wwPDB EM Validation Summary Report (i)

Nov 9, 2022 – 02:55 AM JST

PDB ID	:	6AHF
EMDB ID	:	EMD-9625
Title	:	CryoEM Reconstruction of Hsp104 N728A Hexamer
Authors	:	Zhang, X.; Zhang, L.; Zhang, S.
Deposited on	:	2018-08-17
Resolution	:	6.78 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 (i)) were used in the production of this report:

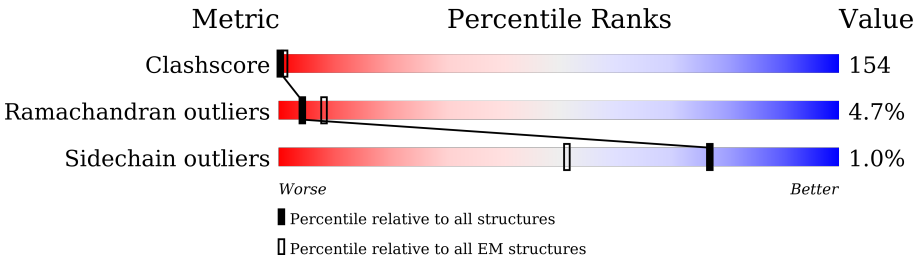
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.78 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	908	6% 7% 51% 6% 36%
1	B	908	9% 17% 56% 8% 19%
1	C	908	14% 19% 66% 9% • 5%
1	D	908	14% 19% 67% 8% • 5%
1	E	908	6% 5% 64% 8% 22%
1	F	908	6% 7% 48% 7% 37%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AGS	C	1001	-	-	X	-
2	AGS	D	1001	-	-	X	-
2	AGS	E	1001	-	-	X	-
2	AGS	E	1002	-	-	X	-
2	AGS	F	1001	-	-	X	-
2	AGS	F	1002	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 32108 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.

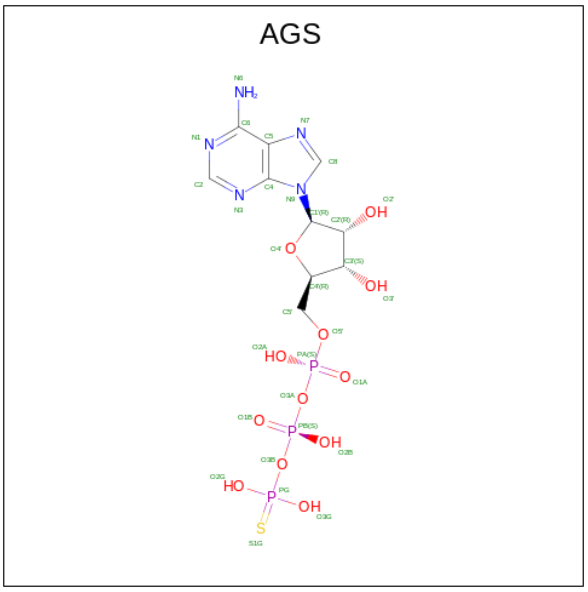
- Molecule 1 is a protein called Heat shock protein 104.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total 4456	C 2803	N 773	O 862	S 18	0	0
1	B	737	Total 5142	C 3152	N 948	O 1024	S 18	0	0
1	C	865	Total 6162	C 3769	N 1133	O 1241	S 19	0	0
1	D	865	Total 6170	C 3778	N 1133	O 1240	S 19	0	0
1	E	705	Total 5512	C 3443	N 973	O 1078	S 18	0	0
1	F	574	Total 4480	C 2821	N 783	O 858	S 18	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	728	ALA	ASN	engineered mutation	UNP P31539
B	728	ALA	ASN	engineered mutation	UNP P31539
C	728	ALA	ASN	engineered mutation	UNP P31539
D	728	ALA	ASN	engineered mutation	UNP P31539
E	728	ALA	ASN	engineered mutation	UNP P31539
F	728	ALA	ASN	engineered mutation	UNP P31539

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



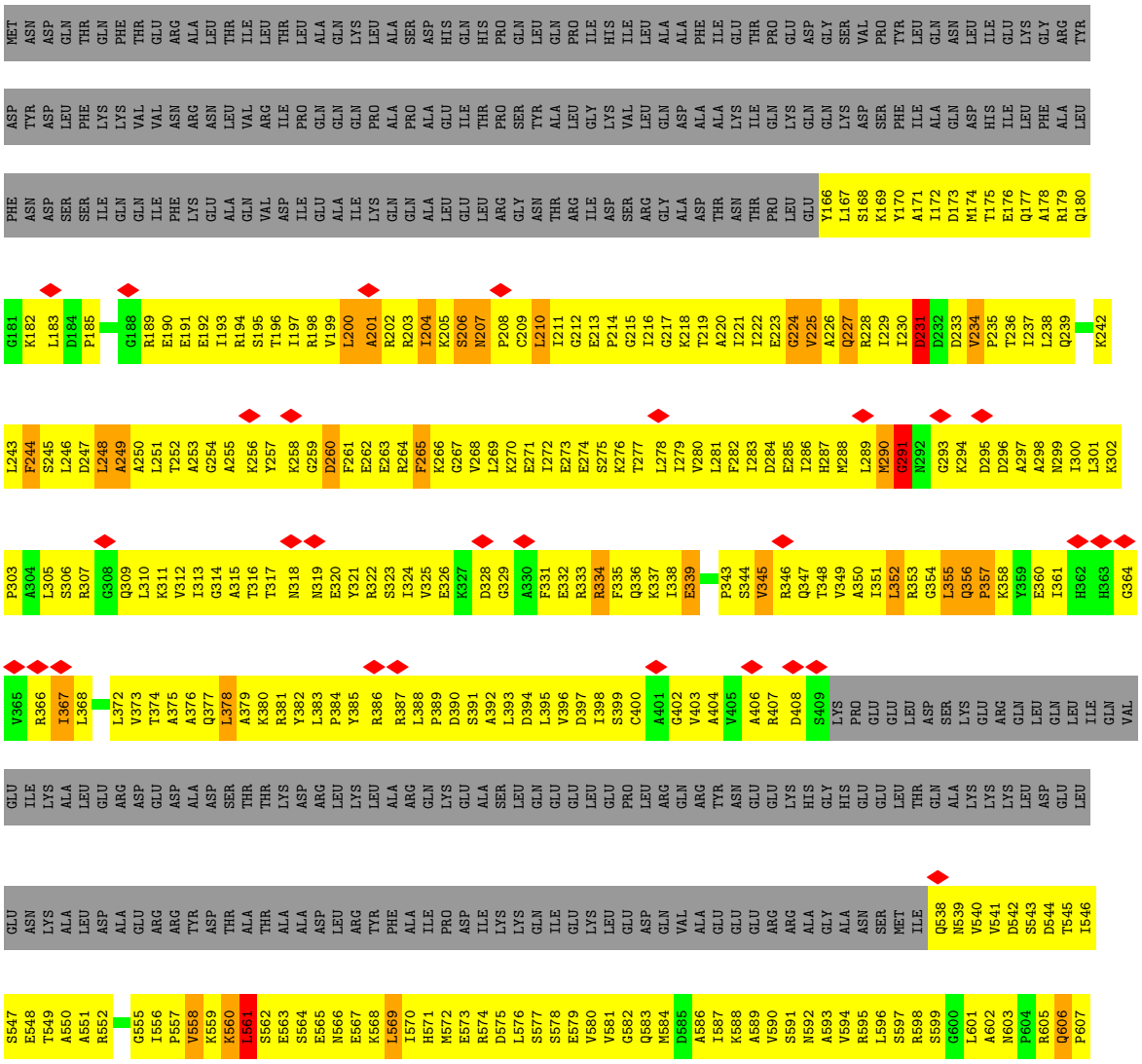
Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

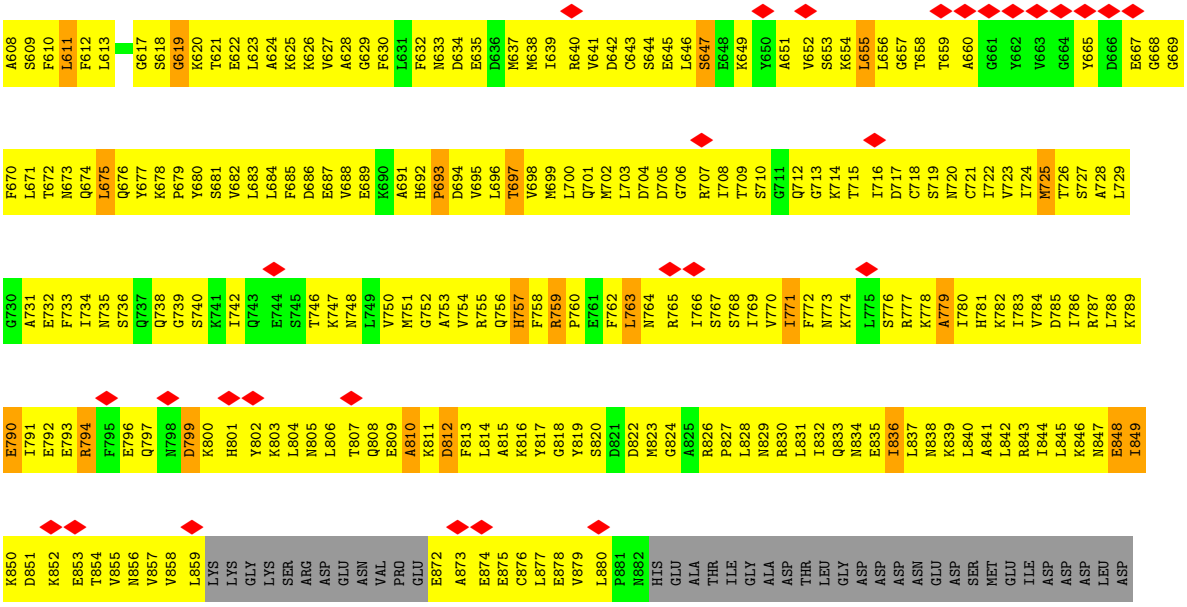
3 Residue-property plots (i)

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

- Molecule 1: Heat shock protein 104

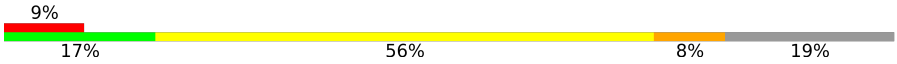
Chain A:

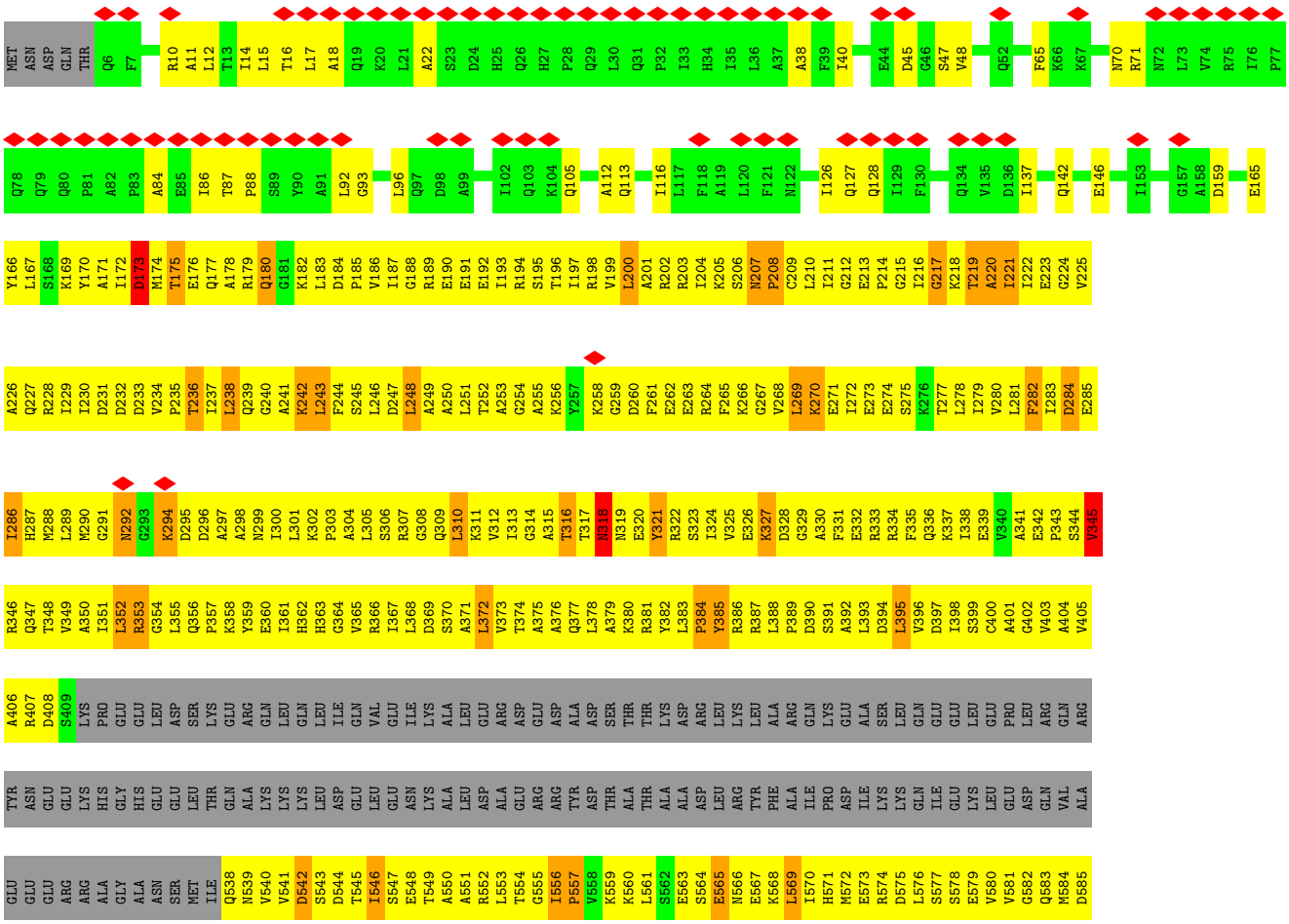


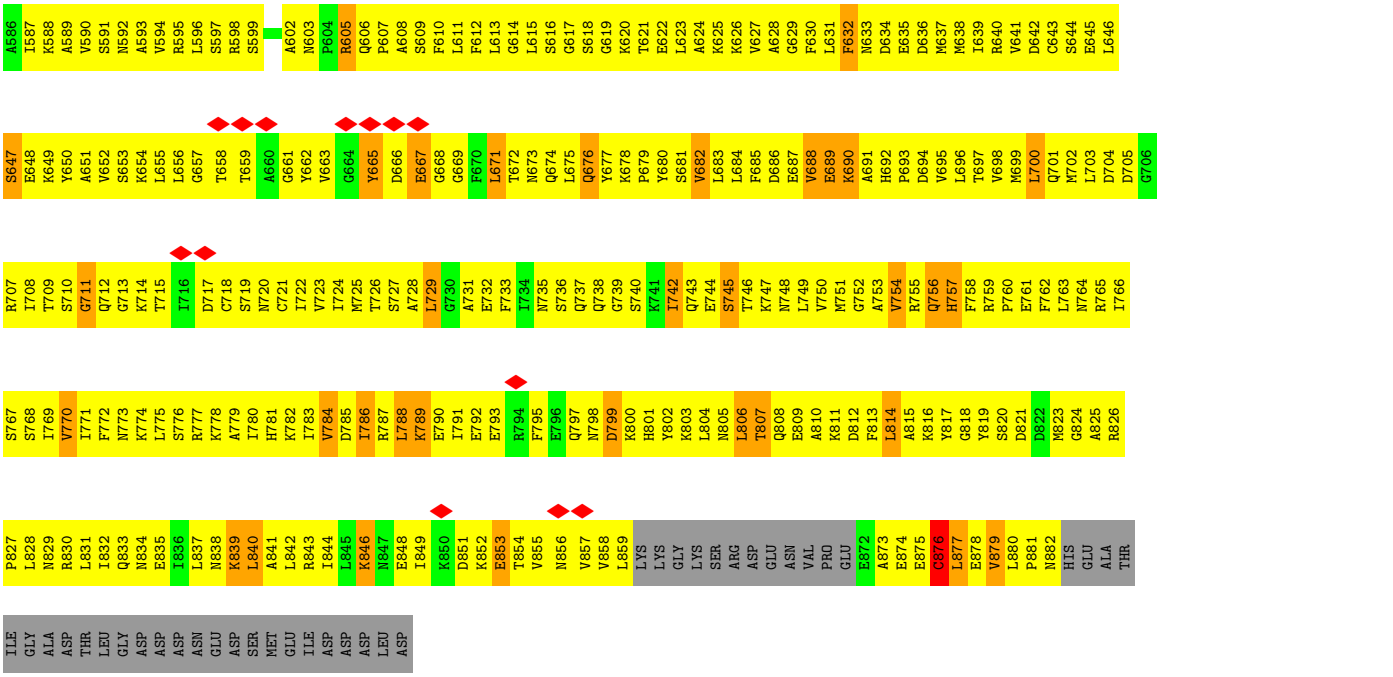


• Molecule 1: Heat shock protein 104

Chain B:

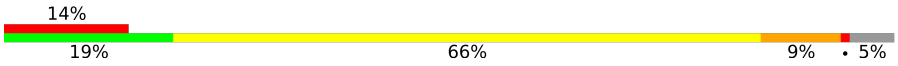


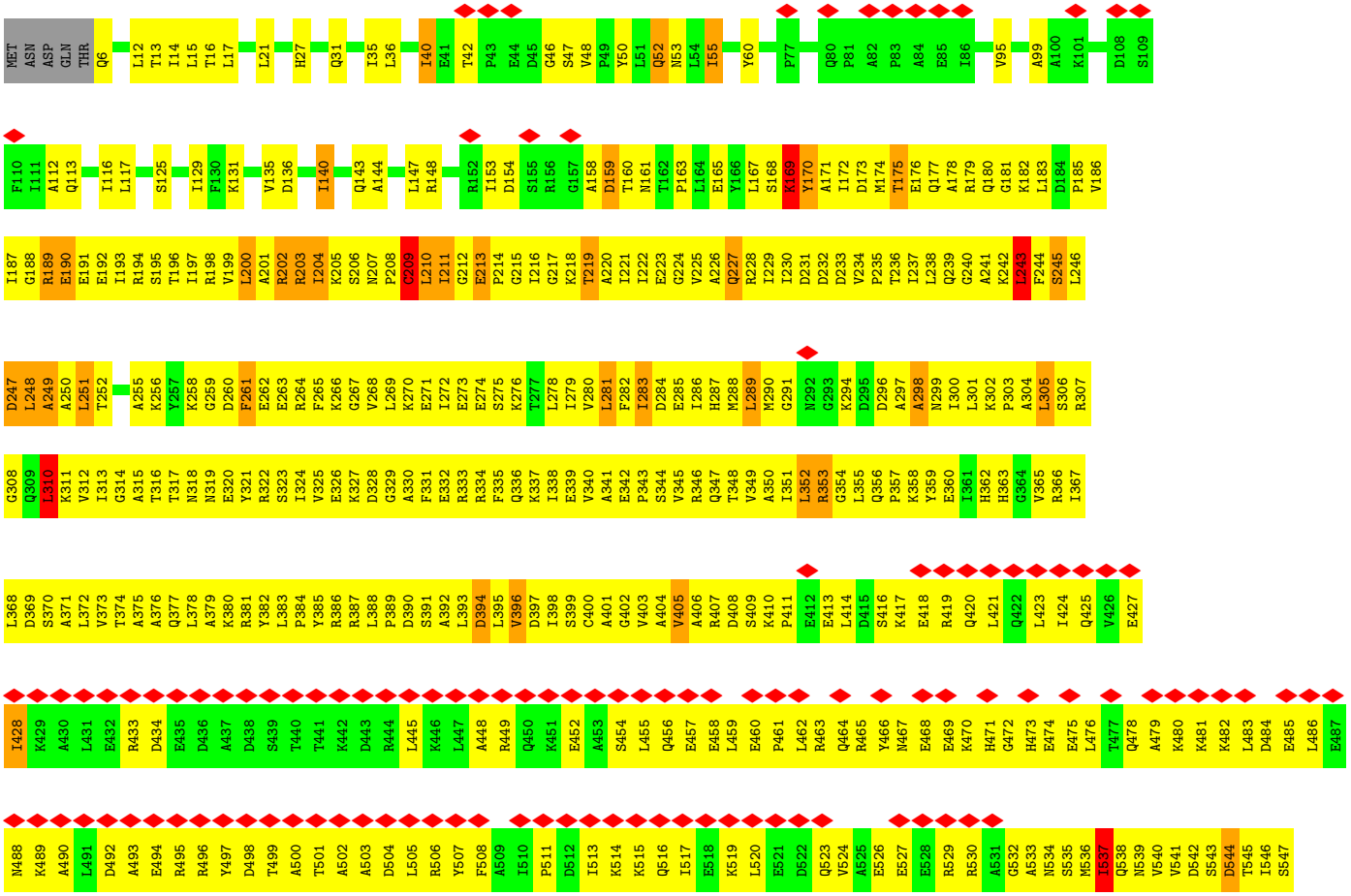


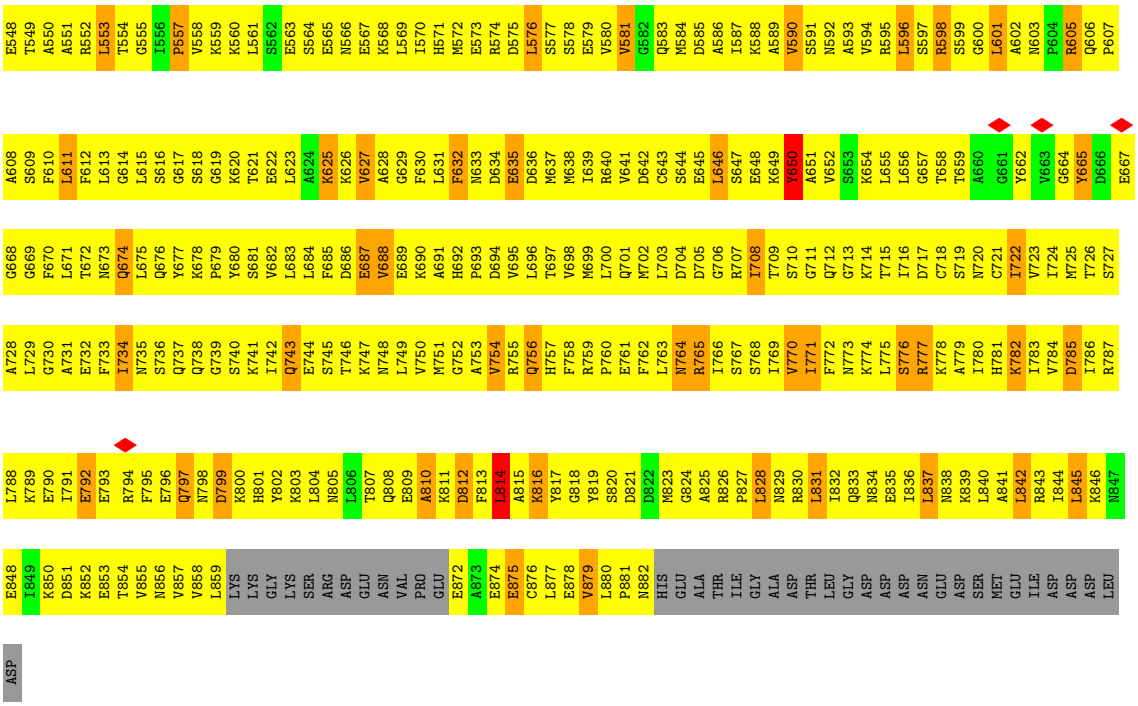


• Molecule 1: Heat shock protein 104

Chain C:

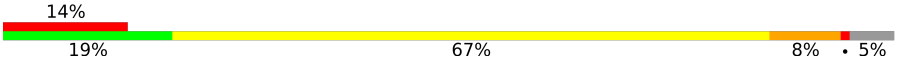


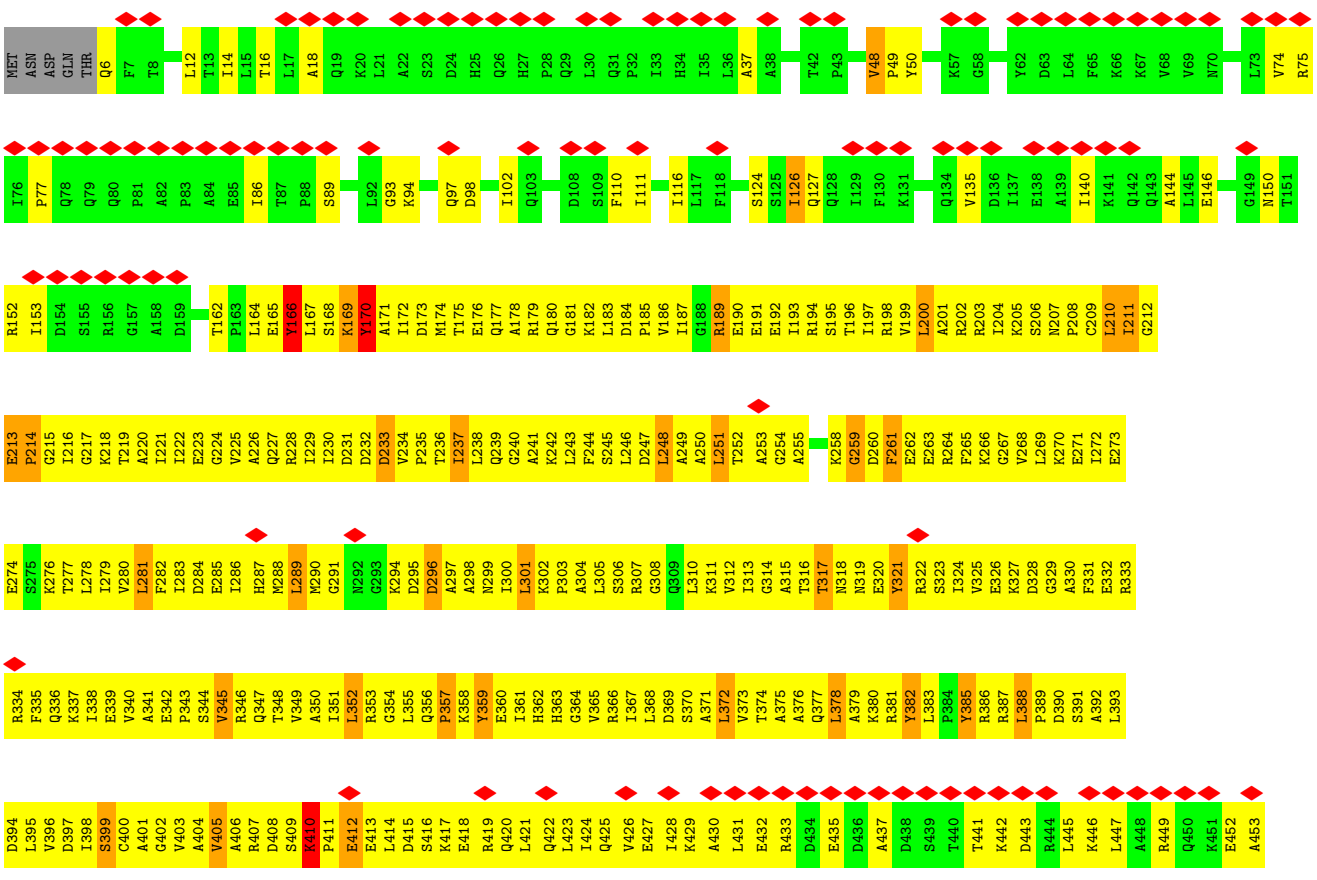


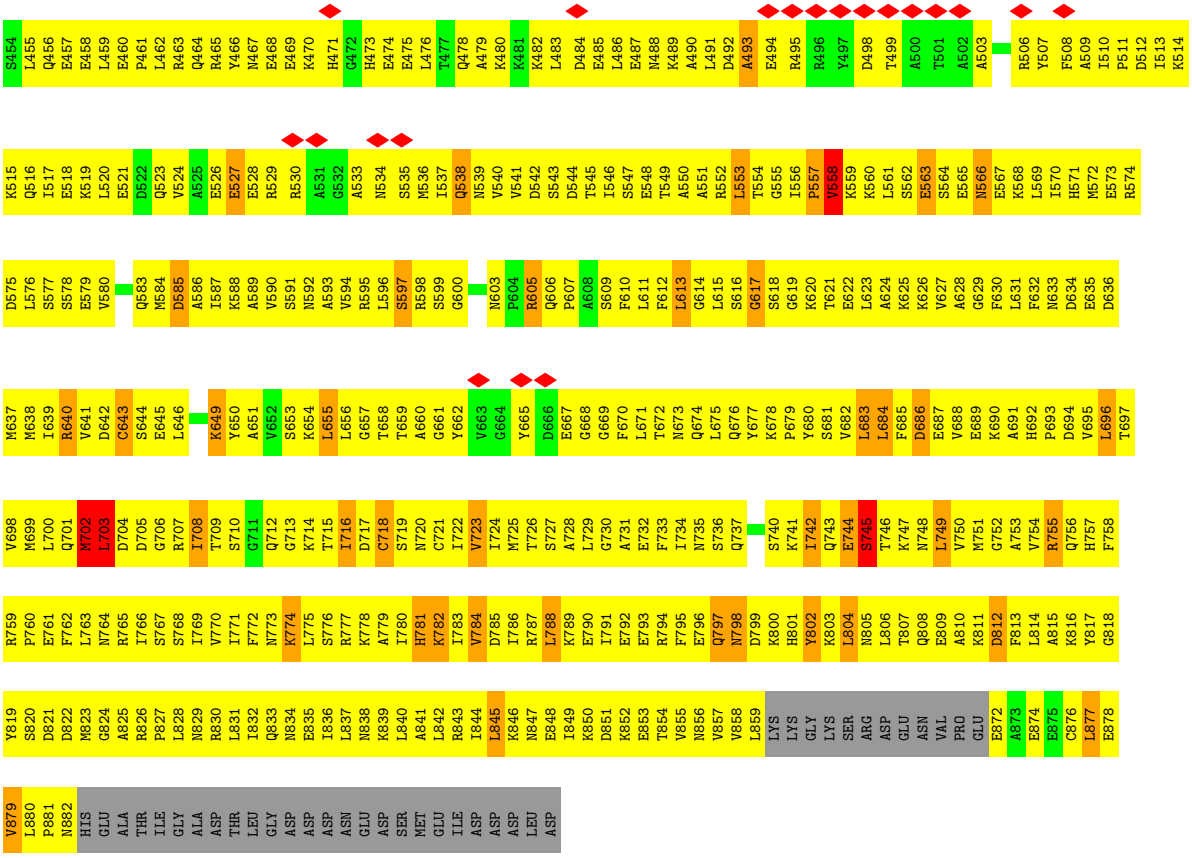


• Molecule 1: Heat shock protein 104

Chain D:

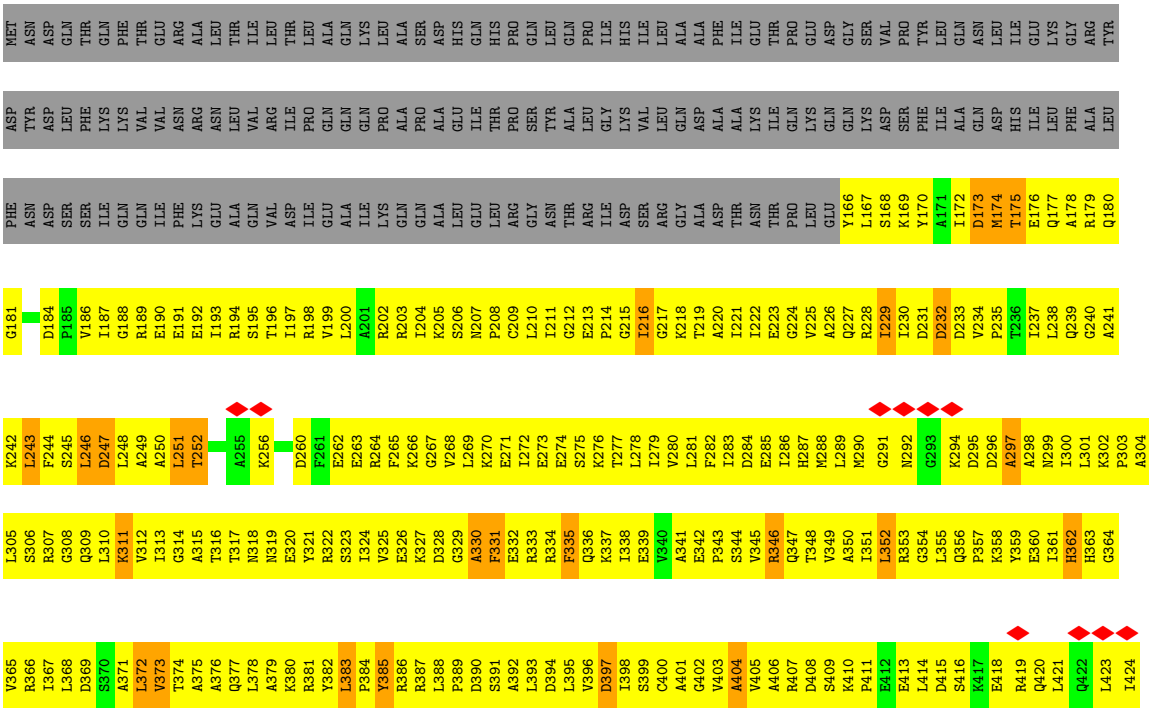


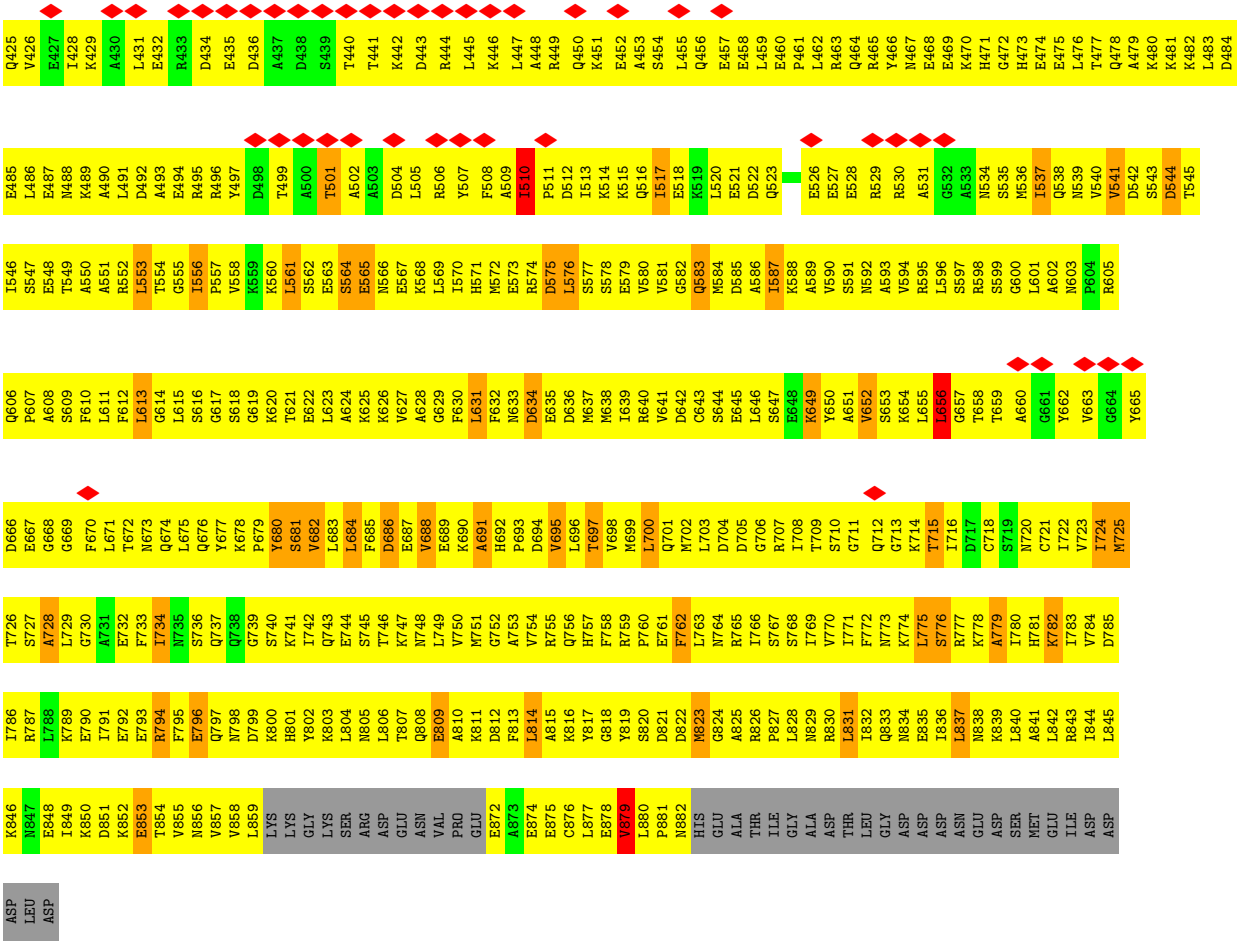




• Molecule 1: Heat shock protein 104

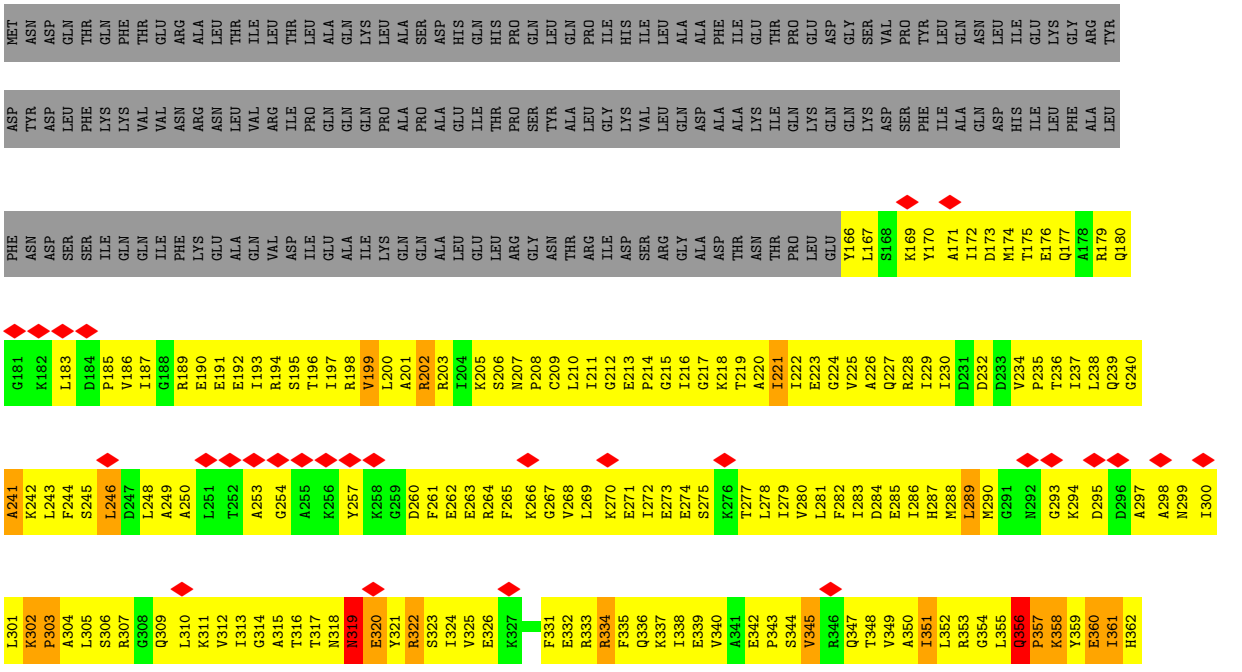
Chain E:

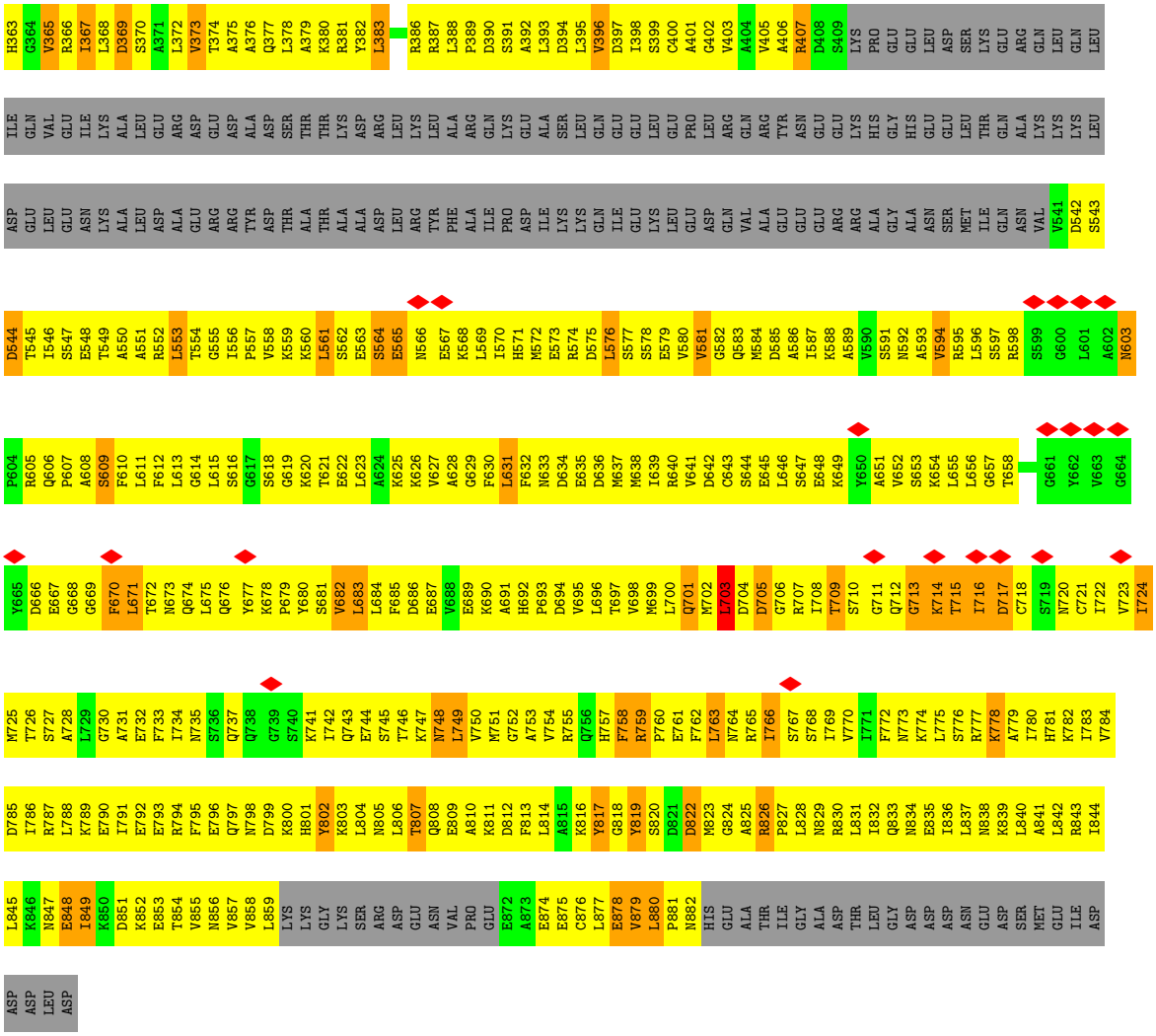




• Molecule 1: Heat shock protein 104

Chain F:




H363 G364 V365 R366 I367 L368 D369 S370 A371 L372 V373 T374 A375 A376 Q377 L378 A379 K380 R381 Y382 L383 R386 R387 L388 P389 D390 S391 A392 L393 D394 L395 V396 D397 I398 S399 C400 A401 G402 V403 A404 V405 A406 R407 D408 S409 LYS PRO GLU GLU LEU ASP SER LYS GLU ARG GLN LEU GLN LEU
ILE GLN VAL GLU ILE LYS ALA LEU GLU ARG ASP GLU ASP ALA ASP SER THR THR LYS ASP ARG LEU LYS LEU ALA ARG GLN LYS GLU ALA SER LEU GLN GLU GLU LEU GLU PRO LEU ARG GLN ARG TYR ASN GLU GLU LYS HIS GLY HIS GLU GLU LEU THR GLN ALA LYS LYS LYS LEU
ASP GLU LEU GLU ASN LYS ALA LEU ASP ALA GLU ARG ARG TYR ASP THR ALA THR ALA ALA ASP LEU ARG TYR PHE ALA ILE PRO ASP ILE LYS LYS GLN ILE GLU GLU LYS LEU GLU ASP GLN VAL ALA GLU GLU GLU ARG ARG ALA GLY ALA ASN SER MET ILE GLN ASN VAL V541 D542 S543
D544 T545 I546 S547 E548 T549 A550 A551 R552 L553 T554 G555 I556 P557 V558 K559 K560 L561 S562 E563 S564 E565 N566 E567 K568 L569 I570 H571 M572 E573 R574 D575 L576 S577 S578 E579 V580 V581 G582 Q583 M584 D585 A586 I587 K588 A589 V590 S591 N592 A593 V594 R595 L596 S597 R598 S599 G600 L601 A602 N603
P604 R605 Q606 P607 A608 S609 F610 L611 F612 L613 G614 L615 S616 G617 S618 G619 K620 T621 E622 L623 A624 K625 K626 V627 A628 G629 F630 L631 F632 N633 D634 E635 D636 M637 M638 I639 R640 V641 D642 C643 S644 E645 L646 S647 E648 K649 Y650 A651 V652 S653 K654 L655 L656 G657 T658 G661 Y662 V663 G664
Y665 D666 E667 G668 G669 F670 L671 T672 N673 Q674 L675 Q676 Y677 K678 P679 Y680 S681 V682 L683 L684 F685 D686 E687 V688 E689 K690 A691 H692 P693 D694 V695 L696 T697 V698 M699 L700 Q701 M702 L703 D704 D705 G706 R707 I708 T709 S710 G711 Q712 G713 K714 T715 I716 D717 C718 S719 N720 C721 I722 V723 I724
M725 T726 S727 A728 L729 G730 A731 E732 F733 I734 N735 S736 Q737 Q738 G739 S740 K741 I742 Q743 E744 S745 T746 K747 N748 L749 V750 M751 G752 A753 V754 R755 Q756 H757 F758 R759 P760 E761 F762 L763 N764 R765 I766 S767 S768 I769 V770 I771 F772 N773 K774 L775 S776 R777 K778 A779 I780 H781 K782 I783 V784
D785 I786 R787 L788 K789 E790 I791 E792 E793 R794 F795 E796 Q797 N798 D799 K800 H801 Y802 K803 L804 N805 L806 T807 Q808 E809 A810 K811 D812 F813 L814 A815 K816 Y817 G818 Y819 S820 D821 D822 M823 G824 A825 R826 P827 L828 N829 R830 L831 I832 Q833 N834 E835 I836 L837 N838 K839 L840 A841 L842 R843 I844
L845 K846 N847 E848 I849 K850 D851 K852 E853 T854 V855 N856 V857 V858 L859 LYS LYS GLY LYS SER ARG ASP GLU ASN VAL PRO GLU E872 A873 E874 E875 C876 L877 E878 V879 L880 P881 N882 HIS GLU ALA THR ILE GLY ALA ASP THR LEU GLY ASP ASP ASP ASN GLU ASP SER MET GLU ILE ASP
ASP ASP LEU ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69537	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.506	Depositor
Minimum map value	-0.223	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	285.12003, 285.12003, 285.12003	wwPDB
Map dimensions	108, 108, 108	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.6400003, 2.6400003, 2.6400003	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.59	0/4509	0.83	4/6077 (0.1%)
1	B	0.67	0/5196	0.93	15/6932 (0.2%)
1	C	0.72	1/6223 (0.0%)	1.00	28/8312 (0.3%)
1	D	1.61	10/6233 (0.2%)	1.00	22/8325 (0.3%)
1	E	0.73	5/5573 (0.1%)	0.96	17/7501 (0.2%)
1	F	0.59	1/4535 (0.0%)	0.84	12/6103 (0.2%)
All	All	0.93	17/32269 (0.1%)	0.94	98/43250 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	30
1	B	0	43
1	C	0	28
1	D	0	41
1	E	0	22
1	F	0	20
All	All	0	184

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	321	TYR	CD2-CE2	63.02	2.33	1.39
1	D	321	TYR	CD1-CE1	59.39	2.28	1.39
1	D	321	TYR	CE2-CZ	39.66	1.90	1.38
1	D	321	TYR	CE1-CZ	39.48	1.89	1.38
1	D	321	TYR	CG-CD1	30.30	1.78	1.39

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	613	LEU	CA-CB-CG	-9.59	93.25	115.30
1	E	553	LEU	CA-CB-CG	-9.56	93.32	115.30
1	C	210	LEU	CA-CB-CG	8.83	135.61	115.30
1	D	200	LEU	CA-CB-CG	-8.80	95.07	115.30
1	C	646	LEU	CA-CB-CG	-8.48	95.79	115.30

There are no chirality outliers.

5 of 184 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	LEU	Peptide
1	A	206	SER	Peptide
1	A	210	LEU	Peptide
1	A	224	GLY	Peptide
1	A	231	ASP	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	4456	0	4540	1177	0
1	B	5142	0	4785	1578	0
1	C	6162	0	5790	1935	0
1	D	6170	0	5790	1953	0
1	E	5512	0	5602	1902	0
1	F	4480	0	4597	1382	0
2	C	31	0	12	29	0
2	D	31	0	12	39	0
2	E	62	0	24	64	0
2	F	62	0	24	37	0
All	All	32108	0	31176	9740	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 154.

The worst 5 of 9740 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:700:LEU:HD23	1:F:703:LEU:CD2	1.21	1.66
1:C:169:LYS:CE	1:C:264:ARG:HD2	1.23	1.62
1:D:321:TYR:CD1	1:D:321:TYR:CG	1.78	1.62
1:F:331:PHE:HA	1:F:334:ARG:CG	1.24	1.62
1:C:169:LYS:HE3	1:C:264:ARG:CB	1.21	1.60

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	571/908 (63%)	408 (72%)	141 (25%)	22 (4%)	3	23
1	B	731/908 (80%)	492 (67%)	204 (28%)	35 (5%)	2	21
1	C	861/908 (95%)	591 (69%)	220 (26%)	50 (6%)	1	18
1	D	861/908 (95%)	584 (68%)	246 (29%)	31 (4%)	3	25
1	E	701/908 (77%)	496 (71%)	170 (24%)	35 (5%)	2	20
1	F	568/908 (63%)	426 (75%)	112 (20%)	30 (5%)	2	19
All	All	4293/5448 (79%)	2997 (70%)	1093 (26%)	203 (5%)	4	21

5 of 203 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ILE
1	B	137	ILE
1	C	159	ASP
1	C	161	ASN
1	C	163	PRO

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	484/782 (62%)	483 (100%)	1 (0%)	93 96
1	B	493/782 (63%)	490 (99%)	3 (1%)	86 92
1	C	599/782 (77%)	593 (99%)	6 (1%)	76 86
1	D	599/782 (77%)	595 (99%)	4 (1%)	84 90
1	E	595/782 (76%)	593 (100%)	2 (0%)	92 95
1	F	490/782 (63%)	475 (97%)	15 (3%)	40 62
All	All	3260/4692 (70%)	3229 (99%)	31 (1%)	77 86

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	544	ASP
1	F	703	LEU
1	F	320	GLU
1	F	709	THR
1	F	365	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	309	GLN
1	F	583	GLN
1	F	797	GLN
1	C	633	ASN
1	C	583	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AGS	E	1001	-	26,33,33	0.88	1 (3%)	26,52,52	2.01	2 (7%)
2	AGS	D	1001	-	26,33,33	1.05	2 (7%)	26,52,52	1.34	2 (7%)
2	AGS	F	1001	-	26,33,33	0.78	0	26,52,52	1.29	1 (3%)
2	AGS	C	1001	-	26,33,33	0.88	1 (3%)	26,52,52	2.33	4 (15%)
2	AGS	F	1002	-	26,33,33	0.87	2 (7%)	26,52,52	1.25	2 (7%)
2	AGS	E	1002	-	26,33,33	0.90	1 (3%)	26,52,52	1.53	2 (7%)

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
2	AGS	E	1001	-	-	4/17/38/38	0/3/3/3
2	AGS	D	1001	-	-	8/17/38/38	0/3/3/3
2	AGS	F	1001	-	-	7/17/38/38	0/3/3/3
2	AGS	C	1001	-	-	4/17/38/38	0/3/3/3
2	AGS	F	1002	-	-	5/17/38/38	0/3/3/3
2	AGS	E	1002	-	-	6/17/38/38	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)
2	D	1001	AGS	C4-N3	-2.52	1.32	1.35
2	F	1002	AGS	C8-N7	-2.40	1.30	1.34
2	E	1002	AGS	C8-N7	-2.38	1.30	1.34
2	C	1001	AGS	PB-O2B	-2.19	1.45	1.55
2	D	1001	AGS	PA-O2A	-2.18	1.45	1.55

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	AGS	PA-O3A-PB	-10.20	97.83	132.83
2	E	1001	AGS	PA-O3A-PB	-9.19	101.31	132.83
2	E	1002	AGS	PA-O3A-PB	-6.17	111.64	132.83
2	D	1001	AGS	PA-O3A-PB	-5.11	115.31	132.83
2	F	1001	AGS	PA-O3A-PB	-4.88	116.08	132.83

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1001	AGS	C4'-C5'-O5'-PA
2	D	1001	AGS	C5'-O5'-PA-O1A
2	D	1001	AGS	C5'-O5'-PA-O2A
2	D	1001	AGS	C3'-C4'-C5'-O5'
2	E	1001	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

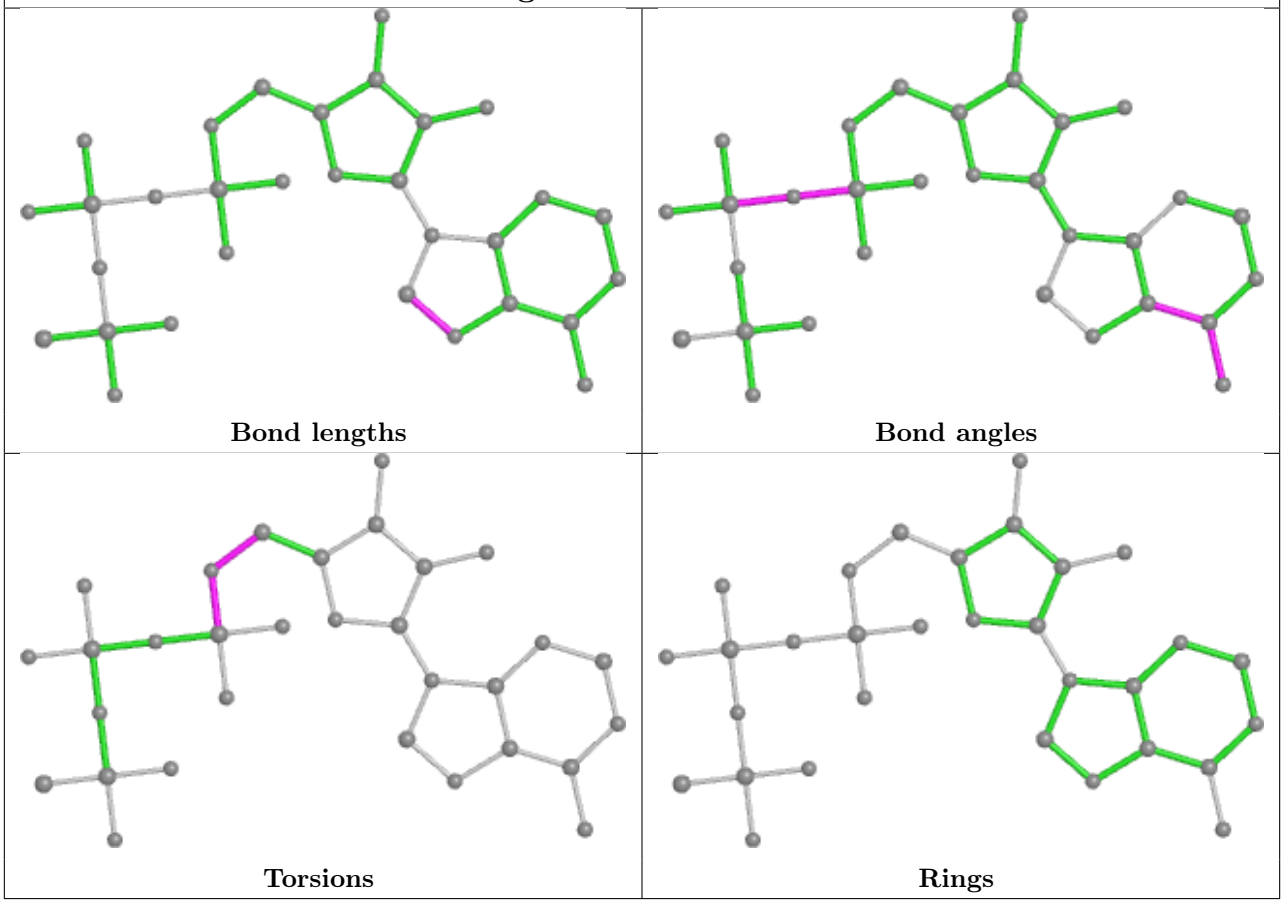
6 monomers are involved in 169 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1001	AGS	29	0
2	D	1001	AGS	39	0
2	F	1001	AGS	18	0
2	C	1001	AGS	29	0
2	F	1002	AGS	19	0
2	E	1002	AGS	35	0

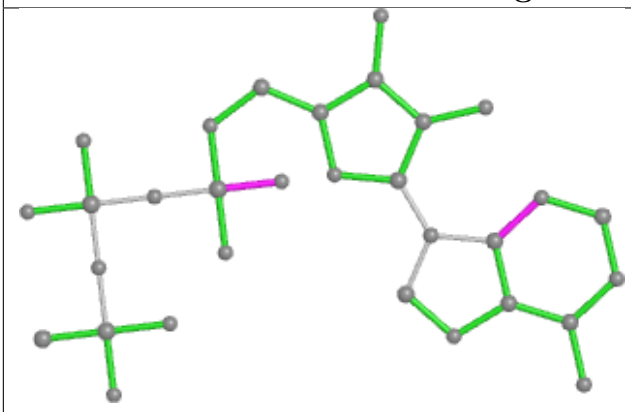
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

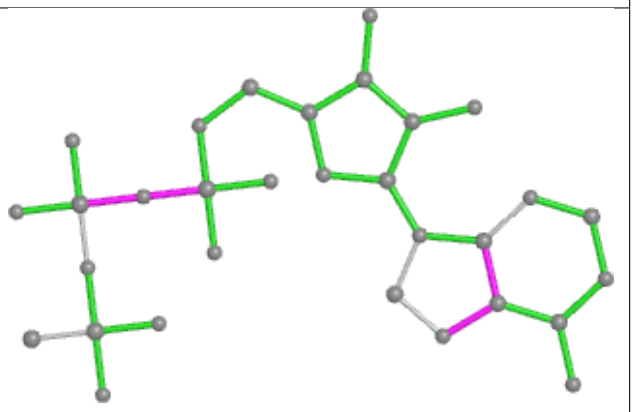
Ligand AGS E 1001



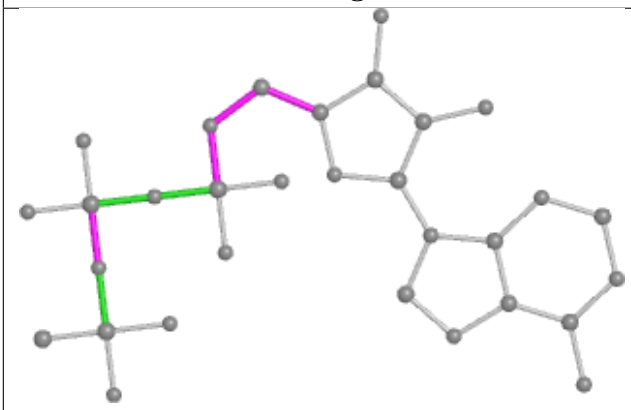
Ligand AGS D 1001



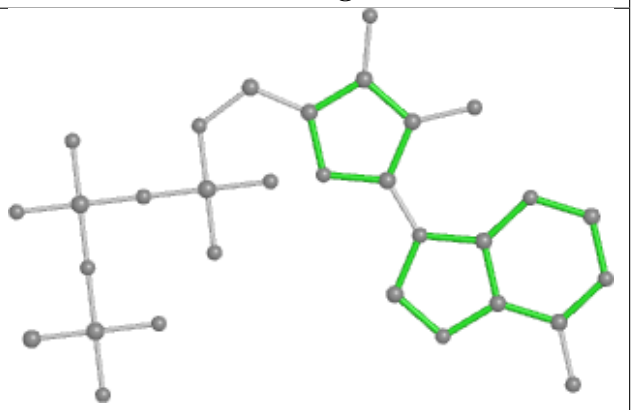
Bond lengths



Bond angles

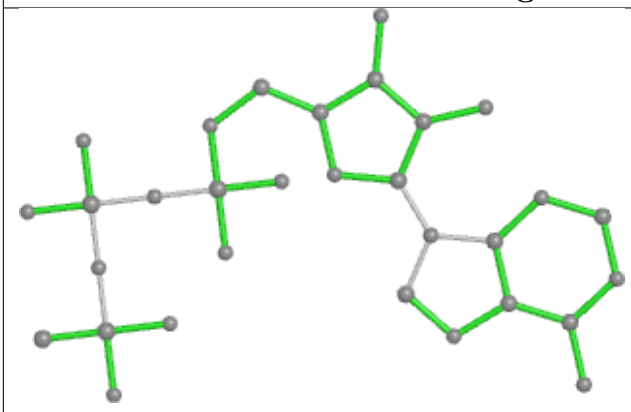


Torsions

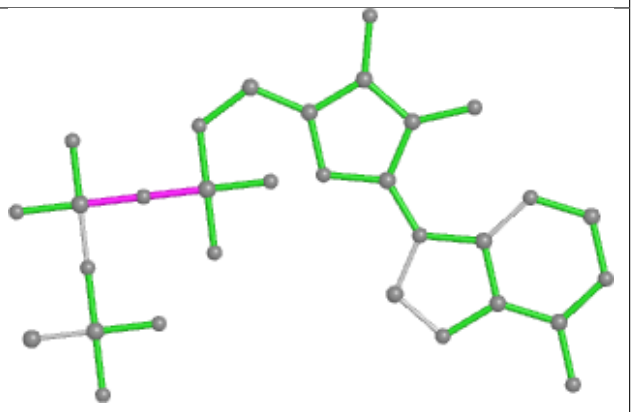


Rings

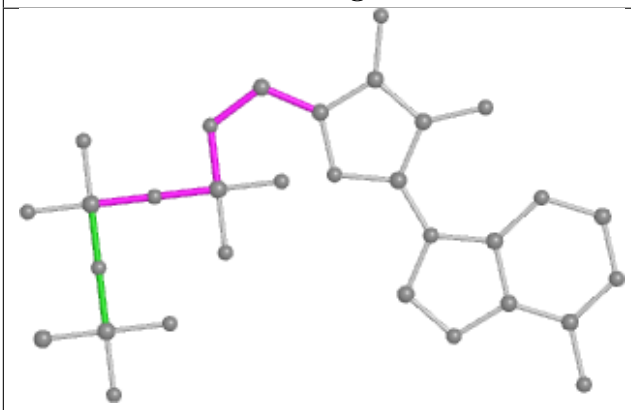
Ligand AGS F 1001



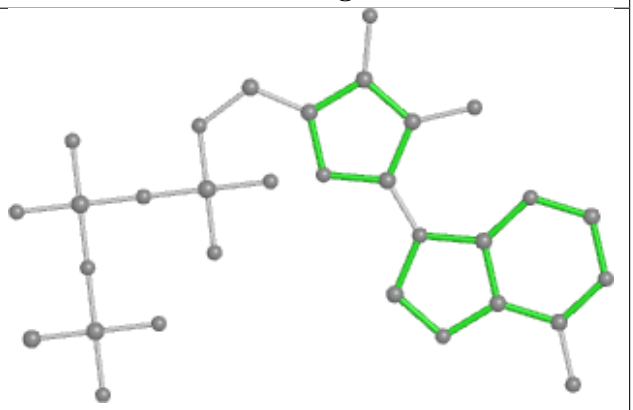
Bond lengths



Bond angles

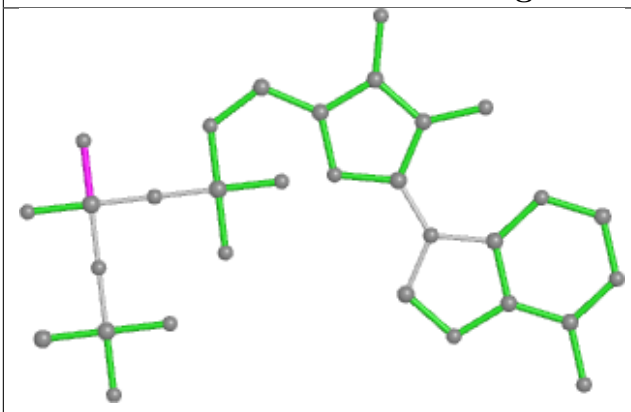


Torsions

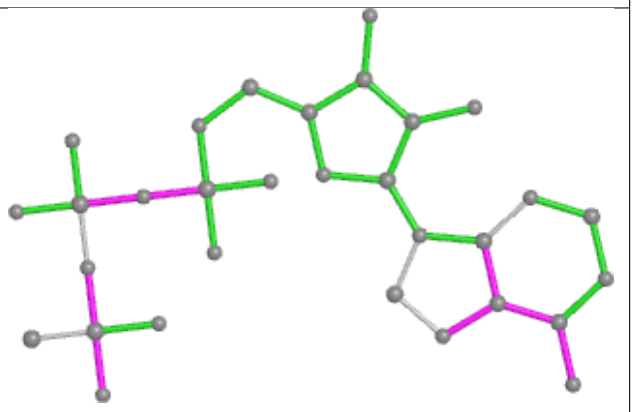


Rings

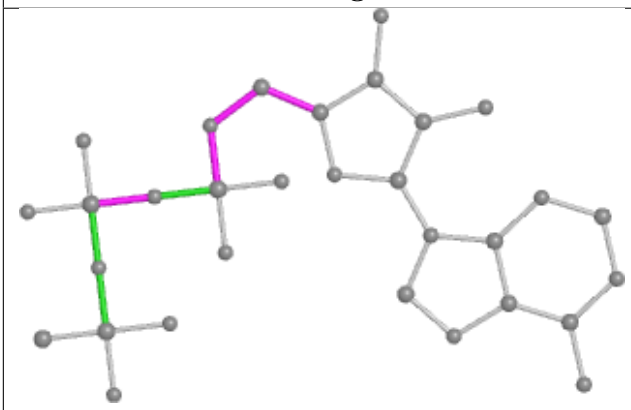
Ligand AGS C 1001



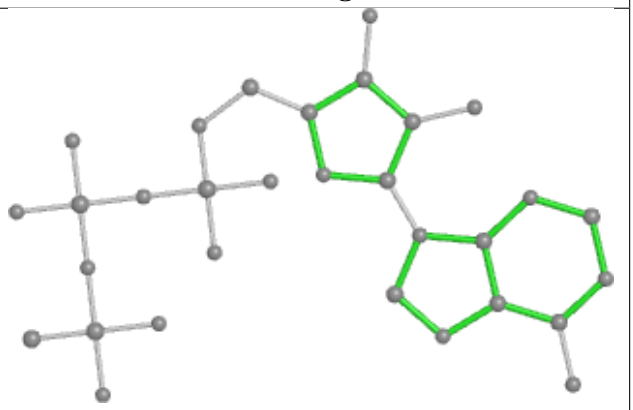
Bond lengths



Bond angles

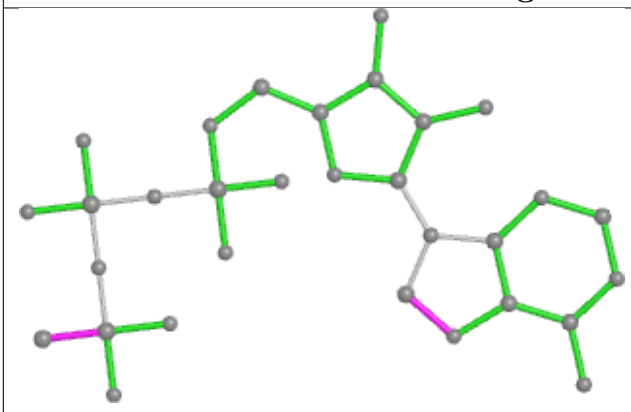


Torsions

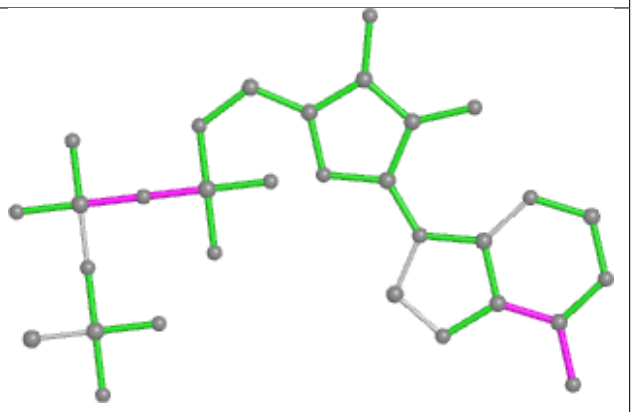


Rings

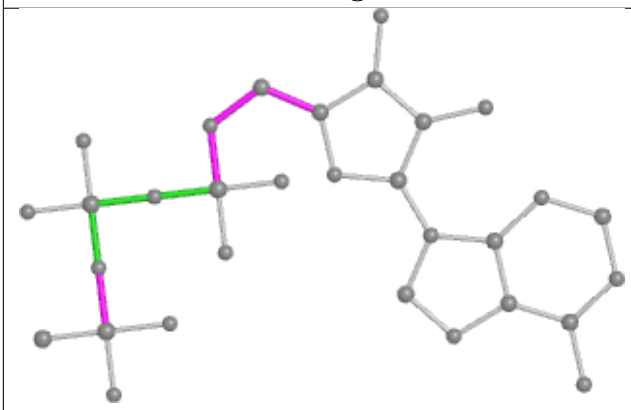
Ligand AGS F 1002



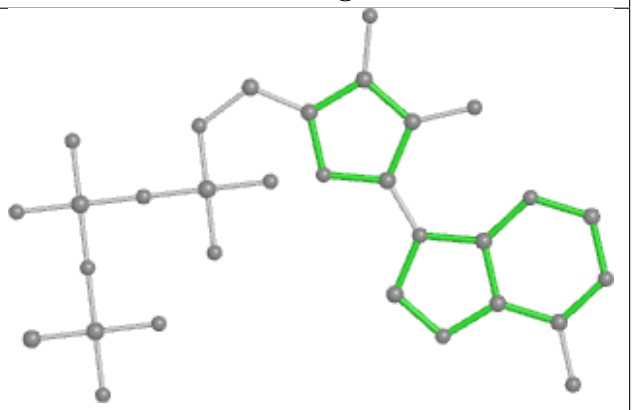
Bond lengths



Bond angles

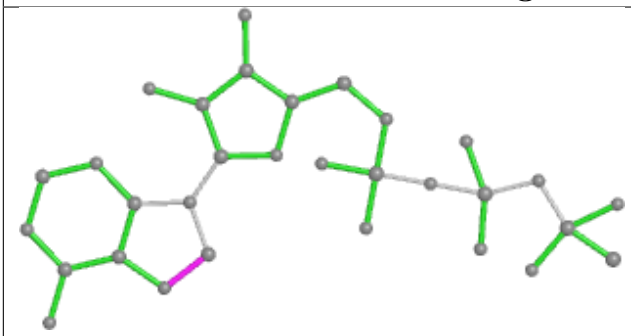


Torsions

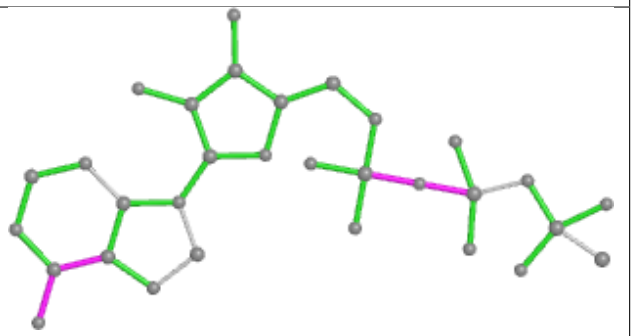


Rings

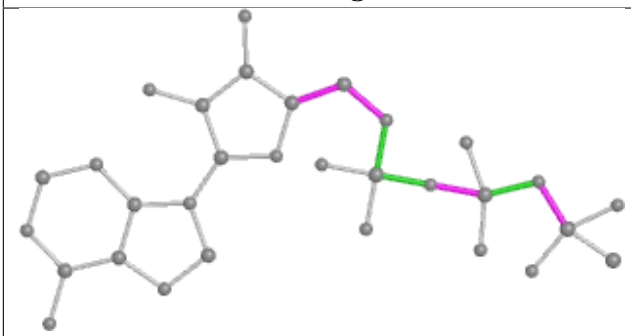
Ligand AGS E 1002



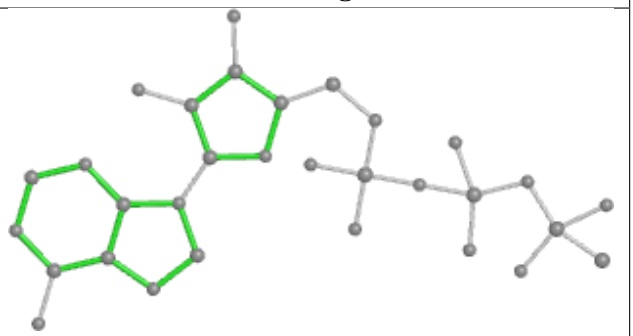
Bond lengths



Bond angles



Torsions



Rings

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.

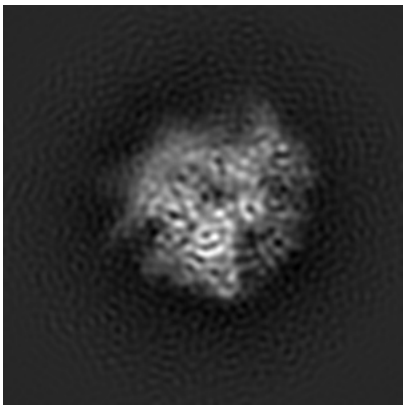
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9625. These allow visual inspection of the internal detail of the map and identification of artifacts.

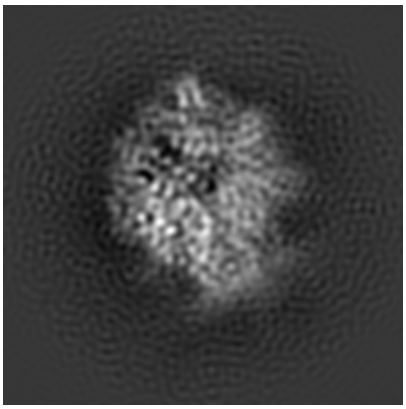
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

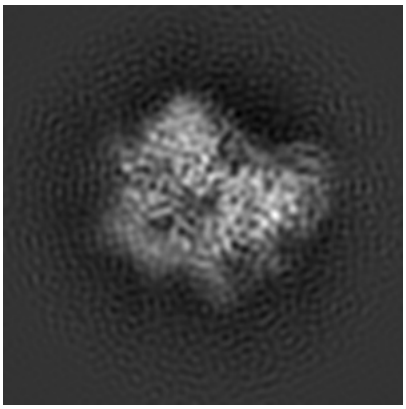
6.1.1 Primary map



X

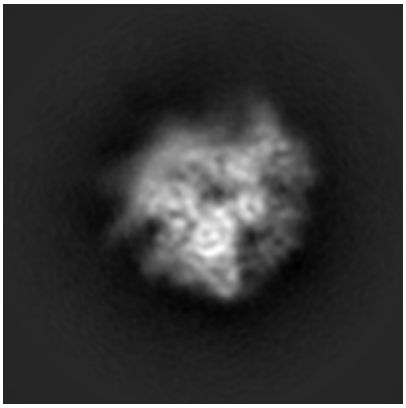


Y

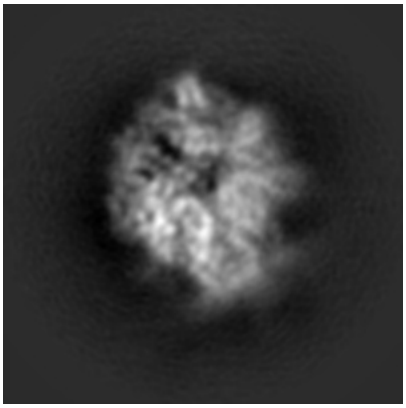


Z

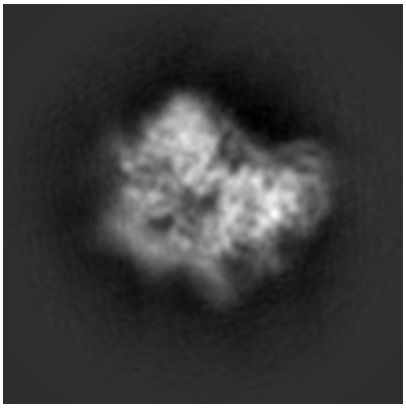
6.1.2 Raw map



X



Y

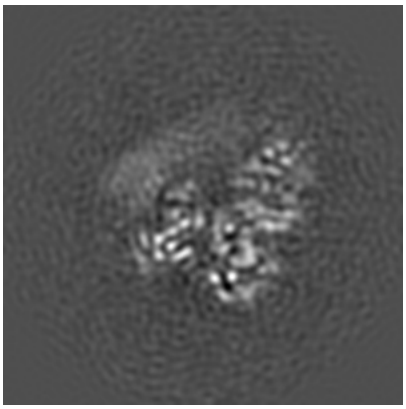


Z

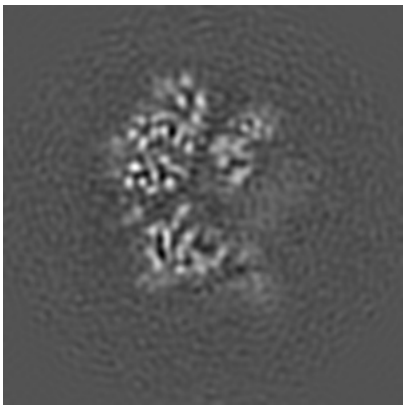
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

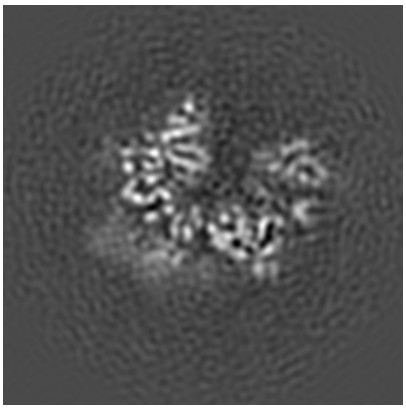
6.2.1 Primary map



X Index: 54

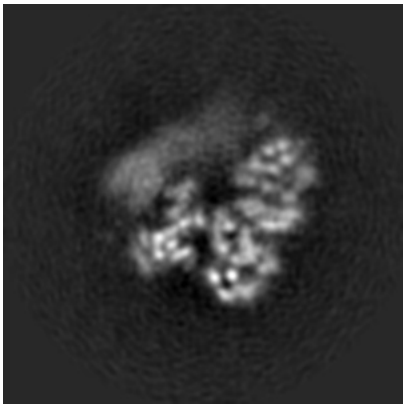


Y Index: 54

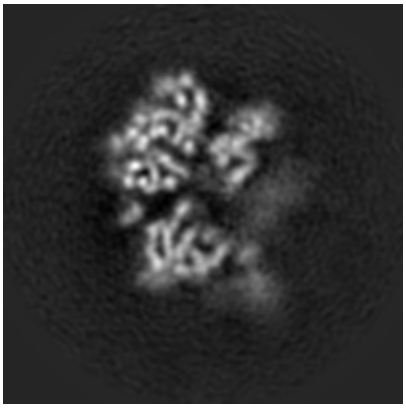


Z Index: 54

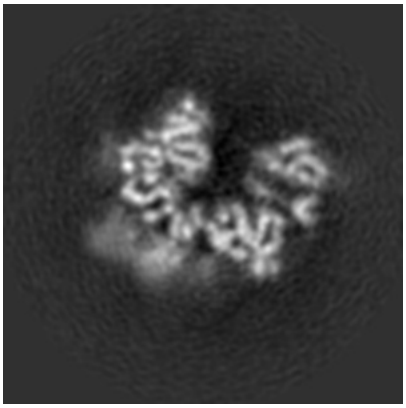
6.2.2 Raw map



X Index: 54



Y Index: 54

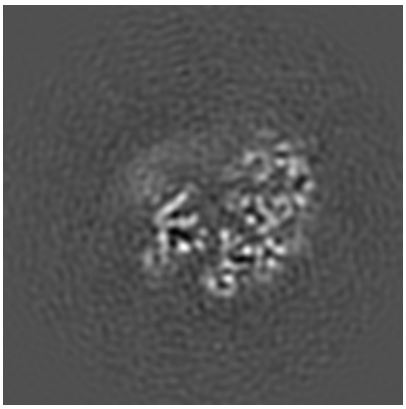


Z Index: 54

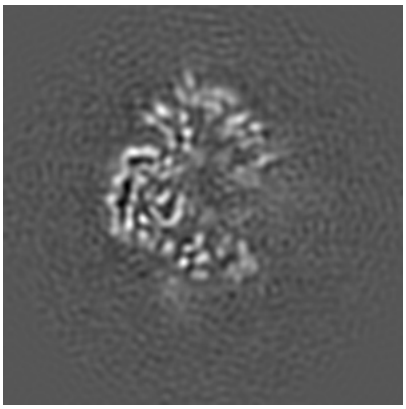
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

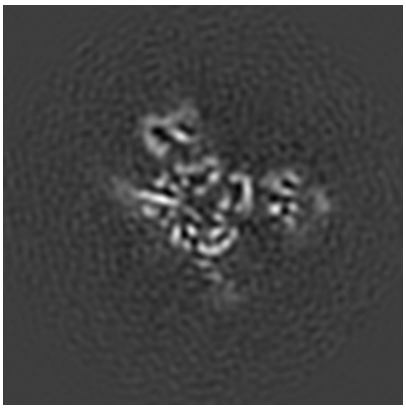
6.3.1 Primary map



X Index: 49

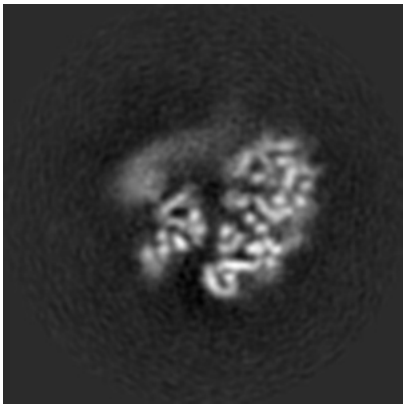


Y Index: 60

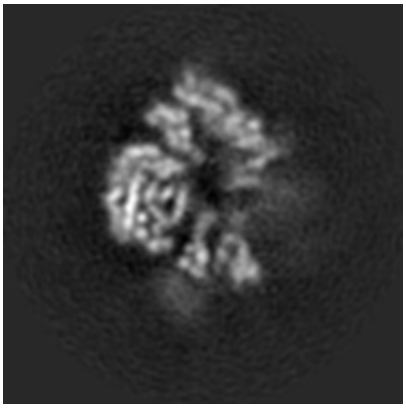


Z Index: 44

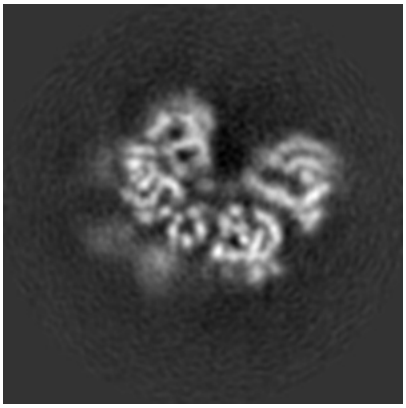
6.3.2 Raw map



X Index: 50



Y Index: 61

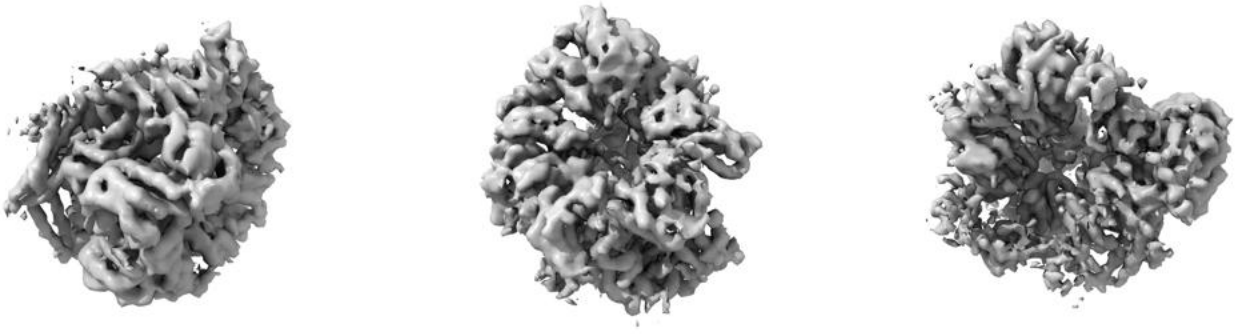


Z Index: 52

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

6.4 Orthogonal surface views (i)

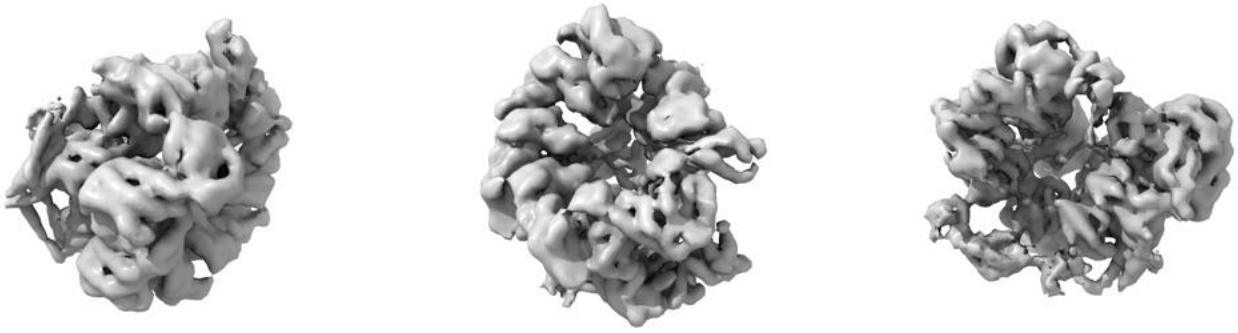
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

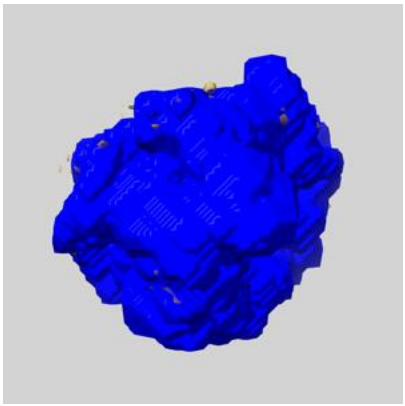
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

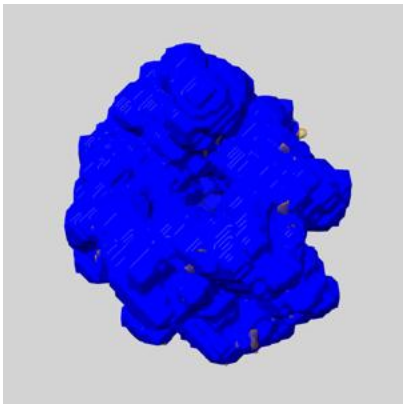
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

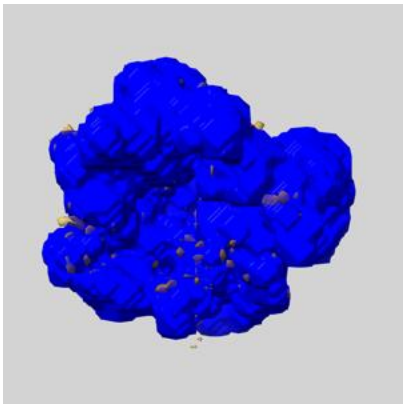
6.5.1 emd_9625_msk_1.map (i)



X



Y

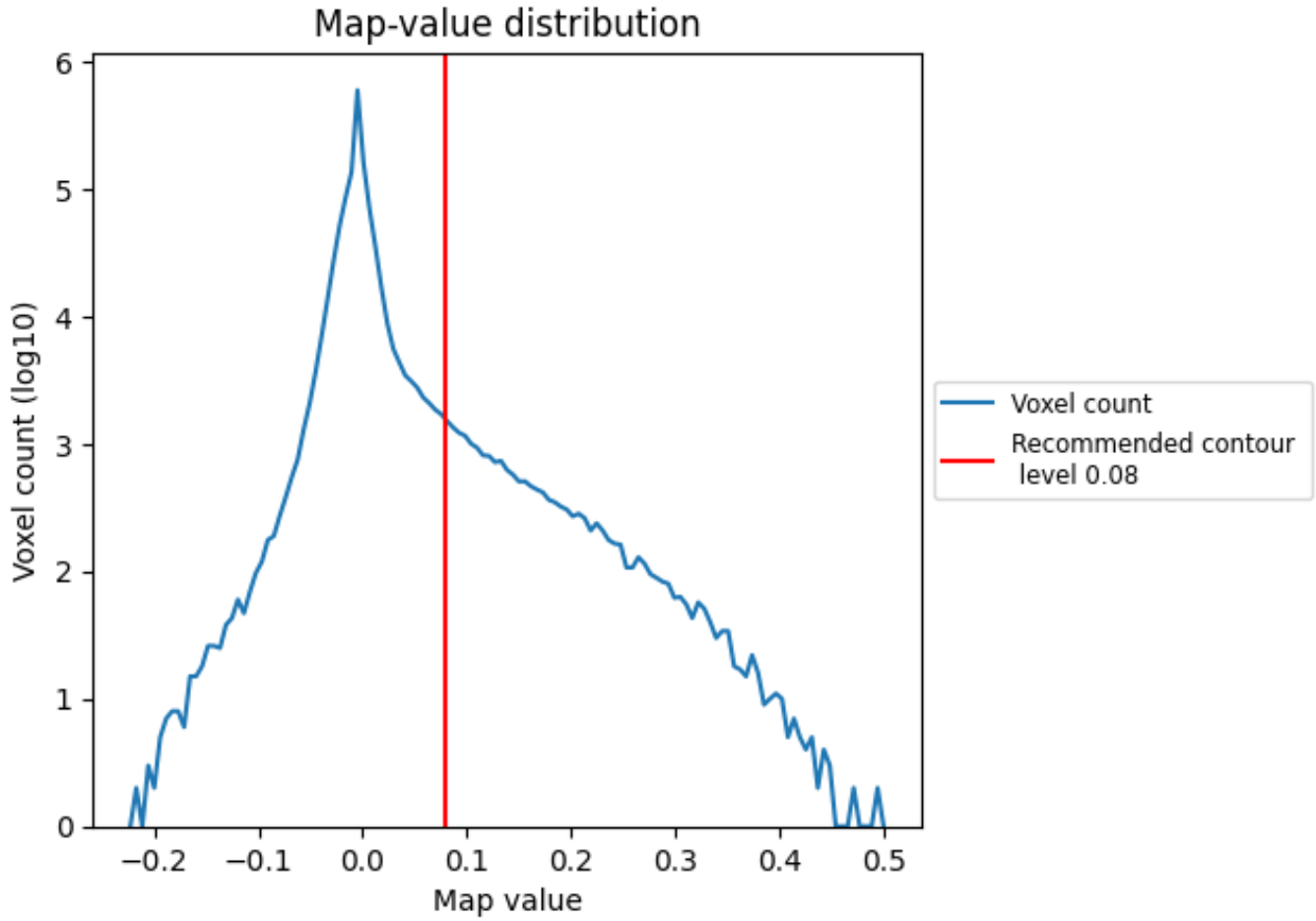


Z

7 Map analysis

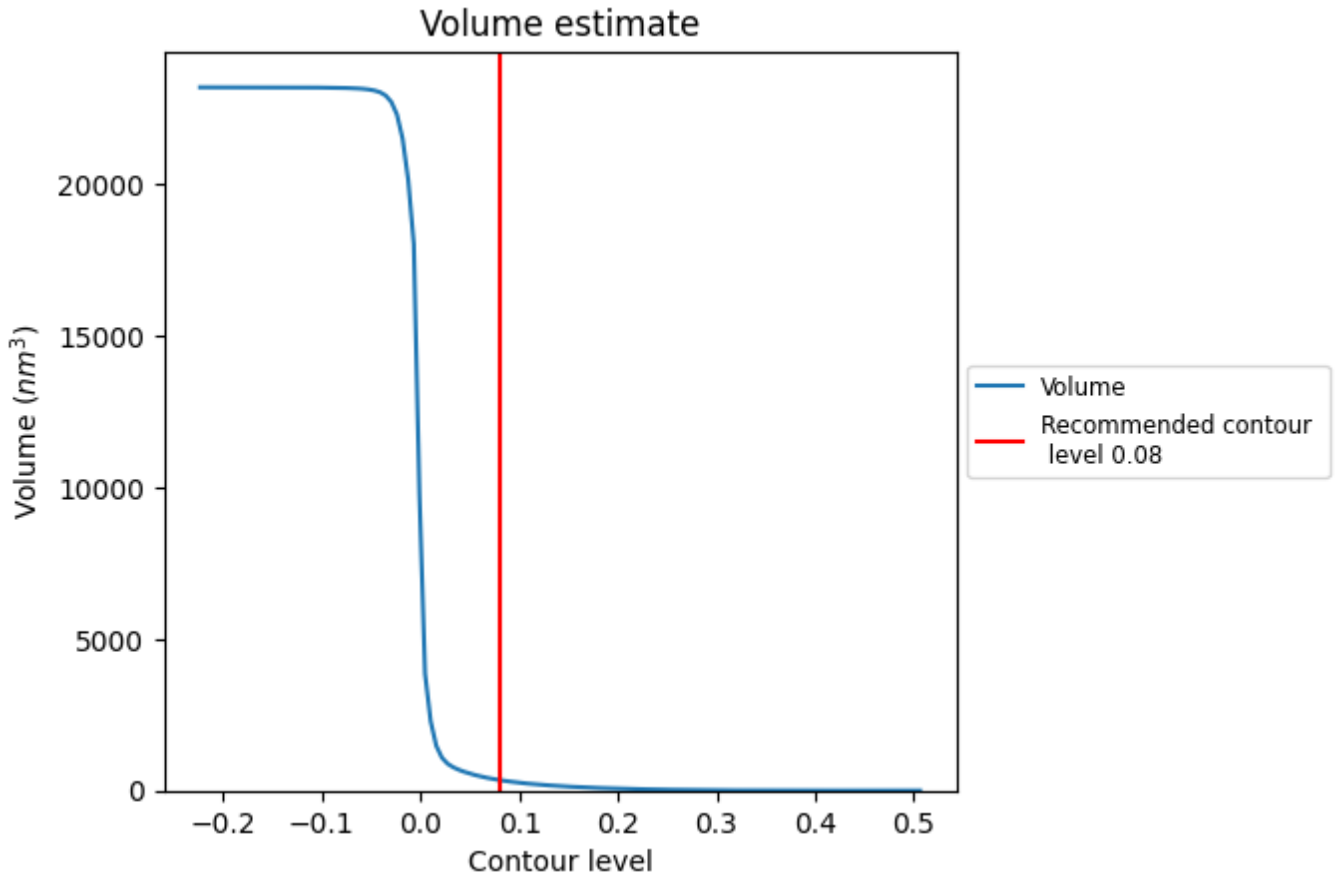
This section contains the results of statistical analysis of the map.

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.

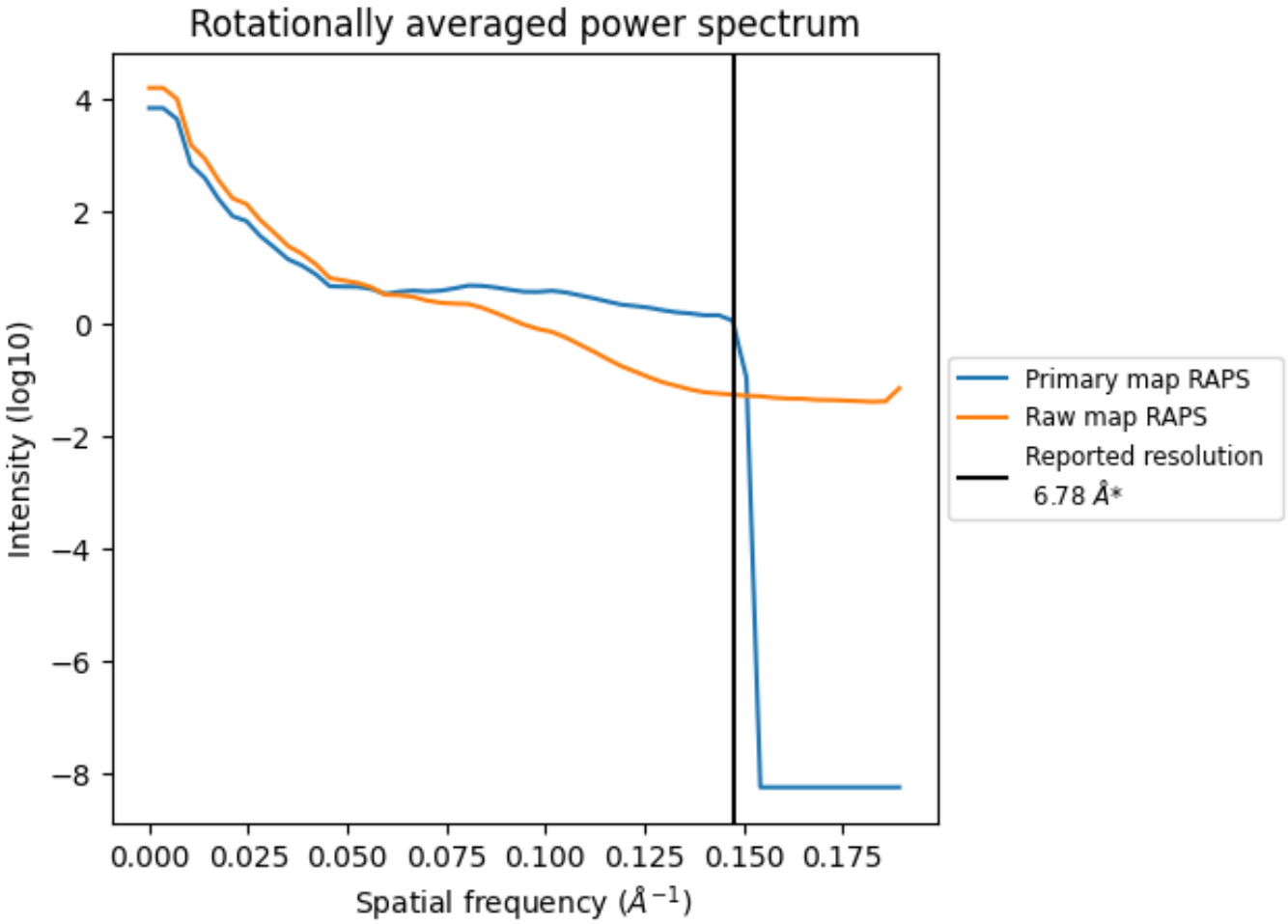
7.2 Volume estimate (i)



The volume at the recommended contour level is 346 nm^3; this corresponds to an approximate mass of 313 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)

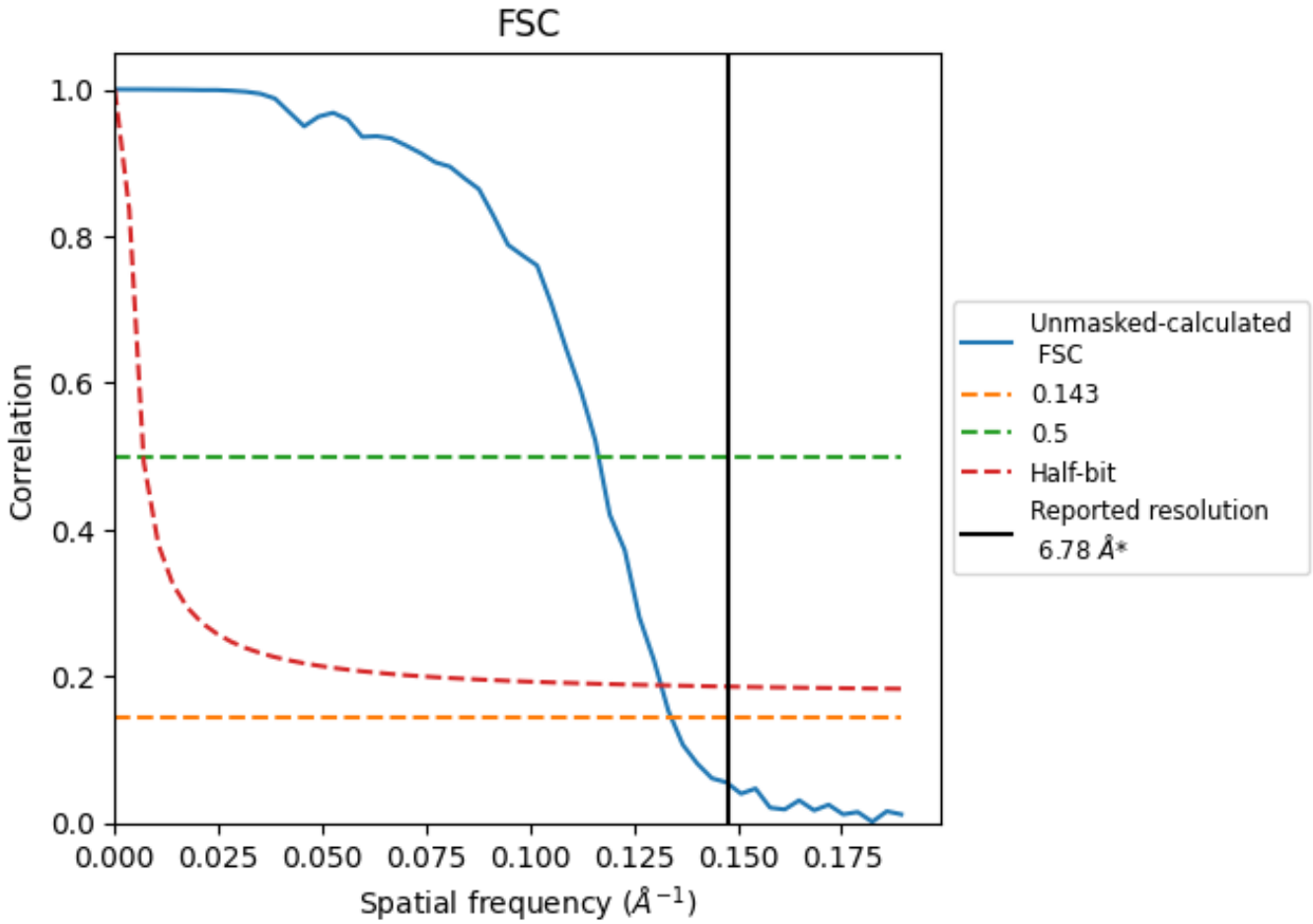


*Reported resolution corresponds to spatial frequency of 0.147 Å^{-1}

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 0.147 Å^{-1}

8.2 Resolution estimates (i)

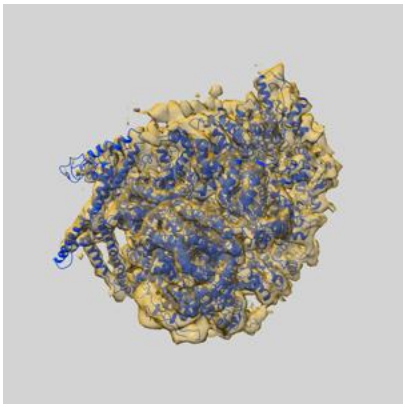
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.46	8.58	7.60

*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 7.46 differs from the reported value 6.78 by more than 10 %

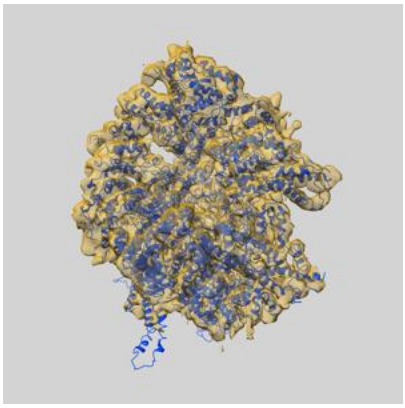
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9625 and PDB model 6AHF. Per-residue inclusion information can be found in section 3 on page 6.

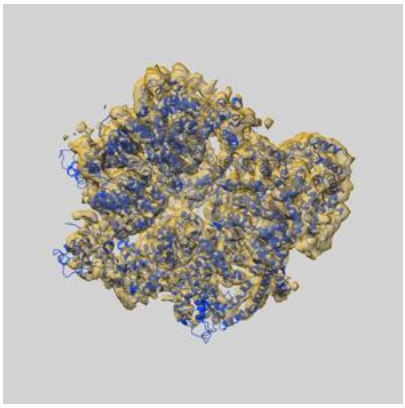
9.1 Map-model overlay



X



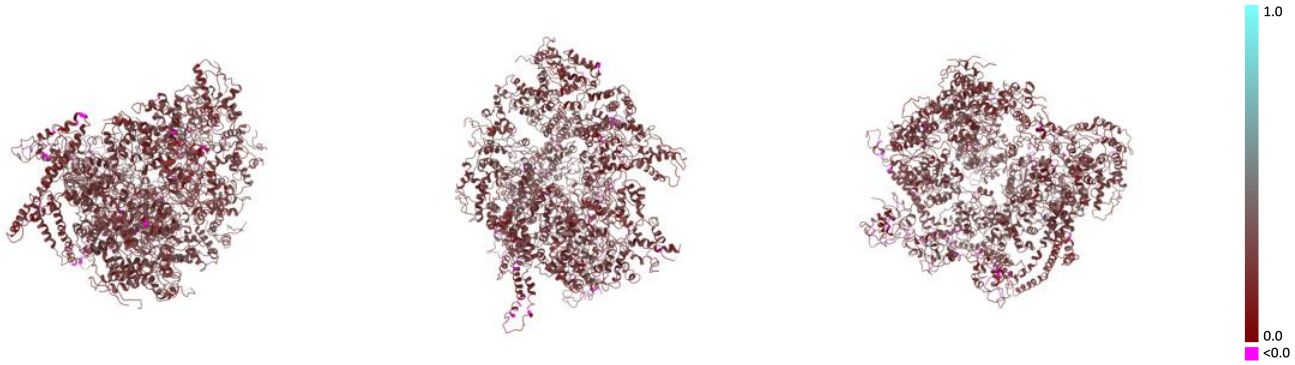
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

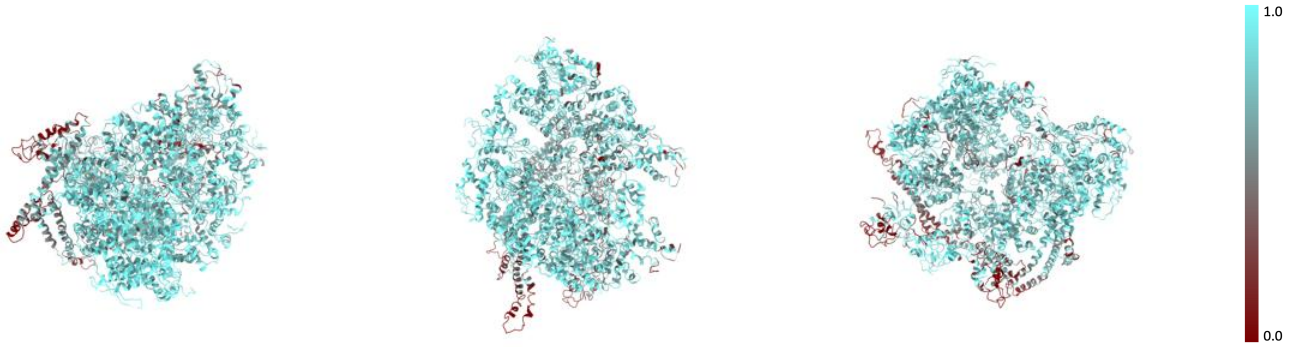
9.2 Q-score mapped to coordinate model



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.

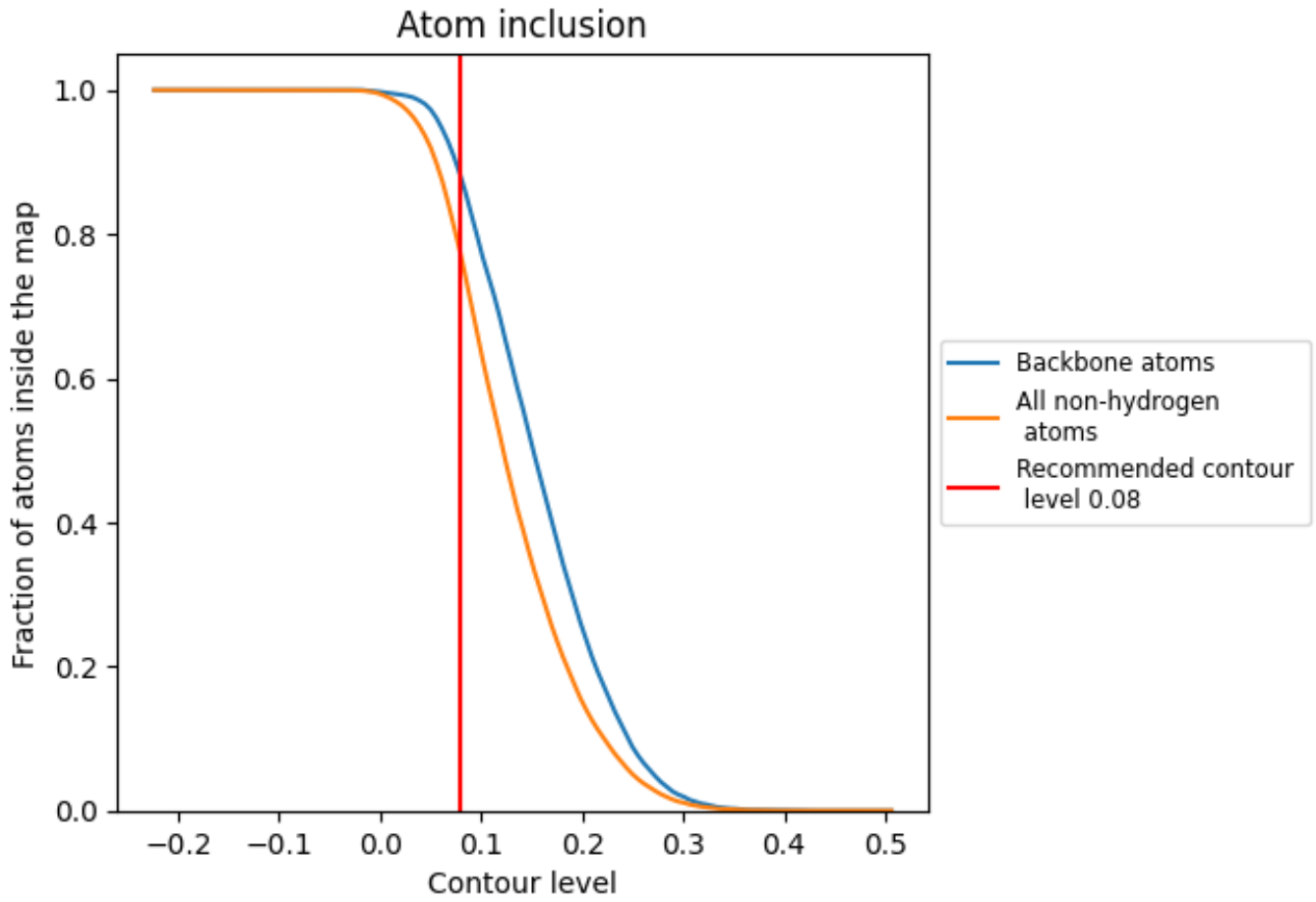
9.3 Atom inclusion mapped to coordinate model



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.2430
A	0.7287	0.2380
B	0.7940	0.2480
C	0.7521	0.2460
D	0.7683	0.2500
E	0.8062	0.2450
F	0.7797	0.2310