



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:57 PM UTC

PDB ID : 7NEP / pdb_00007nep
EMDB ID : EMD-12289
Title : Homology model of the in situ actomyosin complex from the A-band of mouse
psoas muscle sarcomere in the rigor state
Authors : Wang, Z.; Grange, M.; Wagner, T.; Kho, A.L.; Gautel, M.; Raunser, S.
Deposited on : 2021-02-04
Resolution : 10.20 Å (reported)
Based on initial models : 5JLH, 6KN8, 3I5G

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:

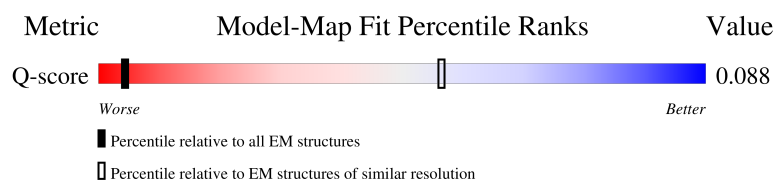
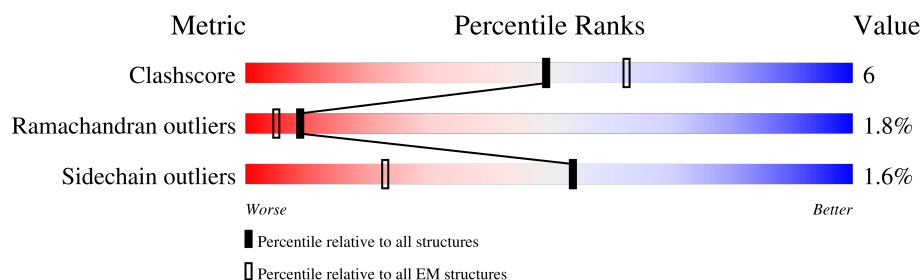
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 10.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	119 (9.70 - 10.70)

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	374	50% 86% 13% .
1	B	374	50% 88% 10% .
1	C	374	48% 83% 16% .
1	D	374	48% 83% 16% .

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Mol	Chain	Length	Quality of chain
1	E	374	42% 82% 16% .
1	F	374	45% 80% 18% .
1	G	374	47% 86% 12% .
1	H	374	56% 84% 14% .
1	I	374	46% 83% 15% .
1	J	374	67% 83% 15% .
1	K	374	53% 84% 13% .
2	P	251	10% 67% 22% . 7%
2	Q	251	9% 66% 22% . 7%
2	T	251	6% 71% 21% . .
2	U	251	12% 71% 23% . .
3	L	813	43% 90% 9% .
3	M	813	47% 90% 9% .
4	N	148	42% 87% 13%
4	O	148	36% 86% 14%
5	R	144	98% 84% 13% ..
5	S	144	91% 84% 13% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 57453 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, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	B	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	C	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	D	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	E	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	F	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	G	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	H	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	I	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	J	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
1	K	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	233	Total	C	N	O	S	0	0
			1881	1149	319	410	3		
2	Q	233	Total	C	N	O	S	0	0
			1881	1149	319	410	3		
2	T	243	Total	C	N	O	S	0	0
			1952	1190	336	423	3		
2	U	243	Total	C	N	O	S	0	0
			1952	1190	336	423	3		

- Molecule 3 is a protein called Myosin-4.

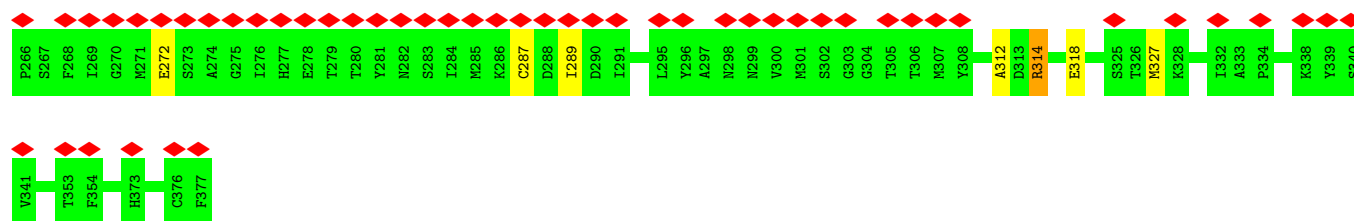
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	813	Total	C	N	O	S	0	0
			6503	4167	1094	1205	37		
3	M	813	Total	C	N	O	S	0	0
			6503	4167	1094	1205	37		

- Molecule 4 is a protein called Myosin light chain 1/3, skeletal muscle isoform.

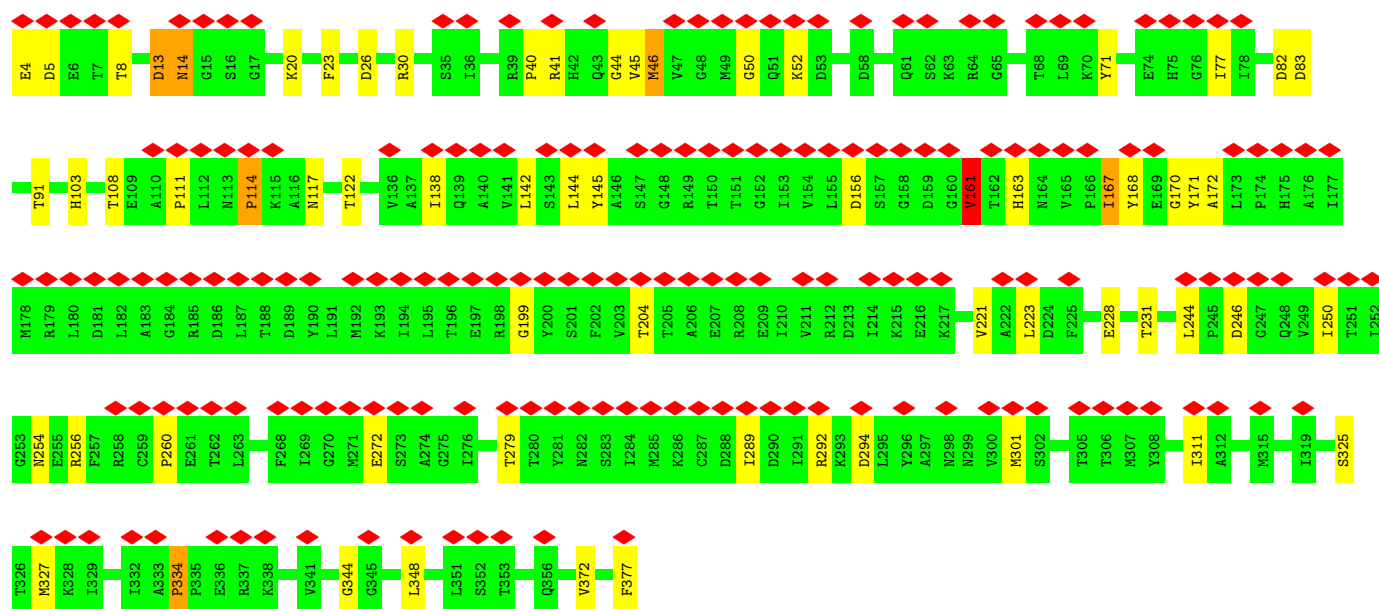
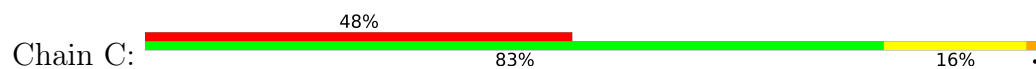
Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	148	Total	C	N	O	S	0	0
			1159	722	193	236	8		
4	O	148	Total	C	N	O	S	0	0
			1159	722	193	236	8		

- Molecule 5 is a protein called Myosin regulatory light chain 2, skeletal muscle isoform.

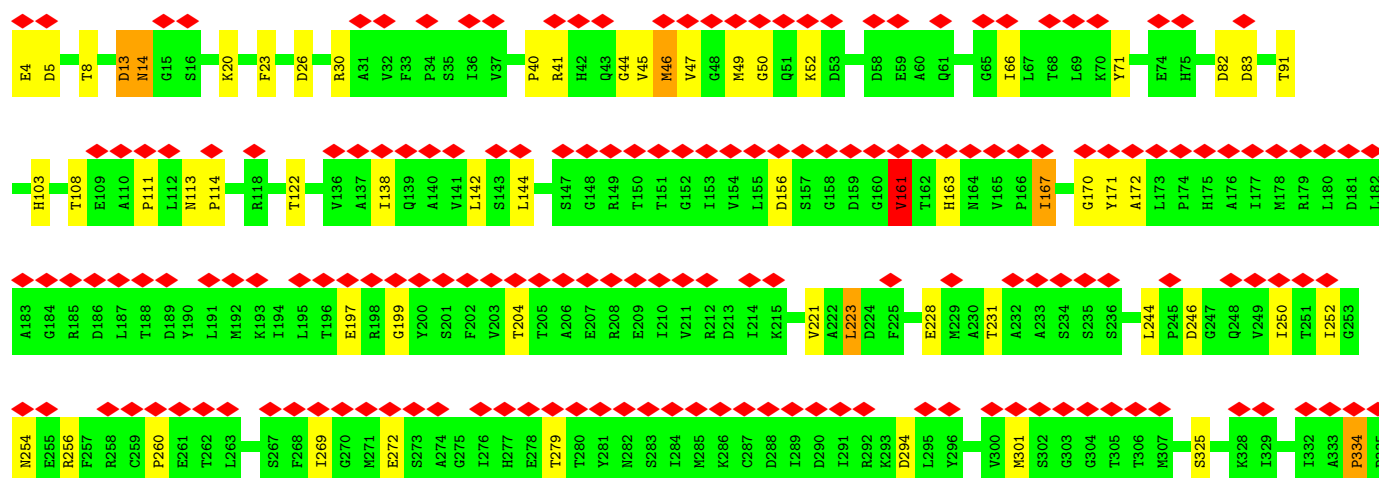
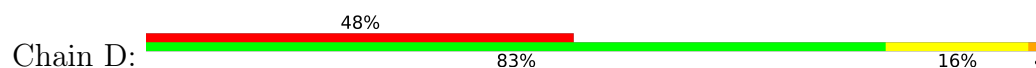
Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	144	Total	C	N	O	S	0	0
			1144	724	185	227	8		
5	S	144	Total	C	N	O	S	0	0
			1144	724	185	227	8		

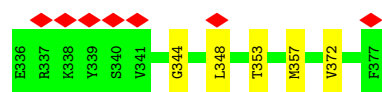


- Molecule 1: Actin, alpha skeletal muscle

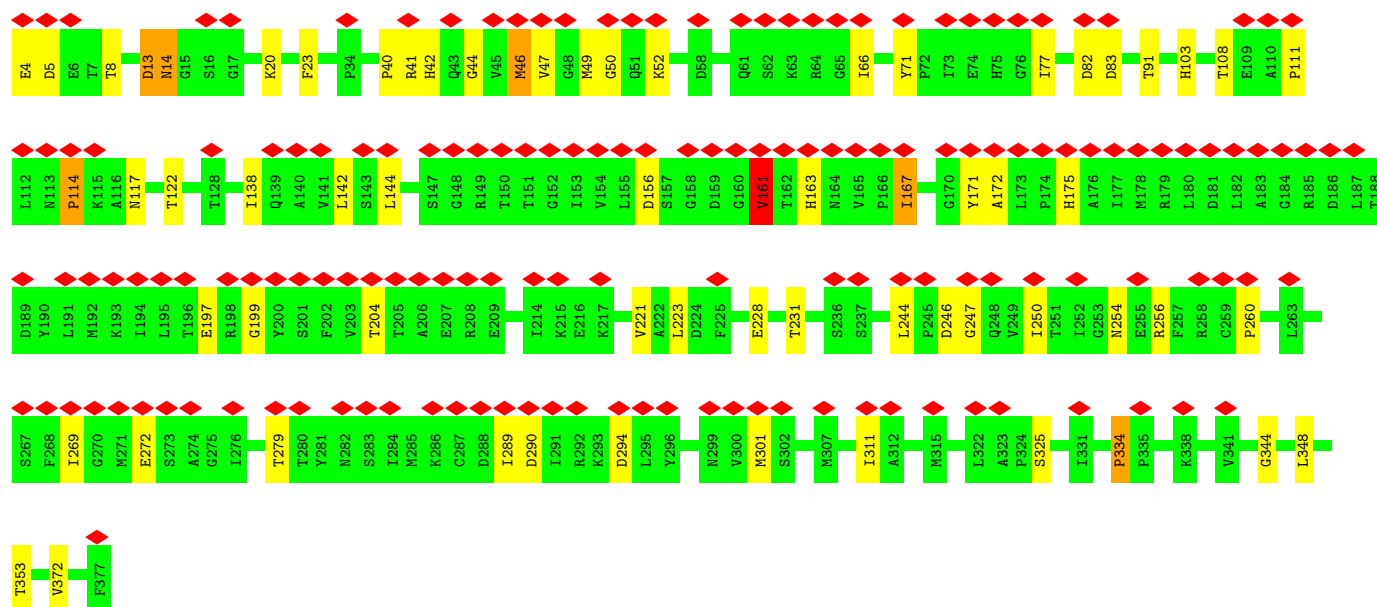
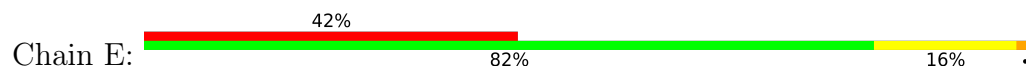


- Molecule 1: Actin, alpha skeletal muscle

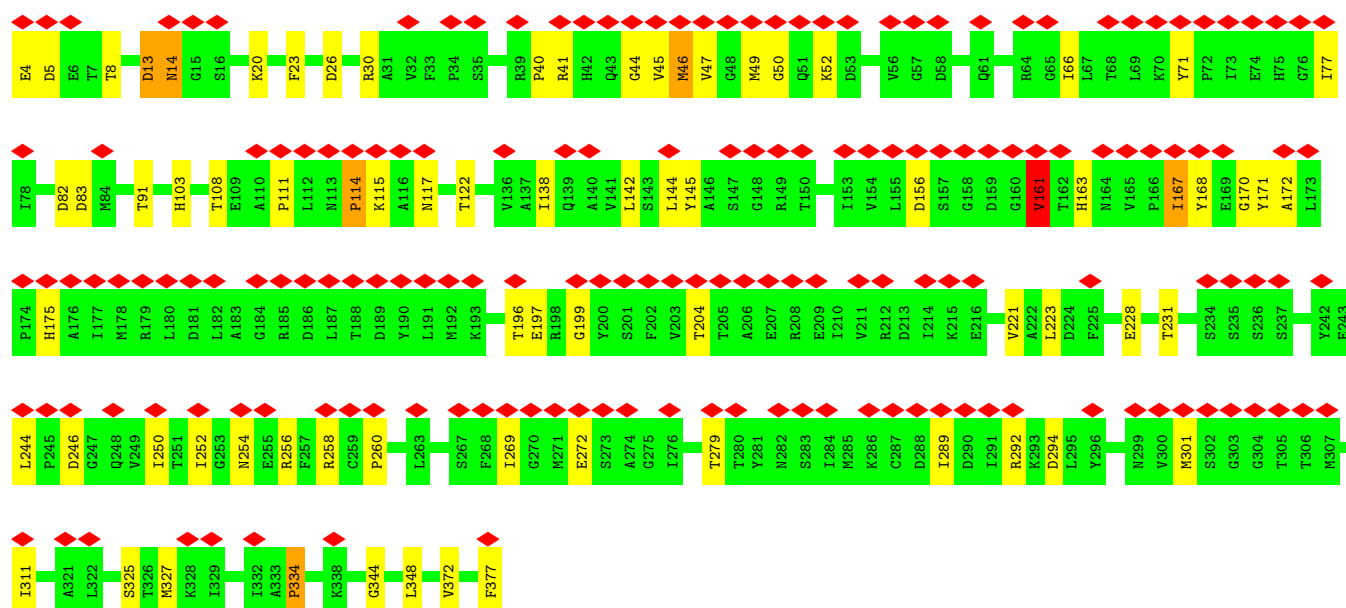




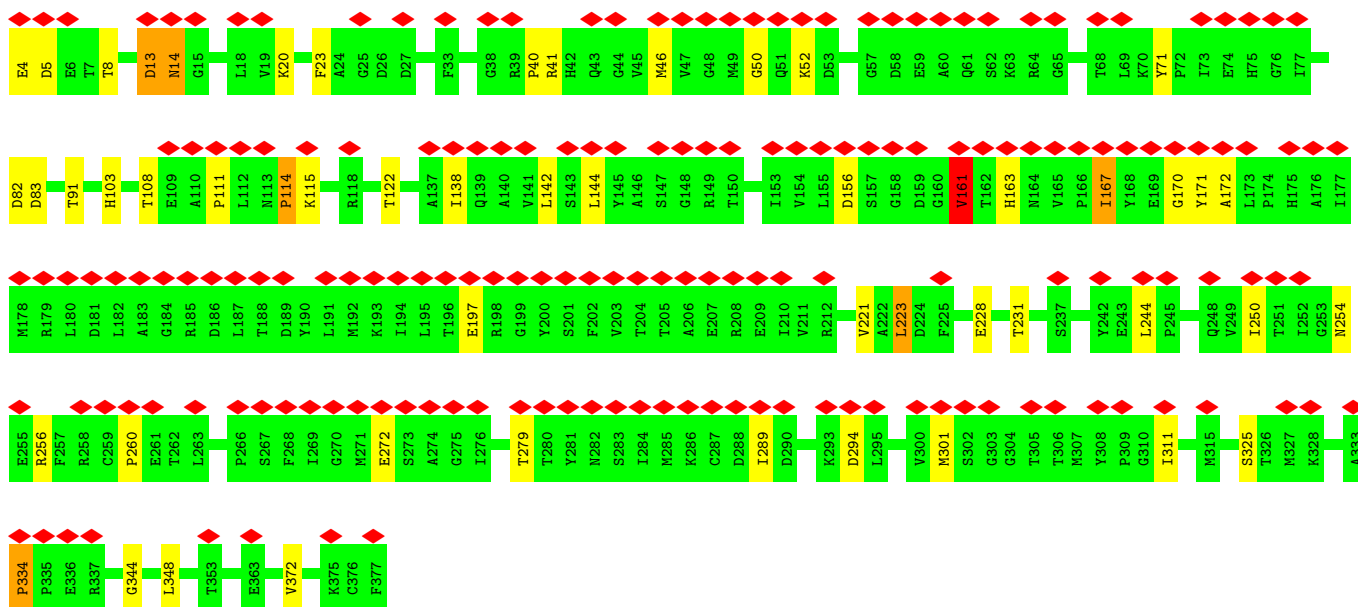
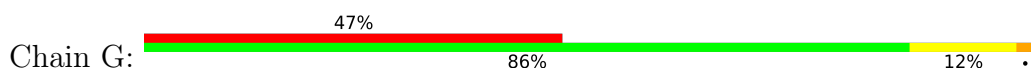
- Molecule 1: Actin, alpha skeletal muscle



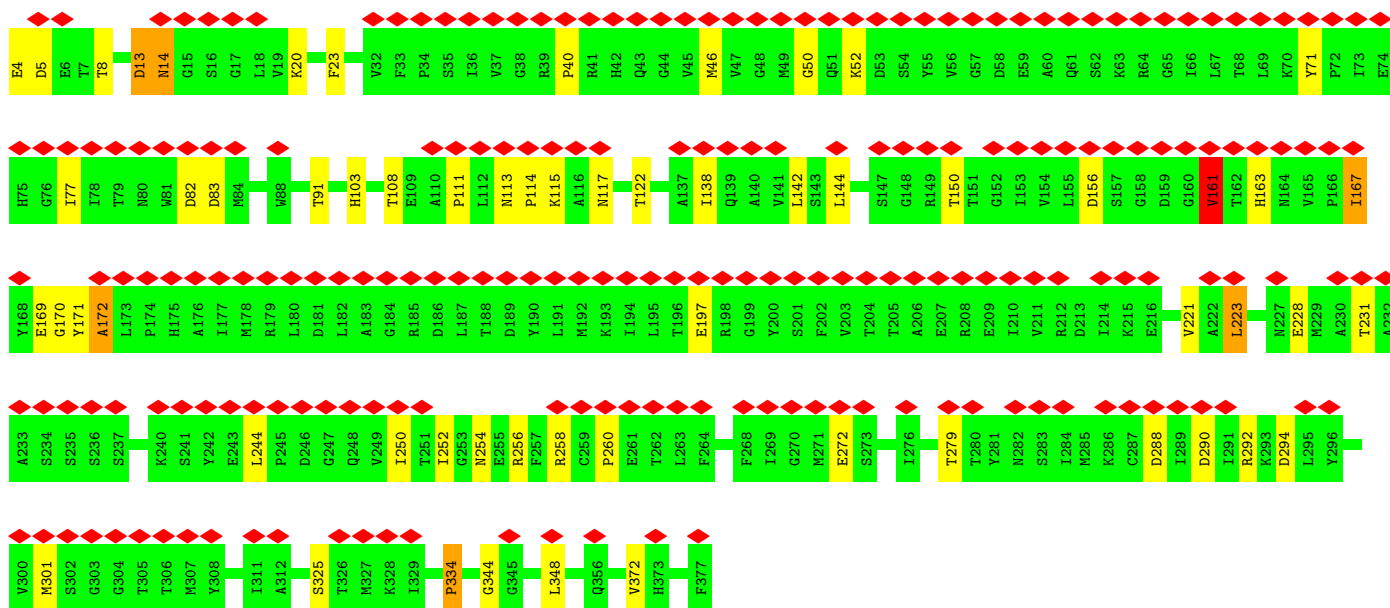
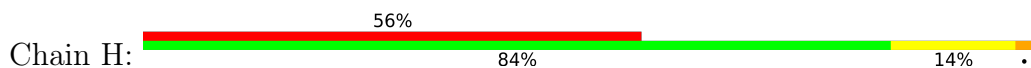
- Molecule 1: Actin, alpha skeletal muscle



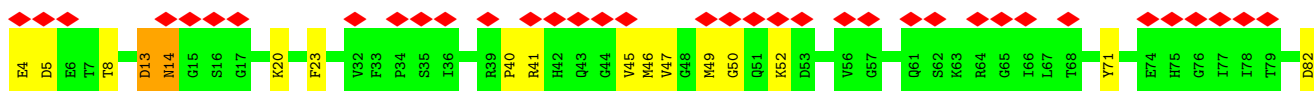
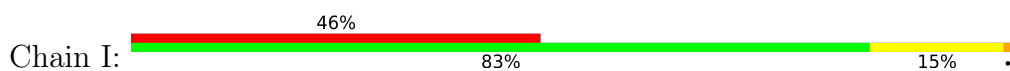
- Molecule 1: Actin, alpha skeletal muscle

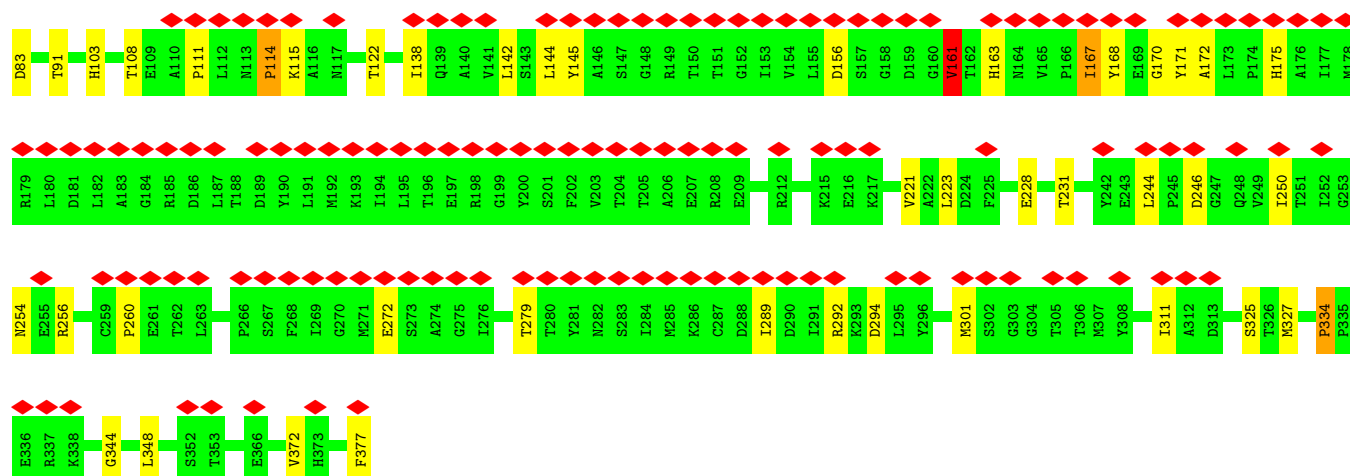


- Molecule 1: Actin, alpha skeletal muscle

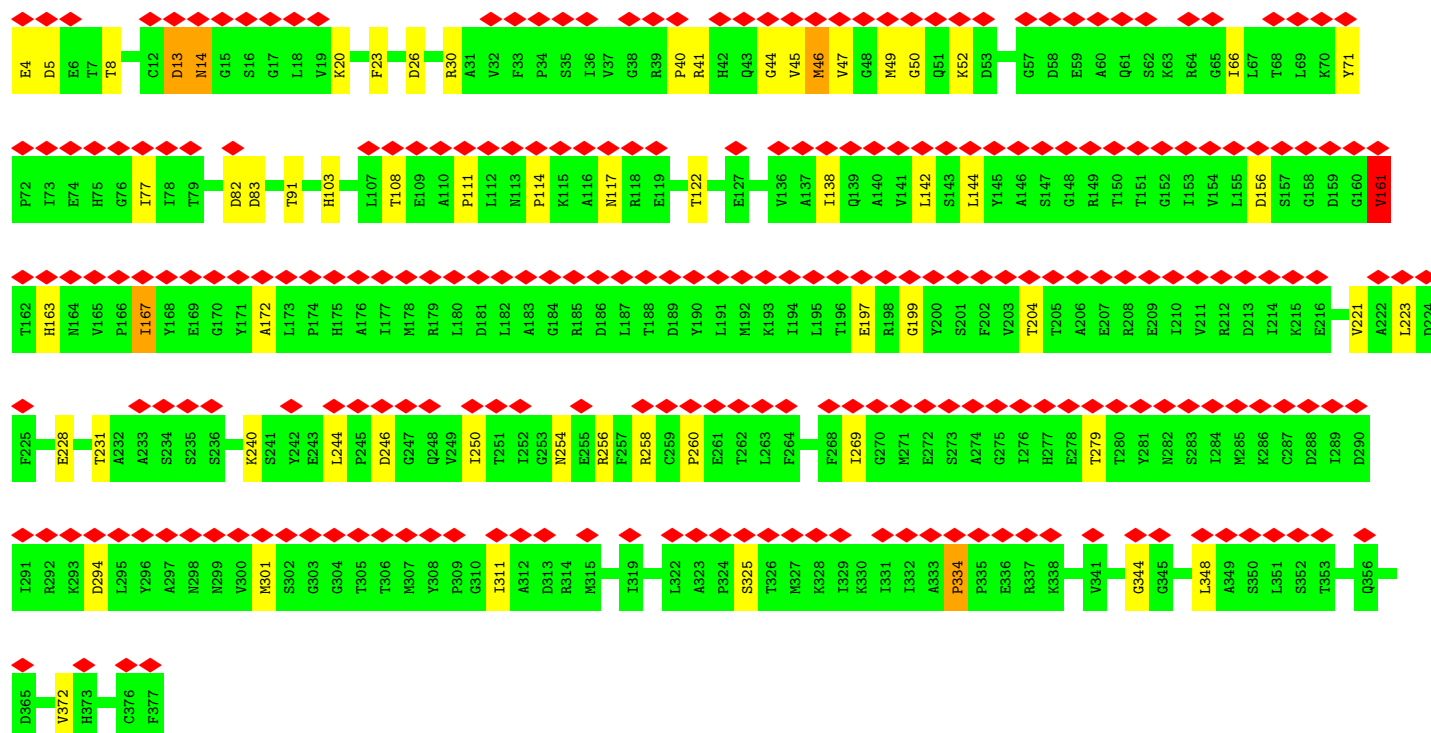
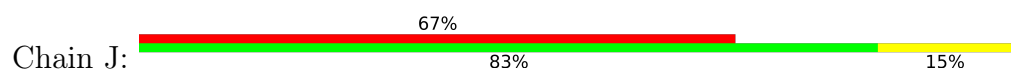


- Molecule 1: Actin, alpha skeletal muscle

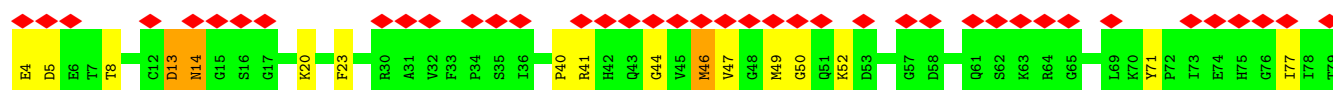
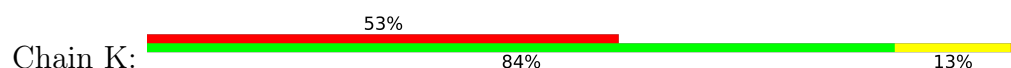


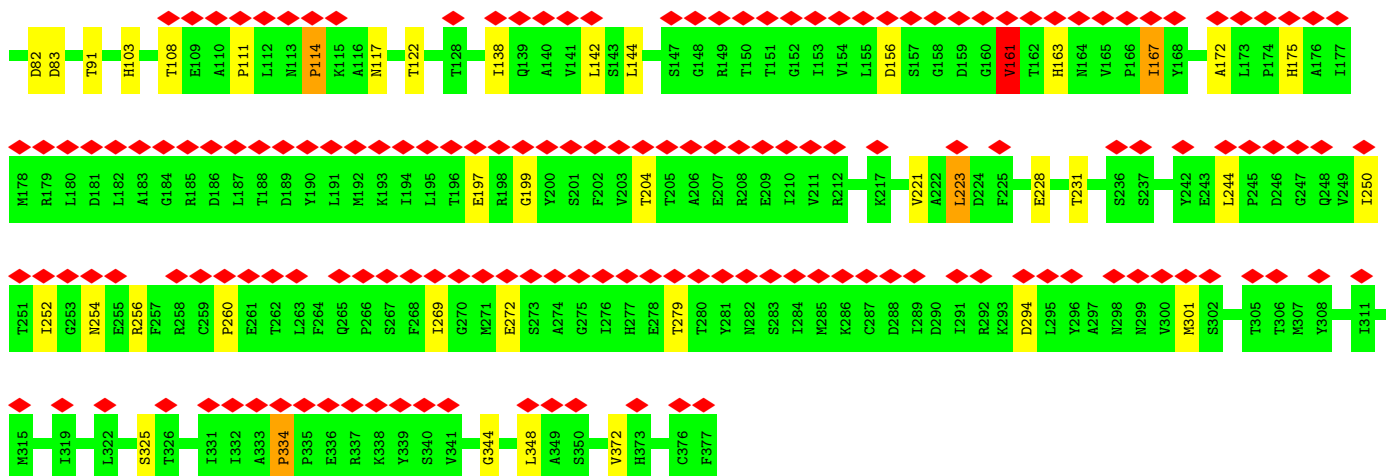


- Molecule 1: Actin, alpha skeletal muscle

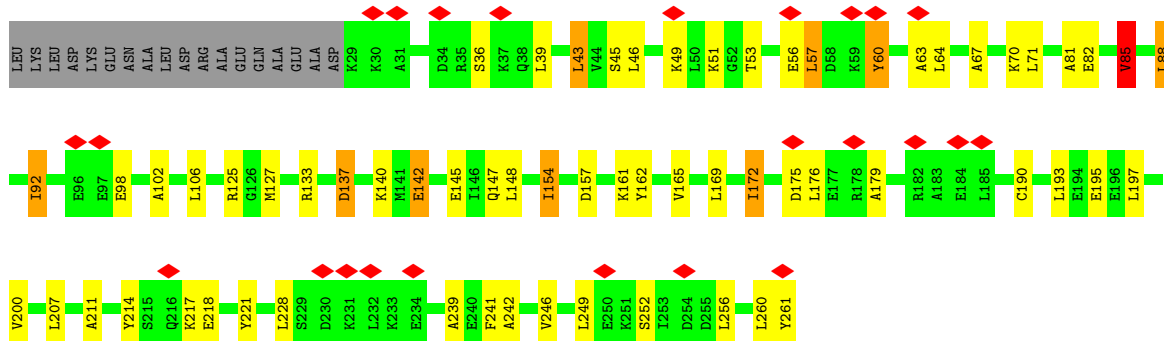


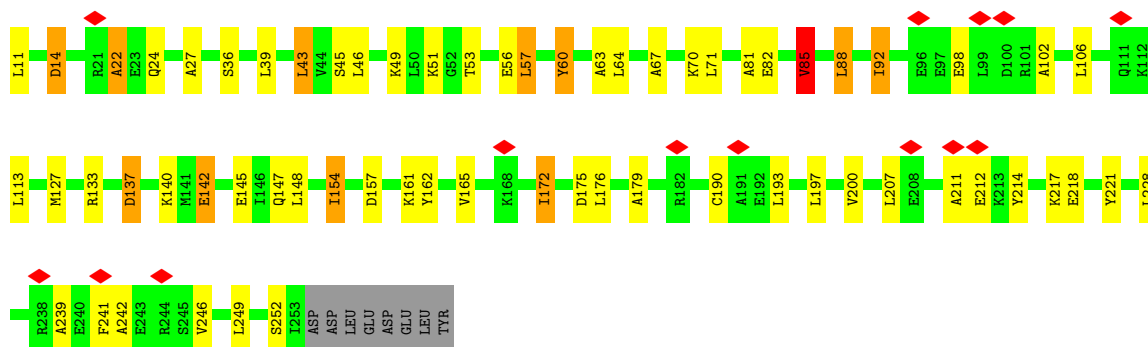
- Molecule 1: Actin, alpha skeletal muscle



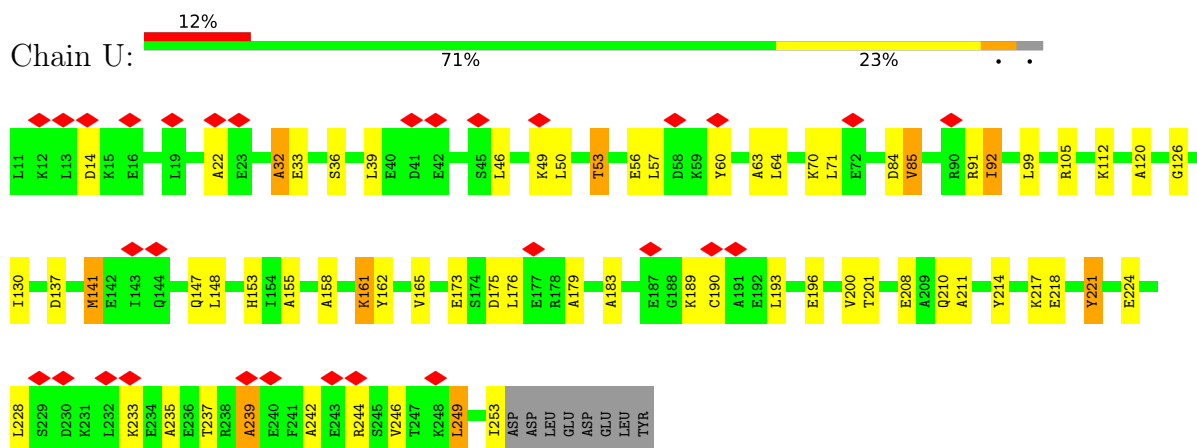


• Molecule 2: Tropomyosin alpha-1 chain

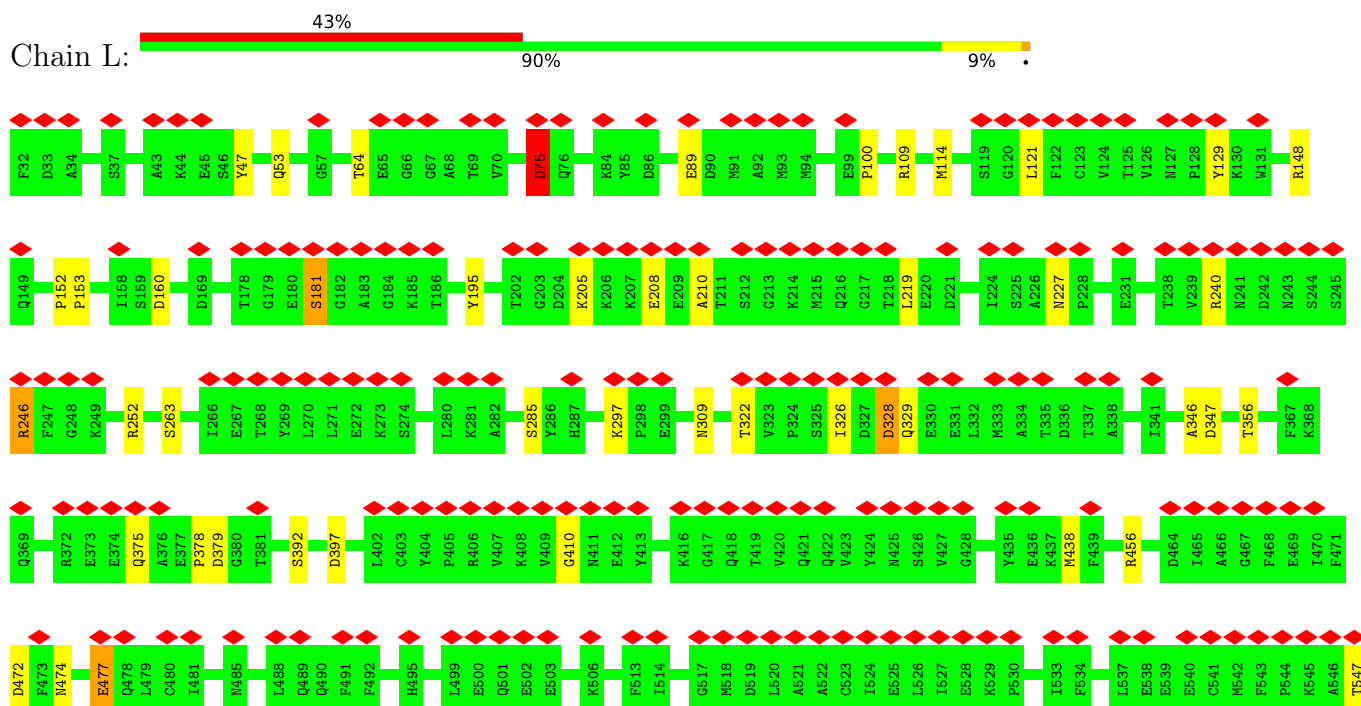


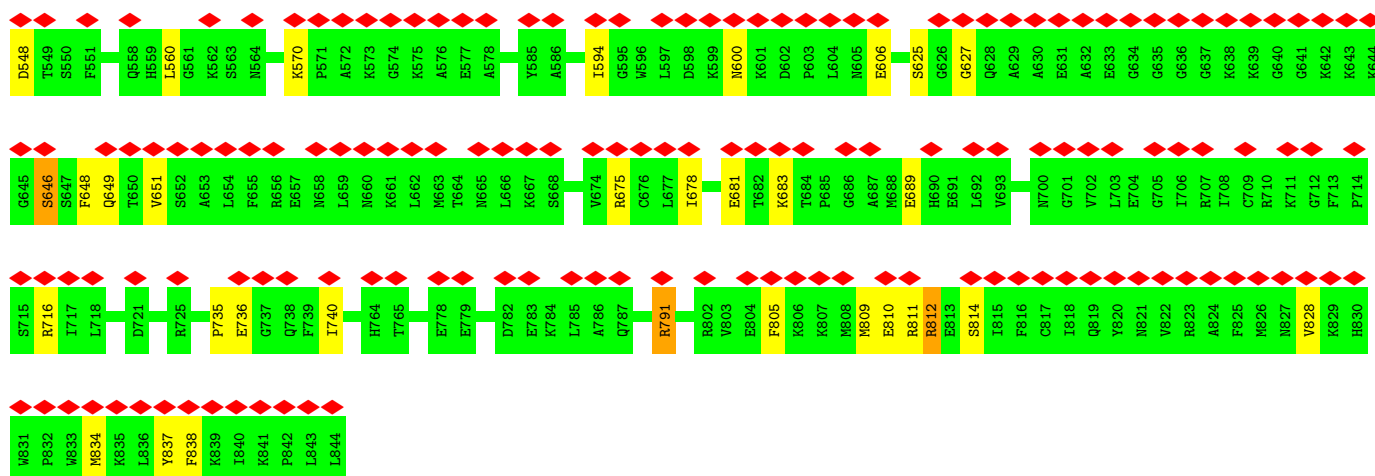


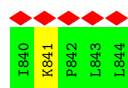
• Molecule 2: Tropomyosin alpha-1 chain



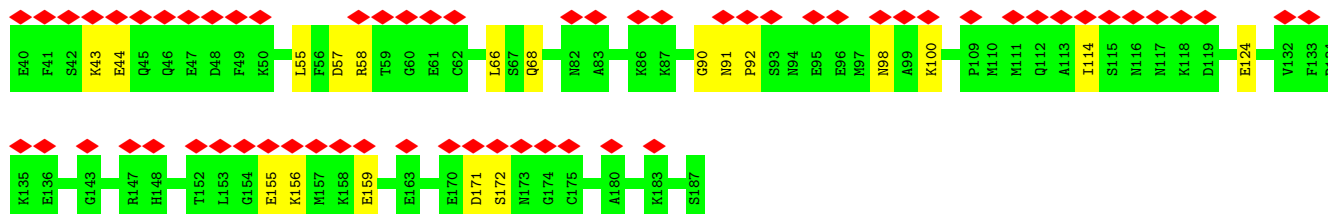
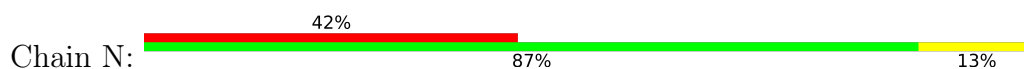
• Molecule 3: Myosin-4



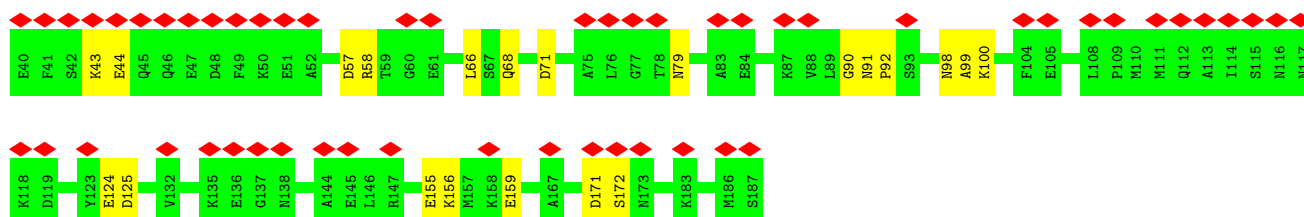
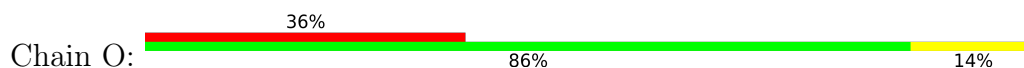




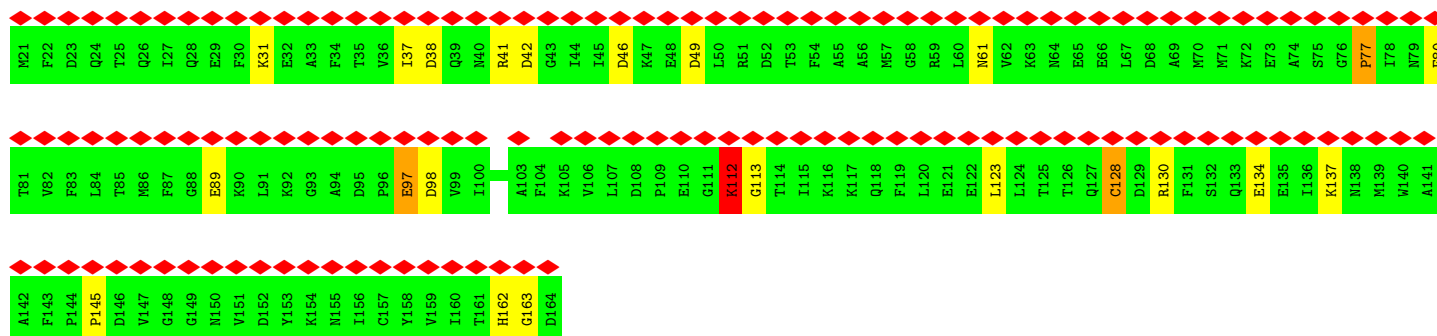
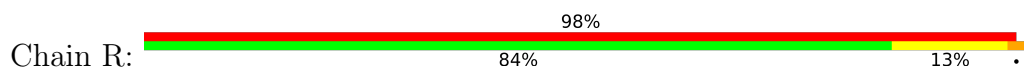
- Molecule 4: Myosin light chain 1/3, skeletal muscle isoform



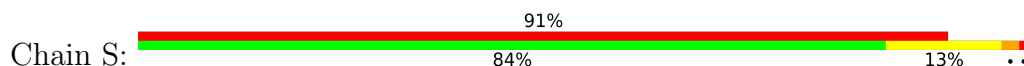
- Molecule 4: Myosin light chain 1/3, skeletal muscle isoform



- Molecule 5: Myosin regulatory light chain 2, skeletal muscle isoform



- Molecule 5: Myosin regulatory light chain 2, skeletal muscle isoform





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	18090	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	3.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	28409	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	351.0, 351.0, 351.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.755, 1.755, 1.755	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	0.87	0/2988	1.53	18/4047 (0.4%)
1	B	0.87	0/2988	1.54	15/4047 (0.4%)
1	C	1.01	0/2988	1.64	24/4047 (0.6%)
1	D	1.01	0/2988	1.64	25/4047 (0.6%)
1	E	1.01	0/2988	1.64	25/4047 (0.6%)
1	F	1.01	0/2988	1.64	24/4047 (0.6%)
1	G	1.01	0/2988	1.64	24/4047 (0.6%)
1	H	1.01	0/2988	1.64	25/4047 (0.6%)
1	I	1.01	0/2988	1.64	24/4047 (0.6%)
1	J	1.01	0/2988	1.64	24/4047 (0.6%)
1	K	1.01	0/2988	1.64	24/4047 (0.6%)
2	P	1.11	0/1887	1.95	36/2515 (1.4%)
2	Q	1.14	2/1887 (0.1%)	2.01	48/2515 (1.9%)
2	T	1.11	0/1957	1.95	40/2607 (1.5%)
2	U	1.13	2/1957 (0.1%)	2.00	48/2607 (1.8%)
3	L	0.87	0/6643	1.53	31/8946 (0.3%)
3	M	0.86	0/6643	1.53	40/8946 (0.4%)
4	N	0.86	0/1174	1.58	14/1571 (0.9%)
4	O	0.86	0/1174	1.57	18/1571 (1.1%)
5	R	0.87	0/1164	1.64	11/1565 (0.7%)
5	S	0.84	0/1164	1.63	10/1565 (0.6%)
All	All	0.97	4/58518 (0.0%)	1.65	548/78925 (0.7%)

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	6
1	B	0	5
1	C	0	5
1	D	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	5
1	F	0	5
1	G	0	5
1	H	0	5
1	I	0	5
1	J	0	5
1	K	0	5
2	P	0	2
2	Q	0	1
2	T	0	1
2	U	0	1
3	L	1	11
3	M	1	12
5	R	0	2
5	S	0	2
All	All	2	88

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	221	TYR	C-O	-5.77	1.17	1.24
2	U	221	TYR	C-O	-5.71	1.17	1.24
2	U	246	VAL	C-O	-5.54	1.17	1.24
2	Q	246	VAL	C-O	-5.50	1.18	1.24

All (548) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	14	ASP	CA-CB-CG	-9.32	103.28	112.60
2	U	224	GLU	CA-C-N	8.73	131.74	120.56
2	U	224	GLU	C-N-CA	8.73	131.74	120.56
2	Q	224	GLU	CA-C-N	8.69	131.69	120.56
2	Q	224	GLU	C-N-CA	8.69	131.69	120.56
3	L	75	ASP	CA-CB-CG	8.18	120.78	112.60
3	L	181	SER	CA-C-N	8.12	136.31	121.70
3	L	181	SER	C-N-CA	8.12	136.31	121.70
3	M	181	SER	CA-C-N	7.99	136.08	121.70
3	M	181	SER	C-N-CA	7.99	136.08	121.70
3	M	75	ASP	CA-CB-CG	7.96	120.56	112.60
1	B	8	THR	N-CA-CB	7.93	123.89	110.49
1	D	334	PRO	O-C-N	-7.58	117.59	121.15
1	C	334	PRO	O-C-N	-7.56	117.60	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	334	PRO	O-C-N	-7.50	117.62	121.15
1	H	334	PRO	O-C-N	-7.50	117.63	121.15
1	F	334	PRO	O-C-N	-7.48	117.63	121.15
1	G	334	PRO	O-C-N	-7.43	117.66	121.15
1	J	334	PRO	O-C-N	-7.43	117.66	121.15
1	E	334	PRO	O-C-N	-7.37	117.69	121.15
1	I	334	PRO	O-C-N	-7.32	117.71	121.15
2	Q	253	ILE	N-CA-CB	7.25	119.03	110.55
3	M	791	ARG	NE-CZ-NH2	7.21	125.69	119.20
1	C	254	ASN	CA-C-N	7.17	130.21	120.38
1	C	254	ASN	C-N-CA	7.17	130.21	120.38
1	H	254	ASN	CA-C-N	7.16	130.19	120.38
1	H	254	ASN	C-N-CA	7.16	130.19	120.38
1	E	254	ASN	CA-C-N	7.16	130.18	120.38
1	E	254	ASN	C-N-CA	7.16	130.18	120.38
1	D	254	ASN	CA-C-N	7.15	130.18	120.38
1	D	254	ASN	C-N-CA	7.15	130.18	120.38
1	J	254	ASN	CA-C-N	7.15	130.18	120.38
1	J	254	ASN	C-N-CA	7.15	130.18	120.38
1	G	254	ASN	CA-C-N	7.15	130.18	120.38
1	G	254	ASN	C-N-CA	7.15	130.18	120.38
1	I	254	ASN	CA-C-N	7.14	130.16	120.38
1	I	254	ASN	C-N-CA	7.14	130.16	120.38
1	F	254	ASN	CA-C-N	7.14	130.16	120.38
1	F	254	ASN	C-N-CA	7.14	130.16	120.38
1	K	254	ASN	CA-C-N	7.09	130.09	120.38
1	K	254	ASN	C-N-CA	7.09	130.09	120.38
2	P	92	ILE	N-CA-CB	7.06	118.81	110.55
2	T	92	ILE	N-CA-CB	7.04	118.79	110.55
1	A	255	GLU	N-CA-CB	-7.00	98.66	110.49
2	P	157	ASP	CA-CB-CG	-6.99	105.61	112.60
2	T	157	ASP	CA-C-N	6.99	129.94	120.44
2	T	157	ASP	C-N-CA	6.99	129.94	120.44
3	M	240	ARG	NE-CZ-NH2	6.98	125.48	119.20
3	L	791	ARG	NE-CZ-NH2	6.98	125.48	119.20
2	P	157	ASP	CA-C-N	6.92	129.85	120.44
2	P	157	ASP	C-N-CA	6.92	129.85	120.44
2	T	157	ASP	CA-CB-CG	-6.88	105.72	112.60
1	A	312	ALA	CA-C-N	6.85	129.34	120.44
1	A	312	ALA	C-N-CA	6.85	129.34	120.44
2	P	57	LEU	CB-CA-C	-6.84	100.14	110.88
1	B	255	GLU	N-CA-CB	-6.81	98.99	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	57	LEU	CB-CA-C	-6.80	100.20	110.88
5	R	89	GLU	CA-C-N	6.77	129.35	120.28
5	R	89	GLU	C-N-CA	6.77	129.35	120.28
2	P	133	ARG	CA-C-N	6.75	129.33	120.28
2	P	133	ARG	C-N-CA	6.75	129.33	120.28
3	L	397	ASP	CA-CB-CG	-6.75	105.85	112.60
2	T	133	ARG	CA-C-N	6.75	129.32	120.28
2	T	133	ARG	C-N-CA	6.75	129.32	120.28
2	T	22	ALA	CA-C-N	6.71	129.56	120.44
2	T	22	ALA	C-N-CA	6.71	129.56	120.44
5	S	113	GLY	N-CA-C	-6.66	105.99	113.79
3	M	397	ASP	CA-CB-CG	-6.63	105.97	112.60
3	M	114	MET	CA-C-N	6.62	129.53	120.46
3	M	114	MET	C-N-CA	6.62	129.53	120.46
3	L	240	ARG	NE-CZ-NH2	6.58	125.12	119.20
3	L	375	GLN	N-CA-C	6.56	118.43	111.28
2	T	154	ILE	N-CA-CB	6.56	119.46	110.54
1	B	312	ALA	CA-C-N	6.55	128.96	120.44
1	B	312	ALA	C-N-CA	6.55	128.96	120.44
2	T	179	ALA	CA-C-N	6.55	129.59	120.29
2	T	179	ALA	C-N-CA	6.55	129.59	120.29
2	P	154	ILE	N-CA-CB	6.54	119.44	110.54
1	E	13	ASP	CA-CB-CG	6.53	119.13	112.60
5	S	89	GLU	CA-C-N	6.53	129.03	120.28
5	S	89	GLU	C-N-CA	6.53	129.03	120.28
1	I	13	ASP	CA-CB-CG	6.53	119.13	112.60
1	K	13	ASP	CA-CB-CG	6.52	119.12	112.60
4	N	44	GLU	N-CA-CB	-6.52	100.56	110.01
1	F	13	ASP	CA-CB-CG	6.52	119.12	112.60
2	P	179	ALA	CA-C-N	6.51	129.54	120.29
2	P	179	ALA	C-N-CA	6.51	129.54	120.29
1	C	13	ASP	CA-CB-CG	6.51	119.11	112.60
1	J	13	ASP	CA-CB-CG	6.50	119.10	112.60
1	G	13	ASP	CA-CB-CG	6.50	119.10	112.60
1	H	13	ASP	CA-CB-CG	6.50	119.10	112.60
1	D	13	ASP	CA-CB-CG	6.50	119.09	112.60
3	L	114	MET	CA-C-N	6.47	129.33	120.46
3	L	114	MET	C-N-CA	6.47	129.33	120.46
2	P	85	VAL	N-CA-CB	6.46	119.33	110.54
2	T	85	VAL	N-CA-CB	6.46	119.32	110.54
2	Q	249	LEU	CA-C-N	6.45	129.21	120.44
2	Q	249	LEU	C-N-CA	6.45	129.21	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	249	LEU	CA-C-N	6.42	129.17	120.44
2	U	249	LEU	C-N-CA	6.42	129.17	120.44
3	M	203	GLY	CA-C-N	6.39	128.85	120.28
3	M	203	GLY	C-N-CA	6.39	128.85	120.28
2	U	120	ALA	CA-C-N	6.32	128.66	120.44
2	U	120	ALA	C-N-CA	6.32	128.66	120.44
2	U	235	ALA	CA-C-N	6.32	129.26	120.29
2	U	235	ALA	C-N-CA	6.32	129.26	120.29
2	Q	120	ALA	CA-C-N	6.29	128.62	120.44
2	Q	120	ALA	C-N-CA	6.29	128.62	120.44
4	N	91	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	245	PRO	CA-C-N	6.26	128.66	120.28
1	A	245	PRO	C-N-CA	6.26	128.66	120.28
2	Q	235	ALA	CA-C-N	6.25	129.17	120.29
2	Q	235	ALA	C-N-CA	6.25	129.17	120.29
5	R	113	GLY	N-CA-C	-6.25	106.48	113.79
4	N	90	GLY	CA-C-N	6.24	130.14	120.60
4	N	90	GLY	C-N-CA	6.24	130.14	120.60
3	M	75	ASP	N-CA-CB	-6.24	99.95	110.49
3	L	181	SER	O-C-N	-6.21	114.33	122.59
1	C	83	ASP	CA-CB-CG	6.20	118.80	112.60
2	Q	91	ARG	CA-C-N	6.20	128.37	120.56
2	Q	91	ARG	C-N-CA	6.20	128.37	120.56
3	M	181	SER	O-C-N	-6.19	114.36	122.59
2	T	175	ASP	CA-C-N	6.19	128.48	120.44
2	T	175	ASP	C-N-CA	6.19	128.48	120.44
1	I	83	ASP	CA-CB-CG	6.18	118.78	112.60
1	J	83	ASP	CA-CB-CG	6.18	118.78	112.60
2	U	91	ARG	CA-C-N	6.18	128.35	120.56
2	U	91	ARG	C-N-CA	6.18	128.35	120.56
1	G	83	ASP	CA-CB-CG	6.17	118.77	112.60
2	U	85	VAL	N-CA-CB	6.16	117.76	110.55
1	K	83	ASP	CA-CB-CG	6.16	118.76	112.60
2	U	126	GLY	CA-C-N	6.13	128.81	120.54
2	U	126	GLY	C-N-CA	6.13	128.81	120.54
1	E	83	ASP	CA-CB-CG	6.12	118.72	112.60
1	D	83	ASP	CA-CB-CG	6.12	118.72	112.60
2	P	175	ASP	CA-C-N	6.12	128.40	120.44
2	P	175	ASP	C-N-CA	6.12	128.40	120.44
1	H	83	ASP	CA-CB-CG	6.12	118.72	112.60
2	Q	85	VAL	N-CA-CB	6.12	117.71	110.55
2	P	142	GLU	CA-C-N	6.12	128.39	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	142	GLU	C-N-CA	6.12	128.39	120.56
2	P	57	LEU	N-CA-CB	6.11	118.87	110.01
2	T	57	LEU	N-CA-CB	6.09	118.84	110.01
2	T	142	GLU	CA-C-N	6.09	128.35	120.56
2	T	142	GLU	C-N-CA	6.09	128.35	120.56
1	F	83	ASP	CA-CB-CG	6.07	118.67	112.60
1	D	279	THR	N-CA-CB	6.07	119.04	110.12
1	B	159	ASP	N-CA-C	-6.07	106.13	112.93
2	Q	137	ASP	CA-C-N	6.07	128.69	120.44
2	Q	137	ASP	C-N-CA	6.07	128.69	120.44
1	I	279	THR	N-CA-CB	6.06	119.03	110.12
1	G	279	THR	N-CA-CB	6.06	119.02	110.12
1	E	279	THR	N-CA-CB	6.05	119.02	110.12
1	K	279	THR	N-CA-CB	6.05	119.01	110.12
4	O	57	ASP	CA-C-N	6.04	133.09	121.54
4	O	57	ASP	C-N-CA	6.04	133.09	121.54
2	Q	126	GLY	CA-C-N	6.03	128.68	120.54
2	Q	126	GLY	C-N-CA	6.03	128.68	120.54
1	F	279	THR	N-CA-CB	6.03	118.98	110.12
1	C	279	THR	N-CA-CB	6.03	118.98	110.12
1	H	279	THR	N-CA-CB	6.03	118.98	110.12
1	J	279	THR	N-CA-CB	6.01	118.96	110.12
2	U	137	ASP	CA-C-N	6.00	128.61	120.44
2	U	137	ASP	C-N-CA	6.00	128.61	120.44
3	M	821	ASN	CA-CB-CG	-5.99	106.61	112.60
3	L	152	PRO	N-CA-C	5.98	118.00	110.70
2	Q	33	GLU	CA-C-N	5.97	128.20	120.44
2	Q	33	GLU	C-N-CA	5.97	128.20	120.44
2	Q	92	ILE	N-CA-CB	5.96	117.52	110.55
4	O	90	GLY	CA-C-N	5.95	129.70	120.60
4	O	90	GLY	C-N-CA	5.95	129.70	120.60
2	Q	161	LYS	CA-C-N	5.94	128.56	120.54
2	Q	161	LYS	C-N-CA	5.94	128.56	120.54
2	U	92	ILE	N-CA-CB	5.94	117.50	110.55
4	N	43	LYS	CA-C-N	5.94	128.16	120.44
4	N	43	LYS	C-N-CA	5.94	128.16	120.44
2	U	33	GLU	CA-C-N	5.92	128.21	120.28
2	U	33	GLU	C-N-CA	5.92	128.21	120.28
1	J	91	THR	N-CA-CB	5.90	118.57	110.01
2	U	161	LYS	CA-C-N	5.90	128.51	120.54
2	U	161	LYS	C-N-CA	5.90	128.51	120.54
5	R	98	ASP	CA-CB-CG	-5.89	106.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	629	ALA	CA-C-N	5.89	128.45	120.38
3	M	629	ALA	C-N-CA	5.89	128.45	120.38
1	B	245	PRO	CA-C-N	5.89	128.65	120.29
1	B	245	PRO	C-N-CA	5.89	128.65	120.29
1	F	325	SER	CA-C-N	5.89	128.76	120.28
1	F	325	SER	C-N-CA	5.89	128.76	120.28
4	O	44	GLU	N-CA-CB	-5.89	101.47	110.01
1	E	325	SER	CA-C-N	5.88	128.75	120.28
1	E	325	SER	C-N-CA	5.88	128.75	120.28
1	K	325	SER	CA-C-N	5.88	128.75	120.28
1	K	325	SER	C-N-CA	5.88	128.75	120.28
1	J	325	SER	CA-C-N	5.87	128.73	120.28
1	J	325	SER	C-N-CA	5.87	128.73	120.28
1	E	91	THR	N-CA-CB	5.87	118.52	110.01
1	F	91	THR	N-CA-CB	5.86	118.51	110.01
1	K	91	THR	N-CA-CB	5.86	118.50	110.01
1	D	91	THR	N-CA-CB	5.86	118.50	110.01
1	I	91	THR	N-CA-CB	5.86	118.50	110.01
1	C	91	THR	N-CA-CB	5.85	118.50	110.01
1	H	325	SER	CA-C-N	5.85	128.71	120.28
1	H	325	SER	C-N-CA	5.85	128.71	120.28
1	G	325	SER	CA-C-N	5.85	128.70	120.28
1	G	325	SER	C-N-CA	5.85	128.70	120.28
2	Q	32	ALA	CA-C-N	5.84	128.59	120.29
2	Q	32	ALA	C-N-CA	5.84	128.59	120.29
1	K	156	ASP	CA-CB-CG	5.84	118.44	112.60
1	H	91	THR	N-CA-CB	5.83	118.47	110.01
1	C	325	SER	CA-C-N	5.83	128.68	120.28
1	C	325	SER	C-N-CA	5.83	128.68	120.28
1	G	91	THR	N-CA-CB	5.83	118.46	110.01
1	E	294	ASP	CA-CB-CG	5.82	118.42	112.60
1	I	325	SER	CA-C-N	5.82	128.66	120.28
1	I	325	SER	C-N-CA	5.82	128.66	120.28
1	E	156	ASP	CA-CB-CG	5.82	118.42	112.60
3	L	646	SER	N-CA-CB	5.82	120.32	110.49
1	D	325	SER	CA-C-N	5.81	128.65	120.28
1	D	325	SER	C-N-CA	5.81	128.65	120.28
2	T	14	ASP	CA-CB-CG	-5.81	106.79	112.60
4	O	91	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	64	ARG	N-CA-C	5.81	117.61	111.28
4	O	171	ASP	CA-C-N	5.81	132.63	121.54
4	O	171	ASP	C-N-CA	5.81	132.63	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	156	ASP	CA-CB-CG	5.80	118.40	112.60
2	Q	158	ALA	CA-C-N	5.80	128.05	120.28
2	Q	158	ALA	C-N-CA	5.80	128.05	120.28
2	U	32	ALA	CA-C-N	5.80	128.53	120.29
2	U	32	ALA	C-N-CA	5.80	128.53	120.29
1	D	156	ASP	CA-CB-CG	5.80	118.40	112.60
3	M	181	SER	CB-CA-C	5.80	121.95	110.42
1	G	156	ASP	CA-CB-CG	5.79	118.39	112.60
1	I	156	ASP	CA-CB-CG	5.79	118.39	112.60
1	I	294	ASP	CA-CB-CG	5.78	118.38	112.60
1	J	294	ASP	CA-CB-CG	5.78	118.38	112.60
2	Q	53	THR	CA-C-N	5.78	128.30	120.44
2	Q	53	THR	C-N-CA	5.78	128.30	120.44
1	J	156	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	156	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	294	ASP	CA-CB-CG	5.77	118.37	112.60
1	H	156	ASP	CA-CB-CG	5.77	118.37	112.60
1	G	294	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	159	ASP	N-CA-C	-5.76	106.48	112.93
4	N	171	ASP	CA-C-N	5.76	132.53	121.54
4	N	171	ASP	C-N-CA	5.76	132.53	121.54
1	H	294	ASP	CA-CB-CG	5.75	118.35	112.60
3	M	152	PRO	N-CA-C	5.75	117.71	110.70
1	D	294	ASP	CA-CB-CG	5.75	118.34	112.60
1	F	294	ASP	CA-CB-CG	5.74	118.34	112.60
2	U	53	THR	CA-C-N	5.74	128.25	120.44
2	U	53	THR	C-N-CA	5.74	128.25	120.44
3	L	75	ASP	N-CA-CB	-5.74	100.80	110.49
5	S	46	ASP	CA-C-N	5.74	127.89	120.44
5	S	46	ASP	C-N-CA	5.74	127.89	120.44
2	Q	244	ARG	CA-C-N	5.73	128.23	120.44
2	Q	244	ARG	C-N-CA	5.73	128.23	120.44
1	A	318	GLU	CB-CG-CD	5.72	122.33	112.60
2	U	158	ALA	CA-C-N	5.72	127.95	120.28
2	U	158	ALA	C-N-CA	5.72	127.95	120.28
1	E	103	HIS	CB-CG-ND1	-5.71	114.13	122.70
1	K	294	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	64	ARG	N-CA-C	5.70	117.49	111.28
1	H	103	HIS	CB-CG-ND1	-5.70	114.16	122.70
1	D	103	HIS	CB-CG-ND1	-5.69	114.16	122.70
1	J	103	HIS	CB-CG-ND1	-5.69	114.16	122.70
1	F	103	HIS	CB-CG-ND1	-5.69	114.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	367	PHE	CA-CB-CG	-5.69	108.11	113.80
1	G	103	HIS	CB-CG-ND1	-5.68	114.18	122.70
2	Q	141	MET	CG-SD-CE	-5.68	88.40	100.90
1	C	103	HIS	CB-CG-ND1	-5.68	114.19	122.70
1	K	103	HIS	CB-CG-ND1	-5.67	114.19	122.70
1	I	103	HIS	CB-CG-ND1	-5.66	114.20	122.70
2	U	141	MET	CG-SD-CE	-5.66	88.44	100.90
1	H	301	MET	CG-SD-CE	-5.63	88.52	100.90
1	C	301	MET	CG-SD-CE	-5.62	88.53	100.90
1	F	301	MET	CG-SD-CE	-5.62	88.54	100.90
5	R	37	ILE	CA-C-N	5.62	132.27	121.54
5	R	37	ILE	C-N-CA	5.62	132.27	121.54
2	Q	217	LYS	CA-C-N	5.62	127.80	120.28
2	Q	217	LYS	C-N-CA	5.62	127.80	120.28
2	U	244	ARG	CA-C-N	5.62	128.26	120.29
2	U	244	ARG	C-N-CA	5.62	128.26	120.29
3	L	227	ASN	CA-C-O	-5.61	113.23	118.73
1	D	301	MET	CG-SD-CE	-5.61	88.56	100.90
1	E	301	MET	CG-SD-CE	-5.61	88.57	100.90
1	G	301	MET	CG-SD-CE	-5.61	88.57	100.90
1	J	301	MET	CG-SD-CE	-5.60	88.57	100.90
2	U	217	LYS	CA-C-N	5.60	127.79	120.28
2	U	217	LYS	C-N-CA	5.60	127.79	120.28
4	O	99	ALA	N-CA-C	5.60	117.39	111.28
1	K	301	MET	CG-SD-CE	-5.59	88.59	100.90
2	P	45	SER	N-CA-CB	5.59	118.12	110.01
4	O	71	ASP	CA-CB-CG	-5.59	107.00	112.60
3	L	181	SER	CB-CA-C	5.59	121.55	110.42
1	I	301	MET	CG-SD-CE	-5.59	88.60	100.90
3	L	346	ALA	CA-C-N	5.59	127.77	120.28
3	L	346	ALA	C-N-CA	5.59	127.77	120.28
3	M	548	ASP	N-CA-CB	-5.58	101.91	110.12
3	M	346	ALA	CA-C-N	5.58	127.76	120.28
3	M	346	ALA	C-N-CA	5.58	127.76	120.28
2	T	45	SER	N-CA-CB	5.57	118.09	110.01
4	O	43	LYS	CA-C-N	5.57	127.67	120.44
4	O	43	LYS	C-N-CA	5.57	127.67	120.44
1	G	46	MET	N-CA-C	-5.56	100.90	108.24
1	C	46	MET	N-CA-C	-5.56	100.90	108.24
5	R	46	ASP	CA-C-N	5.54	127.65	120.44
5	R	46	ASP	C-N-CA	5.54	127.65	120.44
5	S	37	ILE	CA-C-N	5.54	132.13	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	37	ILE	C-N-CA	5.54	132.13	121.54
1	K	46	MET	N-CA-C	-5.53	100.94	108.24
3	L	246	ARG	CD-NE-CZ	-5.53	116.66	124.40
3	M	227	ASN	CA-C-O	-5.53	113.31	118.73
1	A	13	ASP	CA-CB-CG	5.53	118.12	112.60
1	F	46	MET	N-CA-C	-5.52	100.95	108.24
1	D	46	MET	N-CA-C	-5.52	100.95	108.24
1	J	91	THR	CB-CA-C	-5.52	102.22	110.88
1	J	46	MET	N-CA-C	-5.51	100.96	108.24
3	L	548	ASP	N-CA-CB	-5.51	102.02	110.12
1	H	46	MET	N-CA-C	-5.51	100.97	108.24
3	M	648	PHE	CA-C-N	5.51	132.06	121.54
3	M	648	PHE	C-N-CA	5.51	132.06	121.54
2	Q	49	LYS	CA-C-N	5.51	127.60	120.44
2	Q	49	LYS	C-N-CA	5.51	127.60	120.44
1	E	46	MET	N-CA-C	-5.50	100.97	108.24
1	I	46	MET	N-CA-C	-5.50	100.97	108.24
4	N	57	ASP	CA-C-N	5.50	132.05	121.54
4	N	57	ASP	C-N-CA	5.50	132.05	121.54
1	H	91	THR	CB-CA-C	-5.50	102.24	110.88
1	F	91	THR	CB-CA-C	-5.50	102.25	110.88
1	K	91	THR	CB-CA-C	-5.49	102.27	110.88
5	S	48	GLU	CA-C-N	5.49	127.57	120.44
5	S	48	GLU	C-N-CA	5.49	127.57	120.44
2	U	49	LYS	CA-C-N	5.48	127.56	120.44
2	U	49	LYS	C-N-CA	5.48	127.56	120.44
2	P	102	ALA	CA-C-N	5.47	127.62	120.28
2	P	102	ALA	C-N-CA	5.47	127.62	120.28
3	M	246	ARG	CD-NE-CZ	-5.47	116.74	124.40
1	C	91	THR	CB-CA-C	-5.47	102.30	110.88
1	I	91	THR	CB-CA-C	-5.46	102.30	110.88
3	M	806	LYS	N-CA-C	5.46	117.31	111.36
1	D	91	THR	CB-CA-C	-5.46	102.31	110.88
2	T	102	ALA	CA-C-N	5.46	127.59	120.28
2	T	102	ALA	C-N-CA	5.46	127.59	120.28
2	P	60	TYR	CA-C-N	5.46	128.04	120.29
2	P	60	TYR	C-N-CA	5.46	128.04	120.29
1	G	91	THR	CB-CA-C	-5.43	102.35	110.88
2	T	51	LYS	CA-C-N	5.43	125.97	119.94
2	T	51	LYS	C-N-CA	5.43	125.97	119.94
1	E	91	THR	CB-CA-C	-5.43	102.36	110.88
2	T	43	LEU	N-CA-CB	5.42	118.18	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	60	TYR	CA-C-N	5.42	127.98	120.29
2	T	60	TYR	C-N-CA	5.42	127.98	120.29
2	P	88	LEU	CA-C-N	5.41	127.97	120.29
2	P	88	LEU	C-N-CA	5.41	127.97	120.29
2	P	51	LYS	CA-C-N	5.40	125.94	119.94
2	P	51	LYS	C-N-CA	5.40	125.94	119.94
2	P	43	LEU	N-CA-CB	5.38	118.12	110.16
1	F	91	THR	CA-CB-OG1	5.38	117.66	109.60
2	T	88	LEU	CA-C-N	5.37	127.91	120.29
2	T	88	LEU	C-N-CA	5.37	127.91	120.29
1	D	91	THR	CA-CB-OG1	5.36	117.64	109.60
1	J	91	THR	CA-CB-OG1	5.36	117.64	109.60
1	C	91	THR	CA-CB-OG1	5.35	117.62	109.60
2	Q	210	GLN	CA-C-N	5.34	127.43	120.28
2	Q	210	GLN	C-N-CA	5.34	127.43	120.28
1	G	91	THR	CA-CB-OG1	5.34	117.61	109.60
2	Q	221	TYR	N-CA-CB	5.34	117.75	110.01
1	K	91	THR	CA-CB-OG1	5.34	117.61	109.60
1	H	91	THR	CA-CB-OG1	5.33	117.60	109.60
1	E	91	THR	CA-CB-OG1	5.33	117.59	109.60
3	L	410	GLY	CA-C-N	5.33	131.29	121.70
3	L	410	GLY	C-N-CA	5.33	131.29	121.70
4	N	155	GLU	CA-C-N	5.33	131.71	121.54
4	N	155	GLU	C-N-CA	5.33	131.71	121.54
1	I	91	THR	CA-CB-OG1	5.32	117.58	109.60
1	K	161	VAL	CA-C-N	5.30	129.67	122.19
1	K	161	VAL	C-N-CA	5.30	129.67	122.19
2	U	221	TYR	N-CA-CB	5.30	117.70	110.01
1	H	161	VAL	CA-C-N	5.30	129.67	122.19
1	H	161	VAL	C-N-CA	5.30	129.67	122.19
1	J	161	VAL	CA-C-N	5.30	129.66	122.19
1	J	161	VAL	C-N-CA	5.30	129.66	122.19
1	C	161	VAL	CA-C-N	5.29	129.66	122.19
1	C	161	VAL	C-N-CA	5.29	129.66	122.19
1	I	161	VAL	CA-C-N	5.29	129.65	122.19
1	I	161	VAL	C-N-CA	5.29	129.65	122.19
1	H	14	ASN	CA-CB-CG	-5.29	107.31	112.60
1	E	161	VAL	CA-C-N	5.28	129.64	122.19
1	E	161	VAL	C-N-CA	5.28	129.64	122.19
2	U	210	GLN	CA-C-N	5.28	127.36	120.28
2	U	210	GLN	C-N-CA	5.28	127.36	120.28
1	K	14	ASN	CA-CB-CG	-5.27	107.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	VAL	CA-C-N	5.27	129.62	122.19
1	D	161	VAL	C-N-CA	5.27	129.62	122.19
3	M	810	GLU	CB-CG-CD	5.26	121.55	112.60
1	F	161	VAL	CA-C-N	5.26	129.60	122.19
1	F	161	VAL	C-N-CA	5.26	129.60	122.19
3	M	803	VAL	CA-C-N	5.25	127.27	120.44
3	M	803	VAL	C-N-CA	5.25	127.27	120.44
2	T	137	ASP	CA-C-N	5.25	127.58	120.44
2	T	137	ASP	C-N-CA	5.25	127.58	120.44
2	P	137	ASP	CA-C-N	5.24	127.57	120.44
2	P	137	ASP	C-N-CA	5.24	127.57	120.44
1	C	14	ASN	CA-CB-CG	-5.23	107.37	112.60
1	G	161	VAL	CA-C-N	5.23	129.56	122.19
1	G	161	VAL	C-N-CA	5.23	129.56	122.19
1	J	14	ASN	CA-CB-CG	-5.23	107.37	112.60
5	R	128	CYS	CB-CA-C	-5.23	108.99	115.89
1	I	14	ASN	CA-CB-CG	-5.23	107.37	112.60
5	R	42	ASP	N-CA-C	5.23	118.54	111.17
2	U	239	ALA	CA-C-N	5.23	127.28	120.28
2	U	239	ALA	C-N-CA	5.23	127.28	120.28
1	A	63	LYS	CA-C-N	5.22	127.28	120.28
1	A	63	LYS	C-N-CA	5.22	127.28	120.28
2	Q	196	GLU	CA-C-N	5.22	127.23	120.44
2	Q	196	GLU	C-N-CA	5.22	127.23	120.44
3	L	735	PRO	CA-C-N	5.22	131.51	121.54
3	L	735	PRO	C-N-CA	5.22	131.51	121.54
1	D	14	ASN	CA-CB-CG	-5.22	107.38	112.60
1	C	82	ASP	CA-CB-CG	5.22	117.82	112.60
4	O	159	GLU	CA-C-N	5.22	127.53	120.38
4	O	159	GLU	C-N-CA	5.22	127.53	120.38
1	K	5	ASP	CA-CB-CG	-5.21	107.39	112.60
4	N	159	GLU	CA-C-N	5.21	127.58	120.54
4	N	159	GLU	C-N-CA	5.21	127.58	120.54
1	D	5	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	254	ASN	CA-C-N	5.20	131.47	121.54
1	A	254	ASN	C-N-CA	5.20	131.47	121.54
2	Q	183	ALA	CA-C-N	5.20	127.25	120.28
2	Q	183	ALA	C-N-CA	5.20	127.25	120.28
2	U	196	GLU	CA-C-N	5.20	127.20	120.44
2	U	196	GLU	C-N-CA	5.20	127.20	120.44
1	F	5	ASP	CA-CB-CG	-5.20	107.40	112.60
2	Q	239	ALA	CA-C-N	5.20	127.25	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	239	ALA	C-N-CA	5.20	127.25	120.28
1	I	5	ASP	CA-CB-CG	-5.19	107.41	112.60
2	U	183	ALA	CA-C-N	5.19	127.23	120.28
2	U	183	ALA	C-N-CA	5.19	127.23	120.28
3	M	297	LYS	CG-CD-CE	5.19	123.23	111.30
1	C	5	ASP	CA-CB-CG	-5.18	107.42	112.60
1	F	14	ASN	CA-CB-CG	-5.18	107.42	112.60
1	B	63	LYS	CA-C-N	5.18	127.22	120.28
1	B	63	LYS	C-N-CA	5.18	127.22	120.28
1	C	8	THR	N-CA-CB	5.18	119.24	110.49
1	I	8	THR	N-CA-CB	5.18	119.24	110.49
1	H	8	THR	N-CA-CB	5.17	119.23	110.49
1	F	8	THR	N-CA-CB	5.17	119.23	110.49
1	D	8	THR	N-CA-CB	5.17	119.22	110.49
1	E	14	ASN	CA-CB-CG	-5.17	107.43	112.60
1	J	82	ASP	CA-CB-CG	5.17	117.77	112.60
1	G	8	THR	N-CA-CB	5.17	119.22	110.49
1	E	8	THR	N-CA-CB	5.16	119.22	110.49
4	O	125	ASP	CB-CA-C	-5.16	102.71	110.92
1	K	82	ASP	CA-CB-CG	5.16	117.76	112.60
1	G	14	ASN	CA-CB-CG	-5.16	107.44	112.60
1	K	8	THR	N-CA-CB	5.16	119.21	110.49
2	T	172	ILE	CA-C-N	5.16	127.19	120.28
2	T	172	ILE	C-N-CA	5.16	127.19	120.28
1	G	5	ASP	CA-CB-CG	-5.15	107.45	112.60
1	E	82	ASP	CA-CB-CG	5.15	117.75	112.60
1	F	82	ASP	CA-CB-CG	5.15	117.75	112.60
1	G	82	ASP	CA-CB-CG	5.14	117.75	112.60
2	T	27	ALA	CA-C-N	5.14	128.13	120.31
2	T	27	ALA	C-N-CA	5.14	128.13	120.31
1	E	23	PHE	CA-CB-CG	-5.14	108.66	113.80
5	S	112	LYS	N-CA-CB	5.14	119.17	110.49
1	H	82	ASP	CA-CB-CG	5.14	117.74	112.60
2	Q	179	ALA	CA-C-N	5.13	127.58	120.29
2	Q	179	ALA	C-N-CA	5.13	127.58	120.29
1	B	254	ASN	CA-C-N	5.13	131.34	121.54
1	B	254	ASN	C-N-CA	5.13	131.34	121.54
1	E	5	ASP	CA-CB-CG	-5.13	107.47	112.60
1	J	8	THR	N-CA-CB	5.13	119.16	110.49
1	J	23	PHE	CA-CB-CG	-5.13	108.67	113.80
3	L	689	GLU	CA-C-N	5.13	127.15	120.28
3	L	689	GLU	C-N-CA	5.13	127.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	5	ASP	CA-CB-CG	-5.12	107.47	112.60
1	I	23	PHE	CA-CB-CG	-5.12	108.68	113.80
2	P	172	ILE	CA-C-N	5.12	127.14	120.28
2	P	172	ILE	C-N-CA	5.12	127.14	120.28
5	R	112	LYS	N-CA-CB	5.12	119.14	110.49
3	M	684	THR	O-C-N	-5.12	118.27	121.85
1	H	5	ASP	CA-CB-CG	-5.12	107.48	112.60
1	I	82	ASP	CA-CB-CG	5.12	117.72	112.60
3	M	735	PRO	CA-C-N	5.12	131.32	121.54
3	M	735	PRO	C-N-CA	5.12	131.32	121.54
1	A	287	CYS	CA-C-N	5.12	128.93	121.31
1	A	287	CYS	C-N-CA	5.12	128.93	121.31
2	U	237	THR	N-CA-CB	5.11	117.64	110.12
2	U	179	ALA	CA-C-N	5.11	127.55	120.29
2	U	179	ALA	C-N-CA	5.11	127.55	120.29
1	F	23	PHE	CA-CB-CG	-5.11	108.69	113.80
1	C	23	PHE	CA-CB-CG	-5.10	108.70	113.80
3	L	297	LYS	CG-CD-CE	5.10	123.04	111.30
1	D	82	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	111	PRO	N-CA-C	5.08	119.29	111.21
1	H	111	PRO	N-CA-C	5.08	119.29	111.21
1	K	23	PHE	CA-CB-CG	-5.08	108.72	113.80
1	H	23	PHE	CA-CB-CG	-5.08	108.72	113.80
2	Q	237	THR	N-CA-CB	5.08	117.58	110.12
1	B	7	THR	N-CA-CB	5.07	119.05	110.49
1	I	111	PRO	N-CA-C	5.07	119.26	111.21
3	M	630	ALA	N-CA-C	5.06	117.45	111.33
1	D	23	PHE	CA-CB-CG	-5.06	108.74	113.80
1	D	111	PRO	N-CA-C	5.06	119.26	111.21
2	U	153	HIS	CA-C-N	5.06	126.93	120.56
2	U	153	HIS	C-N-CA	5.06	126.93	120.56
3	M	375	GLN	N-CA-C	5.06	116.79	111.28
1	F	111	PRO	N-CA-C	5.05	119.25	111.21
1	E	111	PRO	N-CA-C	5.05	119.24	111.21
2	T	212	GLU	O-C-N	-5.05	116.63	122.09
1	J	111	PRO	N-CA-C	5.05	119.24	111.21
3	L	547	THR	CA-C-N	5.05	127.05	120.28
3	L	547	THR	C-N-CA	5.05	127.05	120.28
2	T	49	LYS	CA-C-N	5.05	127.04	120.28
2	T	49	LYS	C-N-CA	5.05	127.04	120.28
2	P	125	ARG	CA-C-N	5.04	125.69	119.99
2	P	125	ARG	C-N-CA	5.04	125.69	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	153	HIS	CA-C-N	5.04	126.91	120.56
2	Q	153	HIS	C-N-CA	5.04	126.91	120.56
3	M	689	GLU	CA-C-N	5.04	127.03	120.28
3	M	689	GLU	C-N-CA	5.04	127.03	120.28
1	K	111	PRO	N-CA-C	5.04	119.22	111.21
1	G	111	PRO	N-CA-C	5.04	119.22	111.21
2	T	67	ALA	CA-C-N	5.03	127.44	120.29
2	T	67	ALA	C-N-CA	5.03	127.44	120.29
1	G	23	PHE	CA-CB-CG	-5.03	108.77	113.80
2	P	67	ALA	CA-C-N	5.03	127.43	120.29
2	P	67	ALA	C-N-CA	5.03	127.43	120.29
3	L	560	LEU	N-CA-C	5.03	116.76	111.28
1	H	113	ASN	CB-CA-C	5.02	115.95	108.87
4	O	155	GLU	CA-C-N	5.02	131.13	121.54
4	O	155	GLU	C-N-CA	5.02	131.13	121.54
1	B	287	CYS	CA-C-N	5.02	128.79	121.31
1	B	287	CYS	C-N-CA	5.02	128.79	121.31
2	P	49	LYS	CA-C-N	5.02	127.00	120.28
2	P	49	LYS	C-N-CA	5.02	127.00	120.28
1	A	91	THR	N-CA-CB	5.01	117.28	110.01
1	D	113	ASN	CB-CA-C	5.01	115.93	108.87
1	E	290	ASP	CA-CB-CG	-5.01	107.59	112.60
1	A	100	PRO	CA-C-N	5.00	127.49	120.28
1	A	100	PRO	C-N-CA	5.00	127.49	120.28
4	O	79	ASN	CA-CB-CG	-5.00	107.59	112.60
3	L	681	GLU	CA-C-N	5.00	126.98	120.28
3	L	681	GLU	C-N-CA	5.00	126.98	120.28
3	M	598	ASP	CA-CB-CG	-5.00	107.60	112.60
3	M	727	LYS	CA-C-N	5.00	128.83	120.62
3	M	727	LYS	C-N-CA	5.00	128.83	120.62

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	L	64	THR	CA
3	M	64	THR	CA

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain
1	A	258	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	30	ARG	Sidechain
1	A	314	ARG	Sidechain
1	A	39	ARG	Sidechain
1	A	41	ARG	Sidechain
1	B	242	TYR	Sidechain
1	B	25	GLY	Peptide
1	B	314	ARG	Sidechain
1	B	39	ARG	Sidechain
1	B	41	ARG	Sidechain
1	C	14	ASN	Peptide
1	C	223	LEU	Peptide
1	C	256	ARG	Sidechain
1	C	334	PRO	Peptide
1	C	71	TYR	Sidechain
1	D	14	ASN	Peptide
1	D	223	LEU	Peptide
1	D	256	ARG	Sidechain
1	D	334	PRO	Peptide
1	D	71	TYR	Sidechain
1	E	14	ASN	Peptide
1	E	223	LEU	Peptide
1	E	256	ARG	Sidechain
1	E	334	PRO	Peptide
1	E	71	TYR	Sidechain
1	F	14	ASN	Peptide
1	F	223	LEU	Peptide
1	F	256	ARG	Sidechain
1	F	334	PRO	Peptide
1	F	71	TYR	Sidechain
1	G	14	ASN	Peptide
1	G	223	LEU	Peptide
1	G	256	ARG	Sidechain
1	G	334	PRO	Peptide
1	G	71	TYR	Sidechain
1	H	14	ASN	Peptide
1	H	223	LEU	Peptide
1	H	256	ARG	Sidechain
1	H	334	PRO	Peptide
1	H	71	TYR	Sidechain
1	I	14	ASN	Peptide
1	I	223	LEU	Peptide
1	I	256	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	334	PRO	Peptide
1	I	71	TYR	Sidechain
1	J	14	ASN	Peptide
1	J	223	LEU	Peptide
1	J	256	ARG	Sidechain
1	J	334	PRO	Peptide
1	J	71	TYR	Sidechain
1	K	14	ASN	Peptide
1	K	223	LEU	Peptide
1	K	256	ARG	Sidechain
1	K	334	PRO	Peptide
1	K	71	TYR	Sidechain
3	L	129	TYR	Sidechain
3	L	148	ARG	Sidechain
3	L	195	TYR	Sidechain
3	L	246	ARG	Sidechain
3	L	252	ARG	Sidechain
3	L	456	ARG	Sidechain
3	L	675	ARG	Sidechain
3	L	716	ARG	Sidechain
3	L	791	ARG	Sidechain
3	L	812	ARG	Sidechain
3	L	837	TYR	Sidechain
3	M	104	TYR	Sidechain
3	M	148	ARG	Sidechain
3	M	195	TYR	Sidechain
3	M	246	ARG	Sidechain
3	M	252	ARG	Sidechain
3	M	456	ARG	Sidechain
3	M	504	TYR	Sidechain
3	M	675	ARG	Sidechain
3	M	716	ARG	Sidechain
3	M	791	ARG	Sidechain
3	M	811	ARG	Sidechain
3	M	837	TYR	Sidechain
2	P	241	PHE	Sidechain
2	P	261	TYR	Sidechain
2	Q	60	TYR	Sidechain
5	R	112	LYS	Peptide
5	R	163	GLY	Peptide
5	S	112	LYS	Peptide
5	S	163	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	T	241	PHE	Sidechain
2	U	60	TYR	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	2925	0	2887	81	0
1	B	2925	0	2887	105	0
1	C	2925	0	2886	71	0
1	D	2925	0	2887	67	0
1	E	2925	0	2887	62	0
1	F	2925	0	2887	70	0
1	G	2925	0	2887	54	0
1	H	2925	0	2887	70	0
1	I	2925	0	2885	43	0
1	J	2925	0	2887	38	0
1	K	2925	0	2887	63	0
2	P	1881	0	1879	93	0
2	Q	1881	0	1879	108	0
2	T	1952	0	1960	94	0
2	U	1952	0	1960	91	0
3	L	6503	0	6511	12	0
3	M	6503	0	6511	12	0
4	N	1159	0	1124	1	0
4	O	1159	0	1124	1	0
5	R	1144	0	1109	15	0
5	S	1144	0	1111	16	0
All	All	57453	0	56922	654	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 6.

All (654) 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:B:44:GLY:CA	1:H:171:TYR:HD1	0.83	1.46
1:B:272:GLU:HG2	1:C:41:ARG:CD	1.52	1.38
1:B:49:MET:SD	1:H:171:TYR:CD2	2.17	1.38
1:B:44:GLY:HA3	1:H:171:TYR:CD1	0.79	1.32
1:A:46:MET:HG3	1:B:170:GLY:CA	1.61	1.30
1:B:49:MET:CG	1:H:169:GLU:O	1.87	1.23
1:C:46:MET:SD	1:G:170:GLY:HA2	1.78	1.23
1:C:246:ASP:HB2	1:G:289:ILE:CG2	1.70	1.20
1:D:170:GLY:HA3	1:K:46:MET:CE	1.70	1.19
1:B:49:MET:HG2	1:H:169:GLU:O	1.38	1.18
1:A:44:GLY:CA	1:B:171:TYR:CD1	2.27	1.18
1:C:44:GLY:HA2	1:G:171:TYR:HD1	1.11	1.14
1:B:272:GLU:HG2	1:C:41:ARG:HD3	1.26	1.13
1:B:272:GLU:OE2	1:C:41:ARG:CZ	1.73	1.13
1:A:46:MET:HG3	1:B:170:GLY:HA2	1.16	1.12
1:B:44:GLY:HA3	1:H:171:TYR:CG	1.85	1.12
1:C:44:GLY:CA	1:G:171:TYR:CD1	2.33	1.12
1:D:170:GLY:CA	1:K:46:MET:SD	2.37	1.12
1:C:246:ASP:HB2	1:G:289:ILE:HG23	1.28	1.12
1:B:49:MET:SD	1:H:169:GLU:O	2.09	1.11
1:D:170:GLY:HA3	1:K:46:MET:SD	1.91	1.10
1:A:44:GLY:HA3	1:B:171:TYR:CD1	1.87	1.10
1:G:41:ARG:HD3	1:H:272:GLU:OE2	1.53	1.09
1:C:46:MET:HG3	1:G:170:GLY:CA	1.81	1.09
1:D:170:GLY:HA3	1:K:46:MET:HE2	1.32	1.09
5:R:80:PHE:CD2	5:S:51:ARG:HD2	1.86	1.09
1:K:223:LEU:HB3	2:Q:244:ARG:HH12	1.11	1.09
1:C:46:MET:CG	1:G:170:GLY:CA	2.31	1.08
1:A:46:MET:CG	1:B:170:GLY:HA2	1.83	1.07
1:C:44:GLY:HA2	1:G:171:TYR:CD1	1.88	1.07
1:B:45:VAL:O	1:H:171:TYR:O	1.70	1.06
1:C:46:MET:HG3	1:G:170:GLY:HA3	1.13	1.06
1:D:170:GLY:CA	1:K:46:MET:CE	2.33	1.05
1:D:357:MET:SD	1:K:47:VAL:HG21	1.97	1.05
1:A:171:TYR:HA	1:E:44:GLY:HA2	1.34	1.04
1:B:45:VAL:N	1:H:171:TYR:HA	1.70	1.04
1:K:223:LEU:CB	2:Q:244:ARG:HH12	1.71	1.04
1:C:46:MET:CG	1:G:170:GLY:HA3	1.87	1.03
1:D:171:TYR:CZ	1:K:49:MET:SD	2.53	1.01
1:B:49:MET:SD	1:H:171:TYR:CE2	2.53	1.01
1:A:292:ARG:HD2	1:E:246:ASP:OD1	1.62	1.00
1:B:272:GLU:HG2	1:C:41:ARG:HD2	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:MET:HG3	1:B:170:GLY:HA3	1.45	0.99
5:R:80:PHE:HD2	5:S:51:ARG:CD	1.76	0.98
1:C:44:GLY:HA3	1:G:171:TYR:CE1	2.00	0.97
1:I:292:ARG:HD2	1:J:246:ASP:OD1	1.64	0.96
1:C:292:ARG:HD2	1:F:246:ASP:OD1	1.63	0.96
1:A:46:MET:CG	1:B:170:GLY:CA	2.41	0.96
1:B:46:MET:SD	1:H:167:ILE:HG12	2.04	0.96
1:K:223:LEU:HD22	2:Q:237:THR:HG23	1.47	0.96
2:T:165:VAL:HG13	2:U:165:VAL:HG23	1.47	0.95
2:P:165:VAL:HG13	2:Q:165:VAL:HG23	1.48	0.95
1:A:170:GLY:HA3	1:E:49:MET:SD	2.06	0.95
1:D:246:ASP:OD1	1:F:292:ARG:HD2	1.64	0.94
1:C:246:ASP:CB	1:G:289:ILE:HG23	1.96	0.94
1:C:44:GLY:CA	1:G:171:TYR:HD1	1.75	0.93
1:A:41:ARG:HH11	1:C:272:GLU:HG3	1.33	0.93
1:A:41:ARG:HD3	1:C:272:GLU:HG2	1.51	0.93
1:B:41:ARG:HH11	1:G:272:GLU:HG3	1.35	0.92
1:B:44:GLY:HA3	1:H:171:TYR:CE1	1.98	0.92
1:B:46:MET:HE2	1:H:150:THR:O	1.67	0.92
1:B:272:GLU:CG	1:C:41:ARG:CD	2.46	0.91
1:B:44:GLY:CA	1:H:171:TYR:CD1	1.75	0.91
1:B:41:ARG:HD3	1:G:272:GLU:HG2	1.53	0.90
1:A:44:GLY:HA2	1:B:171:TYR:CD1	2.06	0.90
1:A:44:GLY:CA	1:B:171:TYR:HD1	1.75	0.90
1:C:44:GLY:HA3	1:G:171:TYR:CD1	2.04	0.89
1:A:199:GLY:HA2	1:C:114:PRO:HG3	1.55	0.88
1:K:223:LEU:HB3	2:Q:244:ARG:NH1	1.87	0.88
1:B:199:GLY:HA2	1:G:114:PRO:HG3	1.56	0.88
1:B:45:VAL:H	1:H:171:TYR:C	1.82	0.88
5:R:31:LYS:HE2	5:S:52:ASP:OD1	1.73	0.87
1:C:46:MET:CG	1:G:170:GLY:HA2	2.00	0.87
1:A:246:ASP:HB2	1:B:289:ILE:CG2	2.04	0.86
1:B:46:MET:HE2	1:H:170:GLY:H	1.39	0.86
1:K:223:LEU:HD22	2:Q:237:THR:CG2	2.06	0.85
1:A:145:TYR:OH	1:E:46:MET:HB3	1.76	0.85
2:T:165:VAL:HG13	2:U:165:VAL:CG2	2.06	0.85
2:P:165:VAL:HG13	2:Q:165:VAL:CG2	2.06	0.85
2:P:53:THR:HA	2:Q:57:LEU:HD11	1.56	0.85
2:T:53:THR:HA	2:U:57:LEU:HD11	1.56	0.84
1:C:170:GLY:HA3	1:F:49:MET:SD	2.17	0.84
1:C:171:TYR:HA	1:F:44:GLY:HA2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:OE1	1:F:204:THR:HG23	1.77	0.84
1:B:49:MET:SD	1:H:171:TYR:N	2.51	0.84
2:P:57:LEU:N	2:Q:57:LEU:HD21	1.93	0.84
2:T:57:LEU:N	2:U:57:LEU:HD21	1.93	0.83
1:C:145:TYR:OH	1:F:47:VAL:N	2.10	0.83
1:B:49:MET:SD	1:H:171:TYR:CG	2.71	0.83
1:C:289:ILE:HG23	1:F:246:ASP:HB2	1.60	0.82
1:B:49:MET:HE1	1:H:171:TYR:CD1	2.14	0.82
1:A:171:TYR:HA	1:E:44:GLY:CA	2.09	0.82
1:D:47:VAL:N	1:F:145:TYR:OH	2.12	0.81
5:R:80:PHE:CE2	5:S:51:ARG:HD2	2.15	0.81
1:A:272:GLU:HG3	1:F:41:ARG:HH11	1.46	0.81
1:D:44:GLY:HA2	1:F:171:TYR:HA	1.62	0.81
1:I:171:TYR:HA	1:J:44:GLY:HA2	1.62	0.81
1:B:44:GLY:C	1:H:171:TYR:HA	2.05	0.81
1:A:272:GLU:HG2	1:F:41:ARG:HD3	1.61	0.81
1:I:289:ILE:HG23	1:J:246:ASP:HB2	1.62	0.81
1:D:246:ASP:HB2	1:F:289:ILE:HG23	1.62	0.81
1:A:170:GLY:HA2	1:E:46:MET:HG3	1.64	0.80
1:B:44:GLY:N	1:H:171:TYR:HD1	1.77	0.80
1:I:145:TYR:OH	1:J:47:VAL:N	2.12	0.80
1:D:170:GLY:HA2	1:K:46:MET:SD	2.22	0.79
1:D:49:MET:SD	1:F:170:GLY:HA3	2.22	0.79
1:I:170:GLY:HA3	1:J:49:MET:SD	2.22	0.78
1:K:223:LEU:HD22	2:Q:244:ARG:HH22	1.47	0.78
1:A:292:ARG:CD	1:E:246:ASP:OD1	2.33	0.77
1:B:114:PRO:HG3	1:C:199:GLY:HA2	1.66	0.77
2:P:88:LEU:O	2:Q:92:ILE:HD11	1.85	0.77
2:T:88:LEU:O	2:U:92:ILE:HD11	1.85	0.77
5:R:31:LYS:CE	5:S:51:ARG:HH22	1.98	0.77
1:B:45:VAL:C	1:H:171:TYR:O	2.28	0.76
1:G:223:LEU:HD22	2:Q:66:ASP:CG	2.10	0.76
1:D:170:GLY:CA	1:K:46:MET:HE2	2.08	0.76
5:R:31:LYS:CE	5:S:52:ASP:OD1	2.32	0.76
1:B:49:MET:CE	1:H:171:TYR:H	1.99	0.76
1:A:289:ILE:HG23	1:E:246:ASP:HB2	1.68	0.75
2:P:57:LEU:HA	2:Q:57:LEU:HD23	1.69	0.75
2:T:57:LEU:HA	2:U:57:LEU:HD23	1.69	0.75
1:B:272:GLU:OE2	1:C:41:ARG:NH2	2.18	0.75
1:C:246:ASP:HB2	1:G:289:ILE:HG22	1.68	0.74
1:K:223:LEU:CD2	2:Q:237:THR:CG2	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:TYR:CZ	1:I:49:MET:SD	2.80	0.74
1:B:44:GLY:N	1:H:171:TYR:CD1	2.54	0.74
1:E:171:TYR:CD1	1:I:45:VAL:N	2.48	0.74
1:D:171:TYR:OH	1:K:49:MET:SD	2.46	0.74
1:A:114:PRO:HG3	1:F:199:GLY:HA2	1.69	0.73
1:B:45:VAL:H	1:H:171:TYR:HA	1.48	0.73
2:P:165:VAL:CG1	2:Q:165:VAL:HG23	2.19	0.73
1:K:223:LEU:CD2	2:Q:244:ARG:HH22	2.02	0.73
1:C:44:GLY:CA	1:G:171:TYR:CE1	2.68	0.72
1:J:199:GLY:HA2	1:K:114:PRO:HG3	1.71	0.72
1:A:272:GLU:HG3	1:F:41:ARG:NH1	2.04	0.72
5:R:31:LYS:HE2	5:S:51:ARG:HH22	1.54	0.72
2:T:165:VAL:CG1	2:U:165:VAL:HG23	2.19	0.72
1:D:199:GLY:HA2	1:E:114:PRO:HG3	1.71	0.71
1:A:246:ASP:HB2	1:B:289:ILE:HG22	1.72	0.71
2:P:56:GLU:C	2:Q:57:LEU:HD21	2.15	0.71
1:D:170:GLY:HA2	1:K:46:MET:CE	2.19	0.71
1:B:45:VAL:H	1:H:171:TYR:CA	2.04	0.71
1:B:45:VAL:N	1:H:171:TYR:CA	2.50	0.71
1:B:46:MET:CE	1:H:150:THR:O	2.39	0.70
1:B:272:GLU:CG	1:C:41:ARG:HD3	2.13	0.70
2:P:218:GLU:OE1	2:Q:214:TYR:CE1	2.44	0.70
2:T:218:GLU:OE1	2:U:214:TYR:CE1	2.44	0.70
1:C:246:ASP:CG	1:G:289:ILE:HG23	2.16	0.70
2:T:56:GLU:C	2:U:57:LEU:HD21	2.15	0.70
2:T:57:LEU:N	2:U:57:LEU:CD2	2.55	0.69
1:D:171:TYR:HE1	1:K:44:GLY:HA3	1.55	0.69
2:P:57:LEU:N	2:Q:57:LEU:CD2	2.55	0.69
1:A:41:ARG:HH11	1:C:272:GLU:CG	2.04	0.69
1:A:44:GLY:HA2	1:B:171:TYR:HD1	1.45	0.68
1:A:246:ASP:O	1:B:327:MET:HE1	1.93	0.68
1:B:46:MET:HE1	1:H:144:LEU:HD21	1.75	0.68
1:D:47:VAL:H	1:F:145:TYR:HH	1.39	0.68
2:T:53:THR:OG1	2:U:53:THR:OG1	2.08	0.68
1:B:44:GLY:CA	1:H:171:TYR:HA	2.24	0.68
1:A:114:PRO:CG	1:F:199:GLY:HA2	2.23	0.68
1:D:171:TYR:CE1	1:K:49:MET:SD	2.86	0.67
1:A:44:GLY:HA3	1:B:171:TYR:CE1	2.29	0.67
1:C:170:GLY:HA2	1:F:46:MET:HG3	1.75	0.67
1:B:46:MET:HE2	1:H:170:GLY:N	2.08	0.67
1:B:41:ARG:HH11	1:G:272:GLU:CG	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:80:PHE:CD2	5:S:51:ARG:CD	2.58	0.66
1:I:114:PRO:HG3	1:K:199:GLY:HA2	1.76	0.66
1:B:65:GLY:HA3	1:H:288:ASP:HB3	1.78	0.66
1:E:199:GLY:HA2	1:F:114:PRO:HG3	1.76	0.66
2:P:56:GLU:C	2:Q:57:LEU:CD2	2.69	0.66
5:R:80:PHE:HD2	5:S:51:ARG:NE	1.93	0.65
1:A:45:VAL:H	1:B:171:TYR:HA	1.60	0.65
1:A:246:ASP:OD1	1:B:289:ILE:HG23	1.95	0.65
2:T:56:GLU:C	2:U:57:LEU:CD2	2.69	0.65
1:G:197:GLU:HB2	1:H:115:LYS:HD2	1.79	0.65
1:E:289:ILE:CG2	1:I:246:ASP:CG	2.70	0.64
1:A:41:ARG:CD	1:C:272:GLU:HG2	2.25	0.64
1:I:145:TYR:HH	1:J:47:VAL:H	1.42	0.64
1:A:41:ARG:NH1	1:C:272:GLU:HG3	2.10	0.64
1:H:223:LEU:HD22	2:T:24:GLN:OE1	1.98	0.64
2:P:53:THR:OG1	2:Q:53:THR:OG1	2.08	0.64
1:C:145:TYR:HH	1:F:47:VAL:N	1.96	0.64
1:A:327:MET:HE3	1:E:247:GLY:HA3	1.81	0.63
1:B:41:ARG:NH1	1:G:272:GLU:HG3	2.10	0.63
1:A:272:GLU:OE1	1:F:204:THR:CG2	2.45	0.63
1:A:246:ASP:O	1:B:327:MET:CE	2.47	0.63
1:C:46:MET:CE	1:G:170:GLY:HA2	2.29	0.63
2:P:36:SER:O	2:Q:39:LEU:HD13	1.99	0.62
1:A:44:GLY:HA2	1:B:171:TYR:HA	1.80	0.62
1:B:272:GLU:OE1	1:C:204:THR:CG2	2.48	0.62
1:B:272:GLU:OE1	1:C:204:THR:HG23	2.00	0.62
2:T:36:SER:O	2:U:39:LEU:HD13	1.99	0.62
1:B:41:ARG:CD	1:G:272:GLU:HG2	2.27	0.62
1:D:46:MET:HG3	1:F:170:GLY:HA2	1.82	0.61
1:A:327:MET:CE	1:E:246:ASP:O	2.48	0.61
1:A:173:LEU:CD2	1:E:42:HIS:CD2	2.83	0.61
1:D:47:VAL:N	1:F:145:TYR:HH	1.95	0.60
1:A:246:ASP:CG	1:B:289:ILE:HG23	2.26	0.60
1:D:171:TYR:HE1	1:K:44:GLY:CA	2.13	0.60
1:I:170:GLY:HA2	1:J:46:MET:HG3	1.82	0.60
2:P:256:LEU:HD11	2:Q:257:GLU:OE2	2.02	0.60
1:E:171:TYR:CE2	1:I:49:MET:SD	2.95	0.59
1:D:269:ILE:O	1:E:175:HIS:HB3	2.01	0.59
1:J:269:ILE:O	1:K:175:HIS:HB3	2.01	0.59
5:R:31:LYS:HE2	5:S:51:ARG:NH2	2.17	0.59
5:R:31:LYS:CE	5:S:51:ARG:NH2	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:MET:HE3	1:E:247:GLY:CA	2.33	0.59
2:T:57:LEU:HD21	2:U:53:THR:O	2.03	0.59
1:C:246:ASP:CB	1:G:289:ILE:CG2	2.60	0.59
1:D:357:MET:SD	1:K:47:VAL:CG2	2.84	0.59
1:I:145:TYR:HH	1:J:47:VAL:N	1.96	0.59
1:A:292:ARG:HD2	1:E:246:ASP:CG	2.26	0.58
1:D:170:GLY:C	1:K:46:MET:SD	2.86	0.58
1:G:228:GLU:OE2	2:Q:65:LYS:HE2	2.04	0.58
1:E:269:ILE:O	1:F:175:HIS:HB3	2.03	0.58
2:P:57:LEU:HD21	2:Q:53:THR:O	2.03	0.58
1:B:44:GLY:C	1:H:171:TYR:CD1	2.75	0.58
1:J:204:THR:HG23	1:K:272:GLU:CD	2.29	0.57
1:I:175:HIS:HB3	1:K:269:ILE:O	2.03	0.57
2:T:98:GLU:C	2:U:99:LEU:HD13	2.29	0.57
1:G:197:GLU:O	1:H:115:LYS:HG3	2.03	0.57
2:T:53:THR:CA	2:U:57:LEU:HD11	2.33	0.57
1:A:170:GLY:HA2	1:E:46:MET:CG	2.34	0.57
2:P:221:TYR:HB3	2:Q:221:TYR:CB	2.35	0.57
5:R:31:LYS:NZ	5:S:51:ARG:HH22	2.02	0.57
1:B:45:VAL:N	1:H:171:TYR:C	2.58	0.57
1:C:46:MET:SD	1:G:170:GLY:CA	2.68	0.57
1:B:46:MET:SD	1:H:167:ILE:CG1	2.86	0.57
2:T:221:TYR:HB3	2:U:221:TYR:CB	2.35	0.57
2:P:127:MET:O	2:Q:130:ILE:HD11	2.04	0.57
2:P:98:GLU:C	2:Q:99:LEU:HD13	2.29	0.56
1:B:46:MET:CE	1:H:170:GLY:H	2.14	0.56
1:D:204:THR:HG23	1:E:272:GLU:CD	2.29	0.56
1:E:41:ARG:HD3	1:F:272:GLU:HG2	1.87	0.56
2:P:43:LEU:HD21	2:Q:39:LEU:O	2.06	0.56
2:T:127:MET:O	2:U:130:ILE:HD11	2.04	0.56
2:P:162:TYR:CE1	2:Q:165:VAL:HG11	2.40	0.56
2:P:214:TYR:HB3	2:Q:214:TYR:CB	2.36	0.56
1:B:246:ASP:OD1	1:H:292:ARG:NH1	2.38	0.56
2:T:214:TYR:HB3	2:U:214:TYR:HB2	1.88	0.56
1:D:246:ASP:O	1:F:327:MET:CE	2.54	0.56
2:P:218:GLU:OE1	2:Q:214:TYR:CD1	2.60	0.55
1:B:45:VAL:HB	1:H:172:ALA:CB	2.37	0.55
1:A:44:GLY:N	1:B:171:TYR:HD1	2.04	0.55
1:I:327:MET:CE	1:J:246:ASP:O	2.54	0.55
2:T:162:TYR:CE1	2:U:165:VAL:HG11	2.40	0.55
2:T:218:GLU:OE1	2:U:214:TYR:CD1	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:109:ARG:HH22	3:L:153:PRO:HG2	1.71	0.55
1:I:272:GLU:HG2	1:K:41:ARG:HD3	1.88	0.55
2:T:214:TYR:HB3	2:U:214:TYR:CB	2.36	0.55
2:P:214:TYR:HB3	2:Q:214:TYR:HB2	1.88	0.55
2:T:43:LEU:HD21	2:U:39:LEU:O	2.05	0.55
1:B:272:GLU:CG	1:C:41:ARG:HD2	2.30	0.54
1:A:44:GLY:N	1:B:171:TYR:CD1	2.74	0.54
2:T:36:SER:HB3	2:U:32:ALA:O	2.08	0.54
2:P:36:SER:HB3	2:Q:32:ALA:O	2.08	0.54
1:A:145:TYR:OH	1:E:47:VAL:N	2.28	0.54
1:B:49:MET:CE	1:H:171:TYR:CD1	2.90	0.54
1:C:170:GLY:HA2	1:F:46:MET:CG	2.37	0.54
1:A:48:GLY:HA3	3:M:543:PHE:CZ	2.42	0.54
1:A:327:MET:HE1	1:E:246:ASP:C	2.33	0.53
2:T:64:LEU:HD13	2:U:63:ALA:C	2.33	0.53
1:E:171:TYR:OH	1:I:49:MET:SD	2.64	0.53
1:B:44:GLY:CA	1:H:171:TYR:CB	2.86	0.53
2:P:53:THR:CA	2:Q:57:LEU:HD11	2.33	0.53
5:R:31:LYS:NZ	5:S:52:ASP:OD1	2.42	0.53
1:B:44:GLY:HA2	1:H:171:TYR:CB	2.39	0.53
1:A:173:LEU:HD23	1:E:42:HIS:CD2	2.43	0.53
1:D:171:TYR:N	1:K:46:MET:SD	2.82	0.53
1:A:246:ASP:HB2	1:B:289:ILE:HG23	1.88	0.53
1:B:46:MET:CE	1:H:170:GLY:N	2.71	0.53
2:P:162:TYR:HE1	2:Q:165:VAL:CG1	2.22	0.53
1:E:289:ILE:HG23	1:I:246:ASP:CG	2.34	0.52
2:T:162:TYR:HE1	2:U:165:VAL:CG1	2.22	0.52
1:B:44:GLY:HA2	1:H:171:TYR:HB3	1.91	0.52
1:G:197:GLU:O	1:H:115:LYS:CG	2.56	0.52
1:J:197:GLU:O	1:K:114:PRO:HA	2.09	0.52
1:K:223:LEU:CD2	2:Q:237:THR:HG23	2.27	0.52
2:P:64:LEU:HD13	2:Q:63:ALA:C	2.33	0.52
1:D:197:GLU:O	1:E:114:PRO:HA	2.10	0.52
2:P:70:LYS:C	2:Q:71:LEU:HD23	2.35	0.52
2:T:70:LYS:C	2:U:71:LEU:HD23	2.35	0.52
3:M:109:ARG:HH22	3:M:153:PRO:HG2	1.75	0.52
2:P:88:LEU:O	2:Q:92:ILE:CD1	2.58	0.51
5:R:80:PHE:CD2	5:S:51:ARG:NE	2.77	0.51
1:B:44:GLY:CA	1:H:171:TYR:CG	2.65	0.51
1:D:170:GLY:HA2	1:K:46:MET:HE1	1.92	0.51
2:T:64:LEU:HD13	2:U:64:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:TYR:CE1	1:K:44:GLY:CA	2.94	0.51
1:K:223:LEU:HB2	2:Q:244:ARG:HH12	1.70	0.51
1:B:49:MET:HE1	1:H:171:TYR:CE1	2.46	0.51
1:D:170:GLY:CA	1:K:46:MET:HE1	2.37	0.51
1:G:223:LEU:HD22	2:Q:66:ASP:OD1	2.11	0.51
2:T:193:LEU:HD13	2:U:190:CYS:O	2.11	0.51
1:A:46:MET:SD	1:B:170:GLY:HA2	2.49	0.51
2:T:71:LEU:HD13	2:U:70:LYS:C	2.36	0.51
2:T:81:ALA:O	2:U:85:VAL:CG2	2.59	0.51
1:B:49:MET:CE	1:H:171:TYR:CE1	2.93	0.51
2:P:81:ALA:O	2:Q:85:VAL:CG2	2.59	0.51
1:A:45:VAL:N	1:B:171:TYR:HA	2.26	0.51
1:A:168:TYR:HB3	1:E:66:ILE:HD11	1.92	0.51
1:C:168:TYR:HB3	1:F:66:ILE:HD11	1.93	0.51
2:P:64:LEU:HD13	2:Q:64:LEU:N	2.26	0.51
2:P:193:LEU:HD13	2:Q:190:CYS:O	2.11	0.51
1:J:41:ARG:HD3	1:K:272:GLU:HG2	1.92	0.50
2:T:214:TYR:CD2	2:U:211:ALA:HB1	2.47	0.50
2:P:71:LEU:HD13	2:Q:70:LYS:C	2.36	0.50
1:D:66:ILE:HD11	1:F:168:TYR:HB3	1.93	0.50
2:T:57:LEU:HD21	2:U:56:GLU:HB3	1.94	0.50
1:C:377:PHE:CD1	1:F:45:VAL:HG21	2.46	0.50
1:D:41:ARG:HD3	1:E:272:GLU:HG2	1.92	0.50
1:A:144:LEU:HD23	1:E:46:MET:HE1	1.93	0.50
5:S:47:LYS:HZ3	5:S:68:ASP:CG	2.18	0.50
1:C:122:THR:HG21	1:C:372:VAL:HG22	1.94	0.49
1:F:122:THR:HG21	1:F:372:VAL:HG22	1.94	0.49
1:C:292:ARG:HH11	1:F:246:ASP:CG	2.19	0.49
1:K:122:THR:HG21	1:K:372:VAL:HG22	1.95	0.49
2:P:57:LEU:HD21	2:Q:56:GLU:HB3	1.94	0.49
2:T:60:TYR:HD1	2:U:57:LEU:HD22	1.77	0.49
1:I:145:TYR:OH	1:J:46:MET:HB3	2.12	0.49
2:T:190:CYS:SG	2:U:189:LYS:HG3	2.53	0.49
2:P:214:TYR:CD2	2:Q:211:ALA:HB1	2.47	0.49
1:D:122:THR:HG21	1:D:372:VAL:HG22	1.95	0.49
2:T:46:LEU:HD13	2:U:50:LEU:HD13	1.95	0.49
1:G:122:THR:HG21	1:G:372:VAL:HG22	1.95	0.49
1:I:168:TYR:HB3	1:J:66:ILE:HD11	1.93	0.49
2:P:60:TYR:HD1	2:Q:57:LEU:HD22	1.78	0.49
2:P:70:LYS:O	2:Q:71:LEU:HD23	2.13	0.49
2:P:88:LEU:HB3	2:Q:92:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:834:MET:HE3	3:M:838:PHE:CZ	2.48	0.49
1:D:223:LEU:HD22	2:P:195:GLU:HG2	1.94	0.49
2:P:221:TYR:HB3	2:Q:221:TYR:HB2	1.95	0.49
1:A:175:HIS:HB3	1:F:269:ILE:O	2.13	0.49
1:B:49:MET:HE1	1:H:171:TYR:CG	2.47	0.49
2:P:46:LEU:HD13	2:Q:50:LEU:HD13	1.95	0.49
5:R:134:GLU:CD	5:R:134:GLU:H	2.21	0.49
1:B:45:VAL:HB	1:H:172:ALA:HB2	1.95	0.48
1:C:377:PHE:CG	1:F:45:VAL:HG21	2.48	0.48
1:D:45:VAL:HG21	1:F:377:PHE:CG	2.48	0.48
1:D:46:MET:HB3	1:F:145:TYR:OH	2.12	0.48
1:G:41:ARG:CD	1:H:272:GLU:OE2	2.43	0.48
2:T:88:LEU:HB3	2:U:92:ILE:HD13	1.95	0.48
1:A:115:LYS:HG3	1:F:197:GLU:HB2	1.94	0.48
2:T:221:TYR:HB3	2:U:221:TYR:HB2	1.95	0.48
2:T:70:LYS:O	2:U:71:LEU:HD23	2.13	0.48
1:E:289:ILE:HG23	1:I:246:ASP:OD1	2.12	0.48
2:P:172:ILE:HG21	2:Q:173:GLU:HA	1.94	0.48
1:D:46:MET:CG	1:F:170:GLY:HA2	2.43	0.48
1:H:122:THR:HG21	1:H:372:VAL:HG22	1.95	0.48
1:I:122:THR:HG21	1:I:372:VAL:HG22	1.94	0.48
1:I:377:PHE:CG	1:J:45:VAL:HG21	2.48	0.48
2:T:172:ILE:HG21	2:U:173:GLU:HA	1.94	0.48
1:I:170:GLY:HA2	1:J:46:MET:CG	2.43	0.48
1:J:122:THR:HG21	1:J:372:VAL:HG22	1.95	0.48
2:T:88:LEU:O	2:U:92:ILE:CD1	2.58	0.48
2:P:190:CYS:SG	2:Q:189:LYS:HG3	2.53	0.48
2:P:211:ALA:O	2:Q:214:TYR:CE2	2.67	0.48
2:T:211:ALA:O	2:U:214:TYR:CE2	2.67	0.48
1:A:44:GLY:CA	1:B:171:TYR:HA	2.44	0.48
1:A:114:PRO:HA	1:F:197:GLU:HA	1.96	0.48
1:B:62:SER:O	1:H:290:ASP:OD1	2.32	0.48
1:C:170:GLY:CA	1:F:46:MET:HG3	2.42	0.48
1:E:122:THR:HG21	1:E:372:VAL:HG22	1.94	0.48
2:P:228:LEU:HB3	2:Q:228:LEU:HB3	1.96	0.48
1:A:327:MET:HE1	1:E:246:ASP:O	2.13	0.48
2:P:53:THR:O	2:Q:57:LEU:HD21	2.14	0.48
2:P:98:GLU:O	2:Q:99:LEU:HD13	2.14	0.48
2:P:140:LYS:HB2	2:Q:141:MET:SD	2.54	0.48
2:P:217:LYS:HB2	2:Q:218:GLU:OE2	2.14	0.48
2:T:140:LYS:HB2	2:U:141:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:CD	1:F:204:THR:HG23	2.38	0.47
1:E:197:GLU:HB2	1:F:115:LYS:HG3	1.96	0.47
1:I:115:LYS:HG3	1:K:197:GLU:HB2	1.96	0.47
1:I:272:GLU:CD	1:K:204:THR:HG23	2.40	0.47
4:N:66:LEU:HD22	4:N:100:LYS:HB3	1.97	0.47
2:T:98:GLU:O	2:U:99:LEU:HD13	2.14	0.47
3:L:834:MET:HE3	3:L:838:PHE:CZ	2.49	0.47
1:E:204:THR:HG23	1:F:272:GLU:CD	2.40	0.47
1:A:357:MET:SD	1:E:47:VAL:HG22	2.54	0.47
1:E:353:THR:HG21	1:I:47:VAL:HG11	1.95	0.47
1:G:228:GLU:OE2	2:Q:65:LYS:NZ	2.46	0.47
1:I:377:PHE:CD1	1:J:45:VAL:HG21	2.50	0.47
2:T:53:THR:O	2:U:57:LEU:HD21	2.14	0.47
2:T:228:LEU:HB3	2:U:228:LEU:HB3	1.96	0.47
1:A:4:GLU:N	1:A:4:GLU:CD	2.73	0.47
1:A:170:GLY:CA	1:E:46:MET:HG3	2.41	0.47
2:P:148:LEU:HD13	2:Q:148:LEU:N	2.30	0.47
2:T:148:LEU:HD13	2:U:148:LEU:N	2.30	0.47
1:D:41:ARG:NH1	1:E:272:GLU:HG3	2.30	0.47
2:P:46:LEU:HB3	2:Q:46:LEU:HB3	1.97	0.47
2:P:197:LEU:HD12	2:Q:200:VAL:HG21	1.96	0.47
1:A:327:MET:CE	1:E:246:ASP:C	2.87	0.47
1:C:161:VAL:HG12	1:C:163:HIS:CE1	2.51	0.46
1:D:269:ILE:O	1:E:175:HIS:CB	2.63	0.46
1:A:289:ILE:CG2	1:E:246:ASP:HB2	2.39	0.46
2:P:165:VAL:HG13	2:Q:165:VAL:HG21	1.93	0.46
1:D:161:VAL:HG12	1:D:163:HIS:CE1	2.51	0.46
1:G:161:VAL:HG12	1:G:163:HIS:CE1	2.51	0.46
1:J:41:ARG:NH1	1:K:272:GLU:HG3	2.30	0.46
1:A:102:GLU:HB2	1:A:103:HIS:CD2	2.50	0.46
1:A:114:PRO:HG3	1:F:199:GLY:CA	2.42	0.46
1:A:246:ASP:CB	1:B:289:ILE:HG23	2.45	0.46
2:T:214:TYR:HD2	2:U:211:ALA:O	1.99	0.46
2:T:217:LYS:HB2	2:U:218:GLU:OE2	2.14	0.46
1:D:45:VAL:HG21	1:F:377:PHE:CD1	2.50	0.46
1:F:161:VAL:HG12	1:F:163:HIS:CE1	2.51	0.46
1:H:228:GLU:HA	1:H:231:THR:HG22	1.98	0.46
1:I:161:VAL:HG12	1:I:163:HIS:CE1	2.51	0.46
1:J:161:VAL:HG12	1:J:163:HIS:CE1	2.51	0.46
1:K:161:VAL:HG12	1:K:163:HIS:CE1	2.51	0.46
2:T:249:LEU:HB3	2:U:249:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:600:ASN:HA	3:L:651:VAL:HG22	1.98	0.46
1:G:228:GLU:OE2	2:Q:65:LYS:CE	2.63	0.46
1:K:223:LEU:HD22	2:Q:244:ARG:NH2	2.25	0.46
2:P:249:LEU:HB3	2:Q:249:LEU:HB3	1.98	0.46
2:P:252:SER:HB3	2:Q:253:ILE:HD11	1.98	0.46
1:B:102:GLU:HB2	1:B:103:HIS:CD2	2.50	0.46
1:E:161:VAL:HG12	1:E:163:HIS:CE1	2.50	0.46
1:K:228:GLU:HA	1:K:231:THR:HG22	1.98	0.46
2:T:197:LEU:HD12	2:U:200:VAL:HG21	1.96	0.46
3:L:812:ARG:HD3	3:L:814:SER:H	1.80	0.46
1:A:114:PRO:HG3	1:F:196:THR:O	2.15	0.46
1:E:228:GLU:HA	1:E:231:THR:HG22	1.98	0.46
2:T:147:GLN:HB3	2:U:148:LEU:HD11	1.98	0.46
1:A:66:ILE:HD11	1:B:168:TYR:HD2	1.80	0.46
2:T:46:LEU:HB3	2:U:46:LEU:HB3	1.97	0.46
1:D:353:THR:HG21	1:K:47:VAL:CG1	2.46	0.45
1:F:228:GLU:HA	1:F:231:THR:HG22	1.98	0.45
2:P:190:CYS:O	2:Q:193:LEU:HD13	2.17	0.45
2:T:162:TYR:HE1	2:U:165:VAL:HG11	1.80	0.45
2:P:53:THR:HG22	2:Q:57:LEU:HD12	1.99	0.45
2:T:165:VAL:CG1	2:U:165:VAL:CG2	2.84	0.45
2:P:214:TYR:HD2	2:Q:211:ALA:O	1.99	0.45
2:T:239:ALA:HA	2:U:239:ALA:HA	1.98	0.45
1:E:244:LEU:HD13	1:E:250:ILE:HG12	1.99	0.45
1:H:161:VAL:HG12	1:H:163:HIS:CE1	2.51	0.45
2:P:60:TYR:CD1	2:Q:57:LEU:HD22	2.52	0.45
1:D:272:GLU:HG2	1:I:41:ARG:HD2	1.97	0.45
1:F:244:LEU:HD13	1:F:250:ILE:HG12	1.99	0.45
1:J:228:GLU:HA	1:J:231:THR:HG22	1.98	0.45
1:J:244:LEU:HD13	1:J:250:ILE:HG12	1.99	0.45
2:P:239:ALA:HA	2:Q:239:ALA:HA	1.98	0.45
1:C:244:LEU:HD13	1:C:250:ILE:HG12	1.99	0.45
1:H:244:LEU:HD13	1:H:250:ILE:HG12	1.99	0.45
1:I:244:LEU:HD13	1:I:250:ILE:HG12	1.99	0.45
2:T:22:ALA:HA	2:U:22:ALA:HA	1.99	0.45
1:A:354:PHE:HD1	1:E:47:VAL:HG21	1.82	0.45
1:D:228:GLU:HA	1:D:231:THR:HG22	1.98	0.45
1:D:244:LEU:HD13	1:D:250:ILE:HG12	1.99	0.45
1:G:244:LEU:HD13	1:G:250:ILE:HG12	1.99	0.45
1:K:244:LEU:HD13	1:K:250:ILE:HG12	1.99	0.45
2:P:92:ILE:HB	2:Q:92:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:147:GLN:HB3	2:Q:148:LEU:HD11	1.98	0.45
2:T:190:CYS:O	2:U:193:LEU:HD13	2.16	0.45
4:O:66:LEU:HD22	4:O:100:LYS:HB3	1.97	0.45
2:T:57:LEU:CA	2:U:57:LEU:HD23	2.44	0.45
1:I:228:GLU:HA	1:I:231:THR:HG22	1.98	0.45
2:P:127:MET:O	2:Q:130:ILE:CD1	2.65	0.45
2:T:148:LEU:HD13	2:U:147:GLN:C	2.42	0.45
2:T:252:SER:HB3	2:U:253:ILE:HD11	1.98	0.45
1:A:41:ARG:NH1	1:C:272:GLU:CG	2.75	0.44
1:I:292:ARG:HH11	1:J:246:ASP:CG	2.25	0.44
2:T:60:TYR:CD1	2:U:57:LEU:HD22	2.52	0.44
1:G:228:GLU:HA	1:G:231:THR:HG22	1.98	0.44
1:J:269:ILE:O	1:K:175:HIS:CB	2.63	0.44
1:B:41:ARG:NH1	1:G:272:GLU:CG	2.75	0.44
2:P:148:LEU:HD13	2:Q:147:GLN:C	2.42	0.44
2:P:165:VAL:CG1	2:Q:165:VAL:CG2	2.84	0.44
1:B:49:MET:CE	1:H:171:TYR:CG	2.99	0.44
2:T:63:ALA:C	2:U:64:LEU:HD13	2.42	0.44
1:C:228:GLU:HA	1:C:231:THR:HG22	1.98	0.44
2:T:53:THR:HG22	2:U:57:LEU:HD12	1.99	0.44
1:D:246:ASP:CB	1:F:289:ILE:HG23	2.41	0.44
2:P:63:ALA:C	2:Q:64:LEU:HD13	2.42	0.44
1:B:4:GLU:CD	1:B:4:GLU:N	2.76	0.44
1:B:44:GLY:HA2	1:H:171:TYR:CD1	2.23	0.44
1:D:272:GLU:CG	1:I:41:ARG:HD2	2.48	0.44
2:P:57:LEU:CA	2:Q:57:LEU:HD23	2.44	0.44
2:P:176:LEU:N	2:Q:176:LEU:HD13	2.33	0.44
2:T:92:ILE:HB	2:U:92:ILE:CD1	2.47	0.44
2:T:161:LYS:HG3	2:U:162:TYR:CD1	2.53	0.44
1:K:223:LEU:HD21	2:Q:237:THR:CG2	2.47	0.44
1:C:145:TYR:OH	1:F:46:MET:HB3	2.18	0.43
1:H:142:LEU:O	1:H:344:GLY:HA3	2.18	0.43
2:P:190:CYS:O	2:Q:193:LEU:CD1	2.66	0.43
2:T:190:CYS:O	2:U:193:LEU:CD1	2.66	0.43
1:D:171:TYR:CE1	1:K:44:GLY:HA2	2.52	0.43
1:D:246:ASP:CG	1:F:292:ARG:HH11	2.25	0.43
1:F:142:LEU:O	1:F:344:GLY:HA3	2.18	0.43
1:K:142:LEU:O	1:K:344:GLY:HA3	2.18	0.43
2:P:161:LYS:HG3	2:Q:162:TYR:CD1	2.53	0.43
2:T:11:LEU:N	2:T:14:ASP:OD2	2.51	0.43
2:T:127:MET:O	2:U:130:ILE:CD1	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:137:ASP:HA	2:U:141:MET:SD	2.58	0.43
1:C:46:MET:HE2	1:G:170:GLY:HA2	1.99	0.43
1:C:142:LEU:O	1:C:344:GLY:HA3	2.18	0.43
1:E:142:LEU:O	1:E:344:GLY:HA3	2.18	0.43
2:T:176:LEU:HD11	2:U:175:ASP:CB	2.49	0.43
3:M:828:VAL:HG21	3:M:834:MET:HE2	1.99	0.43
1:C:289:ILE:HG23	1:F:246:ASP:CB	2.41	0.43
1:G:142:LEU:O	1:G:344:GLY:HA3	2.18	0.43
3:M:500:GLU:CD	3:M:716:ARG:HH22	2.26	0.43
1:D:46:MET:HG3	1:F:170:GLY:CA	2.49	0.43
1:K:223:LEU:CD2	2:Q:244:ARG:NH2	2.77	0.43
2:P:85:VAL:HG21	2:Q:84:ASP:HB3	2.00	0.43
2:T:165:VAL:HG13	2:U:165:VAL:HG21	1.93	0.43
1:D:142:LEU:O	1:D:344:GLY:HA3	2.18	0.43
2:T:85:VAL:HG21	2:U:84:ASP:HB3	2.00	0.43
1:J:144:LEU:HD22	1:J:167:ILE:HG21	2.01	0.43
2:P:176:LEU:HD11	2:Q:175:ASP:CB	2.49	0.43
1:E:144:LEU:HD22	1:E:167:ILE:HG21	2.01	0.43
1:I:142:LEU:O	1:I:344:GLY:HA3	2.18	0.43
2:P:39:LEU:HD13	2:Q:36:SER:O	2.19	0.43
3:M:356:THR:HG23	3:M:438:MET:HE1	2.01	0.43
1:A:114:PRO:HG2	1:F:199:GLY:HA2	2.00	0.42
1:G:144:LEU:HD22	1:G:167:ILE:HG21	2.01	0.42
1:J:142:LEU:O	1:J:344:GLY:HA3	2.18	0.42
3:L:828:VAL:HG21	3:L:834:MET:HE2	2.01	0.42
3:M:600:ASN:HA	3:M:651:VAL:HG22	2.00	0.42
1:B:45:VAL:HB	1:H:172:ALA:HB3	2.00	0.42
1:B:197:GLU:HB2	1:G:115:LYS:HG3	2.01	0.42
1:I:144:LEU:HD22	1:I:167:ILE:HG21	2.01	0.42
1:I:221:VAL:HG22	1:I:260:PRO:HB2	2.01	0.42
2:P:137:ASP:HA	2:Q:141:MET:SD	2.58	0.42
3:L:678:ILE:HD13	3:L:678:ILE:HA	1.94	0.42
3:M:477:GLU:CD	3:M:477:GLU:H	2.26	0.42
2:P:56:GLU:CB	2:Q:57:LEU:HD21	2.49	0.42
3:L:356:THR:HG23	3:L:438:MET:HE1	2.02	0.42
3:M:698:ARG:HG2	3:M:703:LEU:HD12	2.01	0.42
1:C:327:MET:CE	1:F:246:ASP:O	2.68	0.42
1:H:144:LEU:HD22	1:H:167:ILE:HG21	2.01	0.42
2:P:82:GLU:HA	2:P:85:VAL:HG12	2.02	0.42
2:P:207:LEU:HD12	2:Q:208:GLU:HA	2.01	0.42
1:C:144:LEU:HD22	1:C:167:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:TYR:H	1:K:46:MET:CG	2.33	0.42
2:T:39:LEU:HD13	2:U:36:SER:O	2.19	0.42
2:T:176:LEU:N	2:U:176:LEU:HD13	2.33	0.42
3:L:47:TYR:CD1	3:L:100:PRO:HG3	2.55	0.42
3:L:805:PHE:HA	3:L:809:MET:HB2	2.00	0.42
1:A:324:PRO:HB3	1:E:247:GLY:O	2.18	0.42
1:D:223:LEU:CD2	2:P:195:GLU:HG2	2.50	0.42
2:P:36:SER:O	2:Q:39:LEU:CD1	2.66	0.42
2:P:197:LEU:HD12	2:Q:200:VAL:CG2	2.50	0.42
2:P:200:VAL:HG11	2:Q:201:THR:HA	2.02	0.42
3:M:47:TYR:CD1	3:M:100:PRO:HG3	2.54	0.42
1:D:353:THR:HG21	1:K:47:VAL:HG11	2.02	0.42
1:E:4:GLU:N	1:E:4:GLU:OE1	2.53	0.42
1:E:221:VAL:HG22	1:E:260:PRO:HB2	2.02	0.42
1:F:144:LEU:HD22	1:F:167:ILE:HG21	2.01	0.42
2:P:176:LEU:HD11	2:Q:175:ASP:HB3	2.01	0.42
2:T:82:GLU:HA	2:T:85:VAL:HG12	2.02	0.42
1:J:221:VAL:HG22	1:J:260:PRO:HB2	2.02	0.42
3:L:477:GLU:H	3:L:477:GLU:CD	2.28	0.42
1:A:145:TYR:HH	1:E:47:VAL:H	1.61	0.41
1:C:46:MET:HE2	1:G:170:GLY:CA	2.50	0.41
1:E:197:GLU:O	1:F:114:PRO:HA	2.20	0.41
2:T:106:LEU:HD13	2:U:105:ARG:C	2.45	0.41
1:D:4:GLU:OE1	1:D:4:GLU:N	2.53	0.41
1:D:353:THR:CG2	1:K:47:VAL:HG11	2.50	0.41
1:F:4:GLU:N	1:F:4:GLU:OE1	2.53	0.41
1:I:327:MET:HE3	1:J:246:ASP:O	2.20	0.41
2:P:57:LEU:HD22	2:Q:56:GLU:HG2	2.02	0.41
2:P:260:LEU:N	2:Q:260:LEU:HD13	2.35	0.41
1:A:272:GLU:CD	1:F:204:THR:CG2	2.93	0.41
1:B:161:VAL:HG12	1:B:163:HIS:CE1	2.56	0.41
1:C:13:ASP:OD2	1:C:20:LYS:HE3	2.20	0.41
1:G:13:ASP:OD2	1:G:20:LYS:HE3	2.21	0.41
1:J:4:GLU:N	1:J:4:GLU:OE1	2.53	0.41
1:J:13:ASP:OD2	1:J:20:LYS:HE3	2.21	0.41
2:P:106:LEU:HD13	2:Q:105:ARG:C	2.45	0.41
2:T:57:LEU:HD22	2:U:56:GLU:HG2	2.02	0.41
2:T:197:LEU:HD12	2:U:200:VAL:CG2	2.50	0.41
3:M:678:ILE:HD13	3:M:678:ILE:HA	1.94	0.41
1:K:13:ASP:OD2	1:K:20:LYS:HE3	2.21	0.41
1:D:144:LEU:HD22	1:D:167:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:GLU:OE1	1:G:4:GLU:N	2.53	0.41
1:H:4:GLU:N	1:H:4:GLU:OE1	2.53	0.41
1:I:289:ILE:HG23	1:J:246:ASP:CB	2.41	0.41
2:P:246:VAL:HG13	2:Q:249:LEU:CD1	2.51	0.41
2:T:176:LEU:HD11	2:U:175:ASP:HB3	2.01	0.41
2:T:200:VAL:CG1	2:U:200:VAL:HG23	2.50	0.41
1:D:221:VAL:HG22	1:D:260:PRO:HB2	2.02	0.41
1:H:13:ASP:OD2	1:H:20:LYS:HE3	2.21	0.41
1:H:221:VAL:HG22	1:H:260:PRO:HB2	2.02	0.41
2:T:56:GLU:CB	2:U:57:LEU:HD21	2.49	0.41
2:T:200:VAL:HG11	2:U:201:THR:HA	2.01	0.41
1:B:204:THR:HG23	1:G:272:GLU:CD	2.46	0.41
1:I:4:GLU:OE1	1:I:4:GLU:N	2.53	0.41
2:T:36:SER:O	2:U:39:LEU:CD1	2.66	0.41
1:C:4:GLU:N	1:C:4:GLU:OE1	2.53	0.41
1:C:45:VAL:H	1:G:171:TYR:HA	1.86	0.41
1:C:221:VAL:HG22	1:C:260:PRO:HB2	2.02	0.41
1:D:13:ASP:OD2	1:D:20:LYS:HE3	2.21	0.41
1:I:114:PRO:HA	1:K:197:GLU:O	2.20	0.41
1:K:144:LEU:HD22	1:K:167:ILE:HG21	2.01	0.41
2:P:200:VAL:CG1	2:Q:200:VAL:HG23	2.50	0.41
2:T:246:VAL:HG13	2:U:249:LEU:CD1	2.51	0.41
1:B:314:ARG:HE	1:B:318:GLU:CD	2.28	0.41
1:D:246:ASP:O	1:F:327:MET:HE3	2.20	0.41
1:E:77:ILE:HG23	1:E:117:ASN:HD21	1.86	0.41
1:F:13:ASP:OD2	1:F:20:LYS:HE3	2.20	0.41
1:K:223:LEU:CB	2:Q:244:ARG:NH1	2.56	0.41
1:K:250:ILE:HG22	1:K:252:ILE:HG23	2.03	0.41
2:P:43:LEU:HD11	2:Q:39:LEU:HD23	2.02	0.41
2:P:242:ALA:CB	2:Q:242:ALA:HB1	2.51	0.41
2:T:113:LEU:HD13	2:U:112:LYS:C	2.46	0.41
2:T:207:LEU:HD12	2:U:208:GLU:HA	2.01	0.41
1:C:77:ILE:HG23	1:C:117:ASN:HD21	1.86	0.41
1:D:204:THR:CG2	1:E:272:GLU:CD	2.93	0.41
1:E:13:ASP:OD2	1:E:20:LYS:HE3	2.21	0.41
1:F:221:VAL:HG22	1:F:260:PRO:HB2	2.02	0.41
1:F:250:ILE:HG22	1:F:252:ILE:HG23	2.02	0.41
1:J:77:ILE:HG23	1:J:117:ASN:HD21	1.86	0.41
1:J:240:LYS:CE	2:U:233:LYS:NZ	2.84	0.41
1:K:4:GLU:OE1	1:K:4:GLU:N	2.53	0.41
1:K:77:ILE:HG23	1:K:117:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:VAL:HG22	1:K:260:PRO:HB2	2.02	0.41
2:P:169:LEU:N	2:Q:169:LEU:HD13	2.36	0.41
2:T:43:LEU:HD11	2:U:39:LEU:HD23	2.02	0.41
2:T:162:TYR:CE1	2:U:161:LYS:HB3	2.56	0.41
3:L:326:ILE:HG12	3:L:328:ASP:H	1.87	0.41
3:L:810:GLU:HG3	3:L:811:ARG:N	2.35	0.41
1:A:204:THR:HG23	1:C:272:GLU:CD	2.46	0.40
1:D:250:ILE:HG22	1:D:252:ILE:HG23	2.03	0.40
1:F:26:ASP:OD2	1:F:30:ARG:NH2	2.54	0.40
1:F:77:ILE:HG23	1:F:117:ASN:HD21	1.86	0.40
1:C:26:ASP:OD2	1:C:30:ARG:NH2	2.54	0.40
1:D:26:ASP:OD2	1:D:30:ARG:NH2	2.54	0.40
1:H:77:ILE:HG23	1:H:117:ASN:HD21	1.86	0.40
1:J:221:VAL:HG21	1:J:311:ILE:HG12	2.04	0.40
2:P:142:GLU:HA	2:P:145:GLU:HG2	2.03	0.40
2:T:154:ILE:HG22	2:U:155:ALA:HB1	2.03	0.40
1:C:221:VAL:HG21	1:C:311:ILE:HG12	2.04	0.40
1:D:199:GLY:CA	1:E:114:PRO:HG3	2.48	0.40
1:E:269:ILE:O	1:F:175:HIS:CB	2.69	0.40
1:F:197:GLU:OE2	1:F:258:ARG:NH2	2.55	0.40
1:F:221:VAL:HG21	1:F:311:ILE:HG12	2.04	0.40
2:P:154:ILE:HG22	2:Q:155:ALA:HB1	2.03	0.40
2:T:242:ALA:CB	2:U:242:ALA:HB1	2.51	0.40
1:B:41:ARG:HD3	1:G:272:GLU:CG	2.39	0.40
1:G:221:VAL:HG22	1:G:260:PRO:HB2	2.02	0.40
1:I:13:ASP:OD2	1:I:20:LYS:HE3	2.21	0.40
1:J:26:ASP:OD2	1:J:30:ARG:NH2	2.54	0.40
1:J:197:GLU:OE2	1:J:258:ARG:NH2	2.55	0.40
2:T:142:GLU:HA	2:T:145:GLU:HG2	2.03	0.40
1:A:66:ILE:HD11	1:B:168:TYR:CD2	2.56	0.40
1:E:221:VAL:HG21	1:E:311:ILE:HG12	2.04	0.40
1:G:221:VAL:HG21	1:G:311:ILE:HG12	2.04	0.40
1:H:197:GLU:OE2	1:H:258:ARG:NH2	2.55	0.40
1:H:250:ILE:HG22	1:H:252:ILE:HG23	2.02	0.40
1:I:221:VAL:HG21	1:I:311:ILE:HG12	2.04	0.40
2:P:260:LEU:CA	2:Q:260:LEU:HD13	2.51	0.40
2:T:193:LEU:HD12	2:U:190:CYS:HB2	2.03	0.40
3:M:841:LYS:HE3	5:S:29:GLU:CD	2.46	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	372/374 (100%)	343 (92%)	25 (7%)	4 (1%)	11	46
1	B	372/374 (100%)	345 (93%)	22 (6%)	5 (1%)	9	42
1	C	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	9	42
1	D	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	9	42
1	E	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	9	42
1	F	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	9	42
1	G	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	9	42
1	H	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	9	42
1	I	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	9	42
1	J	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	9	42
1	K	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	9	42
2	P	231/251 (92%)	231 (100%)	0	0	100	100
2	Q	231/251 (92%)	231 (100%)	0	0	100	100
2	T	241/251 (96%)	241 (100%)	0	0	100	100
2	U	241/251 (96%)	241 (100%)	0	0	100	100
3	L	811/813 (100%)	728 (90%)	57 (7%)	26 (3%)	3	21
3	M	811/813 (100%)	725 (89%)	61 (8%)	25 (3%)	3	22
4	N	146/148 (99%)	136 (93%)	4 (3%)	6 (4%)	2	18
4	O	146/148 (99%)	137 (94%)	4 (3%)	5 (3%)	3	21
5	R	142/144 (99%)	121 (85%)	13 (9%)	8 (6%)	1	14
5	S	142/144 (99%)	121 (85%)	13 (9%)	8 (6%)	1	14
All	All	7234/7328 (99%)	6786 (94%)	316 (4%)	132 (2%)	9	34

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	THR
3	L	53	GLN
3	L	64	THR
3	L	329	GLN
3	L	570	LYS
3	L	625	SER
3	L	646	SER
3	L	649	GLN
3	L	736	GLU
4	N	58	ARG
4	N	172	SER
5	R	38	ASP
5	R	77	PRO
5	R	145	PRO
3	M	53	GLN
3	M	64	THR
3	M	329	GLN
3	M	570	LYS
3	M	643	LYS
3	M	649	GLN
3	M	736	GLU
4	O	58	ARG
4	O	172	SER
5	S	38	ASP
5	S	77	PRO
5	S	97	GLU
5	S	145	PRO
1	C	50	GLY
1	C	172	ALA
1	D	50	GLY
1	D	172	ALA
1	E	50	GLY
1	E	172	ALA
1	F	50	GLY
1	F	172	ALA
1	G	50	GLY
1	G	172	ALA
1	H	50	GLY
1	H	172	ALA
1	I	50	GLY
1	I	172	ALA
1	J	50	GLY
1	J	172	ALA

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Mol	Chain	Res	Type
1	K	50	GLY
1	K	172	ALA
3	L	474	ASN
4	N	92	PRO
4	N	156	LYS
5	R	97	GLU
3	M	410	GLY
3	M	474	ASN
3	M	625	SER
3	M	648	PHE
1	A	172	ALA
1	A	236	SER
1	A	255	GLU
1	B	172	ALA
1	B	236	SER
1	B	255	GLU
3	L	181	SER
3	L	205	LYS
3	L	210	ALA
3	L	219	LEU
3	L	285	SER
3	L	378	PRO
3	L	392	SER
3	L	648	PHE
5	R	41	ARG
5	R	112	LYS
5	R	130	ARG
5	R	162	HIS
3	M	207	LYS
3	M	263	SER
3	M	285	SER
3	M	378	PRO
3	M	392	SER
4	O	92	PRO
4	O	156	LYS
5	S	41	ARG
5	S	112	LYS
5	S	130	ARG
5	S	162	HIS
1	C	52	LYS
1	D	52	LYS
1	E	52	LYS

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Mol	Chain	Res	Type
1	F	52	LYS
1	G	52	LYS
1	H	52	LYS
1	I	52	LYS
1	J	52	LYS
1	K	52	LYS
3	L	263	SER
3	M	181	SER
3	M	219	LEU
4	O	98	ASN
1	A	52	LYS
1	B	52	LYS
1	C	40	PRO
1	E	40	PRO
3	L	75	ASP
3	L	208	GLU
3	L	328	ASP
3	L	627	GLY
4	N	98	ASN
3	M	75	ASP
3	M	214	LYS
1	D	40	PRO
1	F	40	PRO
1	G	40	PRO
1	H	40	PRO
1	I	40	PRO
1	J	40	PRO
1	K	40	PRO
3	L	683	LYS
3	L	740	ILE
3	M	135	TYR
3	M	328	ASP
3	M	740	ILE
1	C	114	PRO
1	D	114	PRO
1	E	114	PRO
1	F	114	PRO
1	G	114	PRO
1	H	114	PRO
1	I	114	PRO
1	J	114	PRO
1	K	114	PRO

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Mol	Chain	Res	Type
3	L	309	ASN
3	L	594	ILE
3	M	309	ASN
3	M	594	ILE
4	N	114	ILE

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	317/317 (100%)	308 (97%)	9 (3%)	38	60
1	B	317/317 (100%)	309 (98%)	8 (2%)	42	63
1	C	317/317 (100%)	312 (98%)	5 (2%)	55	70
1	D	317/317 (100%)	312 (98%)	5 (2%)	55	70
1	E	317/317 (100%)	312 (98%)	5 (2%)	55	70
1	F	317/317 (100%)	312 (98%)	5 (2%)	55	70
1	G	317/317 (100%)	312 (98%)	5 (2%)	55	70
1	H	317/317 (100%)	312 (98%)	5 (2%)	55	70
1	I	317/317 (100%)	312 (98%)	5 (2%)	55	70
1	J	317/317 (100%)	312 (98%)	5 (2%)	55	70
1	K	317/317 (100%)	312 (98%)	5 (2%)	55	70
2	P	202/216 (94%)	201 (100%)	1 (0%)	81	83
2	Q	202/216 (94%)	202 (100%)	0	100	100
2	T	208/216 (96%)	207 (100%)	1 (0%)	81	83
2	U	208/216 (96%)	208 (100%)	0	100	100
3	L	699/699 (100%)	689 (99%)	10 (1%)	59	72
3	M	699/699 (100%)	690 (99%)	9 (1%)	61	74
4	N	125/125 (100%)	122 (98%)	3 (2%)	43	64
4	O	125/125 (100%)	123 (98%)	2 (2%)	55	70
5	R	124/124 (100%)	117 (94%)	7 (6%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	124/124 (100%)	117 (94%)	7 (6%)	19	40
All	All	6203/6247 (99%)	6101 (98%)	102 (2%)	54	70

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	53	ASP
1	A	82	ASP
1	A	108	THR
1	A	114	PRO
1	A	159	ASP
1	A	161	VAL
1	A	167	ILE
1	A	205	THR
1	B	27	ASP
1	B	53	ASP
1	B	108	THR
1	B	114	PRO
1	B	159	ASP
1	B	161	VAL
1	B	167	ILE
1	B	205	THR
1	C	108	THR
1	C	138	ILE
1	C	161	VAL
1	C	167	ILE
1	C	348	LEU
1	D	108	THR
1	D	138	ILE
1	D	161	VAL
1	D	167	ILE
1	D	348	LEU
1	E	108	THR
1	E	138	ILE
1	E	161	VAL
1	E	167	ILE
1	E	348	LEU
1	F	108	THR
1	F	138	ILE
1	F	161	VAL
1	F	167	ILE

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Mol	Chain	Res	Type
1	F	348	LEU
1	G	108	THR
1	G	138	ILE
1	G	161	VAL
1	G	167	ILE
1	G	348	LEU
1	H	108	THR
1	H	138	ILE
1	H	161	VAL
1	H	167	ILE
1	H	348	LEU
1	I	108	THR
1	I	138	ILE
1	I	161	VAL
1	I	167	ILE
1	I	348	LEU
1	J	108	THR
1	J	138	ILE
1	J	161	VAL
1	J	167	ILE
1	J	348	LEU
1	K	108	THR
1	K	138	ILE
1	K	161	VAL
1	K	167	ILE
1	K	348	LEU
2	P	85	VAL
2	T	85	VAL
3	L	75	ASP
3	L	89	GLU
3	L	121	LEU
3	L	160	ASP
3	L	322	THR
3	L	347	ASP
3	L	379	ASP
3	L	472	ASP
3	L	477	GLU
3	L	606	GLU
4	N	55	LEU
4	N	68	GLN
4	N	124	GLU
5	R	49	ASP

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Mol	Chain	Res	Type
5	R	61	ASN
5	R	77	PRO
5	R	97	GLU
5	R	123	LEU
5	R	128	CYS
5	R	137	LYS
3	M	75	ASP
3	M	121	LEU
3	M	160	ASP
3	M	322	THR
3	M	347	ASP
3	M	379	ASP
3	M	472	ASP
3	M	477	GLU
3	M	778	GLU
4	O	68	GLN
4	O	124	GLU
5	S	29	GLU
5	S	49	ASP
5	S	61	ASN
5	S	77	PRO
5	S	97	GLU
5	S	123	LEU
5	S	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	103	HIS
1	A	163	HIS
1	B	42	HIS
1	B	103	HIS
1	B	163	HIS
1	C	61	GLN
1	C	90	HIS
1	C	117	ASN
1	C	123	GLN
1	C	139	GLN
1	C	298	ASN
1	D	90	HIS
1	D	94	ASN

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Mol	Chain	Res	Type
1	D	117	ASN
1	D	298	ASN
1	E	61	GLN
1	E	117	ASN
1	E	123	GLN
1	E	298	ASN
1	F	90	HIS
1	F	117	ASN
1	F	123	GLN
1	F	139	GLN
1	F	298	ASN
1	G	61	GLN
1	G	90	HIS
1	G	94	ASN
1	G	117	ASN
1	G	123	GLN
1	G	139	GLN
1	G	298	ASN
1	G	373	HIS
1	H	61	GLN
1	H	90	HIS
1	H	94	ASN
1	H	117	ASN
1	H	123	GLN
1	H	298	ASN
1	I	61	GLN
1	I	90	HIS
1	I	94	ASN
1	I	117	ASN
1	I	139	GLN
1	I	298	ASN
1	J	90	HIS
1	J	94	ASN
1	J	117	ASN
1	J	123	GLN
1	J	139	GLN
1	J	298	ASN
1	K	90	HIS
1	K	94	ASN
1	K	117	ASN
1	K	123	GLN
1	K	139	GLN

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Mol	Chain	Res	Type
1	K	298	ASN
2	P	210	GLN
2	Q	47	GLN
2	T	210	GLN
2	U	47	GLN
3	L	96	HIS
3	L	98	HIS
3	L	164	GLN
3	L	235	ASN
3	L	485	ASN
3	L	558	GLN
3	L	559	HIS
3	L	670	HIS
4	N	45	GLN
5	R	127	GLN
3	M	96	HIS
3	M	98	HIS
3	M	235	ASN
3	M	411	ASN
3	M	485	ASN
3	M	559	HIS
3	M	670	HIS
4	O	45	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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-12289. These allow visual inspection of the internal detail of the map and identification of artifacts.

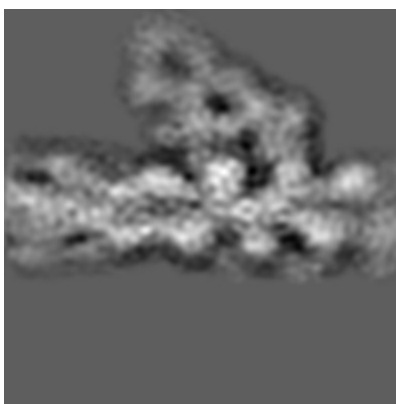
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

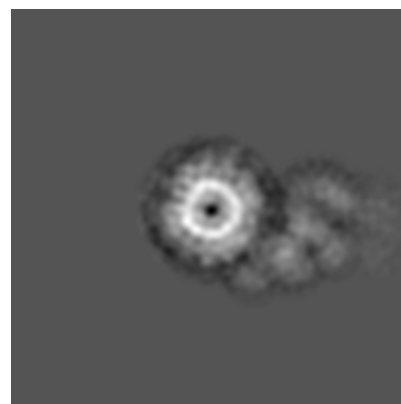
6.1.1 Primary map



X

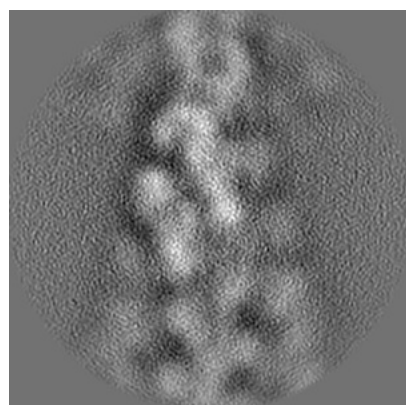


Y

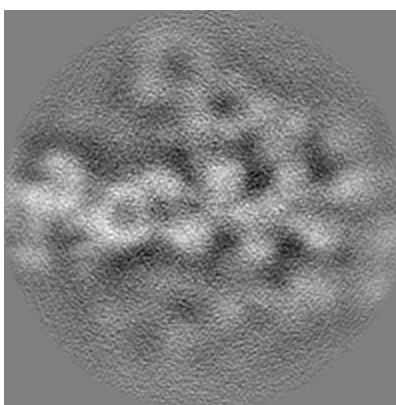


Z

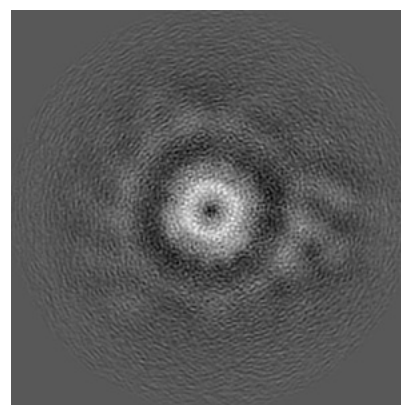
6.1.2 Raw map



X



Y



Z

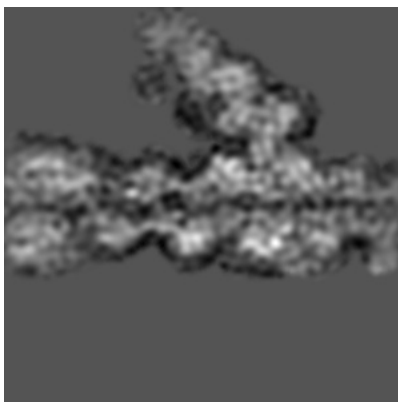
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

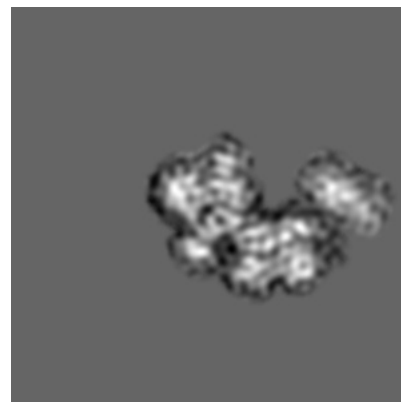
6.2.1 Primary map



X Index: 100

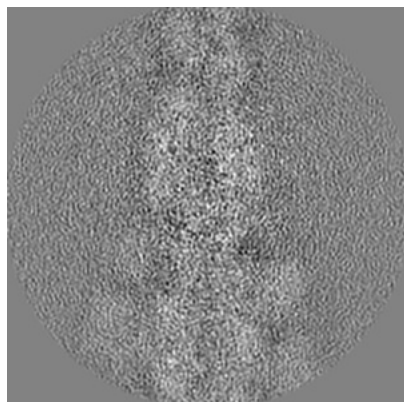


Y Index: 100

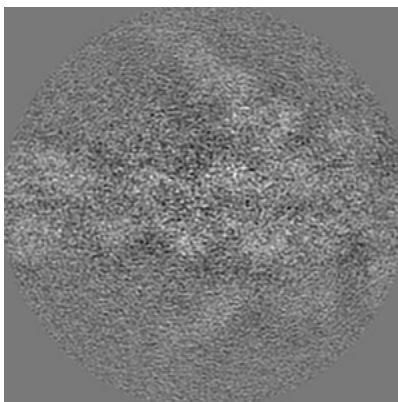


Z Index: 100

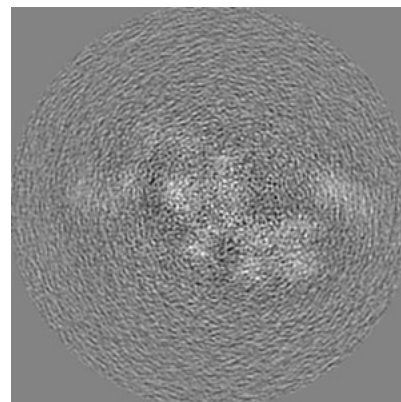
6.2.2 Raw map



X Index: 100



Y Index: 100



Z Index: 100

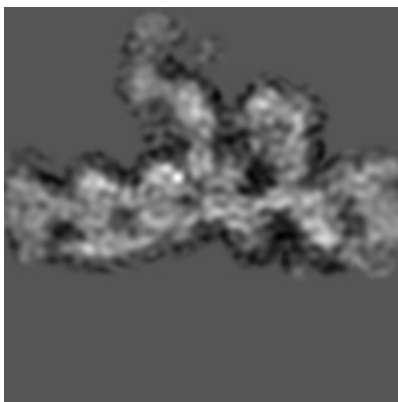
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

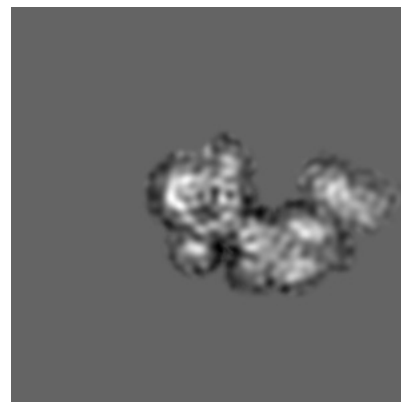
6.3.1 Primary map



X Index: 113

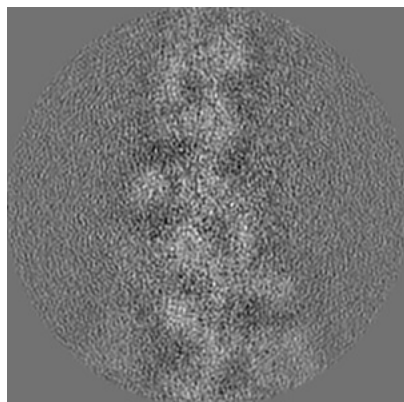


Y Index: 87

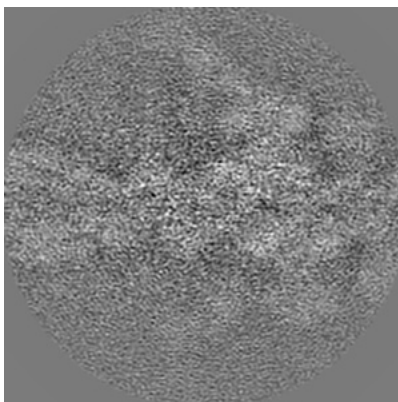


Z Index: 96

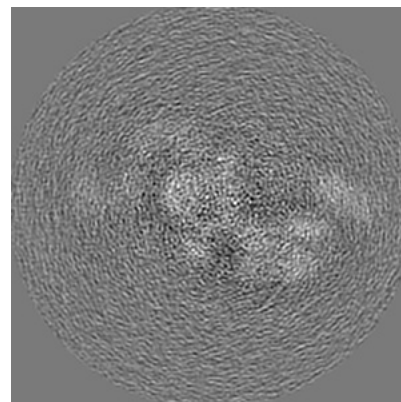
6.3.2 Raw map



X Index: 112



Y Index: 97

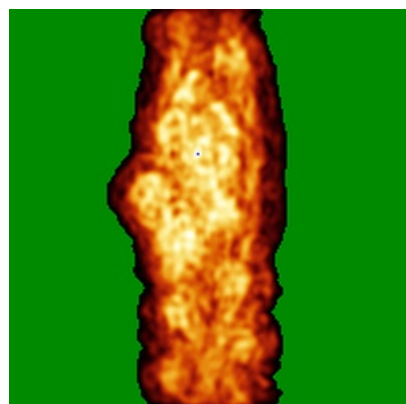


Z Index: 97

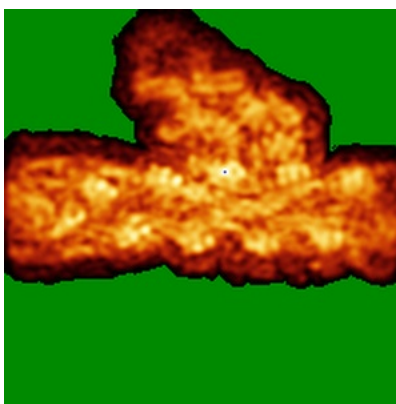
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

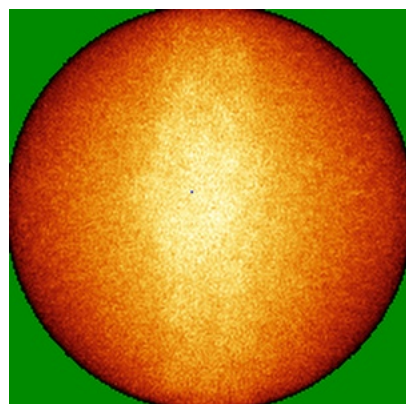


Y

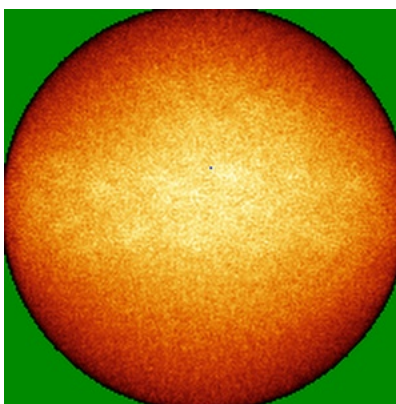


Z

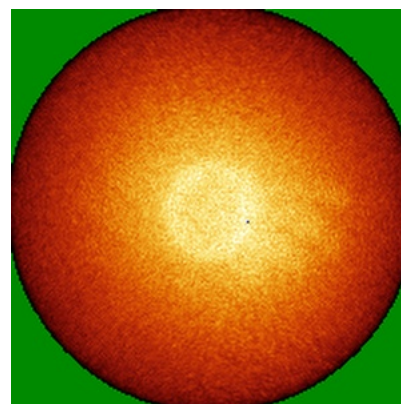
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

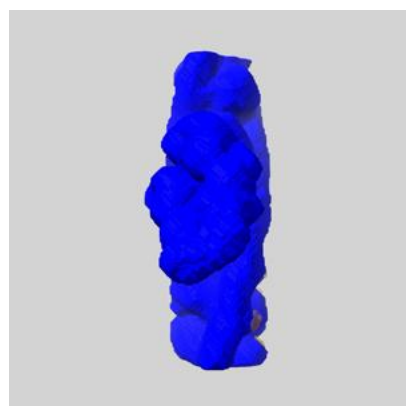
6.6 Mask visualisation [i](#)

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

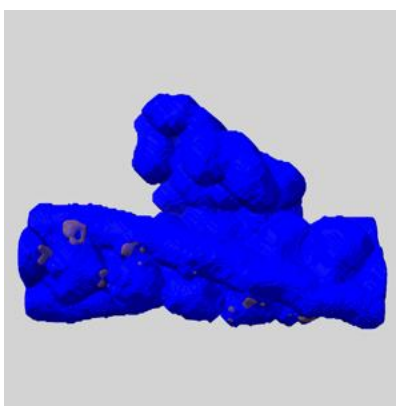
A mask typically either:

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

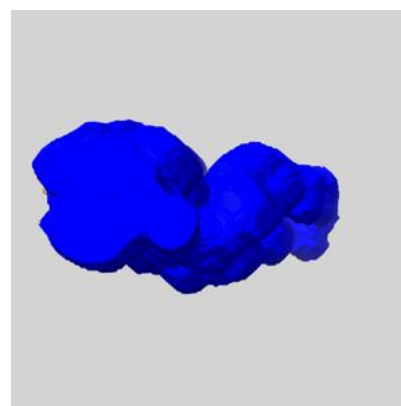
6.6.1 emd_12289_msk_1.map [i](#)



X



Y

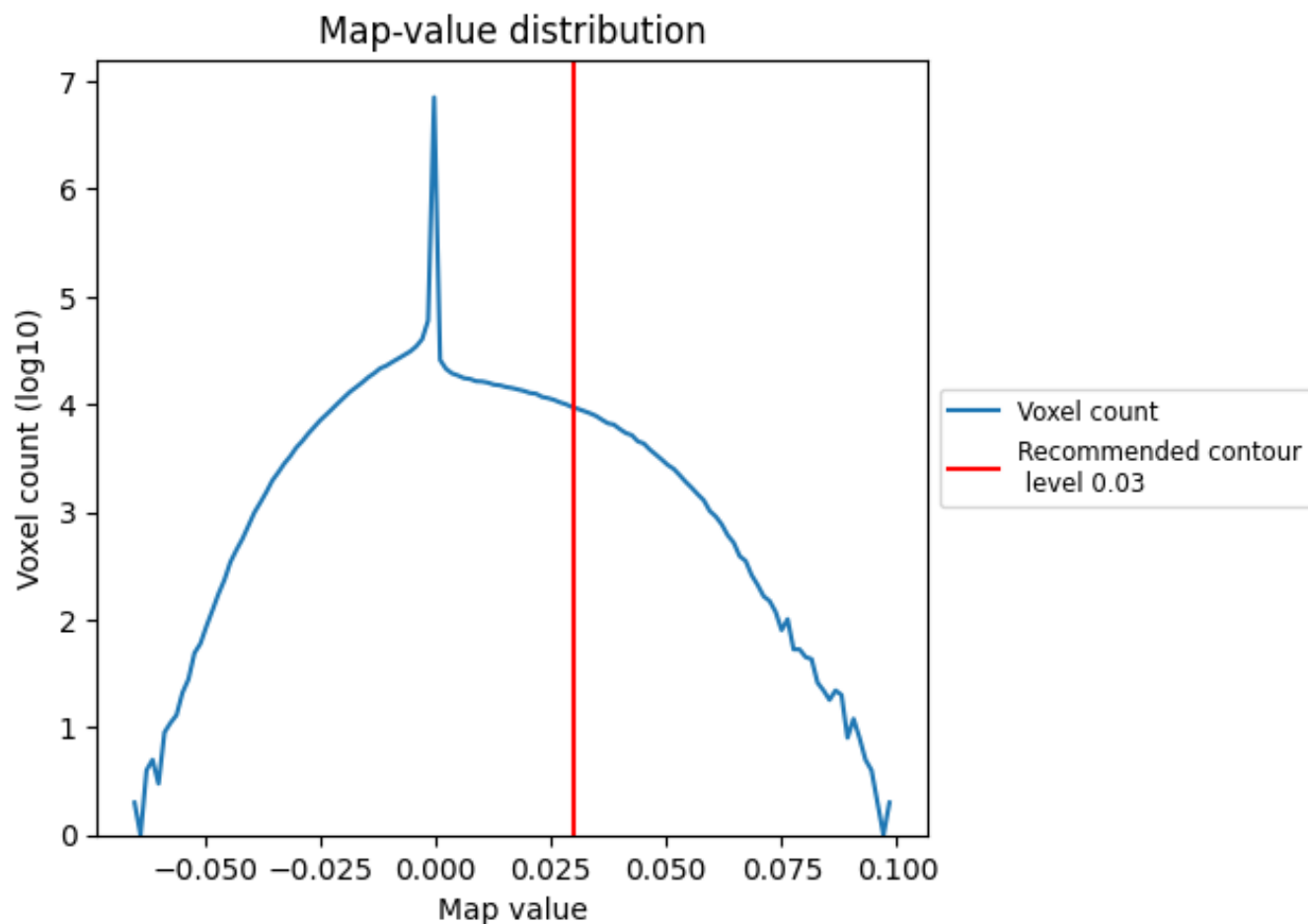


Z

7 Map analysis [i](#)

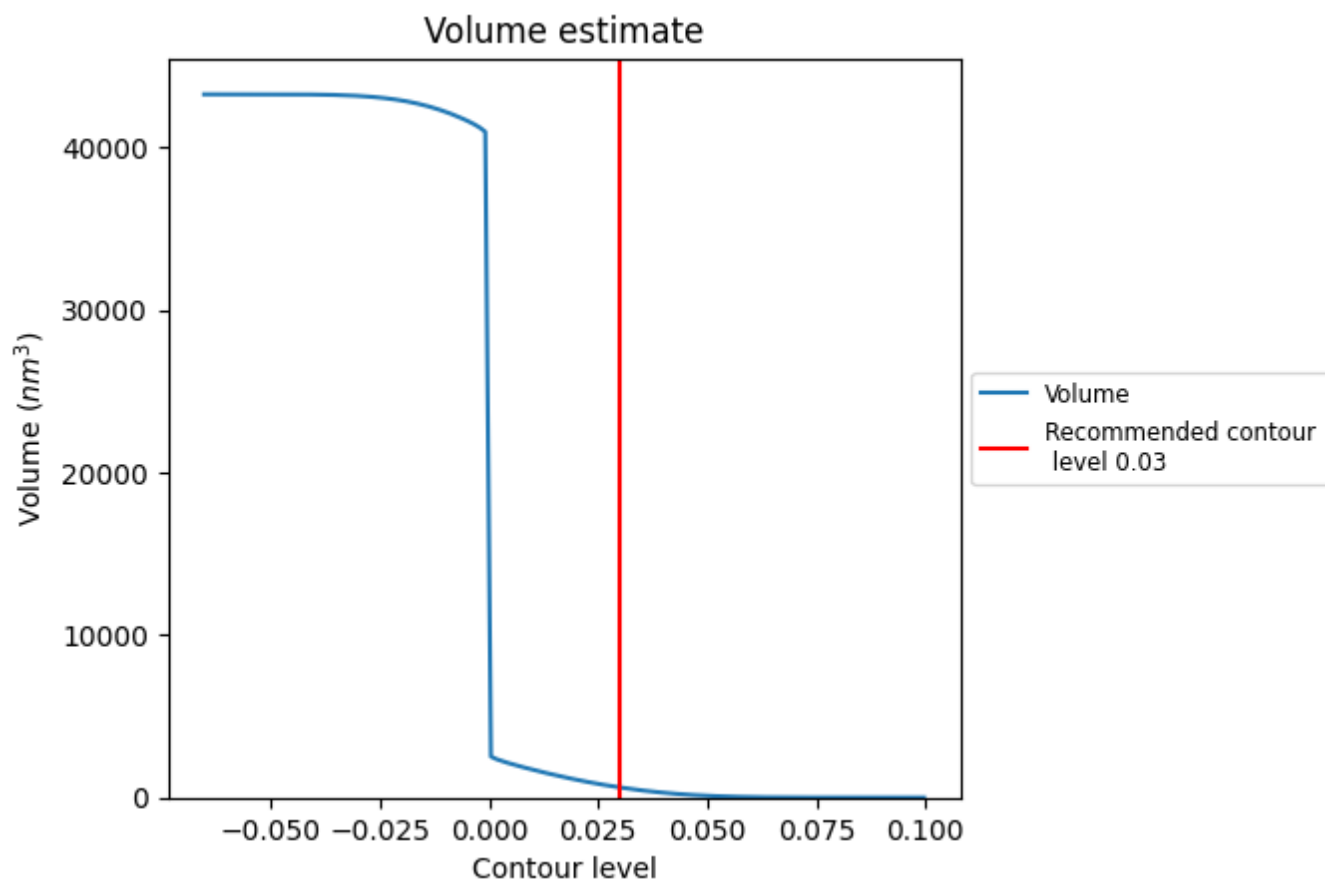
This section contains the results of statistical analysis of the map.

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.

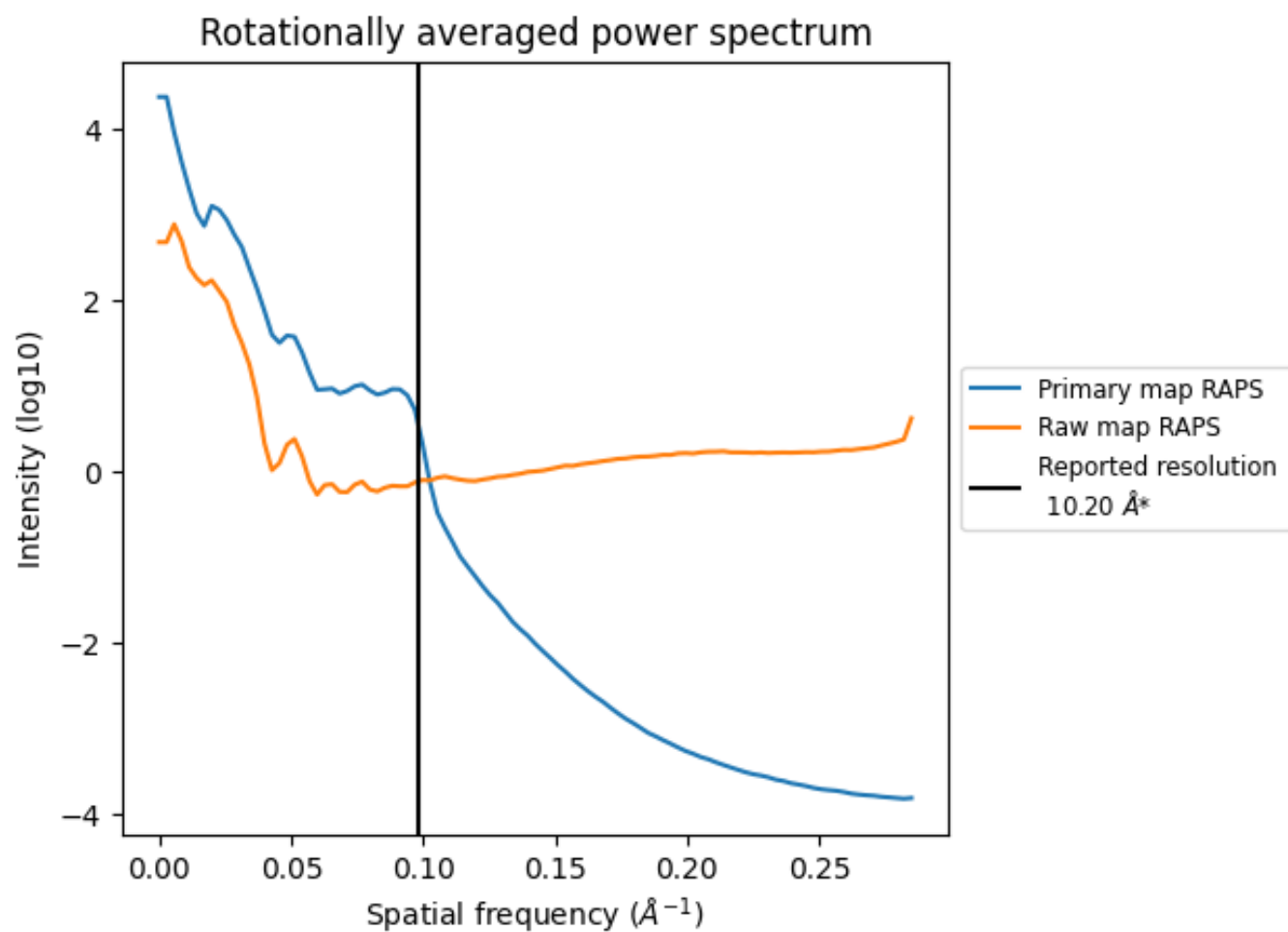
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 624 nm³; this corresponds to an approximate mass of 564 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 ⓘ

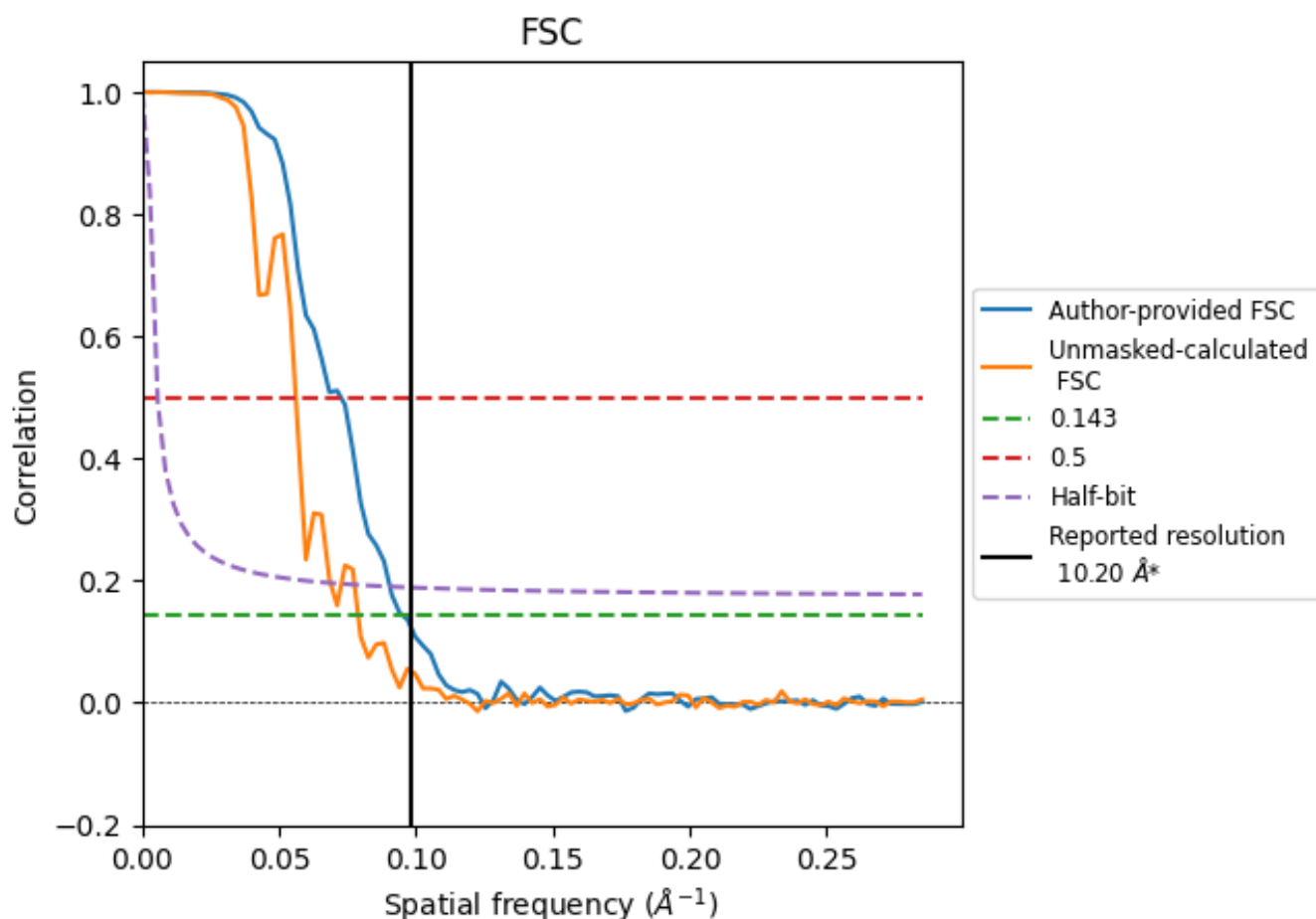


*Reported resolution corresponds to spatial frequency of 0.098 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.098 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

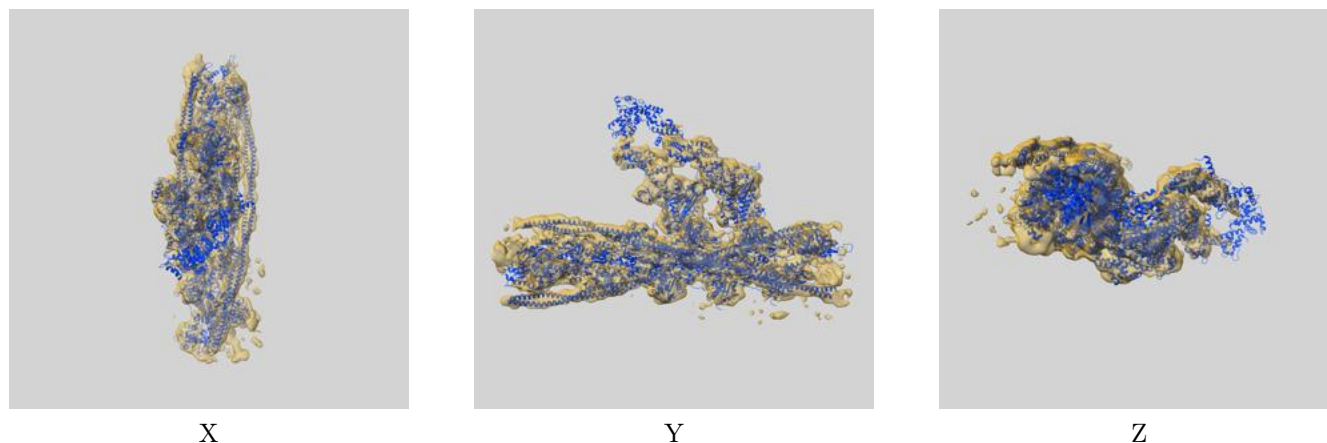
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.20	-	-
Author-provided FSC curve	10.52	13.77	11.05
Unmasked-calculated*	12.67	17.83	14.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 12.67 differs from the reported value 10.2 by more than 10 %

9 Map-model fit [i](#)

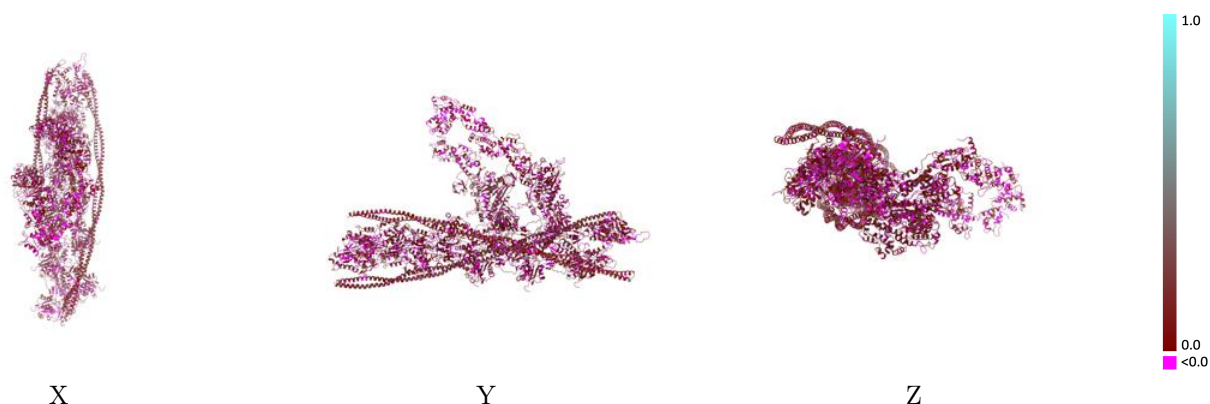
This section contains information regarding the fit between EMDB map EMD-12289 and PDB model 7NEP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 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](#)

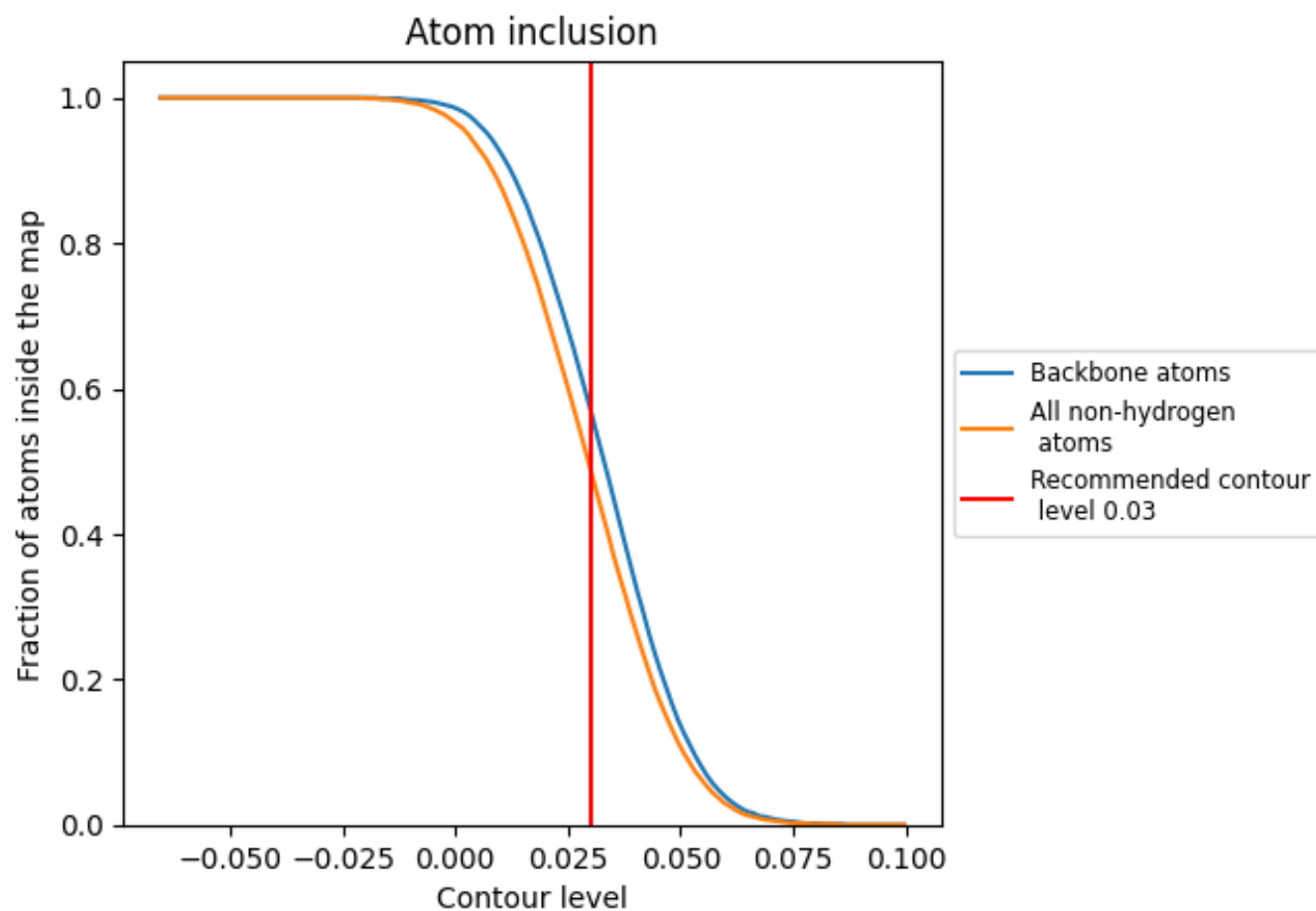


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 49% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4890	 0.0880
A	 0.4480	 0.0930
B	 0.4600	 0.0910
C	 0.4750	 0.0840
D	 0.4660	 0.0880
E	 0.5210	 0.0970
F	 0.4910	 0.0900
G	 0.4830	 0.0920
H	 0.3970	 0.0860
I	 0.4800	 0.0890
J	 0.3240	 0.0700
K	 0.4270	 0.0840
L	 0.5120	 0.0790
M	 0.4770	 0.0690
N	 0.5290	 0.0690
O	 0.5750	 0.0660
P	 0.7530	 0.1300
Q	 0.7480	 0.1430
R	 0.0160	 0.0250
S	 0.0940	 0.0410
T	 0.7700	 0.1340
U	 0.7220	 0.1350

