 (1%)	10	15
8	W	171/174 (98%)	134 (78%)	34 (20%)	3 (2%)	6	8
8	X	171/174 (98%)	139 (81%)	31 (18%)	1 (1%)	21	30
8	l	171/174 (98%)	138 (81%)	32 (19%)	1 (1%)	21	30
8	m	171/174 (98%)	131 (77%)	39 (23%)	1 (1%)	21	30
8	n	171/174 (98%)	139 (81%)	32 (19%)	0	100	100
8	o	171/174 (98%)	138 (81%)	33 (19%)	0	100	100
8	p	171/174 (98%)	135 (79%)	34 (20%)	2 (1%)	10	15
8	q	171/174 (98%)	134 (78%)	36 (21%)	1 (1%)	21	30
8	r	171/174 (98%)	138 (81%)	32 (19%)	1 (1%)	21	30
8	s	171/174 (98%)	137 (80%)	32 (19%)	2 (1%)	10	15
8	t	171/174 (98%)	132 (77%)	37 (22%)	2 (1%)	10	15
8	w	171/174 (98%)	137 (80%)	33 (19%)	1 (1%)	21	30
8	x	171/174 (98%)	129 (75%)	41 (24%)	1 (1%)	21	30
9	K	1005/1037 (97%)	892 (89%)	111 (11%)	2 (0%)	43	57
All	All	7409/7559 (98%)	6265 (85%)	1111 (15%)	33 (0%)	31	42

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	161	LYS
8	W	35	GLU
5	J	303	ILE

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Mol	Chain	Res	Type
8	Q	51	GLU
8	S	51	GLU

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	134/136 (98%)	134 (100%)	0	100	100
1	B	135/136 (99%)	135 (100%)	0	100	100
1	C	135/136 (99%)	133 (98%)	2 (2%)	57	75
2	D	252/253 (100%)	252 (100%)	0	100	100
2	E	252/253 (100%)	251 (100%)	1 (0%)	84	92
2	F	252/253 (100%)	251 (100%)	1 (0%)	84	92
2	G	251/253 (99%)	250 (100%)	1 (0%)	84	92
3	H	272/280 (97%)	272 (100%)	0	100	100
4	I	255/266 (96%)	255 (100%)	0	100	100
5	J	442/445 (99%)	441 (100%)	1 (0%)	87	94
8	L	159/160 (99%)	159 (100%)	0	100	100
8	M	159/160 (99%)	159 (100%)	0	100	100
8	N	159/160 (99%)	158 (99%)	1 (1%)	78	88
8	O	159/160 (99%)	159 (100%)	0	100	100
8	P	159/160 (99%)	159 (100%)	0	100	100
8	Q	159/160 (99%)	159 (100%)	0	100	100
8	R	159/160 (99%)	159 (100%)	0	100	100
8	S	159/160 (99%)	158 (99%)	1 (1%)	78	88
8	T	159/160 (99%)	159 (100%)	0	100	100
8	W	159/160 (99%)	159 (100%)	0	100	100
8	X	159/160 (99%)	159 (100%)	0	100	100
8	l	159/160 (99%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	m	159/160 (99%)	158 (99%)	1 (1%)	78 88
8	n	159/160 (99%)	159 (100%)	0	100 100
8	o	159/160 (99%)	159 (100%)	0	100 100
8	p	159/160 (99%)	159 (100%)	0	100 100
8	q	159/160 (99%)	159 (100%)	0	100 100
8	r	159/160 (99%)	159 (100%)	0	100 100
8	s	159/160 (99%)	159 (100%)	0	100 100
8	t	159/160 (99%)	159 (100%)	0	100 100
8	w	159/160 (99%)	159 (100%)	0	100 100
8	x	159/160 (99%)	159 (100%)	0	100 100
9	K	921/949 (97%)	917 (100%)	4 (0%)	84 92
All	All	6799/6880 (99%)	6786 (100%)	13 (0%)	85 94

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	S	3	THR
8	m	86	LEU
9	K	774	ILE
9	K	208	ILE
9	K	212	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
8	S	32	ASN
9	K	875	ASN
8	m	101	ASN
9	K	846	ASN
8	x	136	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	U	43/46 (93%)	16 (37%)	3 (6%)
7	V	48/51 (94%)	9 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	91/97 (93%)	25 (27%)	3 (3%)

5 of 25 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	U	3	U
6	U	4	U
6	U	5	A
6	U	6	A
6	U	7	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	U	5	A
6	U	41	A
6	U	42	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
11	ANP	K	1103	12	33,33,33	0.89	3 (9%)	45,52,52	0.66	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	ANP	K	1102	12	33,33,33	1.23	4 (12%)	45,52,52	1.47	5 (11%)

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
11	ANP	K	1103	12	-	5/18/38/38	0/3/3/3
11	ANP	K	1102	12	-	9/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	1102	ANP	PG-O2G	-3.31	1.48	1.56
11	K	1102	ANP	PB-O2B	-3.20	1.48	1.56
11	K	1102	ANP	PG-O3G	-2.83	1.49	1.56
11	K	1103	ANP	PB-O3A	-2.74	1.55	1.59
11	K	1103	ANP	PG-O1G	2.19	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	1102	ANP	O1B-PB-N3B	6.13	120.80	111.77
11	K	1102	ANP	O2B-PB-O1B	4.55	119.62	109.87
11	K	1102	ANP	O3A-PB-N3B	-3.36	97.28	106.59
11	K	1102	ANP	O3G-PG-O1G	-2.35	107.55	113.45
11	K	1103	ANP	O2G-PG-O1G	-2.35	107.55	113.45

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1102	ANP	PB-N3B-PG-O1G
11	K	1102	ANP	PG-N3B-PB-O1B
11	K	1102	ANP	C5'-O5'-PA-O1A
11	K	1102	ANP	C5'-O5'-PA-O2A
11	K	1102	ANP	C5'-O5'-PA-O3A

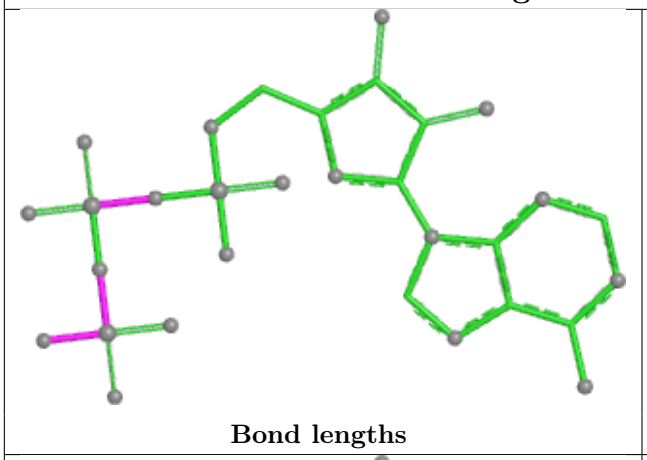
There are no ring outliers.

2 monomers are involved in 9 short contacts:

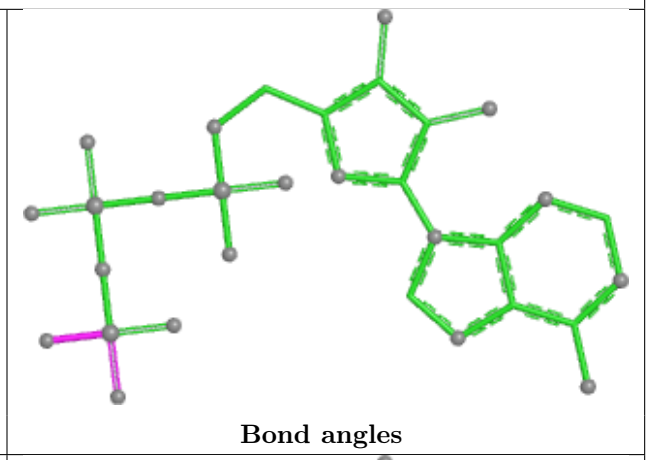
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1103	ANP	3	0
11	K	1102	ANP	6	0

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

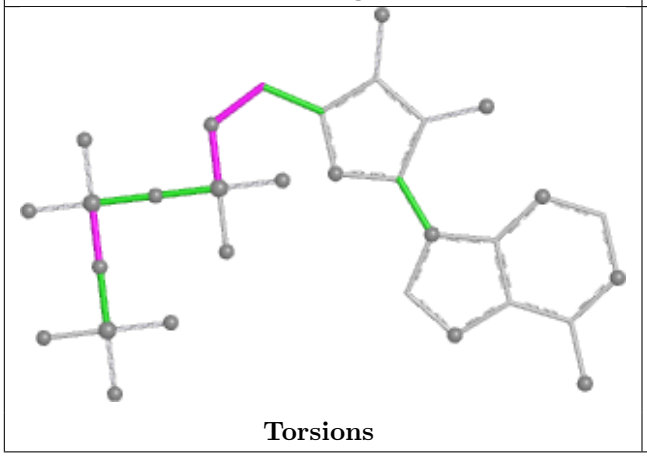
Ligand ANP K 1103



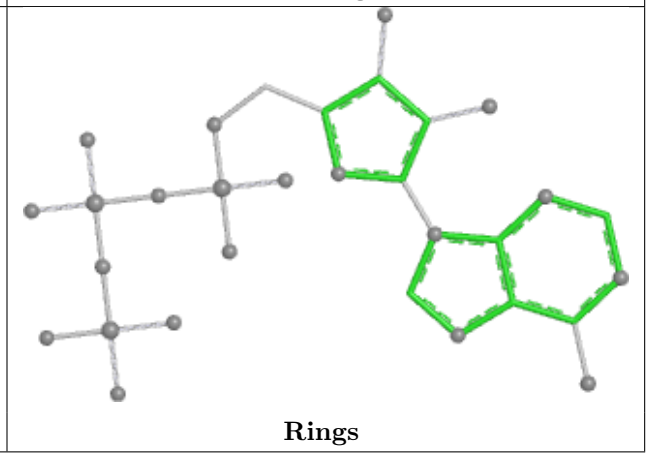
Bond lengths



Bond angles

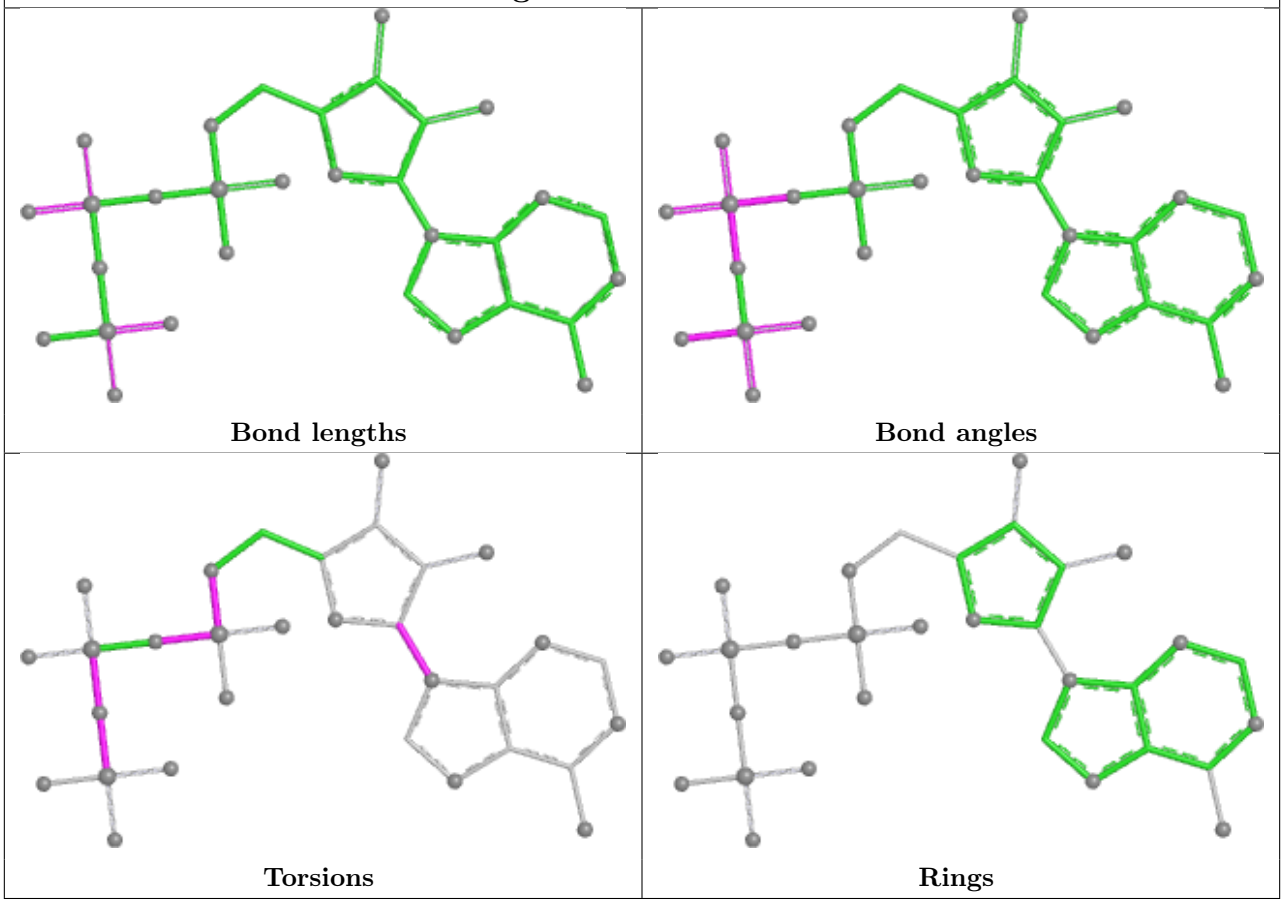


Torsions



Rings

Ligand ANP K 1102



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

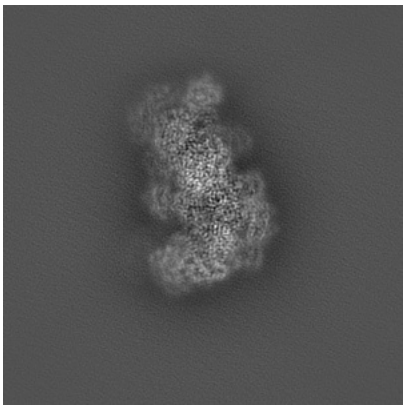
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10117. These allow visual inspection of the internal detail of the map and identification of artifacts.

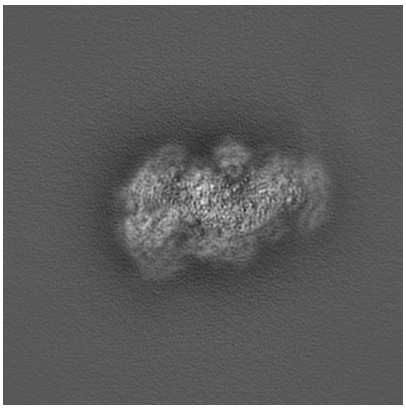
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

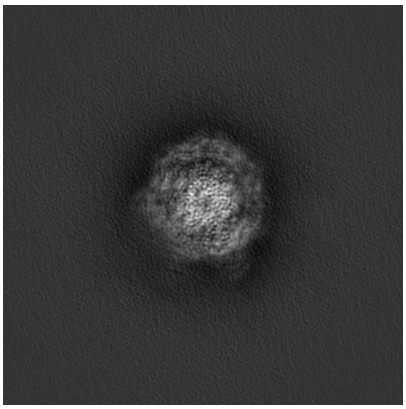
6.1.1 Primary map



X

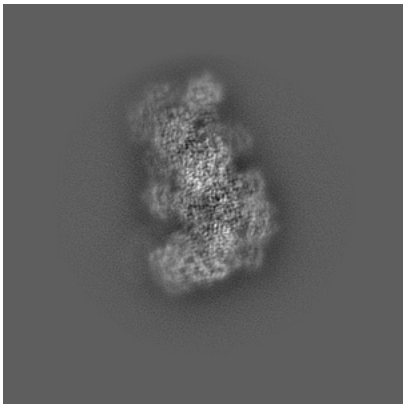


Y

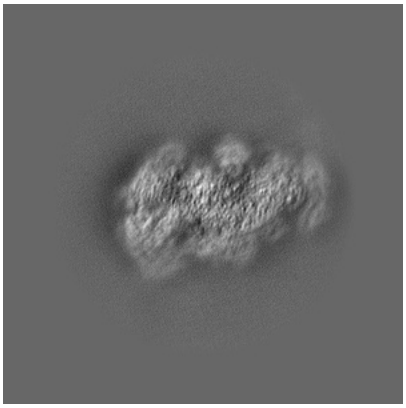


Z

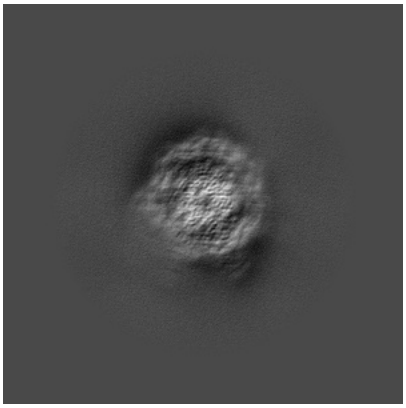
6.1.2 Raw map



X



Y

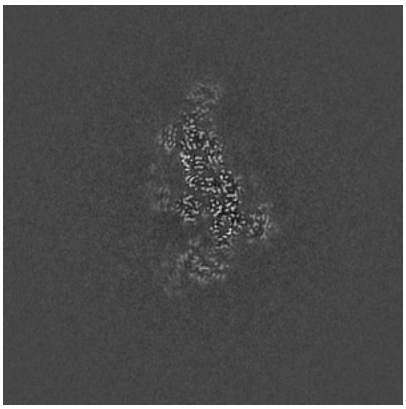


Z

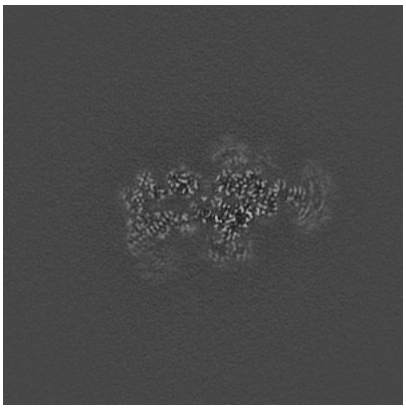
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

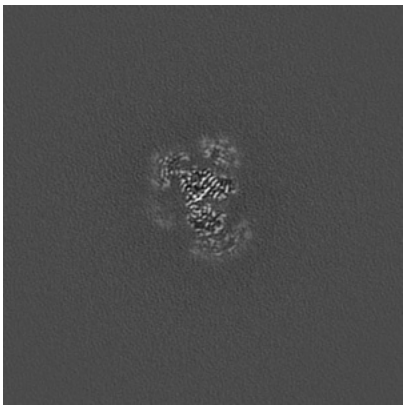
6.2.1 Primary map



X Index: 250

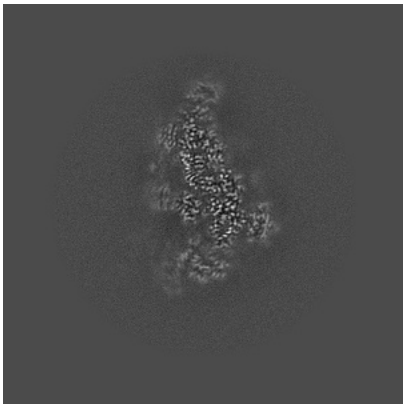


Y Index: 250

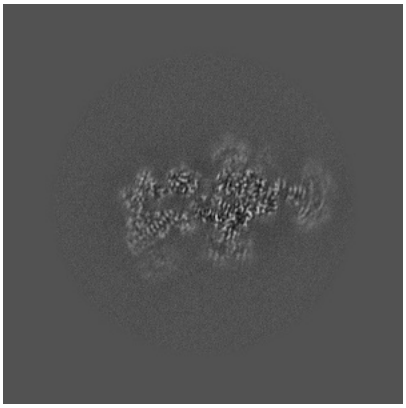


Z Index: 250

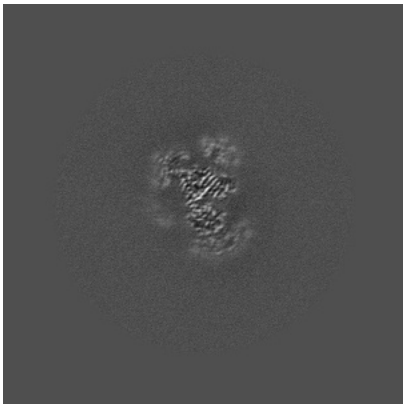
6.2.2 Raw map



X Index: 250



Y Index: 250

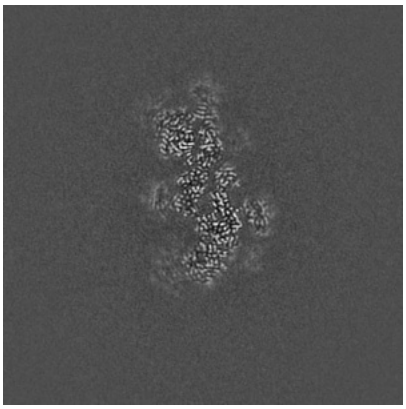


Z Index: 250

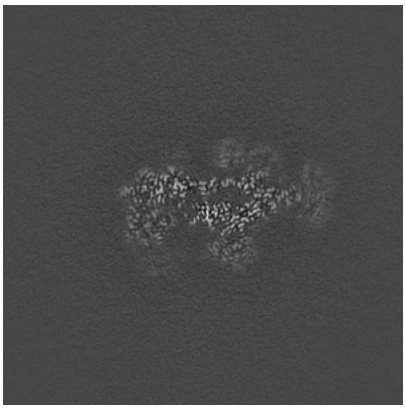
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

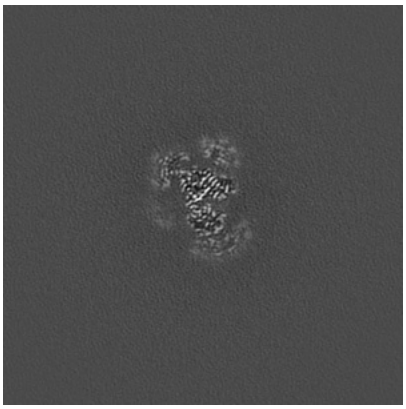
6.3.1 Primary map



X Index: 267

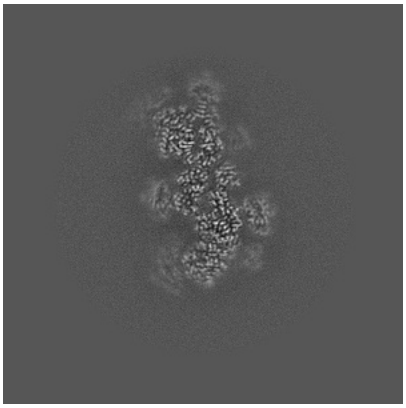


Y Index: 259

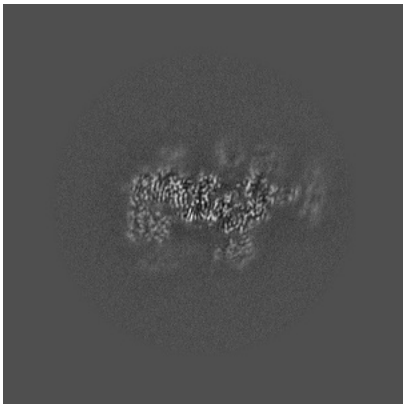


Z Index: 250

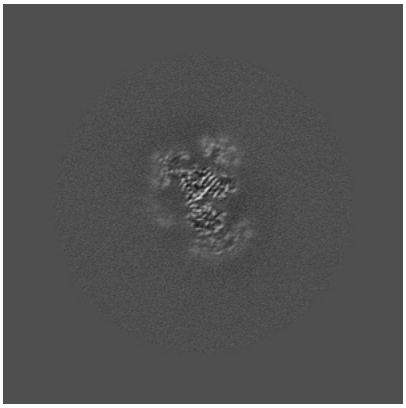
6.3.2 Raw map



X Index: 267



Y Index: 264

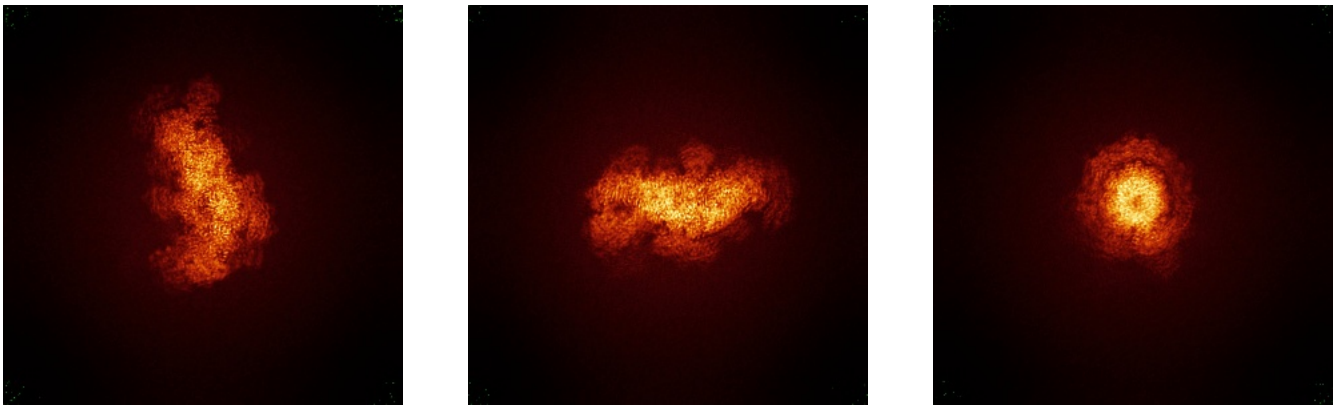


Z Index: 250

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

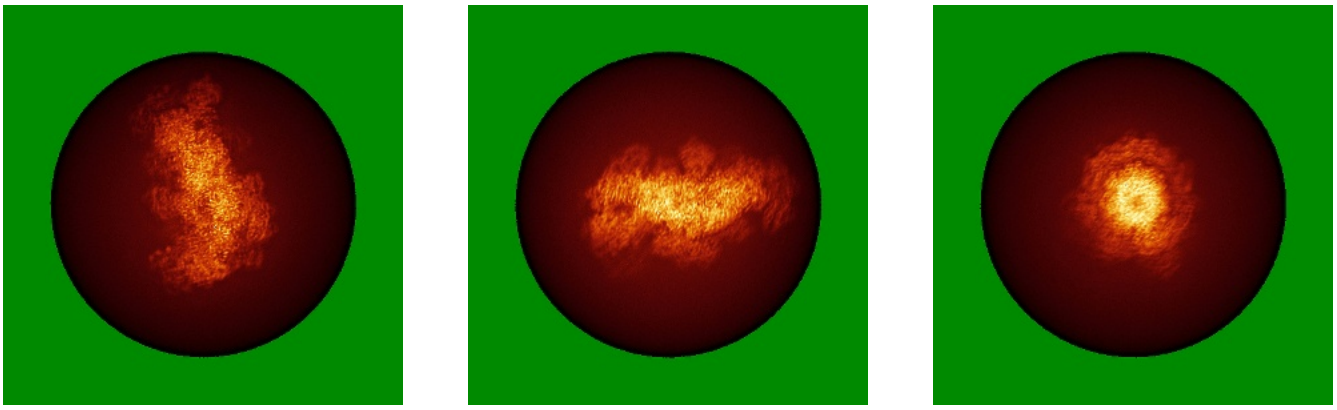
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

6.5 Orthogonal surface views (i)

This section was not generated.

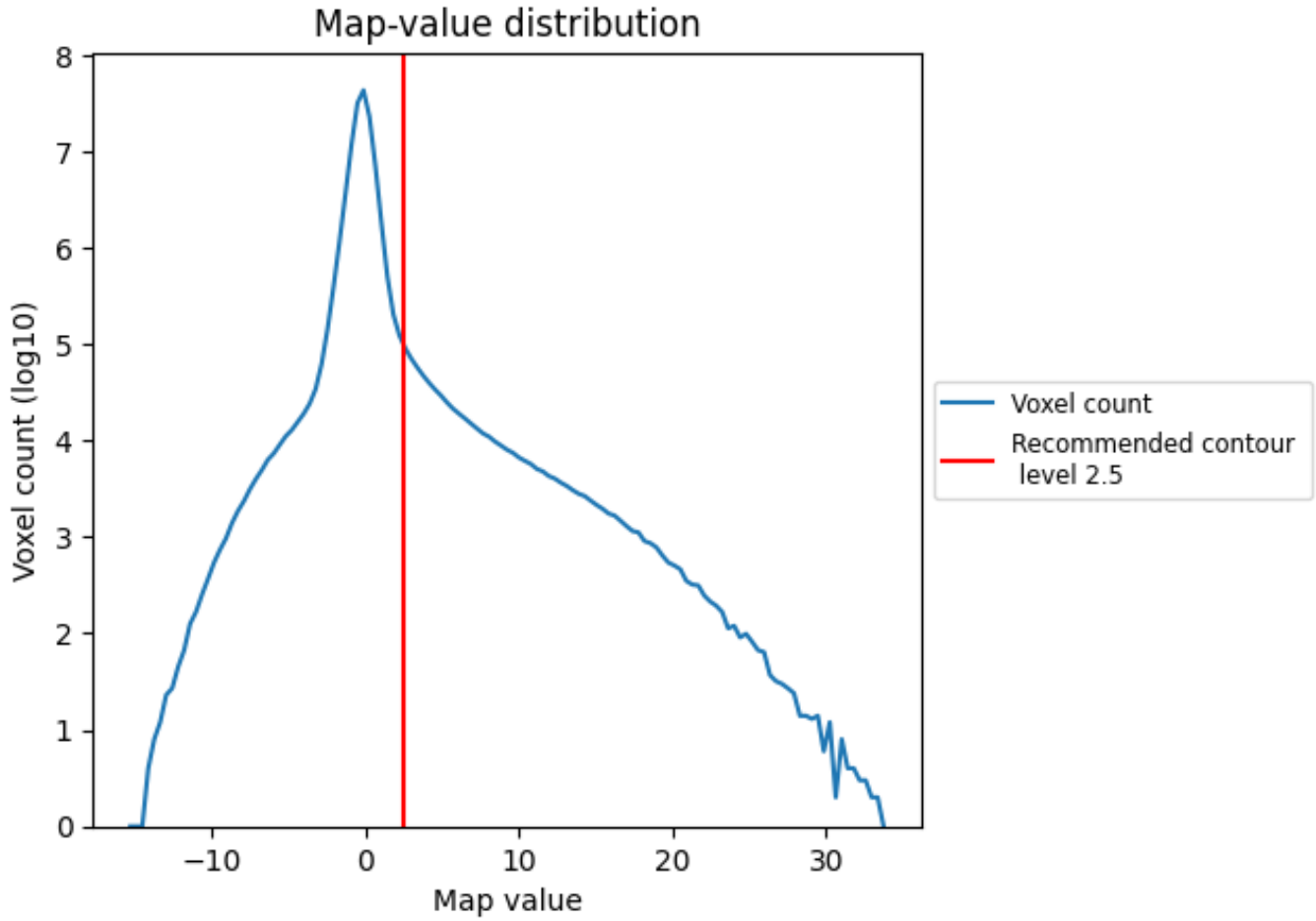
6.6 Mask visualisation (i)

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

7 Map analysis

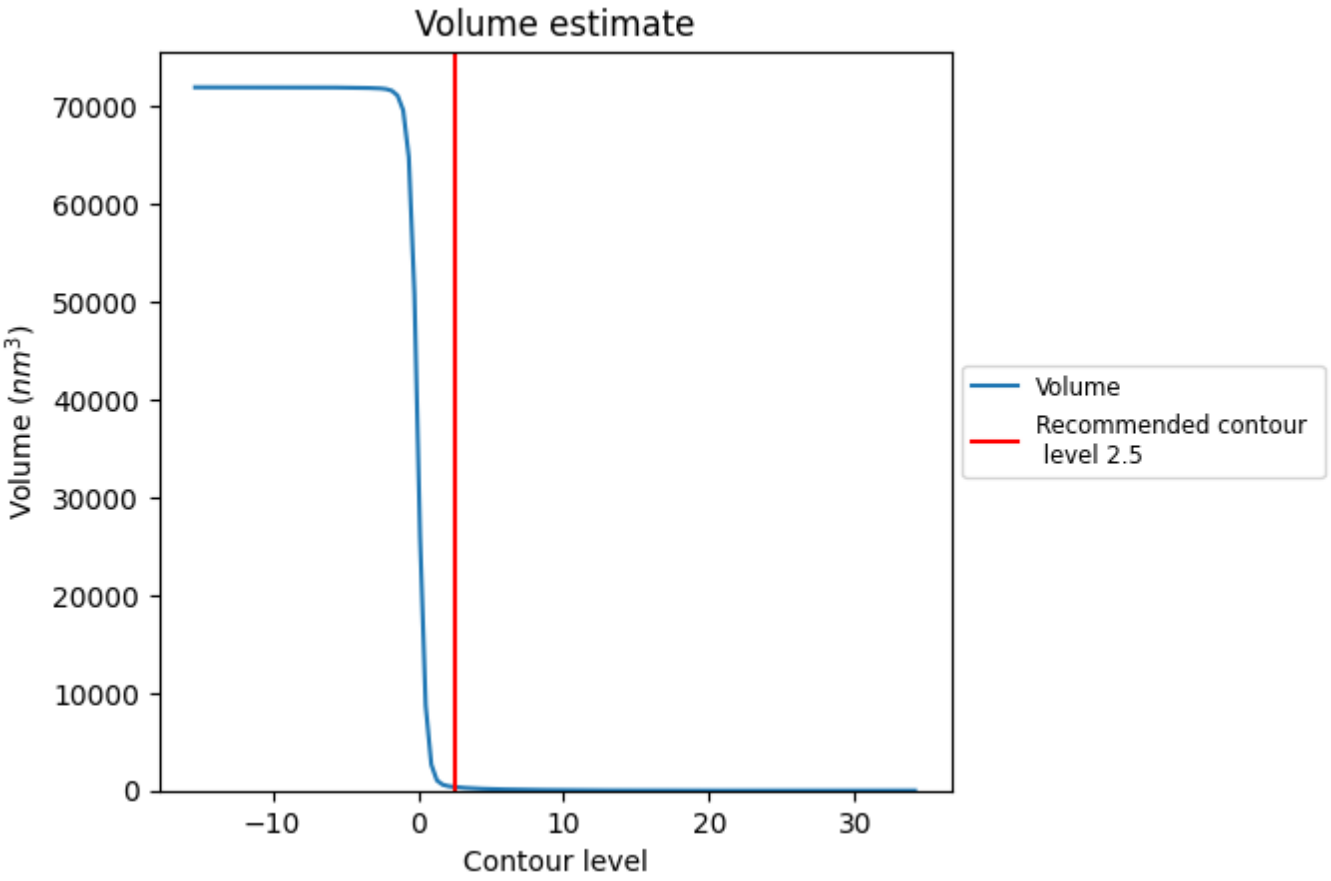
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

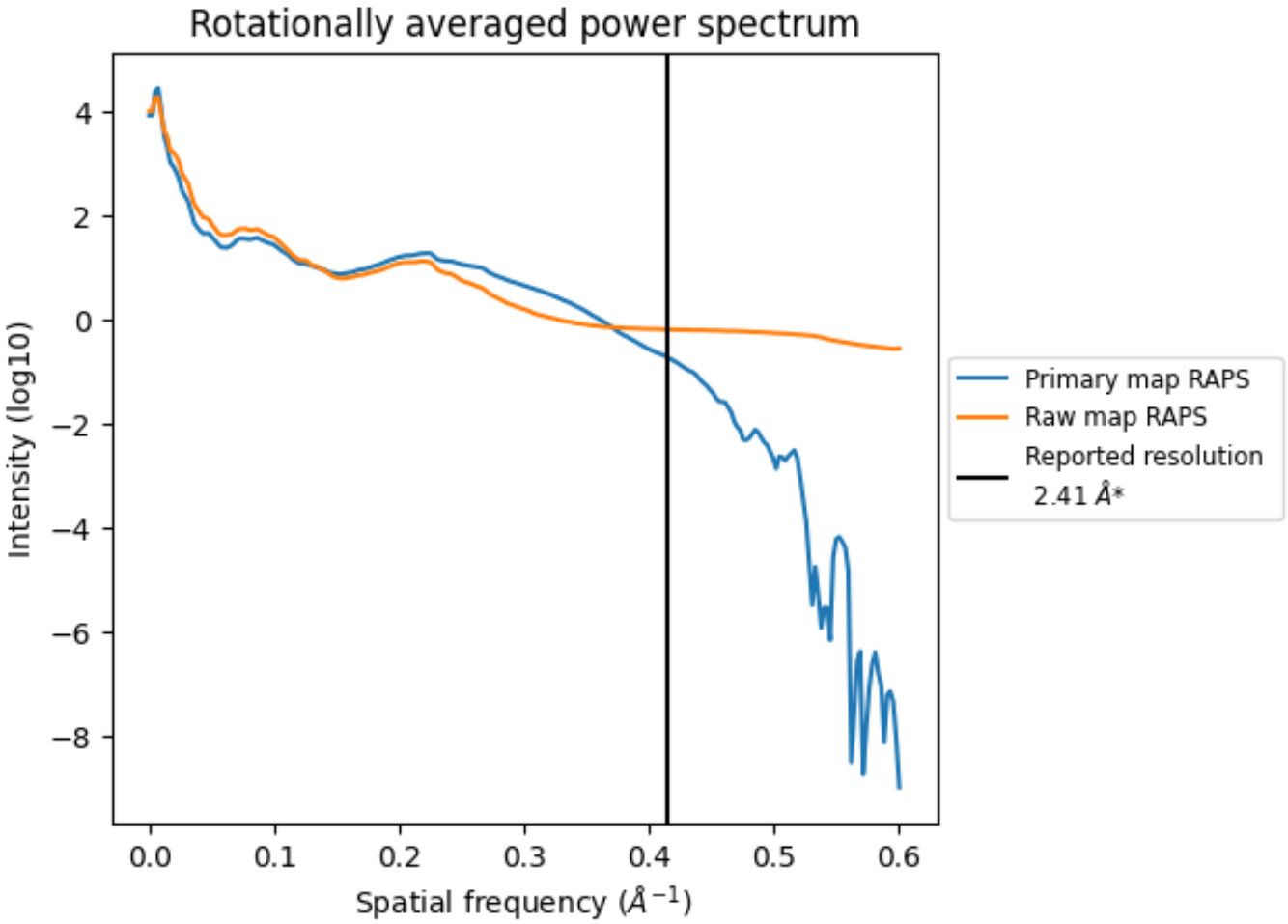
7.2 Volume estimate (i)



The volume at the recommended contour level is 367 nm^3; this corresponds to an approximate mass of 332 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)

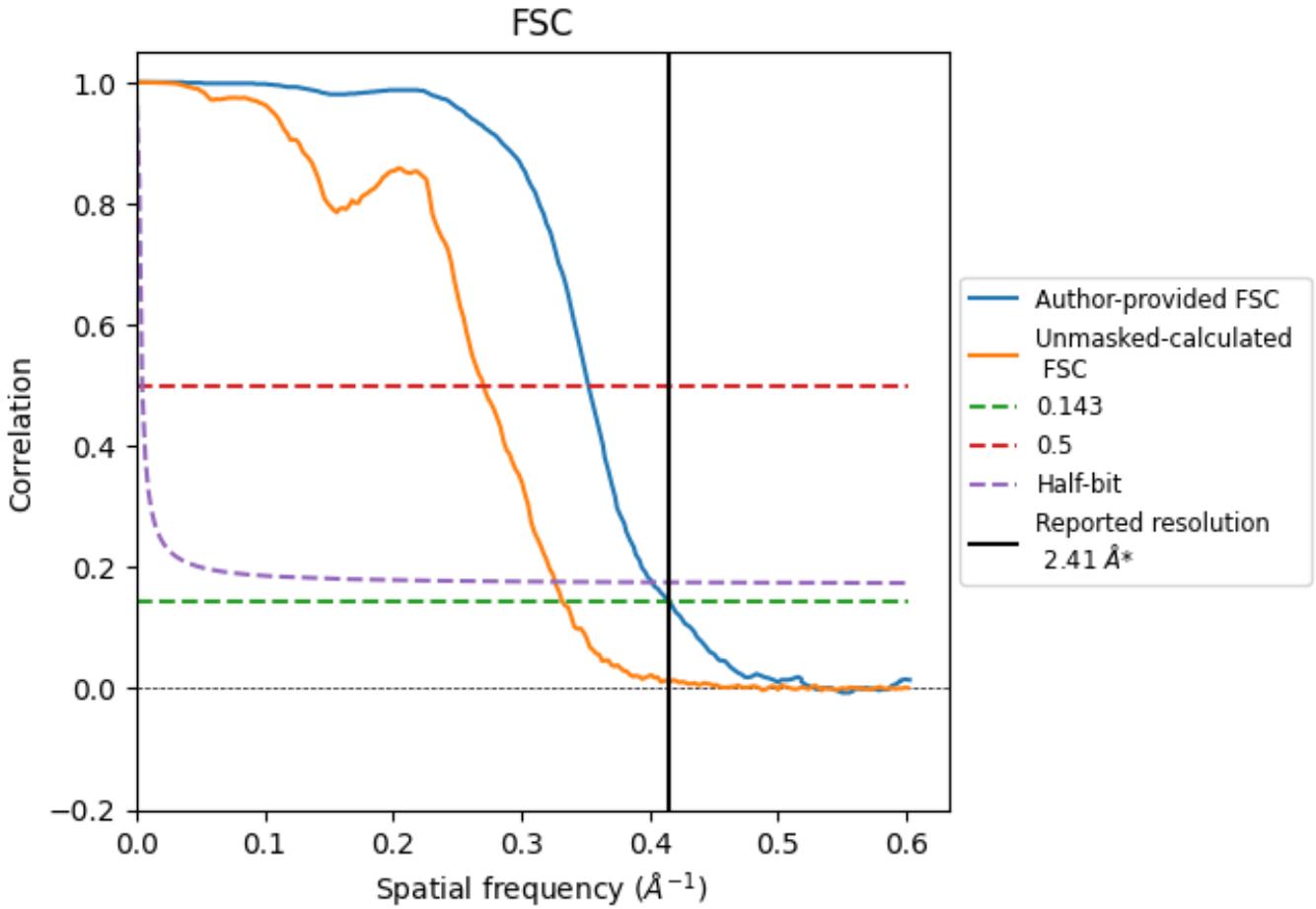


*Reported resolution corresponds to spatial frequency of 0.415 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.415 Å^{-1}

8.2 Resolution estimates (i)

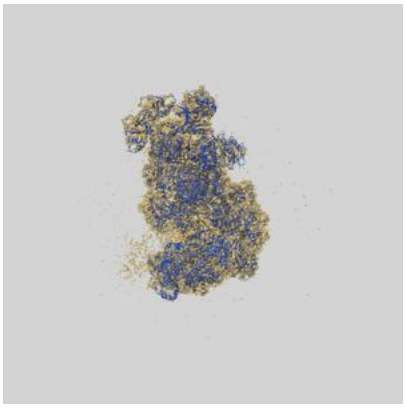
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.84	2.49
Unmasked-calculated*	3.01	3.70	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.01 differs from the reported value 2.41 by more than 10 %

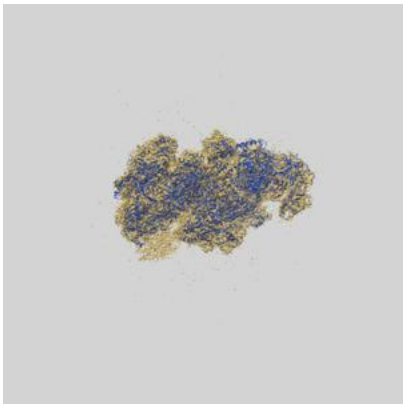
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10117 and PDB model 6S8B. Per-residue inclusion information can be found in section 3 on page 9.

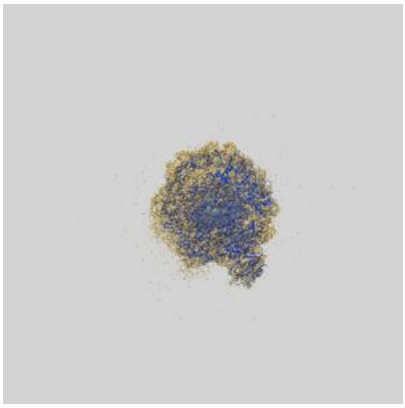
9.1 Map-model overlay



X



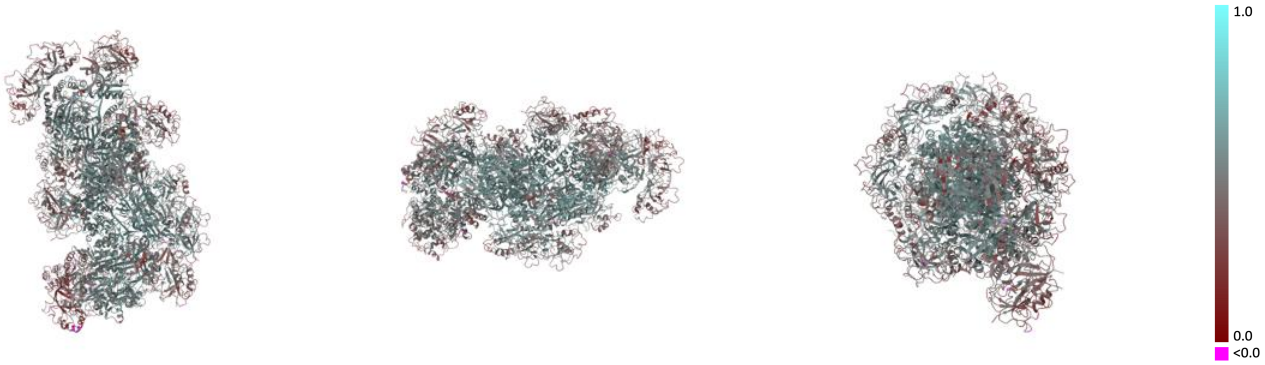
Y



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.

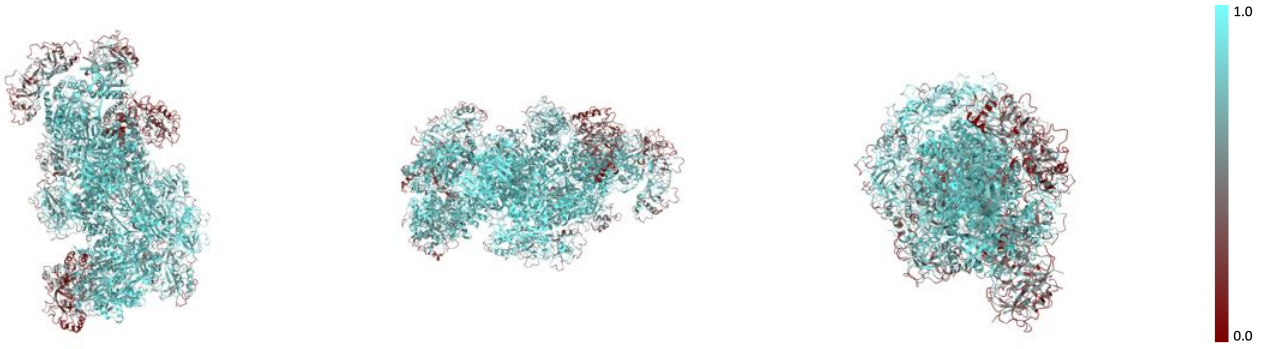
9.2 Q-score mapped to coordinate model (i)



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.

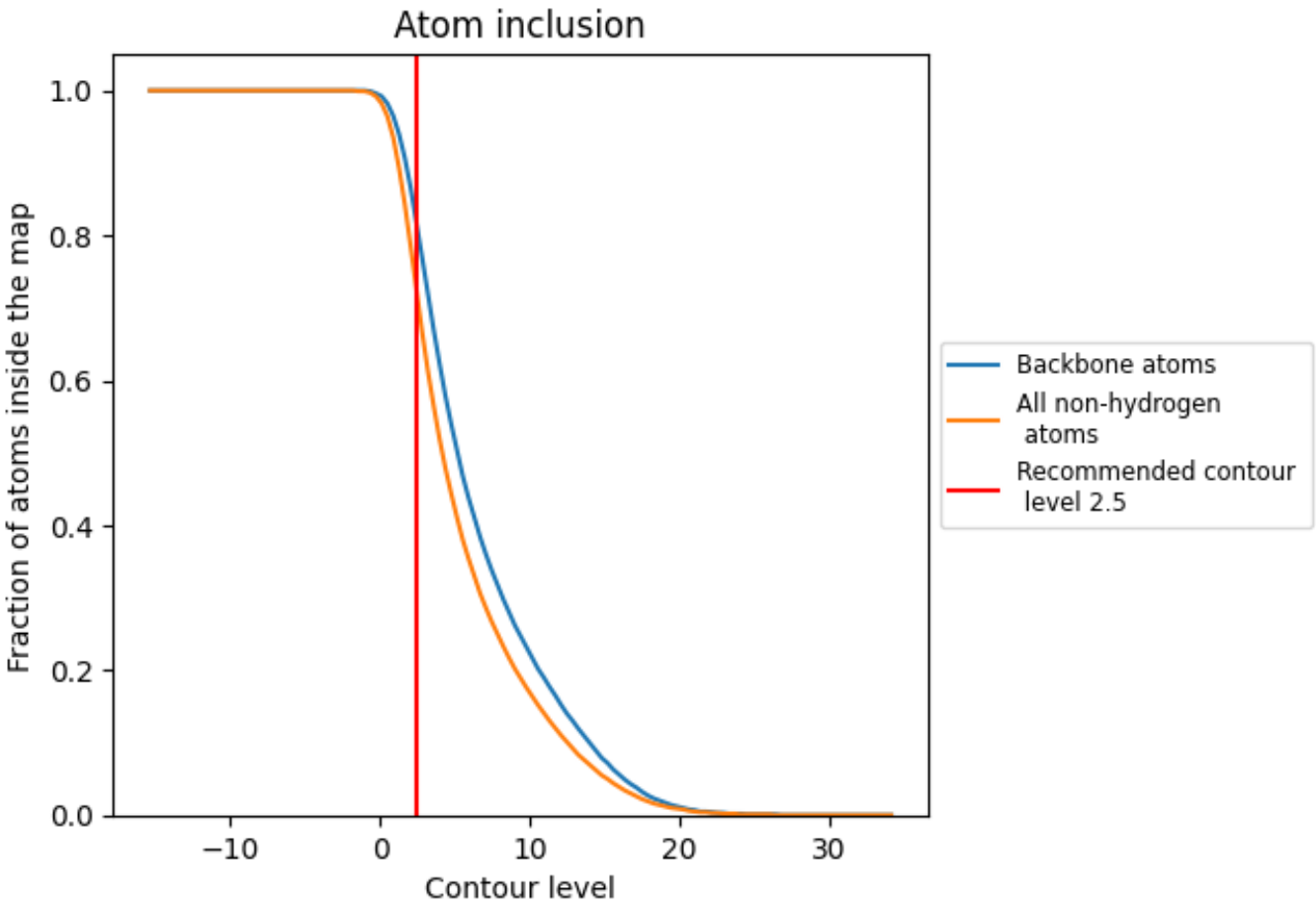
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 72% 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	0.7180	0.4800
A	0.9120	0.5820
B	0.9190	0.5870
C	0.9150	0.5820
D	0.9340	0.5970
E	0.9240	0.5950
F	0.9300	0.5920
G	0.9060	0.5720
H	0.8890	0.5450
I	0.9160	0.5850
J	0.8340	0.5320
K	0.7500	0.4600
L	0.8030	0.4670
M	0.8180	0.4750
N	0.6180	0.4050
O	0.6900	0.4550
P	0.5410	0.4470
Q	0.6630	0.4240
R	0.6800	0.4240
S	0.2460	0.3730
T	0.5560	0.3890
U	0.8870	0.5720
V	0.9620	0.6020
W	0.3900	0.3870
X	0.2530	0.3200
l	0.8030	0.4730
m	0.8400	0.4810
n	0.6010	0.3830
o	0.6860	0.4550
p	0.5820	0.4470
q	0.6750	0.4250
r	0.7120	0.4340
s	0.2540	0.3800
t	0.4470	0.3670
w	0.3870	0.3600
x	0.2030	0.3260

