



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:21 AM UTC

PDB ID : 8Q6T / pdb_00008q6t
EMDB ID : EMD-18198
Title : Helical reconstruction of the relaxed thick filament from FIB milled left ventricular mouse myofibrils
Authors : Tamborrini, D.; Raunser, S.
Deposited on : 2023-08-14
Resolution : 18.00 Å(reported)
Based on initial model : .

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

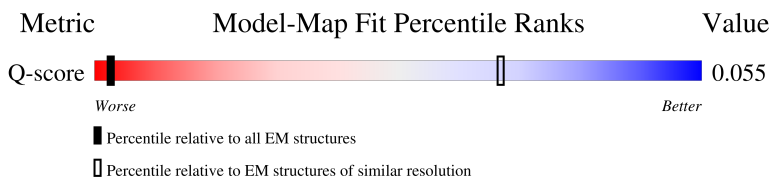
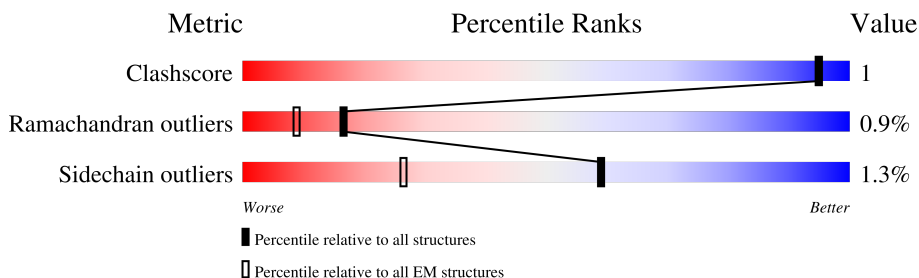
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 18.00 Å.

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



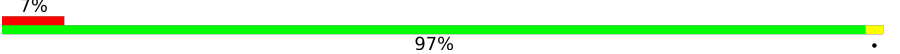
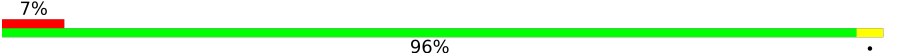
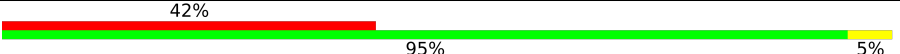
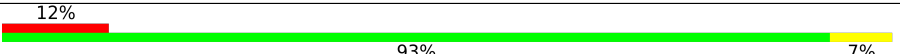
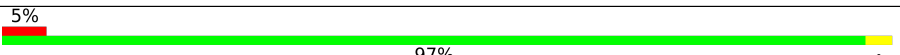
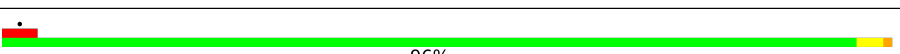
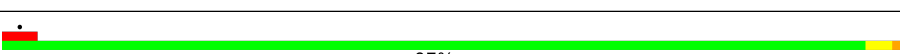
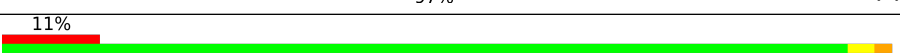
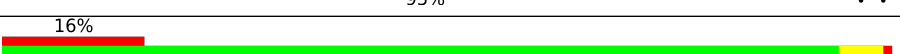
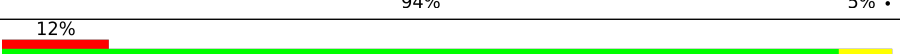
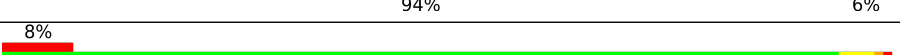
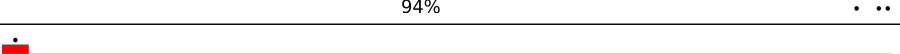
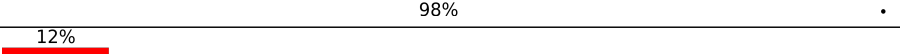
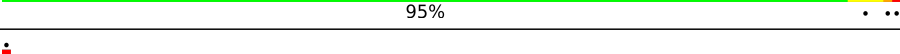
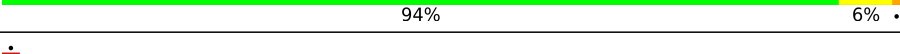
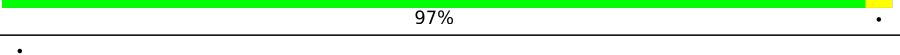
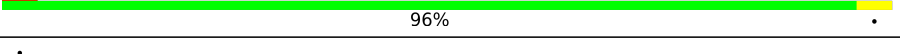
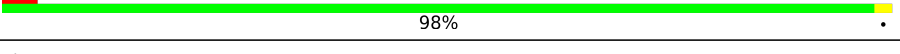
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	24 (17.50 - 18.30)

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

Mol	Chain	Length	Quality of chain
1	A	1935	14% 97%
1	B	1935	9% 96%
1	H	1935	10% 96%
1	N	1935	8% 97%

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Mol	Chain	Length	Quality of chain
1	O	1935	
1	Q	1935	
2	C	152	
2	D	152	
2	J	152	
2	K	152	
2	R	152	
2	S	152	
3	E	160	
3	F	160	
3	L	160	
3	M	160	
3	T	160	
3	U	160	
4	G	400	
4	V	400	
5	I	1079	
5	P	1079	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 131418 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 Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1926	Total	C	N	O	S	0	0
			15571	9670	2761	3076	64		
1	B	1926	Total	C	N	O	S	0	0
			15571	9670	2761	3076	64		
1	H	1930	Total	C	N	O	S	0	0
			15600	9690	2765	3080	65		
1	N	1930	Total	C	N	O	S	0	0
			15600	9690	2765	3080	65		
1	O	1926	Total	C	N	O	S	0	0
			15571	9670	2761	3076	64		
1	Q	1926	Total	C	N	O	S	0	0
			15571	9670	2761	3076	64		

- Molecule 2 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	152	Total	C	N	O	S	0	0
			1206	758	200	239	9		
2	D	152	Total	C	N	O	S	0	0
			1206	758	200	239	9		
2	J	152	Total	C	N	O	S	0	0
			1206	758	200	239	9		
2	K	152	Total	C	N	O	S	0	0
			1206	758	200	239	9		
2	R	152	Total	C	N	O	S	0	0
			1206	758	200	239	9		
2	S	152	Total	C	N	O	S	0	0
			1206	758	200	239	9		

- Molecule 3 is a protein called Myosin regulatory light chain 2, ventricular/cardiac muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	160	Total	C	N	O	S	0	0
			1283	811	211	255	6		
3	F	160	Total	C	N	O	S	0	0
			1283	811	211	255	6		
3	L	160	Total	C	N	O	S	0	0
			1283	811	211	255	6		
3	M	160	Total	C	N	O	S	0	0
			1283	811	211	255	6		
3	T	160	Total	C	N	O	S	0	0
			1283	811	211	255	6		
3	U	160	Total	C	N	O	S	0	0
			1283	811	211	255	6		

- Molecule 4 is a protein called Myosin binding protein C, cardiac.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	400	Total	C	N	O	S	0	0
			3151	2002	556	579	14		
4	V	400	Total	C	N	O	S	0	0
			3151	2002	556	579	14		

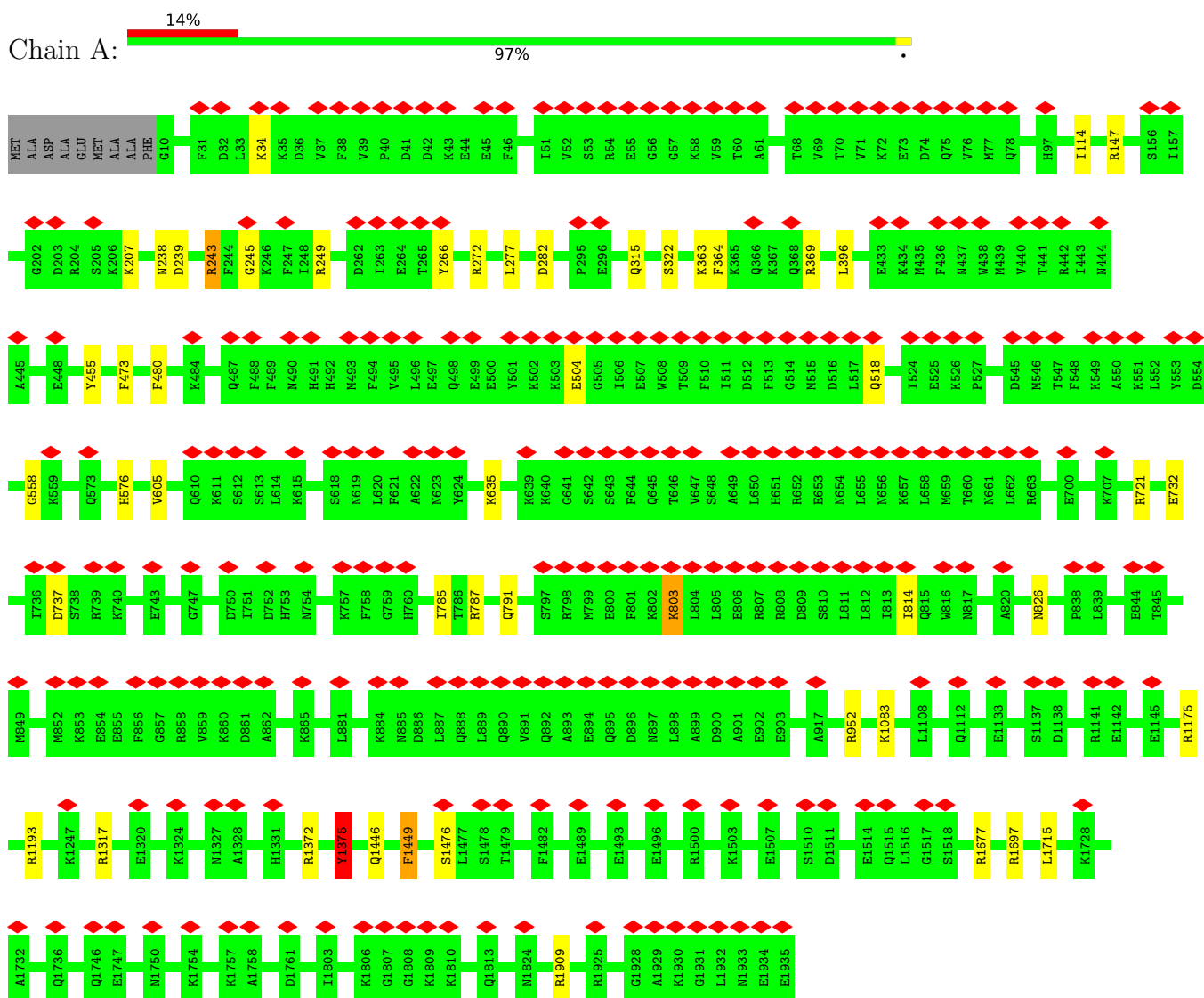
- Molecule 5 is a protein called Titin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	1079	Total	C	N	O	S	0	0
			8349	5261	1424	1637	27		
5	P	1079	Total	C	N	O	S	0	0
			8349	5261	1424	1637	27		

3 Residue-property plots [i](#)

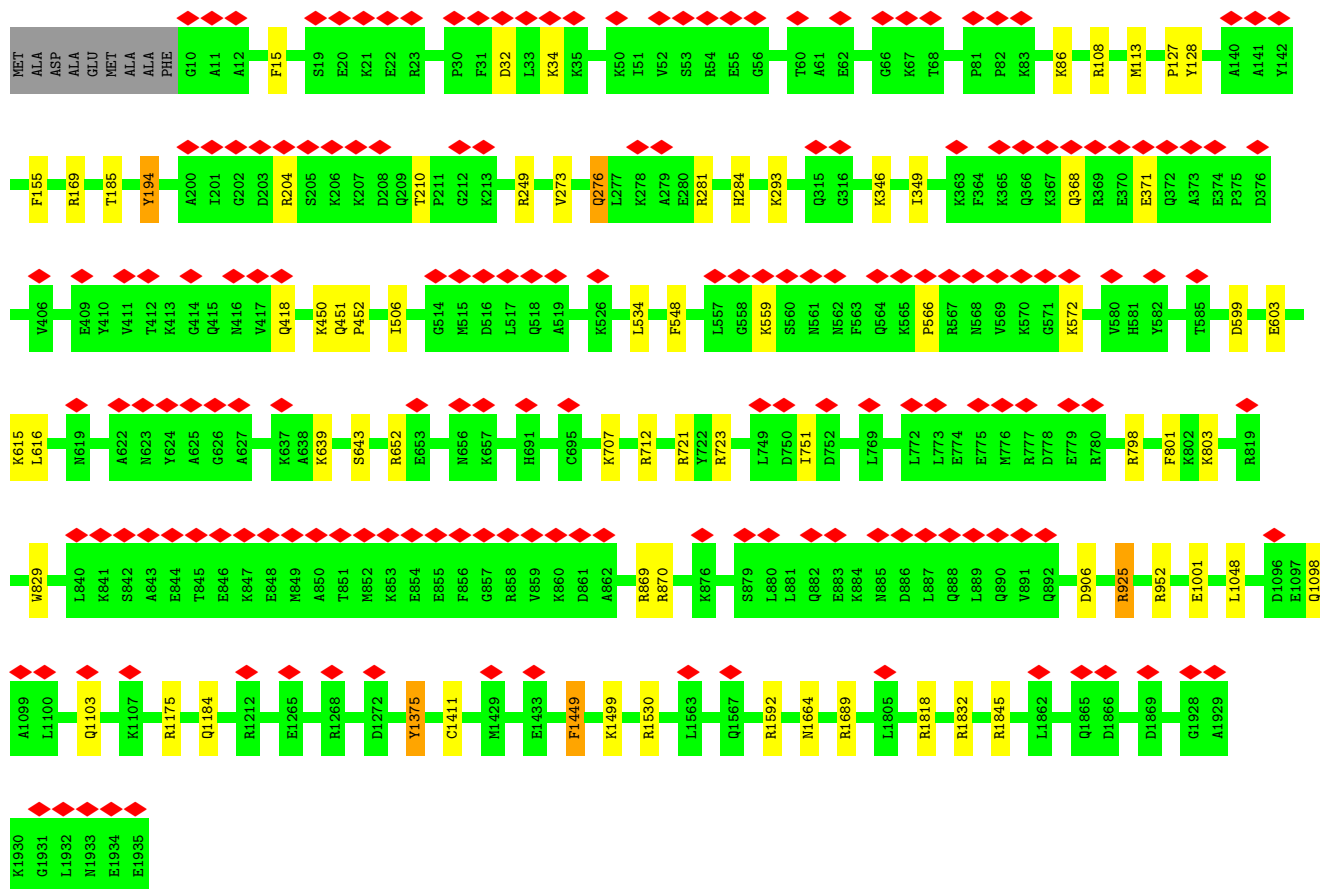
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Myosin-7

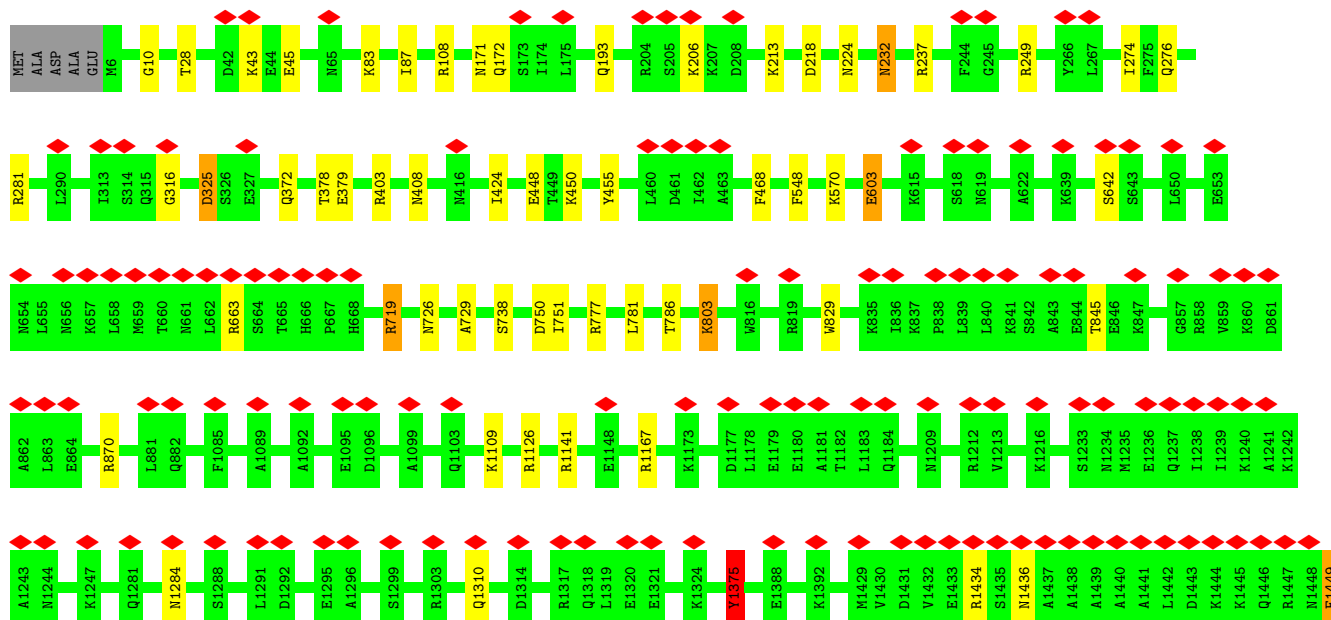


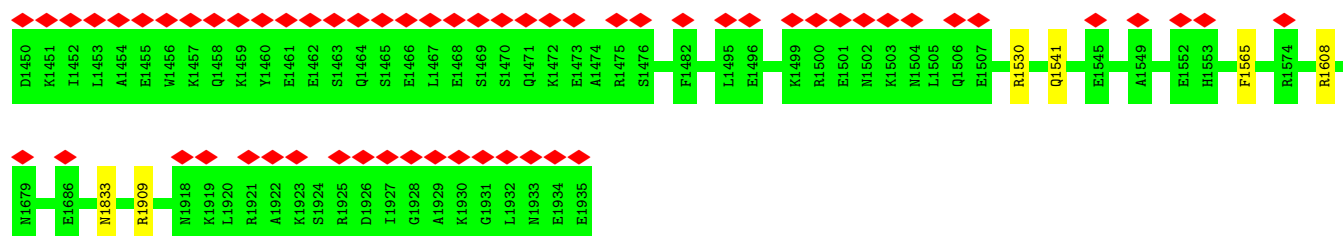
• Molecule 1: Myosin-7



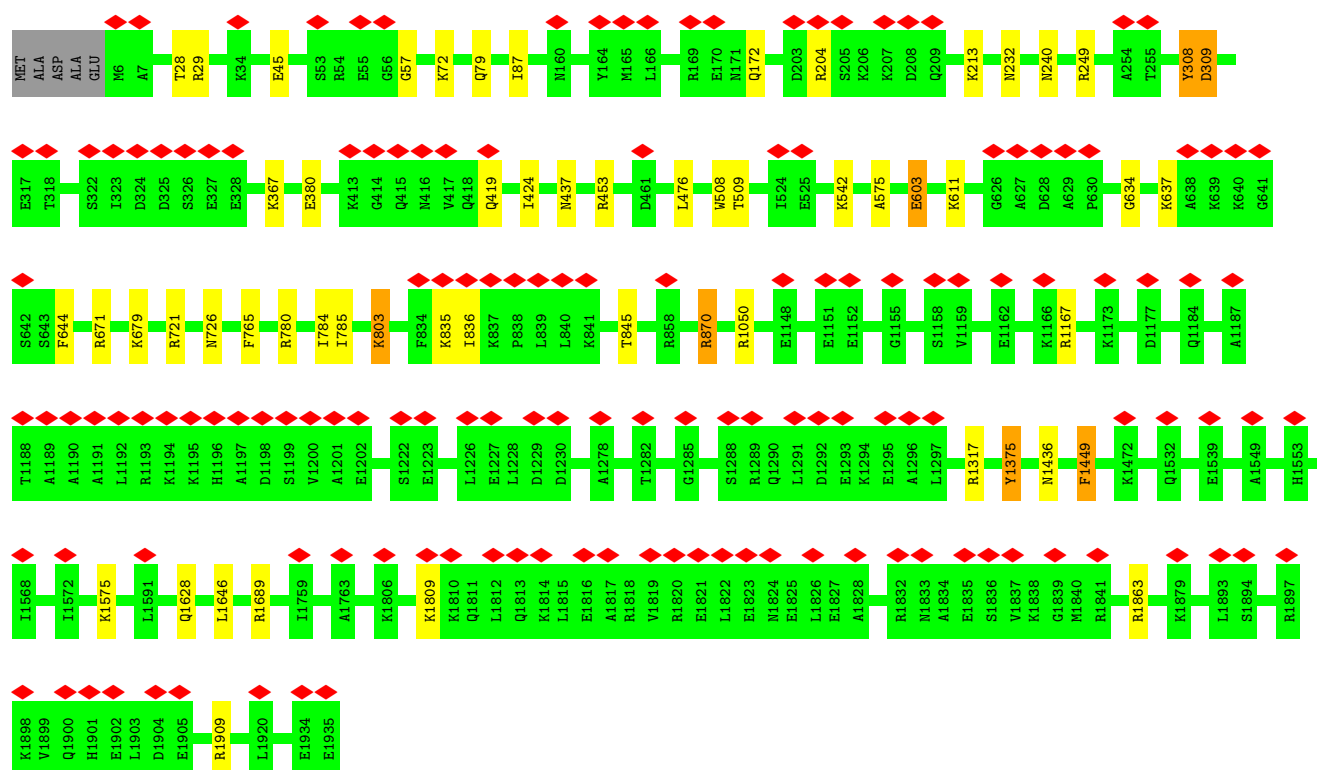


• Molecule 1: Myosin-7

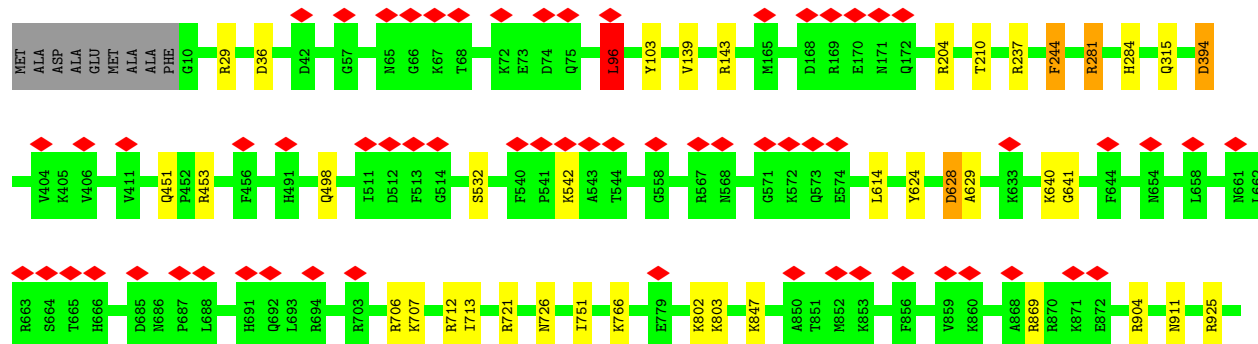


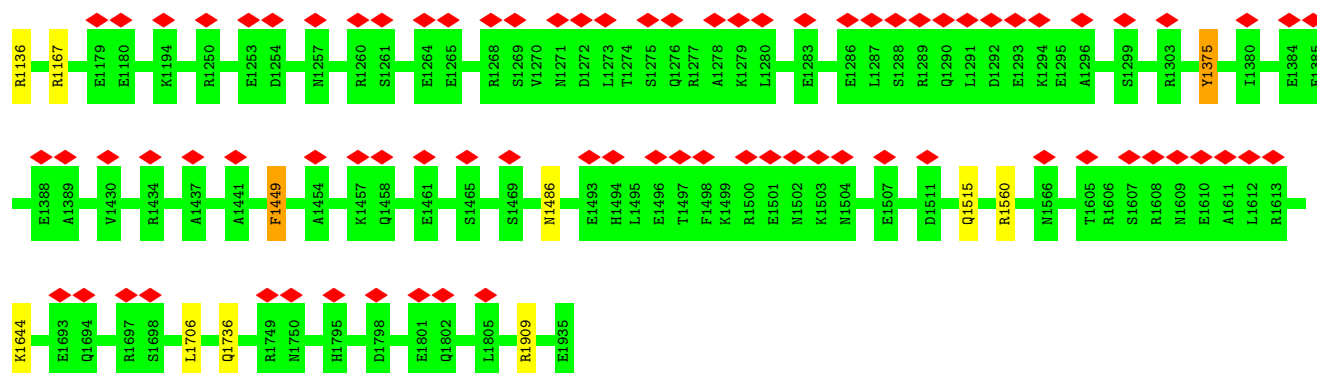


• Molecule 1: Myosin-7

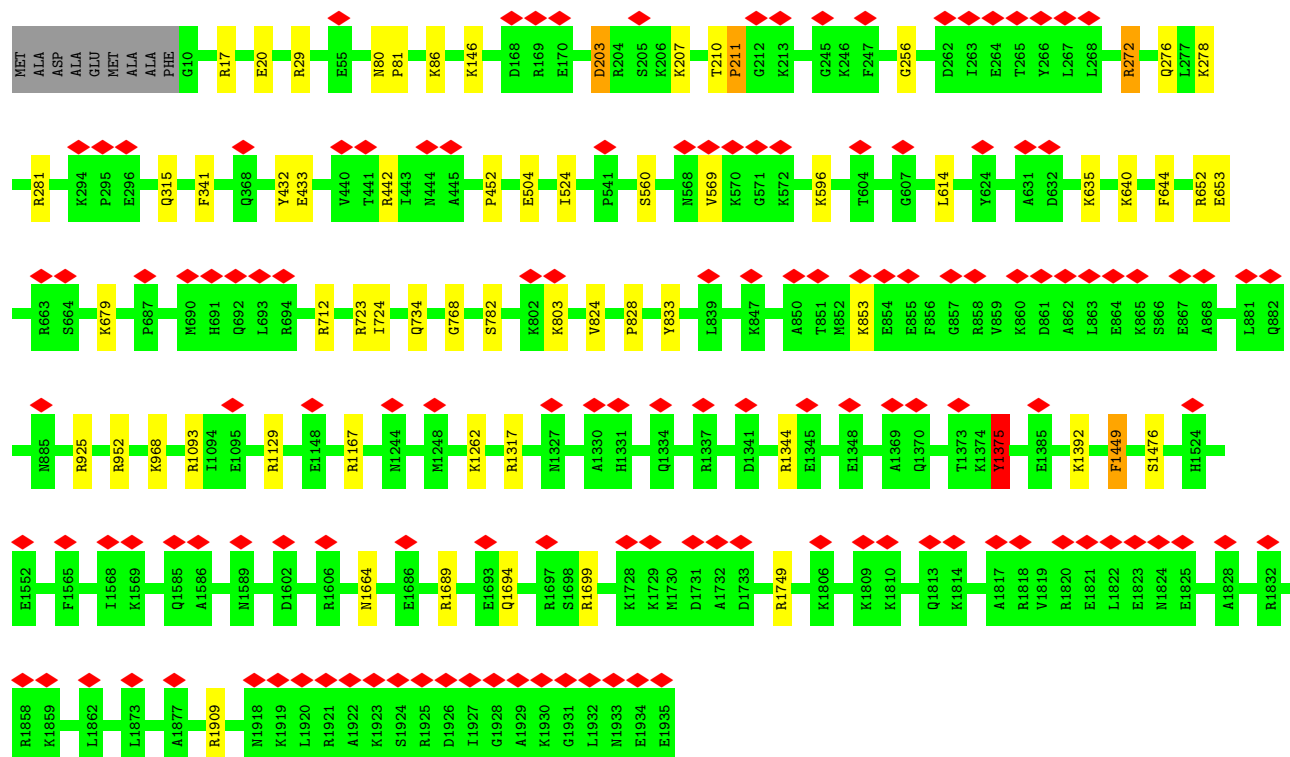


• Molecule 1: Myosin-7

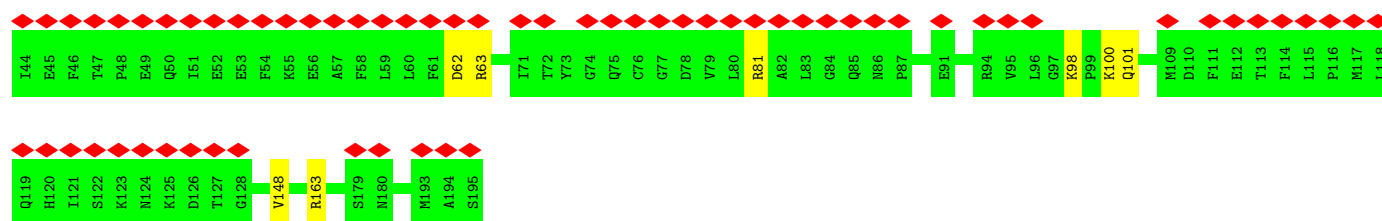
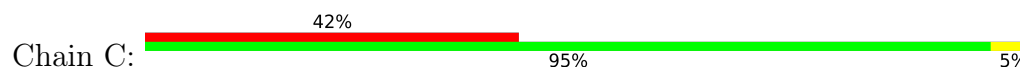




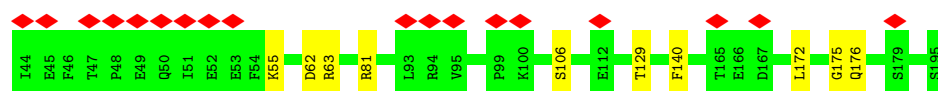
• Molecule 1: Myosin-7



• Molecule 2: Myosin light chain 3



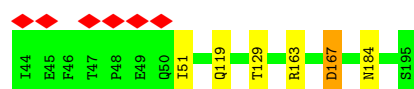
• Molecule 2: Myosin light chain 3



- Molecule 2: Myosin light chain 3



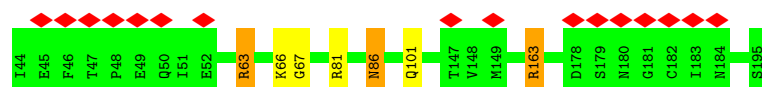
- Molecule 2: Myosin light chain 3



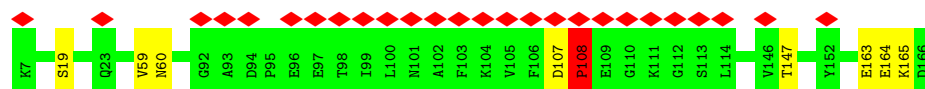
- Molecule 2: Myosin light chain 3



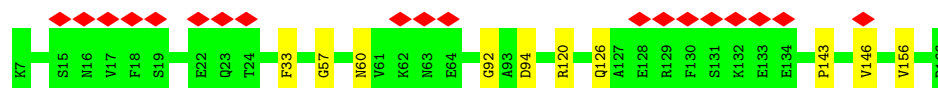
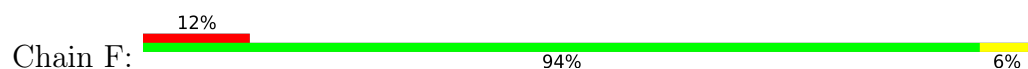
- Molecule 2: Myosin light chain 3



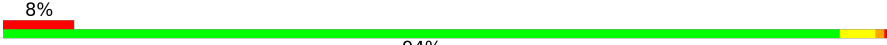
- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform



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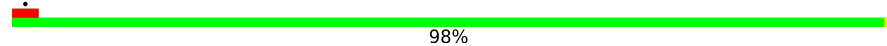


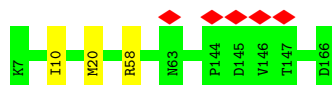
- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform

Chain L:  8% 94%



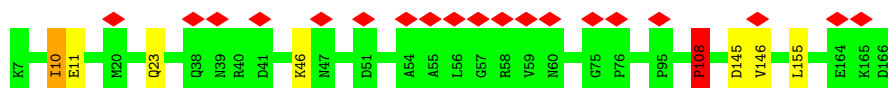
- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform

Chain M:  98%

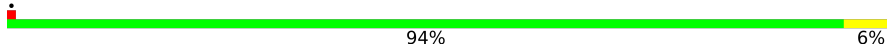


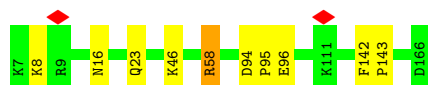
- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform

Chain T:  12% 95%

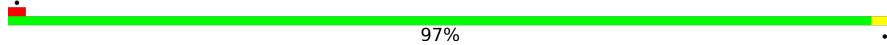


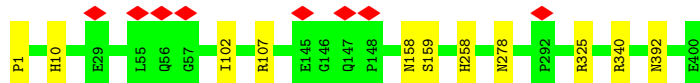
- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform

Chain U:  94% 6%

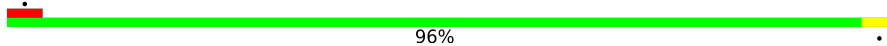


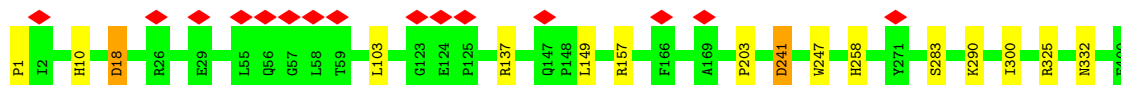
- Molecule 4: Myosin binding protein C, cardiac

Chain G:  97%

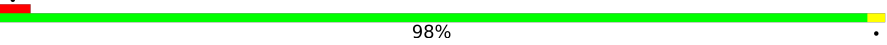


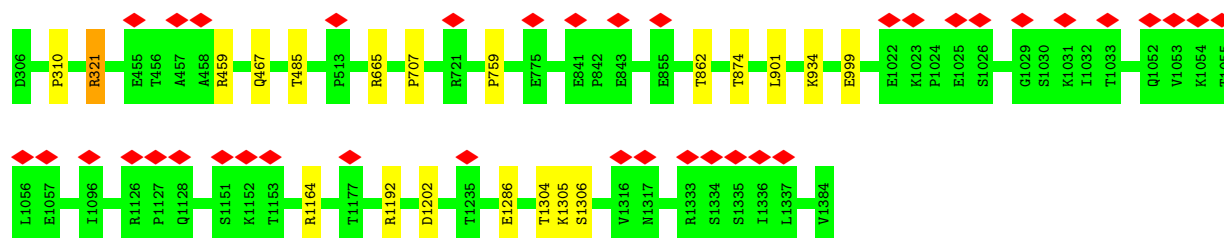
- Molecule 4: Myosin binding protein C, cardiac

Chain V:  96%



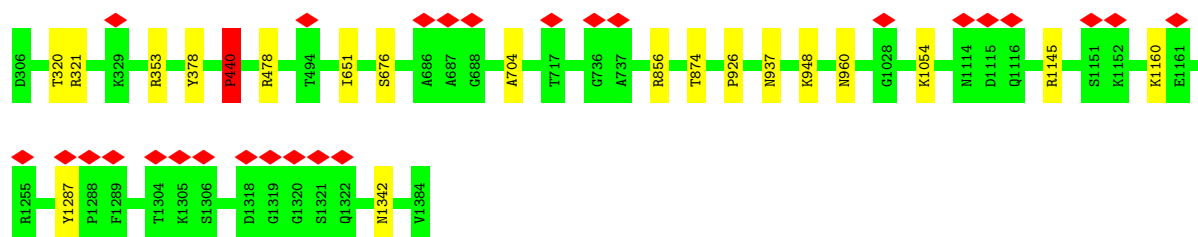
- Molecule 5: Titin

Chain I:  98%



• Molecule 5: Titin

Chain P: 98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=430 Å, axial sym=C3	Depositor
Number of subtomograms used	1589	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 ($e^-/\text{\AA}^2$)	140	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	13.522	Depositor
Minimum map value	0.000	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.387	Depositor
Recommended contour level	2.41	Depositor
Map size (Å)	2168.76, 2168.76, 2168.76	wwPDB
Map dimensions	372, 372, 372	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	5.83, 5.83, 5.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.06	13/15751 (0.1%)	1.33	22/21093 (0.1%)
1	B	0.99	12/15751 (0.1%)	1.34	27/21093 (0.1%)
1	H	1.06	13/15781 (0.1%)	1.33	27/21133 (0.1%)
1	N	1.06	13/15781 (0.1%)	1.33	24/21133 (0.1%)
1	O	0.99	12/15751 (0.1%)	1.34	28/21093 (0.1%)
1	Q	0.99	12/15751 (0.1%)	1.33	29/21093 (0.1%)
2	C	0.86	0/1225	1.35	2/1643 (0.1%)
2	D	0.89	0/1225	1.35	3/1643 (0.2%)
2	J	0.88	0/1225	1.33	0/1643
2	K	0.89	0/1225	1.36	3/1643 (0.2%)
2	R	0.87	0/1225	1.29	2/1643 (0.1%)
2	S	0.89	0/1225	1.37	3/1643 (0.2%)
3	E	2.04	5/1306 (0.4%)	1.37	3/1752 (0.2%)
3	F	0.92	1/1306 (0.1%)	1.42	5/1752 (0.3%)
3	L	2.05	5/1306 (0.4%)	1.38	3/1752 (0.2%)
3	M	0.93	0/1306	1.37	0/1752
3	T	2.05	5/1306 (0.4%)	1.35	0/1752
3	U	0.90	0/1306	1.41	3/1752 (0.2%)
4	G	0.91	0/3233	1.38	7/4398 (0.2%)
4	V	0.92	1/3233 (0.0%)	1.41	5/4398 (0.1%)
5	I	0.88	2/8525 (0.0%)	1.31	6/11602 (0.1%)
5	P	0.87	1/8525 (0.0%)	1.31	7/11602 (0.1%)
All	All	1.04	95/133268 (0.1%)	1.34	209/179008 (0.1%)

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	1
1	B	0	2
1	H	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
1	Q	0	5
2	S	0	1
3	L	0	1
5	I	0	1
5	P	0	1
All	All	0	15

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	803	LYS	CD-CE	49.20	3.00	1.52
1	A	803	LYS	CD-CE	49.16	3.00	1.52
1	H	803	LYS	CD-CE	49.10	2.99	1.52
3	T	108	PRO	CA-CB	38.57	2.08	1.53
3	E	108	PRO	CA-CB	38.53	2.08	1.53
3	L	108	PRO	N-CA	38.46	1.96	1.47
3	L	108	PRO	CA-CB	38.45	2.08	1.53
3	T	108	PRO	N-CA	38.33	1.96	1.47
3	E	108	PRO	N-CA	38.16	1.96	1.47
1	A	1449	PHE	CD1-CE1	37.95	2.52	1.38
1	Q	1449	PHE	CD1-CE1	37.91	2.52	1.38
1	H	1375	TYR	CD2-CE2	37.86	2.52	1.38
1	O	1375	TYR	CD2-CE2	37.84	2.52	1.38
1	A	1375	TYR	CD2-CE2	37.80	2.52	1.38
1	O	1449	PHE	CD1-CE1	37.79	2.52	1.38
1	B	1375	TYR	CD2-CE2	37.78	2.52	1.38
1	N	1375	TYR	CD2-CE2	37.77	2.52	1.38
1	H	1449	PHE	CD2-CE2	37.75	2.51	1.38
1	N	1449	PHE	CD2-CE2	37.75	2.51	1.38
1	Q	1375	TYR	CD1-CE1	37.75	2.52	1.38
1	B	1449	PHE	CD2-CE2	37.69	2.51	1.38
3	T	108	PRO	N-CD	33.39	1.94	1.47
3	L	108	PRO	N-CD	32.24	1.92	1.47
3	E	108	PRO	N-CD	32.19	1.92	1.47
3	E	108	PRO	CG-CD	17.04	2.08	1.50
3	L	108	PRO	CG-CD	16.96	2.08	1.50
3	T	108	PRO	CG-CD	16.24	2.06	1.50
1	N	1449	PHE	CG-CD2	15.79	1.72	1.38
1	H	1449	PHE	CG-CD2	15.75	1.72	1.38
1	A	1449	PHE	CG-CD1	15.70	1.71	1.38
1	H	1375	TYR	CG-CD2	15.68	1.72	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1449	PHE	CG-CD2	15.67	1.71	1.38
1	B	1375	TYR	CG-CD2	15.67	1.72	1.39
1	N	1375	TYR	CG-CD2	15.65	1.72	1.39
1	O	1449	PHE	CG-CD1	15.61	1.71	1.38
1	Q	1449	PHE	CG-CD1	15.59	1.71	1.38
1	O	1375	TYR	CG-CD2	15.55	1.72	1.39
1	A	1375	TYR	CG-CD2	15.48	1.71	1.39
1	Q	1375	TYR	CG-CD1	15.40	1.71	1.39
1	H	1449	PHE	CG-CD1	14.87	1.70	1.38
1	B	1449	PHE	CG-CD1	14.86	1.70	1.38
1	N	1449	PHE	CG-CD1	14.82	1.70	1.38
1	A	1449	PHE	CG-CD2	14.82	1.70	1.38
1	Q	1449	PHE	CG-CD2	14.81	1.70	1.38
1	O	1449	PHE	CG-CD2	14.76	1.69	1.38
1	B	1375	TYR	CG-CD1	14.59	1.70	1.39
1	N	1375	TYR	CG-CD1	14.57	1.70	1.39
1	Q	1375	TYR	CG-CD2	14.52	1.69	1.39
1	H	1375	TYR	CG-CD1	14.47	1.69	1.39
1	A	1375	TYR	CG-CD1	14.39	1.69	1.39
1	O	1375	TYR	CG-CD1	14.35	1.69	1.39
1	H	1375	TYR	CE2-CZ	14.24	1.72	1.38
1	A	1375	TYR	CE2-CZ	14.23	1.72	1.38
1	O	1375	TYR	CE2-CZ	14.21	1.72	1.38
1	Q	1375	TYR	CE1-CZ	14.18	1.72	1.38
1	B	1375	TYR	CE2-CZ	14.18	1.72	1.38
1	N	1375	TYR	CE2-CZ	14.11	1.72	1.38
1	Q	1375	TYR	CE2-CZ	13.44	1.70	1.38
1	N	1375	TYR	CE1-CZ	13.42	1.70	1.38
1	A	1375	TYR	CE1-CZ	13.31	1.70	1.38
1	O	1375	TYR	CE1-CZ	13.27	1.70	1.38
1	H	1375	TYR	CE1-CZ	13.26	1.70	1.38
1	B	1375	TYR	CE1-CZ	13.22	1.70	1.38
3	T	108	PRO	CB-CG	11.43	2.06	1.49
3	L	108	PRO	CB-CG	11.41	2.06	1.49
3	E	108	PRO	CB-CG	11.35	2.06	1.49
1	O	1449	PHE	CE1-CZ	11.07	1.71	1.38
1	A	1449	PHE	CE1-CZ	11.04	1.71	1.38
1	Q	1449	PHE	CE1-CZ	11.02	1.71	1.38
1	N	1449	PHE	CE2-CZ	11.01	1.71	1.38
1	B	1449	PHE	CE2-CZ	10.94	1.71	1.38
1	H	1449	PHE	CE2-CZ	10.93	1.71	1.38
1	A	1449	PHE	CD2-CE2	10.66	1.70	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1449	PHE	CD1-CE1	10.66	1.70	1.38
1	Q	1449	PHE	CD2-CE2	10.66	1.70	1.38
1	B	1449	PHE	CD1-CE1	10.64	1.70	1.38
1	O	1449	PHE	CD2-CE2	10.63	1.70	1.38
1	Q	1375	TYR	CD2-CE2	10.62	1.70	1.38
1	N	1375	TYR	CD1-CE1	10.56	1.70	1.38
1	N	1449	PHE	CD1-CE1	10.54	1.70	1.38
1	A	1375	TYR	CD1-CE1	10.51	1.70	1.38
1	O	1375	TYR	CD1-CE1	10.49	1.70	1.38
1	B	1375	TYR	CD1-CE1	10.46	1.70	1.38
1	Q	1449	PHE	CE2-CZ	10.46	1.70	1.38
1	N	1449	PHE	CE1-CZ	10.43	1.70	1.38
1	H	1375	TYR	CD1-CE1	10.42	1.69	1.38
1	B	1449	PHE	CE1-CZ	10.40	1.69	1.38
1	A	1449	PHE	CE2-CZ	10.40	1.69	1.38
1	O	1449	PHE	CE2-CZ	10.39	1.69	1.38
1	H	1449	PHE	CE1-CZ	10.39	1.69	1.38
5	P	926	PRO	CA-C	5.80	1.55	1.51
4	V	203	PRO	CA-C	5.66	1.54	1.51
5	I	310	PRO	CA-C	5.42	1.54	1.51
3	F	143	PRO	CA-C	5.42	1.54	1.51
5	I	759	PRO	CA-C	5.05	1.54	1.51

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	803	LYS	CG-CD-CE	10.04	134.40	111.30
1	H	803	LYS	CG-CD-CE	9.93	134.14	111.30
1	N	803	LYS	CG-CD-CE	9.79	133.81	111.30
1	H	325	ASP	CA-CB-CG	7.63	120.23	112.60
1	O	244	PHE	CA-CB-CG	7.53	121.33	113.80
1	O	712	ARG	NE-CZ-NH2	7.35	125.81	119.20
1	O	1909	ARG	NE-CZ-NH2	7.11	125.60	119.20
1	B	712	ARG	NE-CZ-NH2	7.08	125.57	119.20
5	P	440	PRO	CA-N-CD	-6.98	102.23	112.00
1	H	1909	ARG	NE-CZ-NH2	6.83	125.35	119.20
2	R	191	HIS	CA-CB-CG	6.83	120.63	113.80
1	B	281	ARG	NE-CZ-NH2	6.75	125.28	119.20
2	D	81	ARG	NE-CZ-NH2	6.69	125.22	119.20
1	B	108	ARG	NE-CZ-NH2	6.67	125.21	119.20
4	V	1	PRO	CA-N-CD	-6.63	102.71	112.00
1	H	1375	TYR	CG-CD2-CE2	-6.63	111.25	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1141	ARG	NE-CZ-NH2	6.62	125.15	119.20
1	H	237	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	O	1375	TYR	CG-CD2-CE2	-6.59	111.31	121.20
1	O	1736	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	A	1375	TYR	CG-CD2-CE2	-6.59	111.32	121.20
1	B	1375	TYR	CG-CD2-CE2	-6.58	111.33	121.20
4	G	1	PRO	CA-N-CD	-6.57	102.80	112.00
1	N	1375	TYR	CG-CD2-CE2	-6.56	111.36	121.20
2	D	62	ASP	CA-CB-CG	6.52	119.12	112.60
1	Q	1375	TYR	CG-CD1-CE1	-6.45	111.53	121.20
1	O	628	ASP	CA-CB-CG	6.44	119.04	112.60
3	L	60	ASN	CA-CB-CG	6.39	118.99	112.60
1	Q	1909	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	B	707	LYS	CA-C-N	6.29	125.96	119.92
1	B	707	LYS	C-N-CA	6.29	125.96	119.92
1	H	468	PHE	CA-CB-CG	6.26	120.06	113.80
1	O	1167	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	N	803	LYS	CD-CE-NZ	6.18	131.67	111.90
1	O	281	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	Q	952	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	H	803	LYS	CD-CE-NZ	6.11	131.47	111.90
1	A	1909	ARG	NE-CZ-NH2	6.07	124.66	119.20
5	P	856	ARG	NE-CZ-NH2	6.06	124.66	119.20
2	K	184	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	A	803	LYS	CD-CE-NZ	6.05	131.27	111.90
1	O	237	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	N	765	PHE	CA-CB-CG	6.02	119.82	113.80
1	H	1126	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	N	309	ASP	CA-CB-CG	5.90	118.50	112.60
1	Q	1664	ASN	CA-CB-CG	5.88	118.48	112.60
1	Q	1167	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	H	1167	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	B	1818	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	H	1565	PHE	CA-CB-CG	5.83	119.63	113.80
4	G	158	ASN	CA-CB-CG	5.83	118.42	112.60
1	B	155	PHE	CA-CB-CG	5.82	119.62	113.80
1	B	1530	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	N	1167	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	B	798	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	B	548	PHE	CA-CB-CG	5.81	119.61	113.80
3	F	60	ASN	CA-CB-CG	5.79	118.39	112.60
3	U	58	ARG	NE-CZ-NH2	5.79	124.41	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	652	ARG	NE-CZ-NH2	5.79	124.41	119.20
2	K	167	ASP	CA-CB-CG	5.75	118.35	112.60
1	N	308	TYR	CA-CB-CG	5.75	124.25	113.90
1	N	870	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	A	1193	ARG	NE-CZ-NH2	5.73	124.36	119.20
3	E	60	ASN	CA-CB-CG	5.73	118.33	112.60
5	P	321	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	K	163	ARG	NE-CZ-NH2	5.71	124.34	119.20
3	F	120	ARG	NE-CZ-NH2	5.70	124.33	119.20
5	I	321	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	N	249	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	O	394	ASP	CA-CB-CG	5.66	118.26	112.60
1	Q	203	ASP	CA-CB-CG	5.64	118.24	112.60
1	Q	210	THR	CA-C-N	5.62	126.87	119.84
1	Q	210	THR	C-N-CA	5.62	126.87	119.84
1	N	671	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	B	1664	ASN	CA-CB-CG	5.60	118.20	112.60
1	O	869	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	H	1541	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	Q	712	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	H	1530	ARG	NE-CZ-NH2	5.56	124.21	119.20
5	P	926	PRO	N-CA-C	5.56	115.81	110.47
1	O	451	GLN	CA-C-N	5.55	125.22	119.56
1	O	451	GLN	C-N-CA	5.55	125.22	119.56
1	H	249	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	A	243	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	S	86	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	1449	PHE	CG-CD1-CE1	-5.53	111.30	120.70
1	N	721	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	B	276	GLN	OE1-CD-NE2	-5.53	117.08	122.60
1	H	1284	ASN	CA-CB-CG	5.52	118.12	112.60
1	Q	652	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	A	1697	ARG	NE-CZ-NH2	5.52	124.16	119.20
1	N	1689	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	Q	1449	PHE	CG-CD1-CE1	-5.50	111.36	120.70
1	A	787	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	B	1449	PHE	CG-CD2-CE2	-5.49	111.36	120.70
5	P	353	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	H	1449	PHE	CG-CD2-CE2	-5.49	111.37	120.70
1	N	1449	PHE	CG-CD2-CE2	-5.49	111.38	120.70
1	O	721	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	1175	ARG	NE-CZ-NH2	5.48	124.13	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1145	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	H	548	PHE	CA-CB-CG	5.46	119.26	113.80
1	O	1449	PHE	CG-CD1-CE1	-5.46	111.41	120.70
1	A	1677	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	O	143	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	N	1628	GLN	OE1-CD-NE2	-5.43	117.17	122.60
3	F	143	PRO	N-CA-CB	5.39	106.21	103.19
1	A	1372	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	Q	1129	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	Q	276	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	H	403	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	O	453	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	H	1434	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	369	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	576	HIS	CB-CG-CD2	-5.33	124.28	131.20
4	V	241	ASP	CA-CB-CG	5.33	117.93	112.60
1	Q	272	ARG	NE-CZ-NH2	5.31	123.98	119.20
4	V	258	HIS	CB-CG-CD2	-5.31	124.30	131.20
3	E	108	PRO	N-CA-CB	5.31	108.83	103.25
1	Q	81	PRO	CA-C-N	5.29	125.01	119.82
1	Q	81	PRO	C-N-CA	5.29	125.01	119.82
4	V	137	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	N	1050	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	O	29	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	O	1486	ASN	CA-CB-CG	5.28	117.88	112.60
3	L	108	PRO	N-CA-CB	5.28	108.79	103.25
4	G	278	ASN	CA-CB-CG	5.28	117.88	112.60
1	O	204	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	Q	1689	ARG	NE-CZ-NH2	5.27	123.95	119.20
1	H	108	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	B	1845	ARG	NE-CZ-NH2	5.26	123.93	119.20
4	G	107	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	Q	782	SER	CA-C-N	5.25	127.63	120.54
1	Q	782	SER	C-N-CA	5.25	127.63	120.54
1	B	1175	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	B	1592	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	H	232	ASN	CA-CB-CG	5.25	117.85	112.60
5	I	1202	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	204	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	C	62	ASP	CA-CB-CG	5.24	117.84	112.60
3	F	33	PHE	CA-CB-CG	5.24	119.04	113.80
2	S	81	ARG	NE-CZ-NH2	5.23	123.91	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	707	PRO	N-CA-CB	5.23	106.12	103.19
5	I	459	ARG	NE-CZ-NH2	5.23	123.90	119.20
3	E	107	ASP	CA-CB-CG	5.21	117.81	112.60
1	Q	1317	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	1317	ARG	NE-CZ-NH2	5.21	123.88	119.20
1	A	480	PHE	CA-CB-CG	5.20	119.00	113.80
1	H	281	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	O	36	ASP	CA-CB-CG	5.19	117.79	112.60
1	Q	281	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	Q	341	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	147	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	H	218	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	1689	ARG	NE-CZ-NH2	5.17	123.85	119.20
2	R	138	ARG	NE-CZ-NH2	5.17	123.85	119.20
5	I	1164	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	B	925	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	Q	1749	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	H	663	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	N	1909	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	B	1832	ARG	NE-CZ-NH2	5.15	123.83	119.20
2	D	140	PHE	N-CA-C	5.15	116.89	111.28
4	G	258	HIS	CB-CG-CD2	-5.15	124.51	131.20
5	P	478	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	H	719	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	O	1515	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	H	1310	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	737	ASP	CA-CB-CG	5.12	117.72	112.60
1	N	1317	ARG	NE-CZ-NH2	5.12	123.80	119.20
1	Q	29	ARG	NE-CZ-NH2	5.12	123.80	119.20
1	Q	17	ARG	NE-CZ-NH2	5.11	123.80	119.20
4	V	18	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	473	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	249	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	O	925	ARG	NE-CZ-NH2	5.10	123.79	119.20
3	U	8	LYS	N-CA-C	5.10	117.58	111.71
1	B	721	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	284	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	N	29	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	Q	1699	ARG	NE-CZ-NH2	5.08	123.77	119.20
4	G	392	ASN	CA-CB-CG	5.08	117.68	112.60
2	C	81	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	Q	925	ARG	NE-CZ-NH2	5.07	123.76	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	836	ILE	CA-C-N	5.07	126.09	120.06
1	N	836	ILE	C-N-CA	5.07	126.09	120.06
3	F	126	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	272	ARG	NE-CZ-NH2	5.06	123.75	119.20
4	G	340	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	O	1136	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	721	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	Q	1093	ARG	NE-CZ-NH2	5.04	123.74	119.20
3	L	106	PHE	CA-CB-CG	5.04	118.84	113.80
1	O	1560	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	B	249	ARG	NE-CZ-NH2	5.03	123.73	119.20
5	I	467	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	169	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	N	1436	ASN	CA-CB-CG	5.03	117.63	112.60
3	U	142	PHE	CA-CB-CG	5.03	118.83	113.80
1	N	437	ASN	CA-CB-CG	5.02	117.62	112.60
1	N	780	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	O	802	LYS	CA-C-N	5.02	131.13	121.54
1	O	802	LYS	C-N-CA	5.02	131.13	121.54
2	S	163	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	N	1863	ARG	NE-CZ-NH2	5.02	123.71	119.20
1	Q	1344	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	H	1436	ASN	CA-CB-CG	5.01	117.61	112.60
1	B	870	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	O	904	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1375	TYR	Sidechain
1	B	194	TYR	Sidechain
1	B	925	ARG	Sidechain
1	H	1375	TYR	Sidechain
1	H	1608	ARG	Sidechain
5	I	1192	ARG	Sidechain
3	L	40	ARG	Sidechain
1	O	103	TYR	Sidechain
5	P	378	TYR	Sidechain
1	Q	1375	TYR	Sidechain
1	Q	272	ARG	Sidechain
1	Q	432	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	Q	442	ARG	Sidechain
1	Q	833	TYR	Sidechain
2	S	63	ARG	Sidechain

5.2 Too-close contacts

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	15571	0	15684	84	0
1	B	15571	0	15684	53	0
1	H	15600	0	15711	83	0
1	N	15600	0	15712	86	0
1	O	15571	0	15683	57	0
1	Q	15571	0	15684	54	0
2	C	1206	0	1182	0	0
2	D	1206	0	1182	0	0
2	J	1206	0	1182	0	0
2	K	1206	0	1182	0	0
2	R	1206	0	1182	0	0
2	S	1206	0	1182	0	0
3	E	1283	0	1245	36	0
3	F	1283	0	1245	0	0
3	L	1283	0	1245	35	0
3	M	1283	0	1245	0	0
3	T	1283	0	1245	36	0
3	U	1283	0	1245	0	0
4	G	3151	0	3155	0	0
4	V	3151	0	3155	0	0
5	I	8349	0	8362	0	0
5	P	8349	0	8362	0	0
All	All	131418	0	131754	281	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 1.

All (281) 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:A:1375:TYR:CE2	1:B:1375:TYR:CE2	2.12	1.38
1:A:1375:TYR:CD2	1:B:1375:TYR:CE2	2.12	1.38
1:A:1449:PHE:CD1	1:B:1449:PHE:CD2	2.12	1.38
1:A:1375:TYR:CE2	1:B:1375:TYR:CD2	2.12	1.38
1:A:1375:TYR:CD2	1:B:1375:TYR:CD2	2.12	1.38
1:A:1449:PHE:CE1	1:B:1449:PHE:CD2	2.12	1.38
1:A:1449:PHE:CE1	1:B:1449:PHE:CE2	2.12	1.37
1:H:1449:PHE:CD2	1:O:1449:PHE:CD1	2.12	1.37
1:H:1449:PHE:CE2	1:O:1449:PHE:CE1	2.12	1.37
1:N:1375:TYR:CE2	1:Q:1375:TYR:CD1	2.12	1.37
1:N:1449:PHE:CE2	1:Q:1449:PHE:CD1	2.12	1.37
1:H:1375:TYR:CE2	1:O:1375:TYR:CD2	2.12	1.37
1:H:1375:TYR:CE2	1:O:1375:TYR:CE2	2.12	1.37
1:N:1375:TYR:CD2	1:Q:1375:TYR:CD1	2.12	1.37
1:N:1449:PHE:CD2	1:Q:1449:PHE:CD1	2.12	1.37
1:H:1449:PHE:CD2	1:O:1449:PHE:CE1	2.12	1.36
1:H:1375:TYR:CD2	1:O:1375:TYR:CD2	2.12	1.36
1:H:1449:PHE:CE2	1:O:1449:PHE:CD1	2.12	1.36
1:N:1449:PHE:CE2	1:Q:1449:PHE:CE1	2.12	1.36
1:H:1375:TYR:CD2	1:O:1375:TYR:CE2	2.12	1.36
1:A:1449:PHE:CD1	1:B:1449:PHE:CE2	2.12	1.35
1:N:1375:TYR:CD2	1:Q:1375:TYR:CE1	2.12	1.35
1:N:1375:TYR:CE2	1:Q:1375:TYR:CE1	2.12	1.35
1:N:1449:PHE:CD2	1:Q:1449:PHE:CE1	2.12	1.34
3:T:108:PRO:CD	3:T:108:PRO:CG	2.06	1.34
3:L:108:PRO:CB	3:L:108:PRO:CG	2.06	1.32
3:L:108:PRO:CG	3:L:108:PRO:CD	2.08	1.32
3:E:108:PRO:CA	3:E:108:PRO:CB	2.08	1.31
3:T:108:PRO:CB	3:T:108:PRO:CA	2.08	1.31
3:T:108:PRO:CG	3:T:108:PRO:CB	2.06	1.31
3:L:108:PRO:CB	3:L:108:PRO:CA	2.08	1.31
3:E:108:PRO:CB	3:E:108:PRO:CG	2.06	1.30
3:E:108:PRO:N	3:E:108:PRO:CD	1.92	1.30
3:E:108:PRO:CG	3:E:108:PRO:CD	2.08	1.30
3:L:108:PRO:CD	3:L:108:PRO:N	1.92	1.30
3:E:108:PRO:CA	3:E:108:PRO:N	1.96	1.29
3:T:108:PRO:CD	3:T:108:PRO:N	1.94	1.29
3:T:108:PRO:CA	3:T:108:PRO:N	1.96	1.29
3:L:108:PRO:CA	3:L:108:PRO:N	1.96	1.28
1:A:1375:TYR:CG	1:B:1375:TYR:CE2	2.30	1.20
1:A:1449:PHE:CE1	1:B:1449:PHE:CG	2.30	1.20
1:H:1375:TYR:CG	1:O:1375:TYR:CE2	2.30	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1449:PHE:CG	1:B:1449:PHE:CE2	2.30	1.19
1:H:1375:TYR:CZ	1:O:1375:TYR:CE2	2.31	1.19
1:N:1449:PHE:CE2	1:Q:1449:PHE:CG	2.30	1.19
1:N:1449:PHE:CG	1:Q:1449:PHE:CE1	2.30	1.19
1:A:1449:PHE:CE1	1:B:1449:PHE:CZ	2.31	1.19
1:H:1449:PHE:CZ	1:O:1449:PHE:CD1	2.31	1.19
1:N:1375:TYR:CZ	1:Q:1375:TYR:CE1	2.31	1.19
1:A:1375:TYR:CD2	1:B:1375:TYR:CZ	2.31	1.19
1:H:1375:TYR:CD2	1:O:1375:TYR:CG	2.31	1.19
1:H:1449:PHE:CG	1:O:1449:PHE:CD1	2.31	1.19
1:N:1375:TYR:CD2	1:Q:1375:TYR:CZ	2.31	1.19
1:A:1375:TYR:CE2	1:B:1375:TYR:CZ	2.31	1.19
1:A:1449:PHE:CZ	1:B:1449:PHE:CE2	2.31	1.19
1:H:1449:PHE:CG	1:O:1449:PHE:CE1	2.31	1.19
1:N:1449:PHE:CE2	1:Q:1449:PHE:CZ	2.31	1.19
1:A:1375:TYR:CD2	1:B:1375:TYR:CG	2.31	1.19
1:H:1375:TYR:CD2	1:O:1375:TYR:CZ	2.31	1.19
1:H:1375:TYR:CZ	1:O:1375:TYR:CD2	2.31	1.19
1:H:1375:TYR:CE2	1:O:1375:TYR:CG	2.30	1.18
1:H:1449:PHE:CE2	1:O:1449:PHE:CZ	2.31	1.18
1:N:1375:TYR:CE2	1:Q:1375:TYR:CG	2.30	1.18
1:N:1375:TYR:CD2	1:Q:1375:TYR:CG	2.31	1.18
1:H:1449:PHE:CD2	1:O:1449:PHE:CG	2.31	1.18
1:H:1449:PHE:CD2	1:O:1449:PHE:CZ	2.31	1.18
1:H:1449:PHE:CE2	1:O:1449:PHE:CG	2.30	1.18
1:N:1375:TYR:CZ	1:Q:1375:TYR:CD1	2.30	1.18
1:N:1375:TYR:CG	1:Q:1375:TYR:CD1	2.31	1.18
1:H:1375:TYR:CE2	1:O:1375:TYR:CZ	2.31	1.18
1:A:1375:TYR:CZ	1:B:1375:TYR:CD2	2.31	1.18
1:A:1449:PHE:CD1	1:B:1449:PHE:CG	2.31	1.18
1:A:1449:PHE:CZ	1:B:1449:PHE:CD2	2.31	1.18
1:N:1449:PHE:CD2	1:Q:1449:PHE:CG	2.31	1.18
1:A:1375:TYR:CG	1:B:1375:TYR:CD2	2.31	1.17
1:A:1375:TYR:CZ	1:B:1375:TYR:CE2	2.30	1.17
1:N:1375:TYR:CG	1:Q:1375:TYR:CE1	2.31	1.17
1:N:1375:TYR:CE2	1:Q:1375:TYR:CZ	2.31	1.17
1:N:1449:PHE:CD2	1:Q:1449:PHE:CZ	2.31	1.17
1:N:1449:PHE:CZ	1:Q:1449:PHE:CD1	2.31	1.17
1:A:1375:TYR:CE2	1:B:1375:TYR:CG	2.31	1.17
1:A:1449:PHE:CD1	1:B:1449:PHE:CZ	2.31	1.17
1:H:1375:TYR:CG	1:O:1375:TYR:CD2	2.31	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1449:PHE:CG	1:Q:1449:PHE:CD1	2.31	1.17
1:N:1449:PHE:CZ	1:Q:1449:PHE:CE1	2.31	1.17
1:A:1449:PHE:CG	1:B:1449:PHE:CD2	2.31	1.17
1:H:1449:PHE:CZ	1:O:1449:PHE:CE1	2.31	1.16
1:N:1449:PHE:CE2	1:Q:1449:PHE:CD2	2.35	1.15
1:A:1449:PHE:CD2	1:B:1449:PHE:CD2	2.35	1.15
1:A:1375:TYR:CE2	1:B:1375:TYR:CD1	2.35	1.15
1:A:1375:TYR:CD2	1:B:1375:TYR:CE1	2.35	1.15
1:A:1375:TYR:CD1	1:B:1375:TYR:CD2	2.35	1.15
1:A:1449:PHE:CE1	1:B:1449:PHE:CE1	2.35	1.15
1:A:1449:PHE:CD2	1:B:1449:PHE:CE2	2.35	1.15
1:H:1449:PHE:CD2	1:O:1449:PHE:CE2	2.35	1.15
1:N:1375:TYR:CD1	1:Q:1375:TYR:CD1	2.35	1.15
1:N:1449:PHE:CE2	1:Q:1449:PHE:CE2	2.35	1.15
1:N:1449:PHE:CD1	1:Q:1449:PHE:CD1	2.35	1.15
1:H:1449:PHE:CE1	1:O:1449:PHE:CE1	2.35	1.15
1:N:1375:TYR:CD1	1:Q:1375:TYR:CE1	2.35	1.15
1:N:1449:PHE:CD2	1:Q:1449:PHE:CD2	2.35	1.15
1:N:1449:PHE:CD1	1:Q:1449:PHE:CE1	2.35	1.15
1:H:1375:TYR:CD1	1:O:1375:TYR:CD2	2.35	1.15
1:H:1449:PHE:CE1	1:O:1449:PHE:CD1	2.35	1.15
1:A:1375:TYR:CE1	1:B:1375:TYR:CD2	2.35	1.14
1:N:1375:TYR:CE1	1:Q:1375:TYR:CE1	2.35	1.14
1:A:803:LYS:CE	3:E:108:PRO:CA	2.25	1.14
1:A:1375:TYR:CE2	1:B:1375:TYR:CE1	2.35	1.14
1:A:1375:TYR:CD1	1:B:1375:TYR:CE2	2.35	1.14
1:A:1449:PHE:CD1	1:B:1449:PHE:CE1	2.35	1.14
1:H:1375:TYR:CE2	1:O:1375:TYR:CD1	2.35	1.14
1:H:1375:TYR:CD2	1:O:1375:TYR:CE1	2.35	1.14
1:H:1375:TYR:CE1	1:O:1375:TYR:CE2	2.35	1.14
1:H:1449:PHE:CD1	1:O:1449:PHE:CD1	2.34	1.14
1:N:1449:PHE:CD2	1:Q:1449:PHE:CE2	2.35	1.14
1:A:1449:PHE:CE2	1:B:1449:PHE:CE2	2.35	1.14
1:H:1375:TYR:CD2	1:O:1375:TYR:CD1	2.35	1.14
1:N:1375:TYR:CE1	1:Q:1375:TYR:CD1	2.35	1.14
1:N:1449:PHE:CE1	1:Q:1449:PHE:CE1	2.35	1.14
1:A:1449:PHE:CD1	1:B:1449:PHE:CD1	2.35	1.14
1:H:803:LYS:CD	3:L:108:PRO:CA	2.26	1.14
1:N:1375:TYR:CE2	1:Q:1375:TYR:CD2	2.35	1.14
1:N:1449:PHE:CE1	1:Q:1449:PHE:CD1	2.35	1.14
1:A:803:LYS:CD	3:E:108:PRO:CA	2.26	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1449:PHE:CD2	1:O:1449:PHE:CD2	2.35	1.14
1:N:803:LYS:CE	3:T:108:PRO:CA	2.26	1.14
1:N:1375:TYR:CE2	1:Q:1375:TYR:CE2	2.35	1.14
1:A:1375:TYR:CD2	1:B:1375:TYR:CD1	2.35	1.13
1:A:1449:PHE:CE2	1:B:1449:PHE:CD2	2.35	1.13
1:H:803:LYS:CE	3:L:108:PRO:CB	2.26	1.13
1:H:1375:TYR:CE1	1:O:1375:TYR:CD2	2.35	1.13
1:H:1449:PHE:CE2	1:O:1449:PHE:CD2	2.35	1.13
1:H:1449:PHE:CD1	1:O:1449:PHE:CE1	2.35	1.13
1:N:803:LYS:CD	3:T:108:PRO:CA	2.26	1.13
1:A:803:LYS:CE	3:E:108:PRO:CB	2.26	1.13
1:H:803:LYS:CE	3:L:108:PRO:CA	2.25	1.13
1:N:1375:TYR:CD2	1:Q:1375:TYR:CE2	2.35	1.13
1:H:1375:TYR:CD1	1:O:1375:TYR:CE2	2.35	1.13
1:N:1375:TYR:CD2	1:Q:1375:TYR:CD2	2.35	1.13
1:A:1449:PHE:CE1	1:B:1449:PHE:CD1	2.35	1.13
1:H:1449:PHE:CE2	1:O:1449:PHE:CE2	2.35	1.13
1:A:1375:TYR:CE1	1:B:1375:TYR:CE2	2.35	1.12
1:H:1375:TYR:CE2	1:O:1375:TYR:CE1	2.35	1.12
1:H:803:LYS:CD	3:L:108:PRO:CG	2.27	1.12
1:N:803:LYS:CE	3:T:108:PRO:CB	2.28	1.11
1:N:803:LYS:CE	3:T:108:PRO:CG	2.28	1.11
1:A:803:LYS:CD	3:E:108:PRO:CG	2.27	1.11
1:N:803:LYS:CD	3:T:108:PRO:CB	2.28	1.10
1:A:803:LYS:CE	3:E:108:PRO:CD	2.28	1.10
1:N:803:LYS:CE	3:T:108:PRO:CD	2.29	1.10
1:N:803:LYS:CD	3:T:108:PRO:CD	2.29	1.10
1:A:803:LYS:CD	3:E:108:PRO:CB	2.30	1.09
1:H:803:LYS:CE	3:L:108:PRO:CD	2.28	1.09
1:H:803:LYS:CD	3:L:108:PRO:CB	2.29	1.09
1:N:803:LYS:CD	3:T:108:PRO:CG	2.30	1.09
1:A:803:LYS:CD	3:E:108:PRO:CD	2.31	1.08
1:H:803:LYS:CD	3:L:108:PRO:CD	2.31	1.08
1:H:803:LYS:CE	3:L:108:PRO:CG	2.30	1.08
1:A:803:LYS:CE	3:E:108:PRO:CG	2.30	1.08
1:N:803:LYS:CE	3:T:108:PRO:N	2.26	0.99
1:B:1375:TYR:CE2	1:B:1375:TYR:CD2	2.52	0.98
1:O:1375:TYR:CD2	1:O:1375:TYR:CE2	2.52	0.98
1:A:1375:TYR:CE2	1:A:1375:TYR:CD2	2.52	0.98
1:H:1375:TYR:CE2	1:H:1375:TYR:CD2	2.52	0.98
1:A:1449:PHE:CD1	1:A:1449:PHE:CE1	2.52	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1449:PHE:CD1	1:Q:1449:PHE:CE1	2.52	0.98
1:O:1449:PHE:CD1	1:O:1449:PHE:CE1	2.52	0.98
1:H:1449:PHE:CD2	1:H:1449:PHE:CE2	2.51	0.97
1:A:803:LYS:CE	3:E:108:PRO:N	2.27	0.97
1:N:1375:TYR:CE2	1:N:1375:TYR:CD2	2.52	0.97
1:Q:1375:TYR:CD1	1:Q:1375:TYR:CE1	2.51	0.97
1:B:1449:PHE:CD2	1:B:1449:PHE:CE2	2.51	0.97
1:N:803:LYS:HE2	3:T:108:PRO:CD	1.92	0.97
1:N:803:LYS:HE3	3:T:108:PRO:CA	1.93	0.97
1:N:803:LYS:HD3	3:T:108:PRO:CG	1.94	0.97
1:N:1449:PHE:CE2	1:N:1449:PHE:CD2	2.51	0.97
1:H:803:LYS:CE	3:L:108:PRO:N	2.28	0.96
1:H:803:LYS:CD	3:L:108:PRO:N	2.29	0.96
1:N:803:LYS:CD	3:T:108:PRO:N	2.29	0.96
1:A:803:LYS:CD	3:E:108:PRO:N	2.29	0.95
1:A:803:LYS:HD2	3:E:108:PRO:CD	1.97	0.95
1:H:803:LYS:HD2	3:L:108:PRO:CD	1.95	0.94
1:N:803:LYS:HD2	3:T:108:PRO:CB	1.96	0.93
1:A:803:LYS:HE3	3:E:108:PRO:CB	1.96	0.93
1:H:803:LYS:HE3	3:L:108:PRO:CB	1.98	0.91
1:A:803:LYS:HE2	3:E:108:PRO:N	1.90	0.86
1:H:803:LYS:HE2	3:L:108:PRO:N	1.90	0.83
1:H:803:LYS:HD3	3:L:108:PRO:CA	2.09	0.83
1:A:803:LYS:HD3	3:E:108:PRO:N	1.97	0.79
1:H:803:LYS:HE3	3:L:108:PRO:CA	2.13	0.78
1:A:803:LYS:HD3	3:E:108:PRO:CA	2.13	0.78
1:H:803:LYS:HD3	3:L:108:PRO:N	1.99	0.78
1:N:803:LYS:HD2	3:T:108:PRO:CA	2.17	0.74
1:A:803:LYS:HE3	3:E:108:PRO:CA	2.16	0.74
1:N:803:LYS:HE2	3:T:108:PRO:HD2	1.71	0.73
1:N:803:LYS:HE3	3:T:108:PRO:C	2.14	0.72
1:N:803:LYS:HD3	3:T:108:PRO:HG3	1.72	0.71
1:A:803:LYS:CG	3:E:108:PRO:HB3	2.21	0.70
1:A:803:LYS:HD2	3:E:108:PRO:CG	2.20	0.70
1:H:803:LYS:CG	3:L:108:PRO:HB3	2.21	0.70
1:H:803:LYS:CG	3:L:108:PRO:CB	2.69	0.70
1:A:803:LYS:CG	3:E:108:PRO:CB	2.70	0.69
1:H:803:LYS:HD2	3:L:108:PRO:HD3	1.75	0.67
1:A:803:LYS:HE3	3:E:108:PRO:HB2	1.75	0.67
1:A:803:LYS:HD2	3:E:108:PRO:HD3	1.77	0.67
1:H:803:LYS:HE3	3:L:108:PRO:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:803:LYS:HD2	3:T:108:PRO:HB3	1.76	0.63
1:H:803:LYS:HD2	3:L:108:PRO:CG	2.24	0.63
1:A:803:LYS:HE2	3:E:108:PRO:CA	2.30	0.61
1:N:803:LYS:CD	3:T:108:PRO:HA	2.30	0.60
1:H:803:LYS:NZ	3:L:108:PRO:CG	2.65	0.59
1:N:803:LYS:HD3	3:T:108:PRO:CD	2.27	0.58
1:A:803:LYS:NZ	3:E:108:PRO:CG	2.66	0.58
1:O:96:LEU:HD13	1:O:96:LEU:H	1.68	0.58
1:H:803:LYS:HE2	3:L:108:PRO:CA	2.32	0.57
1:N:803:LYS:NZ	3:T:108:PRO:CB	2.69	0.55
1:N:803:LYS:CG	3:T:108:PRO:N	2.69	0.55
1:H:803:LYS:HD3	3:L:108:PRO:HA	1.86	0.55
1:N:803:LYS:HE3	3:T:108:PRO:N	2.19	0.55
1:H:803:LYS:CD	3:L:108:PRO:HA	2.31	0.54
1:H:803:LYS:NZ	3:L:108:PRO:HG2	2.22	0.53
1:A:803:LYS:NZ	3:E:108:PRO:HG2	2.23	0.53
1:A:803:LYS:HG3	3:E:108:PRO:HB3	1.91	0.53
1:H:803:LYS:HE3	3:L:108:PRO:C	2.34	0.52
1:A:803:LYS:CD	3:E:108:PRO:HA	2.31	0.51
1:H:803:LYS:CE	3:L:108:PRO:C	2.84	0.50
1:A:1449:PHE:CD2	1:B:1449:PHE:HE2	2.22	0.50
1:A:1449:PHE:HD1	1:B:1449:PHE:CD1	2.22	0.49
1:H:1375:TYR:CE1	1:O:1375:TYR:HD2	2.22	0.49
1:N:803:LYS:NZ	3:T:108:PRO:HB2	2.27	0.49
1:H:1449:PHE:HD2	1:O:1449:PHE:CD2	2.22	0.49
1:A:803:LYS:HE3	3:E:108:PRO:C	2.38	0.49
1:H:1449:PHE:HE2	1:O:1449:PHE:CD2	2.22	0.48
1:A:803:LYS:CE	3:E:108:PRO:C	2.85	0.48
1:H:1375:TYR:HE2	1:O:1375:TYR:CD1	2.22	0.47
1:N:803:LYS:NZ	3:T:108:PRO:CG	2.76	0.47
1:A:1449:PHE:CE2	1:B:1449:PHE:HD2	2.23	0.47
1:N:1449:PHE:CD1	1:Q:1449:PHE:HD1	2.22	0.47
1:N:1449:PHE:HD2	1:Q:1449:PHE:CE2	2.22	0.47
1:H:1375:TYR:HE2	1:O:1375:TYR:CE1	2.23	0.47
1:H:803:LYS:CD	3:L:108:PRO:HG3	2.38	0.47
1:A:245:GLY:HA3	1:A:266:TYR:CD2	2.49	0.47
1:B:801:PHE:CE2	1:B:803:LYS:HE2	2.50	0.47
1:A:1375:TYR:CD1	1:B:1375:TYR:HD2	2.23	0.46
1:H:1449:PHE:CE1	1:O:1449:PHE:HD1	2.22	0.46
1:A:803:LYS:HD3	3:E:108:PRO:HA	1.90	0.46
1:H:1449:PHE:HE2	1:O:1449:PHE:CE2	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:508:TRP:CG	1:N:509:THR:H	2.33	0.46
1:H:1449:PHE:HD2	1:O:1449:PHE:CE2	2.22	0.45
1:H:1449:PHE:CD1	1:O:1449:PHE:HD1	2.22	0.45
1:N:1449:PHE:CE1	1:Q:1449:PHE:HD1	2.22	0.45
1:N:1375:TYR:HD2	1:Q:1375:TYR:CE2	2.22	0.45
1:N:1375:TYR:HE2	1:Q:1375:TYR:CE2	2.22	0.45
1:N:1449:PHE:CE1	1:Q:1449:PHE:HE1	2.23	0.44
1:A:1449:PHE:CD2	1:B:1449:PHE:HD2	2.22	0.44
1:N:1375:TYR:HE2	1:Q:1375:TYR:CD2	2.23	0.44
1:O:281:ARG:HH12	1:O:284:HIS:CE1	2.36	0.44
1:N:803:LYS:HE2	3:T:108:PRO:N	2.25	0.44
1:N:803:LYS:HG2	3:T:108:PRO:N	2.33	0.44
1:A:1449:PHE:CE2	1:B:1449:PHE:HE2	2.22	0.43
1:A:1375:TYR:HD2	1:B:1375:TYR:CD1	2.22	0.43
1:A:803:LYS:NZ	3:E:108:PRO:CD	2.82	0.43
1:H:803:LYS:HG3	3:L:108:PRO:HB3	1.97	0.43
1:H:1375:TYR:CD1	1:O:1375:TYR:HD2	2.22	0.43
1:N:1375:TYR:CE1	1:Q:1375:TYR:HD1	2.22	0.43
1:A:1449:PHE:HE1	1:B:1449:PHE:CE1	2.23	0.43
1:B:450:LYS:C	1:B:452:PRO:HD3	2.45	0.42
3:T:10:ILE:HG22	3:T:11:GLU:H	1.85	0.42
1:O:706:ARG:HG3	1:O:707:LYS:H	1.84	0.42
1:N:1449:PHE:HE2	1:Q:1449:PHE:CE2	2.22	0.42
1:N:1449:PHE:CD1	1:Q:1449:PHE:HE1	2.22	0.41
1:O:1644:LYS:HE2	1:O:1644:LYS:HA	2.01	0.41
1:A:1449:PHE:HD1	1:B:1449:PHE:CE1	2.22	0.41
1:N:1375:TYR:CE1	1:Q:1375:TYR:HE1	2.23	0.41
1:N:803:LYS:CD	3:T:108:PRO:HD3	2.40	0.41
1:N:1375:TYR:CD1	1:Q:1375:TYR:HD1	2.22	0.41
1:H:1375:TYR:HD2	1:O:1375:TYR:CE1	2.23	0.41
1:A:803:LYS:CD	3:E:108:PRO:HG3	2.38	0.41
1:N:803:LYS:CE	1:N:803:LYS:CD	3.00	0.40
1:A:803:LYS:CE	1:A:803:LYS:CD	2.99	0.40
1:N:803:LYS:CE	3:T:108:PRO:HG2	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1924/1935 (99%)	1836 (95%)	75 (4%)	13 (1%)	18	56
1	B	1924/1935 (99%)	1810 (94%)	98 (5%)	16 (1%)	16	54
1	H	1928/1935 (100%)	1834 (95%)	78 (4%)	16 (1%)	16	54
1	N	1928/1935 (100%)	1854 (96%)	62 (3%)	12 (1%)	21	59
1	O	1924/1935 (99%)	1825 (95%)	86 (4%)	13 (1%)	18	56
1	Q	1924/1935 (99%)	1827 (95%)	81 (4%)	16 (1%)	16	54
2	C	150/152 (99%)	140 (93%)	6 (4%)	4 (3%)	4	25
2	D	150/152 (99%)	138 (92%)	8 (5%)	4 (3%)	4	25
2	J	150/152 (99%)	138 (92%)	10 (7%)	2 (1%)	9	42
2	K	150/152 (99%)	138 (92%)	12 (8%)	0	100	100
2	R	150/152 (99%)	133 (89%)	16 (11%)	1 (1%)	18	56
2	S	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	6	31
3	E	158/160 (99%)	139 (88%)	14 (9%)	5 (3%)	3	21
3	F	158/160 (99%)	134 (85%)	19 (12%)	5 (3%)	3	21
3	L	158/160 (99%)	141 (89%)	14 (9%)	3 (2%)	6	32
3	M	158/160 (99%)	137 (87%)	19 (12%)	2 (1%)	9	42
3	T	158/160 (99%)	138 (87%)	17 (11%)	3 (2%)	6	32
3	U	158/160 (99%)	139 (88%)	13 (8%)	6 (4%)	2	19
4	G	398/400 (100%)	371 (93%)	25 (6%)	2 (0%)	24	63
4	V	398/400 (100%)	376 (94%)	15 (4%)	7 (2%)	6	34
5	I	1077/1079 (100%)	1036 (96%)	35 (3%)	6 (1%)	21	59
5	P	1077/1079 (100%)	1035 (96%)	40 (4%)	2 (0%)	43	78
All	All	16350/16440 (100%)	15455 (94%)	754 (5%)	141 (1%)	16	51

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	VAL
1	B	451	GLN
3	E	163	GLU
3	F	92	GLY
1	N	575	ALA
1	O	210	THR
5	P	440	PRO
1	Q	211	PRO
4	V	18	ASP
1	A	238	ASN
1	A	455	TYR
1	A	785	ILE
1	B	15	PHE
1	B	128	TYR
1	B	566	PRO
2	D	176	GLN
3	E	59	VAL
3	E	147	THR
1	H	274	ILE
1	H	642	SER
3	L	59	VAL
1	N	603	GLU
1	O	624	TYR
1	O	640	LYS
1	O	803	LYS
1	Q	86	LYS
1	Q	1476	SER
2	R	95	VAL
2	S	67	GLY
3	T	108	PRO
3	T	146	VAL
3	U	16	ASN
4	V	10	HIS
4	V	247	TRP
1	A	322	SER
1	B	273	VAL
1	B	639	LYS
2	C	100	LYS
1	H	455	TYR
1	H	738	SER
1	H	750	ASP
1	H	829	TRP
5	I	901	LEU

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Mol	Chain	Res	Type
5	I	1286	GLU
5	I	1305	LYS
5	I	1306	SER
2	J	163	ARG
1	N	45	GLU
1	N	232	ASN
1	N	367	LYS
1	N	679	LYS
1	O	532	SER
1	O	614	LEU
1	O	713	ILE
1	Q	614	LEU
2	S	163	ARG
3	T	145	ASP
3	U	23	GLN
3	U	96	GLU
4	V	103	LEU
4	V	149	LEU
4	V	300	ILE
4	V	332	ASN
1	A	114	ILE
1	A	277	LEU
1	A	282	ASP
1	A	364	PHE
1	A	396	LEU
1	A	558	GLY
1	A	1476	SER
1	B	86	LYS
1	B	643	SER
2	C	101	GLN
2	C	163	ARG
2	D	106	SER
2	D	172	LEU
3	F	57	GLY
4	G	10	HIS
1	H	45	GLU
1	H	378	THR
1	H	603	GLU
1	H	729	ALA
5	I	321	ARG
2	J	107	LYS
3	L	33	PHE

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Mol	Chain	Res	Type
3	M	20	MET
1	N	644	PHE
1	O	315	GLN
5	P	704	ALA
1	Q	315	GLN
1	Q	560	SER
1	Q	640	LYS
1	Q	644	PHE
1	B	32	ASP
1	B	34	LYS
1	B	293	LYS
1	B	371	GLU
1	B	603	GLU
1	B	751	ILE
1	H	28	THR
1	H	83	LYS
1	H	316	GLY
1	H	379	GLU
3	M	58	ARG
1	N	637	LYS
1	O	96	LEU
1	Q	256	GLY
1	Q	723	ARG
1	Q	803	LYS
1	A	207	LYS
1	B	599	ASP
2	D	175	GLY
3	E	19	SER
3	E	108	PRO
1	H	10	GLY
1	H	372	GLN
3	L	108	PRO
1	N	57	GLY
1	N	835	LYS
1	O	726	ASN
1	Q	768	GLY
3	U	143	PRO
2	C	98	LYS
3	F	156	VAL
4	G	102	ILE
1	Q	452	PRO
1	Q	824	VAL

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Mol	Chain	Res	Type
3	U	94	ASP
3	F	94	ASP
3	F	146	VAL
5	I	999	GLU
2	S	86	ASN
1	N	785	ILE
1	O	629	ALA
1	O	641	GLY
1	Q	569	VAL
3	U	95	PRO
1	B	127	PRO
1	N	634	GLY
1	O	751	ILE
1	Q	828	PRO

5.3.2 Protein sidechains ⓘ

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	1688/1693 (100%)	1672 (99%)	16 (1%)	70	79
1	B	1688/1693 (100%)	1661 (98%)	27 (2%)	55	70
1	H	1690/1693 (100%)	1663 (98%)	27 (2%)	55	70
1	N	1690/1693 (100%)	1665 (98%)	25 (2%)	57	72
1	O	1688/1693 (100%)	1677 (99%)	11 (1%)	76	81
1	Q	1688/1693 (100%)	1667 (99%)	21 (1%)	63	75
2	C	131/131 (100%)	129 (98%)	2 (2%)	57	72
2	D	131/131 (100%)	128 (98%)	3 (2%)	44	64
2	J	131/131 (100%)	128 (98%)	3 (2%)	44	64
2	K	131/131 (100%)	127 (97%)	4 (3%)	35	56
2	R	131/131 (100%)	128 (98%)	3 (2%)	44	64
2	S	131/131 (100%)	128 (98%)	3 (2%)	44	64
3	E	139/139 (100%)	137 (99%)	2 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	139/139 (100%)	139 (100%)	0	100	100
3	L	139/139 (100%)	135 (97%)	4 (3%)	37	58
3	M	139/139 (100%)	138 (99%)	1 (1%)	76	81
3	T	139/139 (100%)	135 (97%)	4 (3%)	37	58
3	U	139/139 (100%)	137 (99%)	2 (1%)	59	72
4	G	344/344 (100%)	342 (99%)	2 (1%)	78	83
4	V	344/344 (100%)	339 (98%)	5 (2%)	57	72
5	I	928/928 (100%)	922 (99%)	6 (1%)	78	83
5	P	928/928 (100%)	916 (99%)	12 (1%)	61	74
All	All	14296/14322 (100%)	14113 (99%)	183 (1%)	59	74

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	239	ASP
1	A	243	ARG
1	A	315	GLN
1	A	363	LYS
1	A	504	GLU
1	A	518	GLN
1	A	635	LYS
1	A	732	GLU
1	A	791	GLN
1	A	814	ILE
1	A	826	ASN
1	A	952	ARG
1	A	1083	LYS
1	A	1446	GLN
1	A	1715	LEU
1	B	113	MET
1	B	185	THR
1	B	194	TYR
1	B	210	THR
1	B	276	GLN
1	B	346	LYS
1	B	349	ILE
1	B	368	GLN
1	B	418	GLN

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Mol	Chain	Res	Type
1	B	506	ILE
1	B	534	LEU
1	B	559	LYS
1	B	572	LYS
1	B	615	LYS
1	B	616	LEU
1	B	723	ARG
1	B	829	TRP
1	B	869	ARG
1	B	906	ASP
1	B	952	ARG
1	B	1001	GLU
1	B	1048	LEU
1	B	1098	GLN
1	B	1103	GLN
1	B	1184	GLN
1	B	1411	CYS
1	B	1499	LYS
2	C	63	ARG
2	C	148	VAL
2	D	55	LYS
2	D	63	ARG
2	D	129	THR
3	E	164	GLU
3	E	165	LYS
4	G	159	SER
4	G	325	ARG
1	H	43	LYS
1	H	87	ILE
1	H	171	ASN
1	H	172	GLN
1	H	193	GLN
1	H	206	LYS
1	H	213	LYS
1	H	224	ASN
1	H	232	ASN
1	H	276	GLN
1	H	325	ASP
1	H	408	ASN
1	H	424	ILE
1	H	448	GLU
1	H	450	LYS

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Mol	Chain	Res	Type
1	H	570	LYS
1	H	603	GLU
1	H	719	ARG
1	H	726	ASN
1	H	751	ILE
1	H	777	ARG
1	H	781	LEU
1	H	786	THR
1	H	845	THR
1	H	870	ARG
1	H	1109	LYS
1	H	1833	ASN
5	I	485	THR
5	I	665	ARG
5	I	862	THR
5	I	874	THR
5	I	934	LYS
5	I	1304	THR
2	J	129	THR
2	J	137	LEU
2	J	185	TYR
2	K	51	ILE
2	K	119	GLN
2	K	129	THR
2	K	167	ASP
3	L	91	LYS
3	L	106	PHE
3	L	142	PHE
3	L	151	ASP
3	M	10	ILE
1	N	28	THR
1	N	72	LYS
1	N	79	GLN
1	N	87	ILE
1	N	172	GLN
1	N	204	ARG
1	N	213	LYS
1	N	240	ASN
1	N	308	TYR
1	N	309	ASP
1	N	380	GLU
1	N	419	GLN

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Mol	Chain	Res	Type
1	N	424	ILE
1	N	453	ARG
1	N	476	LEU
1	N	542	LYS
1	N	603	GLU
1	N	611	LYS
1	N	726	ASN
1	N	784	ILE
1	N	845	THR
1	N	870	ARG
1	N	1575	LYS
1	N	1646	LEU
1	N	1809	LYS
1	O	96	LEU
1	O	139	VAL
1	O	244	PHE
1	O	394	ASP
1	O	498	GLN
1	O	542	LYS
1	O	628	ASP
1	O	766	LYS
1	O	847	LYS
1	O	911	ASN
1	O	1706	LEU
5	P	320	THR
5	P	440	PRO
5	P	651	ILE
5	P	676	SER
5	P	874	THR
5	P	937	ASN
5	P	948	LYS
5	P	960	ASN
5	P	1054	LYS
5	P	1160	LYS
5	P	1287	TYR
5	P	1342	ASN
1	Q	20	GLU
1	Q	80	ASN
1	Q	146	LYS
1	Q	203	ASP
1	Q	207	LYS
1	Q	211	PRO

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Mol	Chain	Res	Type
1	Q	278	LYS
1	Q	433	GLU
1	Q	504	GLU
1	Q	524	ILE
1	Q	596	LYS
1	Q	635	LYS
1	Q	653	GLU
1	Q	679	LYS
1	Q	724	ILE
1	Q	734	GLN
1	Q	853	LYS
1	Q	968	LYS
1	Q	1262	LYS
1	Q	1392	LYS
1	Q	1694	GLN
2	R	102	GLU
2	R	172	LEU
2	R	191	HIS
2	S	63	ARG
2	S	66	LYS
2	S	101	GLN
3	T	10	ILE
3	T	23	GLN
3	T	46	LYS
3	T	155	LEU
3	U	46	LYS
3	U	58	ARG
4	V	157	ARG
4	V	241	ASP
4	V	283	SER
4	V	290	LYS
4	V	325	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (196) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	209	GLN
1	A	222	GLN
1	A	454	GLN
1	A	482	ASN
1	A	487	GLN

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Mol	Chain	Res	Type
1	A	490	ASN
1	A	661	ASN
1	A	817	ASN
1	A	897	ASN
1	A	1160	GLN
1	A	1164	ASN
1	A	1255	GLN
1	A	1267	GLN
1	A	1271	ASN
1	A	1276	GLN
1	A	1346	GLN
1	A	1422	GLN
1	A	1664	ASN
1	A	1678	ASN
1	A	1726	GLN
1	B	172	GLN
1	B	305	ASN
1	B	306	ASN
1	B	315	GLN
1	B	368	GLN
1	B	372	GLN
1	B	391	ASN
1	B	418	GLN
1	B	486	GLN
1	B	602	ASN
1	B	645	GLN
1	B	696	ASN
1	B	815	GLN
1	B	911	ASN
1	B	1160	GLN
1	B	1267	GLN
1	B	1271	ASN
1	B	1502	ASN
1	B	1562	GLN
1	B	1628	GLN
1	B	1664	ASN
1	B	1720	ASN
1	B	1746	GLN
1	B	1750	ASN
2	D	101	GLN
2	D	176	GLN
4	G	45	GLN

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Mol	Chain	Res	Type
4	G	119	GLN
4	G	139	GLN
4	G	253	HIS
4	G	324	ASN
4	G	398	GLN
1	H	97	HIS
1	H	104	ASN
1	H	240	ASN
1	H	276	GLN
1	H	315	GLN
1	H	368	GLN
1	H	401	HIS
1	H	418	GLN
1	H	451	GLN
1	H	486	GLN
1	H	490	ASN
1	H	491	HIS
1	H	518	GLN
1	H	555	ASN
1	H	556	HIS
1	H	564	GLN
1	H	589	ASN
1	H	651	HIS
1	H	686	ASN
1	H	692	GLN
1	H	696	ASN
1	H	755	GLN
1	H	888	GLN
1	H	892	GLN
1	H	1003	HIS
1	H	1160	GLN
1	H	1164	ASN
1	H	1209	ASN
1	H	1259	HIS
1	H	1464	GLN
1	H	1628	GLN
1	H	1647	GLN
1	H	1720	ASN
1	H	1746	GLN
1	H	1750	ASN
1	H	1802	GLN
1	H	1811	GLN

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Mol	Chain	Res	Type
1	H	1833	ASN
5	I	390	ASN
5	I	575	ASN
5	I	602	ASN
5	I	764	GLN
5	I	776	ASN
5	I	1244	GLN
2	J	101	GLN
2	K	119	GLN
2	K	120	HIS
3	L	60	ASN
3	M	16	ASN
3	M	137	GLN
1	N	219	GLN
1	N	306	ASN
1	N	401	HIS
1	N	419	GLN
1	N	471	ASN
1	N	482	ASN
1	N	486	GLN
1	N	589	ASN
1	N	623	ASN
1	N	666	HIS
1	N	676	ASN
1	N	696	ASN
1	N	711	ASN
1	N	817	ASN
1	N	933	ASN
1	N	1003	HIS
1	N	1164	ASN
1	N	1185	HIS
1	N	1338	HIS
1	N	1773	GLN
1	O	79	GLN
1	O	135	ASN
1	O	187	ASN
1	O	209	GLN
1	O	251	HIS
1	O	415	GLN
1	O	418	GLN
1	O	419	GLN
1	O	454	GLN

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Mol	Chain	Res	Type
1	O	475	GLN
1	O	482	ASN
1	O	490	ASN
1	O	589	ASN
1	O	692	GLN
1	O	696	ASN
1	O	760	HIS
1	O	817	ASN
1	O	826	ASN
1	O	933	ASN
1	O	1003	HIS
1	O	1040	GLN
1	O	1164	ASN
1	O	1338	HIS
1	O	1358	GLN
1	O	1395	GLN
1	O	1464	GLN
1	O	1609	ASN
1	O	1633	ASN
1	O	1670	ASN
5	P	451	ASN
5	P	556	GLN
5	P	559	ASN
5	P	776	ASN
5	P	897	ASN
5	P	937	ASN
5	P	1110	ASN
5	P	1244	GLN
5	P	1302	HIS
1	Q	79	GLN
1	Q	172	GLN
1	Q	232	ASN
1	Q	292	ASN
1	Q	305	ASN
1	Q	391	ASN
1	Q	562	ASN
1	Q	666	HIS
1	Q	668	HIS
1	Q	691	HIS
1	Q	711	ASN
1	Q	720	GLN
1	Q	933	ASN

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Mol	Chain	Res	Type
1	Q	1071	ASN
1	Q	1075	GLN
1	Q	1112	GLN
1	Q	1255	GLN
1	Q	1541	GLN
1	Q	1590	HIS
1	Q	1656	GLN
1	Q	1664	ASN
1	Q	1694	GLN
1	Q	1719	GLN
1	Q	1813	GLN
1	Q	1916	GLN
2	S	191	HIS
3	T	23	GLN
3	U	27	GLN
4	V	45	GLN
4	V	83	ASN
4	V	116	GLN
4	V	119	GLN
4	V	196	GLN
4	V	229	ASN
4	V	278	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

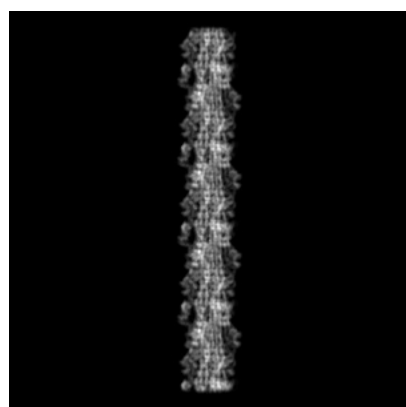
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18198. These allow visual inspection of the internal detail of the map and identification of artifacts.

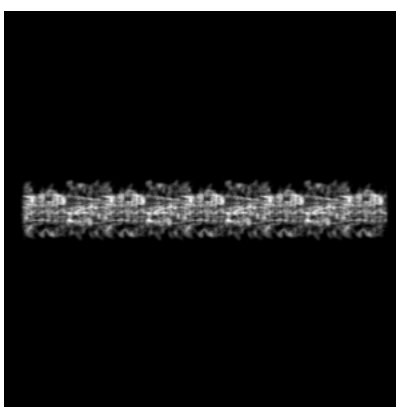
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

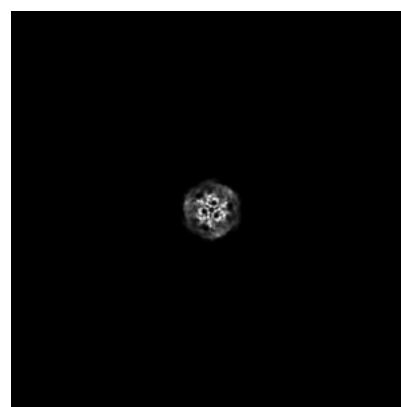
6.1.1 Primary map



X



Y

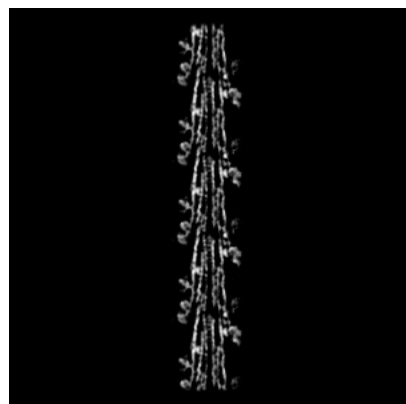


Z

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

6.2 Central slices [i](#)

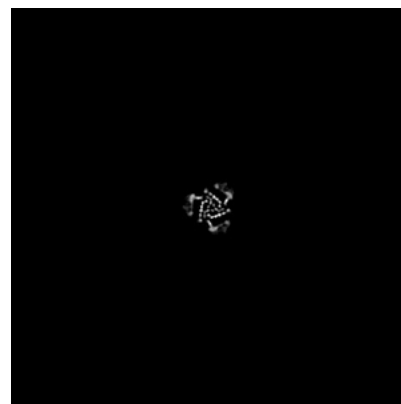
6.2.1 Primary map



X Index: 186



Y Index: 186



Z Index: 186

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: 183



Y Index: 193

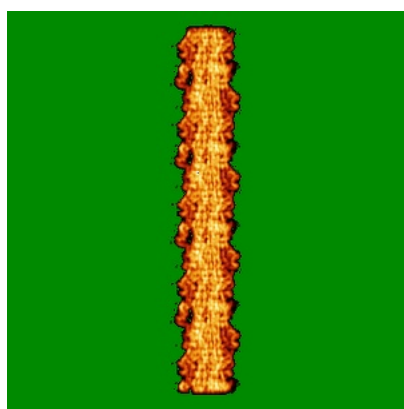


Z Index: 172

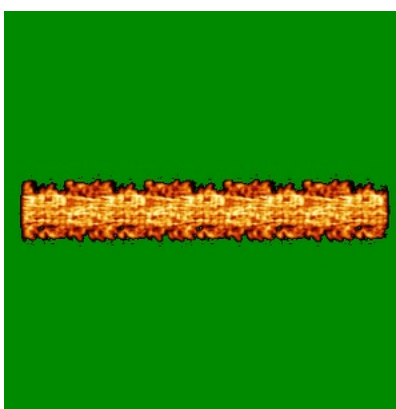
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y

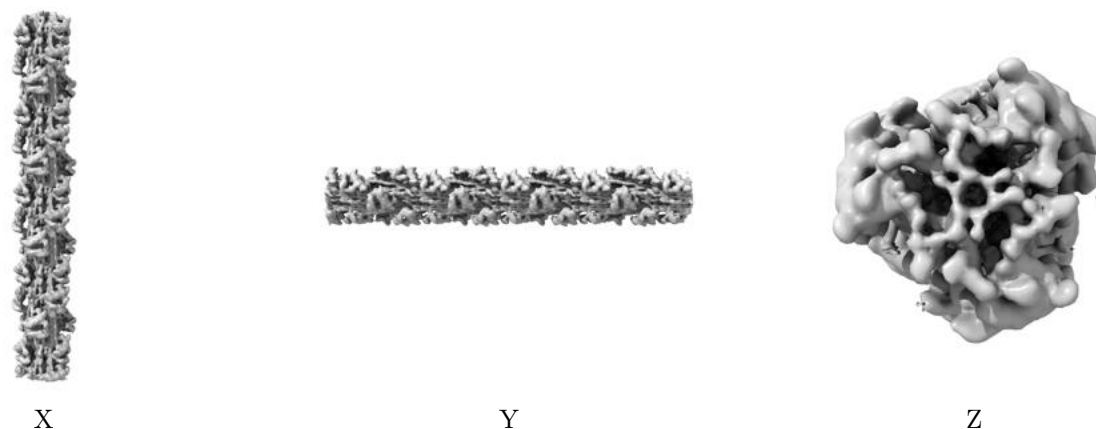


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.41. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

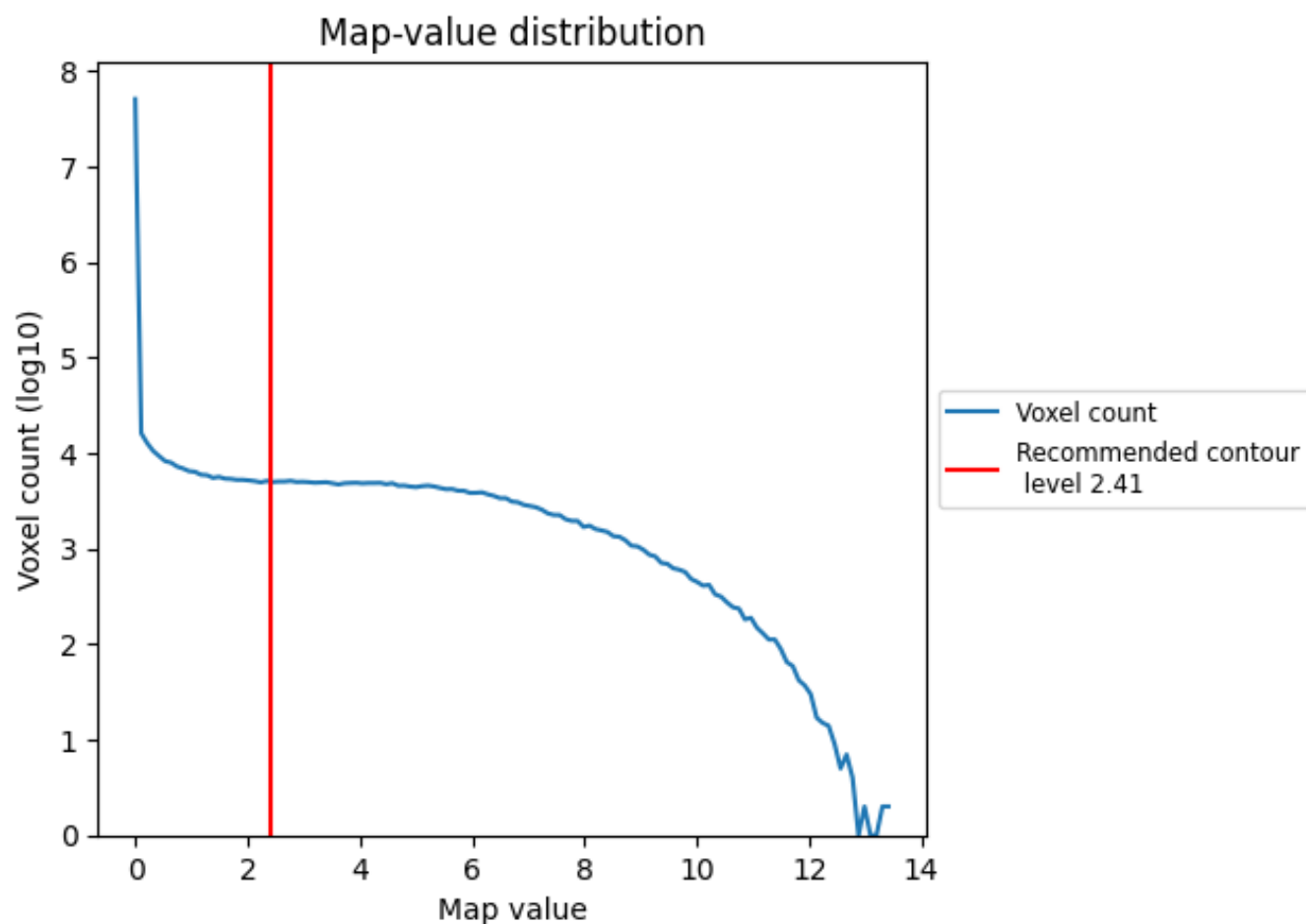
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

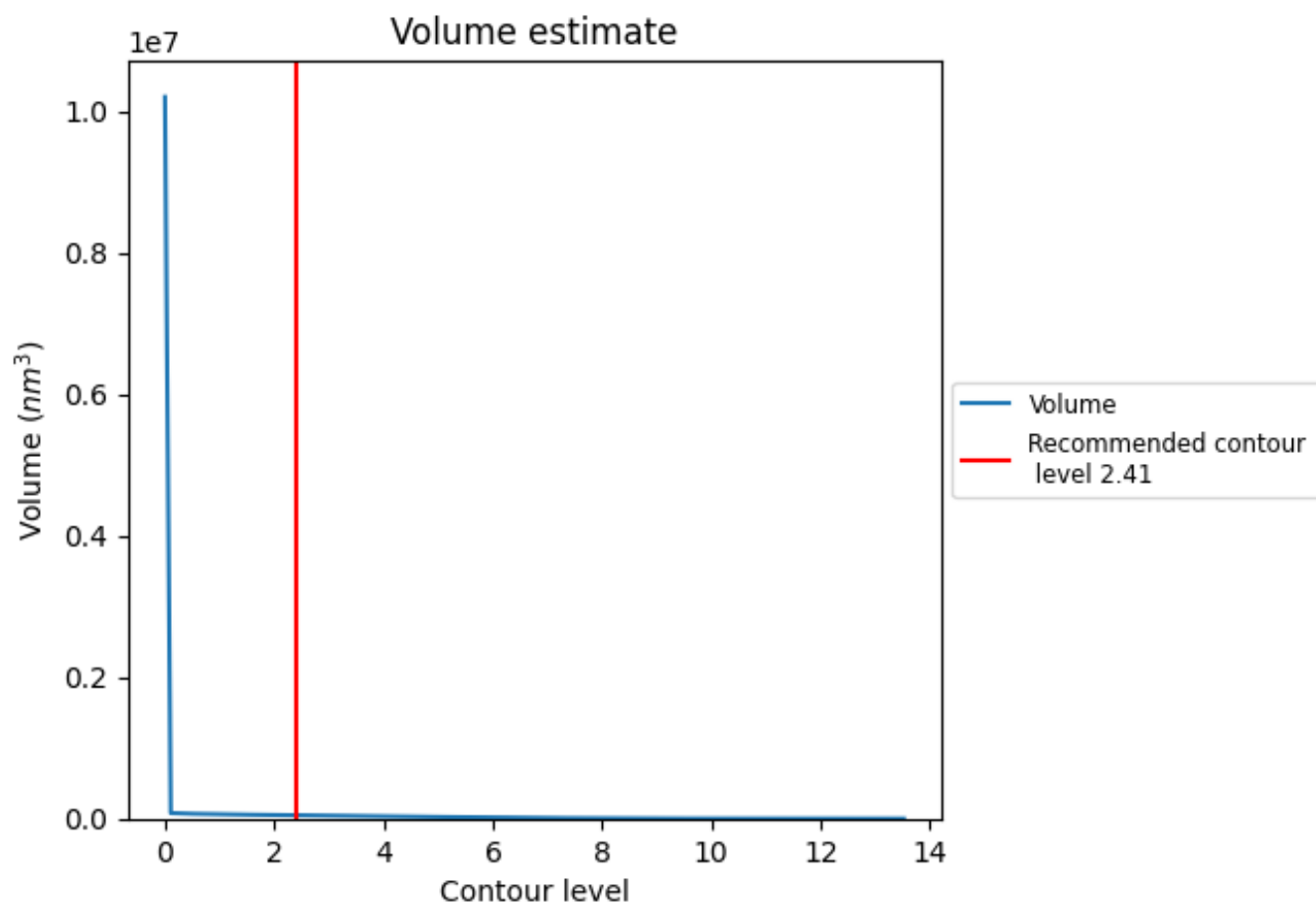
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

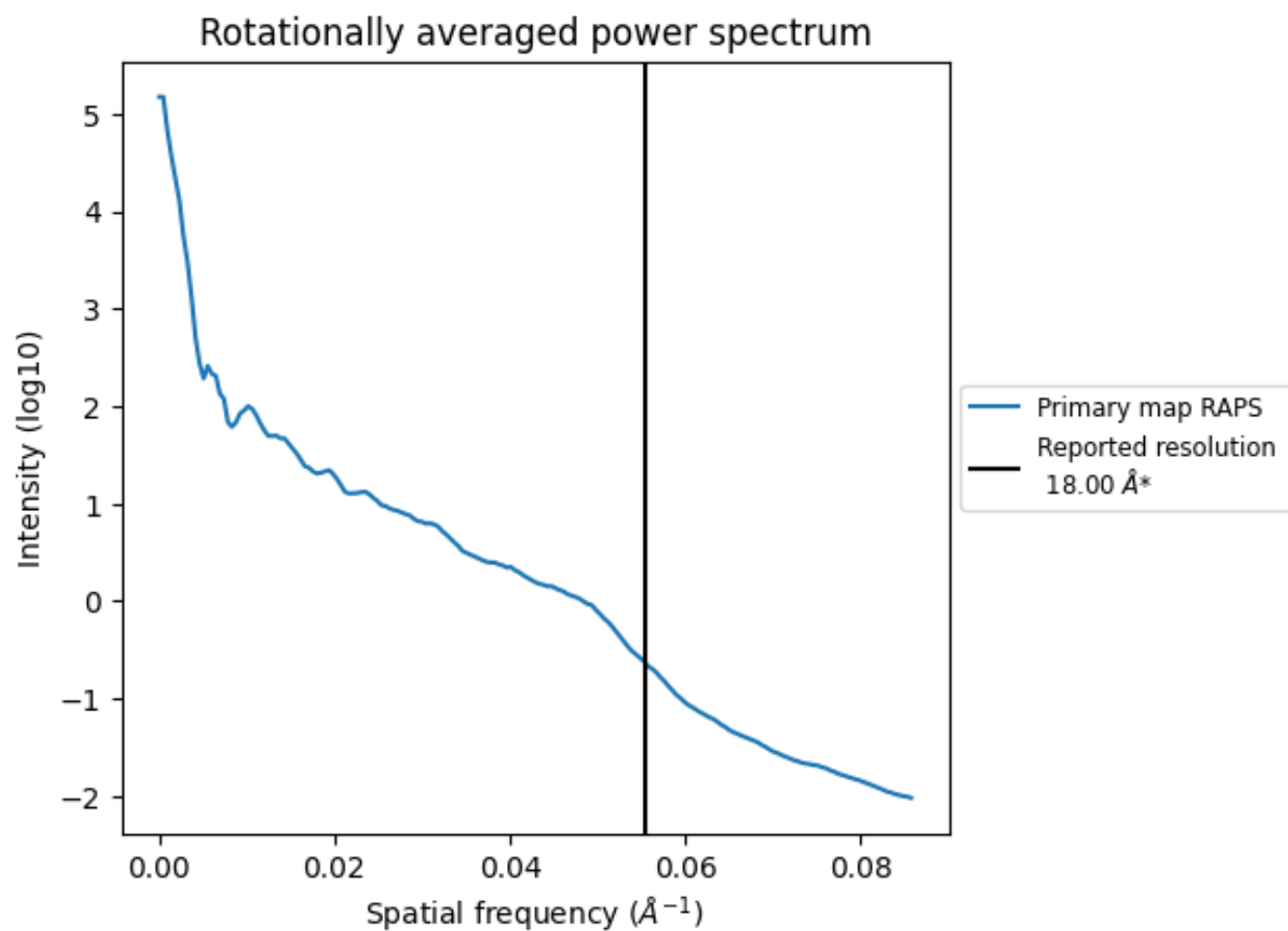
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47100 nm³; this corresponds to an approximate mass of 42547 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.056 $\text{\AA}^{-1}$

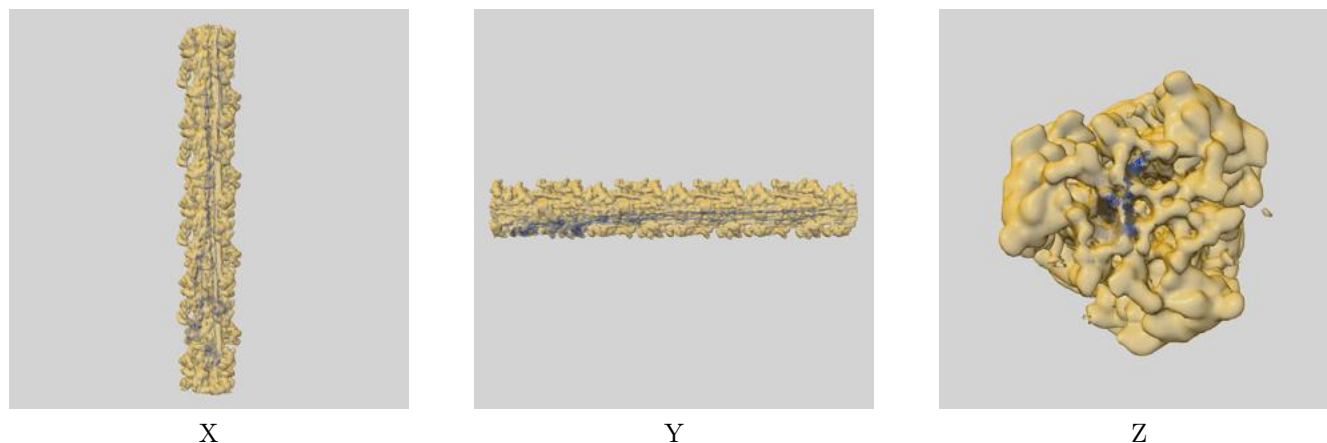
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

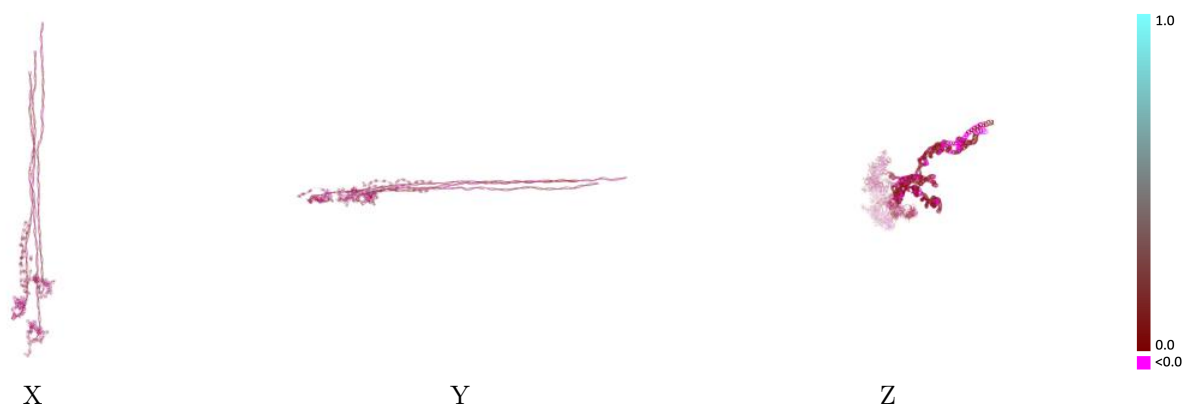
This section contains information regarding the fit between EMDB map EMD-18198 and PDB model 8Q6T. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.41 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



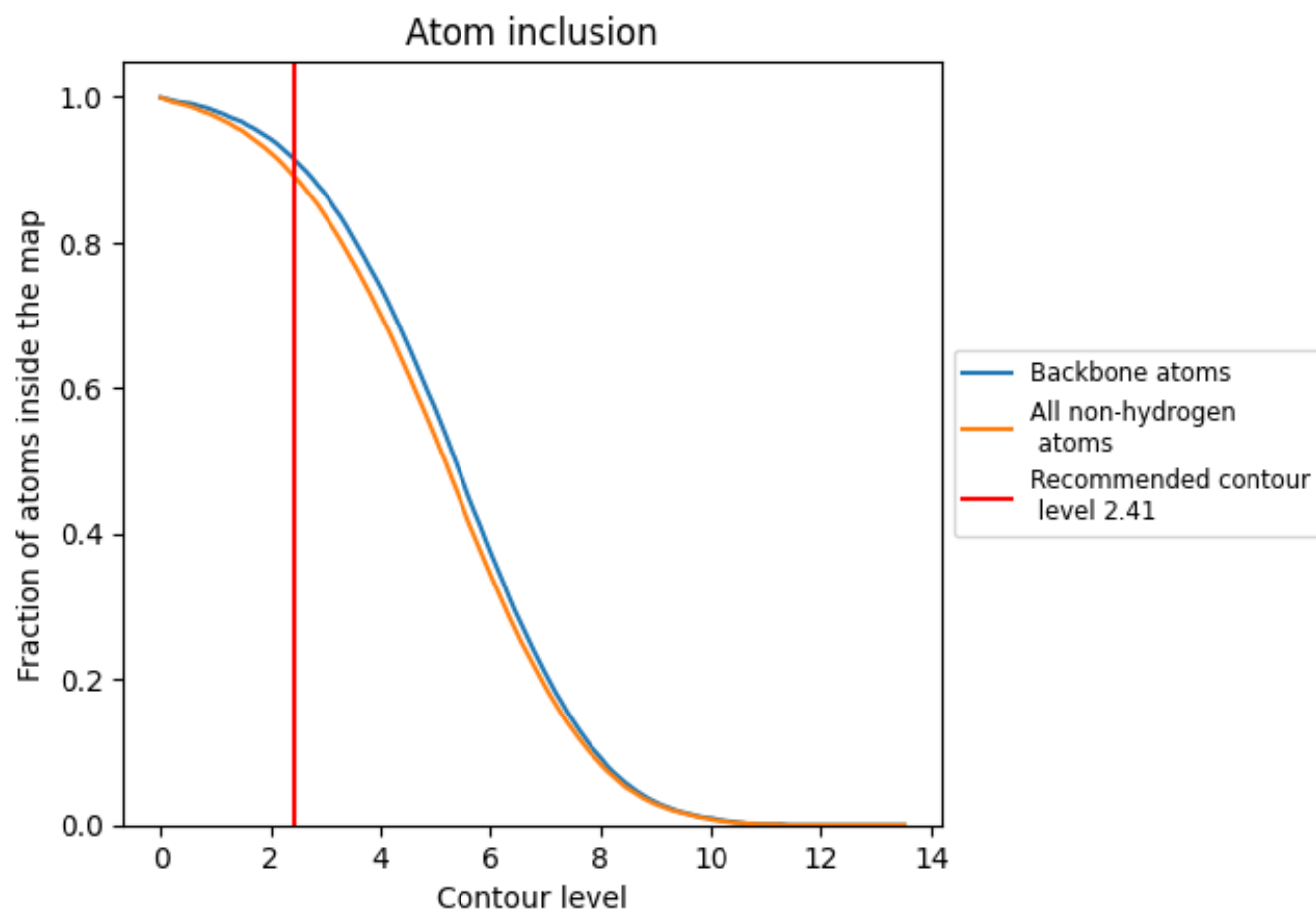
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.41).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.41) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.0550
A	 0.8380	 0.0420
B	 0.8820	 0.0590
C	 0.5730	 0.0040
D	 0.8670	 0.0430
E	 0.8080	 0.0530
F	 0.8500	 0.0410
G	 0.9600	 0.0610
H	 0.8710	 0.0510
I	 0.9420	 0.0680
J	 0.9500	 0.0640
K	 0.9330	 0.0520
L	 0.8900	 0.0630
M	 0.9450	 0.0530
N	 0.9010	 0.0590
O	 0.8910	 0.0600
P	 0.9560	 0.0580
Q	 0.9050	 0.0540
R	 0.9400	 0.0630
S	 0.8980	 0.0540
T	 0.8570	 0.0330
U	 0.9690	 0.0600
V	 0.9470	 0.0550

