Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 09:13 PM EST

PDB ID	:	6VZG
EMDB ID	:	EMD-21489
Title	:	Cryo-EM structure of Sth1-Arp7-Arp9-Rtt102
Authors	:	Leschziner, A.E.; Baker, R.W.
Deposited on	:	2020-02-28
Resolution	:	4.20 Å(reported)
Based on initial models	:	5TGC, 4I6M

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

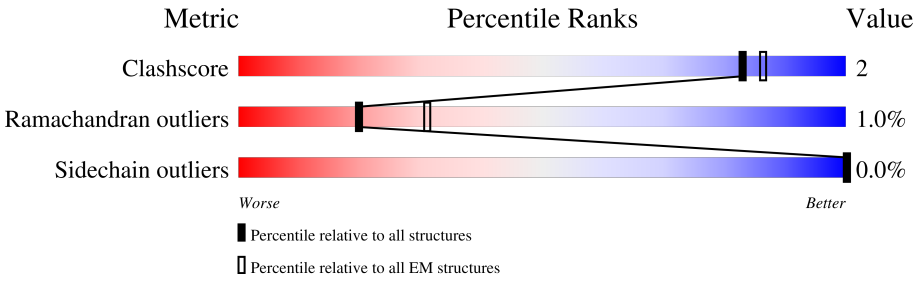
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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	1-L	477	68% 79% · 18%
1	10-L	477	78% · 18%
1	2-L	477	78% · 18%
1	3-L	477	78% · 18%
1	4-L	477	78% · 18%
1	5-L	477	78% · 18%
1	6-L	477	79% · · 18%
1	7-L	477	77% 5% 18%

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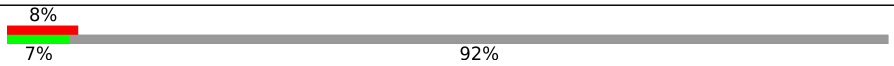
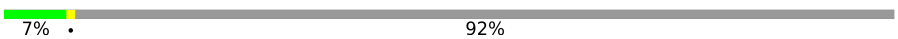
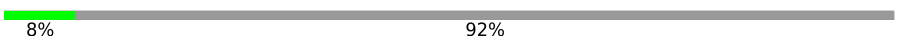
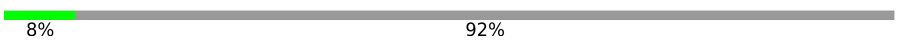
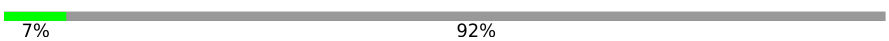
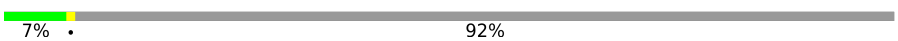
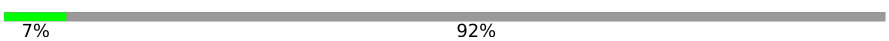
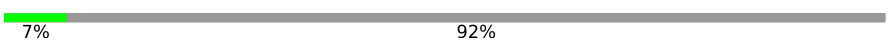
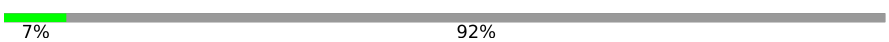
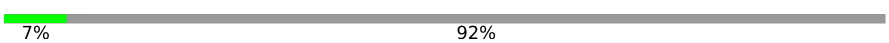
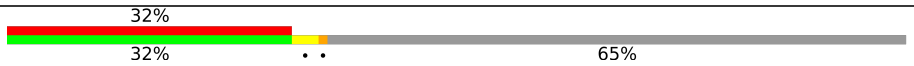
Mol	Chain	Length	Quality of chain
1	8-L	477	
1	9-L	477	
2	1-M	467	
2	10-M	467	
2	2-M	467	
2	3-M	467	
2	4-M	467	
2	5-M	467	
2	6-M	467	
2	7-M	467	
2	8-M	467	
2	9-M	467	
3	1-K	813	
3	10-K	813	
3	2-K	813	
3	3-K	813	
3	4-K	813	
3	5-K	813	
3	6-K	813	
3	7-K	813	
3	8-K	813	
3	9-K	813	
4	1-N	157	
4	10-N	157	
4	2-N	157	

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Mol	Chain	Length	Quality of chain
4	3-N	157	
4	4-N	157	
4	5-N	157	
4	6-N	157	
4	7-N	157	
4	8-N	157	
4	9-N	157	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 74080 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 Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0
1	2-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0
1	3-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0
1	4-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0
1	5-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0
1	6-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0
1	7-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0
1	8-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0
1	9-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0
1	10-L	393	Total 3154	C 2035	N 514	O 590	S 15	0	0

- Molecule 2 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-M	396	Total 3192	C 2048	N 521	O 616	S 7	0	0
2	2-M	396	Total 3192	C 2048	N 521	O 616	S 7	0	0
2	3-M	396	Total 3192	C 2048	N 521	O 616	S 7	0	0
2	4-M	396	Total 3192	C 2048	N 521	O 616	S 7	0	0
2	5-M	396	Total 3192	C 2048	N 521	O 616	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	6-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	7-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	8-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	9-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	10-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		

- Molecule 3 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	2-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	3-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	4-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	5-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	6-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	7-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	8-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	9-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	10-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	285	MET	-	initiating methionine	UNP P32597
K	286	GLY	-	expression tag	UNP P32597
K	287	SER	-	expression tag	UNP P32597
K	288	SER	-	expression tag	UNP P32597

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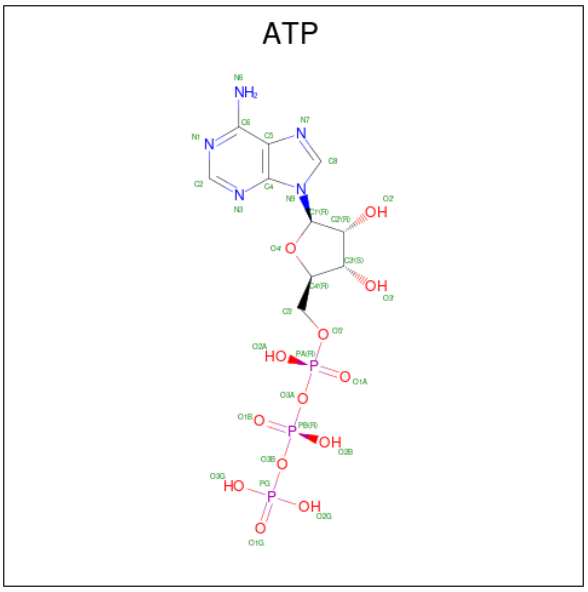
Chain	Residue	Modelled	Actual	Comment	Reference
K	289	HIS	-	expression tag	UNP P32597
K	290	HIS	-	expression tag	UNP P32597
K	291	HIS	-	expression tag	UNP P32597
K	292	HIS	-	expression tag	UNP P32597
K	293	HIS	-	expression tag	UNP P32597
K	294	HIS	-	expression tag	UNP P32597
K	295	SER	-	expression tag	UNP P32597
K	296	GLN	-	expression tag	UNP P32597
K	297	ASP	-	expression tag	UNP P32597
K	298	PRO	-	expression tag	UNP P32597
K	299	ASN	-	expression tag	UNP P32597
K	300	SER	-	expression tag	UNP P32597
K	372	LYS	ARG	conflict	UNP P32597

- Molecule 4 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	2-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	3-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	4-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	5-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	6-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	7-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	8-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	9-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	10-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



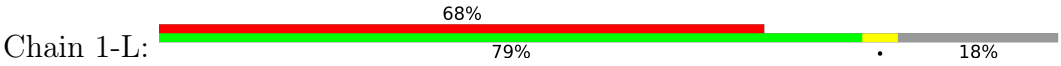
Mol	Chain	Residues	Atoms					AltConf
5	1-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	2-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	3-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	4-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	5-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	6-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	7-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	8-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	9-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	10-L	1	Total	C	N	O	P	0
			31	10	5	13	3	

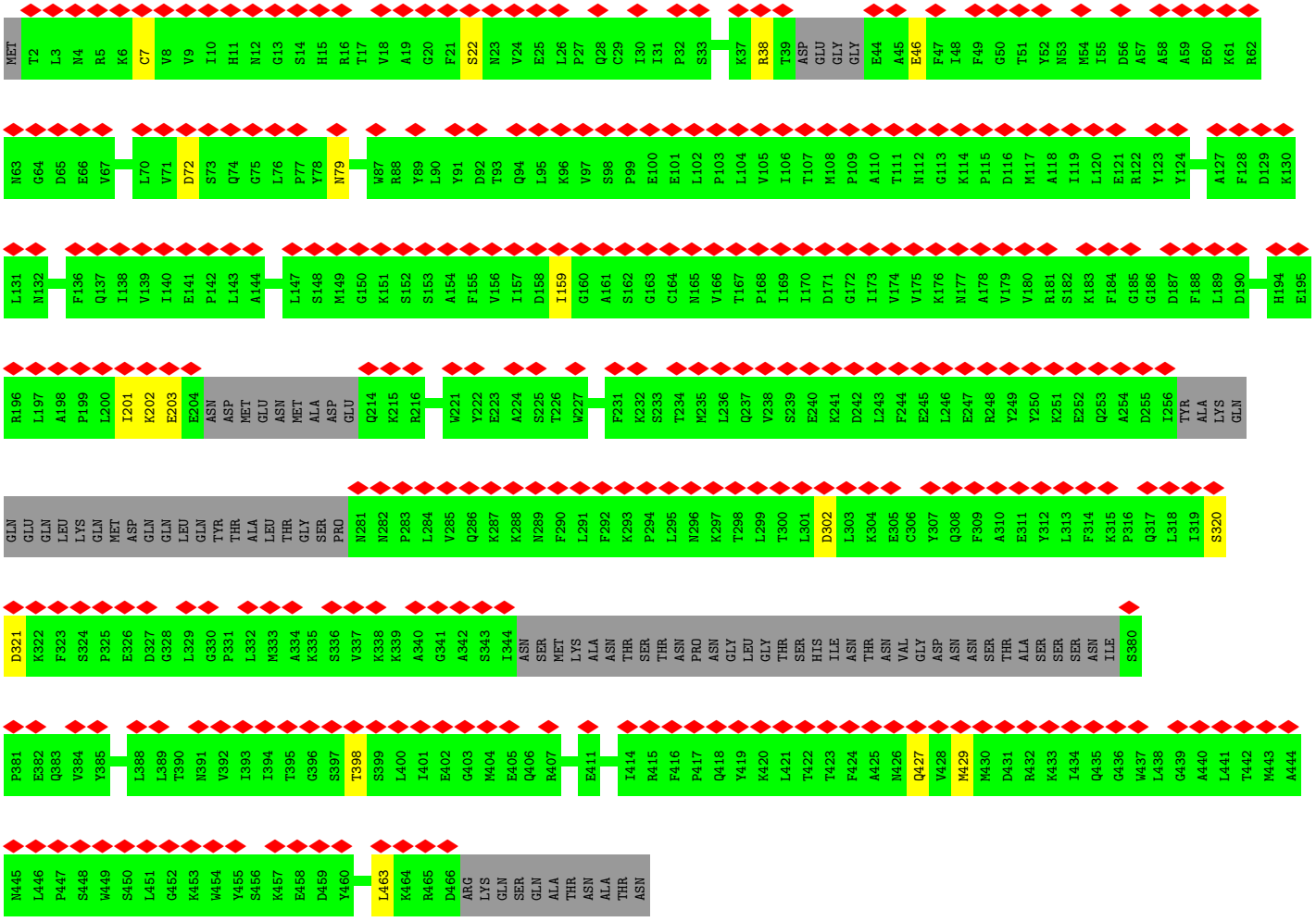
3 Residue-property plots (i)

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: Actin-related protein 7

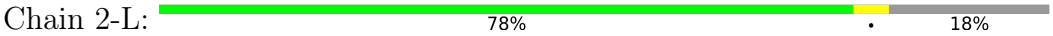
Chain 1-L:

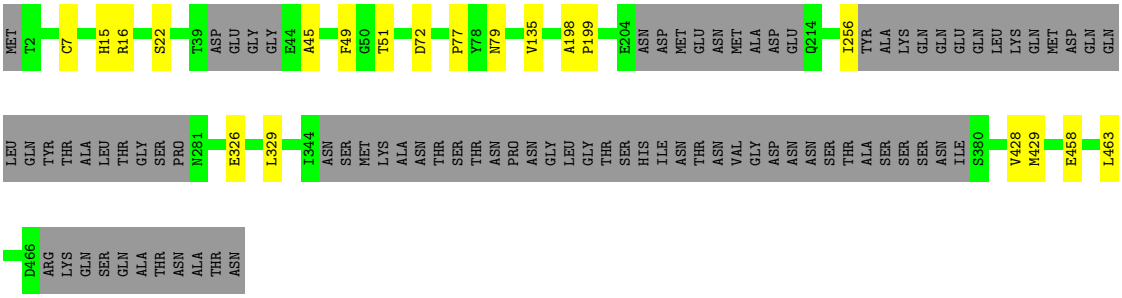




• Molecule 1: Actin-related protein 7

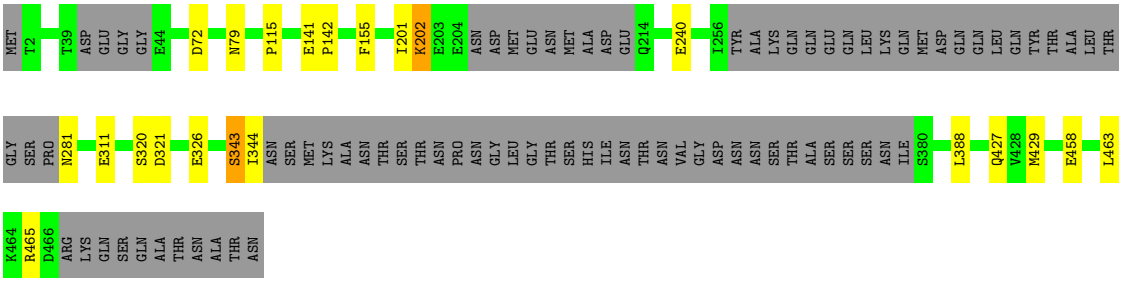
Chain 2-L:





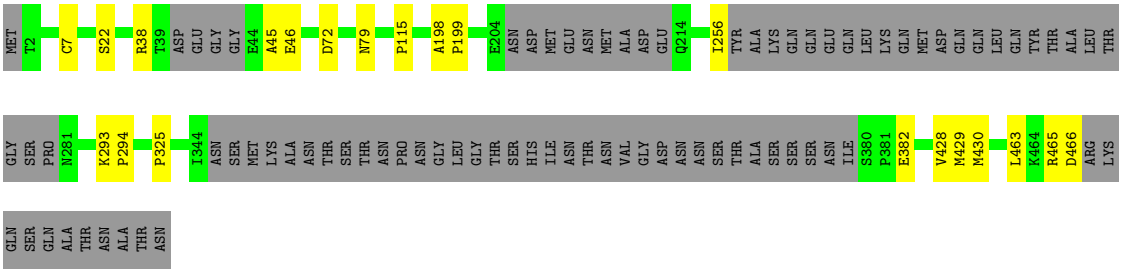
• Molecule 1: Actin-related protein 7

Chain 3-L:



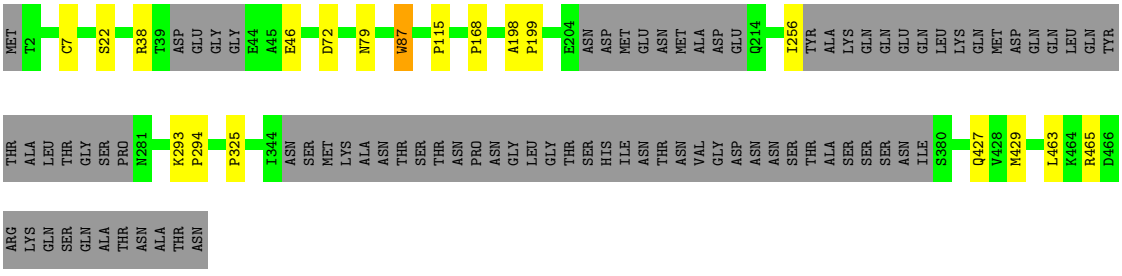
• Molecule 1: Actin-related protein 7

Chain 4-L:



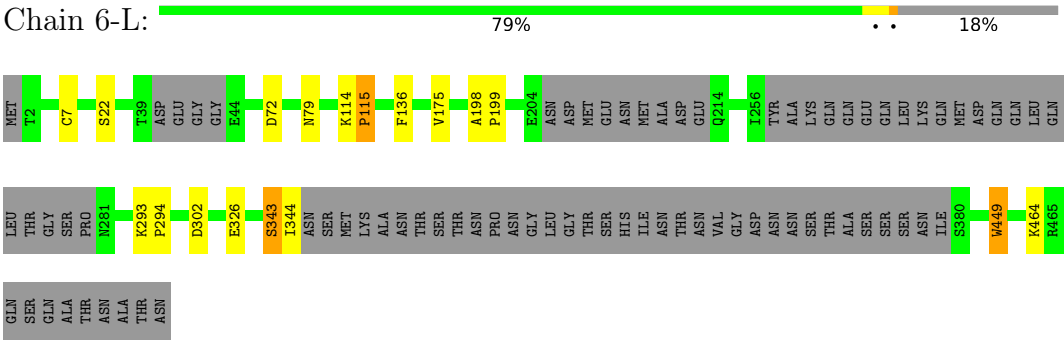
• Molecule 1: Actin-related protein 7

Chain 5-L:



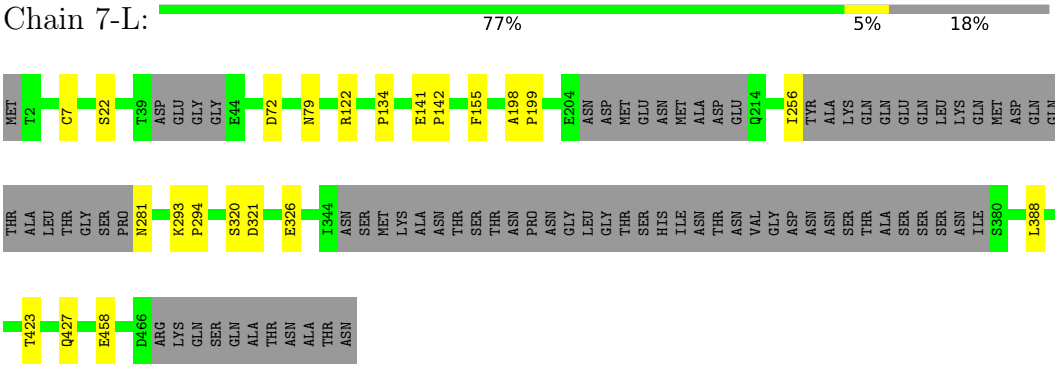
• Molecule 1: Actin-related protein 7

Chain 6-L:



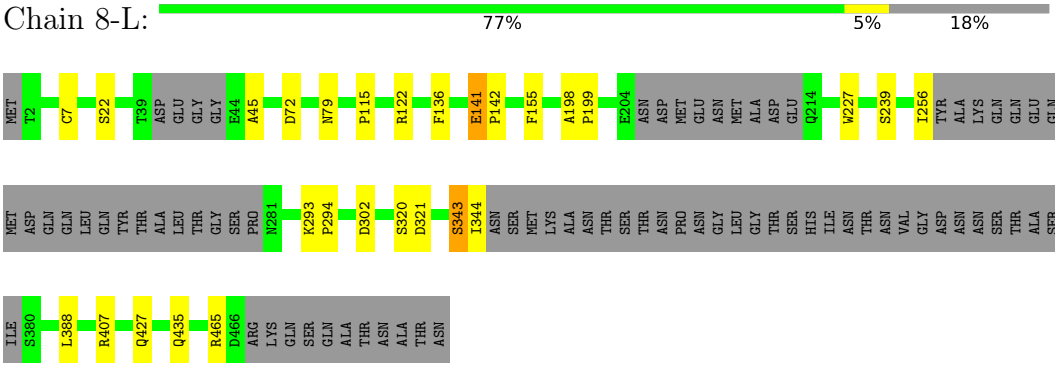
• Molecule 1: Actin-related protein 7

Chain 7-L:



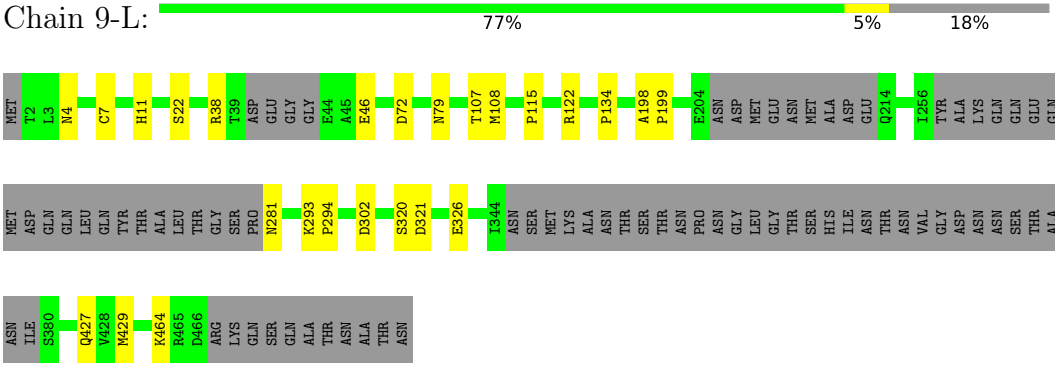
• Molecule 1: Actin-related protein 7

Chain 8-L:



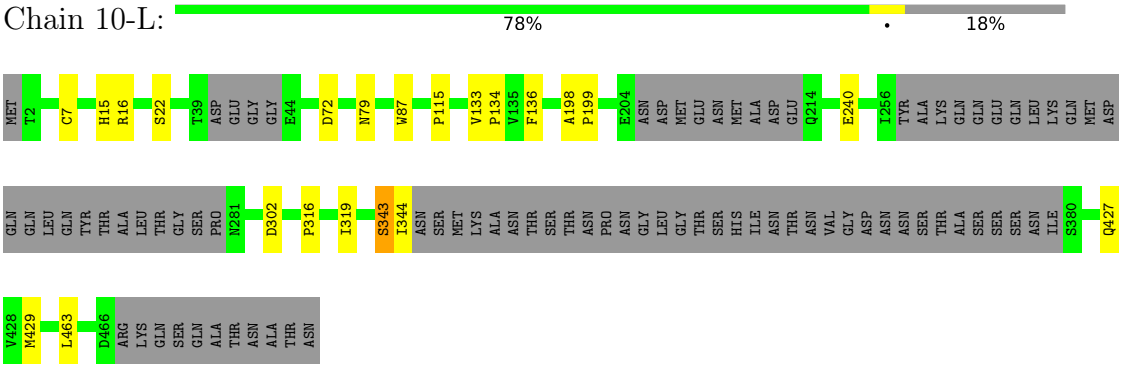
• Molecule 1: Actin-related protein 7

Chain 9-L:



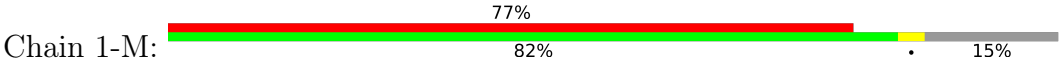
• Molecule 1: Actin-related protein 7

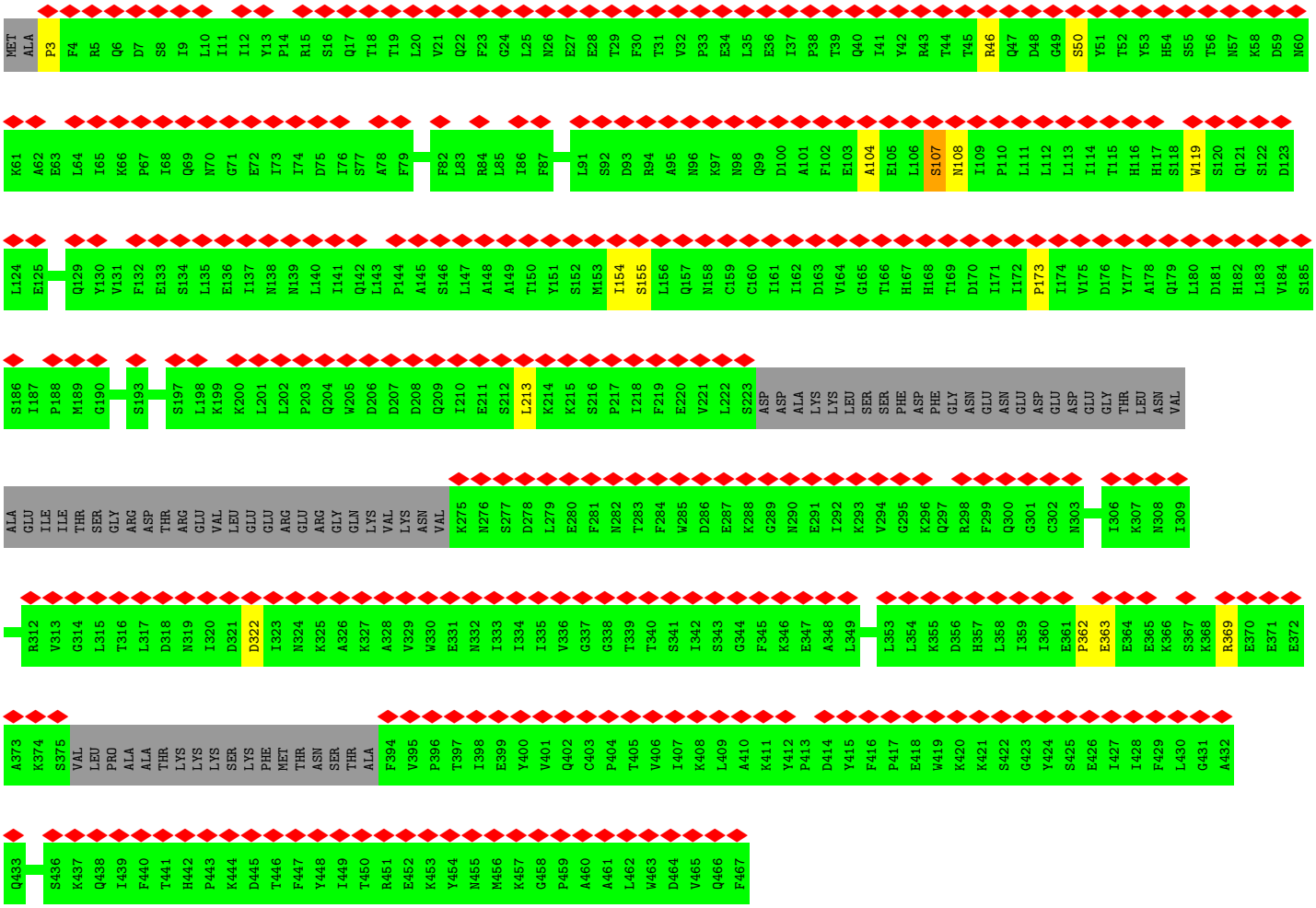
Chain 10-L:



• Molecule 2: Actin-like protein ARP9

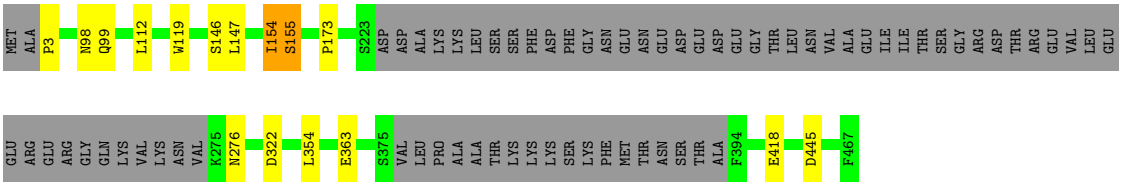
Chain 1-M:





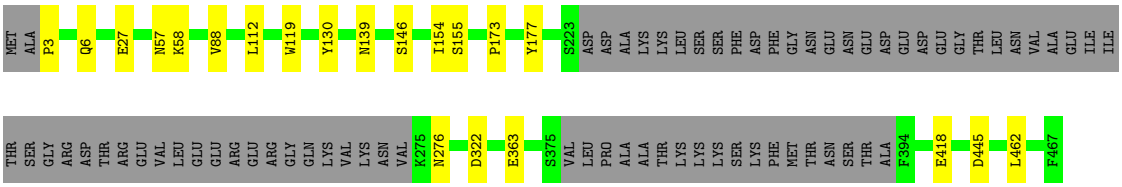
• Molecule 2: Actin-like protein ARP9

Chain 2-M:



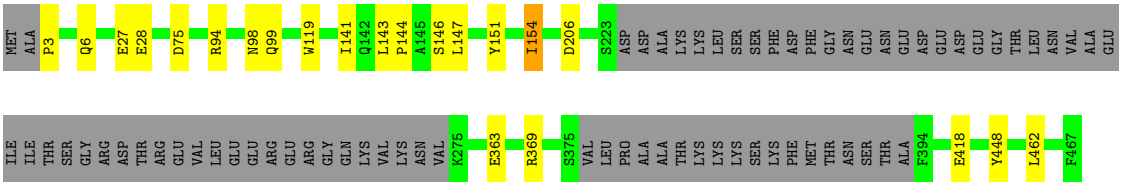
• Molecule 2: Actin-like protein ARP9

Chain 3-M:



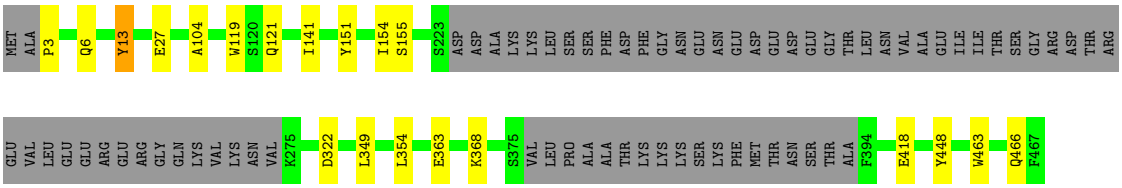
• Molecule 2: Actin-like protein ARP9

Chain 4-M:



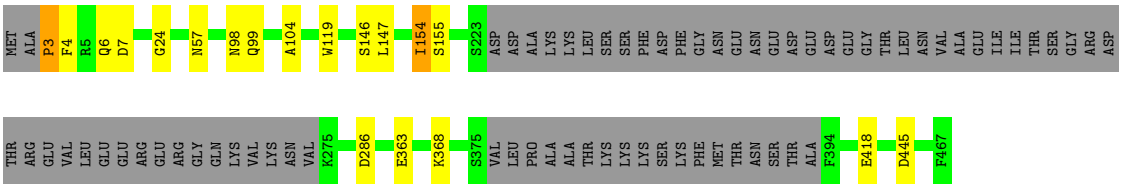
• Molecule 2: Actin-like protein ARP9

Chain 5-M:



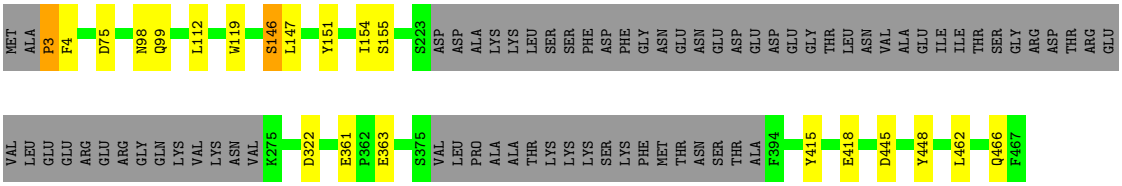
• Molecule 2: Actin-like protein ARP9

Chain 6-M:



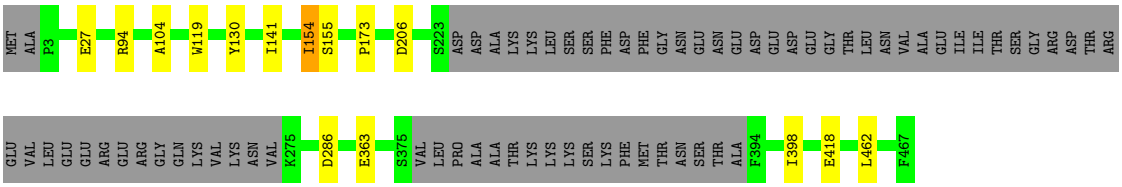
• Molecule 2: Actin-like protein ARP9

Chain 7-M:



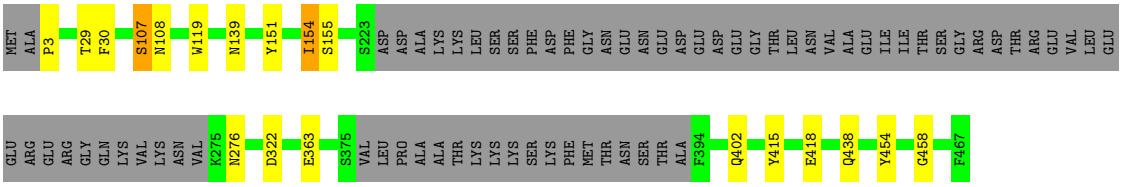
• Molecule 2: Actin-like protein ARP9

Chain 8-M:



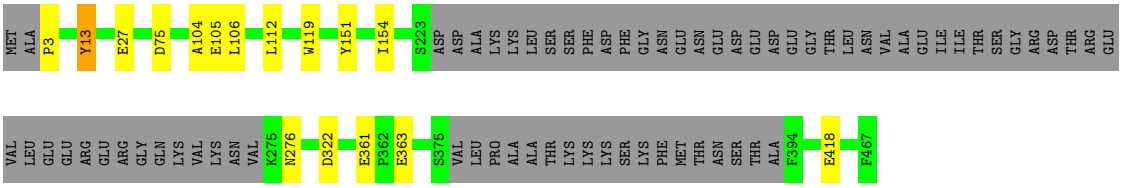
• Molecule 2: Actin-like protein ARP9

Chain 9-M:



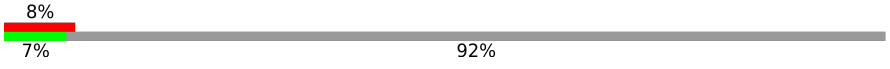
• Molecule 2: Actin-like protein ARP9

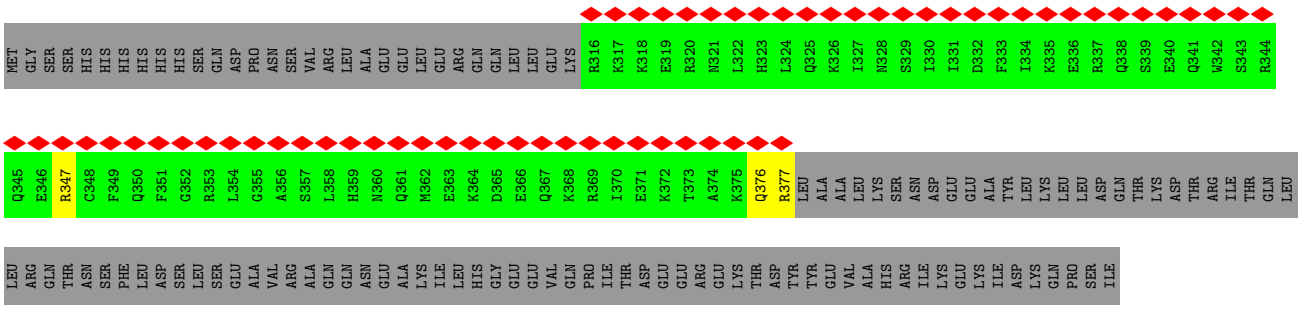
Chain 10-M:

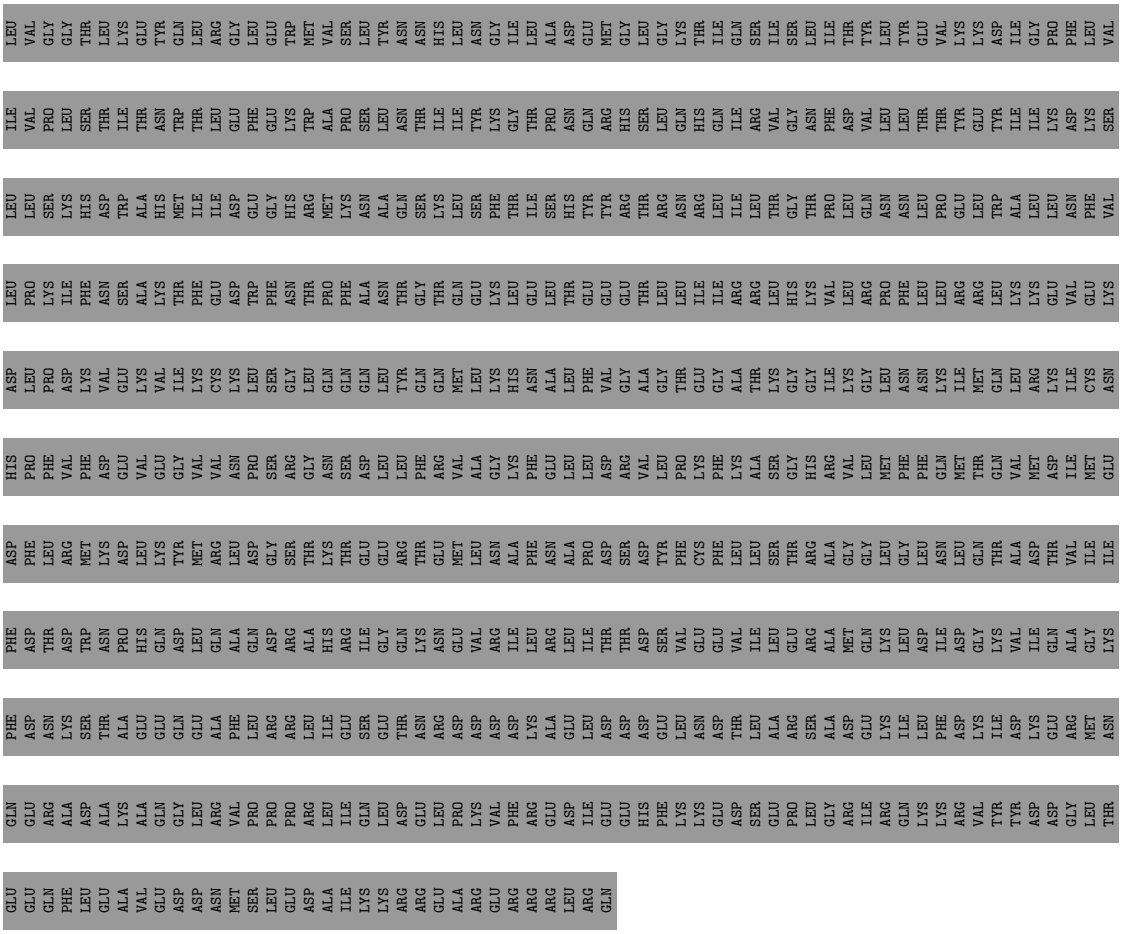


• Molecule 3: Nuclear protein STH1/NPS1

Chain 1-K:

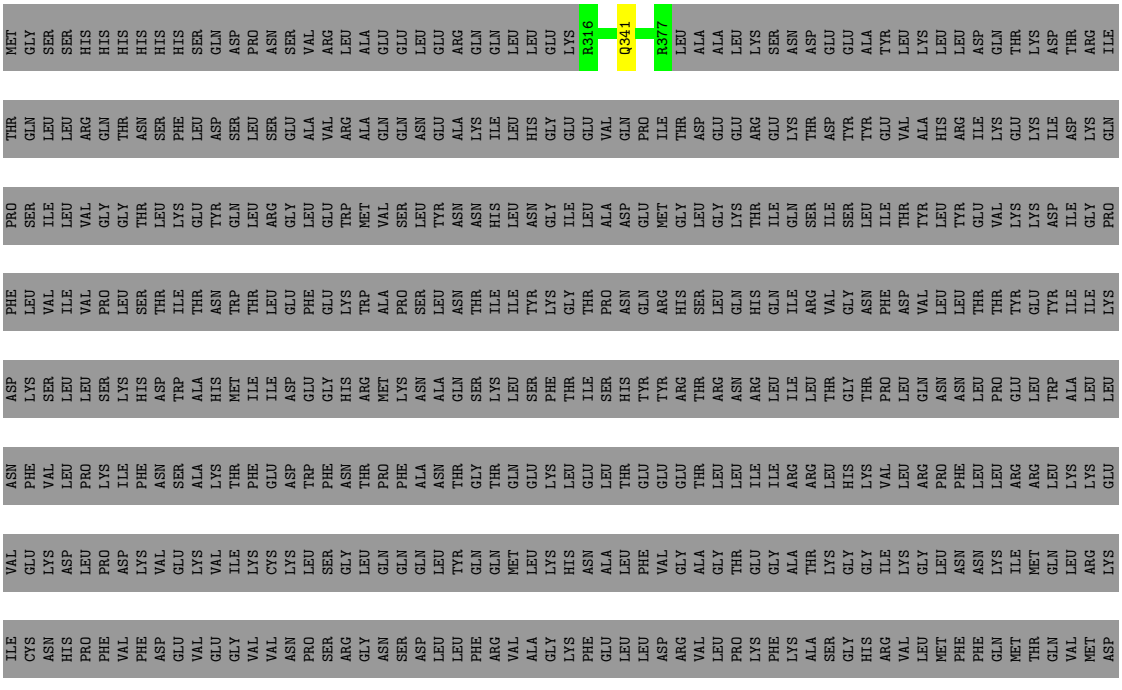


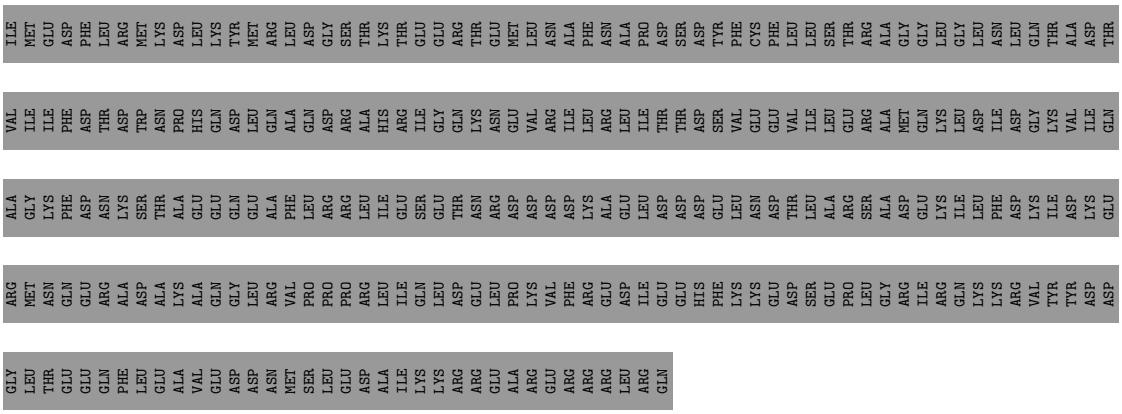




• Molecule 3: Nuclear protein STH1/NPS1

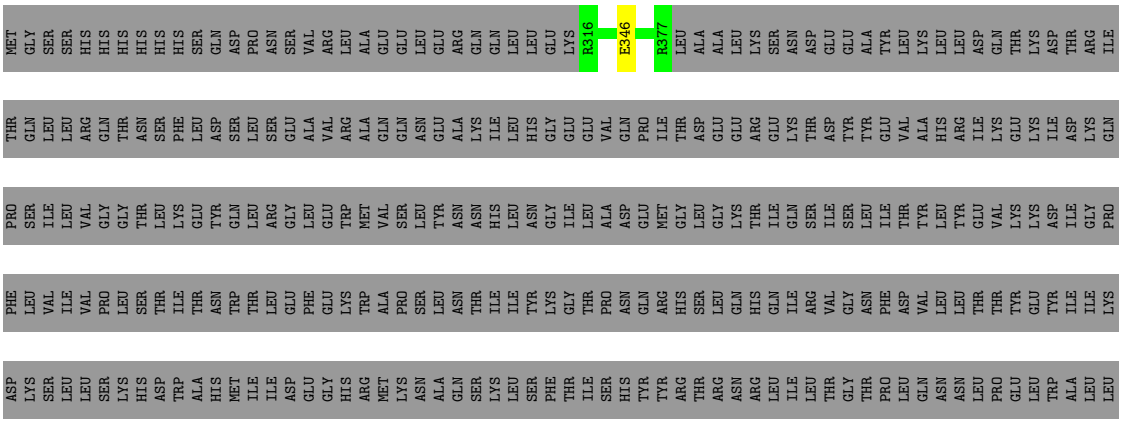
Chain 2-K:





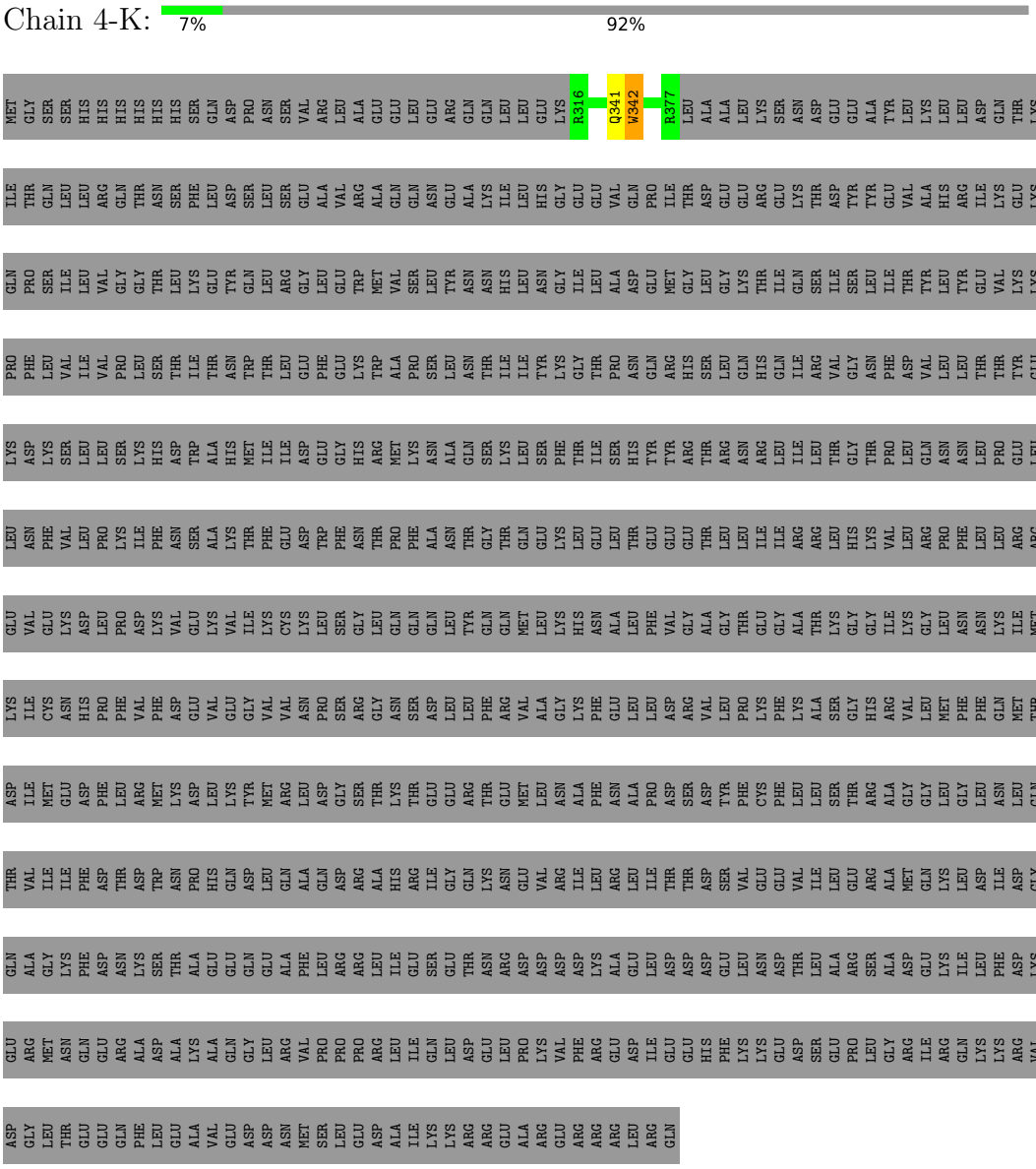
• Molecule 3: Nuclear protein STH1/NPS1

Chain 3-K: 8% 92%



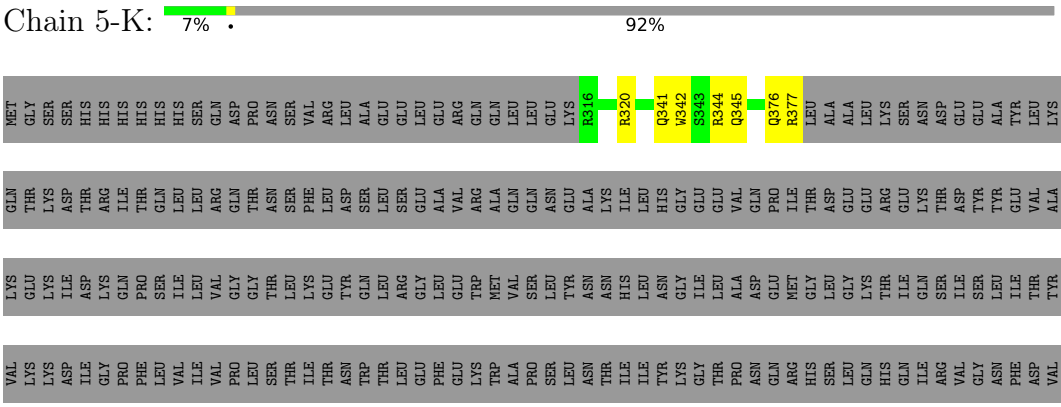
• Molecule 3: Nuclear protein STH1/NPS1

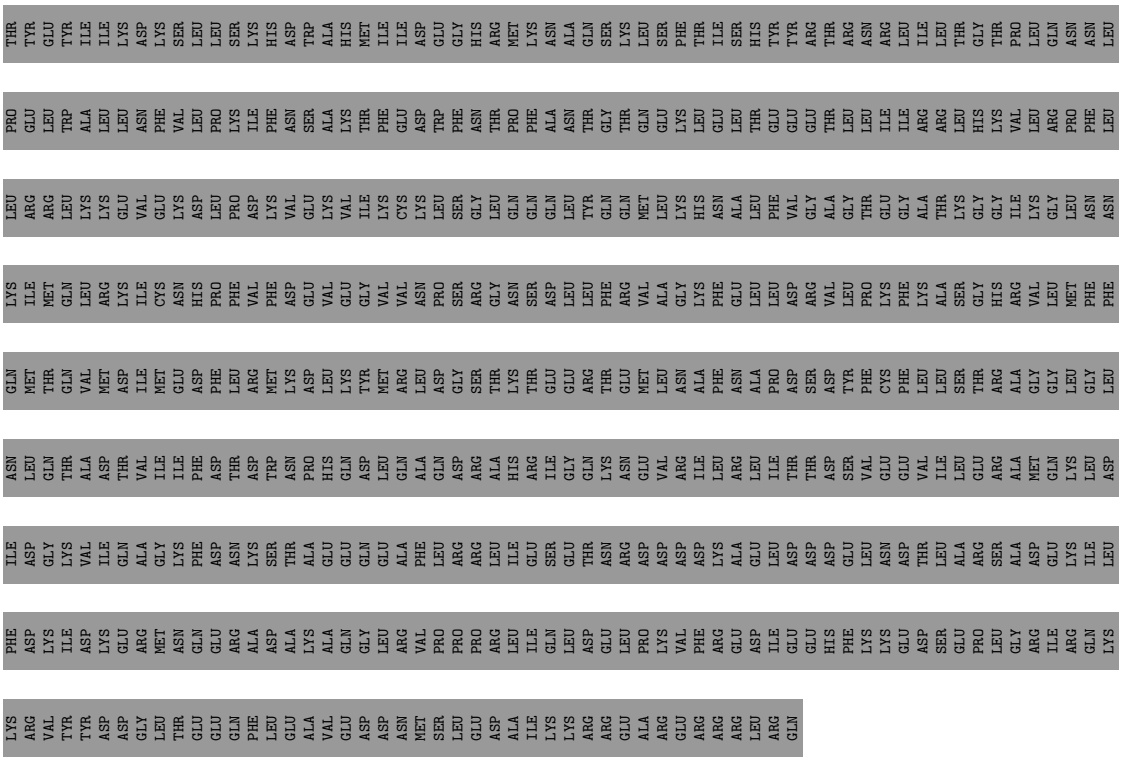
Chain 4-K:



• Molecule 3: Nuclear protein STH1/NPS1

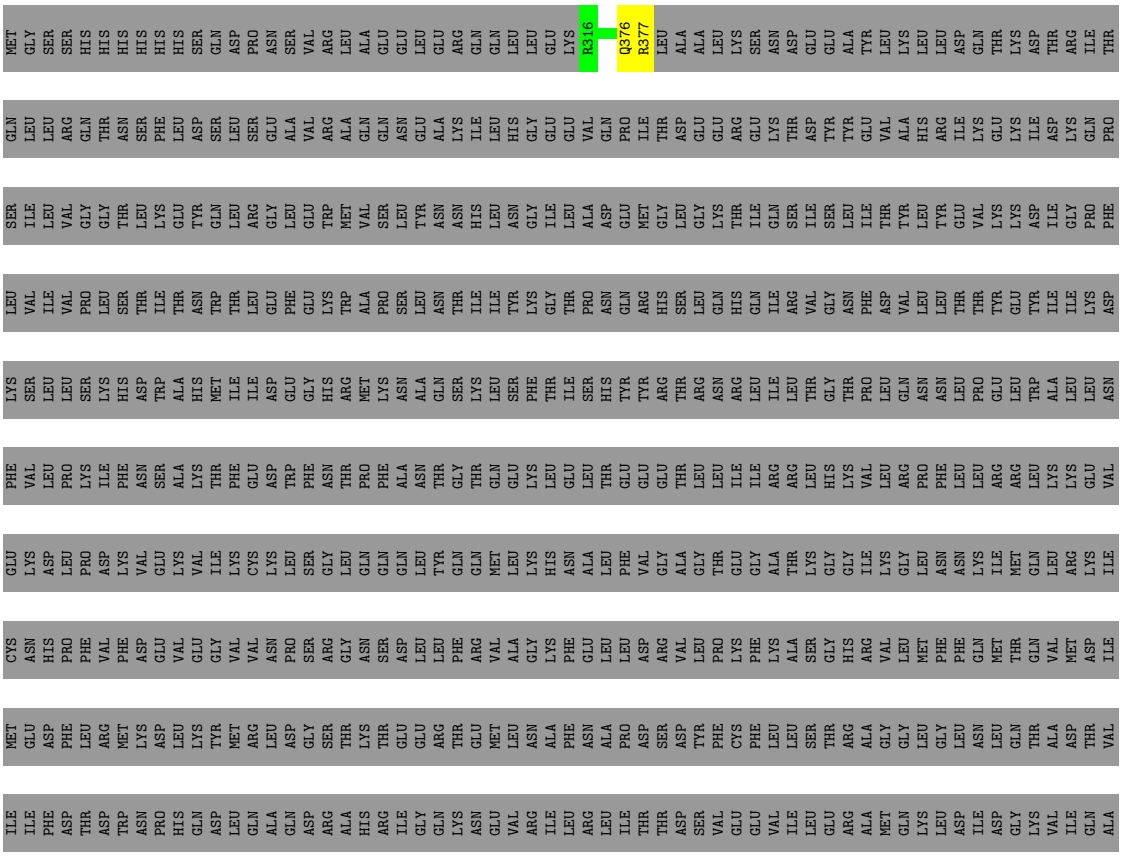
Chain 5-K:





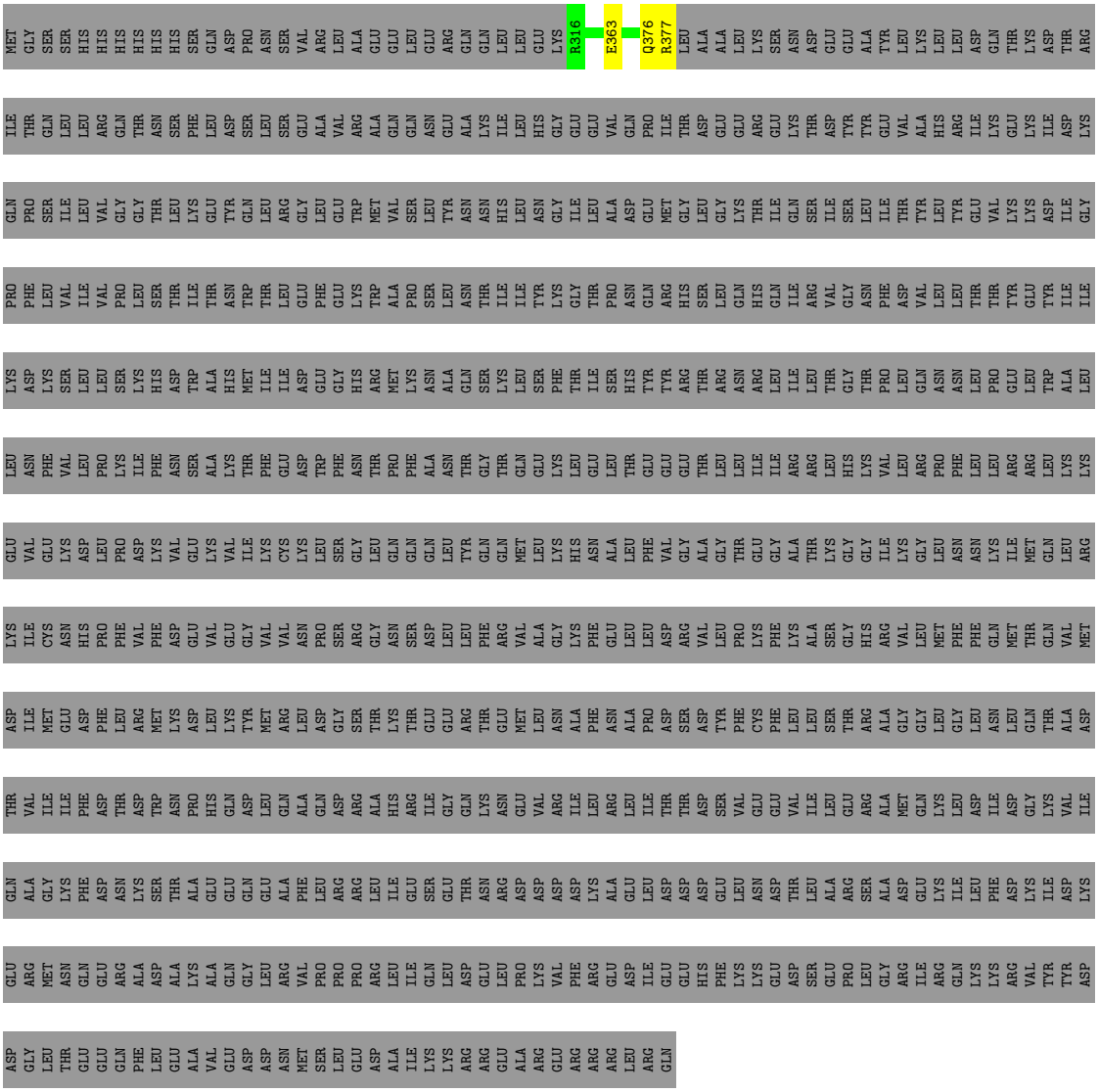
• Molecule 3: Nuclear protein STH1/NPS1

Chain 6-K: 7% 92%



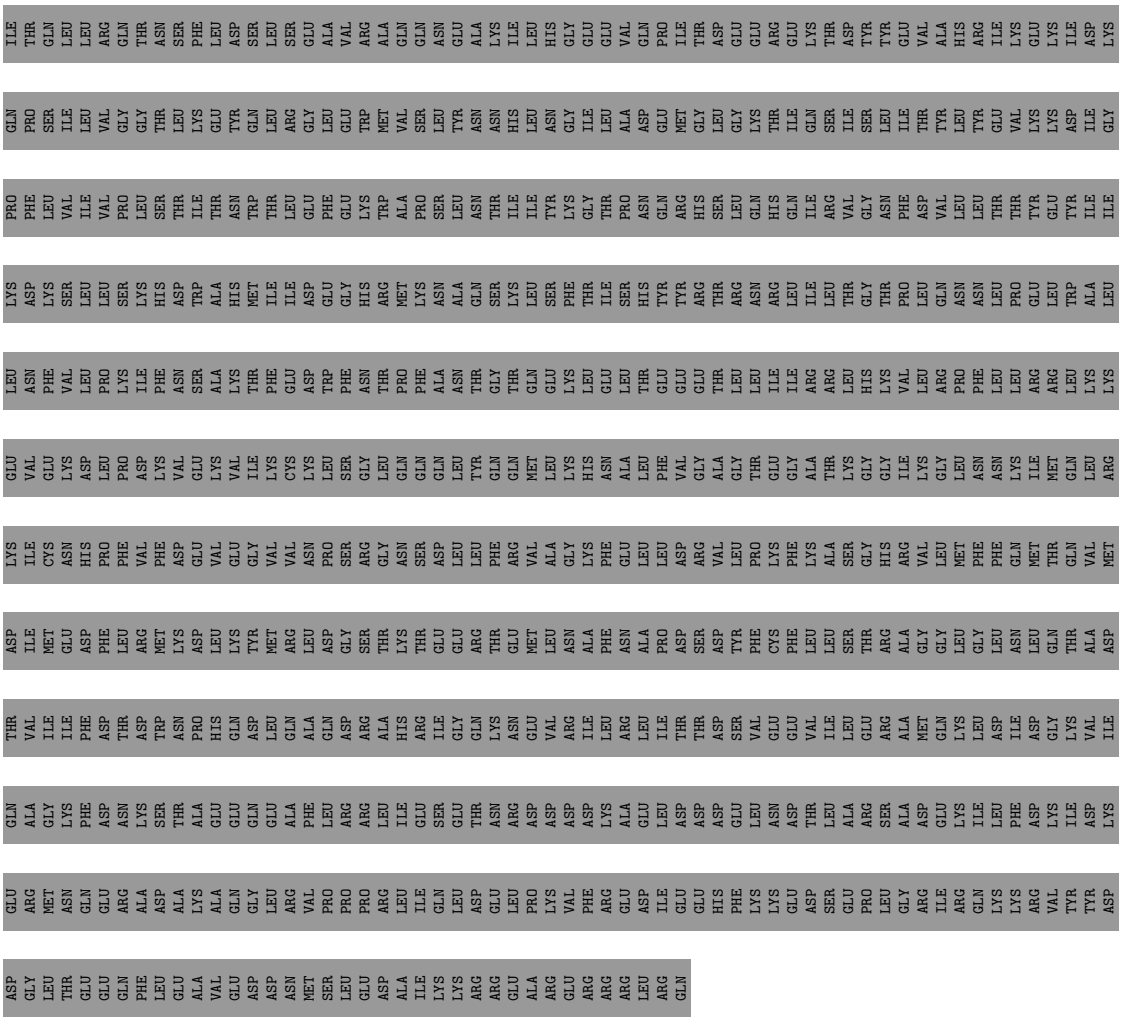
• Molecule 3: Nuclear protein STH1/NPS1

Chain 7-K: 7% 92%



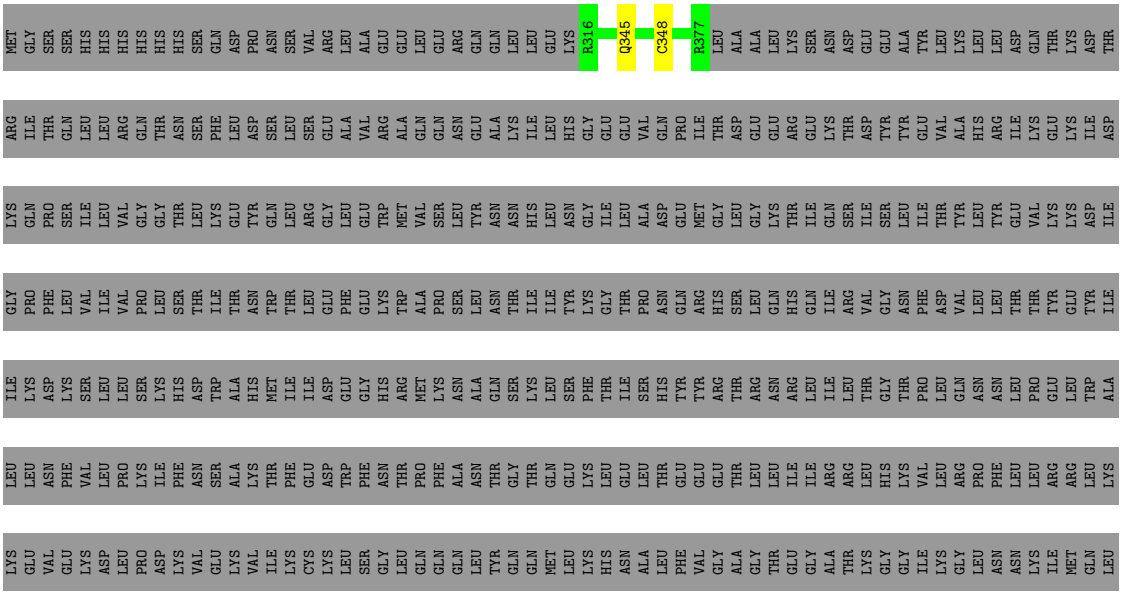
• Molecule 3: Nuclear protein STH1/NPS1

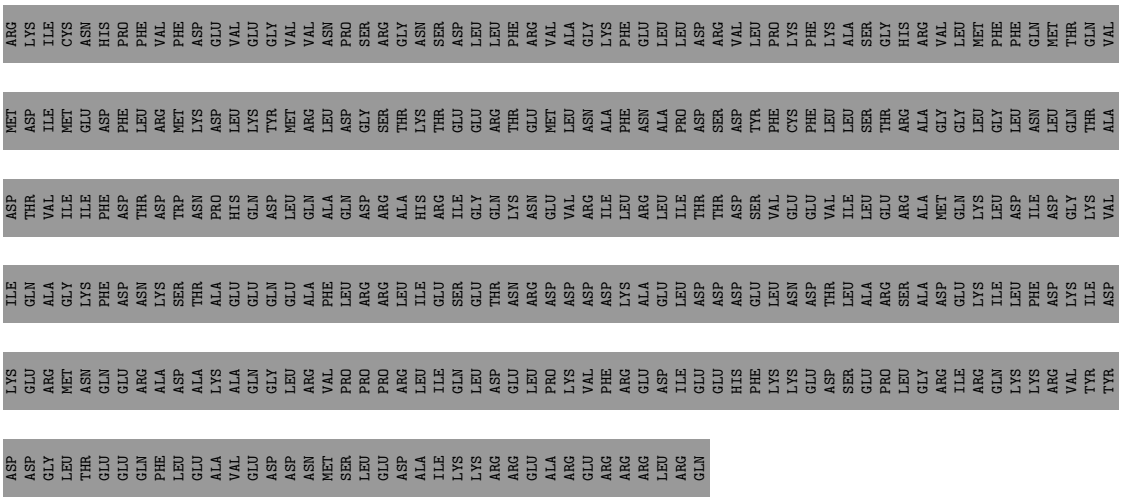
Chain 8-K: 7% 92%



• Molecule 3: Nuclear protein STH1/NPS1

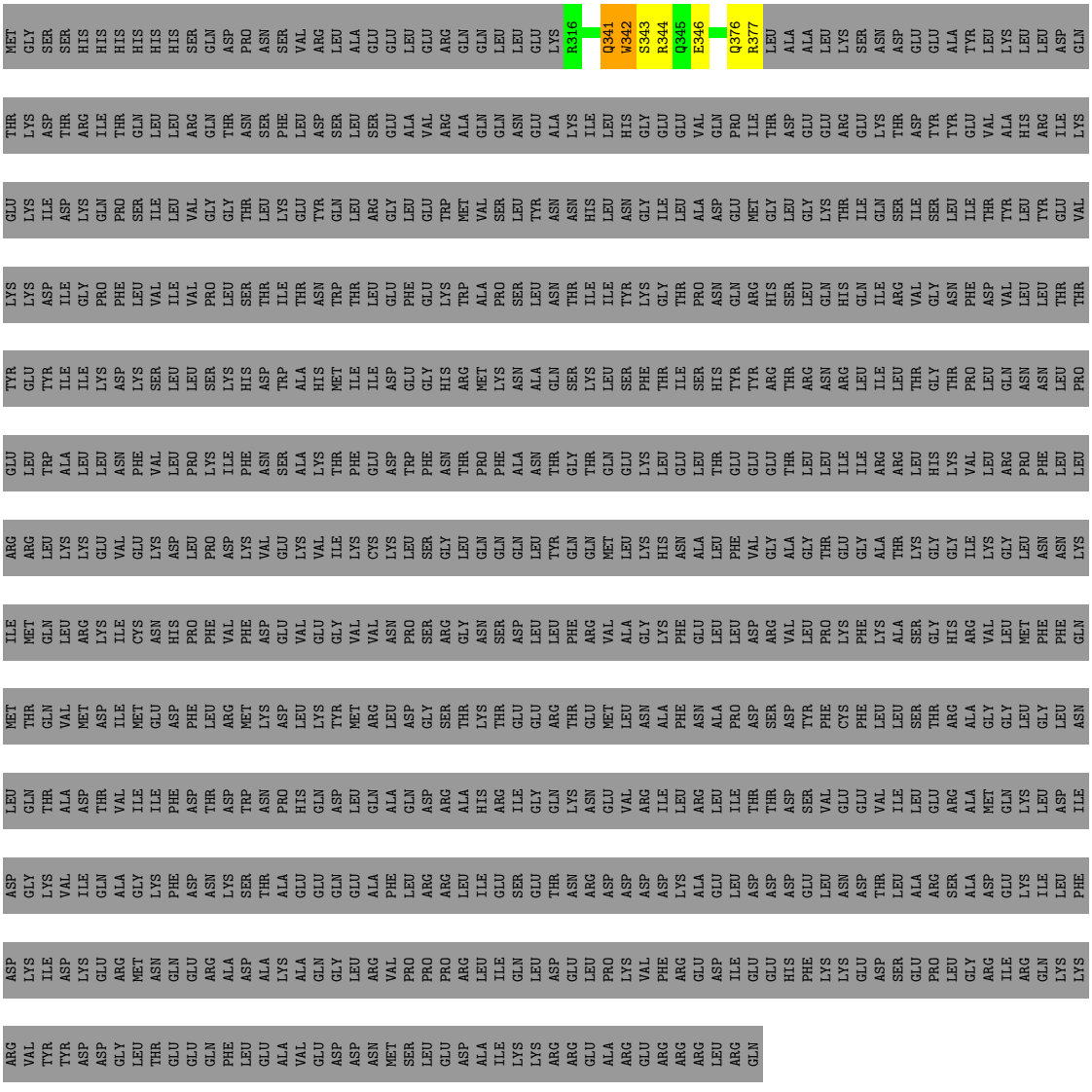
Chain 9-K:





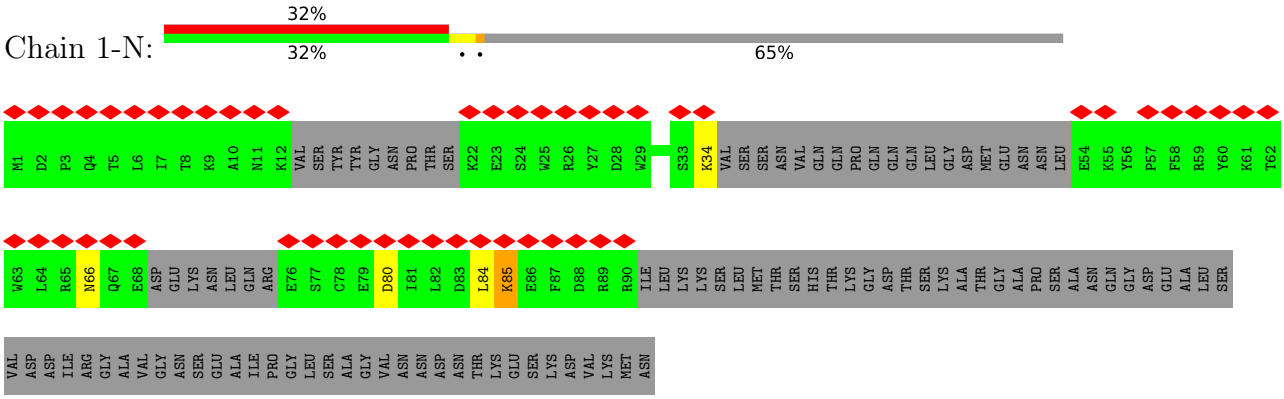
• Molecule 3: Nuclear protein STH1/NPS1

Chain 10-K:



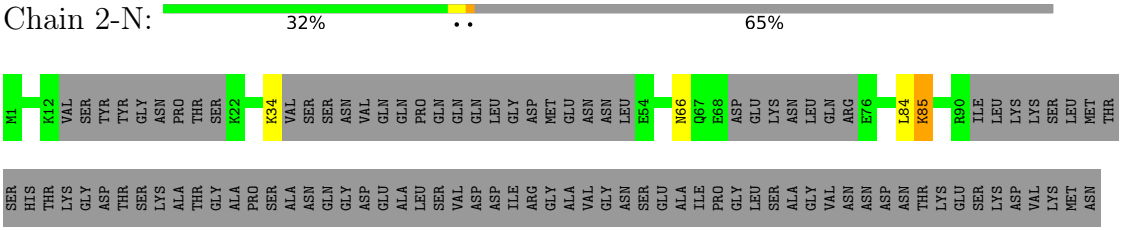
• Molecule 4: Regulator of Ty1 transposition protein 102

Chain 1-N:



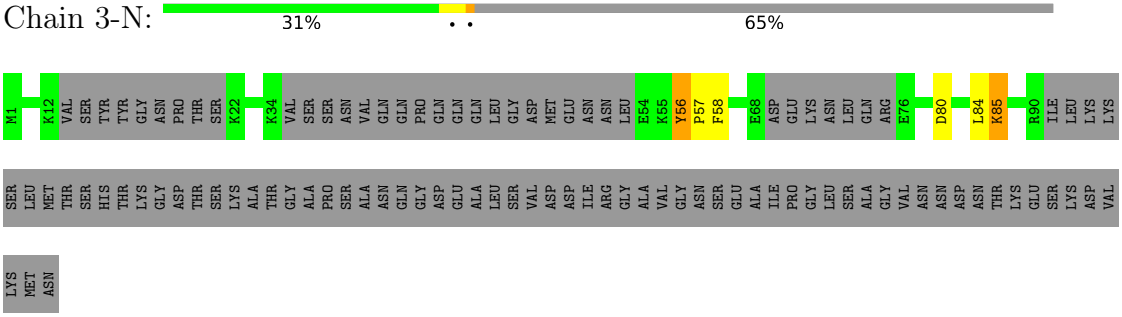
• Molecule 4: Regulator of Ty1 transposition protein 102

Chain 2-N:



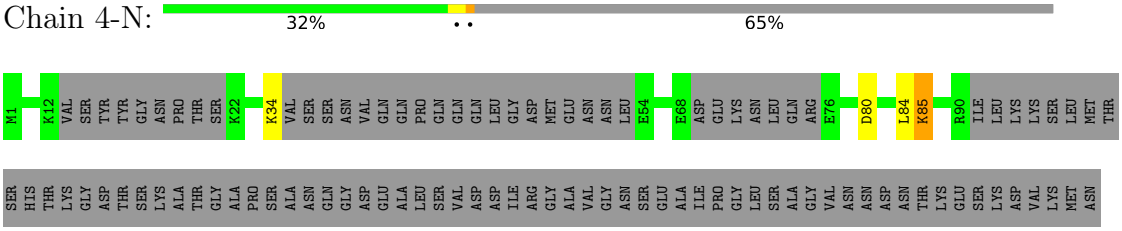
• Molecule 4: Regulator of Ty1 transposition protein 102

Chain 3-N:



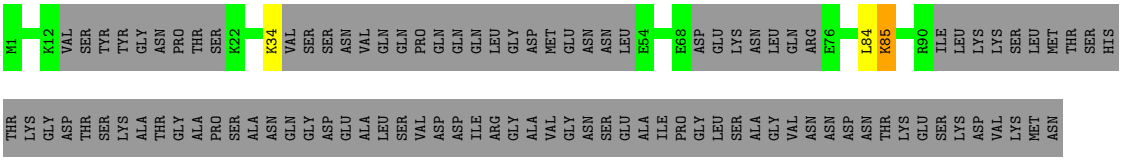
• Molecule 4: Regulator of Ty1 transposition protein 102

Chain 4-N:

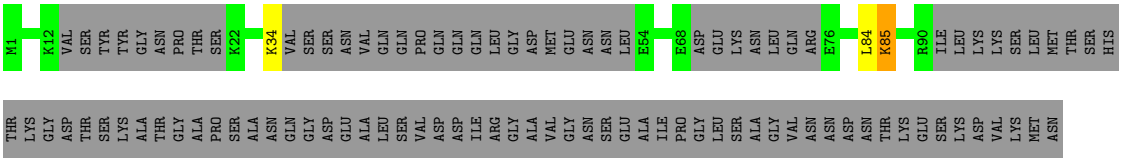


• Molecule 4: Regulator of Ty1 transposition protein 102

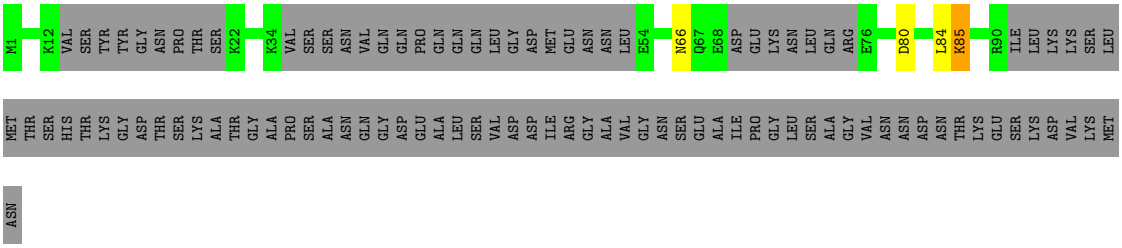
Chain 5-N:



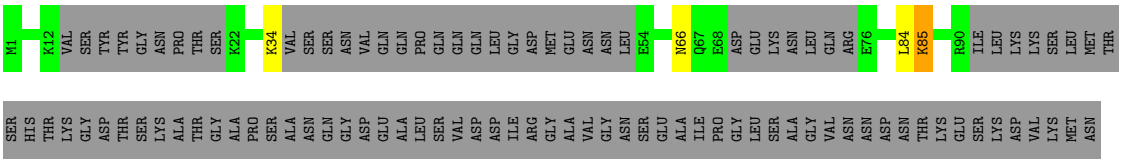
• Molecule 4: Regulator of Ty1 transposition protein 102



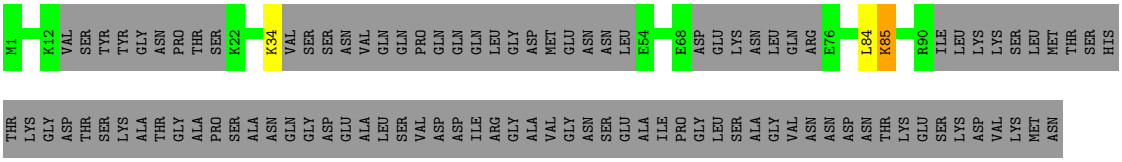
• Molecule 4: Regulator of Ty1 transposition protein 102



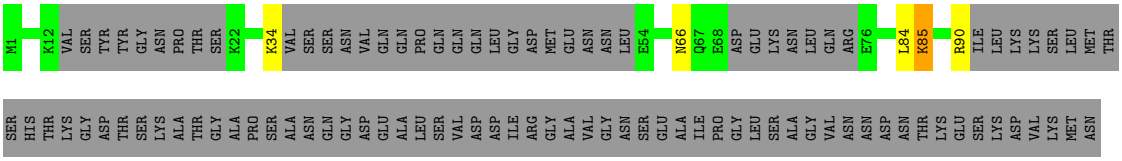
• Molecule 4: Regulator of Ty1 transposition protein 102



• Molecule 4: Regulator of Ty1 transposition protein 102



• Molecule 4: Regulator of Ty1 transposition protein 102


M1 K12 VAL SER TYR TYR GLY ASN PRO THR SER K22 K34 VAL SER SER ASN VAL GLN GLN PRO GLN GLN GLN LEU GLY ASP MET GLU ASN ASN LEU E54 N66 Q67 E68 ASP GLU LYS ASN LEU GLN ARG E76 L84 K85 R90 ILE LEU LYS LYS SER LEU MET THR
SER HIS THR LYS GLY ASP THR SER LYS ALA THR GLY ALA PRO SER ALA ASN GLN GLY ASP GLU ALA LEU SER VAL ASP ASP ILE ARG GLY ALA VAL GLY ASN SER GLU ALA ILE PRO GLY LEU SER ALA GLY VAL ASN ASN ASP ASN THR LYS GLU SER LYS ASP VAL LYS MET ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	415957	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	278.4, 278.4, 278.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1-L	0.85	0/3220	0.70	0/4355
1	2-L	0.86	0/3220	0.71	0/4355
1	3-L	0.86	0/3220	0.72	0/4355
1	4-L	0.85	0/3220	0.70	0/4355
1	5-L	0.86	0/3220	0.71	0/4355
1	6-L	0.86	0/3220	0.71	0/4355
1	7-L	0.86	0/3220	0.70	1/4355 (0.0%)
1	8-L	0.86	0/3220	0.72	0/4355
1	9-L	0.86	0/3220	0.70	0/4355
1	10-L	0.86	0/3220	0.70	0/4355
2	1-M	0.85	0/3259	0.70	0/4417
2	2-M	0.85	0/3259	0.69	0/4417
2	3-M	0.84	0/3259	0.70	2/4417 (0.0%)
2	4-M	0.85	0/3259	0.70	3/4417 (0.1%)
2	5-M	0.86	0/3259	0.71	2/4417 (0.0%)
2	6-M	0.84	0/3259	0.70	0/4417
2	7-M	0.84	0/3259	0.71	2/4417 (0.0%)
2	8-M	0.85	0/3259	0.69	1/4417 (0.0%)
2	9-M	0.84	0/3259	0.71	2/4417 (0.0%)
2	10-M	0.84	0/3259	0.70	1/4417 (0.0%)
3	1-K	0.90	0/543	0.64	0/716
3	2-K	0.88	0/543	0.59	0/716
3	3-K	0.88	0/543	0.59	0/716
3	4-K	0.88	0/543	0.61	0/716
3	5-K	0.87	0/543	0.56	0/716
3	6-K	0.89	0/543	0.60	0/716
3	7-K	0.88	0/543	0.59	0/716
3	8-K	0.87	0/543	0.58	0/716
3	9-K	0.91	0/543	0.62	0/716
3	10-K	0.88	0/543	0.61	0/716
4	1-N	0.89	0/505	0.70	0/674
4	2-N	0.90	0/505	0.68	0/674

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	3-N	0.90	0/505	0.75	1/674 (0.1%)
4	4-N	0.90	0/505	0.76	0/674
4	5-N	0.89	0/505	0.73	0/674
4	6-N	0.88	0/505	0.73	0/674
4	7-N	0.90	0/505	0.75	0/674
4	8-N	0.89	0/505	0.72	0/674
4	9-N	0.90	0/505	0.70	0/674
4	10-N	0.89	0/505	0.74	0/674
All	All	0.86	0/75270	0.70	15/101620 (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	2-L	0	1
1	3-L	0	2
1	6-L	0	2
1	8-L	0	2
1	10-L	0	2
2	1-M	0	2
2	2-M	0	2
2	3-M	0	2
2	4-M	0	2
2	5-M	0	4
2	6-M	0	2
2	7-M	0	4
2	9-M	0	2
2	10-M	0	2
All	All	0	31

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7-M	448	TYR	CB-CG-CD1	-7.84	116.30	121.00
2	4-M	448	TYR	CB-CG-CD1	-6.79	116.92	121.00
2	5-M	151	TYR	CB-CG-CD1	-6.60	117.04	121.00
2	8-M	130	TYR	CB-CG-CD2	-6.20	117.28	121.00
2	5-M	448	TYR	CB-CG-CD1	-6.14	117.31	121.00
2	4-M	151	TYR	CB-CG-CD2	-5.95	117.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	9-M	151	TYR	CB-CG-CD1	-5.83	117.50	121.00
4	3-N	56	TYR	C-N-CD	-5.75	107.95	120.60
2	3-M	177	TYR	CB-CG-CD2	-5.65	117.61	121.00
2	4-M	94	ARG	NE-CZ-NH2	-5.49	117.56	120.30
2	3-M	130	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	7-L	407	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	7-M	151	TYR	CB-CG-CD1	-5.21	117.87	121.00
2	9-M	415	TYR	CB-CG-CD2	-5.20	117.88	121.00
2	10-M	151	TYR	CB-CG-CD1	-5.00	118.00	121.00

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1-M	3	PRO	Mainchain,Peptide
1	10-L	343	SER	Mainchain,Peptide
2	10-M	3	PRO	Mainchain,Peptide
1	2-L	49	PHE	Mainchain
2	2-M	3	PRO	Mainchain,Peptide
1	3-L	343	SER	Mainchain,Peptide
2	3-M	3	PRO	Mainchain,Peptide
2	4-M	3	PRO	Mainchain,Peptide
2	5-M	3	PRO	Mainchain,Peptide
2	5-M	466	GLN	Mainchain,Peptide
1	6-L	343	SER	Mainchain,Peptide
2	6-M	3	PRO	Mainchain,Peptide
2	7-M	3	PRO	Mainchain,Peptide
2	7-M	466	GLN	Mainchain,Peptide
1	8-L	343	SER	Mainchain,Peptide
2	9-M	3	PRO	Mainchain,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	1-L	3154	0	3173	11	0
1	2-L	3154	0	3173	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-L	3154	0	3173	18	0
1	4-L	3154	0	3173	11	0
1	5-L	3154	0	3173	15	0
1	6-L	3154	0	3173	14	0
1	7-L	3154	0	3173	16	0
1	8-L	3154	0	3173	21	0
1	9-L	3154	0	3173	19	0
1	10-L	3154	0	3173	15	0
2	1-M	3192	0	3180	8	0
2	2-M	3192	0	3180	12	0
2	3-M	3192	0	3180	13	0
2	4-M	3192	0	3180	14	0
2	5-M	3192	0	3180	13	0
2	6-M	3192	0	3180	13	0
2	7-M	3192	0	3180	16	0
2	8-M	3192	0	3180	9	0
2	9-M	3192	0	3180	13	0
2	10-M	3192	0	3180	13	0
3	1-K	537	0	546	2	0
3	2-K	537	0	546	0	0
3	3-K	537	0	546	1	0
3	4-K	537	0	546	1	0
3	5-K	537	0	546	4	0
3	6-K	537	0	546	1	0
3	7-K	537	0	546	2	0
3	8-K	537	0	546	1	0
3	9-K	537	0	546	2	0
3	10-K	537	0	546	5	0
4	1-N	494	0	473	6	0
4	2-N	494	0	473	6	0
4	3-N	494	0	473	4	0
4	4-N	494	0	473	5	0
4	5-N	494	0	473	4	0
4	6-N	494	0	473	4	0
4	7-N	494	0	473	4	0
4	8-N	494	0	473	6	0
4	9-N	494	0	473	4	0
4	10-N	494	0	473	7	0
5	1-L	31	0	12	1	0
5	2-L	31	0	12	2	0
5	3-L	31	0	12	1	0
5	4-L	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	5-L	31	0	12	2	0
5	6-L	31	0	12	1	0
5	7-L	31	0	12	1	0
5	8-L	31	0	12	1	0
5	9-L	31	0	12	1	0
5	10-L	31	0	12	2	0
All	All	74080	0	73840	350	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 2.

All (350) 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)
2:M:154:ILE:HG22	2:M:154:ILE:O	1.74	0.86
2:M:154:ILE:HG22	2:M:154:ILE:O	1.76	0.84
1:L:256:ILE:O	1:L:256:ILE:HG23	1.77	0.83
1:L:465:ARG:O	1:L:465:ARG:NH1	2.15	0.76
3:K:346:GLU:N	3:K:346:GLU:OE1	2.19	0.75
2:M:154:ILE:HG22	2:M:154:ILE:O	1.85	0.75
2:M:438:GLN:O	2:M:438:GLN:HG3	1.88	0.74
2:M:154:ILE:HG22	2:M:154:ILE:O	1.87	0.72
2:M:6:GLN:N	2:M:6:GLN:OE1	2.22	0.72
5:L:501:ATP:O1G	5:L:501:ATP:O1B	2.05	0.70
2:M:154:ILE:HG22	2:M:154:ILE:O	1.90	0.70
3:K:346:GLU:N	3:K:346:GLU:OE1	2.26	0.69
5:L:501:ATP:O1G	5:L:501:ATP:O1B	2.08	0.68
5:L:501:ATP:O2B	5:L:501:ATP:O2G	2.12	0.68
2:M:418:GLU:OE1	2:M:418:GLU:N	2.26	0.67
2:M:154:ILE:HG22	2:M:154:ILE:O	1.93	0.67
2:M:363:GLU:OE1	2:M:363:GLU:N	2.27	0.64
2:M:154:ILE:HG22	2:M:154:ILE:O	1.97	0.63
1:L:256:ILE:HG22	1:L:256:ILE:O	1.97	0.63
2:M:6:GLN:N	2:M:6:GLN:OE1	2.29	0.62
2:M:363:GLU:OE1	2:M:363:GLU:N	2.26	0.62
2:M:418:GLU:OE1	2:M:418:GLU:N	2.25	0.62
1:L:256:ILE:O	1:L:256:ILE:HG23	1.99	0.62
2:M:363:GLU:CD	2:M:363:GLU:H	2.03	0.61
2:M:363:GLU:OE1	2:M:363:GLU:N	2.29	0.61
3:K:345:GLN:OE1	3:K:345:GLN:N	2.26	0.61
1:L:87:TRP:HA	1:L:87:TRP:CE3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:34:LYS:O	4:N:34:LYS:HG2	2.01	0.61
2:M:462:LEU:HD12	2:M:462:LEU:O	1.99	0.61
2:M:418:GLU:OE1	2:M:418:GLU:N	2.26	0.61
4:N:34:LYS:O	4:N:34:LYS:HG2	2.00	0.61
4:N:34:LYS:O	4:N:34:LYS:HG2	2.01	0.61
1:L:344:ILE:O	1:L:344:ILE:HG22	2.01	0.60
2:M:363:GLU:OE1	2:M:363:GLU:N	2.26	0.60
2:M:6:GLN:OE1	2:M:6:GLN:N	2.27	0.60
2:M:418:GLU:OE1	2:M:418:GLU:N	2.27	0.60
4:N:34:LYS:O	4:N:34:LYS:HG2	2.02	0.60
4:N:34:LYS:O	4:N:34:LYS:HG2	2.03	0.59
1:L:227:TRP:C	1:L:227:TRP:CD1	2.75	0.59
2:M:6:GLN:OE1	2:M:6:GLN:N	2.31	0.59
2:M:154:ILE:O	2:M:154:ILE:CG2	2.47	0.59
1:L:302:ASP:C	1:L:302:ASP:OD1	2.40	0.59
4:N:34:LYS:O	4:N:34:LYS:HG2	2.03	0.59
1:L:302:ASP:C	1:L:302:ASP:OD1	2.40	0.59
4:N:34:LYS:O	4:N:34:LYS:HG2	2.03	0.59
1:L:302:ASP:C	1:L:302:ASP:OD1	2.42	0.59
1:L:87:TRP:HA	1:L:87:TRP:HE3	1.68	0.59
4:N:34:LYS:O	4:N:34:LYS:HG2	2.04	0.58
5:L:501:ATP:O2B	5:L:501:ATP:O2G	2.22	0.58
1:L:302:ASP:C	1:L:302:ASP:OD1	2.42	0.58
2:M:363:GLU:OE1	2:M:363:GLU:N	2.33	0.57
1:L:427:GLN:OE1	1:L:427:GLN:N	2.32	0.56
1:L:427:GLN:OE1	1:L:427:GLN:N	2.31	0.56
1:L:240:GLU:H	1:L:240:GLU:CD	2.09	0.56
2:M:363:GLU:OE1	2:M:363:GLU:N	2.32	0.56
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.21	0.56
2:M:363:GLU:H	2:M:363:GLU:CD	2.04	0.56
2:M:418:GLU:OE1	2:M:418:GLU:N	2.31	0.56
2:M:276:ASN:OD1	2:M:276:ASN:N	2.38	0.56
2:M:206:ASP:OD1	2:M:206:ASP:C	2.44	0.55
1:L:240:GLU:OE1	1:L:240:GLU:N	2.33	0.55
1:L:326:GLU:OE1	1:L:326:GLU:N	2.38	0.55
2:M:276:ASN:OD1	2:M:276:ASN:N	2.39	0.55
1:L:427:GLN:OE1	1:L:427:GLN:N	2.31	0.55
1:L:458:GLU:OE1	1:L:458:GLU:N	2.35	0.55
1:L:136:PHE:C	1:L:136:PHE:CD2	2.80	0.55
1:L:427:GLN:OE1	1:L:427:GLN:N	2.34	0.55
1:L:427:GLN:OE1	1:L:427:GLN:N	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:276:ASN:OD1	2:M:276:ASN:N	2.39	0.54
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.23	0.54
1:L:427:GLN:OE1	1:L:427:GLN:N	2.33	0.54
1:L:427:GLN:OE1	1:L:427:GLN:N	2.32	0.54
1:L:302:ASP:C	1:L:302:ASP:OD1	2.43	0.54
2:M:276:ASN:OD1	2:M:276:ASN:N	2.40	0.54
2:M:363:GLU:OE1	2:M:363:GLU:N	2.34	0.54
4:N:90:ARG:O	4:N:90:ARG:HG3	2.07	0.54
3:K:343:SER:OG	3:K:344:ARG:N	2.39	0.53
2:M:418:GLU:OE1	2:M:418:GLU:N	2.33	0.53
2:M:141:ILE:HG23	2:M:141:ILE:O	2.08	0.53
2:M:363:GLU:OE1	2:M:363:GLU:N	2.32	0.53
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.27	0.52
2:M:438:GLN:O	2:M:438:GLN:CG	2.56	0.52
1:L:240:GLU:OE1	1:L:240:GLU:N	2.30	0.52
1:L:458:GLU:OE1	1:L:458:GLU:N	2.37	0.52
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.24	0.52
2:M:154:ILE:HG22	2:M:154:ILE:O	2.09	0.52
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.23	0.52
2:M:119:TRP:CD1	2:M:119:TRP:N	2.75	0.52
2:M:361:GLU:OE1	2:M:361:GLU:N	2.41	0.52
2:M:445:ASP:OD1	2:M:445:ASP:C	2.46	0.52
1:L:326:GLU:OE1	1:L:326:GLU:N	2.38	0.52
2:M:363:GLU:OE1	2:M:363:GLU:N	2.36	0.52
2:M:206:ASP:OD1	2:M:206:ASP:C	2.46	0.51
2:M:418:GLU:OE1	2:M:418:GLU:N	2.34	0.51
1:L:122:ARG:NE	1:L:122:ARG:HA	2.25	0.51
2:M:154:ILE:O	2:M:154:ILE:CG2	2.49	0.51
1:L:79:ASN:OD1	1:L:79:ASN:C	2.48	0.51
2:M:107:SER:OG	2:M:108:ASN:N	2.41	0.51
2:M:107:SER:OG	2:M:108:ASN:N	2.41	0.51
3:K:342:TRP:O	3:K:342:TRP:CG	2.64	0.51
1:L:326:GLU:OE1	1:L:326:GLU:N	2.38	0.51
2:M:119:TRP:CD1	2:M:119:TRP:N	2.77	0.51
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.25	0.50
2:M:119:TRP:CD1	2:M:119:TRP:N	2.79	0.50
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.26	0.50
1:L:326:GLU:OE1	1:L:326:GLU:N	2.38	0.50
2:M:119:TRP:CD1	2:M:119:TRP:N	2.77	0.50
1:L:256:ILE:O	1:L:256:ILE:CG2	2.49	0.50
1:L:458:GLU:OE1	1:L:458:GLU:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:119:TRP:CD1	2:M:119:TRP:N	2.78	0.50
2:M:349:LEU:C	2:M:349:LEU:HD23	2.32	0.50
2:M:119:TRP:CD1	2:M:119:TRP:N	2.78	0.50
2:M:119:TRP:CD1	2:M:119:TRP:N	2.78	0.50
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.26	0.49
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.49
2:M:119:TRP:CD1	2:M:119:TRP:N	2.78	0.49
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.27	0.49
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.49
1:L:326:GLU:OE1	1:L:326:GLU:N	2.39	0.49
1:L:72:ASP:C	1:L:72:ASP:OD1	2.50	0.49
2:M:13:TYR:CD1	2:M:13:TYR:C	2.84	0.49
1:L:201:ILE:O	1:L:202:LYS:CB	2.60	0.49
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.49
2:M:119:TRP:CD1	2:M:119:TRP:N	2.79	0.49
2:M:462:LEU:C	2:M:462:LEU:HD12	2.33	0.49
1:L:72:ASP:C	1:L:72:ASP:OD1	2.52	0.48
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.30	0.48
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.48
2:M:418:GLU:OE1	2:M:418:GLU:N	2.31	0.48
2:M:462:LEU:C	2:M:462:LEU:HD12	2.34	0.48
1:L:463:LEU:C	1:L:463:LEU:HD23	2.34	0.48
1:L:72:ASP:C	1:L:72:ASP:OD1	2.52	0.48
2:M:119:TRP:CD1	2:M:119:TRP:N	2.80	0.48
1:L:428:VAL:HG12	1:L:428:VAL:O	2.13	0.48
1:L:136:PHE:C	1:L:136:PHE:CD2	2.86	0.48
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.48
2:M:13:TYR:C	2:M:13:TYR:CD2	2.86	0.48
2:M:112:LEU:C	2:M:112:LEU:HD23	2.34	0.48
1:L:311:GLU:HA	1:L:311:GLU:OE1	2.14	0.48
1:L:343:SER:OG	1:L:344:ILE:HA	2.14	0.48
1:L:428:VAL:O	1:L:430:MET:N	2.47	0.48
1:L:155:PHE:CE1	1:L:388:LEU:HB3	2.49	0.48
5:L:501:ATP:O2A	5:L:501:ATP:O2B	2.31	0.48
1:L:463:LEU:C	1:L:463:LEU:HD23	2.34	0.48
1:L:7:CYS:SG	1:L:22:SER:HB3	2.54	0.48
1:L:87:TRP:CE3	1:L:87:TRP:CA	2.96	0.48
1:L:79:ASN:OD1	1:L:79:ASN:C	2.52	0.48
1:L:343:SER:CB	1:L:344:ILE:HA	2.44	0.48
1:L:79:ASN:OD1	1:L:79:ASN:C	2.52	0.48
4:N:66:ASN:OD1	4:N:66:ASN:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:CYS:SG	1:L:22:SER:HB3	2.54	0.47
1:L:79:ASN:OD1	1:L:79:ASN:C	2.52	0.47
2:M:112:LEU:C	2:M:112:LEU:HD23	2.34	0.47
1:L:79:ASN:OD1	1:L:79:ASN:C	2.50	0.47
2:M:445:ASP:OD1	2:M:445:ASP:C	2.53	0.47
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.27	0.47
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.47
1:L:141:GLU:HB2	1:L:142:PRO:CD	2.45	0.47
1:L:343:SER:CB	1:L:344:ILE:HA	2.45	0.47
2:M:112:LEU:C	2:M:112:LEU:HD23	2.35	0.47
4:N:85:LYS:HB2	4:N:85:LYS:HZ2	1.80	0.47
2:M:154:ILE:O	2:M:154:ILE:CG2	2.58	0.47
1:L:343:SER:OG	1:L:344:ILE:HA	2.15	0.47
2:M:445:ASP:OD1	2:M:445:ASP:C	2.53	0.47
3:K:341:GLN:O	3:K:342:TRP:C	2.52	0.47
1:L:122:ARG:NE	1:L:122:ARG:HA	2.29	0.47
2:M:112:LEU:C	2:M:112:LEU:HD23	2.35	0.47
2:M:462:LEU:C	2:M:462:LEU:HD12	2.36	0.47
1:L:79:ASN:OD1	1:L:79:ASN:C	2.50	0.47
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.30	0.47
3:K:341:GLN:O	3:K:342:TRP:C	2.53	0.47
5:L:501:ATP:O2A	5:L:501:ATP:O2B	2.33	0.47
1:L:72:ASP:C	1:L:72:ASP:OD1	2.52	0.47
2:M:462:LEU:HD12	2:M:462:LEU:C	2.36	0.47
3:K:342:TRP:O	3:K:342:TRP:CD1	2.69	0.46
3:K:376:GLN:O	3:K:377:ARG:HB2	2.15	0.46
3:K:320:ARG:NE	3:K:320:ARG:HA	2.31	0.46
3:K:341:GLN:O	3:K:343:SER:N	2.49	0.46
1:L:79:ASN:OD1	1:L:79:ASN:C	2.54	0.46
3:K:347:ARG:H	3:K:347:ARG:HD2	1.81	0.46
1:L:79:ASN:OD1	1:L:79:ASN:C	2.51	0.46
3:K:376:GLN:O	3:K:377:ARG:HB2	2.16	0.46
1:L:136:PHE:C	1:L:136:PHE:CD2	2.89	0.46
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.31	0.46
2:M:98:ASN:O	2:M:99:GLN:HB2	2.16	0.46
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.31	0.46
1:L:79:ASN:OD1	1:L:79:ASN:C	2.55	0.45
1:L:79:ASN:OD1	1:L:79:ASN:C	2.52	0.45
1:L:463:LEU:C	1:L:463:LEU:HD23	2.37	0.45
2:M:146:SER:OG	2:M:147:LEU:N	2.50	0.45
1:L:463:LEU:C	1:L:463:LEU:HD23	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:418:GLU:OE1	2:M:418:GLU:N	2.37	0.45
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.98	0.45
1:L:449:TRP:C	1:L:449:TRP:CD1	2.89	0.45
1:L:293:LYS:HB3	1:L:294:PRO:HD3	1.98	0.45
2:M:445:ASP:OD1	2:M:445:ASP:C	2.55	0.45
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.32	0.45
1:L:122:ARG:NE	1:L:122:ARG:HA	2.31	0.45
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.98	0.45
1:L:465:ARG:HA	1:L:465:ARG:NE	2.32	0.45
1:L:256:ILE:HG22	1:L:256:ILE:O	2.16	0.45
3:K:376:GLN:O	3:K:377:ARG:HB2	2.16	0.45
2:M:286:ASP:OD1	2:M:286:ASP:C	2.55	0.45
1:L:302:ASP:OD1	1:L:302:ASP:O	2.35	0.45
1:L:11:HIS:C	1:L:11:HIS:ND1	2.70	0.45
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.98	0.45
3:K:376:GLN:O	3:K:377:ARG:HB2	2.16	0.45
2:M:57:ASN:OD1	2:M:57:ASN:C	2.56	0.45
2:M:146:SER:OG	2:M:147:LEU:N	2.50	0.45
2:M:369:ARG:HA	2:M:369:ARG:NE	2.32	0.44
1:L:343:SER:HB3	1:L:344:ILE:HA	1.99	0.44
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.99	0.44
1:L:343:SER:HB3	1:L:344:ILE:HA	1.99	0.44
1:L:201:ILE:O	1:L:202:LYS:HB3	2.17	0.44
1:L:429:MET:SD	2:M:322:ASP:HA	2.58	0.44
1:L:463:LEU:C	1:L:463:LEU:HD23	2.38	0.44
1:L:463:LEU:C	1:L:463:LEU:HD23	2.37	0.44
2:M:98:ASN:O	2:M:99:GLN:HB3	2.18	0.44
2:M:354:LEU:C	2:M:354:LEU:HD23	2.38	0.44
2:M:141:ILE:HG23	2:M:141:ILE:O	2.16	0.44
2:M:13:TYR:HD2	2:M:13:TYR:O	2.01	0.44
1:L:38:ARG:HB2	1:L:46:GLU:HB3	2.00	0.44
2:M:322:ASP:OD1	2:M:322:ASP:C	2.56	0.44
1:L:136:PHE:O	1:L:136:PHE:HD2	2.01	0.44
1:L:87:TRP:CD1	1:L:87:TRP:N	2.83	0.44
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43
1:L:329:LEU:C	1:L:329:LEU:HD23	2.39	0.43
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.99	0.43
2:M:98:ASN:O	2:M:99:GLN:HB3	2.19	0.43
2:M:146:SER:OG	2:M:147:LEU:N	2.51	0.43
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:139:ASN:OD1	2:M:139:ASN:C	2.56	0.43
2:M:146:SER:OG	2:M:147:LEU:N	2.50	0.43
1:L:256:ILE:O	1:L:256:ILE:CG2	2.64	0.43
1:L:281:ASN:OD1	1:L:281:ASN:C	2.56	0.43
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43
1:L:141:GLU:CB	1:L:142:PRO:CD	2.97	0.43
1:L:141:GLU:HB2	1:L:142:PRO:CD	2.49	0.43
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43
1:L:465:ARG:HA	1:L:465:ARG:NE	2.34	0.43
2:M:121:GLN:HG3	2:M:463:TRP:CZ2	2.54	0.43
1:L:7:CYS:SG	1:L:22:SER:HB3	2.58	0.43
1:L:198:ALA:HB3	1:L:199:PRO:HD3	2.00	0.43
2:M:75:ASP:C	2:M:75:ASP:OD1	2.57	0.43
1:L:38:ARG:HB2	1:L:46:GLU:HB3	2.01	0.43
4:N:34:LYS:O	4:N:34:LYS:CG	2.67	0.43
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.00	0.43
1:L:4:ASN:OD1	1:L:4:ASN:C	2.57	0.43
1:L:38:ARG:HB2	1:L:46:GLU:HB3	2.01	0.43
2:M:368:LYS:HA	2:M:368:LYS:HD3	1.87	0.43
1:L:159:ILE:HG22	1:L:398:THR:HB	2.01	0.43
1:L:281:ASN:OD1	1:L:281:ASN:C	2.57	0.43
2:M:75:ASP:C	2:M:75:ASP:OD1	2.57	0.43
4:N:84:LEU:O	4:N:85:LYS:HB2	2.19	0.43
1:L:4:ASN:OD1	1:L:4:ASN:O	2.36	0.43
1:L:429:MET:SD	2:M:322:ASP:HA	2.59	0.43
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.01	0.42
2:M:98:ASN:O	2:M:99:GLN:HB3	2.18	0.42
2:M:94:ARG:HA	2:M:94:ARG:HD3	1.78	0.42
1:L:281:ASN:OD1	1:L:281:ASN:C	2.57	0.42
1:L:7:CYS:SG	1:L:22:SER:HB3	2.59	0.42
2:M:75:ASP:C	2:M:75:ASP:OD1	2.58	0.42
3:K:341:GLN:O	3:K:342:TRP:C	2.58	0.42
1:L:114:LYS:HB3	1:L:115:PRO:HD3	2.01	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.19	0.42
4:N:66:ASN:OD1	4:N:66:ASN:C	2.55	0.42
2:M:454:TYR:O	2:M:458:GLY:N	2.53	0.42
4:N:34:LYS:O	4:N:34:LYS:CG	2.67	0.42
4:N:34:LYS:O	4:N:34:LYS:CG	2.67	0.42
1:L:429:MET:SD	2:M:322:ASP:HA	2.60	0.42
1:L:465:ARG:O	1:L:466:ASP:CB	2.67	0.42
1:L:141:GLU:HB2	1:L:142:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:85:LYS:HB2	4:N:85:LYS:HZ2	1.85	0.42
1:L:7:CYS:SG	1:L:22:SER:HB3	2.60	0.42
2:M:322:ASP:OD1	2:M:322:ASP:C	2.58	0.42
2:M:7:ASP:HA	2:M:24:GLY:HA2	2.01	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.19	0.42
1:L:15:HIS:CD2	1:L:16:ARG:HG3	2.55	0.42
1:L:198:ALA:HB3	1:L:199:PRO:HD3	2.01	0.42
2:M:3:PRO:HA	2:M:4:PHE:HA	1.90	0.42
3:K:345:GLN:HA	3:K:348:CYS:SG	2.59	0.42
4:N:80:ASP:C	4:N:80:ASP:OD1	2.57	0.42
2:M:88:VAL:O	2:M:88:VAL:HG22	2.19	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.42
1:L:198:ALA:HB3	1:L:199:PRO:HD3	2.02	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.19	0.42
1:L:227:TRP:CD1	1:L:227:TRP:O	2.73	0.42
2:M:286:ASP:OD1	2:M:286:ASP:C	2.57	0.42
5:L:501:ATP:O1A	5:L:501:ATP:O2B	2.38	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.42
1:L:256:ILE:O	1:L:256:ILE:HG22	2.19	0.42
2:M:369:ARG:HA	2:M:369:ARG:NE	2.35	0.42
4:N:34:LYS:O	4:N:34:LYS:CG	2.68	0.42
4:N:34:LYS:O	4:N:34:LYS:CG	2.68	0.42
1:L:429:MET:SD	2:M:322:ASP:HA	2.60	0.41
2:M:354:LEU:C	2:M:354:LEU:HD23	2.40	0.41
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.41
2:M:154:ILE:O	2:M:155:SER:C	2.58	0.41
1:L:302:ASP:OD1	1:L:302:ASP:O	2.38	0.41
4:N:66:ASN:OD1	4:N:66:ASN:C	2.58	0.41
1:L:38:ARG:HB2	1:L:46:GLU:HB3	2.02	0.41
1:L:464:LYS:HD3	1:L:464:LYS:HA	1.84	0.41
4:N:66:ASN:OD1	4:N:66:ASN:C	2.58	0.41
2:M:46:ARG:NH2	2:M:50:SER:OG	2.49	0.41
2:M:322:ASP:OD1	2:M:322:ASP:C	2.58	0.41
2:M:322:ASP:OD1	2:M:322:ASP:C	2.58	0.41
1:L:316:PRO:HA	1:L:319:ILE:HD12	2.02	0.41
2:M:104:ALA:O	2:M:106:LEU:N	2.52	0.41
1:L:155:PHE:CE1	1:L:388:LEU:HB3	2.55	0.41
1:L:7:CYS:SG	1:L:22:SER:HB3	2.60	0.41
2:M:213:LEU:C	2:M:213:LEU:HD23	2.41	0.41
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:376:GLN:O	3:K:377:ARG:HB2	2.20	0.41
2:M:57:ASN:C	2:M:57:ASN:OD1	2.59	0.41
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.02	0.41
1:L:392:VAL:HB	1:L:423:THR:HG22	2.03	0.41
1:L:107:THR:OG1	1:L:108:MET:N	2.53	0.41
4:N:80:ASP:C	4:N:80:ASP:OD1	2.59	0.41
1:L:7:CYS:SG	1:L:22:SER:HB3	2.61	0.41
2:M:3:PRO:HB2	2:M:4:PHE:HA	2.03	0.41
1:L:155:PHE:CE1	1:L:388:LEU:HB3	2.56	0.41
1:L:133:VAL:HA	1:L:134:PRO:HD3	1.98	0.41
2:M:322:ASP:OD1	2:M:322:ASP:C	2.58	0.41
1:L:382:GLU:H	1:L:382:GLU:CD	2.23	0.41
2:M:141:ILE:O	2:M:141:ILE:HG23	2.21	0.41
4:N:84:LEU:O	4:N:85:LYS:HB2	2.21	0.41
4:N:80:ASP:C	4:N:80:ASP:OD1	2.59	0.41
1:L:15:HIS:CD2	1:L:16:ARG:HG3	2.56	0.41
4:N:34:LYS:O	4:N:34:LYS:CG	2.68	0.41
2:M:143:LEU:HA	2:M:144:PRO:HD2	1.94	0.41
2:M:415:TYR:CZ	3:K:363:GLU:HG2	2.56	0.41
4:N:66:ASN:OD1	4:N:66:ASN:C	2.57	0.41
1:L:429:MET:SD	2:M:322:ASP:HA	2.61	0.41
2:M:368:LYS:HD3	2:M:368:LYS:HA	1.91	0.41
2:M:139:ASN:OD1	2:M:139:ASN:C	2.59	0.40
4:N:56:TYR:O	4:N:58:PHE:N	2.54	0.40
4:N:34:LYS:O	4:N:34:LYS:CG	2.69	0.40
1:L:239:SER:O	1:L:407:ARG:HD2	2.21	0.40
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.40
1:L:201:ILE:O	1:L:203:GLU:N	2.54	0.40
4:N:80:ASP:C	4:N:80:ASP:OD1	2.60	0.40
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.02	0.40
1:L:7:CYS:SG	1:L:22:SER:HB3	2.62	0.40
4:N:34:LYS:O	4:N:34:LYS:CG	2.69	0.40
2:M:361:GLU:OE1	2:M:361:GLU:N	2.44	0.40
1:L:7:CYS:SG	1:L:22:SER:HB3	2.62	0.40
4:N:84:LEU:O	4:N:85:LYS:CB	2.70	0.40
2:M:29:THR:OG1	2:M:30:PHE:N	2.54	0.40

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	1-L	383/477 (80%)	370 (97%)	12 (3%)	1 (0%)	41	76
1	2-L	383/477 (80%)	368 (96%)	10 (3%)	5 (1%)	12	48
1	3-L	383/477 (80%)	366 (96%)	15 (4%)	2 (0%)	29	68
1	4-L	383/477 (80%)	366 (96%)	13 (3%)	4 (1%)	15	54
1	5-L	383/477 (80%)	368 (96%)	12 (3%)	3 (1%)	19	60
1	6-L	383/477 (80%)	362 (94%)	17 (4%)	4 (1%)	15	54
1	7-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41	76
1	8-L	383/477 (80%)	367 (96%)	12 (3%)	4 (1%)	15	54
1	9-L	383/477 (80%)	369 (96%)	12 (3%)	2 (0%)	29	68
1	10-L	383/477 (80%)	369 (96%)	13 (3%)	1 (0%)	41	76
2	1-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	46
2	2-M	390/467 (84%)	373 (96%)	14 (4%)	3 (1%)	19	60
2	3-M	390/467 (84%)	374 (96%)	10 (3%)	6 (2%)	10	46
2	4-M	390/467 (84%)	367 (94%)	20 (5%)	3 (1%)	19	60
2	5-M	390/467 (84%)	373 (96%)	14 (4%)	3 (1%)	19	60
2	6-M	390/467 (84%)	369 (95%)	18 (5%)	3 (1%)	19	60
2	7-M	390/467 (84%)	368 (94%)	20 (5%)	2 (0%)	29	68
2	8-M	390/467 (84%)	369 (95%)	15 (4%)	6 (2%)	10	46
2	9-M	390/467 (84%)	365 (94%)	21 (5%)	4 (1%)	15	54
2	10-M	390/467 (84%)	370 (95%)	18 (5%)	2 (0%)	29	68
3	1-K	60/813 (7%)	59 (98%)	1 (2%)	0	100	100
3	2-K	60/813 (7%)	59 (98%)	0	1 (2%)	9	44
3	3-K	60/813 (7%)	59 (98%)	1 (2%)	0	100	100
3	4-K	60/813 (7%)	57 (95%)	2 (3%)	1 (2%)	9	44
3	5-K	60/813 (7%)	57 (95%)	0	3 (5%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	6-K	60/813 (7%)	60 (100%)	0	0	100	100
3	7-K	60/813 (7%)	59 (98%)	1 (2%)	0	100	100
3	8-K	60/813 (7%)	59 (98%)	0	1 (2%)	9	44
3	9-K	60/813 (7%)	60 (100%)	0	0	100	100
3	10-K	60/813 (7%)	57 (95%)	1 (2%)	2 (3%)	4	30
4	1-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
4	2-N	47/157 (30%)	45 (96%)	1 (2%)	1 (2%)	7	39
4	3-N	47/157 (30%)	44 (94%)	1 (2%)	2 (4%)	2	25
4	4-N	47/157 (30%)	43 (92%)	3 (6%)	1 (2%)	7	39
4	5-N	47/157 (30%)	43 (92%)	3 (6%)	1 (2%)	7	39
4	6-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
4	7-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
4	8-N	47/157 (30%)	45 (96%)	1 (2%)	1 (2%)	7	39
4	9-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
4	10-N	47/157 (30%)	45 (96%)	1 (2%)	1 (2%)	7	39
All	All	8800/19140 (46%)	8402 (96%)	314 (4%)	84 (1%)	20	54

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-L	202	LYS
2	1-M	155	SER
2	1-M	363	GLU
1	2-L	51	THR
2	3-M	58	LYS
4	3-N	57	PRO
1	4-L	429	MET
3	5-K	341	GLN
1	6-L	175	VAL
2	6-M	104	ALA
1	8-L	435	GLN
2	8-M	27	GLU
2	9-M	402	GLN
3	10-K	342	TRP
4	1-N	85	LYS
1	2-L	45	ALA
1	2-L	429	MET

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Mol	Chain	Res	Type
2	2-M	155	SER
3	2-K	341	GLN
4	2-N	85	LYS
1	3-L	202	LYS
2	3-M	27	GLU
2	3-M	146	SER
2	3-M	155	SER
4	3-N	85	LYS
1	4-L	45	ALA
4	4-N	85	LYS
2	5-M	27	GLU
2	5-M	155	SER
4	5-N	85	LYS
2	6-M	155	SER
4	6-N	85	LYS
1	7-L	134	PRO
2	7-M	155	SER
4	7-N	85	LYS
1	8-L	45	ALA
2	8-M	155	SER
4	8-N	85	LYS
2	9-M	155	SER
4	9-N	85	LYS
2	10-M	27	GLU
2	10-M	105	GLU
4	10-N	85	LYS
2	1-M	104	ALA
2	1-M	107	SER
2	1-M	362	PRO
1	2-L	77	PRO
1	3-L	115	PRO
1	4-L	115	PRO
2	4-M	28	GLU
1	5-L	115	PRO
2	5-M	104	ALA
1	6-L	464	LYS
2	7-M	146	SER
1	8-L	115	PRO
2	8-M	104	ALA
2	8-M	398	ILE
3	8-K	342	TRP
1	9-L	115	PRO

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Mol	Chain	Res	Type
2	9-M	107	SER
1	10-L	115	PRO
2	1-M	173	PRO
2	2-M	173	PRO
2	3-M	173	PRO
1	5-L	168	PRO
3	5-K	345	GLN
1	6-L	115	PRO
1	6-L	449	TRP
2	8-M	173	PRO
2	2-M	154	ILE
2	3-M	154	ILE
3	4-K	342	TRP
1	8-L	141	GLU
2	4-M	27	GLU
3	5-K	344	ARG
1	9-L	134	PRO
3	10-K	341	GLN
2	4-M	154	ILE
2	6-M	154	ILE
2	8-M	154	ILE
2	9-M	154	ILE
1	2-L	135	VAL
1	4-L	325	PRO
1	5-L	325	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	1-L	349/420 (83%)	349 (100%)	0	100 100
1	2-L	349/420 (83%)	349 (100%)	0	100 100
1	3-L	349/420 (83%)	349 (100%)	0	100 100
1	4-L	349/420 (83%)	349 (100%)	0	100 100
1	5-L	349/420 (83%)	348 (100%)	1 (0%)	92 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-L	349/420 (83%)	349 (100%)	0	100	100
1	7-L	349/420 (83%)	349 (100%)	0	100	100
1	8-L	349/420 (83%)	349 (100%)	0	100	100
1	9-L	349/420 (83%)	349 (100%)	0	100	100
1	10-L	349/420 (83%)	349 (100%)	0	100	100
2	1-M	362/423 (86%)	362 (100%)	0	100	100
2	2-M	362/423 (86%)	362 (100%)	0	100	100
2	3-M	362/423 (86%)	362 (100%)	0	100	100
2	4-M	362/423 (86%)	362 (100%)	0	100	100
2	5-M	362/423 (86%)	361 (100%)	1 (0%)	92	95
2	6-M	362/423 (86%)	362 (100%)	0	100	100
2	7-M	362/423 (86%)	362 (100%)	0	100	100
2	8-M	362/423 (86%)	362 (100%)	0	100	100
2	9-M	362/423 (86%)	362 (100%)	0	100	100
2	10-M	362/423 (86%)	361 (100%)	1 (0%)	92	95
3	1-K	58/735 (8%)	58 (100%)	0	100	100
3	2-K	58/735 (8%)	58 (100%)	0	100	100
3	3-K	58/735 (8%)	58 (100%)	0	100	100
3	4-K	58/735 (8%)	58 (100%)	0	100	100
3	5-K	58/735 (8%)	58 (100%)	0	100	100
3	6-K	58/735 (8%)	58 (100%)	0	100	100
3	7-K	58/735 (8%)	58 (100%)	0	100	100
3	8-K	58/735 (8%)	58 (100%)	0	100	100
3	9-K	58/735 (8%)	58 (100%)	0	100	100
3	10-K	58/735 (8%)	58 (100%)	0	100	100
4	1-N	54/140 (39%)	54 (100%)	0	100	100
4	2-N	54/140 (39%)	54 (100%)	0	100	100
4	3-N	54/140 (39%)	54 (100%)	0	100	100
4	4-N	54/140 (39%)	54 (100%)	0	100	100
4	5-N	54/140 (39%)	54 (100%)	0	100	100
4	6-N	54/140 (39%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	7-N	54/140 (39%)	54 (100%)	0	100	100
4	8-N	54/140 (39%)	54 (100%)	0	100	100
4	9-N	54/140 (39%)	54 (100%)	0	100	100
4	10-N	54/140 (39%)	54 (100%)	0	100	100
All	All	8230/17180 (48%)	8227 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5-L	87	TRP
2	5-M	13	TYR
2	10-M	13	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	2-L	11	HIS

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)

10 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	$\#\|Z\| > 2$
5	ATP	1-L	501	-	26,33,33	0.99	0	31,52,52	2.15	6 (19%)
5	ATP	7-L	501	-	26,33,33	1.00	1 (3%)	31,52,52	2.10	7 (22%)
5	ATP	4-L	501	-	26,33,33	0.95	0	31,52,52	1.99	7 (22%)
5	ATP	2-L	501	-	26,33,33	0.97	0	31,52,52	2.02	7 (22%)
5	ATP	9-L	501	-	26,33,33	0.99	0	31,52,52	2.04	7 (22%)
5	ATP	10-L	501	-	26,33,33	1.00	0	31,52,52	2.02	6 (19%)
5	ATP	5-L	501	-	26,33,33	0.98	0	31,52,52	1.99	7 (22%)
5	ATP	8-L	501	-	26,33,33	0.98	0	31,52,52	2.06	6 (19%)
5	ATP	3-L	501	-	26,33,33	0.97	0	31,52,52	2.04	7 (22%)
5	ATP	6-L	501	-	26,33,33	0.98	0	31,52,52	2.09	7 (22%)

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
5	ATP	1-L	501	-	-	1/18/38/38	0/3/3/3
5	ATP	7-L	501	-	-	7/18/38/38	0/3/3/3
5	ATP	4-L	501	-	-	6/18/38/38	0/3/3/3
5	ATP	2-L	501	-	-	7/18/38/38	0/3/3/3
5	ATP	9-L	501	-	-	8/18/38/38	0/3/3/3
5	ATP	10-L	501	-	-	6/18/38/38	0/3/3/3
5	ATP	5-L	501	-	-	5/18/38/38	0/3/3/3
5	ATP	8-L	501	-	-	3/18/38/38	0/3/3/3
5	ATP	3-L	501	-	-	5/18/38/38	0/3/3/3
5	ATP	6-L	501	-	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	7-L	501	ATP	C5-C4	2.01	1.46	1.40

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1-L	501	ATP	PA-O3A-PB	-6.88	109.22	132.83
5	6-L	501	ATP	PA-O3A-PB	-6.50	110.53	132.83
5	3-L	501	ATP	PA-O3A-PB	-6.40	110.86	132.83
5	7-L	501	ATP	PB-O3B-PG	-6.37	110.98	132.83
5	8-L	501	ATP	PA-O3A-PB	-6.36	110.99	132.83
5	2-L	501	ATP	PB-O3B-PG	-6.27	111.33	132.83
5	5-L	501	ATP	PA-O3A-PB	-6.22	111.49	132.83
5	9-L	501	ATP	PB-O3B-PG	-6.20	111.55	132.83
5	10-L	501	ATP	PB-O3B-PG	-6.12	111.81	132.83
5	2-L	501	ATP	PA-O3A-PB	-6.12	111.83	132.83
5	10-L	501	ATP	PA-O3A-PB	-6.08	111.96	132.83
5	4-L	501	ATP	PB-O3B-PG	-6.07	111.99	132.83
5	7-L	501	ATP	PA-O3A-PB	-6.05	112.06	132.83
5	6-L	501	ATP	PB-O3B-PG	-6.04	112.10	132.83
5	1-L	501	ATP	PB-O3B-PG	-6.03	112.14	132.83
5	8-L	501	ATP	PB-O3B-PG	-6.00	112.25	132.83
5	4-L	501	ATP	PA-O3A-PB	-5.85	112.75	132.83
5	9-L	501	ATP	PA-O3A-PB	-5.84	112.78	132.83
5	3-L	501	ATP	PB-O3B-PG	-5.68	113.34	132.83
5	5-L	501	ATP	PB-O3B-PG	-5.58	113.67	132.83
5	1-L	501	ATP	C3'-C2'-C1'	3.41	106.11	100.98
5	6-L	501	ATP	C3'-C2'-C1'	3.16	105.74	100.98
5	7-L	501	ATP	C3'-C2'-C1'	3.11	105.66	100.98
5	9-L	501	ATP	C3'-C2'-C1'	3.11	105.65	100.98
5	2-L	501	ATP	N3-C2-N1	-3.10	123.83	128.68
5	1-L	501	ATP	N3-C2-N1	-3.06	123.89	128.68
5	10-L	501	ATP	N3-C2-N1	-3.04	123.93	128.68
5	9-L	501	ATP	N3-C2-N1	-3.03	123.94	128.68
5	6-L	501	ATP	N3-C2-N1	-3.01	123.97	128.68
5	4-L	501	ATP	N3-C2-N1	-3.00	123.99	128.68
5	5-L	501	ATP	N3-C2-N1	-3.00	123.99	128.68
5	8-L	501	ATP	N3-C2-N1	-2.96	124.06	128.68
5	8-L	501	ATP	C3'-C2'-C1'	2.94	105.41	100.98
5	7-L	501	ATP	N3-C2-N1	-2.93	124.10	128.68
5	3-L	501	ATP	C3'-C2'-C1'	2.92	105.38	100.98
5	5-L	501	ATP	C3'-C2'-C1'	2.91	105.36	100.98
5	3-L	501	ATP	N3-C2-N1	-2.89	124.16	128.68
5	7-L	501	ATP	O3G-PG-O2G	2.78	118.27	107.64
5	3-L	501	ATP	O3G-PG-O2G	2.75	118.16	107.64
5	10-L	501	ATP	C3'-C2'-C1'	2.74	105.11	100.98
5	4-L	501	ATP	O3G-PG-O2G	2.73	118.08	107.64
5	2-L	501	ATP	O3G-PG-O2G	2.66	117.81	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	9-L	501	ATP	O3G-PG-O2G	2.65	117.77	107.64
5	10-L	501	ATP	O3G-PG-O2G	2.64	117.73	107.64
5	6-L	501	ATP	O3G-PG-O2G	2.61	117.60	107.64
5	1-L	501	ATP	O3G-PG-O2G	2.60	117.56	107.64
5	4-L	501	ATP	C3'-C2'-C1'	2.53	104.78	100.98
5	2-L	501	ATP	C3'-C2'-C1'	2.51	104.75	100.98
5	6-L	501	ATP	C4-C5-N7	-2.49	106.81	109.40
5	4-L	501	ATP	C4-C5-N7	-2.43	106.87	109.40
5	1-L	501	ATP	C4-C5-N7	-2.40	106.90	109.40
5	3-L	501	ATP	C4-C5-N7	-2.36	106.94	109.40
5	5-L	501	ATP	C4-C5-N7	-2.36	106.94	109.40
5	8-L	501	ATP	O3G-PG-O2G	2.35	116.62	107.64
5	7-L	501	ATP	C4-C5-N7	-2.35	106.95	109.40
5	5-L	501	ATP	O3G-PG-O2G	2.34	116.59	107.64
5	8-L	501	ATP	C4-C5-N7	-2.32	106.98	109.40
5	9-L	501	ATP	C4-C5-N7	-2.31	106.99	109.40
5	2-L	501	ATP	C4-C5-N7	-2.31	106.99	109.40
5	10-L	501	ATP	C4-C5-N7	-2.24	107.06	109.40
5	9-L	501	ATP	O2B-PB-O1B	2.12	122.71	112.24
5	7-L	501	ATP	O2B-PB-O1B	2.07	122.45	112.24
5	4-L	501	ATP	O2B-PB-O1B	2.06	122.44	112.24
5	5-L	501	ATP	O2B-PB-O1B	2.05	122.39	112.24
5	3-L	501	ATP	O2B-PB-O1B	2.02	122.24	112.24
5	2-L	501	ATP	O2B-PB-O1B	2.02	122.22	112.24
5	6-L	501	ATP	O2B-PB-O1B	2.01	122.16	112.24

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	3-L	501	ATP	PB-O3B-PG-O3G
5	4-L	501	ATP	PB-O3B-PG-O3G
5	6-L	501	ATP	O4'-C4'-C5'-O5'
5	6-L	501	ATP	C3'-C4'-C5'-O5'
5	7-L	501	ATP	C5'-O5'-PA-O1A
5	9-L	501	ATP	PB-O3B-PG-O3G
5	9-L	501	ATP	C5'-O5'-PA-O1A
5	9-L	501	ATP	C5'-O5'-PA-O3A
5	4-L	501	ATP	O4'-C4'-C5'-O5'
5	4-L	501	ATP	C3'-C4'-C5'-O5'
5	5-L	501	ATP	O4'-C4'-C5'-O5'
5	5-L	501	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	7-L	501	ATP	C3'-C4'-C5'-O5'
5	3-L	501	ATP	O4'-C4'-C5'-O5'
5	3-L	501	ATP	C3'-C4'-C5'-O5'
5	7-L	501	ATP	O4'-C4'-C5'-O5'
5	9-L	501	ATP	O4'-C4'-C5'-O5'
5	9-L	501	ATP	C3'-C4'-C5'-O5'
5	8-L	501	ATP	C3'-C4'-C5'-O5'
5	2-L	501	ATP	PA-O3A-PB-O1B
5	10-L	501	ATP	PA-O3A-PB-O1B
5	8-L	501	ATP	O4'-C4'-C5'-O5'
5	7-L	501	ATP	PB-O3B-PG-O3G
5	7-L	501	ATP	C5'-O5'-PA-O3A
5	2-L	501	ATP	C3'-C4'-C5'-O5'
5	10-L	501	ATP	C3'-C4'-C5'-O5'
5	2-L	501	ATP	PA-O3A-PB-O2B
5	3-L	501	ATP	PA-O3A-PB-O2B
5	5-L	501	ATP	PA-O3A-PB-O2B
5	9-L	501	ATP	PA-O3A-PB-O2B
5	10-L	501	ATP	PA-O3A-PB-O2B
5	2-L	501	ATP	O4'-C4'-C5'-O5'
5	10-L	501	ATP	O4'-C4'-C5'-O5'
5	10-L	501	ATP	PB-O3B-PG-O1G
5	2-L	501	ATP	PB-O3B-PG-O3G
5	10-L	501	ATP	PB-O3B-PG-O3G
5	4-L	501	ATP	C5'-O5'-PA-O3A
5	1-L	501	ATP	PA-O3A-PB-O1B
5	3-L	501	ATP	PA-O3A-PB-O1B
5	4-L	501	ATP	PA-O3A-PB-O2B
5	5-L	501	ATP	PA-O3A-PB-O1B
5	7-L	501	ATP	PA-O3A-PB-O2B
5	9-L	501	ATP	PA-O3A-PB-O1B
5	2-L	501	ATP	C5'-O5'-PA-O1A
5	4-L	501	ATP	C5'-O5'-PA-O1A
5	5-L	501	ATP	C5'-O5'-PA-O1A
5	6-L	501	ATP	C5'-O5'-PA-O1A
5	7-L	501	ATP	C5'-O5'-PA-O2A
5	8-L	501	ATP	C5'-O5'-PA-O1A
5	9-L	501	ATP	C5'-O5'-PA-O2A
5	2-L	501	ATP	PB-O3B-PG-O1G

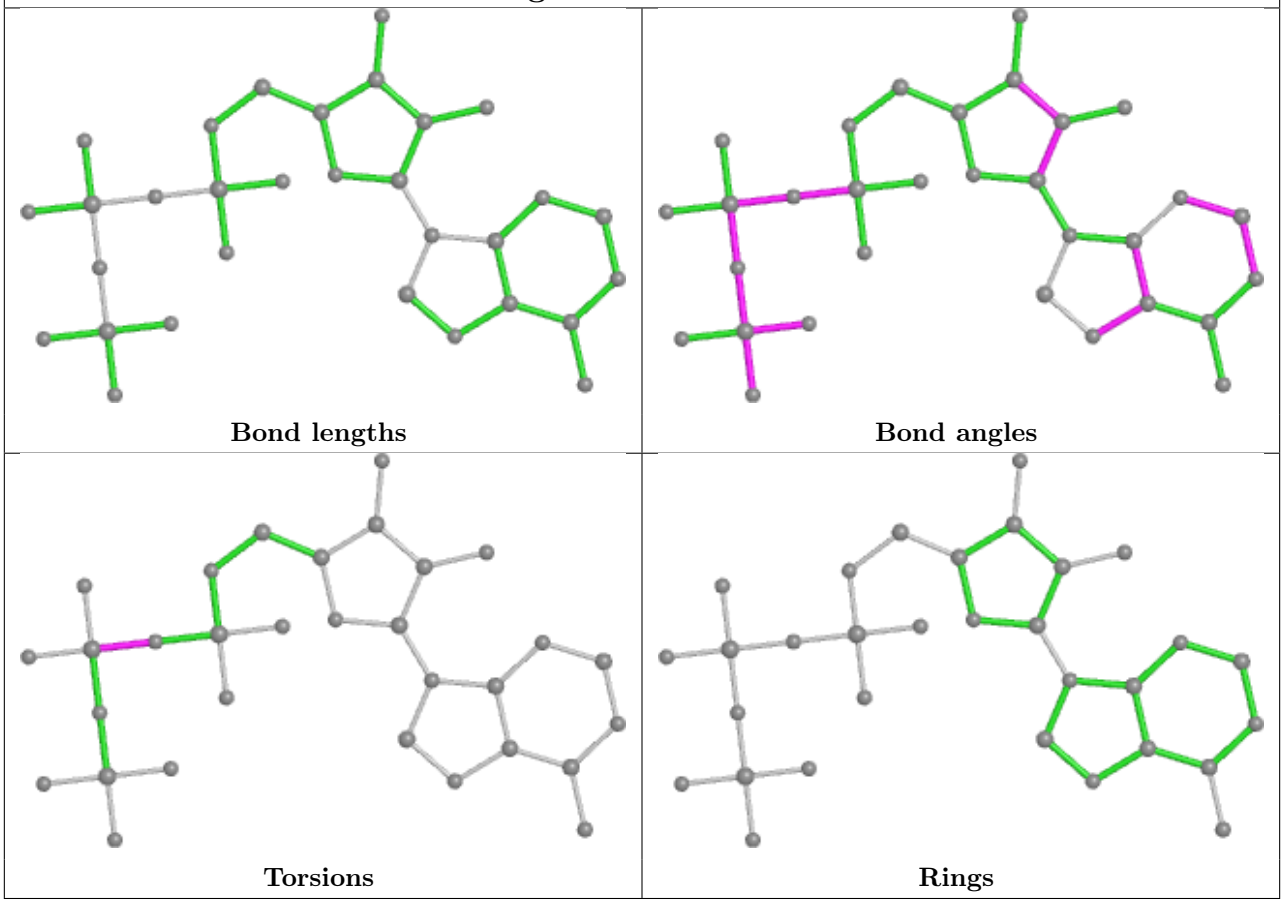
There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1-L	501	ATP	1	0
5	7-L	501	ATP	1	0
5	2-L	501	ATP	2	0
5	9-L	501	ATP	1	0
5	10-L	501	ATP	2	0
5	5-L	501	ATP	2	0
5	8-L	501	ATP	1	0
5	3-L	501	ATP	1	0
5	6-L	501	ATP	1	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 ATP L 501



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.

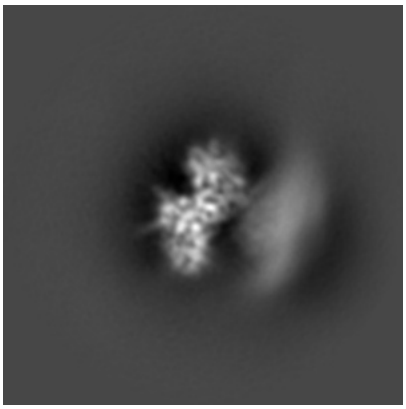
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21489. These allow visual inspection of the internal detail of the map and identification of artifacts.

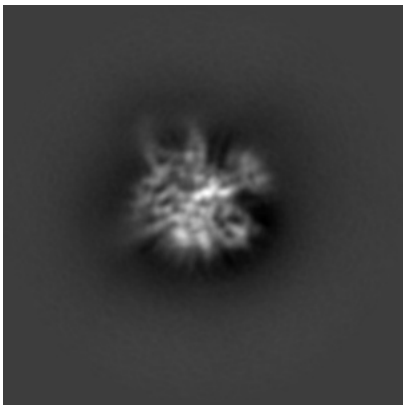
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

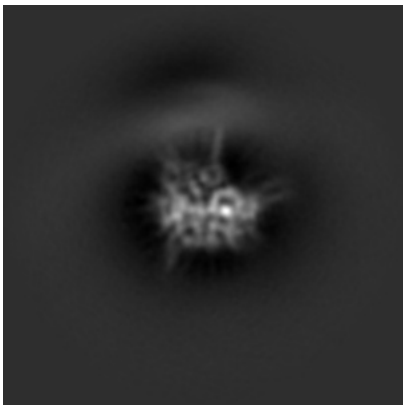
6.1.1 Primary map



X

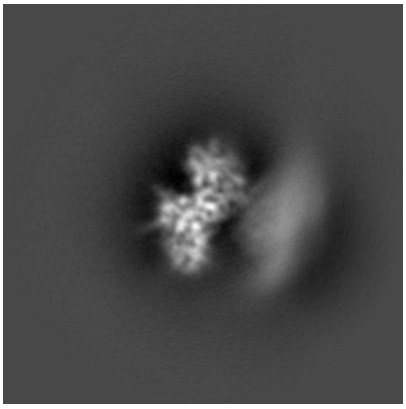


Y

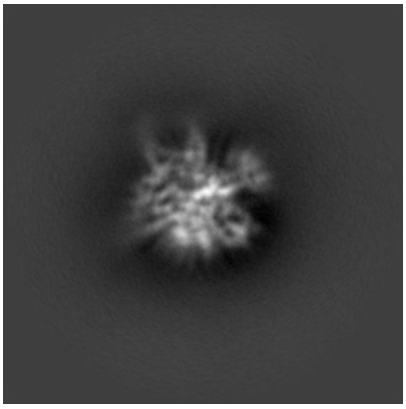


Z

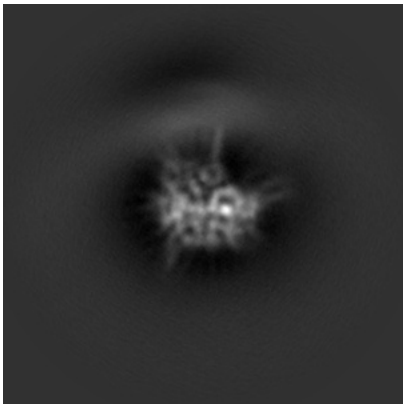
6.1.2 Raw map



X



Y

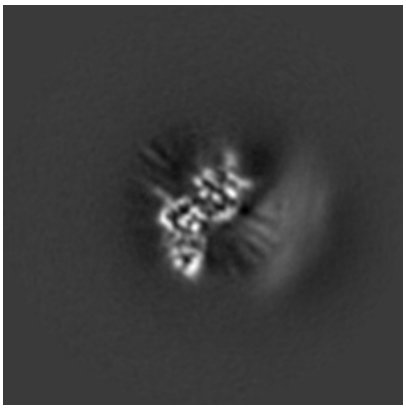


Z

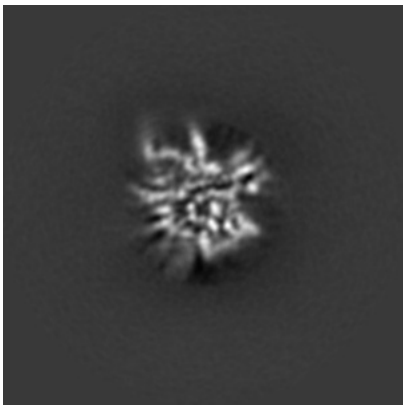
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

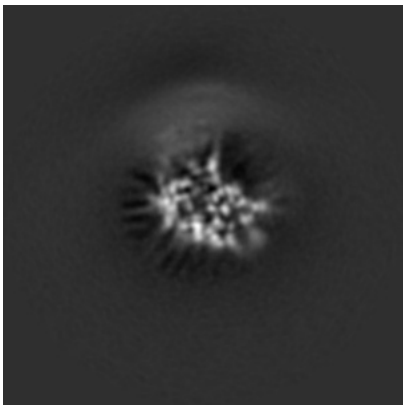
6.2.1 Primary map



X Index: 120

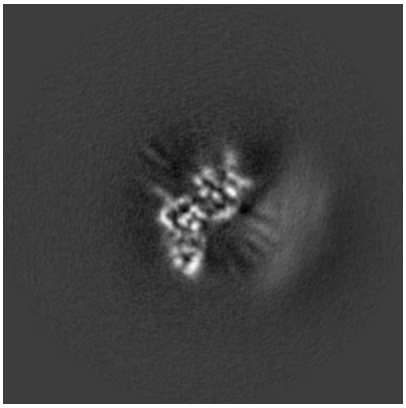


Y Index: 120

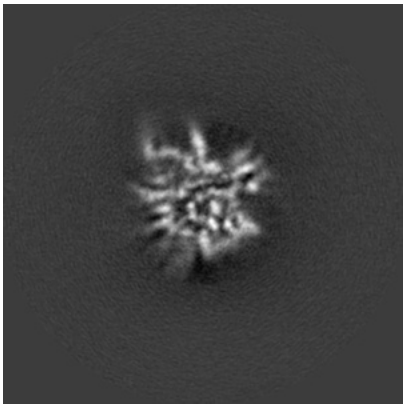


Z Index: 120

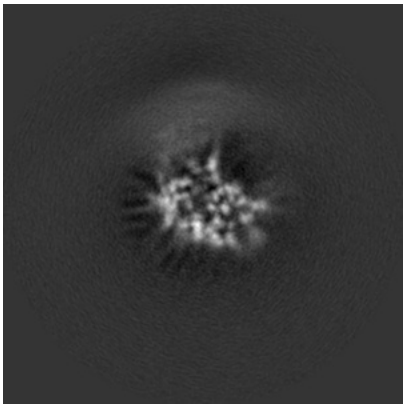
6.2.2 Raw map



X Index: 120



Y Index: 120

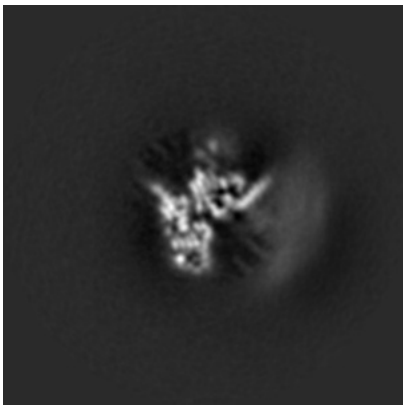


Z Index: 120

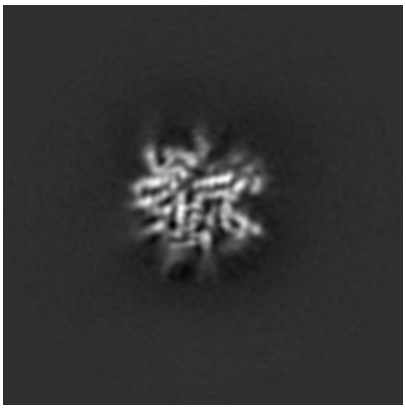
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

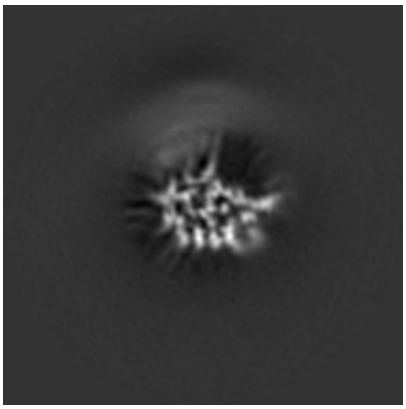
6.3.1 Primary map



X Index: 126

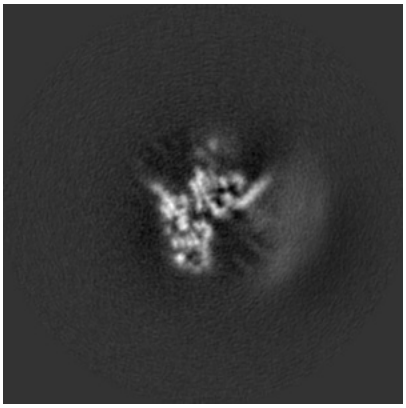


Y Index: 116

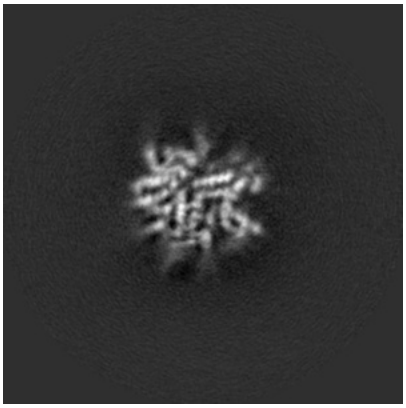


Z Index: 117

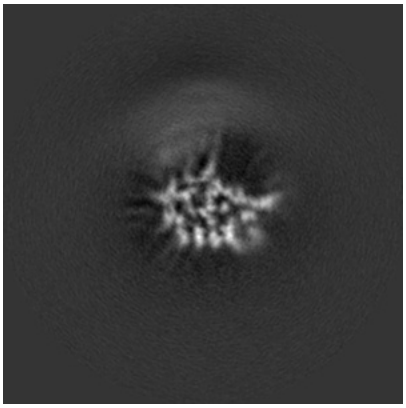
6.3.2 Raw map



X Index: 126



Y Index: 116

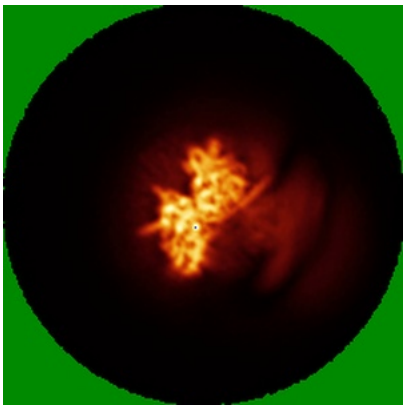


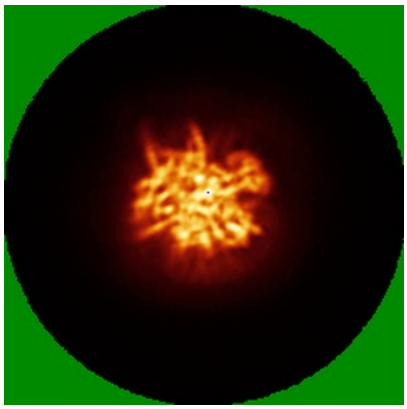
Z Index: 117

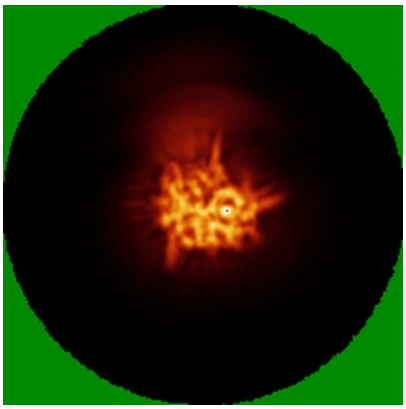
The images above show the largest variance slices of the map in three orthogonal directions.

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

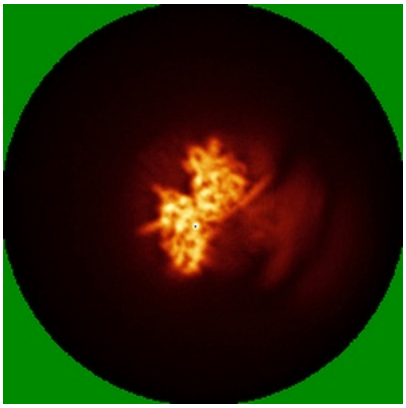
6.4.1 Primary map

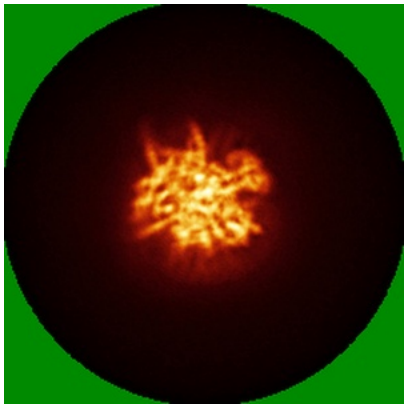

X

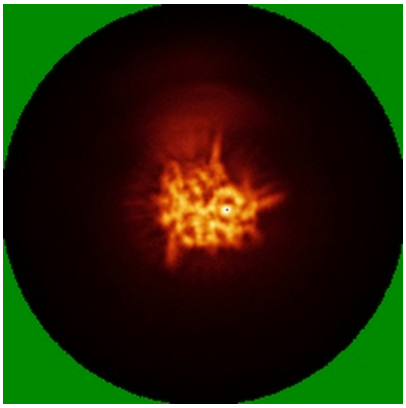

Y


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)

6.5.1 Primary map

X Y Z

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

6.5.2 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.

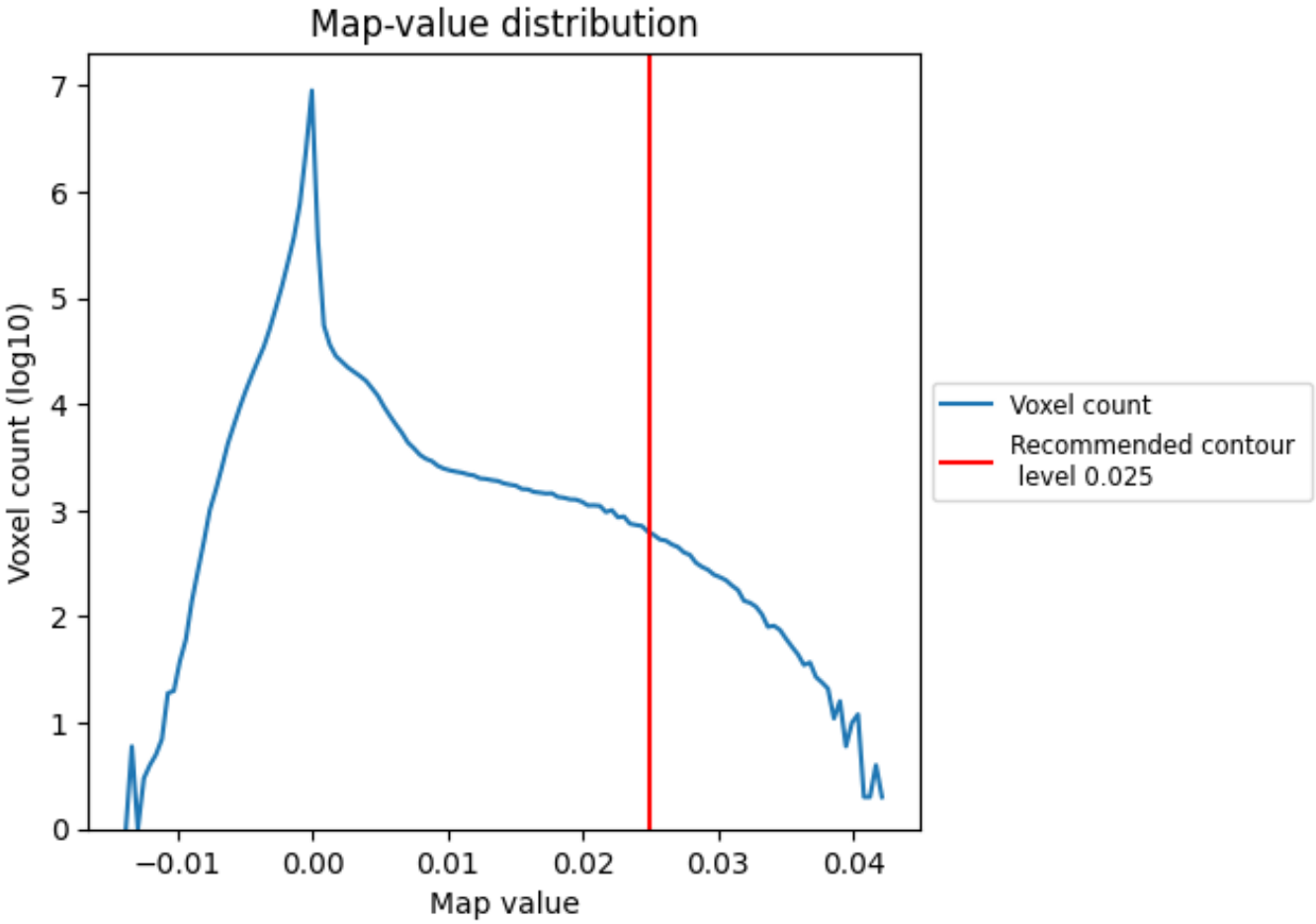
6.6 Mask visualisation (i)

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

7 Map analysis

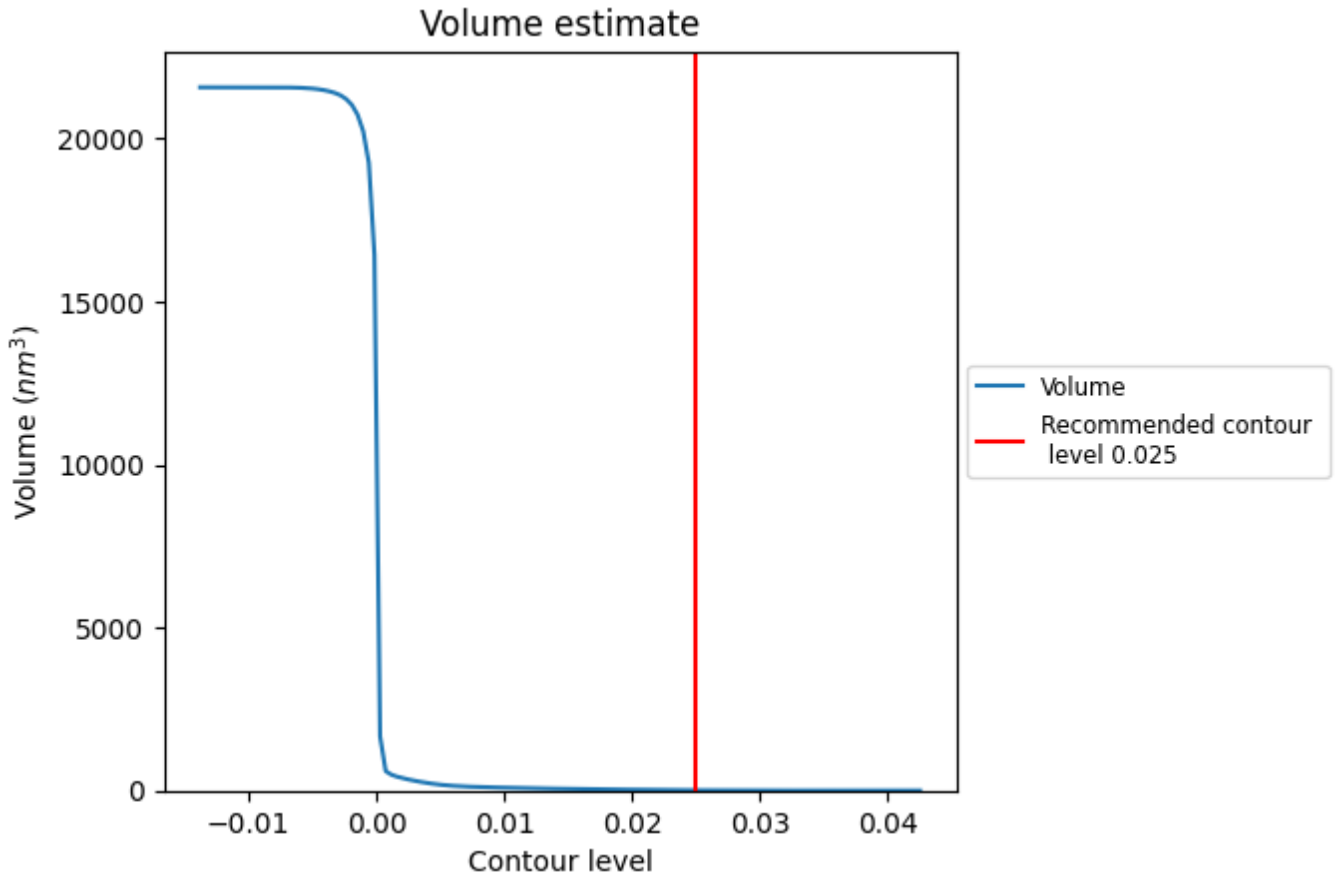
This section contains the results of statistical analysis of the map.

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.

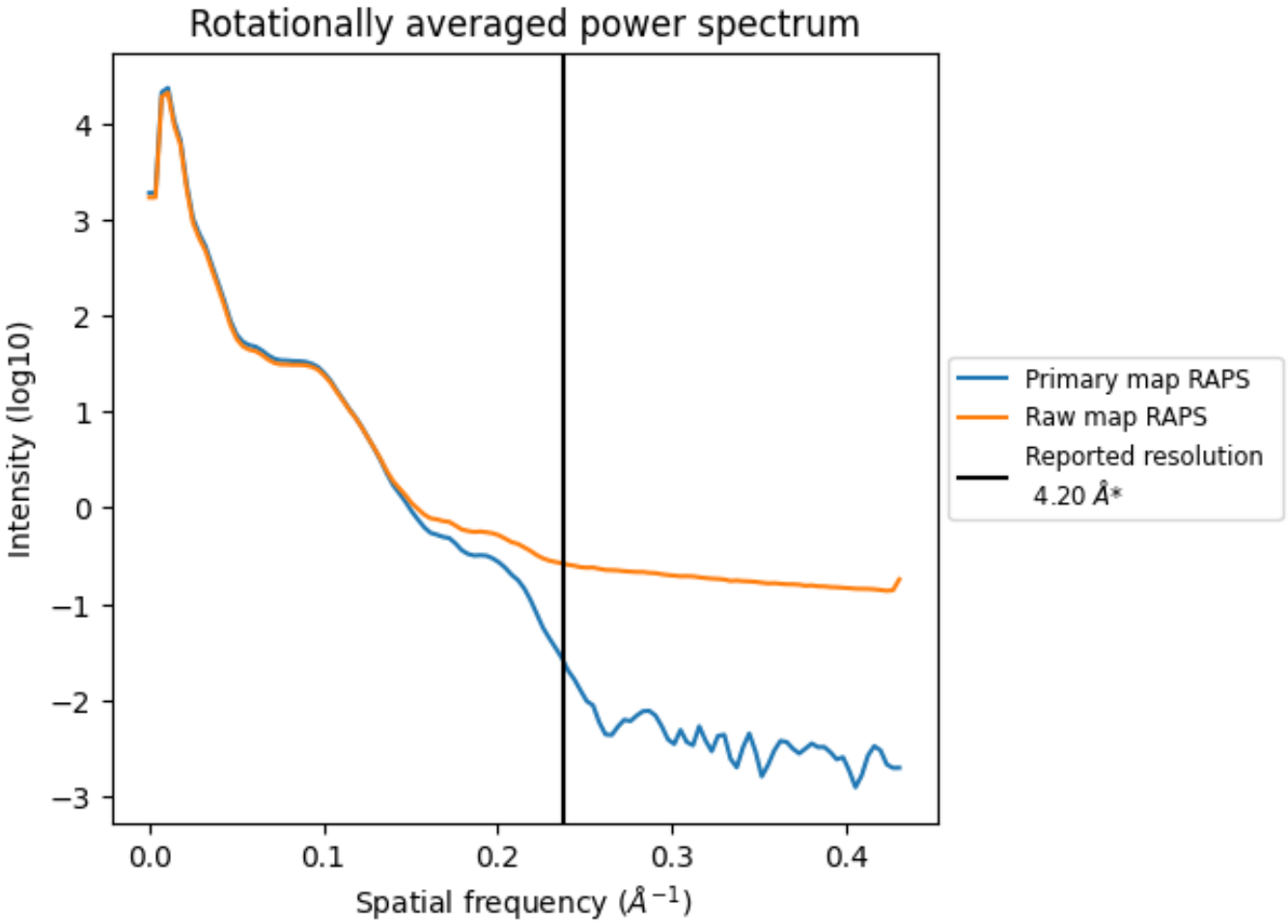
7.2 Volume estimate



The volume at the recommended contour level is 11 nm^3; this corresponds to an approximate mass of 10 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)

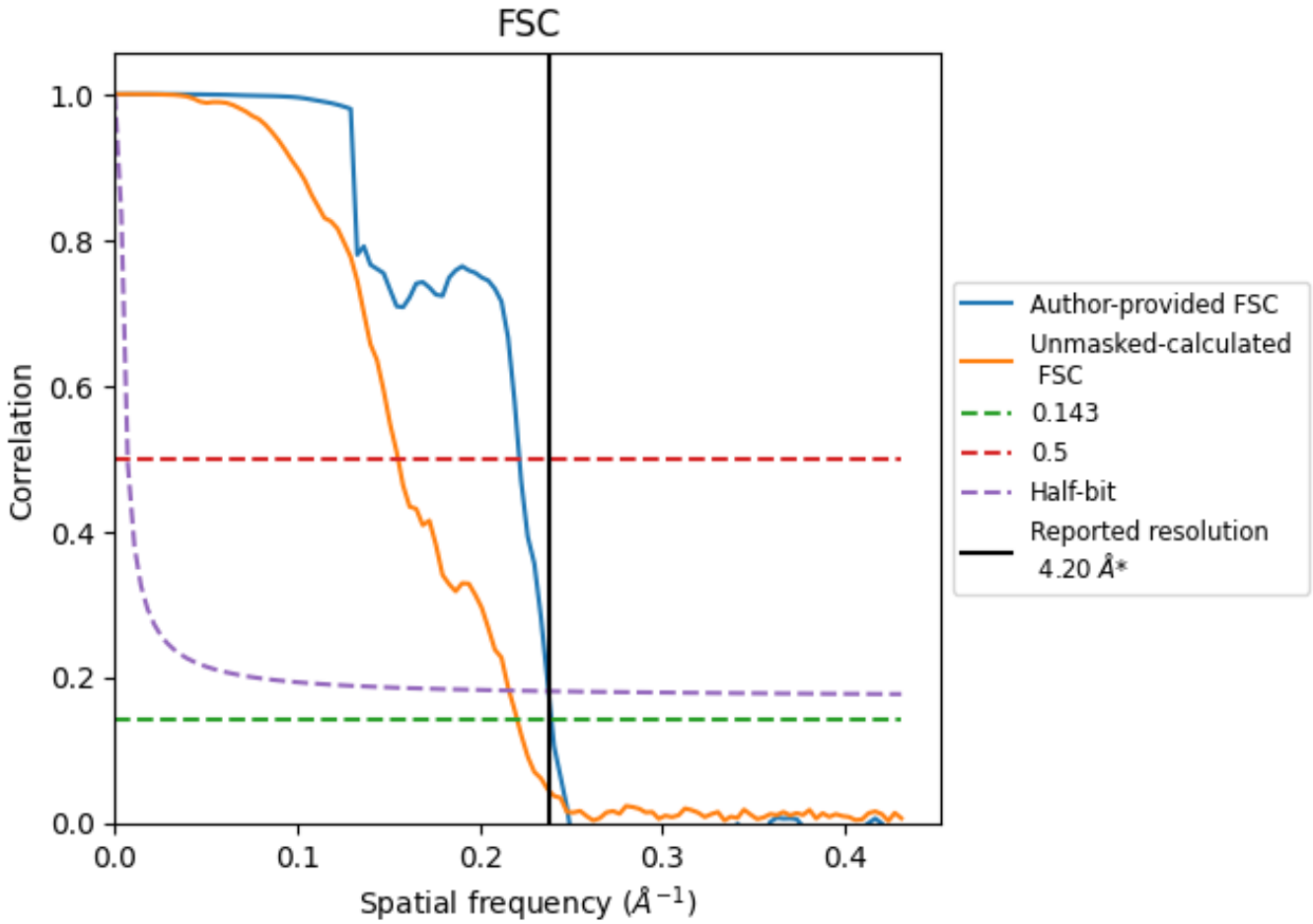


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

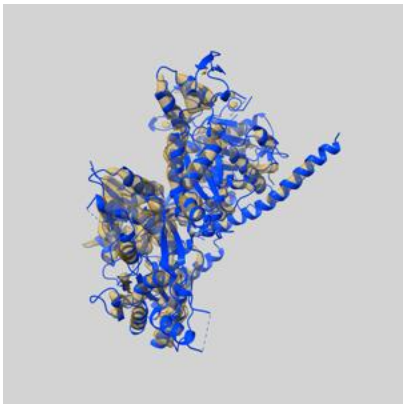
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	4.51	4.21
Unmasked-calculated*	4.54	6.45	4.63

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

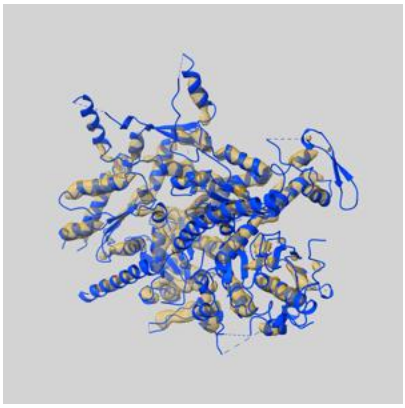
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21489 and PDB model 6VZG. Per-residue inclusion information can be found in section 3 on page 9.

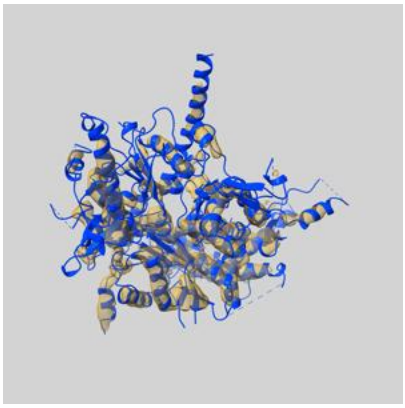
9.1 Map-model overlay



X



Y



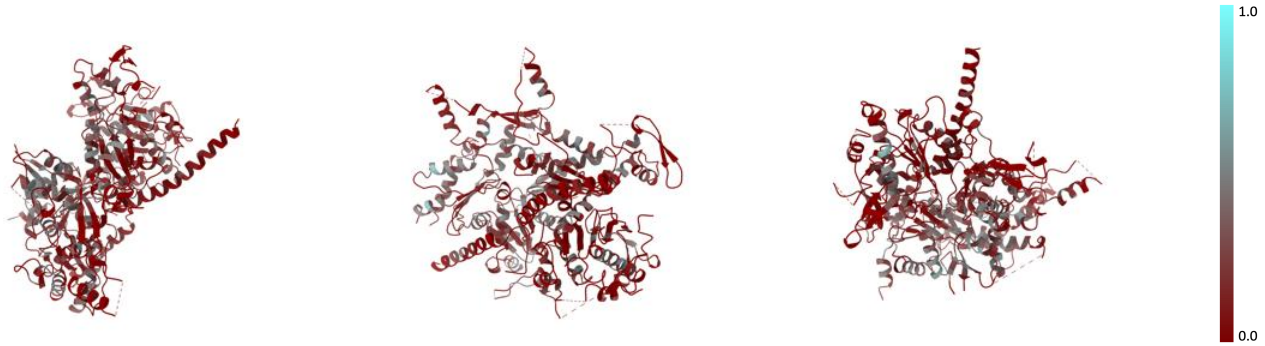
Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

This section was not generated.

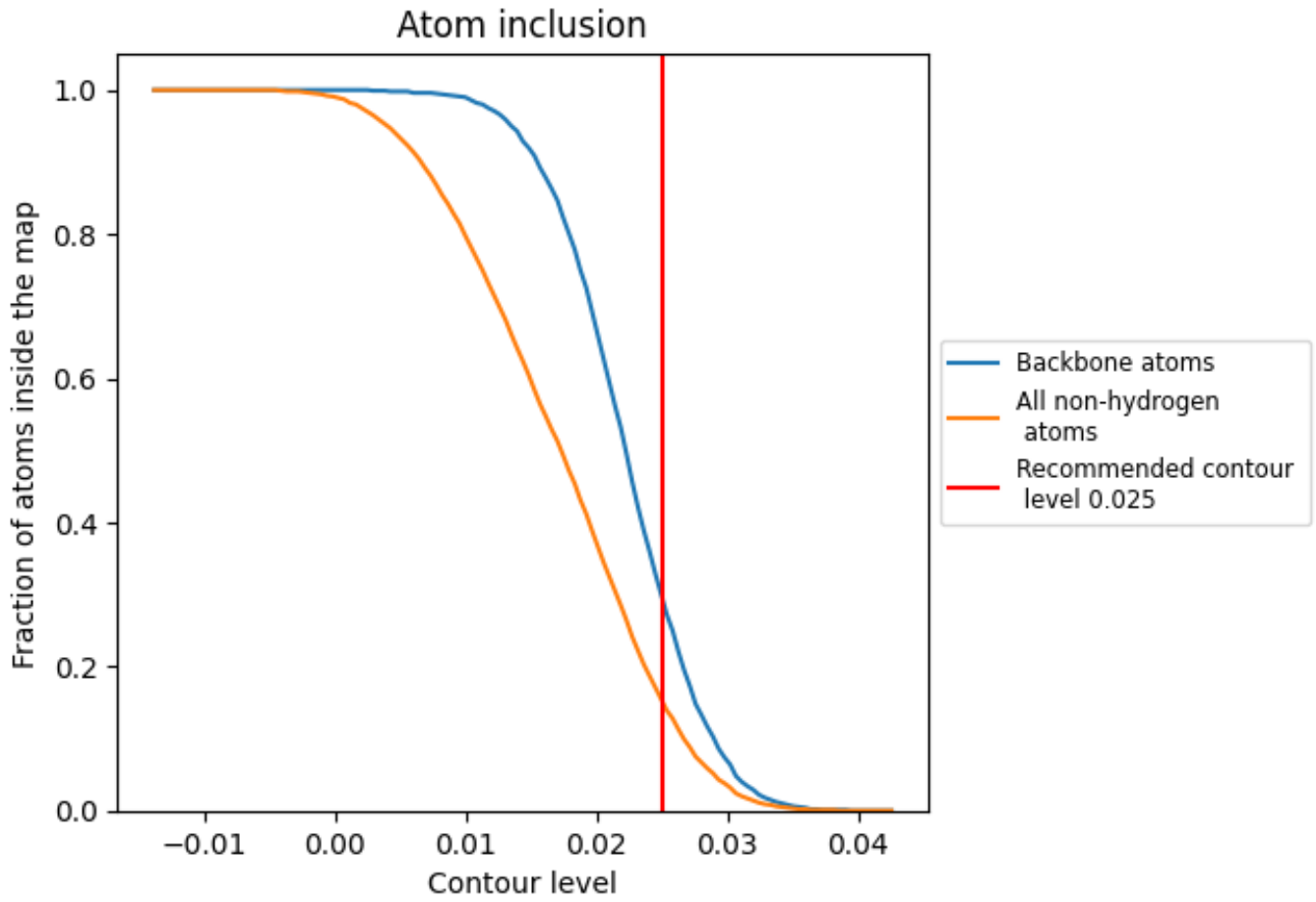
9.3 Atom inclusion mapped to coordinate model



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 30% of all backbone atoms, 15% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.1530
K	0.0540
L	0.2000
M	0.1310
N	0.0960